



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2016 – 07:00 PM EDT

PDB ID : 5J4D
Title : E. coli release factor 1 bound to the 70S ribosome in response to a pseudouridylated stop codon
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2016-03-31
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

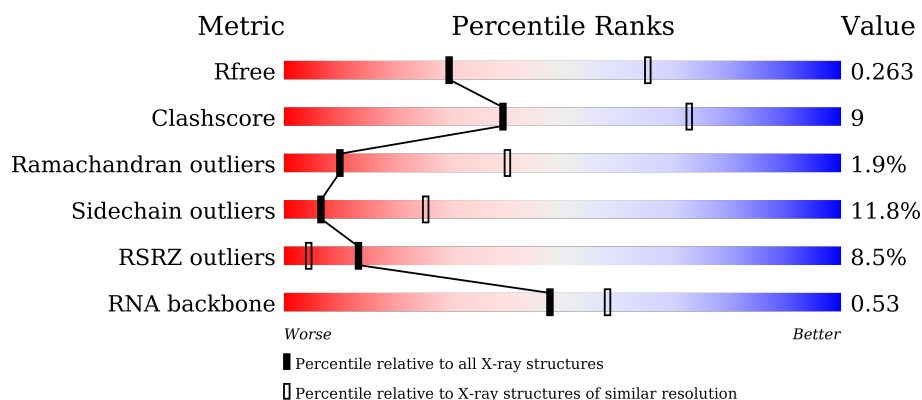
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1507	
1	FB	1507	
2	B	2880	
2	GB	2880	



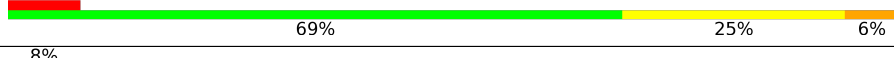

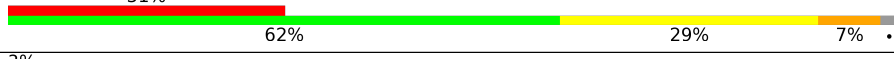
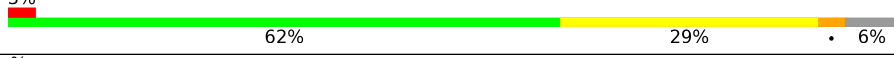




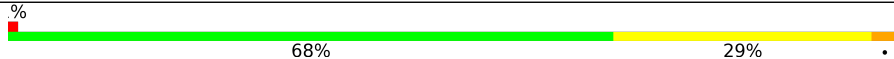
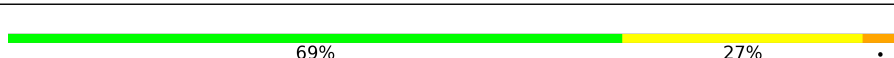
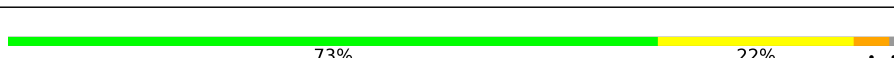
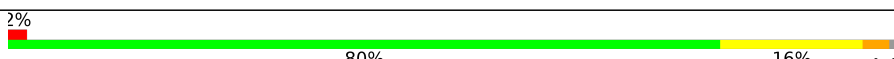
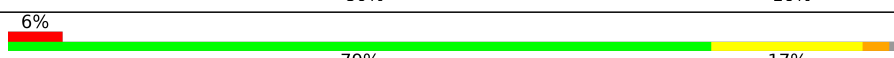
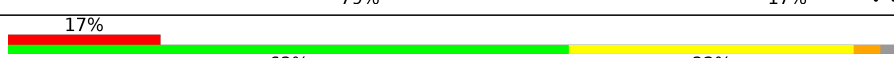





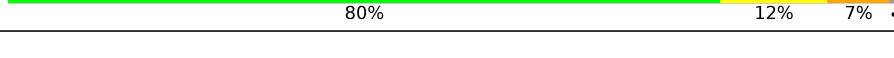



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Mol	Chain	Length	Quality of chain
3	C	120	
3	HB	120	
4	D	77	
4	IA	77	
4	IB	77	
4	NC	77	
5	E	275	
5	JB	275	
6	F	206	
6	KB	206	
7	G	205	
7	LB	205	
8	H	182	
8	MB	182	
9	I	180	
9	NB	180	
10	J	148	
10	OB	148	
11	K	140	
11	PB	140	
12	L	122	
12	QB	122	
13	M	150	
13	RB	150	
14	N	141	

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Mol	Chain	Length	Quality of chain
14	SB	141	
15	O	118	
15	TB	118	
16	P	112	
16	UB	112	
17	Q	146	
17	VB	146	
18	R	118	
18	WB	118	
19	S	101	
19	XB	101	
20	T	113	
20	YB	113	
21	U	96	
21	ZB	96	
22	AC	110	
22	V	110	
23	BC	206	
23	W	206	
24	CC	85	
24	X	85	
25	DC	98	
25	Y	98	
26	EC	72	
26	Z	72	

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Mol	Chain	Length	Quality of chain
27	AA	60	
27	FC	60	
28	BA	71	
28	GC	71	
29	CA	60	
29	HC	60	
30	DA	54	
30	IC	54	
31	EA	49	
31	JC	49	
32	FA	65	
32	KC	65	
33	GA	37	
33	LC	37	
34	HA	27	
34	MC	27	
35	JA	368	
35	OC	368	
36	KA	256	
36	PC	256	
37	LA	239	
37	QC	239	
38	MA	209	
38	RC	209	
39	NA	162	

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Mol	Chain	Length	Quality of chain
39	SC	162	
40	OA	101	
40	TC	101	
41	PA	156	
41	UC	156	
42	QA	138	
42	VC	138	
43	RA	128	
43	WC	128	
44	SA	105	
44	XC	105	
45	TA	129	
45	YC	129	
46	UA	132	
46	ZC	132	
47	AD	126	
47	VA	126	
48	BD	61	
48	WA	61	
49	CD	89	
49	XA	89	
50	DD	88	
50	YA	88	
51	ED	105	
51	ZA	105	

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Mol	Chain	Length	Quality of chain
52	AB	88	
52	FD	88	
53	BB	93	
53	GD	93	
54	CB	106	
54	HD	106	
55	DB	27	
55	ID	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	A	1601	-	-	-	X
56	MG	A	1603	-	-	-	X
56	MG	A	1604	-	-	-	X
56	MG	A	1606	-	-	-	X
56	MG	A	1610	-	-	-	X
56	MG	A	1613	-	-	-	X
56	MG	A	1620	-	-	-	X
56	MG	A	1637	-	-	-	X
56	MG	A	1643	-	-	-	X
56	MG	A	1645	-	-	-	X
56	MG	A	1656	-	-	-	X
56	MG	A	1662	-	-	-	X
56	MG	A	1676	-	-	-	X
56	MG	A	1709	-	-	-	X
56	MG	A	1715	-	-	-	X
56	MG	A	1727	-	-	-	X
56	MG	A	1743	-	-	-	X
56	MG	A	1786	-	-	-	X
56	MG	A	1794	-	-	-	X
56	MG	A	1809	-	-	-	X
56	MG	A	1814	-	-	-	X
56	MG	A	1869	-	-	-	X
56	MG	A	1875	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	A	1886	-	-	-	X
56	MG	AA	101	-	-	-	X
56	MG	AA	102	-	-	-	X
56	MG	B	2904	-	-	-	X
56	MG	B	2909	-	-	-	X
56	MG	B	2911	-	-	-	X
56	MG	B	2912	-	-	-	X
56	MG	B	2914	-	-	-	X
56	MG	B	2916	-	-	-	X
56	MG	B	2920	-	-	-	X
56	MG	B	2921	-	-	-	X
56	MG	B	2922	-	-	-	X
56	MG	B	2923	-	-	-	X
56	MG	B	2924	-	-	-	X
56	MG	B	2927	-	-	-	X
56	MG	B	2928	-	-	-	X
56	MG	B	2929	-	-	-	X
56	MG	B	2930	-	-	-	X
56	MG	B	2931	-	-	-	X
56	MG	B	2937	-	-	-	X
56	MG	B	2950	-	-	-	X
56	MG	B	2951	-	-	-	X
56	MG	B	2953	-	-	-	X
56	MG	B	2961	-	-	-	X
56	MG	B	2964	-	-	-	X
56	MG	B	2965	-	-	-	X
56	MG	B	2970	-	-	-	X
56	MG	B	2975	-	-	-	X
56	MG	B	2979	-	-	-	X
56	MG	B	2980	-	-	-	X
56	MG	B	2988	-	-	-	X
56	MG	B	2990	-	-	-	X
56	MG	B	2991	-	-	-	X
56	MG	B	2992	-	-	-	X
56	MG	B	2993	-	-	-	X
56	MG	B	2995	-	-	-	X
56	MG	B	2996	-	-	-	X
56	MG	B	2999	-	-	-	X
56	MG	B	3001	-	-	-	X
56	MG	B	3002	-	-	-	X
56	MG	B	3013	-	-	-	X
56	MG	B	3019	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	B	3025	-	-	-	X
56	MG	B	3027	-	-	-	X
56	MG	B	3029	-	-	-	X
56	MG	B	3031	-	-	-	X
56	MG	B	3039	-	-	-	X
56	MG	B	3040	-	-	-	X
56	MG	B	3043	-	-	-	X
56	MG	B	3046	-	-	-	X
56	MG	B	3047	-	-	-	X
56	MG	B	3062	-	-	-	X
56	MG	B	3070	-	-	-	X
56	MG	B	3075	-	-	-	X
56	MG	B	3084	-	-	-	X
56	MG	B	3092	-	-	-	X
56	MG	B	3100	-	-	-	X
56	MG	B	3108	-	-	-	X
56	MG	B	3128	-	-	-	X
56	MG	B	3134	-	-	-	X
56	MG	B	3144	-	-	-	X
56	MG	B	3161	-	-	-	X
56	MG	B	3197	-	-	-	X
56	MG	B	3206	-	-	-	X
56	MG	B	3208	-	-	-	X
56	MG	B	3226	-	-	-	X
56	MG	B	3229	-	-	-	X
56	MG	B	3236	-	-	-	X
56	MG	B	3255	-	-	-	X
56	MG	B	3262	-	-	-	X
56	MG	B	3270	-	-	-	X
56	MG	B	3278	-	-	-	X
56	MG	B	3301	-	-	-	X
56	MG	B	3322	-	-	-	X
56	MG	B	3324	-	-	-	X
56	MG	B	3330	-	-	-	X
56	MG	B	3334	-	-	-	X
56	MG	B	3339	-	-	-	X
56	MG	B	3344	-	-	-	X
56	MG	B	3345	-	-	-	X
56	MG	B	3346	-	-	-	X
56	MG	B	3406	-	-	-	X
56	MG	B	3410	-	-	-	X
56	MG	B	3416	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	B	3422	-	-	-	X
56	MG	B	3430	-	-	-	X
56	MG	B	3445	-	-	-	X
56	MG	B	3453	-	-	-	X
56	MG	B	3458	-	-	-	X
56	MG	B	3473	-	-	-	X
56	MG	B	3479	-	-	-	X
56	MG	B	3499	-	-	-	X
56	MG	B	3507	-	-	-	X
56	MG	B	3519	-	-	-	X
56	MG	B	3523	-	-	-	X
56	MG	B	3526	-	-	-	X
56	MG	B	3528	-	-	-	X
56	MG	B	3531	-	-	-	X
56	MG	B	3544	-	-	-	X
56	MG	B	3556	-	-	-	X
56	MG	B	3567	-	-	-	X
56	MG	B	3579	-	-	-	X
56	MG	B	3603	-	-	-	X
56	MG	B	3631	-	-	-	X
56	MG	B	3635	-	-	-	X
56	MG	B	3666	-	-	-	X
56	MG	B	3694	-	-	-	X
56	MG	B	3706	-	-	-	X
56	MG	B	3717	-	-	-	X
56	MG	B	3741	-	-	-	X
56	MG	B	3757	-	-	-	X
56	MG	B	3775	-	-	-	X
56	MG	B	3779	-	-	-	X
56	MG	B	3784	-	-	-	X
56	MG	B	3810	-	-	-	X
56	MG	B	3814	-	-	-	X
56	MG	B	3815	-	-	-	X
56	MG	B	3816	-	-	-	X
56	MG	B	3822	-	-	-	X
56	MG	B	3829	-	-	-	X
56	MG	B	3833	-	-	-	X
56	MG	B	3840	-	-	-	X
56	MG	B	3841	-	-	-	X
56	MG	BC	306	-	-	-	X
56	MG	C	206	-	-	-	X
56	MG	C	209	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	C	233	-	-	-	X
56	MG	C	244	-	-	-	X
56	MG	CB	201	-	-	-	X
56	MG	E	307	-	-	-	X
56	MG	F	301	-	-	-	X
56	MG	F	304	-	-	-	X
56	MG	F	305	-	-	-	X
56	MG	F	308	-	-	-	X
56	MG	F	313	-	-	-	X
56	MG	FA	103	-	-	-	X
56	MG	FB	1601	-	-	-	X
56	MG	FB	1603	-	-	-	X
56	MG	FB	1607	-	-	-	X
56	MG	FB	1608	-	-	-	X
56	MG	FB	1609	-	-	-	X
56	MG	FB	1614	-	-	-	X
56	MG	FB	1620	-	-	-	X
56	MG	FB	1623	-	-	-	X
56	MG	FB	1627	-	-	-	X
56	MG	FB	1636	-	-	-	X
56	MG	FB	1642	-	-	-	X
56	MG	FB	1657	-	-	-	X
56	MG	FB	1680	-	-	-	X
56	MG	FB	1681	-	-	-	X
56	MG	FB	1688	-	-	-	X
56	MG	FB	1690	-	-	-	X
56	MG	FB	1697	-	-	-	X
56	MG	FB	1707	-	-	-	X
56	MG	FB	1713	-	-	-	X
56	MG	FB	1722	-	-	-	X
56	MG	FB	1731	-	-	-	X
56	MG	FB	1738	-	-	-	X
56	MG	FB	1740	-	-	-	X
56	MG	FB	1746	-	-	-	X
56	MG	FB	1750	-	-	-	X
56	MG	FB	1755	-	-	-	X
56	MG	FB	1765	-	-	-	X
56	MG	FB	1787	-	-	-	X
56	MG	FB	1790	-	-	-	X
56	MG	FB	1800	-	-	-	X
56	MG	FB	1827	-	-	-	X
56	MG	FB	1834	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	FB	1845	-	-	-	X
56	MG	FB	1847	-	-	-	X
56	MG	FB	1878	-	-	-	X
56	MG	FB	1889	-	-	-	X
56	MG	FB	1908	-	-	-	X
56	MG	FB	1911	-	-	-	X
56	MG	FB	1927	-	-	-	X
56	MG	FB	1932	-	-	-	X
56	MG	FB	1937	-	-	-	X
56	MG	FB	1949	-	-	-	X
56	MG	G	3201	-	-	-	X
56	MG	G	3202	-	-	-	X
56	MG	GB	2902	-	-	-	X
56	MG	GB	2904	-	-	-	X
56	MG	GB	2906	-	-	-	X
56	MG	GB	2907	-	-	-	X
56	MG	GB	2909	-	-	-	X
56	MG	GB	2911	-	-	-	X
56	MG	GB	2917	-	-	-	X
56	MG	GB	2918	-	-	-	X
56	MG	GB	2922	-	-	-	X
56	MG	GB	2933	-	-	-	X
56	MG	GB	2934	-	-	-	X
56	MG	GB	2935	-	-	-	X
56	MG	GB	2938	-	-	-	X
56	MG	GB	2948	-	-	-	X
56	MG	GB	2954	-	-	-	X
56	MG	GB	2956	-	-	-	X
56	MG	GB	2963	-	-	-	X
56	MG	GB	2969	-	-	-	X
56	MG	GB	2974	-	-	-	X
56	MG	GB	2976	-	-	-	X
56	MG	GB	2978	-	-	-	X
56	MG	GB	2982	-	-	-	X
56	MG	GB	2983	-	-	-	X
56	MG	GB	2989	-	-	-	X
56	MG	GB	3000	-	-	-	X
56	MG	GB	3009	-	-	-	X
56	MG	GB	3011	-	-	-	X
56	MG	GB	3015	-	-	-	X
56	MG	GB	3016	-	-	-	X
56	MG	GB	3021	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	GB	3039	-	-	-	X
56	MG	GB	3043	-	-	-	X
56	MG	GB	3047	-	-	-	X
56	MG	GB	3049	-	-	-	X
56	MG	GB	3051	-	-	-	X
56	MG	GB	3052	-	-	-	X
56	MG	GB	3056	-	-	-	X
56	MG	GB	3057	-	-	-	X
56	MG	GB	3061	-	-	-	X
56	MG	GB	3064	-	-	-	X
56	MG	GB	3069	-	-	-	X
56	MG	GB	3071	-	-	-	X
56	MG	GB	3074	-	-	-	X
56	MG	GB	3081	-	-	-	X
56	MG	GB	3090	-	-	-	X
56	MG	GB	3098	-	-	-	X
56	MG	GB	3103	-	-	-	X
56	MG	GB	3105	-	-	-	X
56	MG	GB	3108	-	-	-	X
56	MG	GB	3128	-	-	-	X
56	MG	GB	3141	-	-	-	X
56	MG	GB	3149	-	-	-	X
56	MG	GB	3169	-	-	-	X
56	MG	GB	3171	-	-	-	X
56	MG	GB	3174	-	-	-	X
56	MG	GB	3176	-	-	-	X
56	MG	GB	3177	-	-	-	X
56	MG	GB	3194	-	-	-	X
56	MG	GB	3203	-	-	-	X
56	MG	GB	3204	-	-	-	X
56	MG	GB	3220	-	-	-	X
56	MG	GB	3222	-	-	-	X
56	MG	GB	3224	-	-	-	X
56	MG	GB	3228	-	-	-	X
56	MG	GB	3230	-	-	-	X
56	MG	GB	3234	-	-	-	X
56	MG	GB	3242	-	-	-	X
56	MG	GB	3268	-	-	-	X
56	MG	GB	3275	-	-	-	X
56	MG	GB	3297	-	-	-	X
56	MG	GB	3304	-	-	-	X
56	MG	GB	3305	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	GB	3309	-	-	-	X
56	MG	GB	3313	-	-	-	X
56	MG	GB	3332	-	-	-	X
56	MG	GB	3349	-	-	-	X
56	MG	GB	3352	-	-	-	X
56	MG	GB	3359	-	-	-	X
56	MG	GB	3362	-	-	-	X
56	MG	GB	3368	-	-	-	X
56	MG	GB	3384	-	-	-	X
56	MG	GB	3421	-	-	-	X
56	MG	GB	3435	-	-	-	X
56	MG	GB	3455	-	-	-	X
56	MG	GB	3489	-	-	-	X
56	MG	GB	3491	-	-	-	X
56	MG	GB	3500	-	-	-	X
56	MG	GB	3503	-	-	-	X
56	MG	GB	3512	-	-	-	X
56	MG	GB	3540	-	-	-	X
56	MG	GB	3593	-	-	-	X
56	MG	GB	3600	-	-	-	X
56	MG	GB	3601	-	-	-	X
56	MG	GB	3604	-	-	-	X
56	MG	GB	3606	-	-	-	X
56	MG	GB	3624	-	-	-	X
56	MG	GB	3626	-	-	-	X
56	MG	GB	3643	-	-	-	X
56	MG	GB	3645	-	-	-	X
56	MG	GB	3650	-	-	-	X
56	MG	GB	3660	-	-	-	X
56	MG	GB	3668	-	-	-	X
56	MG	GB	3673	-	-	-	X
56	MG	GB	3678	-	-	-	X
56	MG	GB	3686	-	-	-	X
56	MG	GB	3695	-	-	-	X
56	MG	GB	3697	-	-	-	X
56	MG	GB	3707	-	-	-	X
56	MG	GB	3710	-	-	-	X
56	MG	GB	3711	-	-	-	X
56	MG	H	202	-	-	-	X
56	MG	HB	202	-	-	-	X
56	MG	HB	205	-	-	-	X
56	MG	HD	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	I	202	-	-	-	X
56	MG	IA	102	-	-	-	X
56	MG	IA	116	-	-	-	X
56	MG	JA	403	-	-	-	X
56	MG	K	204	-	-	-	X
56	MG	KB	301	-	-	-	X
56	MG	KC	102	-	-	-	X
56	MG	L	201	-	-	-	X
56	MG	LA	301	-	-	-	X
56	MG	LB	302	-	-	-	X
56	MG	LB	303	-	-	-	X
56	MG	LB	305	-	-	-	X
56	MG	M	203	-	-	-	X
56	MG	M	207	-	-	-	X
56	MG	MA	301	-	-	-	X
56	MG	MB	201	-	-	-	X
56	MG	N	201	-	-	-	X
56	MG	O	202	-	-	-	X
56	MG	OC	404	-	-	-	X
56	MG	PB	203	-	-	-	X
56	MG	Q	202	-	-	-	X
56	MG	QB	205	-	-	-	X
56	MG	R	202	-	-	-	X
56	MG	RA	202	-	-	-	X
56	MG	RB	205	-	-	-	X
56	MG	RB	206	-	-	-	X
56	MG	RC	303	-	-	-	X
56	MG	RC	306	-	-	-	X
56	MG	RC	311	-	-	-	X
56	MG	SA	203	-	-	-	X
56	MG	SB	203	-	-	-	X
56	MG	SC	201	-	-	-	X
56	MG	TB	202	-	-	-	X
56	MG	VB	205	-	-	-	X
56	MG	VB	207	-	-	-	X
56	MG	WA	101	-	-	-	X
56	MG	WB	202	-	-	-	X
56	MG	X	105	-	-	-	X
56	MG	XB	201	-	-	-	X
56	MG	YB	206	-	-	-	X
56	MG	YC	201	-	-	-	X
56	MG	YC	204	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 300991 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is DNA/RNA hybrid called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	FB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	GB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	HB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	IB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	NC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	JB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	KB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	LB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	MB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	NB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	OB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	PB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	QB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	RB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
14	SB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	TB	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	110	Total	C	N	O		0	0	0
			877	553	175	149				
16	UB	110	Total	C	N	O		0	0	0
			877	553	175	149				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	VB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	WB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	XB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	YB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	ZB	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	AC	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	BC	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	CC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	DC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	EC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	FC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	GC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	HC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	IC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	JC	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	KC	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	LC	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is DNA/RNA hybrid called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	MC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	258	Total	C	N	O	S	0	0	0
			2005	1227	380	390	8			
35	OC	258	Total	C	N	O	S	0	0	0
			2005	1227	380	390	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	361	LEU	-	expression tag	UNP P0A7I0
JA	362	GLU	-	expression tag	UNP P0A7I0
JA	363	HIS	-	expression tag	UNP P0A7I0

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	364	HIS	-	expression tag	UNP P0A7I0
JA	365	HIS	-	expression tag	UNP P0A7I0
JA	366	HIS	-	expression tag	UNP P0A7I0
JA	367	HIS	-	expression tag	UNP P0A7I0
JA	368	HIS	-	expression tag	UNP P0A7I0
OC	361	LEU	-	expression tag	UNP P0A7I0
OC	362	GLU	-	expression tag	UNP P0A7I0
OC	363	HIS	-	expression tag	UNP P0A7I0
OC	364	HIS	-	expression tag	UNP P0A7I0
OC	365	HIS	-	expression tag	UNP P0A7I0
OC	366	HIS	-	expression tag	UNP P0A7I0
OC	367	HIS	-	expression tag	UNP P0A7I0
OC	368	HIS	-	expression tag	UNP P0A7I0

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	PC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	QC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	RC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	SC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	TC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	PA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	UC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	VC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RA	127	Total	C	N	O		0	0	0
			1011	639	198	174				
43	WC	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	SA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	XC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	TA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	YC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	ZC	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	VA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	AD	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	BD	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	CD	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	DD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	ZA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	ED	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	AB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	FD	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	GD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	HD	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	DB	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	ID	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	2	Total	Mg	0	0
			2	2		
56	CA	3	Total	Mg	0	0
			3	3		
56	VC	2	Total	Mg	0	0
			2	2		
56	RC	11	Total	Mg	0	0
			11	11		
56	WB	3	Total	Mg	0	0
			3	3		
56	PA	3	Total	Mg	0	0
			3	3		
56	A	287	Total	Mg	0	0
			287	287		
56	BC	9	Total	Mg	0	0
			9	9		
56	PB	4	Total	Mg	0	0
			4	4		
56	NA	3	Total	Mg	0	0
			3	3		
56	JA	13	Total	Mg	0	0
			13	13		
56	HC	2	Total	Mg	0	0
			2	2		
56	FB	349	Total	Mg	0	0
			349	349		
56	YB	7	Total	Mg	0	0
			7	7		
56	Q	4	Total	Mg	0	0
			4	4		
56	UB	1	Total	Mg	0	0
			1	1		
56	WC	2	Total	Mg	0	0
			2	2		
56	H	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	C	44	Total 44	Mg 44	0	0
56	XC	2	Total 2	Mg 2	0	0
56	OB	2	Total 2	Mg 2	0	0
56	MC	1	Total 1	Mg 1	0	0
56	CD	3	Total 3	Mg 3	0	0
56	YA	1	Total 1	Mg 1	0	0
56	KA	4	Total 4	Mg 4	0	0
56	UA	3	Total 3	Mg 3	0	0
56	GA	1	Total 1	Mg 1	0	0
56	ZC	2	Total 2	Mg 2	0	0
56	X	8	Total 8	Mg 8	0	0
56	SC	7	Total 7	Mg 7	0	0
56	S	8	Total 8	Mg 8	0	0
56	DD	1	Total 1	Mg 1	0	0
56	J	3	Total 3	Mg 3	0	0
56	TA	1	Total 1	Mg 1	0	0
56	E	10	Total 10	Mg 10	0	0
56	GD	1	Total 1	Mg 1	0	0
56	EA	2	Total 2	Mg 2	0	0
56	CC	2	Total 2	Mg 2	0	0
56	XB	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	TB	4	Total 4	Mg 4	0	0
56	VA	3	Total 3	Mg 3	0	0
56	Z	3	Total 3	Mg 3	0	0
56	RA	4	Total 4	Mg 4	0	0
56	DA	3	Total 3	Mg 3	0	0
56	U	2	Total 2	Mg 2	0	0
56	L	5	Total 5	Mg 5	0	0
56	PC	5	Total 5	Mg 5	0	0
56	G	11	Total 11	Mg 11	0	0
56	Y	5	Total 5	Mg 5	0	0
56	NB	3	Total 3	Mg 3	0	0
56	ED	2	Total 2	Mg 2	0	0
56	JB	13	Total 13	Mg 13	0	0
56	FC	1	Total 1	Mg 1	0	0
56	DB	1	Total 1	Mg 1	0	0
56	BA	3	Total 3	Mg 3	0	0
56	W	8	Total 8	Mg 8	0	0
56	N	6	Total 6	Mg 6	0	0
56	OA	4	Total 4	Mg 4	0	0
56	MB	7	Total 7	Mg 7	0	0
56	AA	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	SB	4	Total 4	Mg 4	0	0
56	QC	4	Total 4	Mg 4	0	0
56	AD	1	Total 1	Mg 1	0	0
56	MA	5	Total 5	Mg 5	0	0
56	I	7	Total 7	Mg 7	0	0
56	IB	5	Total 5	Mg 5	0	0
56	KC	5	Total 5	Mg 5	0	0
56	GC	2	Total 2	Mg 2	0	0
56	ZA	3	Total 3	Mg 3	0	0
56	LA	2	Total 2	Mg 2	0	0
56	CB	1	Total 1	Mg 1	0	0
56	HD	1	Total 1	Mg 1	0	0
56	TC	1	Total 1	Mg 1	0	0
56	VB	8	Total 8	Mg 8	0	0
56	RB	6	Total 6	Mg 6	0	0
56	IA	21	Total 21	Mg 21	0	0
56	P	4	Total 4	Mg 4	0	0
56	NC	14	Total 14	Mg 14	0	0
56	K	9	Total 9	Mg 9	0	0
56	LB	5	Total 5	Mg 5	0	0
56	B	944	Total 944	Mg 944	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	HA	2	Total 2	Mg 2	0	0
56	O	3	Total 3	Mg 3	0	0
56	DC	3	Total 3	Mg 3	0	0
56	WA	1	Total 1	Mg 1	0	0
56	T	5	Total 5	Mg 5	0	0
56	R	2	Total 2	Mg 2	0	0
56	HB	32	Total 32	Mg 32	0	0
56	M	8	Total 8	Mg 8	0	0
56	FA	4	Total 4	Mg 4	0	0
56	D	2	Total 2	Mg 2	0	0
56	YC	6	Total 6	Mg 6	0	0
56	BB	1	Total 1	Mg 1	0	0
56	UC	2	Total 2	Mg 2	0	0
56	XA	3	Total 3	Mg 3	0	0
56	SA	3	Total 3	Mg 3	0	0
56	EC	4	Total 4	Mg 4	0	0
56	QB	6	Total 6	Mg 6	0	0
56	OC	7	Total 7	Mg 7	0	0
56	KB	4	Total 4	Mg 4	0	0
56	GB	812	Total 812	Mg 812	0	0
56	ZB	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	F	15	Total	Mg	0	0
			15	15		

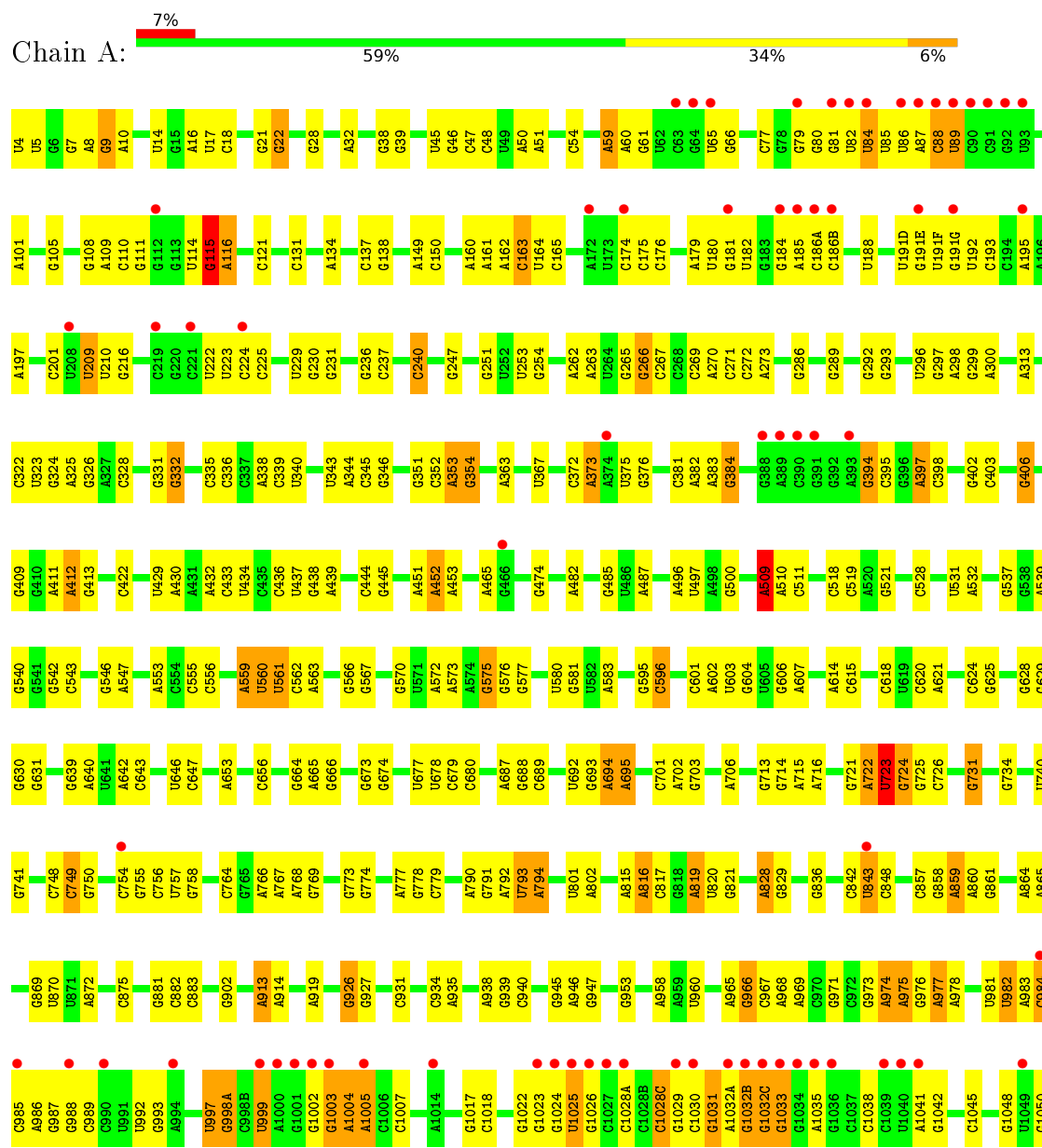
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

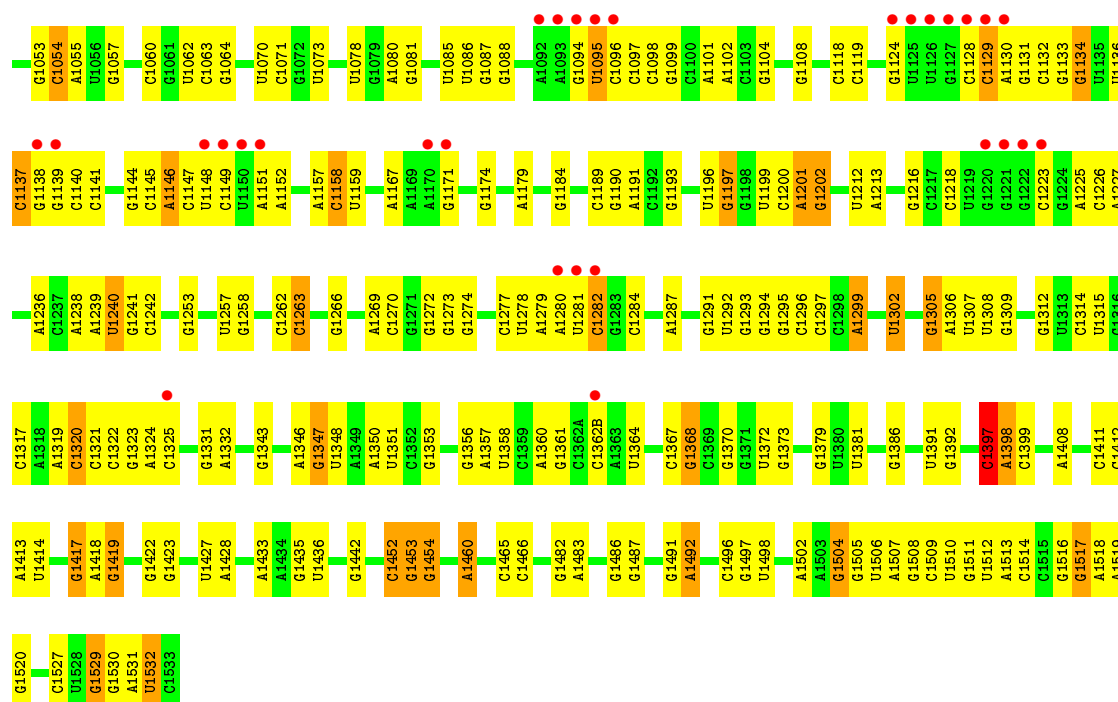
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	1	Total	Zn	0	0
			1	1		
57	CA	1	Total	Zn	0	0
			1	1		
57	AC	1	Total	Zn	0	0
			1	1		
57	V	1	Total	Zn	0	0
			1	1		
57	GA	1	Total	Zn	0	0
			1	1		
57	IC	1	Total	Zn	0	0
			1	1		
57	DA	1	Total	Zn	0	0
			1	1		
57	GC	1	Total	Zn	0	0
			1	1		
57	HC	1	Total	Zn	0	0
			1	1		
57	LC	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

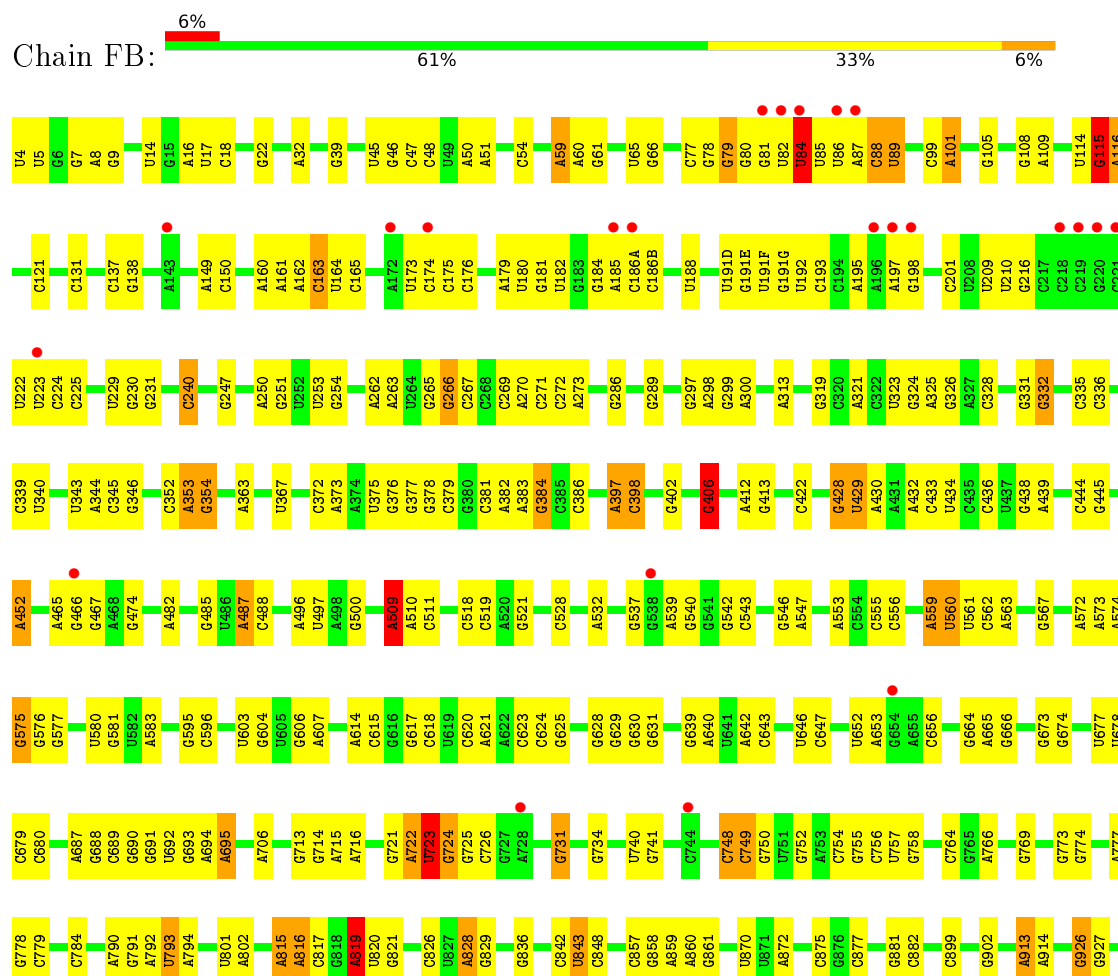
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S ribosomal RNA



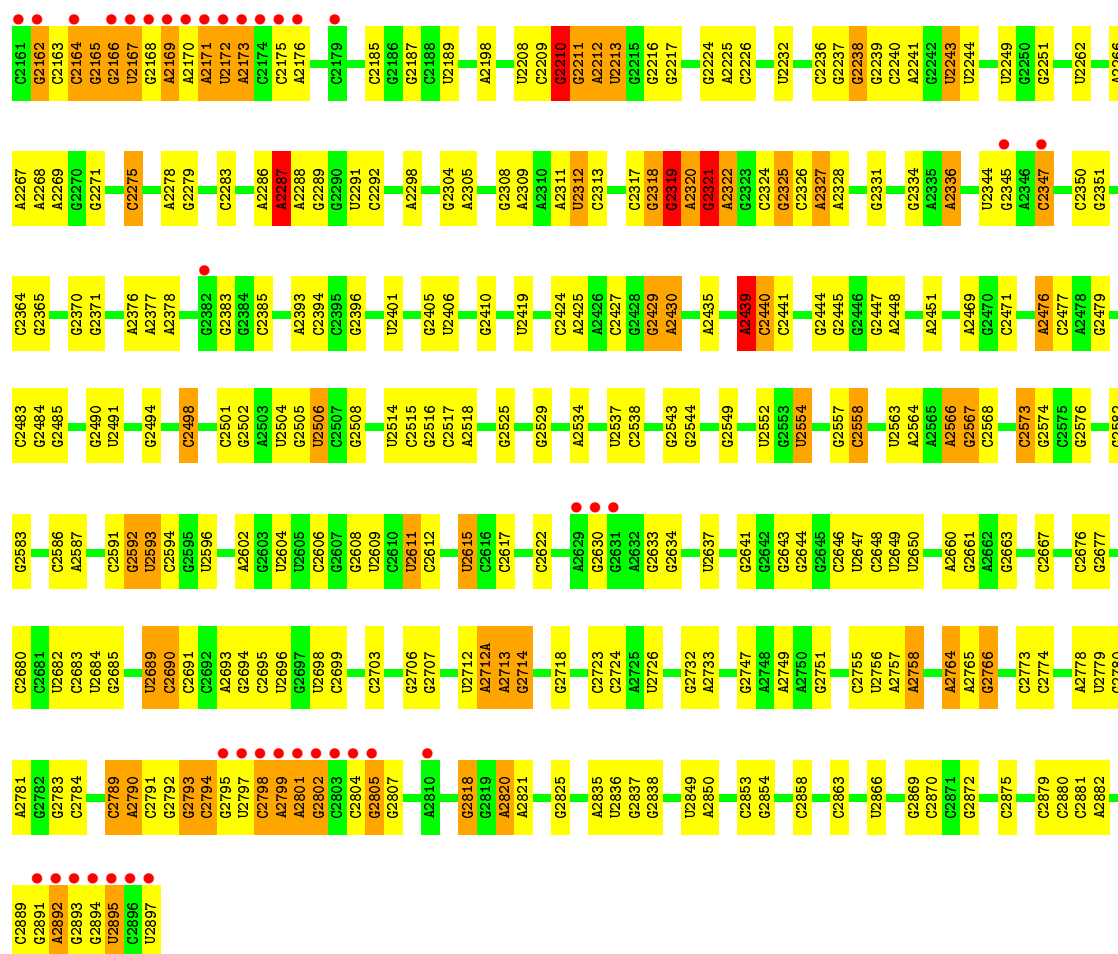


• Molecule 1: 16S ribosomal RNA

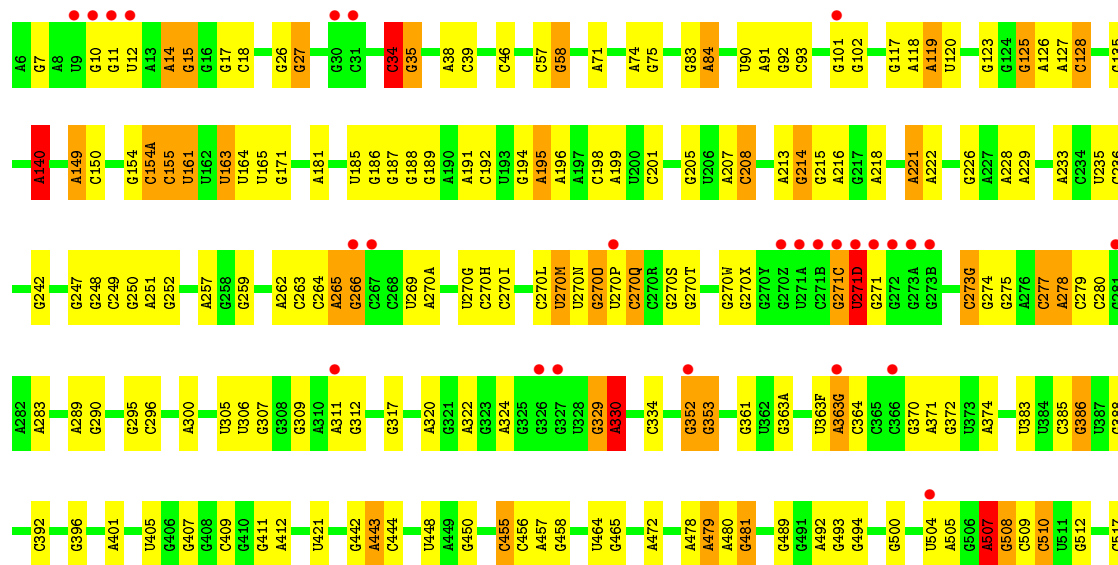


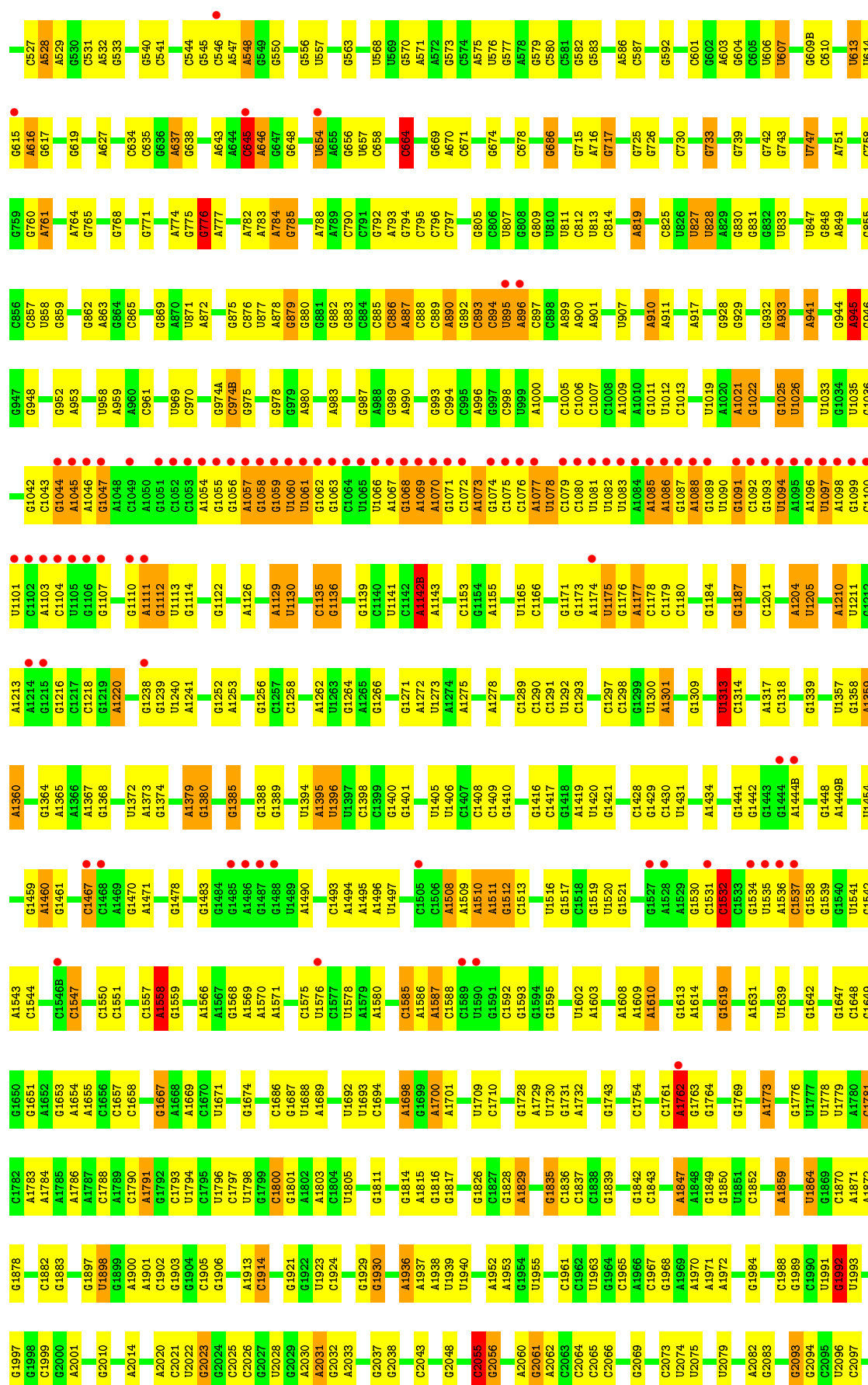


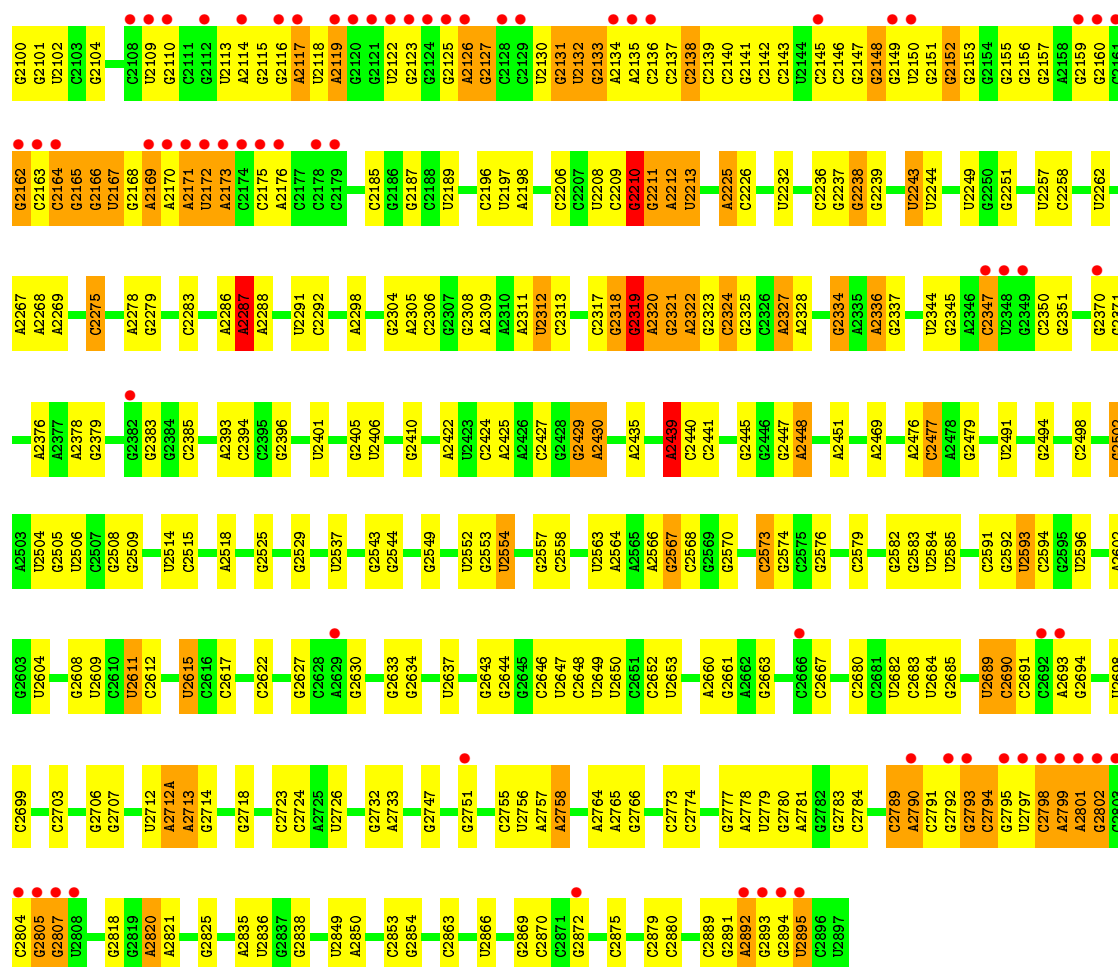
U2096	C1999	U1898	A1784	U1659	C1550	G1459	A1360	G1245	G1131	G1062	A872	A777	G644
C2097	G2000	G1899	A1785	C1660	C1551	A1460	G1364	G1246	C1135	G1063	C876	A782	C645
G2100	A2001	A1900	A1786	C1663	C1557	G1461	A1365	G1252	G1136	C1064	U877	A783	A646
G2101	A2005	A1901	A1787	C1666	C1558	G1466	A1366	A1253	G1139	U1065	A878	A784	G647
U2102	C2006	G1788	C1788	G1667	A1559	C1467	G1368	G1256	G1140	U1066	G879	G785	G648
G2103	A2014	C1905	A1790	A1668	G1559	C1467	G1368	C1257	U1141	G1068	G880	A788	U654
G2104	A2015	C1905	A1791	A1669	A1566	A1471	A1372	C1258	A1142B	A1069	G882	A789	G656
G2110	U2016	G1906	U1796	C1670	A1567	A1472	A1373	C1259	A1143	A1070	G883	C790	U657
G2111	A1913	C1914	C1797	U1671	A1568	A1478	A1379	C1261	G1143	C1072	C884	C791	C658
G2112	A2020	C1914	C1797	U1671	A1569	G1478	G1380	A1262	C1153	A1073	C885	G792	C664
U2113	C2021	U1915	U1799	G1674	A1570	G1483	G1380	U1263	C1153	G1074	C886	C796	
A2114	U2022	A1916	G1800	G1674	A1571	G1483	G1380	G1264	G1154	A887	C888	C797	C671
G2115	G2023	G1801	G1801	G1682	C1577	G1483	G1385	A1265	A1155	C1076	C889	C799	C672
G2116	C2024	A1919	A1802	C1686	C1574	A1490	G1388	C1261	U1165	U1078	A890	A800	C673
A2117	C2025	A1920	A1803	G1687	U1575	G1491	G1389	A1262	C1166	C1079	G892	U803	G674
U2118	C2026	G1921	A1804	U1688	U1576	G1492	G1389	G1264	G1170	U1080	C893	A804	C678
G2119	G2027	U1805	U1805	U1688	C1577	C1493	U1394	C1269	G1171	U1081	C894	A804	
A2120	U2028	U1923	G1811	U1689	U1578	A1494	A1395	C1289	G1173	U1082	A896	C806	G682
G2121	C2031	U1924	G1811	U1692	C1585	A1496	U1397	C1290	A1174	U1083	C897	U807	
U2122	G2032	G1929	A1815	U1693	U1586	U1497	C1398	C1291	U1175	A1085	C898	U811	G686
G2123	A2033	G1930	G1816	C1694	A1587	C1498	C1398	C1292	G1176	A1086	A899	C812	G700
G2124	C2040	U1935	A1821	U1699	C1588	C1499	G1401	C1293	A1177	U1087	A900	U813	
A2126	U2041	A1936	G1826	C1701	G1592	A1508	G1401	C1297	C1178	U1088	A901	C814	G715
G2127	C2042	A1937	U1826	C1710	G1593	A1509	C1403	C1298	C1179	G1089	U907	A819	G717
C2043	A1938	U1939	U1829	U1709	C1594	A1510	U1404	G1299	C1180	U1090	U907	A819	
U2130	U1940	U1940	G1835	C1711	U1602	C1512	U1406	C1301	G1184	C1092	A910	C825	G725
G2131	G1948	U1948	G1839	C1712	A1603	C1513	C1408	A1301	C1185	G1093	A911	U826	G726
U2132	C2048	U1948	G1835	U1709	U1602	U1514	C1409	G1309	G1187	U1094	A917	U827	C730
C2053	A2054	G1839	A1932	G1728	A1608	U1516	C1409	U1309	G1187	A1095	G929	A829	
A2054	C2055	U1952	A1932	C1729	A1609	C1518	G1417	U1317	C1201	U1097	A911	C830	G733
G2056	U1953	A1953	G1842	U1730	A1609	C1518	G1417	C1317	G1099	G831	G932	U832	G742
C2137	G1954	C1843	C1843	G1731	A1610	G1521	A1419	C1302	C1202	C1100	A933	C832	G743
A2059	U1955	U1955	A1847	G1743	A1614	G1522	U1420	A1322	G1203	U1101	A941	U833	
C2060	G2061	U1963	A1848	C1732	U1621	U1522	G1421	A1322	A1204	C1102			
G2061	C2062	G1964	U1849	C1733	A1614	U1522	G1421	A1322	U1205	A1103	U847	U747	
C2063	A1965	C1965	G1850	C1734	U1621	U1522	G1421	A1322	U1205	A1104	G848	A849	A751
C2064	U1966	A1966	U1851	C1735	A1631	U1529	G1428	G1325	A1210	U1105	G944	A849	
C2065	C1967	C1967	C1852	C1736	U1639	A1530	C1429	G1332	C1211	U1106	G946		
C2066	U1968	A1968	A1859	A1762	G1640	C1532	C1430	C1333	G1212	G1107	G947	G855	G758
G2146	A1859	G1969	G1859	G1764	A1641	C1533	U1431	C1333	G1212	U1108	G948	C856	G759
G2147	A1970	A1970	U1864	C1764	A1641	C1533	U1431	A1336	A1213	C1109	A1046	C857	G760
G2148	U1971	A1971	U1864	C1771	G1642	U1534	U1431	A1336	G1216	U1110	G952	U858	A761
U2149	C2073	U1972	G1869	C1772	U1647	U1535	A1434	A1339	C1217	G1111	A953	C859	
U2150	A2077	U1972	C1870	G1772	C1648	U1536	G1441	G1339	C1217	A1111	G944	U860	A764
C2151	G1984	A1871	A1871	A1773	C1648	C1537	G1441	C1218	C1218	G1112	U958	A861	G765
G2152	C2078	A1872	A1872	G1773	G1649	C1538	G1442	U1341	G1219	U1113	A959	G862	
G2153	U2079	G1878	G1878	G1776	G1650	G1539	G1442	U1341	A1220	G1114	A960	A863	G768
G2154	C1988	G1989	C1988	U1777	G1651	G1540	A1444B	C1345	G1235	G1122	C961	G864	
G2155	U1778	U1778	G1882	U1778	A1652	U1541	G1448	U1346	G1236				
G2156	G1992	G1883	A1883	U1779	G1653	U1542	G1448	G1347	G1236	A1126	A1057	U969	A774
G2157	U1993	A1780	A1780	A1953	A1654	A1543	A1449B	G1347	A1237	A1126	G1059	G869	G775
A2158	C1992	C1892	C1892	C1781	A1654	C1544	U1454	U1357	G1238			A870	G776
G2159	U2089	U1997	C1987	C1782	C1657	C1547	U1454	C1358	A1241	A1129	U1060	A870	G775
C2160	G1998	C1998	C1987	A1782	C1658	C1547	U1454	C1358	A1241	U1129	U1061	A871	G776



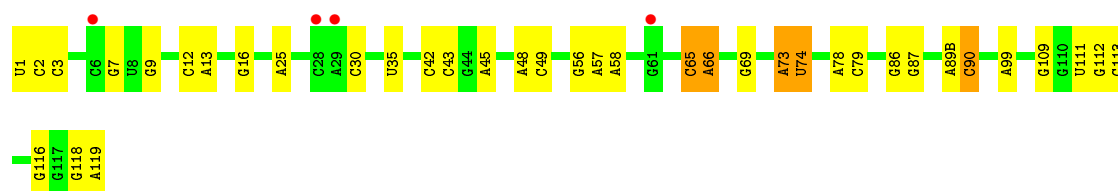
• Molecule 2: 25S ribosomal RNA



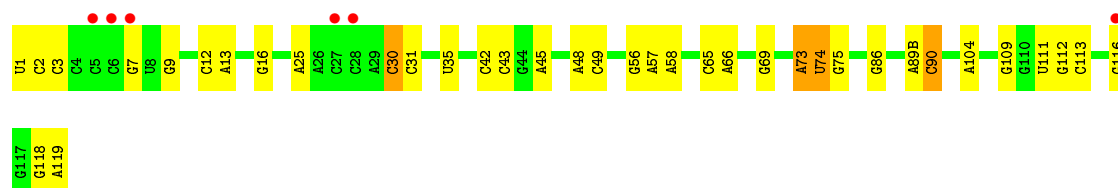




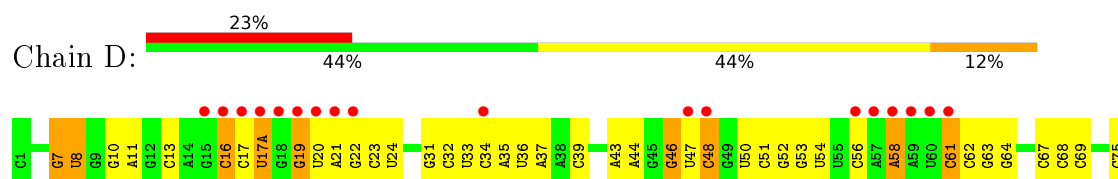
• Molecule 3: 5S ribosomal RNA



• Molecule 3: 5S ribosomal RNA



• Molecule 4: tRNA

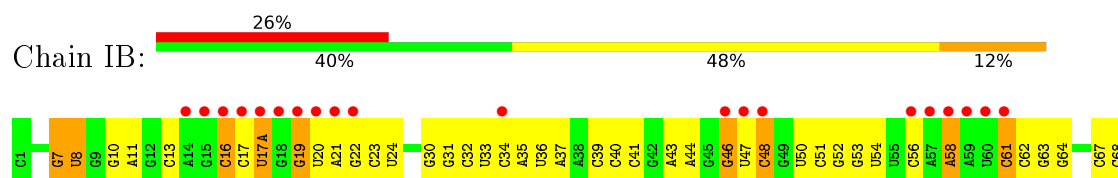


A76

- Molecule 4: tRNA

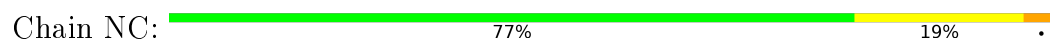


- Molecule 4: tRNA

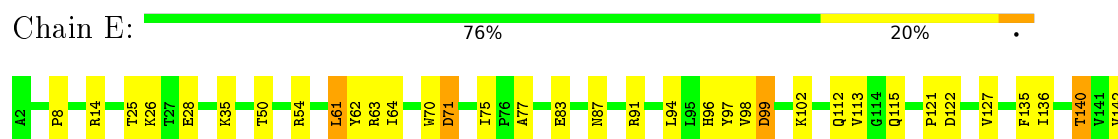


C69
C75
A76

- Molecule 4: tRNA



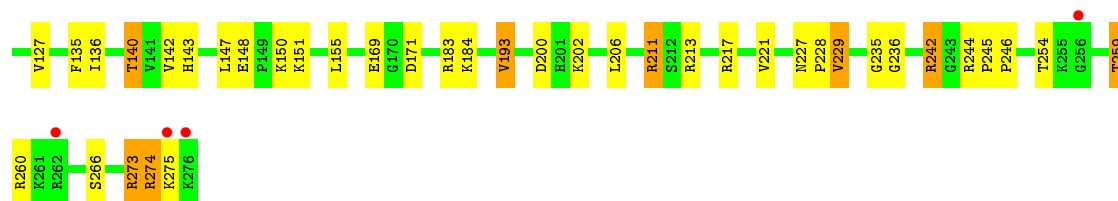
- Molecule 5: 50S ribosomal protein L2



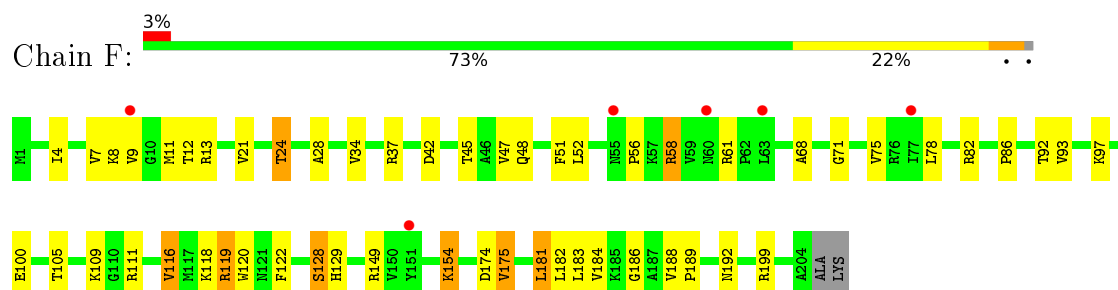
L147
E148
P149
K150
K151
L155
E169
G170
D171
R183
K184
V193
D200
K201
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L206
R211
V221
N227
P228
V229
G235
G236
E237
R242
P246
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K261
R262
R263
K264
R273
R274
K275
K276

- Molecule 5: 50S ribosomal protein L2

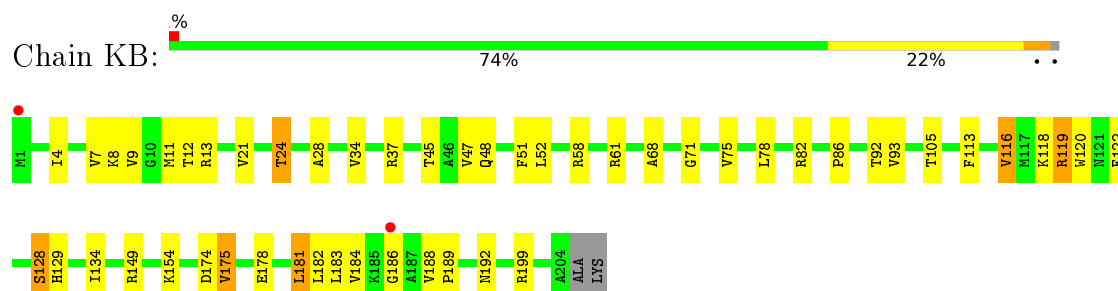




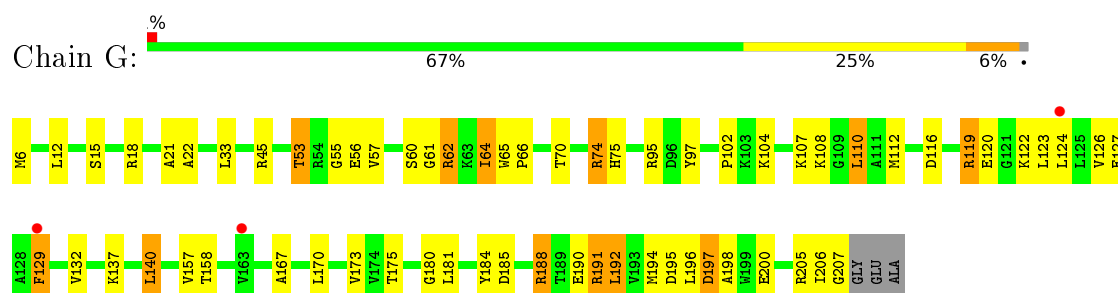
- Molecule 6: 50S ribosomal protein L3



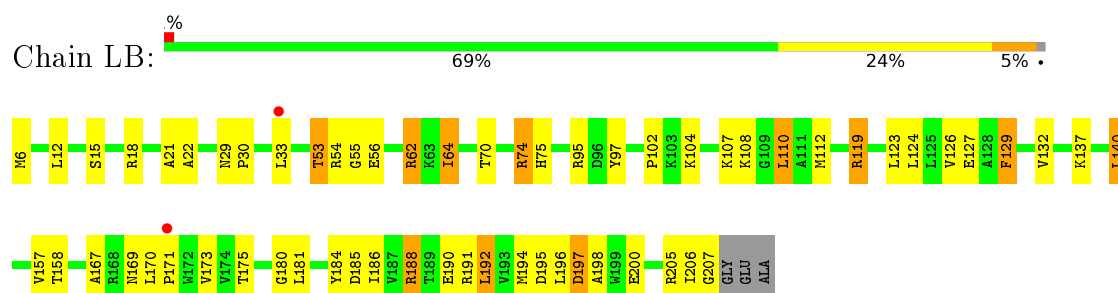
- Molecule 6: 50S ribosomal protein L3



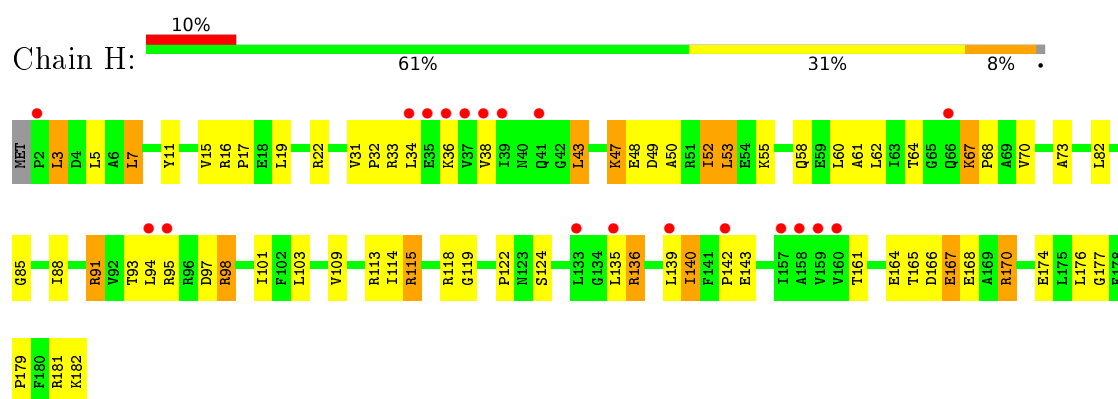
- Molecule 7: 50S ribosomal protein L4



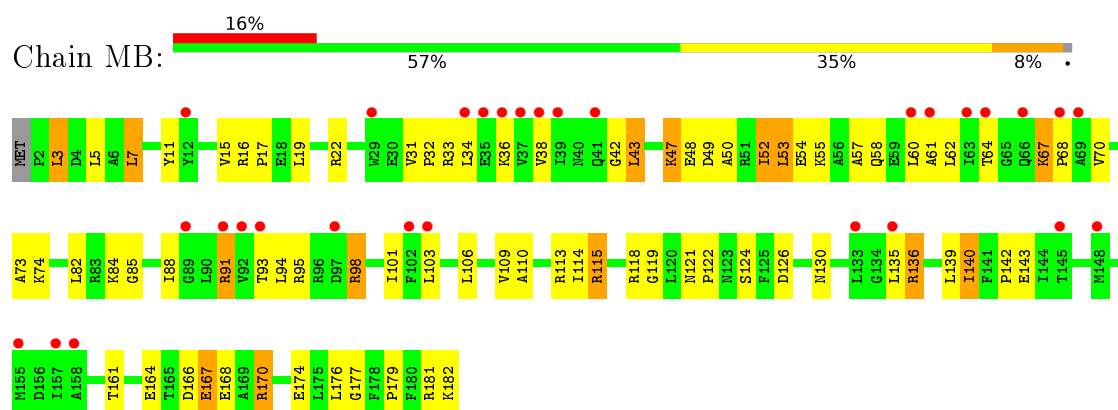
- Molecule 7: 50S ribosomal protein L4



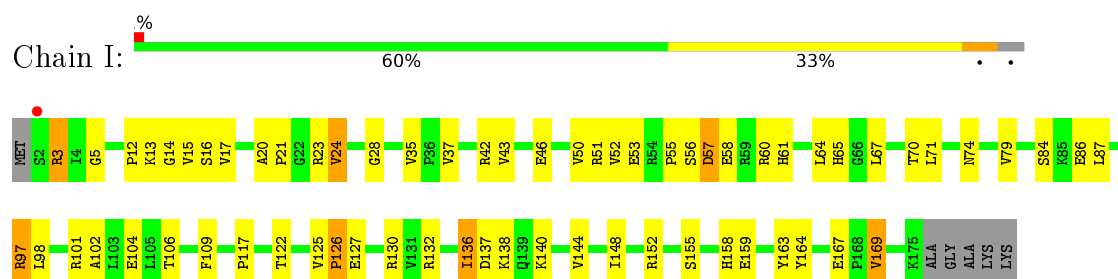
- Molecule 8: 50S ribosomal protein L5



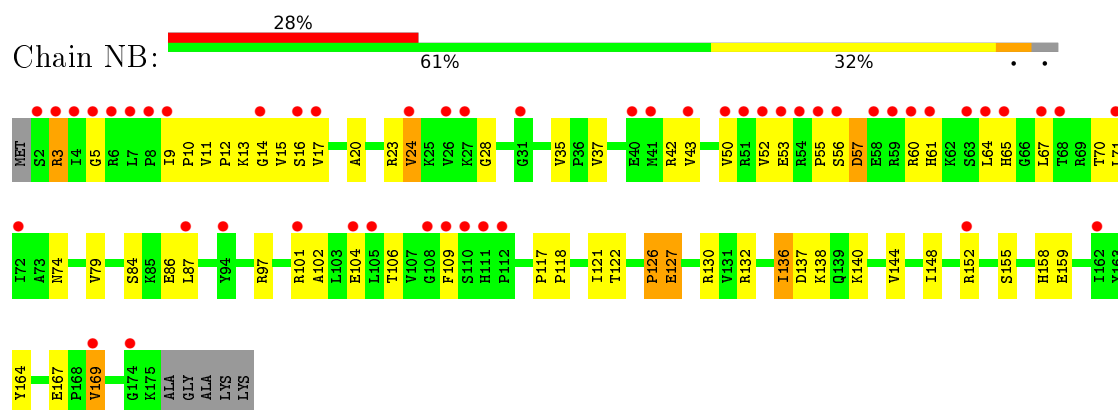
• Molecule 8: 50S ribosomal protein L5



• Molecule 9: 50S ribosomal protein L6

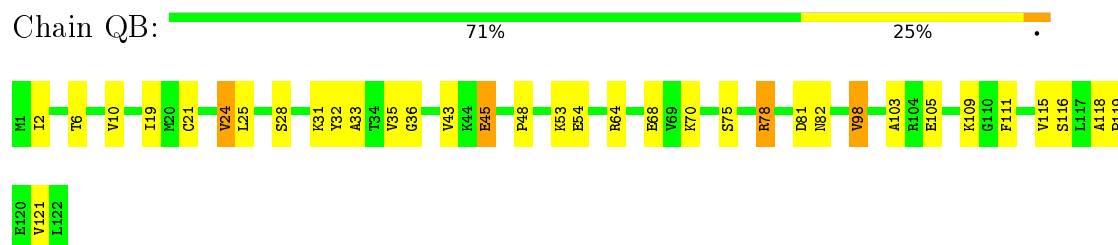


• Molecule 9: 50S ribosomal protein L6

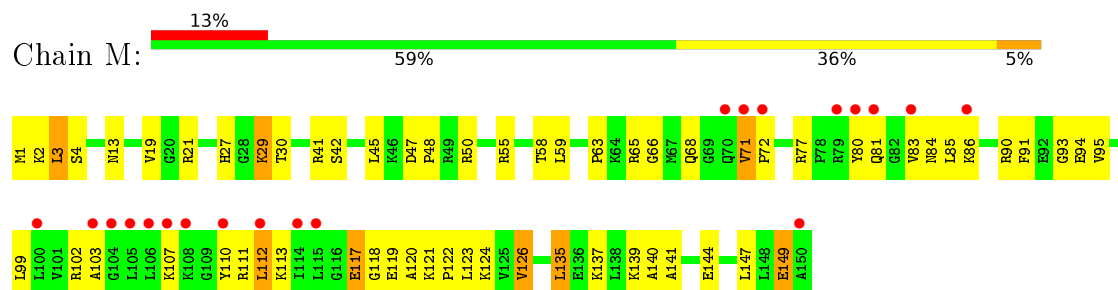


• Molecule 10: 50S ribosomal protein L9

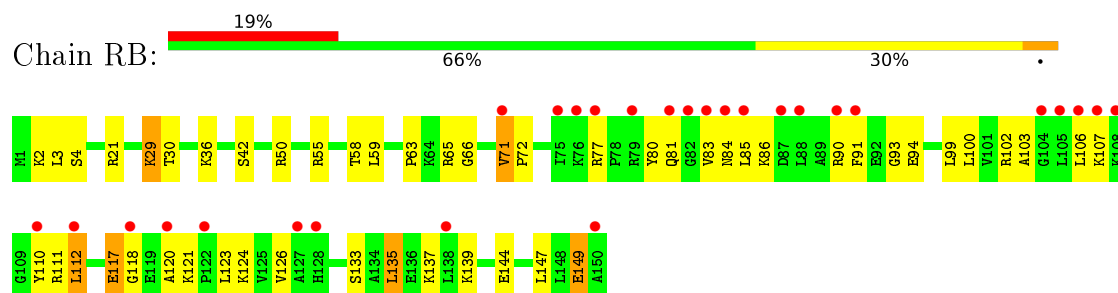
- Molecule 12: 50S ribosomal protein L14



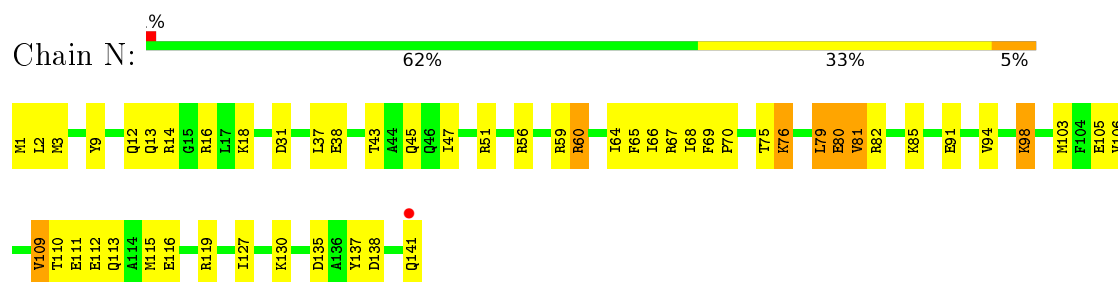
- Molecule 13: 50S ribosomal protein L15



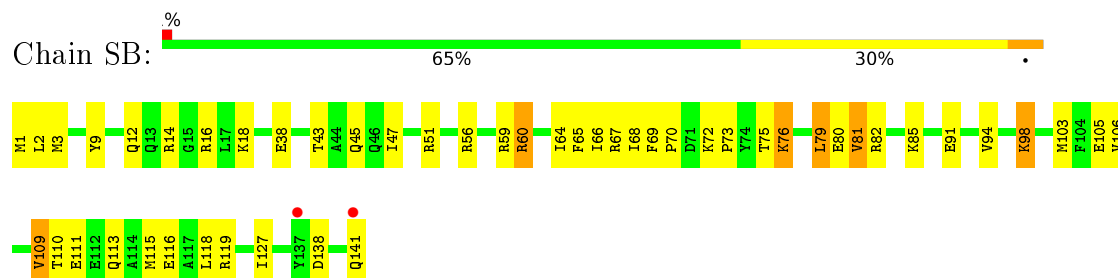
- Molecule 13: 50S ribosomal protein L15



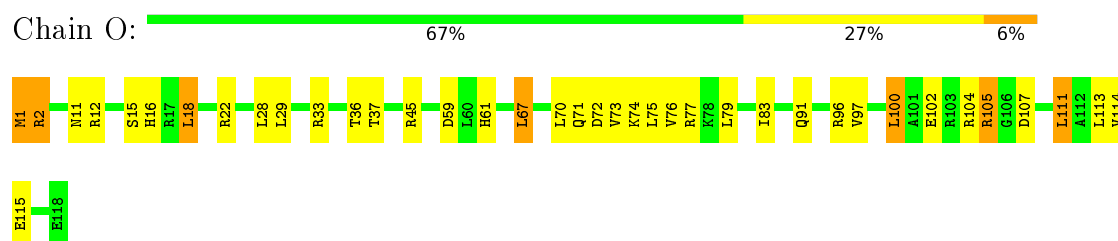
- Molecule 14: 50S ribosomal protein L16



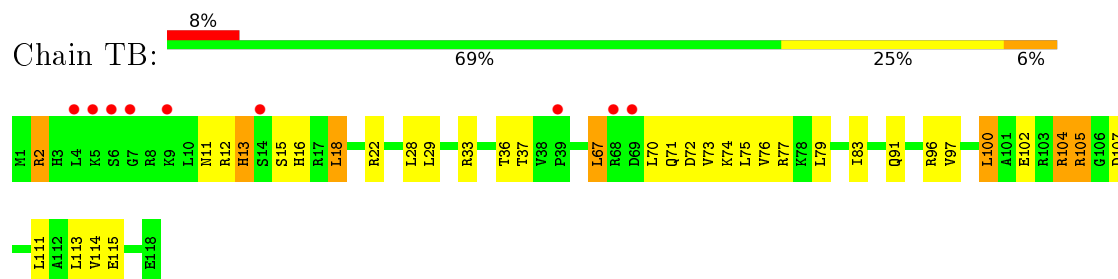
- Molecule 14: 50S ribosomal protein L16



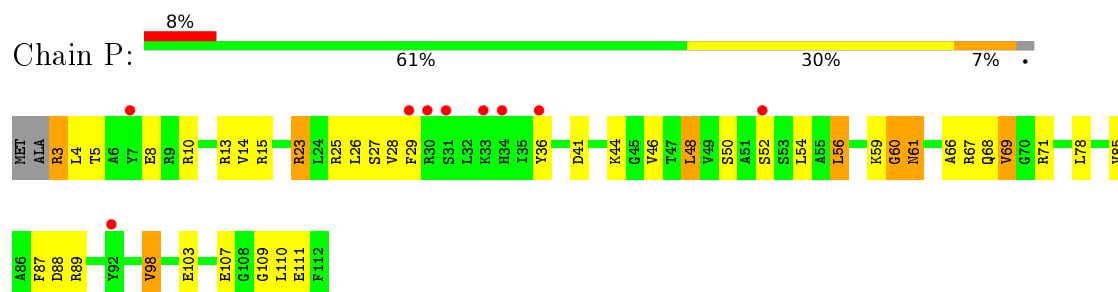
- Molecule 15: 50S ribosomal protein L17



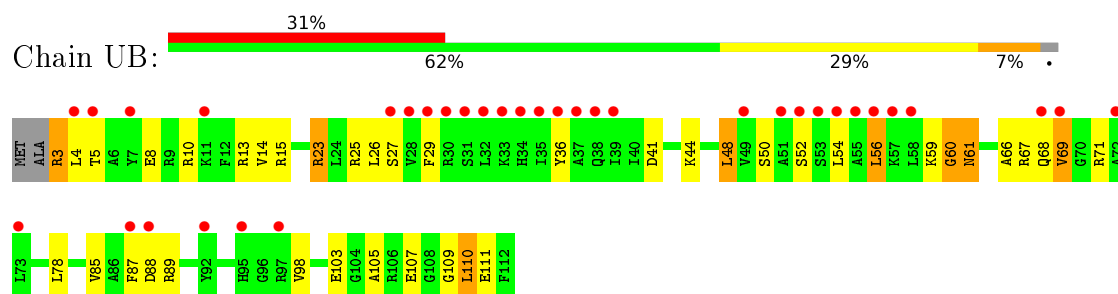
- Molecule 15: 50S ribosomal protein L17



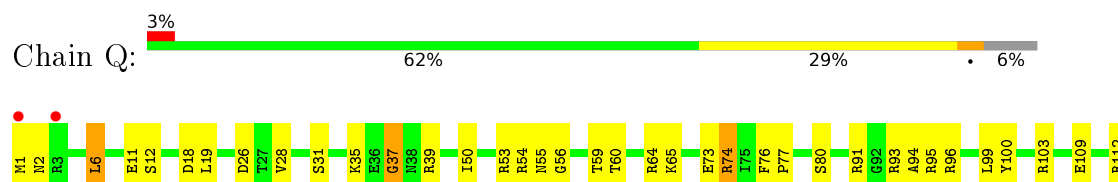
- Molecule 16: 50S ribosomal protein L18

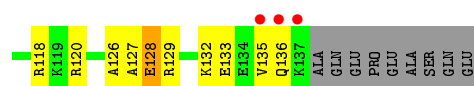


- Molecule 16: 50S ribosomal protein L18

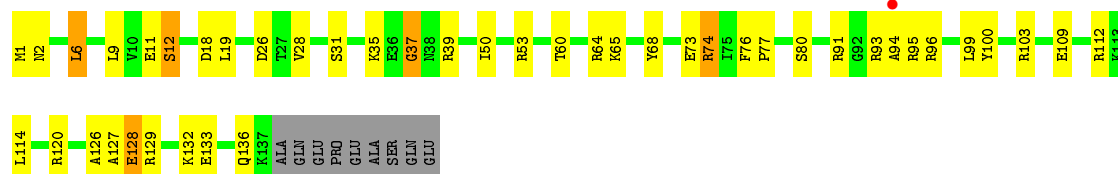


- Molecule 17: 50S ribosomal protein L19

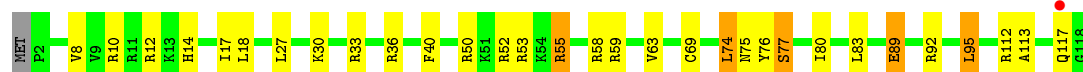




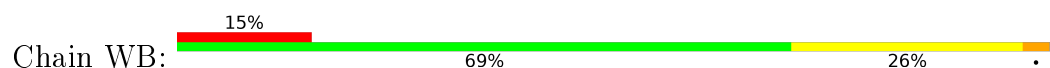
- Molecule 17: 50S ribosomal protein L19



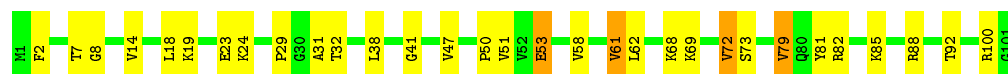
- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21

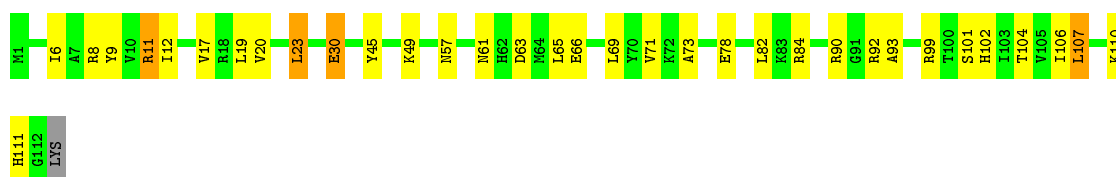


- Molecule 19: 50S ribosomal protein L21



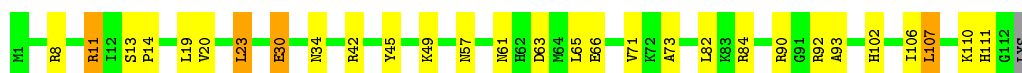
- Molecule 20: 50S ribosomal protein L22





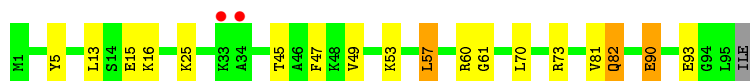
- Molecule 20: 50S ribosomal protein L22

Chain YB: 73% 22%



- Molecule 21: 50S ribosomal protein L23

Chain U: 2% 80% 16%



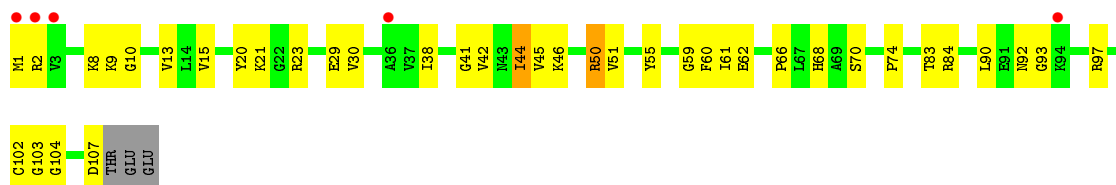
- Molecule 21: 50S ribosomal protein L23

Chain ZB: 6% 79% 17%



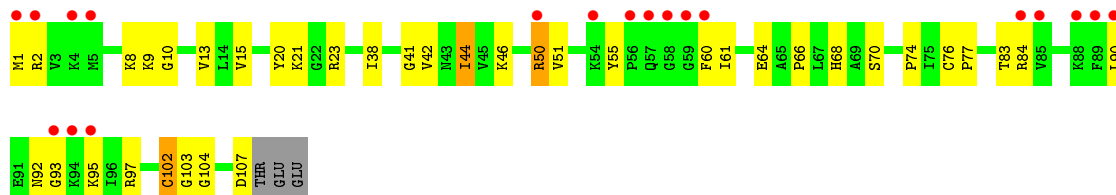
- Molecule 22: 50S ribosomal protein L24

Chain V: 5% 62% 34%

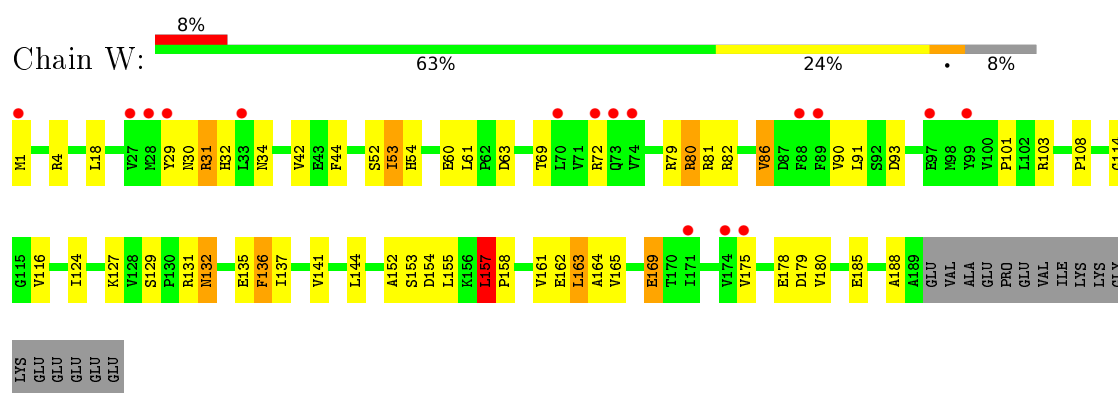


- Molecule 22: 50S ribosomal protein L24

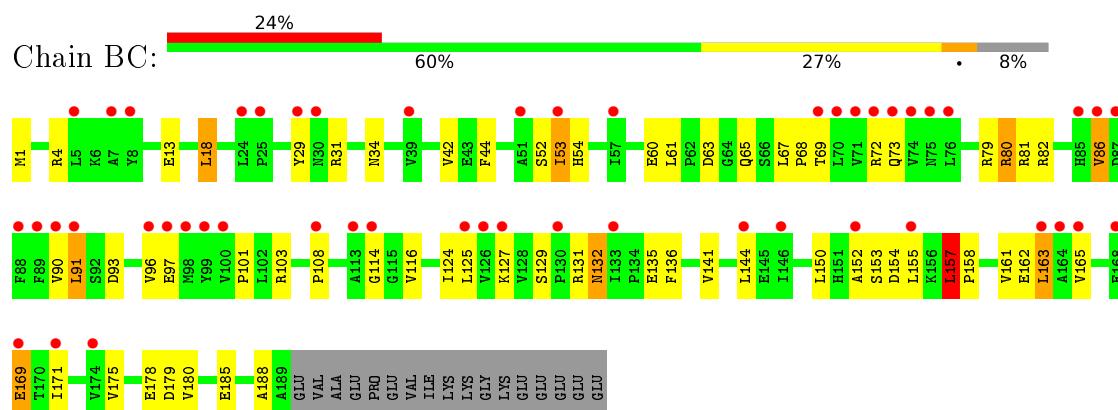
Chain AC: 17% 63% 32%



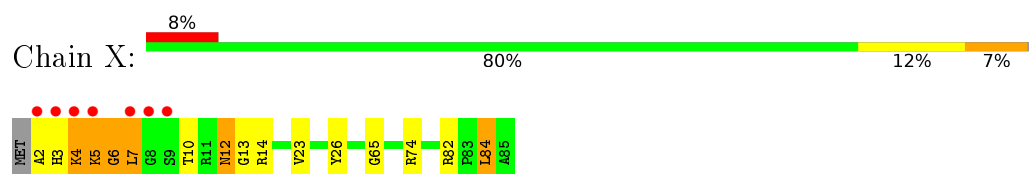
- Molecule 23: 50S ribosomal protein L25



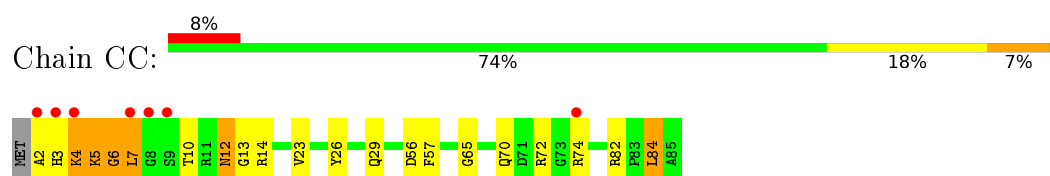
- Molecule 23: 50S ribosomal protein L25



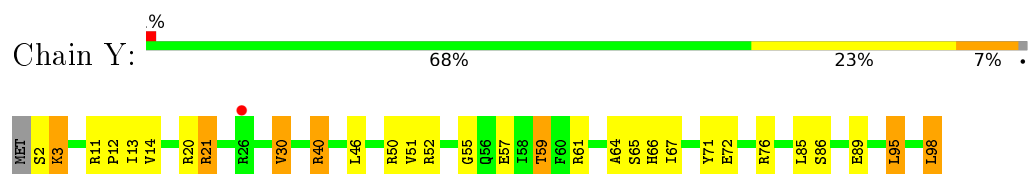
- Molecule 24: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L28





- Molecule 26: 50S ribosomal protein L29

Chain Z: 60% 33%



- Molecule 26: 50S ribosomal protein L29

Chain EC: 28% 64% 29%



- Molecule 27: 50S ribosomal protein L30

Chain AA: 2% 70% 25% 5%



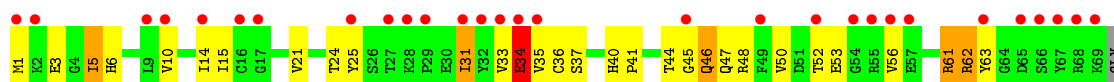
- Molecule 27: 50S ribosomal protein L30

Chain FC: 70% 25% 5%



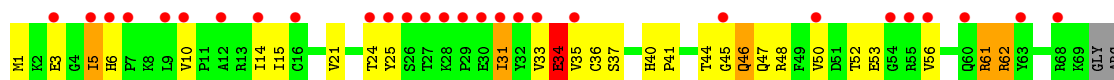
- Molecule 28: 50S ribosomal protein L31

Chain BA: 41% 55% 34% 7%




- Molecule 28: 50S ribosomal protein L31

Chain GC: 39% 56% 32% 7%




- Molecule 29: 50S ribosomal protein L32

Chain CA:  78% 20% .



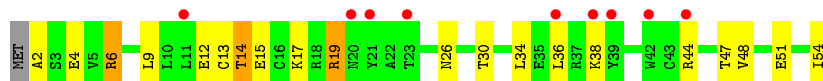
- Molecule 29: 50S ribosomal protein L32

Chain HC:  77% 22% .



- Molecule 30: 50S ribosomal protein L33

Chain DA:  17% 61% 31% 6% .



- Molecule 30: 50S ribosomal protein L33

Chain IC:  35% 63% 28% 7% .




- Molecule 31: 50S ribosomal protein L34

Chain EA:  67% 27% . .



- Molecule 31: 50S ribosomal protein L34

Chain JC:  78% 18% . .




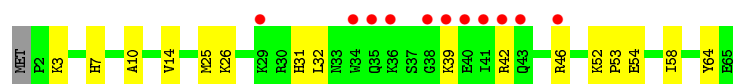
- Molecule 32: 50S ribosomal protein L35

Chain FA:  3% 66% 31% . .

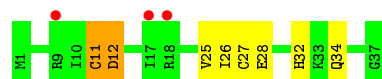
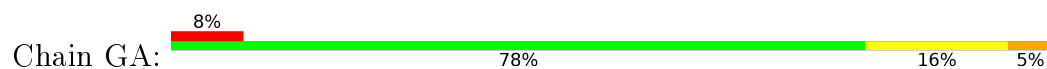


- Molecule 32: 50S ribosomal protein L35

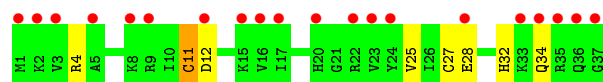
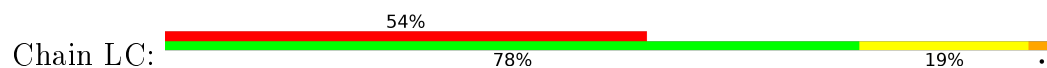
Chain KC:  17% 74% 25% .



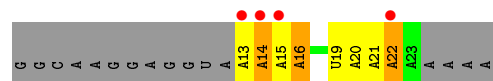
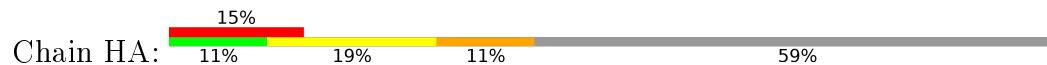
- Molecule 33: 50S ribosomal protein L36



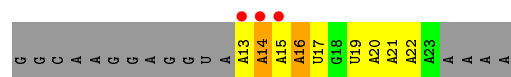
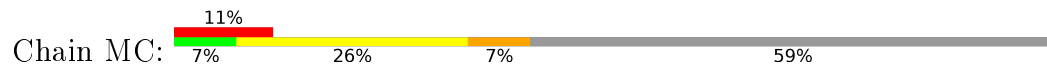
- Molecule 33: 50S ribosomal protein L36



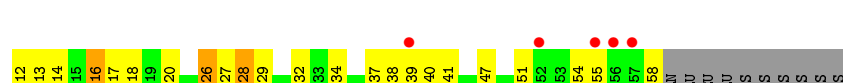
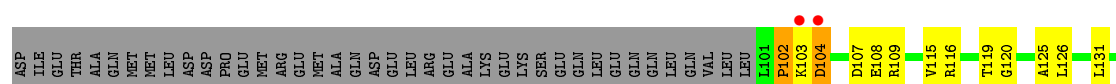
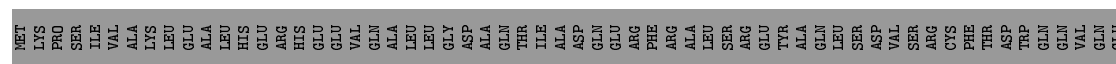
- Molecule 34: mRNA



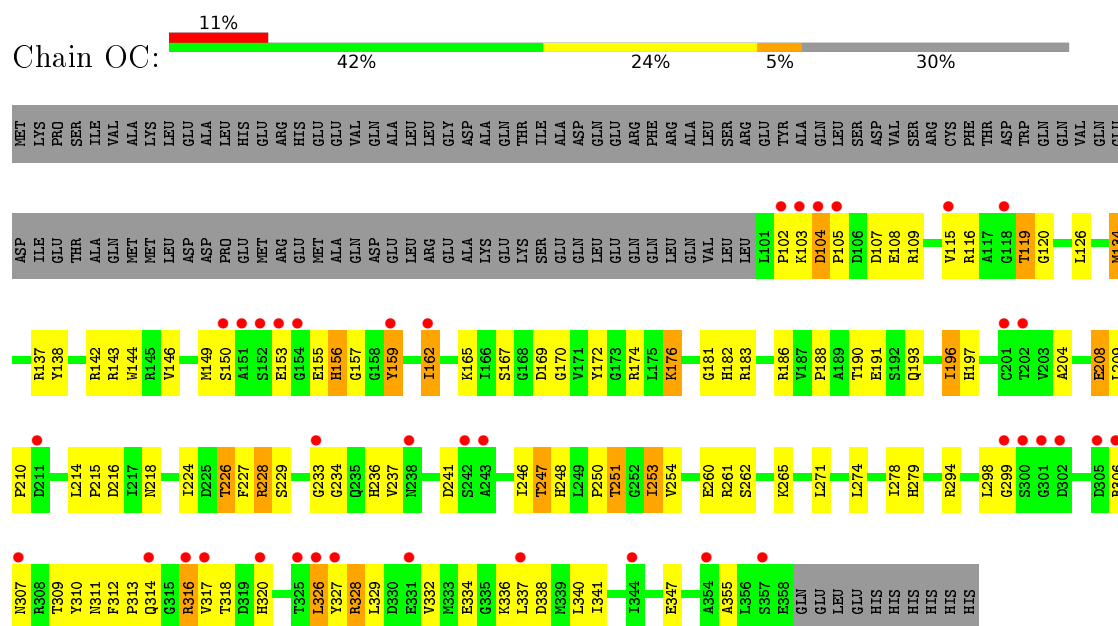
- Molecule 34: mRNA



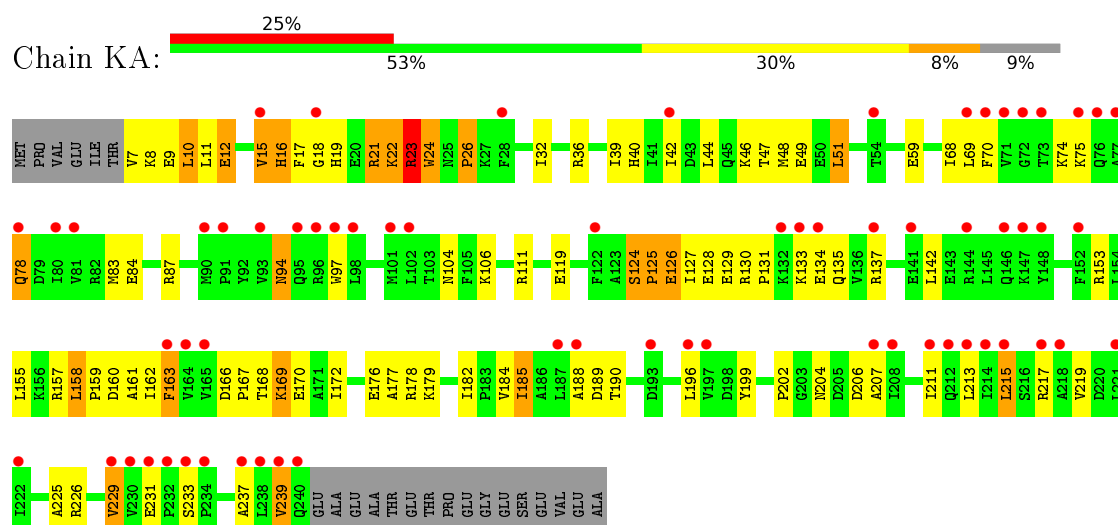
- Molecule 35: Peptide chain release factor 1



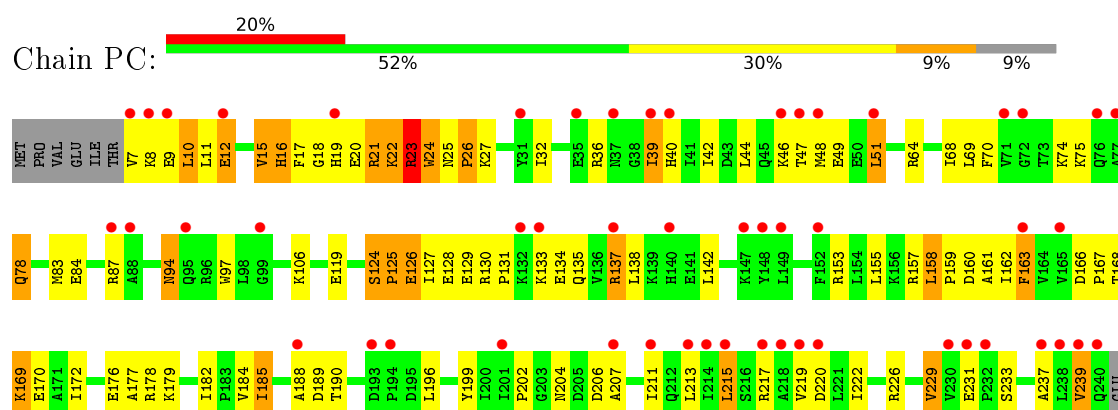
• Molecule 35: Peptide chain release factor 1



• Molecule 36: 30S ribosomal protein S2



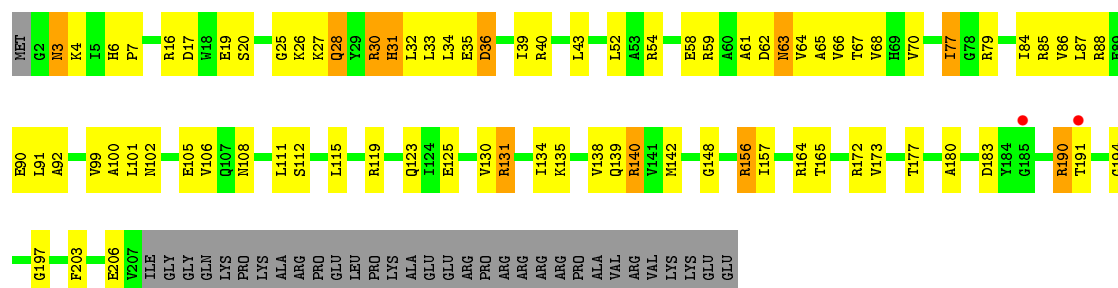
• Molecule 36: 30S ribosomal protein S2



ALA
GLU
ALA
THR
GLU
THR
PRO
GLU
GLY
SER
GLU
VAL
GLU
ALA

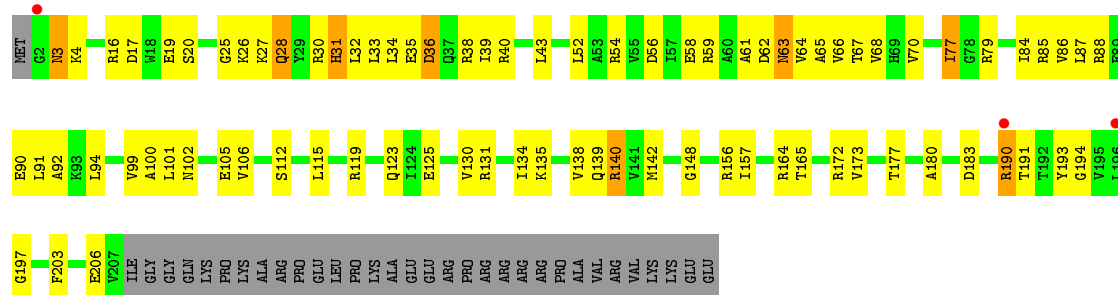
• Molecule 37: 30S ribosomal protein S3

Chain LA: 



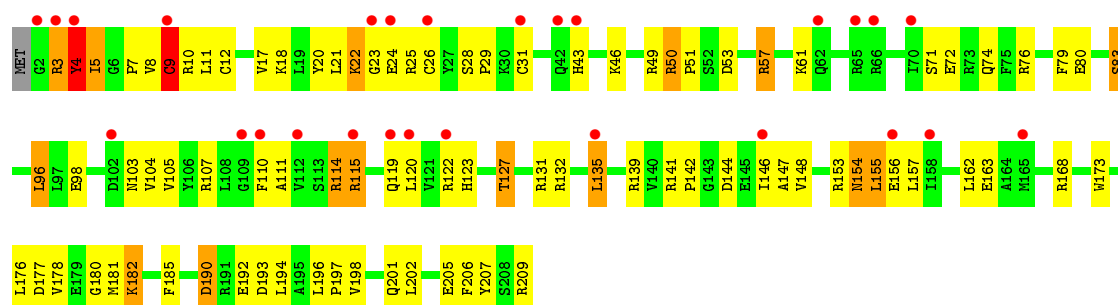
• Molecule 37: 30S ribosomal protein S3

Chain QC: 



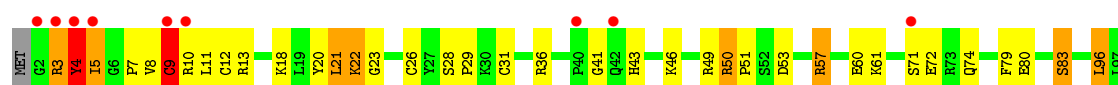
• Molecule 38: 30S ribosomal protein S4

Chain MA: 



• Molecule 38: 30S ribosomal protein S4

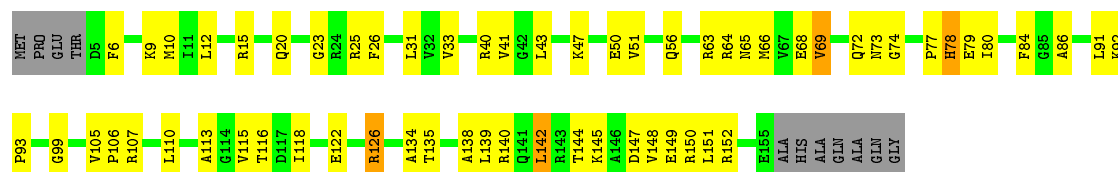
Chain RC: 





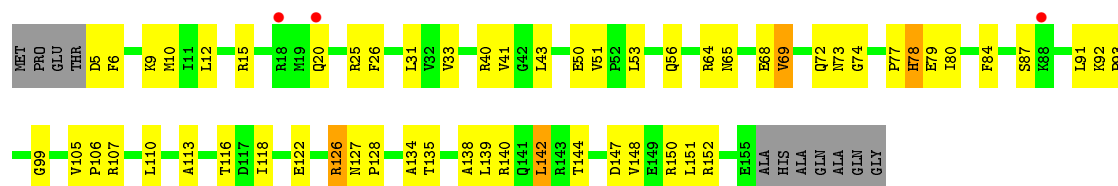
- Molecule 39: 30S ribosomal protein S5

Chain NA: 56% 35% 7%



- Molecule 39: 30S ribosomal protein S5

Chain SC: 57% 33% 7%



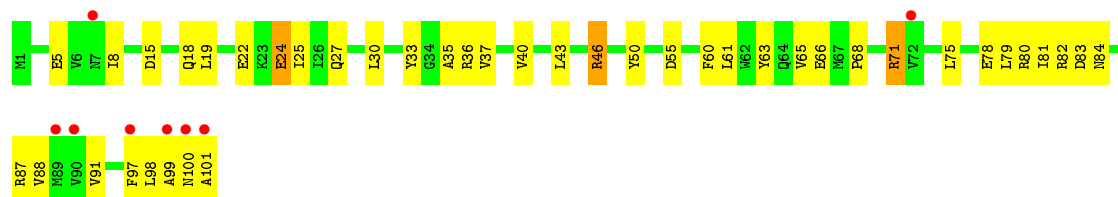
- Molecule 40: 30S ribosomal protein S6

Chain OA: 54% 42% 7%



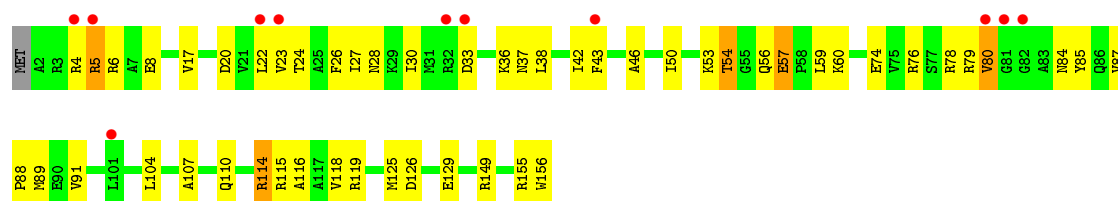
- Molecule 40: 30S ribosomal protein S6

Chain TC: 58% 39% 8%

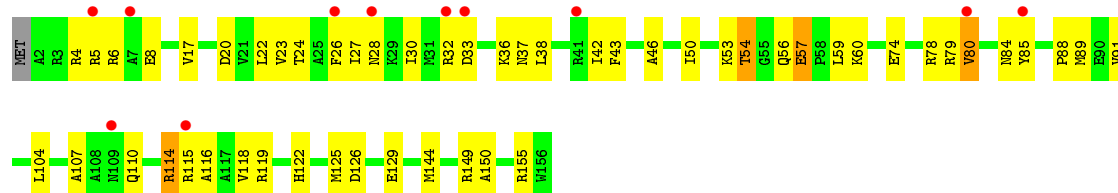


- Molecule 41: 30S ribosomal protein S7

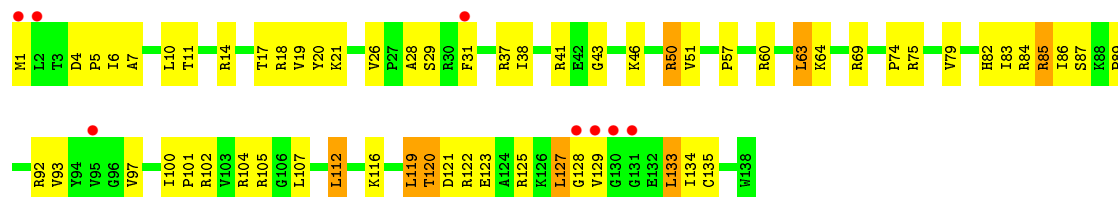
Chain PA: 66% 30% 7%



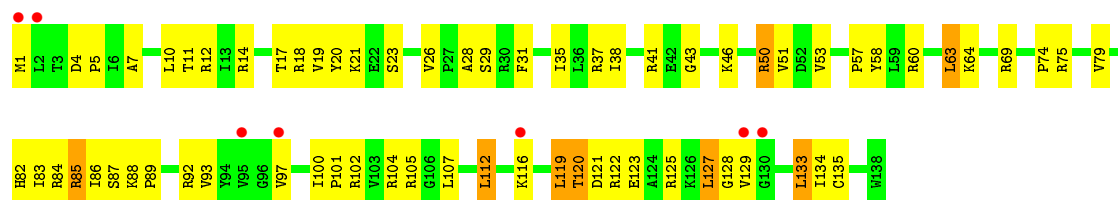
- Molecule 41: 30S ribosomal protein S7



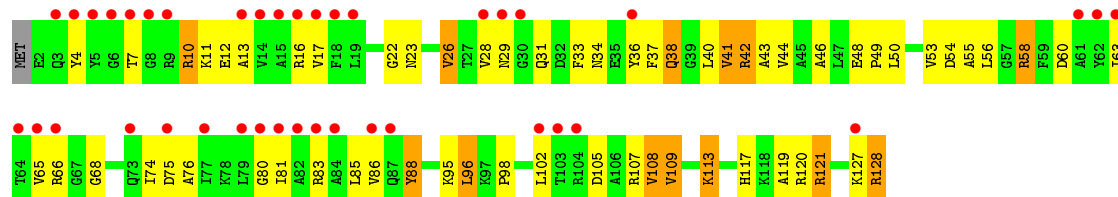
- Molecule 42: 30S ribosomal protein S8



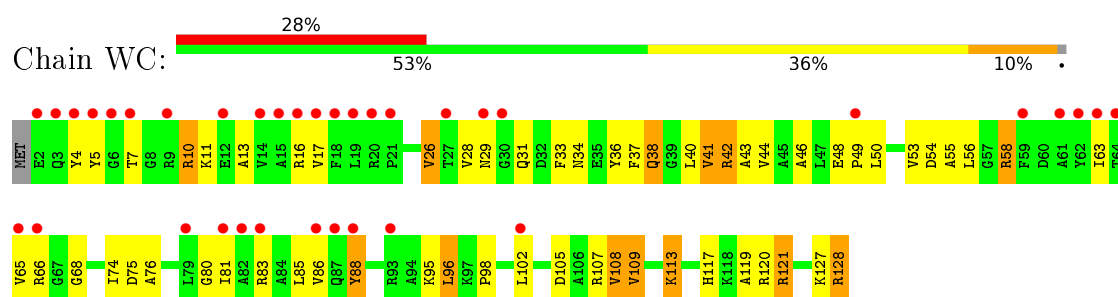
- Molecule 42: 30S ribosomal protein S8



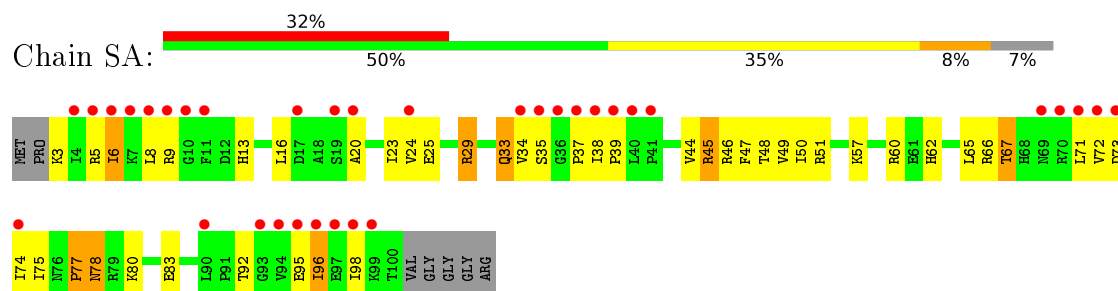
- Molecule 43: 30S ribosomal protein S9



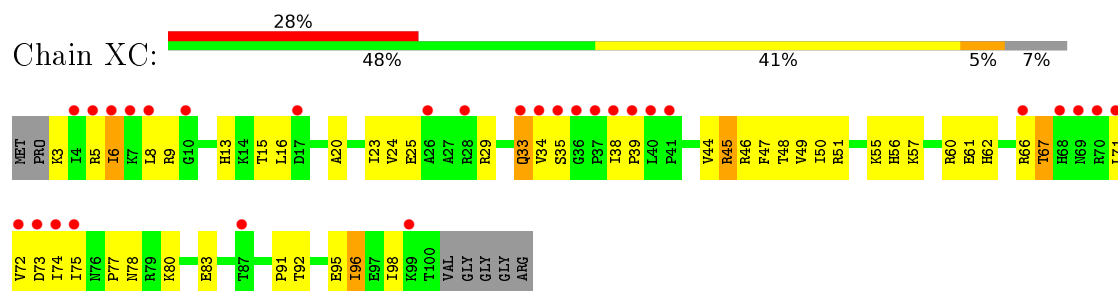
- Molecule 43: 30S ribosomal protein S9



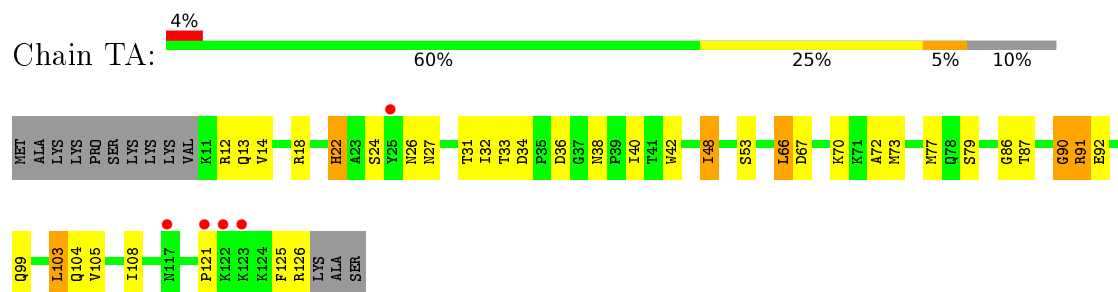
• Molecule 44: 30S ribosomal protein S10



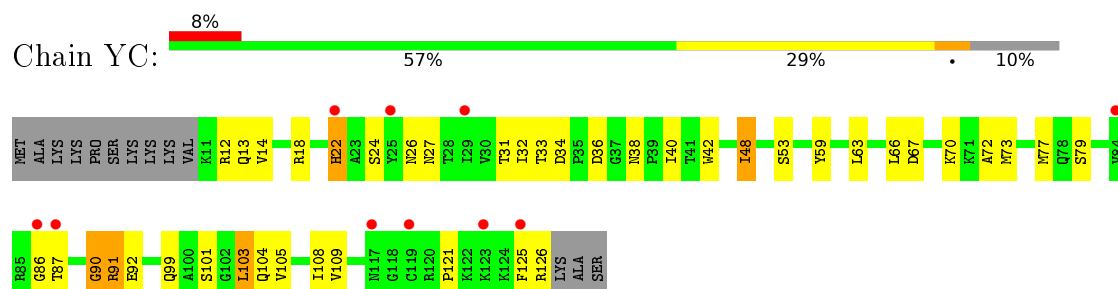
• Molecule 44: 30S ribosomal protein S10



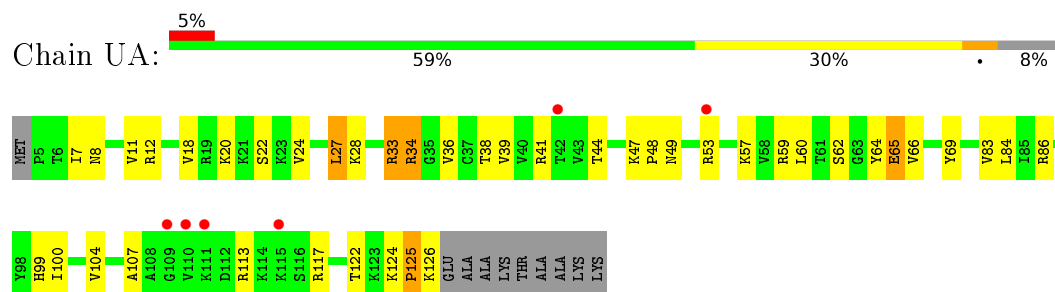
• Molecule 45: 30S ribosomal protein S11



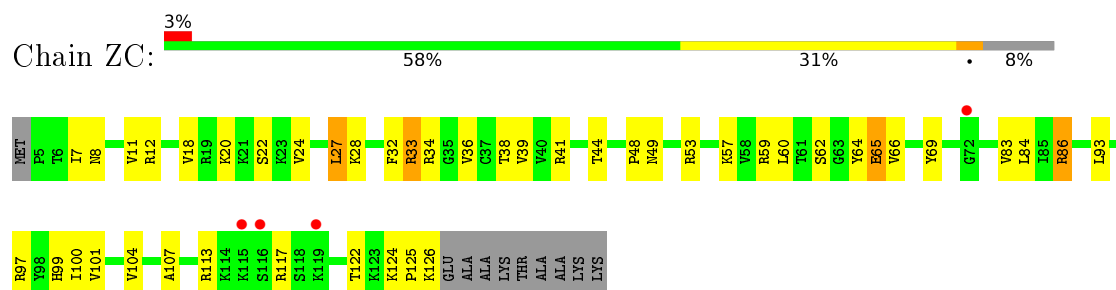
• Molecule 45: 30S ribosomal protein S11



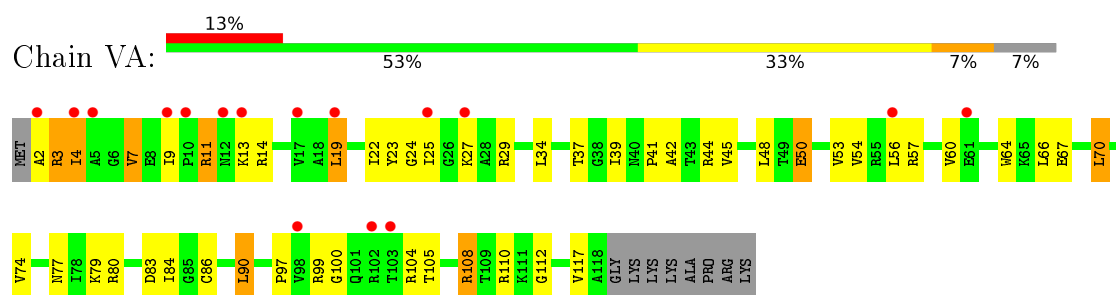
- Molecule 46: 30S ribosomal protein S12



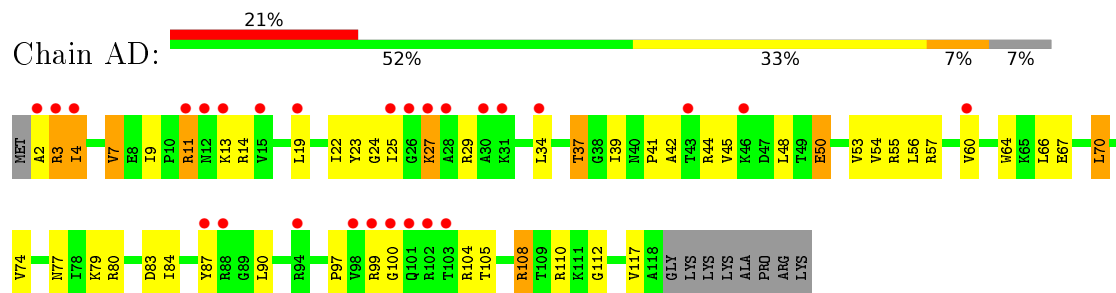
- Molecule 46: 30S ribosomal protein S12



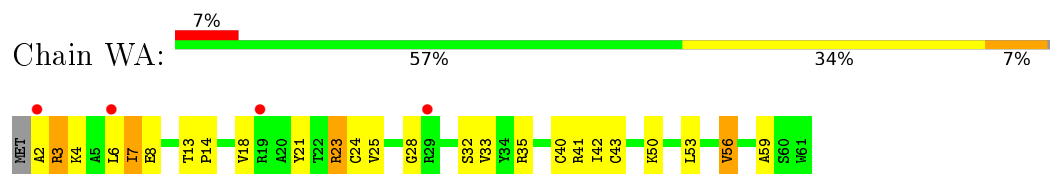
- Molecule 47: 30S ribosomal protein S13



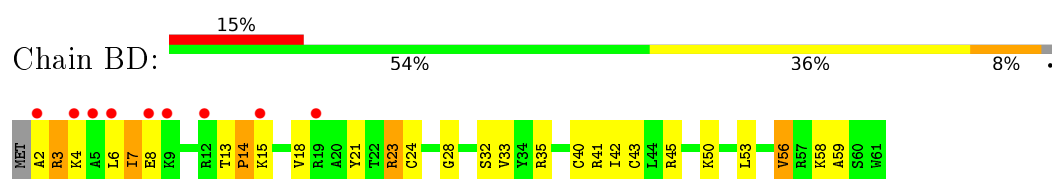
- Molecule 47: 30S ribosomal protein S13



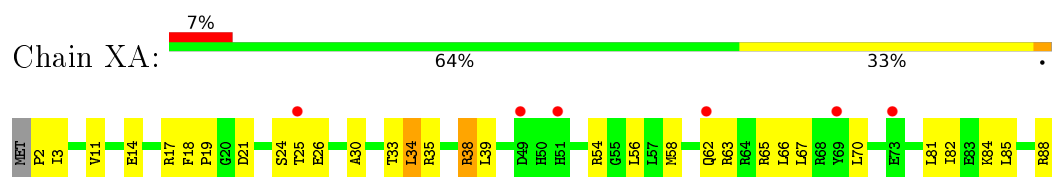
- Molecule 48: 30S ribosomal protein S14 type Z



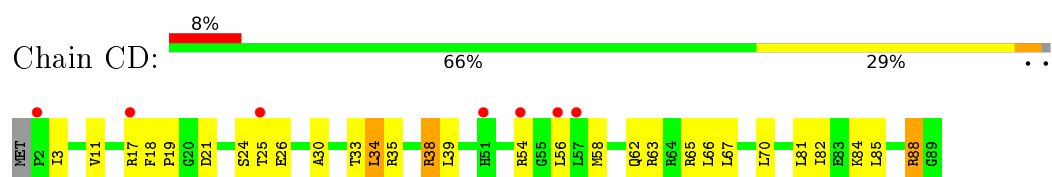
- Molecule 48: 30S ribosomal protein S14 type Z



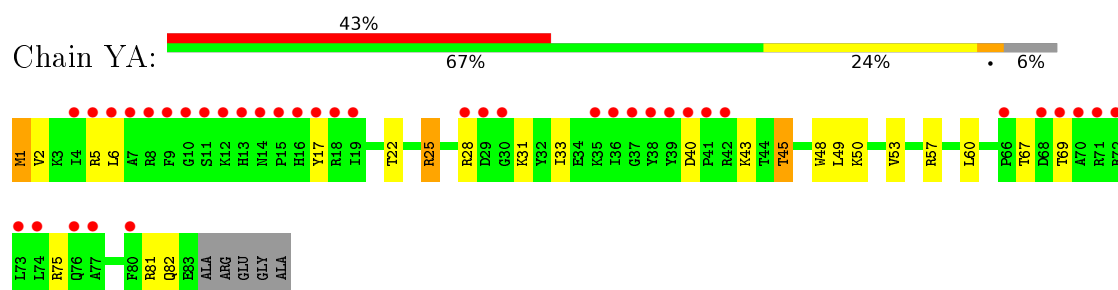
- Molecule 49: 30S ribosomal protein S15



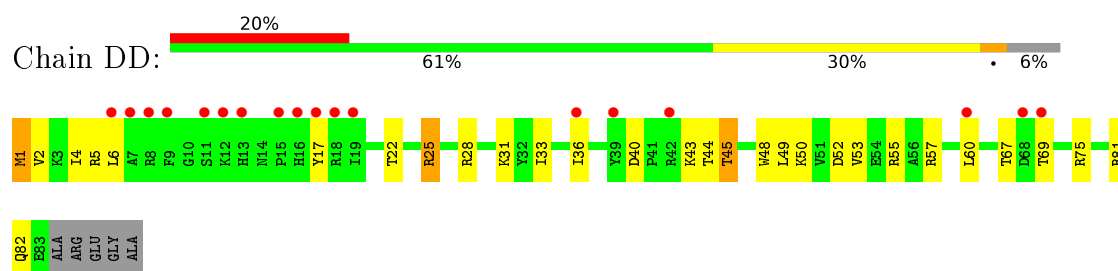
- Molecule 49: 30S ribosomal protein S15



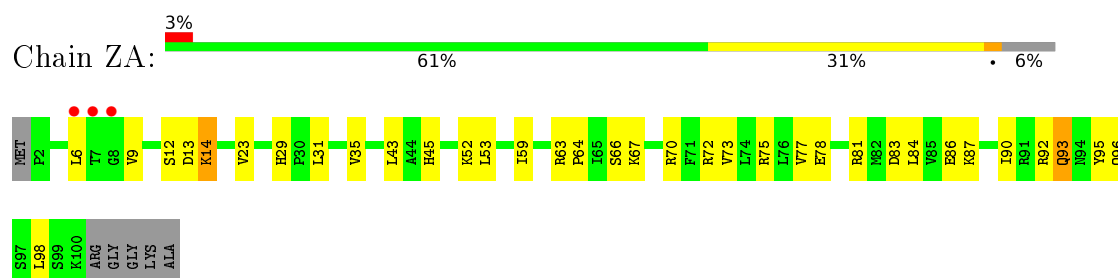
- Molecule 50: 30S ribosomal protein S16



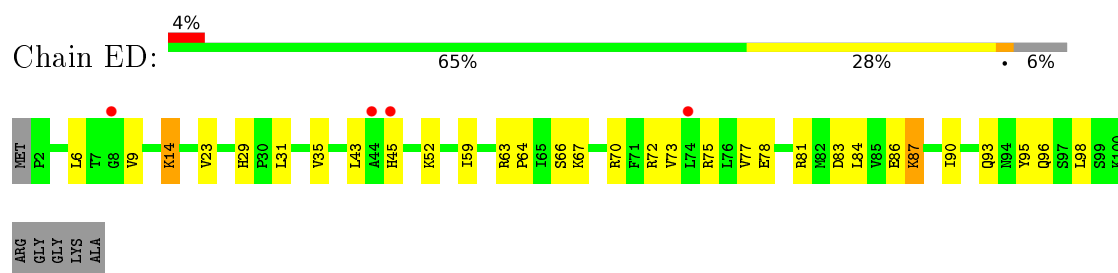
- Molecule 50: 30S ribosomal protein S16



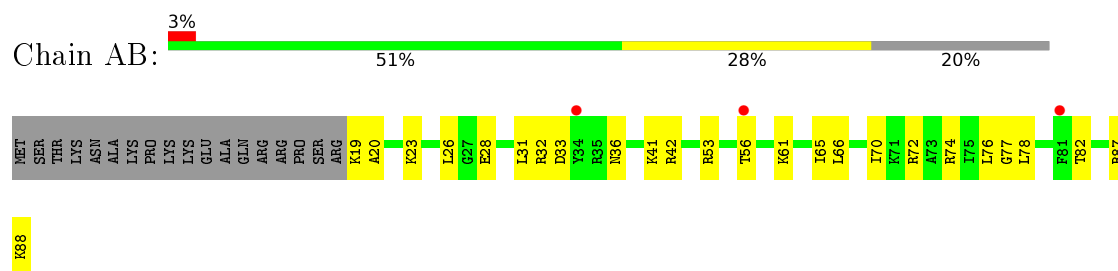
- Molecule 51: 30S ribosomal protein S17



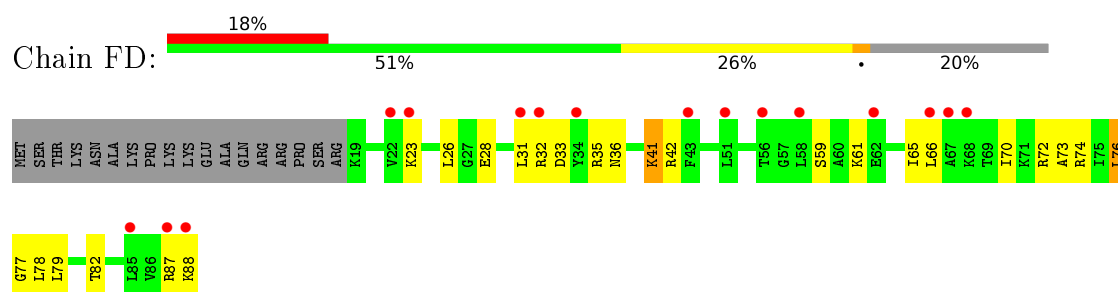
- Molecule 51: 30S ribosomal protein S17



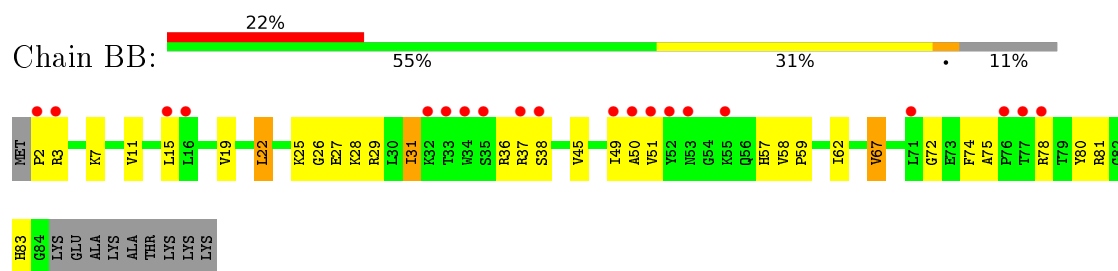
- Molecule 52: 30S ribosomal protein S18



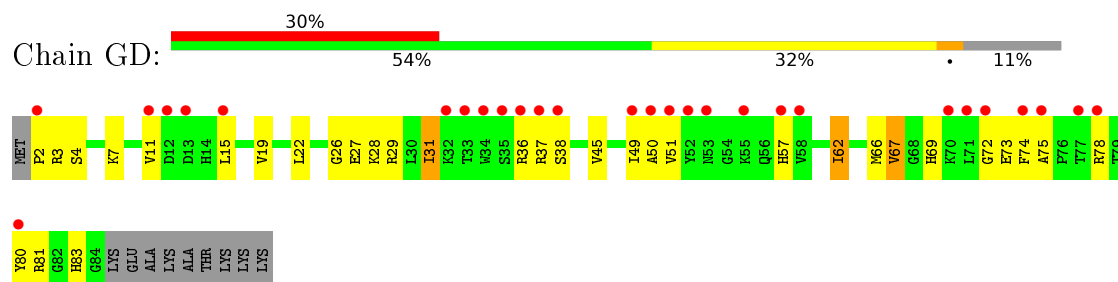
- Molecule 52: 30S ribosomal protein S18



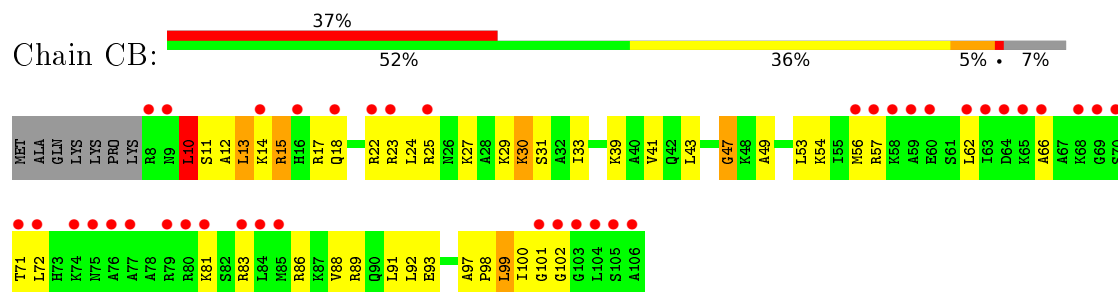
- Molecule 53: 30S ribosomal protein S19



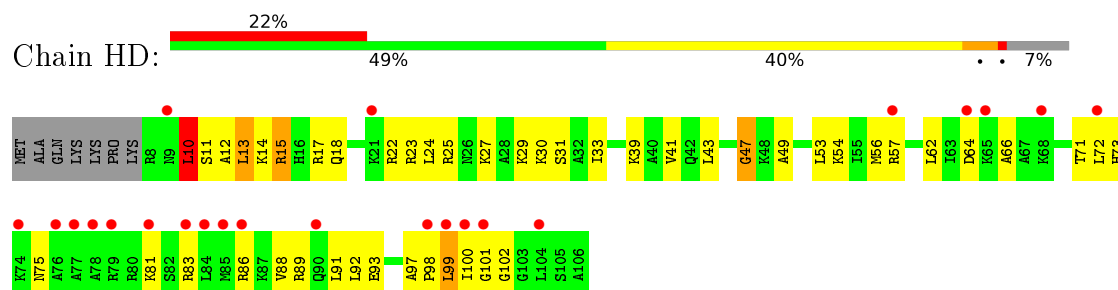
- Molecule 53: 30S ribosomal protein S19



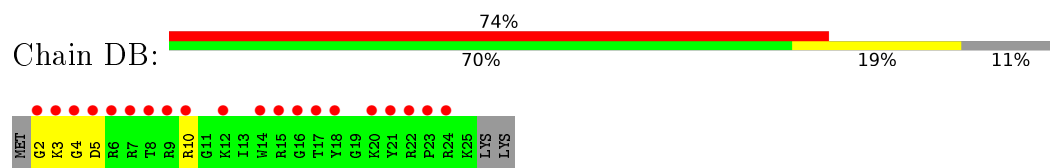
Chain CB:



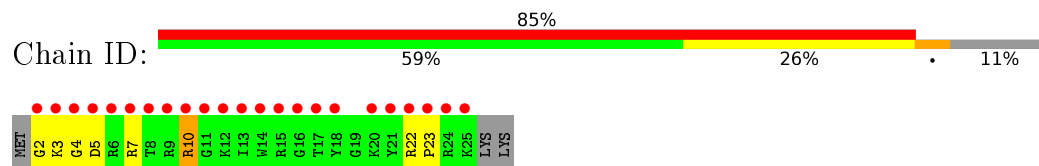
Chain HD:



Chain DB:



Chain ID:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.54Å 454.40Å 619.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 87.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-3.10) 100.0 (87.34-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.221 , 0.256 0.233 , 0.263	Depositor DCC
R_{free} test set	21343 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	300991	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, 2MU, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/35961	0.97	23/56125 (0.0%)
1	FB	0.55	1/35961 (0.0%)	0.99	26/56125 (0.0%)
2	B	0.85	30/69214 (0.0%)	1.22	348/108048 (0.3%)
2	GB	0.70	13/69214 (0.0%)	1.12	225/108048 (0.2%)
3	C	0.59	0/2881	1.00	1/4494 (0.0%)
3	HB	0.49	0/2881	0.92	0/4494
4	D	0.38	0/1744	0.85	1/2719 (0.0%)
4	IA	0.59	0/1744	1.01	2/2719 (0.1%)
4	IB	0.38	0/1744	0.86	1/2719 (0.0%)
4	NC	0.56	0/1744	0.97	1/2719 (0.0%)
5	E	0.66	1/2195 (0.0%)	0.68	0/2955
5	JB	0.55	0/2195	0.63	0/2955
6	F	0.58	0/1596	0.62	0/2153
6	KB	0.50	0/1596	0.60	0/2153
7	G	0.58	0/1621	0.63	0/2194
7	LB	0.49	0/1621	0.59	0/2194
8	H	0.39	0/1496	0.56	1/2013 (0.0%)
8	MB	0.35	0/1496	0.55	1/2013 (0.0%)
9	I	0.48	0/1356	0.57	0/1834
9	NB	0.32	0/1356	0.51	0/1834
10	J	0.45	0/1152	0.57	0/1559
10	OB	0.37	0/1152	0.55	0/1559
11	K	0.55	0/1148	0.59	0/1547
11	PB	0.43	0/1148	0.55	0/1547
12	L	0.55	0/942	0.60	0/1268
12	QB	0.50	0/942	0.57	0/1268
13	M	0.55	0/1162	0.62	0/1544
13	RB	0.47	0/1162	0.60	0/1544
14	N	0.62	2/1142 (0.2%)	0.58	0/1525
14	SB	0.51	0/1142	0.56	0/1525
15	O	0.50	0/982	0.62	0/1312
15	TB	0.43	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	P	0.40	0/887	0.53	0/1180
16	UB	0.35	0/887	0.50	0/1180
17	Q	0.47	0/1157	0.56	0/1544
17	VB	0.43	0/1157	0.56	0/1544
18	R	0.58	0/982	0.61	0/1306
18	WB	0.47	0/982	0.54	0/1306
19	S	0.60	0/790	0.62	0/1057
19	XB	0.49	0/790	0.57	0/1057
20	T	0.60	0/901	0.64	0/1209
20	YB	0.52	0/901	0.62	0/1209
21	U	0.62	0/764	0.63	1/1025 (0.1%)
21	ZB	0.50	0/764	0.61	1/1025 (0.1%)
22	AC	0.49	0/827	0.59	0/1103
22	V	0.56	0/827	0.62	0/1103
23	BC	0.38	0/1527	0.52	0/2073
23	W	0.44	0/1527	0.54	0/2073
24	CC	0.48	0/671	0.61	0/892
24	X	0.59	0/671	0.64	0/892
25	DC	0.49	0/768	0.62	0/1021
25	Y	0.58	0/768	0.64	0/1021
26	EC	0.44	0/594	0.52	0/785
26	Z	0.59	0/594	0.57	0/785
27	AA	0.58	0/482	0.59	0/646
27	FC	0.45	0/482	0.58	0/646
28	BA	0.37	0/565	0.48	0/761
28	GC	0.37	0/565	0.48	0/761
29	CA	0.56	0/474	0.64	0/640
29	HC	0.48	0/474	0.59	0/640
30	DA	0.49	0/460	0.59	0/613
30	IC	0.44	0/460	0.55	0/613
31	EA	0.70	0/426	0.69	0/561
31	JC	0.56	0/426	0.62	0/561
32	FA	0.68	0/525	0.59	0/691
32	KC	0.54	0/525	0.57	0/691
33	GA	0.62	0/310	0.64	0/407
33	LC	0.45	0/310	0.58	0/407
34	HA	0.81	0/225	0.90	0/348
34	MC	0.82	0/225	0.87	0/348
35	JA	0.42	0/2037	0.59	0/2746
35	OC	0.38	0/2037	0.58	0/2746
36	KA	0.35	0/1935	0.53	0/2609
36	PC	0.36	0/1935	0.53	0/2609
37	LA	0.33	0/1636	0.47	0/2205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	QC	0.34	0/1636	0.47	0/2205
38	MA	0.42	1/1733 (0.1%)	0.56	0/2318
38	RC	0.48	1/1733 (0.1%)	0.57	0/2318
39	NA	0.42	0/1171	0.55	0/1576
39	SC	0.47	0/1171	0.55	0/1576
40	OA	0.46	0/856	0.55	0/1154
40	TC	0.42	0/856	0.53	0/1154
41	PA	0.34	0/1276	0.46	0/1709
41	UC	0.33	0/1276	0.47	0/1709
42	QA	0.38	0/1136	0.55	0/1527
42	VC	0.39	0/1136	0.56	0/1527
43	RA	0.32	0/1029	0.47	0/1378
43	WC	0.32	0/1029	0.47	0/1378
44	SA	0.33	0/807	0.50	0/1085
44	XC	0.34	0/807	0.50	0/1085
45	TA	0.43	0/879	0.55	0/1187
45	YC	0.43	0/879	0.55	0/1187
46	UA	0.45	0/963	0.54	0/1287
46	ZC	0.45	0/963	0.54	0/1287
47	AD	0.31	0/943	0.52	0/1265
47	VA	0.32	0/943	0.52	0/1265
48	BD	0.35	0/501	0.50	0/664
48	WA	0.34	0/501	0.49	0/664
49	CD	0.42	0/745	0.53	0/992
49	XA	0.41	0/745	0.53	0/992
50	DD	0.41	0/716	0.52	0/963
50	YA	0.35	0/716	0.49	0/963
51	ED	0.45	0/836	0.53	0/1117
51	ZA	0.43	0/836	0.53	0/1117
52	AB	0.46	0/579	0.57	0/768
52	FD	0.45	0/579	0.57	0/768
53	BB	0.28	0/680	0.51	0/915
53	GD	0.28	0/680	0.51	0/915
54	CB	0.33	0/764	0.52	0/1006
54	HD	0.37	0/764	0.53	0/1006
55	DB	0.32	0/212	0.47	0/277
55	ID	0.31	0/212	0.45	0/277
All	All	0.63	49/322210 (0.0%)	0.98	632/481238 (0.1%)

All (49) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1142(B)	A	N9-C4	-9.19	1.32	1.37
2	B	1762	A	N9-C4	8.08	1.42	1.37
2	B	2249	U	C4-O4	7.73	1.29	1.23
2	B	330	A	N9-C4	-7.25	1.33	1.37
5	E	237	GLU	CG-CD	7.22	1.62	1.51
2	GB	1142(B)	A	N9-C4	-7.18	1.33	1.37
2	GB	330	A	N9-C4	-7.13	1.33	1.37
2	B	2593	U	C4-O4	6.75	1.29	1.23
2	B	530	G	C2-N3	6.67	1.38	1.32
2	GB	2593	U	C4-O4	6.49	1.28	1.23
2	GB	2287	A	N9-C4	-6.34	1.34	1.37
2	B	1021	A	N9-C4	-6.29	1.34	1.37
2	B	945	A	C5-C6	-6.29	1.35	1.41
2	B	1762	A	C5-C4	6.26	1.43	1.38
2	B	1671	U	C2-N3	6.20	1.42	1.37
2	GB	1026	U	N1-C2	6.19	1.44	1.38
2	GB	1762	A	N9-C4	6.03	1.41	1.37
2	B	1026	U	N1-C2	5.96	1.44	1.38
2	B	1021	A	N3-C4	-5.95	1.31	1.34
1	FB	1397	C	N1-C6	5.90	1.40	1.37
2	B	945	A	N9-C4	-5.88	1.34	1.37
2	B	1602	U	C4-O4	5.86	1.28	1.23
14	N	80	GLU	CB-CG	5.83	1.63	1.52
2	B	2287	A	N9-C4	-5.70	1.34	1.37
2	B	1762	A	N3-C4	5.68	1.38	1.34
14	N	80	GLU	CG-CD	5.66	1.60	1.51
2	B	568	U	C4-O4	5.53	1.28	1.23
2	GB	2249	U	C4-O4	5.52	1.28	1.23
2	B	1021	A	N7-C5	-5.51	1.35	1.39
2	B	1671	U	C4-O4	5.49	1.28	1.23
2	GB	945	A	N9-C4	-5.42	1.34	1.37
2	B	570	G	C6-O6	5.42	1.29	1.24
2	B	1142(B)	A	N3-C4	-5.39	1.31	1.34
2	B	2286	A	N7-C5	-5.39	1.36	1.39
2	B	2028	U	C4-O4	5.37	1.27	1.23
2	GB	1021	A	N9-C4	-5.36	1.34	1.37
2	GB	1602	U	C4-O4	5.36	1.27	1.23
2	B	2062	A	N7-C5	5.32	1.42	1.39
2	GB	1671	U	C4-O4	5.32	1.27	1.23
2	B	450	G	N9-C8	-5.31	1.34	1.37
2	B	1187	G	C6-O6	5.29	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	A	N3-C4	-5.27	1.31	1.34
38	RC	9	CYS	CB-SG	5.20	1.91	1.82
2	B	797	C	N1-C6	-5.17	1.34	1.37
38	MA	9	CYS	CB-SG	5.11	1.91	1.82
2	GB	1762	A	C5-C6	5.08	1.45	1.41
2	GB	34	C	N1-C6	5.06	1.40	1.37
2	B	2286	A	N9-C4	-5.03	1.34	1.37
2	B	1762	A	N7-C5	5.00	1.42	1.39

All (632) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1671	U	N3-C4-O4	12.55	128.19	119.40
2	GB	330	A	C2-N3-C4	-11.88	104.66	110.60
2	GB	2593	U	N3-C4-C5	-11.59	107.65	114.60
2	B	1021	A	C2-N3-C4	-11.37	104.92	110.60
2	GB	1021	A	C2-N3-C4	-10.84	105.18	110.60
2	B	330	A	C2-N3-C4	-10.70	105.25	110.60
2	B	2576	G	O5'-P-OP2	-10.45	96.29	105.70
2	B	1602	U	N3-C4-C5	-10.41	108.36	114.60
2	B	945	A	C5-N7-C8	-10.38	98.71	103.90
2	B	570	G	C5-C6-N1	-10.32	106.34	111.50
2	GB	1671	U	N3-C4-O4	10.11	126.47	119.40
2	GB	1187	G	N1-C6-O6	9.90	125.84	119.90
1	FB	1452	C	C6-N1-C2	-9.85	116.36	120.30
2	B	1021	A	C8-N9-C4	-9.76	101.90	105.80
2	B	945	A	C4-C5-N7	9.74	115.57	110.70
2	B	2685	G	C5-C6-N1	-9.69	106.66	111.50
2	B	450	G	C5-C6-N1	-9.64	106.68	111.50
2	B	2593	U	N3-C4-C5	-9.54	108.87	114.60
2	GB	2430	A	O5'-P-OP1	-9.41	97.23	105.70
2	B	2028	U	N3-C4-C5	-9.04	109.18	114.60
2	B	2249	U	N3-C4-C5	-8.95	109.23	114.60
2	B	1671	U	N3-C4-C5	-8.89	109.27	114.60
2	B	568	U	N3-C4-C5	-8.82	109.31	114.60
2	B	265	A	N7-C8-N9	8.82	118.21	113.80
2	GB	1204	A	O4'-C1'-N9	8.82	115.25	108.20
2	GB	2249	U	N3-C4-C5	-8.80	109.32	114.60
2	GB	570	G	C5-C6-N1	-8.78	107.11	111.50
2	GB	945	A	C5-N7-C8	-8.75	99.53	103.90
2	B	2593	U	N3-C4-O4	8.72	125.50	119.40
2	B	1142(B)	A	C2-N3-C4	-8.69	106.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1021	A	N1-C2-N3	8.66	133.63	129.30
2	B	1698	A	C2-N3-C4	-8.57	106.31	110.60
2	B	2593	U	C6-N1-C2	-8.54	115.87	121.00
2	B	570	G	C5-C6-O6	8.53	133.72	128.60
2	B	1021	A	N7-C8-N9	8.52	118.06	113.80
2	B	761	A	C5-N7-C8	-8.45	99.67	103.90
2	B	1026	U	N1-C2-O2	8.38	128.66	122.80
2	B	2447	G	N1-C6-O6	8.34	124.91	119.90
2	GB	450	G	C5-C6-N1	-8.34	107.33	111.50
2	GB	548	A	C8-N9-C4	-8.32	102.47	105.80
2	B	1602	U	C4-C5-C6	8.25	124.65	119.70
2	B	265	A	C5-N7-C8	-8.19	99.80	103.90
2	B	733	G	C5-N7-C8	-8.18	100.21	104.30
2	GB	1026	U	N1-C2-O2	8.17	128.52	122.80
2	B	1558	A	N1-C6-N6	8.16	123.49	118.60
2	B	1187	G	C5-C6-N1	-8.10	107.45	111.50
2	B	2249	U	N3-C4-O4	8.08	125.06	119.40
2	B	1021	A	C5-N7-C8	-8.05	99.88	103.90
2	GB	330	A	N1-C2-N3	8.04	133.32	129.30
2	GB	140	A	N7-C8-N9	8.01	117.80	113.80
2	GB	1602	U	N3-C4-C5	-8.01	109.80	114.60
2	GB	2491	U	C5-C4-O4	-8.00	121.10	125.90
2	GB	1021	A	N1-C2-N3	7.99	133.29	129.30
2	B	2430	A	O5'-P-OP1	-7.97	98.53	105.70
2	B	1187	G	N1-C6-O6	7.95	124.67	119.90
2	B	1204	A	C2-N3-C4	-7.94	106.63	110.60
2	B	570	G	C4-C5-N7	-7.94	107.62	110.80
4	IA	74	C	C6-N1-C2	-7.92	117.13	120.30
2	GB	945	A	C4-C5-N7	7.92	114.66	110.70
2	B	945	A	N1-C6-N6	7.91	123.35	118.60
2	B	2491	U	C5-C4-O4	-7.90	121.16	125.90
2	B	265	A	C8-N9-C4	-7.90	102.64	105.80
2	B	1204	A	O4'-C1'-N9	7.87	114.50	108.20
2	GB	2593	U	N3-C4-O4	7.87	124.91	119.40
2	B	528	A	C2-N3-C4	-7.84	106.68	110.60
2	GB	1698	A	N1-C6-N6	7.79	123.27	118.60
2	GB	2593	U	C4-C5-C6	7.79	124.37	119.70
2	GB	510	C	O5'-P-OP2	-7.79	98.69	105.70
1	A	1452	C	C6-N1-C2	-7.78	117.19	120.30
2	GB	1698	A	C6-C5-N7	-7.73	126.89	132.30
2	B	761	A	C4-C5-C6	-7.72	113.14	117.00
2	B	528	A	N1-C6-N6	7.71	123.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1558	A	C2-N3-C4	-7.67	106.76	110.60
2	GB	1779	U	O5'-P-OP1	-7.65	98.81	105.70
2	B	790	C	O5'-P-OP2	-7.65	98.82	105.70
2	B	330	A	N1-C2-N3	7.64	133.12	129.30
2	B	2028	U	N3-C4-O4	7.63	124.75	119.40
2	B	140	A	N7-C8-N9	7.62	117.61	113.80
2	GB	2593	U	C6-N1-C2	-7.62	116.43	121.00
2	B	2286	A	C5-N7-C8	-7.61	100.10	103.90
2	B	1026	U	N3-C2-O2	-7.56	116.91	122.20
2	B	2286	A	N7-C8-N9	7.55	117.57	113.80
2	GB	528	A	C2-N3-C4	-7.55	106.83	110.60
2	B	2286	A	C8-N9-C4	-7.51	102.79	105.80
2	GB	945	A	N1-C6-N6	7.49	123.10	118.60
2	GB	2838	G	N1-C6-O6	7.48	124.39	119.90
2	B	933	A	C5-N7-C8	-7.47	100.17	103.90
2	B	450	G	C4-C5-N7	-7.44	107.82	110.80
2	B	2210	G	O4'-C1'-N9	7.43	114.14	108.20
2	B	1698	A	N1-C2-N3	7.42	133.01	129.30
2	B	945	A	C6-C5-N7	-7.36	127.15	132.30
2	GB	2491	U	C5-C6-N1	7.36	126.38	122.70
2	B	1698	A	C6-C5-N7	-7.32	127.18	132.30
2	B	948	G	O5'-P-OP1	7.28	119.44	110.70
2	B	1698	A	N7-C8-N9	7.28	117.44	113.80
2	GB	512	G	O4'-C1'-N9	7.26	114.00	108.20
1	FB	1452	C	C5-C6-N1	7.24	124.62	121.00
2	GB	1698	A	C2-N3-C4	-7.24	106.98	110.60
2	GB	761	A	C5-N7-C8	-7.23	100.29	103.90
2	GB	265	A	N7-C8-N9	7.20	117.40	113.80
2	GB	2573	C	C6-N1-C2	7.19	123.18	120.30
2	B	450	G	C4-C5-C6	7.19	123.11	118.80
2	GB	2249	U	N3-C4-O4	7.19	124.43	119.40
2	GB	733	G	C4-C5-N7	7.18	113.67	110.80
2	B	2583	G	N1-C6-O6	7.16	124.20	119.90
1	FB	1399	C	C6-N1-C2	-7.16	117.44	120.30
2	B	1187	G	N3-C2-N2	-7.16	114.89	119.90
2	B	568	U	C4-C5-C6	7.15	123.99	119.70
2	GB	2210	G	O4'-C1'-N9	7.14	113.92	108.20
2	B	512	G	O4'-C1'-N9	7.14	113.91	108.20
2	B	733	G	C4-C5-N7	7.12	113.65	110.80
2	GB	2576	G	O5'-P-OP2	-7.09	99.31	105.70
2	B	751	A	O5'-P-OP2	-7.07	99.33	105.70
2	B	1520	U	C5-C4-O4	7.06	130.14	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	933	A	C5-N7-C8	-7.06	100.37	103.90
2	GB	1021	A	N7-C8-N9	7.04	117.32	113.80
2	GB	733	G	C5-N7-C8	-7.01	100.80	104.30
2	B	1698	A	C8-N9-C4	-7.00	103.00	105.80
2	B	1936	A	N1-C6-N6	7.00	122.80	118.60
2	GB	2838	G	C5-C6-O6	-6.99	124.40	128.60
2	B	1781	C	N3-C4-N4	-6.99	113.11	118.00
2	B	2593	U	N1-C2-O2	-6.99	117.91	122.80
2	B	208	C	C6-N1-C2	6.98	123.09	120.30
2	B	1142(B)	A	N3-C4-C5	6.98	131.68	126.80
2	GB	2028	U	N3-C4-C5	-6.98	110.41	114.60
2	B	2895	U	C5-C6-N1	6.97	126.19	122.70
2	B	2685	G	N1-C6-O6	6.95	124.07	119.90
2	B	645	C	C5-C6-N1	6.95	124.47	121.00
2	GB	259	G	N1-C6-O6	6.93	124.06	119.90
2	B	1210	A	C8-N9-C4	-6.92	103.03	105.80
2	B	1261	C	N3-C4-C5	6.92	124.67	121.90
2	GB	1026	U	N3-C2-O2	-6.92	117.36	122.20
2	GB	1021	A	C8-N9-C4	-6.92	103.03	105.80
2	B	2430	A	O5'-P-OP2	6.91	119.00	110.70
2	GB	548	A	N7-C8-N9	6.90	117.25	113.80
2	B	1992	G	N3-C4-C5	-6.90	125.15	128.60
2	B	945	A	C2-N3-C4	-6.89	107.15	110.60
2	GB	265	A	C5-N7-C8	-6.86	100.47	103.90
2	GB	140	A	C8-N9-C4	-6.85	103.06	105.80
2	B	2241	A	C2-N3-C4	-6.82	107.19	110.60
2	B	1698	A	O4'-C1'-N9	6.82	113.66	108.20
2	B	1142(B)	A	N3-C4-N9	-6.79	121.97	127.40
2	GB	1142(B)	A	C2-N3-C4	-6.77	107.22	110.60
2	GB	1898	U	C5-C4-O4	6.76	129.96	125.90
2	B	2447	G	C5-C6-O6	-6.74	124.56	128.60
2	B	1186	G	O5'-P-OP1	-6.74	99.64	105.70
2	GB	776	G	C5-C6-N1	-6.73	108.14	111.50
2	B	1142(B)	A	C5-C6-N1	-6.72	114.34	117.70
2	GB	645	C	C5-C6-N1	6.72	124.36	121.00
2	B	2061	G	C5-C6-N1	-6.72	108.14	111.50
2	GB	1671	U	N3-C4-C5	-6.69	110.59	114.60
1	FB	1397	C	C5-C6-N1	6.68	124.34	121.00
1	A	754	C	C2-N1-C1'	6.66	126.12	118.80
2	B	214	G	C4-C5-N7	-6.64	108.14	110.80
2	B	570	G	N9-C4-C5	6.64	108.05	105.40
2	B	678	C	N3-C4-C5	6.63	124.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	758	C	C6-N1-C2	6.63	122.95	120.30
3	C	87	G	C8-N9-C4	6.63	109.05	106.40
1	A	1452	C	C5-C6-N1	6.63	124.31	121.00
2	B	1852	C	C6-N1-C2	-6.62	117.65	120.30
2	B	140	A	C8-N9-C4	-6.61	103.16	105.80
2	B	945	A	N7-C8-N9	6.60	117.10	113.80
2	GB	570	G	C4-C5-N7	-6.60	108.16	110.80
2	B	2606	C	C2-N3-C4	-6.60	116.60	119.90
2	B	528	A	C5-C6-N1	-6.59	114.40	117.70
2	B	1671	U	C4-C5-C6	6.56	123.64	119.70
2	GB	2439	A	O4'-C1'-N9	-6.55	102.96	108.20
2	GB	2593	U	N1-C2-O2	-6.52	118.24	122.80
2	B	2685	G	N3-C2-N2	-6.51	115.34	119.90
2	GB	1021	A	C5-N7-C8	-6.51	100.65	103.90
2	GB	1781	C	C5-C6-N1	-6.50	117.75	121.00
2	B	570	G	C8-N9-C4	-6.50	103.80	106.40
2	B	1336	A	N1-C6-N6	-6.50	114.70	118.60
2	GB	1602	U	C4-C5-C6	6.50	123.60	119.70
2	GB	2573	C	C2-N1-C1'	-6.49	111.67	118.80
2	GB	2573	C	C5-C6-N1	-6.47	117.76	121.00
2	GB	1828	G	C5-C6-O6	6.46	132.48	128.60
2	B	1602	U	C6-N1-C2	-6.46	117.12	121.00
2	B	1663	C	N1-C2-O2	-6.46	115.03	118.90
1	FB	754	C	C2-N1-C1'	6.44	125.88	118.80
2	B	933	A	C4-C5-N7	6.43	113.91	110.70
2	B	2020	A	N1-C6-N6	-6.42	114.75	118.60
2	B	2286	A	C2-N3-C4	-6.42	107.39	110.60
2	GB	1698	A	O4'-C1'-N9	6.42	113.33	108.20
2	B	2287	A	C2-N3-C4	-6.41	107.39	110.60
2	B	2444	G	N1-C2-N3	6.41	127.75	123.90
2	B	1602	U	N3-C4-O4	6.41	123.89	119.40
2	GB	214	G	O4'-C1'-N9	6.41	113.32	108.20
2	GB	1847	A	C2-N3-C4	6.41	113.80	110.60
1	FB	945	G	N1-C6-O6	6.40	123.74	119.90
2	GB	128	C	C6-N1-C2	6.38	122.85	120.30
2	B	252	G	N1-C6-O6	6.37	123.72	119.90
2	B	2319	G	N3-C4-C5	6.37	131.78	128.60
2	B	1204	A	N1-C2-N3	6.36	132.48	129.30
2	B	2593	U	C5-C6-N1	6.35	125.87	122.70
2	B	140	A	C5-N7-C8	-6.35	100.73	103.90
2	GB	1769	G	N1-C6-O6	6.33	123.70	119.90
2	B	1781	C	C5-C6-N1	-6.32	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	570	G	C5-C6-O6	6.31	132.39	128.60
2	B	330	A	N3-C4-C5	6.31	131.22	126.80
2	B	2491	U	C5-C6-N1	6.31	125.85	122.70
2	B	1992	G	P-O3'-C3'	6.31	127.27	119.70
2	B	2055	C	OP2-P-O3'	6.30	119.07	105.20
2	GB	2249	U	C4-C5-C6	6.30	123.48	119.70
2	B	330	A	C5-N7-C8	-6.30	100.75	103.90
2	B	2318	G	O4'-C1'-N9	6.30	113.24	108.20
21	ZB	57	LEU	CA-CB-CG	6.29	129.76	115.30
2	B	589	C	N1-C2-O2	-6.28	115.13	118.90
2	GB	1698	A	N7-C8-N9	6.28	116.94	113.80
2	B	761	A	N7-C8-N9	6.28	116.94	113.80
2	B	2059	A	O5'-P-OP2	-6.28	100.05	105.70
2	GB	1532	C	C6-N1-C2	-6.28	117.79	120.30
2	GB	1992	G	P-O3'-C3'	6.27	127.22	119.70
2	GB	1021	A	C5-C6-N1	-6.26	114.57	117.70
2	B	2061	G	OP2-P-O3'	6.26	118.97	105.20
2	GB	1698	A	C4-C5-C6	6.26	120.13	117.00
2	B	800	A	O5'-P-OP2	-6.25	100.07	105.70
2	B	827	U	O5'-P-OP1	6.24	118.19	110.70
2	B	548	A	C8-N9-C4	-6.23	103.31	105.80
2	B	2286	A	C6-C5-N7	-6.22	127.95	132.30
2	B	700	G	C4-C5-N7	6.21	113.28	110.80
2	B	2685	G	N3-C4-N9	-6.21	122.28	126.00
2	GB	865	C	C6-N1-C2	6.21	122.78	120.30
2	B	1992	G	C8-N9-C4	-6.21	103.92	106.40
2	GB	2030	A	C8-N9-C4	6.21	108.28	105.80
2	GB	140	A	C5-N7-C8	-6.20	100.80	103.90
2	GB	1852	C	C6-N1-C2	-6.17	117.83	120.30
2	GB	761	A	C4-C5-C6	-6.17	113.92	117.00
21	U	57	LEU	CA-CB-CG	6.16	129.47	115.30
2	GB	568	U	N3-C4-C5	-6.16	110.90	114.60
2	GB	1187	G	C5-C6-N1	-6.16	108.42	111.50
1	FB	1397	C	O4'-C1'-N1	6.15	113.12	108.20
2	B	2318	G	N7-C8-N9	6.12	116.16	113.10
2	GB	1859	A	C8-N9-C4	6.09	108.23	105.80
2	GB	257	A	C8-N9-C4	6.08	108.23	105.80
2	B	825	C	OP1-P-O3'	6.08	118.58	105.20
2	B	2573	C	C2-N1-C1'	-6.08	112.11	118.80
1	FB	509	A	C8-N9-C4	-6.07	103.37	105.80
2	B	1602	U	N1-C2-N3	6.07	118.54	114.90
2	B	2838	G	C5-C6-O6	-6.06	124.96	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	758	C	N3-C4-C5	6.05	124.32	121.90
2	GB	776	G	C5-C6-O6	6.04	132.22	128.60
2	B	865	C	C6-N1-C2	6.04	122.71	120.30
2	GB	2895	U	C5-C6-N1	6.04	125.72	122.70
2	B	463	G	C5-C6-O6	6.03	132.22	128.60
2	GB	1828	G	C8-N9-C4	-6.03	103.99	106.40
2	GB	761	A	N7-C8-N9	6.01	116.81	113.80
2	GB	1642	G	C5-C6-O6	-6.01	124.99	128.60
1	FB	723	U	P-O3'-C3'	6.01	126.91	119.70
1	FB	748	C	C6-N1-C2	-6.00	117.90	120.30
2	GB	764	A	N1-C6-N6	6.00	122.20	118.60
2	B	2042	A	C8-N9-C4	6.00	108.20	105.80
2	B	582	G	N1-C6-O6	5.99	123.50	119.90
2	B	1698	A	C5-N7-C8	-5.99	100.90	103.90
1	A	1399	C	C6-N1-C2	-5.99	117.90	120.30
2	GB	2430	A	O5'-P-OP2	5.99	117.89	110.70
2	GB	793	A	C2-N3-C4	-5.99	107.61	110.60
2	B	528	A	N3-C4-C5	5.98	130.99	126.80
2	B	785	G	O5'-P-OP2	-5.98	100.32	105.70
2	B	2319	G	C4-C5-N7	5.98	113.19	110.80
2	B	1258	C	C6-N1-C2	5.97	122.69	120.30
2	B	1781	C	C2-N1-C1'	-5.96	112.24	118.80
2	B	570	G	C4-C5-C6	5.95	122.37	118.80
2	B	1026	U	C2-N1-C1'	5.94	124.83	117.70
2	B	1364	G	C5-C6-O6	5.94	132.16	128.60
2	GB	2319	G	N3-C4-C5	5.94	131.57	128.60
2	GB	2028	U	N3-C4-O4	5.93	123.55	119.40
2	B	2271	G	C8-N9-C4	5.93	108.77	106.40
2	B	2714	G	O5'-P-OP2	5.93	117.81	110.70
2	GB	330	A	N3-C4-C5	5.93	130.95	126.80
1	A	913	A	P-O3'-C3'	5.92	126.81	119.70
2	B	1202	C	C6-N1-C2	-5.92	117.93	120.30
2	GB	1698	A	C5-C6-N1	-5.92	114.74	117.70
2	B	2319	G	C5-N7-C8	-5.92	101.34	104.30
2	GB	2055	C	OP2-P-O3'	5.92	118.22	105.20
1	A	1397	C	O4'-C1'-N1	5.92	112.93	108.20
2	B	806	C	N3-C4-C5	5.91	124.26	121.90
2	GB	527	C	N3-C2-O2	-5.91	117.77	121.90
2	GB	1558	A	C2-N3-C4	-5.90	107.65	110.60
2	B	2491	U	C4-C5-C6	-5.90	116.16	119.70
2	GB	678	C	N3-C4-C5	5.89	124.26	121.90
1	A	723	U	P-O3'-C3'	5.89	126.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	1937	A	C8-N9-C4	5.89	108.16	105.80
2	B	1021	A	N3-C4-N9	-5.89	122.69	127.40
2	B	2028	U	N1-C2-O2	-5.88	118.68	122.80
2	B	2224	G	N1-C6-O6	5.87	123.42	119.90
2	B	1395	A	O4'-C1'-N9	5.87	112.89	108.20
1	FB	1397	C	C6-N1-C2	-5.87	117.95	120.30
2	GB	330	A	C5-N7-C8	-5.85	100.97	103.90
2	B	613	U	O4'-C1'-N1	5.85	112.88	108.20
2	GB	1619	G	C5-C6-O6	-5.85	125.09	128.60
2	B	1022	G	C8-N9-C4	-5.85	104.06	106.40
2	B	1313	U	N3-C2-O2	-5.85	118.11	122.20
2	B	2020	A	C4-C5-N7	-5.84	107.78	110.70
2	B	2066	C	C5-C4-N4	-5.83	116.12	120.20
2	GB	265	A	N1-C6-N6	5.83	122.10	118.60
2	GB	195	A	C4-C5-C6	-5.83	114.08	117.00
2	B	305	U	C5-C4-O4	5.82	129.39	125.90
2	B	1779	U	O5'-P-OP1	-5.82	100.46	105.70
2	B	1698	A	O5'-P-OP2	-5.82	100.47	105.70
2	B	385	C	N3-C2-O2	-5.81	117.83	121.90
2	GB	546	C	C6-N1-C2	-5.81	117.98	120.30
2	GB	383	U	O4'-C1'-N1	5.80	112.84	108.20
2	GB	265	A	C8-N9-C4	-5.80	103.48	105.80
1	A	1397	C	C6-N1-C2	-5.80	117.98	120.30
2	B	2439	A	O5'-P-OP2	-5.80	100.48	105.70
2	GB	945	A	N7-C8-N9	5.80	116.70	113.80
2	GB	1187	G	N3-C2-N2	-5.80	115.84	119.90
1	A	509	A	C8-N9-C4	-5.79	103.48	105.80
2	B	1937	A	C8-N9-C4	5.79	108.12	105.80
1	A	1397	C	C5-C6-N1	5.79	123.89	121.00
2	B	265	A	C4-C5-N7	5.79	113.59	110.70
1	A	794	A	O5'-P-OP1	-5.78	100.50	105.70
1	A	1060	C	C6-N1-C2	-5.78	117.99	120.30
2	GB	790	C	O5'-P-OP2	-5.78	100.50	105.70
2	B	2592	G	N7-C8-N9	5.78	115.99	113.10
1	FB	1028(C)	C	C6-N1-C2	-5.78	117.99	120.30
2	GB	2318	G	O4'-C1'-N9	5.78	112.82	108.20
2	B	2573	C	C6-N1-C2	5.77	122.61	120.30
2	GB	1602	U	N3-C4-O4	5.77	123.44	119.40
2	GB	2430	A	O4'-C1'-N9	5.77	112.81	108.20
2	B	566	U	C5-C6-N1	-5.77	119.82	122.70
2	B	764	A	N1-C6-N6	5.76	122.06	118.60
2	B	213	A	N1-C6-N6	5.75	122.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1313	U	C2-N1-C1'	5.75	124.60	117.70
2	GB	613	U	C2-N1-C1'	5.74	124.59	117.70
2	B	548	A	N7-C8-N9	5.74	116.67	113.80
2	B	507	A	OP2-P-O3'	5.74	117.82	105.20
2	GB	1698	A	N1-C2-N3	5.74	132.17	129.30
2	GB	2583	G	N1-C6-O6	5.73	123.34	119.90
2	GB	2048	G	N1-C6-O6	5.72	123.33	119.90
2	B	214	G	C5-N7-C8	5.72	107.16	104.30
4	IB	34	C	C6-N1-C2	-5.71	118.02	120.30
2	B	1666	G	N1-C6-O6	-5.70	116.48	119.90
2	GB	2838	G	C6-C5-N7	-5.70	126.98	130.40
2	B	1621	U	N3-C2-O2	5.70	126.19	122.20
2	B	1347	G	N1-C6-O6	5.70	123.32	119.90
2	B	2016	U	N1-C2-O2	-5.69	118.82	122.80
2	GB	582	G	C8-N9-C4	5.69	108.67	106.40
2	B	945	A	N3-C4-C5	5.68	130.78	126.80
2	GB	213	A	N1-C6-N6	5.68	122.01	118.60
2	GB	512	G	N1-C6-O6	-5.68	116.49	119.90
2	B	1131	G	O4'-C1'-N9	5.68	112.75	108.20
2	GB	945	A	C6-C5-N7	-5.68	128.32	132.30
2	GB	1936	A	N1-C6-N6	5.68	122.01	118.60
2	B	1771	C	N1-C2-O2	-5.68	115.49	118.90
2	GB	1314	C	N1-C2-O2	5.67	122.30	118.90
2	B	2592	G	C8-N9-C4	-5.66	104.14	106.40
2	B	1043	C	C6-N1-C2	-5.66	118.04	120.30
2	GB	2287	A	C5-N7-C8	-5.66	101.07	103.90
2	GB	948	G	O5'-P-OP1	5.65	117.48	110.70
2	B	2558	C	N1-C2-O2	-5.65	115.51	118.90
2	GB	827	U	O5'-P-OP1	5.65	117.48	110.70
1	FB	899	C	N1-C2-O2	5.65	122.29	118.90
1	A	115	G	P-O3'-C3'	5.64	126.47	119.70
2	GB	1026	U	C2-N1-C1'	5.64	124.47	117.70
2	B	958	U	N1-C2-O2	5.64	126.75	122.80
2	GB	933	A	C4-C5-N7	5.64	113.52	110.70
2	B	265	A	C6-C5-N7	-5.63	128.36	132.30
2	B	1142(B)	A	C5-N7-C8	-5.63	101.08	103.90
2	B	2490	G	C5-C6-N1	-5.63	108.68	111.50
2	GB	271(D)	U	N1-C2-O2	5.63	126.75	122.80
2	GB	645	C	C6-N1-C2	-5.63	118.05	120.30
2	B	1021	A	C5-C6-N1	-5.63	114.88	117.70
2	B	1789	A	O5'-P-OP1	-5.63	100.63	105.70
2	B	1022	G	N9-C4-C5	5.62	107.65	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	450	G	C4-C5-C6	5.62	122.17	118.80
2	B	2028	U	C4-C5-C6	5.62	123.07	119.70
1	FB	819	A	N1-C6-N6	5.62	121.97	118.60
2	B	2059	A	O5'-P-OP1	5.62	117.44	110.70
2	GB	208	C	C6-N1-C2	5.62	122.55	120.30
2	GB	747	U	C6-N1-C2	5.61	124.36	121.00
2	GB	507	A	OP2-P-O3'	5.61	117.53	105.20
2	B	1460	A	O4'-C1'-N9	5.60	112.68	108.20
2	B	682	G	C4-C5-N7	5.60	113.04	110.80
2	GB	2553	G	C5-C6-N1	5.60	114.30	111.50
2	B	2048	G	N1-C6-O6	5.59	123.26	119.90
2	B	1671	U	C5-C4-O4	-5.59	122.55	125.90
4	IA	47	U	C5-C6-N1	5.58	125.49	122.70
1	FB	115	G	P-O3'-C3'	5.58	126.40	119.70
2	B	2077	A	C8-N9-C4	-5.58	103.57	105.80
2	B	1781	C	C5-C4-N4	5.57	124.10	120.20
2	B	247	G	N1-C6-O6	-5.57	116.56	119.90
2	GB	528	A	OP1-P-O3'	5.56	117.44	105.20
2	B	2583	G	C6-C5-N7	-5.56	127.06	130.40
2	B	2485	G	N1-C6-O6	5.56	123.24	119.90
2	B	1053	C	C6-N1-C2	-5.56	118.08	120.30
2	B	128	C	C6-N1-C2	5.55	122.52	120.30
2	GB	2286	A	N7-C8-N9	5.55	116.58	113.80
2	GB	1142(B)	A	N3-C4-C5	5.55	130.69	126.80
2	B	672	C	O5'-P-OP2	-5.55	100.70	105.70
2	B	933	A	N7-C8-N9	5.55	116.58	113.80
2	B	2427	C	OP1-P-O3'	5.55	117.40	105.20
2	GB	825	C	OP1-P-O3'	5.54	117.38	105.20
2	B	587	C	N3-C4-C5	-5.54	119.69	121.90
2	B	2430	A	O4'-C1'-N9	5.54	112.63	108.20
2	B	1698	A	C4-C5-C6	5.53	119.76	117.00
2	B	944	G	C6-C5-N7	-5.52	127.09	130.40
2	B	1092	C	C6-N1-C2	-5.52	118.09	120.30
2	GB	2502	G	O5'-P-OP1	-5.52	100.73	105.70
2	B	530	G	C2-N3-C4	5.52	114.66	111.90
2	B	528	A	OP1-P-O3'	5.52	117.34	105.20
1	FB	913	A	P-O3'-C3'	5.51	126.32	119.70
2	B	613	U	C2-N1-C1'	5.51	124.31	117.70
2	B	2016	U	N3-C2-O2	5.50	126.05	122.20
2	B	2538	C	C6-N1-C2	5.50	122.50	120.30
2	B	2213	U	N1-C2-O2	5.50	126.65	122.80
2	B	1698	A	C4-N9-C1'	5.49	136.18	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2566	A	N1-C6-N6	5.48	121.89	118.60
2	GB	1395	A	O4'-C1'-N9	5.48	112.58	108.20
2	B	2429	G	OP2-P-O3'	5.47	117.24	105.20
2	GB	761	A	C8-N9-C4	-5.47	103.61	105.80
2	GB	2593	U	N1-C2-N3	5.47	118.18	114.90
2	B	210	C	C6-N1-C2	5.47	122.49	120.30
2	GB	265	A	C4-C5-N7	5.47	113.43	110.70
2	B	1325	G	N3-C4-N9	5.46	129.28	126.00
1	FB	250	A	O4'-C1'-N9	5.46	112.57	108.20
2	B	1266	G	C5-C6-N1	5.46	114.23	111.50
2	GB	2491	U	C4-C5-C6	-5.46	116.43	119.70
1	A	945	G	C6-C5-N7	-5.45	127.13	130.40
2	GB	1275	A	N1-C6-N6	5.45	121.87	118.60
2	GB	1788	C	OP1-P-O3'	5.45	117.19	105.20
2	B	233	A	O5'-P-OP1	-5.45	100.80	105.70
2	B	480	A	C8-N9-C4	-5.43	103.63	105.80
2	B	1404	C	N1-C2-O2	5.43	122.16	118.90
2	B	2040	C	C6-N1-C2	5.42	122.47	120.30
2	GB	512	G	C5-C6-O6	5.42	131.85	128.60
2	GB	1698	A	C5-N7-C8	-5.42	101.19	103.90
2	B	2491	U	N1-C2-N3	-5.42	111.65	114.90
2	B	1788	C	OP1-P-O3'	5.42	117.12	105.20
2	GB	1043	C	C2-N1-C1'	5.41	124.75	118.80
2	GB	1781	C	C2-N1-C1'	-5.41	112.85	118.80
2	B	733	G	N7-C8-N9	5.41	115.80	113.10
2	GB	528	A	C5-C6-N1	-5.40	115.00	117.70
2	B	450	G	N1-C6-O6	5.40	123.14	119.90
2	B	510	C	O5'-P-OP2	-5.40	100.84	105.70
8	H	53	LEU	CA-CB-CG	5.40	127.71	115.30
2	B	673	C	N3-C4-N4	5.39	121.78	118.00
2	GB	783	A	C8-N9-C4	-5.39	103.64	105.80
2	B	1012	U	C5-C6-N1	-5.39	120.01	122.70
2	GB	670	A	O5'-P-OP2	-5.39	100.85	105.70
2	B	1670	C	N1-C2-O2	-5.38	115.67	118.90
2	GB	669	G	C2-N3-C4	5.38	114.59	111.90
2	GB	214	G	C4-C5-N7	-5.38	108.65	110.80
2	B	2061	G	N1-C6-O6	5.37	123.12	119.90
2	GB	271(D)	U	N3-C2-O2	-5.37	118.44	122.20
2	B	1043	C	C2-N1-C1'	5.37	124.70	118.80
2	B	2685	G	C2-N3-C4	-5.37	109.22	111.90
2	B	383	U	O4'-C1'-N1	5.36	112.49	108.20
2	GB	2427	C	OP1-P-O3'	5.36	116.99	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	1043	C	C6-N1-C2	-5.36	118.16	120.30
2	B	259	G	N1-C6-O6	5.36	123.11	119.90
2	GB	1129	A	C8-N9-C4	5.35	107.94	105.80
2	B	270(L)	C	C6-N1-C2	5.35	122.44	120.30
2	B	814	C	C5-C6-N1	-5.35	118.33	121.00
2	GB	123	G	N1-C6-O6	5.35	123.11	119.90
2	B	2240	C	C6-N1-C2	5.34	122.44	120.30
2	B	803	U	N1-C2-N3	5.34	118.11	114.90
2	GB	2286	A	C5-N7-C8	-5.34	101.23	103.90
2	GB	84	A	C8-N9-C4	5.34	107.94	105.80
2	B	568	U	C5-C4-O4	5.34	129.10	125.90
1	FB	1158	C	N1-C2-O2	5.34	122.10	118.90
1	A	1529	G	C4-N9-C1'	5.33	133.43	126.50
2	B	760	G	OP1-P-O3'	5.33	116.93	105.20
2	GB	2509	G	C5-C6-O6	-5.33	125.40	128.60
2	B	529	A	O5'-P-OP1	-5.33	100.90	105.70
2	B	2439	A	O4'-C1'-N9	-5.32	103.94	108.20
1	A	945	G	N1-C6-O6	5.32	123.09	119.90
2	GB	1961	C	C5-C6-N1	-5.32	118.34	121.00
2	B	2318	G	C8-N9-C4	-5.32	104.27	106.40
2	GB	933	A	N7-C8-N9	5.32	116.46	113.80
2	B	1682	G	N1-C6-O6	5.32	123.09	119.90
2	GB	259	G	C6-C5-N7	-5.31	127.22	130.40
2	GB	1558	A	N1-C6-N6	5.31	121.78	118.60
2	B	90	U	N3-C2-O2	-5.30	118.49	122.20
2	B	458	G	C5-C6-O6	-5.30	125.42	128.60
2	B	1532	C	C6-N1-C2	-5.29	118.18	120.30
2	B	530	G	C5-C6-N1	5.29	114.14	111.50
2	B	1359	A	N1-C2-N3	5.29	131.94	129.30
2	B	1325	G	N3-C2-N2	5.28	123.60	119.90
2	GB	827	U	O5'-P-OP2	-5.28	100.94	105.70
2	B	861	A	OP2-P-O3'	5.28	116.81	105.20
2	B	574	C	C6-N1-C2	5.28	122.41	120.30
2	B	2321	G	N3-C4-C5	-5.28	125.96	128.60
2	GB	2582	G	O5'-P-OP2	5.28	117.03	110.70
8	MB	53	LEU	CA-CB-CG	5.27	127.43	115.30
1	FB	945	G	C6-C5-N7	-5.27	127.24	130.40
2	GB	1642	G	N1-C6-O6	5.27	123.06	119.90
2	B	2685	G	N3-C4-C5	5.27	131.23	128.60
2	GB	768	G	C5-C6-O6	-5.26	125.44	128.60
2	B	645	C	C6-N1-C2	-5.26	118.20	120.30
2	GB	1698	A	C4-N9-C1'	5.26	135.77	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GB	2287	A	C2-N3-C4	-5.26	107.97	110.60
2	GB	944	G	C4-N9-C1'	5.26	133.34	126.50
2	GB	2061	G	OP2-P-O3'	5.26	116.77	105.20
2	B	2447	G	OP1-P-O3'	5.25	116.76	105.20
2	B	1781	C	C6-N1-C2	5.24	122.40	120.30
2	GB	1313	U	C2-N1-C1'	5.24	123.98	117.70
4	NC	46	G	C4-N9-C1'	-5.24	119.69	126.50
1	FB	1397	C	C2-N3-C4	5.23	122.52	119.90
2	GB	201	C	C6-N1-C2	5.23	122.39	120.30
2	B	776	G	C5-C6-N1	-5.23	108.89	111.50
2	GB	2238	G	N3-C4-C5	-5.23	125.98	128.60
2	GB	528	A	N1-C6-N6	5.22	121.73	118.60
2	GB	758	C	C6-N1-C2	5.22	122.39	120.30
2	B	2238	G	N3-C4-N9	5.22	129.13	126.00
2	B	2838	G	N1-C6-O6	5.21	123.03	119.90
2	B	1588	C	C6-N1-C2	-5.21	118.22	120.30
2	B	2447	G	C6-C5-N7	-5.21	127.27	130.40
2	B	1266	G	C5-C6-O6	-5.21	125.47	128.60
2	B	2419	U	N3-C4-C5	-5.21	111.48	114.60
2	B	1762	A	O4'-C1'-N9	5.20	112.36	108.20
1	FB	1256	A	O4'-C1'-N9	5.20	112.36	108.20
2	GB	978	G	C8-N9-C4	5.20	108.48	106.40
2	B	2054	A	C2-N3-C4	-5.20	108.00	110.60
2	B	1204	A	C5-C6-N1	-5.19	115.10	117.70
2	B	2641	G	O5'-P-OP1	-5.19	101.03	105.70
2	B	600	G	C8-N9-C4	5.19	108.47	106.40
2	B	1332	G	O5'-P-OP2	-5.18	101.04	105.70
2	GB	527	C	N1-C2-O2	5.18	122.01	118.90
2	GB	1835	G	C5-C6-N1	5.18	114.09	111.50
2	B	946	G	C8-N9-C4	5.17	108.47	106.40
2	B	1202	C	N3-C4-C5	-5.17	119.83	121.90
2	GB	1992	G	N3-C4-C5	-5.17	126.02	128.60
2	B	271(D)	U	N1-C2-O2	5.17	126.42	122.80
2	B	2319	G	C2-N3-C4	-5.16	109.32	111.90
2	GB	2073	C	N1-C2-O2	-5.16	115.80	118.90
2	GB	2213	U	N1-C2-O2	5.16	126.42	122.80
2	B	2060	A	N1-C6-N6	5.16	121.70	118.60
2	GB	27	G	C8-N9-C4	5.16	108.46	106.40
2	B	527	C	N3-C4-N4	-5.16	114.39	118.00
2	GB	1671	U	N1-C2-O2	-5.16	119.19	122.80
2	GB	654	U	O4'-C1'-N1	5.15	112.32	108.20
2	GB	510	C	OP1-P-OP2	5.14	127.31	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	U	C5-C6-N1	5.14	125.27	122.70
2	GB	1258	C	C6-N1-C2	5.14	122.36	120.30
2	B	2587	A	OP2-P-O3'	5.14	116.50	105.20
2	GB	1836	C	C5-C6-N1	-5.14	118.43	121.00
2	GB	226	G	O4'-C1'-N9	5.13	112.31	108.20
2	B	870	A	N1-C6-N6	5.13	121.68	118.60
2	B	1688	U	C5-C6-N1	-5.13	120.14	122.70
2	B	2324	C	C6-N1-C2	5.13	122.35	120.30
2	GB	2838	G	C4-C5-N7	5.13	112.85	110.80
2	B	2266	A	O5'-P-OP2	-5.12	101.09	105.70
2	GB	739	G	C8-N9-C4	5.12	108.45	106.40
2	GB	664	C	C6-N1-C2	5.12	122.35	120.30
2	B	27	G	C8-N9-C4	5.12	108.45	106.40
2	B	2073	C	N1-C2-O2	-5.12	115.83	118.90
4	D	34	C	C6-N1-C2	-5.11	118.26	120.30
2	GB	1460	A	O4'-C1'-N9	5.11	112.29	108.20
2	GB	1532	C	C5-C6-N1	5.11	123.55	121.00
2	B	1649	G	C8-N9-C4	-5.11	104.36	106.40
2	GB	1301	A	N1-C6-N6	5.11	121.66	118.60
2	B	1341	U	OP2-P-O3'	5.10	116.43	105.20
2	B	2286	A	C4-C5-N7	5.10	113.25	110.70
2	B	2897	U	N1-C2-O2	5.10	126.37	122.80
1	FB	406	G	N1-C6-O6	5.10	122.96	119.90
2	GB	1828	G	C5-C6-N1	-5.10	108.95	111.50
2	GB	2319	G	C4-C5-N7	5.10	112.84	110.80
2	GB	582	G	N1-C6-O6	5.10	122.96	119.90
2	GB	1992	G	O4'-C1'-N9	-5.10	104.12	108.20
2	GB	2491	U	N1-C2-N3	-5.10	111.84	114.90
2	B	1763	G	C8-N9-C4	5.10	108.44	106.40
2	B	2498	C	OP1-P-OP2	5.09	127.24	119.60
2	B	1992	G	N1-C6-O6	-5.09	116.85	119.90
2	GB	1864	U	N3-C2-O2	-5.09	118.64	122.20
2	B	2501	C	N3-C4-C5	5.09	123.94	121.90
2	B	1938	A	C6-N1-C2	-5.09	115.55	118.60
2	B	2053	G	N1-C6-O6	5.09	122.95	119.90
2	GB	1671	U	C4-C5-C6	5.08	122.75	119.70
2	B	208	C	N3-C4-C5	5.08	123.93	121.90
2	B	566	U	C6-N1-C2	5.08	124.05	121.00
2	B	1968	G	C5-C6-O6	-5.08	125.55	128.60
2	GB	945	A	O4'-C1'-N9	5.08	112.27	108.20
2	GB	1619	G	N1-C6-O6	5.08	122.95	119.90
2	GB	2429	G	OP2-P-O3'	5.08	116.38	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1028(C)	C	C6-N1-C2	-5.08	118.27	120.30
2	B	2858	C	C6-N1-C2	5.08	122.33	120.30
2	B	1660	C	C6-N1-C2	-5.08	118.27	120.30
2	B	2897	U	C2-N1-C1'	5.07	123.79	117.70
2	B	523	C	N1-C2-O2	-5.07	115.86	118.90
1	A	394	G	C5-C6-O6	5.07	131.64	128.60
2	B	2286	A	N1-C6-N6	5.07	121.64	118.60
2	GB	2324	C	C6-N1-C2	5.07	122.33	120.30
2	B	1339	G	N9-C4-C5	5.07	107.43	105.40
2	B	2321	G	C4-N9-C1'	5.07	133.08	126.50
2	B	2558	C	N3-C2-O2	5.07	125.45	121.90
2	B	2506	U	O4'-C1'-N1	5.06	112.25	108.20
1	A	322	C	C6-N1-C2	5.06	122.33	120.30
2	B	2020	A	N9-C4-C5	5.06	107.82	105.80
2	B	2238	G	N3-C4-C5	-5.06	126.07	128.60
2	GB	2447	G	OP1-P-O3'	5.06	116.33	105.20
1	A	1158	C	C2-N1-C1'	5.05	124.36	118.80
2	B	1264	G	OP2-P-O3'	5.05	116.32	105.20
2	B	1059	G	N3-C4-C5	-5.05	126.08	128.60
2	B	2593	U	C4-C5-C6	5.05	122.73	119.70
2	GB	2048	G	C5-C6-O6	-5.05	125.57	128.60
2	B	265	A	N1-C6-N6	5.05	121.63	118.60
2	B	783	A	N1-C6-N6	-5.05	115.57	118.60
2	B	2440	C	N3-C4-C5	-5.05	119.88	121.90
2	B	1992	G	C2-N3-C4	5.04	114.42	111.90
2	GB	1266	G	C5-C6-O6	-5.04	125.57	128.60
2	B	179	G	N3-C2-N2	-5.04	116.37	119.90
1	FB	428	G	C5-C6-O6	5.04	131.62	128.60
1	FB	1405	G	N1-C6-O6	5.04	122.92	119.90
2	B	569	U	C5-C6-N1	-5.04	120.18	122.70
2	B	1190	G	N1-C6-O6	5.04	122.92	119.90
2	B	2318	G	C5-N7-C8	-5.04	101.78	104.30
1	FB	84	U	C5-C6-N1	5.03	125.22	122.70
1	FB	945	G	C4-N9-C1'	5.03	133.04	126.50
2	B	1640	C	C5-C6-N1	5.03	123.52	121.00
2	GB	1781	C	N3-C4-N4	-5.03	114.48	118.00
2	GB	2685	G	C5-C6-N1	-5.03	108.99	111.50
2	B	271(D)	U	N3-C2-O2	-5.03	118.68	122.20
2	GB	265	A	C6-C5-N7	-5.03	128.78	132.30
2	GB	2206	C	N3-C4-C5	5.03	123.91	121.90
2	GB	2570	G	N1-C6-O6	5.02	122.91	119.90
1	A	351	G	OP2-P-O3'	5.02	116.25	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	559	G	N1-C6-O6	5.02	122.91	119.90
2	B	1187	G	C4-C5-C6	5.02	121.81	118.80
1	A	1417	G	N1-C6-O6	5.01	122.91	119.90
2	B	1821	A	C8-N9-C4	5.01	107.81	105.80
2	GB	1828	G	N7-C8-N9	5.01	115.61	113.10
2	B	2586	C	C6-N1-C2	5.01	122.31	120.30
2	B	27	G	N7-C8-N9	-5.01	110.59	113.10
2	GB	1204	A	C2-N3-C4	-5.01	108.09	110.60
2	B	1574	C	C6-N1-C2	-5.01	118.30	120.30
2	B	226	G	O4'-C1'-N9	5.01	112.20	108.20
2	B	582	G	C6-C5-N7	-5.01	127.40	130.40
2	B	1558	A	N3-C4-C5	5.00	130.30	126.80
2	B	2249	U	C4-C5-C6	5.00	122.70	119.70
2	B	214	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	372	0
1	FB	32394	0	16366	348	0
2	B	62031	0	31273	576	0
2	GB	62031	0	31269	584	0
3	C	2576	0	1305	19	0
3	HB	2576	0	1305	17	0
4	D	1642	0	841	29	0
4	IA	1642	0	841	20	0
4	IB	1642	0	840	30	0
4	NC	1642	0	841	13	0
5	E	2145	0	2234	43	0
5	JB	2145	0	2234	51	0
6	F	1563	0	1629	36	0
6	KB	1563	0	1629	33	0
7	G	1586	0	1632	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	LB	1586	0	1632	40	0
8	H	1471	0	1526	50	0
8	MB	1471	0	1526	53	0
9	I	1330	0	1407	44	0
9	NB	1330	0	1407	42	0
10	J	1137	0	1225	46	0
10	OB	1137	0	1225	42	0
11	K	1121	0	1195	18	0
11	PB	1121	0	1195	22	0
12	L	932	0	994	21	0
12	QB	932	0	993	18	0
13	M	1145	0	1228	51	0
13	RB	1145	0	1228	43	0
14	N	1121	0	1179	40	0
14	SB	1121	0	1179	37	0
15	O	968	0	1032	26	0
15	TB	968	0	1033	26	0
16	P	877	0	938	31	0
16	UB	877	0	938	28	0
17	Q	1143	0	1211	41	0
17	VB	1143	0	1211	44	0
18	R	964	0	1022	20	0
18	WB	964	0	1022	23	0
19	S	779	0	852	12	0
19	XB	779	0	852	14	0
20	T	890	0	951	23	0
20	YB	890	0	951	20	0
21	U	750	0	814	9	0
21	ZB	750	0	814	10	0
22	AC	814	0	904	20	0
22	V	814	0	904	22	0
23	BC	1495	0	1521	38	0
23	W	1495	0	1521	34	0
24	CC	662	0	688	20	0
24	X	662	0	688	18	0
25	DC	761	0	837	23	0
25	Y	761	0	837	24	0
26	EC	592	0	654	15	0
26	Z	592	0	654	16	0
27	AA	477	0	529	13	0
27	FC	477	0	529	13	0
28	BA	552	0	537	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	GC	552	0	537	17	0
29	CA	460	0	480	9	0
29	HC	460	0	480	10	0
30	DA	453	0	473	13	0
30	IC	453	0	473	13	0
31	EA	418	0	467	14	0
31	JC	418	0	467	12	0
32	FA	517	0	582	15	0
32	KC	517	0	582	10	0
33	GA	307	0	335	5	0
33	LC	307	0	335	5	0
34	HA	220	0	108	7	0
34	MC	220	0	108	7	0
35	JA	2005	0	1964	61	0
35	OC	2005	0	1964	59	0
36	KA	1900	0	1951	66	0
36	PC	1900	0	1951	69	0
37	LA	1612	0	1677	50	0
37	QC	1612	0	1676	51	0
38	MA	1703	0	1767	71	0
38	RC	1703	0	1766	66	0
39	NA	1155	0	1213	33	0
39	SC	1155	0	1213	29	0
40	OA	843	0	857	34	0
40	TC	843	0	857	31	0
41	PA	1257	0	1296	29	0
41	UC	1257	0	1296	30	0
42	QA	1116	0	1177	52	0
42	VC	1116	0	1177	55	0
43	RA	1011	0	1043	45	0
43	WC	1011	0	1043	45	0
44	SA	794	0	840	36	0
44	XC	794	0	840	35	0
45	TA	864	0	881	30	0
45	YC	864	0	881	34	0
46	UA	958	0	1047	31	0
46	ZC	958	0	1047	29	0
47	AD	933	0	992	40	0
47	VA	933	0	992	44	0
48	BD	492	0	533	21	0
48	WA	492	0	533	20	0
49	CD	734	0	771	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	XA	734	0	771	22	0
50	DD	700	0	720	19	0
50	YA	700	0	720	15	0
51	ED	823	0	893	18	0
51	ZA	823	0	893	21	0
52	AB	574	0	644	16	0
52	FD	574	0	644	18	0
53	BB	665	0	686	19	0
53	GD	665	0	686	20	0
54	CB	762	0	859	32	0
54	HD	762	0	859	34	0
55	DB	208	0	221	3	0
55	ID	208	0	221	5	0
56	A	287	0	0	0	0
56	AA	4	0	0	0	0
56	AD	1	0	0	0	0
56	B	944	0	0	0	0
56	BA	3	0	0	0	0
56	BB	1	0	0	0	0
56	BC	9	0	0	0	0
56	C	44	0	0	0	0
56	CA	3	0	0	0	0
56	CB	1	0	0	0	0
56	CC	2	0	0	0	0
56	CD	3	0	0	0	0
56	D	2	0	0	0	0
56	DA	3	0	0	0	0
56	DB	1	0	0	0	0
56	DC	3	0	0	0	0
56	DD	1	0	0	0	0
56	E	10	0	0	0	0
56	EA	2	0	0	0	0
56	EC	4	0	0	0	0
56	ED	2	0	0	0	0
56	F	15	0	0	0	0
56	FA	4	0	0	0	0
56	FB	349	0	0	0	0
56	FC	1	0	0	0	0
56	G	11	0	0	0	0
56	GA	1	0	0	0	0
56	GB	812	0	0	0	0
56	GC	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	GD	1	0	0	0	0
56	H	3	0	0	0	0
56	HA	2	0	0	0	0
56	HB	32	0	0	0	0
56	HC	2	0	0	0	0
56	HD	1	0	0	0	0
56	I	7	0	0	0	0
56	IA	21	0	0	0	0
56	IB	5	0	0	0	0
56	J	3	0	0	0	0
56	JA	13	0	0	0	0
56	JB	13	0	0	0	0
56	K	9	0	0	0	0
56	KA	4	0	0	0	0
56	KB	4	0	0	0	0
56	KC	5	0	0	0	0
56	L	5	0	0	0	0
56	LA	2	0	0	0	0
56	LB	5	0	0	0	0
56	M	8	0	0	0	0
56	MA	5	0	0	0	0
56	MB	7	0	0	0	0
56	MC	1	0	0	0	0
56	N	6	0	0	0	0
56	NA	3	0	0	0	0
56	NB	3	0	0	0	0
56	NC	14	0	0	0	0
56	O	3	0	0	0	0
56	OA	4	0	0	0	0
56	OB	2	0	0	0	0
56	OC	7	0	0	0	0
56	P	4	0	0	0	0
56	PA	3	0	0	0	0
56	PB	4	0	0	0	0
56	PC	5	0	0	0	0
56	Q	4	0	0	0	0
56	QA	2	0	0	0	0
56	QB	6	0	0	0	0
56	QC	4	0	0	0	0
56	R	2	0	0	0	0
56	RA	4	0	0	0	0
56	RB	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RC	11	0	0	0	0
56	S	8	0	0	0	0
56	SA	3	0	0	0	0
56	SB	4	0	0	0	0
56	SC	7	0	0	0	0
56	T	5	0	0	0	0
56	TA	1	0	0	0	0
56	TB	4	0	0	0	0
56	TC	1	0	0	0	0
56	U	2	0	0	0	0
56	UA	3	0	0	0	0
56	UB	1	0	0	0	0
56	UC	2	0	0	0	0
56	VA	3	0	0	0	0
56	VB	8	0	0	0	0
56	VC	2	0	0	0	0
56	W	8	0	0	0	0
56	WA	1	0	0	0	0
56	WB	3	0	0	0	0
56	WC	2	0	0	0	0
56	X	8	0	0	0	0
56	XA	3	0	0	0	0
56	XB	4	0	0	0	0
56	XC	2	0	0	0	0
56	Y	5	0	0	0	0
56	YA	1	0	0	0	0
56	YB	7	0	0	0	0
56	YC	6	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	3	0	0	0	0
56	ZB	1	0	0	0	0
56	ZC	2	0	0	0	0
57	AC	1	0	0	0	0
57	BA	1	0	0	0	0
57	CA	1	0	0	0	0
57	DA	1	0	0	0	0
57	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	HC	1	0	0	0	0
57	IC	1	0	0	0	0
57	LC	1	0	0	0	0
57	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	300991	0	203678	4336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RC:9:CYS:SG	38:RC:18:LYS:NZ	2.06	1.28
38:MA:9:CYS:SG	38:MA:18:LYS:NZ	2.09	1.26
38:MA:18:LYS:NZ	38:MA:26:CYS:SG	2.12	1.20
38:RC:18:LYS:NZ	38:RC:26:CYS:SG	2.15	1.20
42:VC:50:ARG:HH11	42:VC:50:ARG:HB3	1.21	1.03
42:QA:50:ARG:HH11	42:QA:50:ARG:HB3	1.22	1.02
2:GB:1019:U:HO2'	2:GB:1021:A:H2	1.02	1.01
2:B:84:A:OP2	22:V:8:LYS:NZ	1.95	1.00
8:MB:98:ARG:HH11	8:MB:98:ARG:HG3	1.26	0.99
15:O:105:ARG:HG2	15:O:105:ARG:HH11	1.27	0.97
15:TB:105:ARG:HH11	15:TB:105:ARG:HG2	1.26	0.97
1:A:1309:G:OP2	47:VA:99:ARG:NH1	1.97	0.97
2:GB:2133:G:HO2'	2:GB:2157:G:H1	1.09	0.96
8:H:98:ARG:HG3	8:H:98:ARG:HH11	1.26	0.96
1:FB:176:C:OP1	54:HD:29:LYS:NZ	1.98	0.96
11:K:123:TYR:HH	11:K:130:HIS:HE2	1.07	0.95
1:FB:1309:G:OP2	47:AD:99:ARG:NH1	1.98	0.94
2:GB:84:A:OP2	22:AC:8:LYS:NZ	2.01	0.94
2:B:2298:A:H62	2:B:2318:G:H8	1.14	0.93
29:CA:16:ARG:HH11	29:CA:16:ARG:HG2	1.34	0.93
14:SB:85:LYS:HD3	24:CC:7:LEU:HD22	1.51	0.92
2:B:2133:G:HO2'	2:B:2157:G:H1	0.98	0.92
2:B:1019:U:HO2'	2:B:1021:A:H2	1.02	0.92
1:A:176:C:OP1	54:CB:29:LYS:NZ	2.03	0.91
11:PB:123:TYR:HH	11:PB:130:HIS:HE2	1.09	0.91
12:L:35:VAL:HG11	12:L:103:ALA:HB3	1.53	0.91
35:OC:153:GLU:HA	35:OC:159:TYR:H	1.35	0.91
2:GB:2298:A:H62	2:GB:2318:G:H8	1.10	0.91
35:JA:153:GLU:HA	35:JA:159:TYR:H	1.36	0.91
29:HC:16:ARG:NH1	29:HC:17:ASP:OD1	2.03	0.91
38:RC:18:LYS:NZ	38:RC:31:CYS:SG	2.43	0.91
2:GB:1798:U:H5'	5:JB:259:THR:HG22	1.51	0.90
23:W:79:ARG:HD2	23:W:80:ARG:HH11	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QB:35:VAL:HG11	12:QB:103:ALA:HB3	1.52	0.88
16:P:3:ARG:HH11	16:P:3:ARG:HA	1.36	0.88
43:RA:55:ALA:HB1	43:RA:58:ARG:HB2	1.54	0.88
43:WC:55:ALA:HB1	43:WC:58:ARG:HB2	1.56	0.88
2:B:1359:A:H2	2:B:1372:U:H3	1.22	0.88
23:BC:79:ARG:HD2	23:BC:80:ARG:HH11	1.39	0.88
16:UB:3:ARG:HH11	16:UB:3:ARG:HA	1.36	0.87
8:MB:136:ARG:HE	8:MB:136:ARG:H	1.23	0.86
14:N:85:LYS:HD3	24:X:7:LEU:HD22	1.58	0.86
2:B:1798:U:H5'	5:E:259:THR:HG22	1.54	0.86
1:FB:1266:G:N2	1:FB:1269:A:OP2	2.09	0.86
21:U:60:ARG:NH1	31:EA:47:ARG:HH22	1.73	0.86
29:HC:16:ARG:HG2	29:HC:16:ARG:HH11	1.40	0.86
2:GB:1359:A:H2	2:GB:1372:U:H3	1.23	0.86
38:MA:18:LYS:NZ	38:MA:31:CYS:SG	2.48	0.86
44:SA:33:GLN:HG2	44:SA:75:ILE:HG22	1.58	0.86
1:A:1266:G:N2	1:A:1269:A:OP2	2.09	0.85
54:HD:100:ILE:HG12	54:HD:102:GLY:H	1.42	0.85
1:A:542:G:OP1	38:MA:10:ARG:NH2	2.09	0.85
47:VA:3:ARG:HG2	47:VA:3:ARG:HH11	1.40	0.85
2:B:2469:A:H4'	14:N:56:ARG:HG2	1.58	0.85
2:B:1530:G:H1	2:B:1541:U:H3	1.25	0.84
30:DA:12:GLU:OE1	30:DA:19:ARG:NH1	2.09	0.84
2:B:1216:G:OP2	18:R:12:ARG:NH2	2.10	0.84
30:IC:12:GLU:OE1	30:IC:19:ARG:NH1	2.11	0.84
36:KA:87:ARG:NH1	36:KA:233:SER:HB2	1.93	0.84
29:CA:16:ARG:NH1	29:CA:17:ASP:OD1	2.10	0.84
2:GB:1530:G:H1	2:GB:1541:U:H3	1.25	0.83
2:B:1761:C:H5'	2:B:1762:A:OP2	1.78	0.83
2:GB:2637:U:OP1	6:KB:82:ARG:NH1	2.11	0.83
36:PC:87:ARG:NH1	36:PC:233:SER:HB2	1.94	0.83
42:VC:69:ARG:NH1	42:VC:75:ARG:O	2.13	0.82
44:XC:33:GLN:HG2	44:XC:75:ILE:HG22	1.60	0.82
40:TC:46:ARG:HH11	40:TC:46:ARG:HB3	1.44	0.82
2:GB:2287:A:H62	2:GB:2344:U:H3	1.27	0.82
8:H:136:ARG:HE	8:H:136:ARG:H	1.24	0.82
36:PC:155:LEU:HD21	36:PC:159:PRO:HD3	1.61	0.82
39:SC:78:HIS:HD1	42:VC:104:ARG:HD2	1.45	0.82
2:B:1379:A:H4'	2:B:1380:G:OP2	1.77	0.82
8:H:170:ARG:NH1	8:H:174:GLU:OE2	2.12	0.81
42:QA:69:ARG:NH1	42:QA:75:ARG:O	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1761:C:H5'	2:GB:1762:A:OP2	1.79	0.81
36:KA:155:LEU:HD21	36:KA:159:PRO:HD3	1.60	0.81
37:QC:77:ILE:HA	37:QC:84:ILE:HB	1.62	0.81
2:GB:1216:G:OP2	18:WB:12:ARG:NH2	2.12	0.81
22:V:102:CYS:SG	22:V:103:GLY:N	2.53	0.81
47:AD:3:ARG:HG2	47:AD:3:ARG:HH11	1.44	0.80
2:B:847:U:O4	2:B:933:A:N6	2.14	0.80
2:GB:1379:A:H4'	2:GB:1380:G:OP2	1.79	0.80
8:MB:170:ARG:NH1	8:MB:174:GLU:OE2	2.12	0.80
41:UC:57:GLU:H	41:UC:60:LYS:HZ3	1.30	0.80
2:GB:2319:G:H22	16:UB:3:ARG:NH1	1.80	0.80
2:GB:847:U:O4	2:GB:933:A:N6	2.13	0.80
6:F:47:VAL:HG11	6:F:86:PRO:HD2	1.65	0.79
36:PC:9:GLU:HG3	36:PC:217:ARG:NH1	1.97	0.79
38:RC:18:LYS:HZ3	38:RC:31:CYS:HG	1.26	0.79
2:B:2287:A:H62	2:B:2344:U:H3	1.28	0.79
2:B:993:G:OP1	18:R:50:ARG:NH2	2.16	0.79
2:B:2637:U:OP1	6:F:82:ARG:NH1	2.16	0.79
36:KA:130:ARG:NH1	36:KA:134:GLU:HB3	1.98	0.79
40:OA:46:ARG:HH11	40:OA:46:ARG:HB3	1.48	0.79
1:FB:1295:G:O2'	47:AD:14:ARG:NH1	2.16	0.79
7:G:119:ARG:HH11	7:G:119:ARG:HB2	1.48	0.79
2:GB:819:A:OP2	2:GB:1187:G:N2	2.14	0.79
7:LB:119:ARG:HH11	7:LB:119:ARG:HB2	1.46	0.79
2:B:2319:G:H22	16:P:3:ARG:NH1	1.81	0.79
1:FB:706:A:H4'	45:YC:22:HIS:HD2	1.48	0.78
8:H:115:ARG:HD3	47:VA:7:VAL:HG22	1.65	0.78
2:GB:1264:G:OP1	29:HC:19:ARG:NH2	2.16	0.78
37:LA:77:ILE:HA	37:LA:84:ILE:HB	1.63	0.78
40:TC:46:ARG:NH1	40:TC:46:ARG:HB3	1.99	0.78
9:I:137:ASP:HB3	9:I:140:LYS:HE2	1.64	0.78
6:KB:47:VAL:HG11	6:KB:86:PRO:HD2	1.65	0.78
1:FB:656:C:H4'	49:CD:62:GLN:HE22	1.47	0.78
2:GB:1204:A:H2	2:GB:1241:A:H62	1.32	0.78
41:PA:57:GLU:H	41:PA:60:LYS:HZ3	1.32	0.78
4:IA:76:A:H3'	35:JA:234:GLY:HA3	1.66	0.77
1:A:1295:G:O2'	47:VA:14:ARG:NH1	2.17	0.77
36:KA:9:GLU:HG3	36:KA:217:ARG:NH1	1.98	0.77
36:PC:9:GLU:HG3	36:PC:217:ARG:HH12	1.50	0.77
51:ZA:66:SER:O	51:ZA:70:ARG:NH1	2.17	0.77
2:GB:320:A:OP2	7:LB:137:LYS:HE2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1262:A:N3	29:CA:10:LYS:NZ	2.33	0.77
54:CB:100:ILE:HG12	54:CB:102:GLY:H	1.47	0.77
2:GB:2469:A:H4'	14:SB:56:ARG:HG2	1.65	0.77
39:NA:78:HIS:HD1	42:QA:104:ARG:HD2	1.49	0.77
42:QA:10:LEU:HD22	42:QA:83:ILE:HD11	1.65	0.77
43:RA:117:HIS:HB2	43:RA:121:ARG:HG2	1.67	0.77
21:ZB:60:ARG:NH1	31:JC:47:ARG:HH22	1.83	0.77
42:VC:50:ARG:HB3	42:VC:50:ARG:NH1	1.98	0.77
2:GB:1262:A:N3	29:HC:10:LYS:NZ	2.33	0.77
9:I:56:SER:OG	9:I:57:ASP:N	2.17	0.77
36:PC:130:ARG:NH1	36:PC:134:GLU:HB3	1.99	0.77
2:B:1264:G:OP1	29:CA:19:ARG:NH2	2.16	0.76
5:E:71:ASP:OD2	5:E:71:ASP:N	2.16	0.76
16:P:15:ARG:NH1	16:P:25:ARG:HH21	1.83	0.76
42:QA:50:ARG:HB3	42:QA:50:ARG:NH1	1.97	0.76
2:B:1434:A:H61	2:B:1558:A:H62	1.30	0.76
38:RC:7:PRO:HB2	38:RC:10:ARG:HD2	1.66	0.76
2:B:648:G:H21	32:FA:46:ARG:HH12	1.34	0.76
38:MA:7:PRO:HB2	38:MA:10:ARG:HD2	1.68	0.76
2:B:2792:G:H1	2:B:2805:G:H1'	1.49	0.76
8:MB:5:LEU:HD22	8:MB:101:ILE:HD11	1.67	0.76
2:GB:1434:A:H61	2:GB:1558:A:H62	1.32	0.75
8:H:98:ARG:CG	8:H:98:ARG:HH11	1.98	0.75
8:H:5:LEU:HD22	8:H:101:ILE:HD11	1.68	0.75
35:OC:233:GLY:HA3	35:OC:237:VAL:HB	1.69	0.75
4:NC:19:G:H4'	4:NC:20:U:OP2	1.84	0.75
2:GB:2792:G:H1	2:GB:2805:G:H1'	1.51	0.75
46:ZC:39:VAL:HG12	46:ZC:57:LYS:HB2	1.68	0.75
47:AD:3:ARG:HH12	47:AD:9:ILE:HG12	1.51	0.75
1:A:656:C:H4'	49:XA:62:GLN:HE22	1.50	0.75
8:MB:98:ARG:HH11	8:MB:98:ARG:CG	1.99	0.75
4:IA:19:G:H4'	4:IA:20:U:OP2	1.86	0.75
42:VC:10:LEU:HD22	42:VC:83:ILE:HD11	1.67	0.75
38:RC:127:THR:HA	38:RC:132:ARG:HA	1.69	0.74
49:CD:18:PHE:HB2	49:CD:19:PRO:HD2	1.69	0.74
5:JB:71:ASP:OD2	5:JB:71:ASP:N	2.19	0.74
6:KB:128:SER:OG	6:KB:129:HIS:N	2.20	0.74
2:GB:797:C:OP2	7:LB:62:ARG:HG3	1.86	0.74
36:KA:9:GLU:HG3	36:KA:217:ARG:HH12	1.51	0.74
15:O:12:ARG:HH11	15:O:12:ARG:HG3	1.53	0.74
5:E:112:GLN:HB2	5:E:115:GLN:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:3:ARG:HA	16:P:3:ARG:NH1	2.03	0.74
16:UB:15:ARG:NH1	16:UB:25:ARG:HH21	1.86	0.74
15:TB:105:ARG:NH1	15:TB:105:ARG:HG2	2.01	0.73
5:E:35:LYS:HD3	5:E:64:ILE:HD11	1.69	0.73
7:G:185:ASP:HA	7:G:188:ARG:HD2	1.69	0.73
23:W:93:ASP:HB2	23:W:131:ARG:HH22	1.54	0.73
2:B:1060:U:O2'	2:B:1061:U:OP2	2.06	0.73
53:GD:22:LEU:HD21	53:GD:29:ARG:HB2	1.71	0.73
38:MA:127:THR:HA	38:MA:132:ARG:HA	1.70	0.73
46:UA:33:ARG:HE	46:UA:62:SER:HB3	1.52	0.73
47:AD:54:VAL:HA	47:AD:57:ARG:NH1	2.04	0.73
2:GB:1055:G:N2	2:GB:1104:C:O2	2.22	0.73
9:NB:56:SER:OG	9:NB:57:ASP:N	2.22	0.73
2:B:2210:G:H3'	2:B:2211:G:C8	2.24	0.73
40:OA:46:ARG:HB3	40:OA:46:ARG:NH1	2.03	0.73
35:OC:142:ARG:NH2	35:OC:174:ARG:HH11	1.87	0.73
43:WC:117:HIS:HB2	43:WC:121:ARG:HG2	1.69	0.73
49:XA:18:PHE:HB2	49:XA:19:PRO:HD2	1.71	0.73
53:BB:36:ARG:NH2	53:BB:75:ALA:O	2.22	0.73
1:FB:1024:G:N7	1:FB:1025:U:O2'	2.22	0.73
47:VA:13:LYS:HA	47:VA:44:ARG:HH11	1.53	0.73
2:B:1204:A:H2	2:B:1241:A:H62	1.35	0.72
2:B:797:C:OP2	7:G:62:ARG:HG3	1.89	0.72
50:DD:22:THR:HA	50:DD:33:ILE:HG12	1.71	0.72
4:IB:50:U:H3	4:IB:64:G:H1	1.36	0.72
22:AC:102:CYS:SG	22:AC:103:GLY:N	2.62	0.72
53:BB:22:LEU:HD21	53:BB:29:ARG:HB2	1.70	0.72
2:GB:2138:C:N3	2:GB:2153:G:N2	2.34	0.72
50:YA:22:THR:HA	50:YA:33:ILE:HG12	1.72	0.72
2:B:363(F):U:H3'	2:B:363(G):A:H8	1.55	0.72
17:VB:100:TYR:HB3	17:VB:103:ARG:HH11	1.55	0.72
1:A:1024:G:N7	1:A:1025:U:O2'	2.23	0.72
15:TB:13:HIS:CD2	15:TB:16:HIS:H	2.07	0.72
46:UA:39:VAL:HG12	46:UA:57:LYS:HB2	1.70	0.72
1:FB:1356:G:H2'	1:FB:1357:A:C8	2.24	0.72
47:VA:54:VAL:HA	47:VA:57:ARG:NH1	2.05	0.72
47:VA:3:ARG:HH12	47:VA:9:ILE:HG12	1.53	0.72
1:A:1356:G:H2'	1:A:1357:A:C8	2.25	0.72
17:VB:74:ARG:HG2	17:VB:74:ARG:HH11	1.53	0.72
2:B:2138:C:N3	2:B:2153:G:N2	2.33	0.72
2:GB:2210:G:H3'	2:GB:2211:G:C8	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:OC:188:PRO:HG2	35:OC:191:GLU:HB2	1.71	0.72
9:I:130:ARG:HH12	9:I:132:ARG:HH21	1.35	0.72
1:FB:1453:G:H4'	1:FB:1454:G:OP2	1.90	0.71
35:JA:233:GLY:HA3	35:JA:237:VAL:HB	1.72	0.71
35:OC:107:ASP:HB3	35:OC:109:ARG:HG2	1.72	0.71
15:TB:12:ARG:HH11	15:TB:12:ARG:HG3	1.55	0.71
17:VB:129:ARG:HA	17:VB:132:LYS:NZ	2.04	0.71
23:BC:93:ASP:HB2	23:BC:131:ARG:HH22	1.55	0.71
16:UB:3:ARG:NH1	16:UB:3:ARG:HA	2.04	0.71
47:VA:3:ARG:CG	47:VA:3:ARG:HH11	2.04	0.71
2:B:1055:G:N2	2:B:1104:C:O2	2.24	0.71
2:B:547:A:H3'	2:B:548:A:C8	2.25	0.71
2:GB:547:A:H3'	2:GB:548:A:C8	2.25	0.71
17:Q:129:ARG:HA	17:Q:132:LYS:NZ	2.04	0.71
4:D:50:U:H3	4:D:64:G:H1	1.36	0.71
35:JA:188:PRO:HG2	35:JA:191:GLU:HB2	1.72	0.71
45:YC:79:SER:HA	45:YC:104:GLN:HB3	1.73	0.71
47:AD:13:LYS:HA	47:AD:44:ARG:HH11	1.56	0.71
6:F:61:ARG:HG2	6:F:61:ARG:HH11	1.56	0.71
37:LA:139:GLN:HG3	37:LA:140:ARG:NH1	2.05	0.71
2:B:1815:A:P	5:E:54:ARG:HH22	2.14	0.70
45:TA:79:SER:HA	45:TA:104:GLN:HB3	1.73	0.70
2:GB:1092:C:O2	2:GB:1099:G:N2	2.24	0.70
2:GB:993:G:OP1	18:WB:50:ARG:NH2	2.24	0.70
53:BB:11:VAL:HG23	53:BB:38:SER:HB2	1.73	0.70
2:GB:1761:C:H3'	2:GB:1762:A:H5''	1.72	0.70
36:PC:74:LYS:NZ	36:PC:166:ASP:HB2	2.07	0.70
36:KA:74:LYS:NZ	36:KA:166:ASP:HB2	2.07	0.70
23:W:79:ARG:HD2	23:W:80:ARG:NH1	2.07	0.70
51:ED:66:SER:O	51:ED:70:ARG:NH1	2.24	0.70
1:FB:1381:U:H1'	41:UC:79:ARG:HG2	1.72	0.70
35:JA:107:ASP:HB3	35:JA:109:ARG:HG2	1.73	0.70
5:JB:112:GLN:HB2	5:JB:115:GLN:HB3	1.72	0.70
6:KB:61:ARG:HH11	6:KB:61:ARG:HG2	1.57	0.70
38:MA:96:LEU:HG	38:MA:139:ARG:HH12	1.57	0.70
9:NB:137:ASP:HB3	9:NB:140:LYS:HE2	1.73	0.70
41:PA:57:GLU:N	41:PA:60:LYS:HZ3	1.89	0.69
15:O:105:ARG:HG2	15:O:105:ARG:NH1	2.02	0.69
37:QC:139:GLN:HG3	37:QC:140:ARG:NH1	2.07	0.69
38:MA:18:LYS:HD3	38:MA:31:CYS:SG	2.32	0.69
17:Q:100:TYR:HB3	17:Q:103:ARG:HH11	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:VC:86:ILE:HG21	42:VC:133:LEU:HD13	1.73	0.69
53:GD:11:VAL:HG23	53:GD:38:SER:HB2	1.74	0.69
10:OB:10:GLU:N	10:OB:10:GLU:OE2	2.24	0.69
1:A:1064:G:O2'	1:A:1190:G:N2	2.25	0.69
1:FB:1028(A):C:O2	1:FB:1033:G:N2	2.19	0.69
53:GD:36:ARG:NH2	53:GD:75:ALA:O	2.26	0.69
2:B:833:U:O2	13:M:55:ARG:NH2	2.25	0.69
46:ZC:33:ARG:HE	46:ZC:62:SER:HB3	1.58	0.69
39:SC:40:ARG:NH1	39:SC:68:GLU:HB2	2.08	0.69
22:V:83:THR:OG1	22:V:84:ARG:N	2.26	0.69
2:B:1689:A:H62	2:B:1698:A:H2	1.40	0.69
2:GB:10:G:O2'	2:GB:2801:A:N7	2.25	0.69
36:PC:162:ILE:HD11	36:PC:184:VAL:HG22	1.74	0.69
1:A:1381:U:H1'	41:PA:79:ARG:HG2	1.74	0.69
33:GA:11:CYS:SG	33:GA:12:ASP:N	2.66	0.69
17:Q:60:THR:HG22	17:Q:77:PRO:HA	1.74	0.69
25:Y:52:ARG:NH1	25:Y:57:GLU:HB2	2.07	0.69
1:A:953:G:H5'	1:A:965:A:H61	1.57	0.69
2:GB:1669:A:O2'	2:GB:2549:G:OP1	2.11	0.69
17:Q:91:ARG:HG2	17:Q:91:ARG:HH11	1.58	0.69
41:UC:57:GLU:N	41:UC:60:LYS:HZ3	1.90	0.69
2:B:1092:C:O2	2:B:1099:G:N2	2.26	0.69
2:B:307:G:H21	2:B:330:A:H62	1.41	0.69
25:DC:52:ARG:NH1	25:DC:57:GLU:HB2	2.09	0.69
9:I:159:GLU:HG3	9:I:169:VAL:HG11	1.75	0.69
2:GB:1815:A:P	5:JB:54:ARG:HH22	2.15	0.69
2:GB:833:U:O2	13:RB:55:ARG:NH2	2.26	0.69
1:FB:677:U:H3	1:FB:713:G:H22	1.41	0.68
25:Y:65:SER:HG	25:Y:66:HIS:HD1	1.37	0.68
5:E:142:VAL:HG23	5:E:193:VAL:HA	1.75	0.68
5:E:75:ILE:HD13	5:E:99:ASP:OD2	1.94	0.68
2:GB:1060:U:O2'	2:GB:1061:U:OP2	2.10	0.68
8:MB:113:ARG:HH12	8:MB:142:PRO:HA	1.59	0.68
13:RB:85:LEU:HD13	13:RB:120:ALA:HB2	1.75	0.68
9:NB:130:ARG:HH12	9:NB:132:ARG:HH21	1.41	0.68
38:RC:96:LEU:HG	38:RC:139:ARG:HH12	1.58	0.68
41:UC:20:ASP:OD2	41:UC:22:LEU:HB3	1.92	0.68
17:VB:60:THR:HG22	17:VB:77:PRO:HA	1.74	0.68
1:A:677:U:H3	1:A:713:G:H22	1.41	0.68
2:GB:1173:G:H2'	2:GB:1175:U:H5''	1.74	0.68
5:JB:35:LYS:HD3	5:JB:64:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1173:G:H2'	2:B:1175:U:H5''	1.74	0.68
49:CD:35:ARG:HH11	49:CD:35:ARG:HG3	1.59	0.68
2:B:1021:A:H62	2:B:1141:U:H3	1.42	0.68
2:B:2131:G:H4'	2:B:2132:U:OP2	1.94	0.68
35:JA:142:ARG:NH2	35:JA:174:ARG:HH11	1.90	0.68
1:FB:542:G:OP1	38:RC:10:ARG:NH2	2.27	0.68
49:XA:35:ARG:HH11	49:XA:35:ARG:HG3	1.59	0.68
2:B:330:A:H2	2:B:1210:A:HO2'	1.42	0.68
2:GB:2104:G:H1	2:GB:2185:C:H42	1.42	0.68
2:B:2163:C:H5'	2:B:2165:G:H21	1.59	0.68
8:MB:73:ALA:HB3	8:MB:85:GLY:H	1.57	0.68
35:OC:116:ARG:HD2	35:OC:298:LEU:HD21	1.75	0.68
38:RC:190:ASP:OD2	38:RC:190:ASP:N	2.25	0.68
41:UC:126:ASP:HA	41:UC:129:GLU:HB2	1.76	0.68
1:A:664:G:H22	1:A:741:G:H1	1.42	0.67
2:GB:363(F):U:H3'	2:GB:363(G):A:H8	1.59	0.67
7:LB:185:ASP:HA	7:LB:188:ARG:HD2	1.75	0.67
37:QC:70:VAL:O	37:QC:106:VAL:N	2.27	0.67
2:GB:1398:C:O3'	21:ZB:25:LYS:NZ	2.26	0.67
33:LC:11:CYS:SG	33:LC:12:ASP:N	2.67	0.67
38:MA:18:LYS:HZ3	38:MA:31:CYS:HG	1.40	0.67
36:PC:18:GLY:HA2	36:PC:42:ILE:HG13	1.75	0.67
47:AD:3:ARG:CG	47:AD:3:ARG:HH11	2.07	0.67
2:GB:1021:A:H62	2:GB:1141:U:H3	1.42	0.67
36:KA:18:GLY:HA2	36:KA:42:ILE:HG13	1.76	0.67
14:N:138:ASP:OD1	23:W:81:ARG:NH1	2.27	0.67
1:A:1453:G:H4'	1:A:1454:G:OP2	1.94	0.67
12:L:115:VAL:HG13	12:L:121:VAL:HG21	1.77	0.67
42:QA:7:ALA:HB2	42:QA:85:ARG:HD2	1.74	0.67
47:VA:3:ARG:HG2	47:VA:4:ILE:HG22	1.76	0.67
2:B:91:A:H2'	2:B:92:G:H8	1.59	0.67
2:GB:155:C:H5	2:GB:171:G:H22	1.42	0.67
32:KC:39:LYS:HA	32:KC:42:ARG:NH1	2.10	0.67
39:NA:40:ARG:NH1	39:NA:68:GLU:HB2	2.09	0.67
47:AD:3:ARG:HH11	47:AD:4:ILE:HG22	1.60	0.67
2:B:1385:G:O2'	2:B:1396:U:O2	2.12	0.67
2:B:155:C:H5	2:B:171:G:H22	1.42	0.67
1:FB:664:G:H22	1:FB:741:G:H1	1.40	0.67
38:MA:26:CYS:HA	38:MA:31:CYS:HB2	1.76	0.67
12:QB:115:VAL:HG13	12:QB:121:VAL:HG21	1.77	0.67
2:GB:1689:A:H62	2:GB:1698:A:H2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:JA:107:ASP:HB2	35:JA:172:TYR:HD1	1.58	0.67
35:JA:224:ILE:HG12	35:JA:246:ILE:HG12	1.77	0.67
7:LB:157:VAL:HB	7:LB:194:MET:HG2	1.76	0.67
41:PA:126:ASP:HA	41:PA:129:GLU:HB2	1.77	0.67
43:RA:96:LEU:H	43:RA:98:PRO:HD2	1.60	0.67
2:B:1019:U:H3	2:B:1142(B):A:H62	1.41	0.67
2:B:1754:C:OP1	17:Q:96:ARG:NH1	2.28	0.67
1:FB:1422:G:H5''	12:QB:48:PRO:HB3	1.77	0.67
2:GB:1754:C:OP1	17:VB:96:ARG:NH1	2.28	0.67
2:GB:2126:A:H4'	2:GB:2127:G:H5'	1.76	0.67
5:JB:75:ILE:HD13	5:JB:99:ASP:OD2	1.95	0.67
7:LB:12:LEU:HG	7:LB:124:LEU:HD11	1.76	0.67
8:MB:115:ARG:HD3	47:AD:7:VAL:HG22	1.77	0.67
2:B:11:G:H2'	2:B:12:U:H5'	1.77	0.67
2:B:645:C:H4'	2:B:646:A:OP2	1.93	0.67
49:CD:39:LEU:HD12	49:CD:56:LEU:HB2	1.75	0.67
6:F:128:SER:OG	6:F:129:HIS:N	2.28	0.67
2:GB:2143:C:O2	2:GB:2148:G:N2	2.27	0.67
11:K:123:TYR:OH	11:K:130:HIS:NE2	2.17	0.67
4:NC:76:A:H3'	35:OC:234:GLY:HA3	1.77	0.67
2:GB:1044:G:H5'	2:GB:1045:A:OP2	1.95	0.66
37:LA:27:LYS:HG3	37:LA:28:GLN:HG3	1.78	0.66
17:Q:74:ARG:HG2	17:Q:74:ARG:HH11	1.59	0.66
1:FB:1454:G:OP1	54:HD:39:LYS:NZ	2.24	0.66
2:GB:2131:G:H4'	2:GB:2132:U:OP2	1.93	0.66
5:JB:142:VAL:HG23	5:JB:193:VAL:HA	1.77	0.66
41:PA:20:ASP:OD2	41:PA:22:LEU:HB3	1.95	0.66
47:VA:3:ARG:HH11	47:VA:4:ILE:HG22	1.60	0.66
8:H:113:ARG:HH12	8:H:142:PRO:HA	1.59	0.66
1:A:630:G:H5'	1:A:631:G:OP2	1.95	0.66
27:AA:3:ARG:HH11	27:AA:60:GLU:HB2	1.60	0.66
37:QC:20:SER:OG	37:QC:40:ARG:NH2	2.28	0.66
44:SA:80:LYS:HA	44:SA:83:GLU:HB2	1.78	0.66
43:WC:96:LEU:H	43:WC:98:PRO:HD2	1.60	0.66
2:B:2267:A:H5''	2:B:2268:A:H5'	1.77	0.66
42:VC:7:ALA:HB2	42:VC:85:ARG:HD2	1.77	0.66
1:A:1028(A):C:O2	1:A:1033:G:N2	2.19	0.66
47:AD:3:ARG:HG2	47:AD:4:ILE:HG22	1.77	0.66
32:FA:39:LYS:HA	32:FA:42:ARG:NH1	2.11	0.66
1:FB:1064:G:O2'	1:FB:1190:G:N2	2.28	0.66
1:FB:630:G:H5'	1:FB:631:G:OP2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1358:G:O2'	2:GB:1373:A:N6	2.27	0.66
35:OC:107:ASP:HB2	35:OC:172:TYR:HD1	1.59	0.66
38:RC:154:ASN:OD1	38:RC:154:ASN:N	2.27	0.66
38:RC:18:LYS:HD3	38:RC:31:CYS:SG	2.36	0.66
1:FB:953:G:H5'	1:FB:965:A:H61	1.61	0.66
2:B:1044:G:H5'	2:B:1045:A:OP2	1.96	0.66
1:FB:773:G:O3'	5:JB:202:LYS:NZ	2.28	0.66
2:GB:1019:U:H3	2:GB:1142(B):A:H62	1.44	0.66
2:B:2104:G:H1	2:B:2185:C:H42	1.44	0.66
2:GB:2508:G:OP1	35:OC:228:ARG:NH2	2.25	0.66
1:A:706:A:H4'	45:TA:22:HIS:HD2	1.61	0.65
38:MA:3:ARG:HD2	38:MA:5:ILE:HG23	1.77	0.65
14:N:109:VAL:HG13	14:N:113:GLN:HB3	1.78	0.65
1:A:1454:G:OP1	54:CB:39:LYS:NZ	2.27	0.65
2:B:2126:A:H4'	2:B:2127:G:H5'	1.77	0.65
2:GB:2163:C:H5'	2:GB:2165:G:H21	1.62	0.65
35:JA:116:ARG:HD2	35:JA:298:LEU:HD21	1.77	0.65
17:Q:133:GLU:OE2	17:Q:133:GLU:N	2.28	0.65
14:SB:109:VAL:HG13	14:SB:113:GLN:HB3	1.78	0.65
2:B:10:G:O2'	2:B:2801:A:N7	2.28	0.65
2:B:127:A:H5''	2:B:128:C:C6	2.31	0.65
1:FB:1130:A:H2'	1:FB:1131:G:C8	2.31	0.65
2:GB:771:G:OP1	31:JC:10:ARG:NH1	2.29	0.65
38:MA:154:ASN:N	38:MA:154:ASN:OD1	2.28	0.65
2:B:2291:U:H2'	2:B:2292:C:C6	2.30	0.65
2:B:2784:C:H1'	6:F:37:ARG:HH12	1.61	0.65
2:GB:155:C:H41	2:GB:171:G:H1	1.45	0.65
8:H:167:GLU:N	8:H:167:GLU:OE2	2.30	0.65
36:KA:162:ILE:HD11	36:KA:184:VAL:HG22	1.77	0.65
2:B:1669:A:O2'	2:B:2549:G:OP1	2.12	0.65
42:VC:89:PRO:HA	42:VC:92:ARG:HH12	1.61	0.65
1:FB:723:U:O2'	1:FB:724:G:O5'	2.15	0.65
10:J:10:GLU:N	10:J:10:GLU:OE2	2.29	0.65
25:Y:86:SER:N	25:Y:89:GLU:OE2	2.21	0.65
16:P:78:LEU:HD11	16:P:109:GLY:HA3	1.79	0.65
42:QA:86:ILE:HG21	42:QA:133:LEU:HD13	1.78	0.65
48:WA:24:CYS:HB3	48:WA:28:GLY:H	1.62	0.65
2:B:1761:C:H3'	2:B:1762:A:H5''	1.77	0.65
2:GB:11:G:H2'	2:GB:12:U:H5'	1.79	0.65
36:PC:23:ARG:HB2	36:PC:23:ARG:NH1	2.11	0.65
2:B:1803:A:O2'	5:E:259:THR:HG21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:1130:A:H2'	1:FB:1131:G:H8	1.62	0.65
2:B:1398:C:O3'	21:U:25:LYS:NZ	2.30	0.65
1:A:1130:A:H2'	1:A:1131:G:C8	2.32	0.65
2:B:155:C:H41	2:B:171:G:H1	1.43	0.65
2:GB:140:A:H8	2:GB:1408:C:HO2'	1.42	0.65
15:O:67:LEU:HD22	15:O:76:VAL:HG21	1.78	0.65
1:A:1498:UR3:OP2	34:HA:16:A:O2'	2.15	0.64
1:FB:820:U:H4'	1:FB:821:G:OP2	1.97	0.64
2:GB:127:A:H5''	2:GB:128:C:C6	2.32	0.64
2:GB:2287:A:N6	2:GB:2344:U:H3	1.96	0.64
6:KB:24:THR:HG23	6:KB:184:VAL:HG23	1.78	0.64
44:XC:80:LYS:HA	44:XC:83:GLU:HB2	1.78	0.64
2:GB:91:A:H2'	2:GB:92:G:H8	1.61	0.64
8:H:73:ALA:HB3	8:H:85:GLY:H	1.63	0.64
37:LA:64:VAL:HG22	37:LA:99:VAL:HA	1.78	0.64
7:LB:167:ALA:HB1	7:LB:173:VAL:HG11	1.79	0.64
7:LB:64:ILE:HD11	7:LB:75:HIS:HB2	1.79	0.64
36:PC:69:LEU:HB3	36:PC:162:ILE:HG22	1.79	0.64
2:GB:2291:U:H2'	2:GB:2292:C:C6	2.33	0.64
37:LA:70:VAL:O	37:LA:106:VAL:N	2.28	0.64
15:O:104:ARG:NH1	15:O:107:ASP:OD2	2.30	0.64
35:OC:224:ILE:HG12	35:OC:246:ILE:HG12	1.80	0.64
3:C:57:A:OP2	3:C:58:A:OP2	2.16	0.64
2:GB:2267:A:H5''	2:GB:2268:A:H5'	1.80	0.64
2:GB:307:G:H21	2:GB:330:A:H62	1.44	0.64
16:P:3:ARG:HH11	16:P:3:ARG:CA	2.07	0.64
38:RC:3:ARG:HD2	38:RC:5:ILE:HG23	1.78	0.64
1:A:1005:A:N6	1:A:1024:G:HO2'	1.95	0.64
4:D:31:G:H1	4:D:39:C:H42	1.45	0.64
1:FB:1412:C:H2'	1:FB:1413:A:C8	2.33	0.64
3:HB:57:A:OP2	3:HB:58:A:OP2	2.15	0.64
24:X:6:GLY:HA3	4:IA:1:C:O2	1.97	0.64
10:OB:118:LYS:NZ	10:OB:121:LYS:HG3	2.12	0.64
53:BB:50:ALA:HB1	53:BB:57:HIS:HB3	1.78	0.64
13:M:77:ARG:HB2	13:M:77:ARG:NH1	2.12	0.64
37:QC:58:GLU:HB3	44:XC:92:THR:HG21	1.80	0.64
23:BC:80:ARG:HB3	23:BC:82:ARG:NH1	2.13	0.64
53:GD:50:ALA:HB1	53:GD:57:HIS:HB3	1.78	0.64
49:XA:39:LEU:HD12	49:XA:56:LEU:HB2	1.78	0.64
6:KB:48:GLN:HG2	6:KB:78:LEU:HD12	1.79	0.64
38:RC:201:GLN:NE2	39:SC:116:THR:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:UB:3:ARG:CA	16:UB:3:ARG:HH11	2.08	0.64
2:B:140:A:H8	2:B:1408:C:HO2'	1.45	0.64
47:VA:54:VAL:HA	47:VA:57:ARG:HH12	1.62	0.64
6:F:24:THR:HG23	6:F:184:VAL:HG23	1.80	0.63
2:B:2445:G:OP1	7:G:74:ARG:NH2	2.30	0.63
37:LA:20:SER:OG	37:LA:40:ARG:NH2	2.31	0.63
9:NB:159:GLU:HG3	9:NB:169:VAL:HG11	1.79	0.63
54:CB:43:LEU:O	54:CB:47:GLY:N	2.30	0.63
5:E:122:ASP:OD1	5:E:122:ASP:N	2.28	0.63
2:GB:2394:C:N3	4:IB:76:A:O2'	2.29	0.63
7:LB:197:ASP:N	7:LB:197:ASP:OD1	2.29	0.63
1:A:8:A:C6	38:MA:209:ARG:HB2	2.33	0.63
40:OA:46:ARG:HB2	40:OA:60:PHE:CE1	2.34	0.63
37:QC:27:LYS:HG3	37:QC:28:GLN:HG3	1.78	0.63
9:NB:24:VAL:HG13	9:NB:35:VAL:HB	1.81	0.63
1:A:1422:G:H5''	12:L:48:PRO:HB3	1.81	0.63
12:QB:19:ILE:HG22	12:QB:43:VAL:HA	1.80	0.63
38:RC:178:VAL:O	38:RC:180:GLY:N	2.31	0.63
16:UB:78:LEU:HD11	16:UB:109:GLY:HA3	1.79	0.63
47:VA:108:ARG:NH1	47:VA:112:GLY:O	2.32	0.63
47:VA:34:LEU:HD13	47:VA:41:PRO:HA	1.80	0.63
2:GB:1047:G:H2'	2:GB:1110:G:H1	1.63	0.63
2:GB:648:G:H21	32:KC:46:ARG:HH12	1.43	0.63
38:MA:190:ASP:N	38:MA:190:ASP:OD2	2.31	0.63
47:VA:24:GLY:HA3	47:VA:66:LEU:HD23	1.81	0.63
2:B:1047:G:H2'	2:B:1110:G:H1	1.63	0.63
44:XC:13:HIS:HA	44:XC:16:LEU:HB3	1.81	0.63
2:B:1864:U:OP1	2:B:2410:G:O2'	2.14	0.63
48:BD:24:CYS:HB3	48:BD:28:GLY:H	1.64	0.63
13:RB:77:ARG:NH1	13:RB:77:ARG:HB2	2.14	0.63
40:TC:68:PRO:HG2	40:TC:71:ARG:HH21	1.64	0.63
1:FB:1460:A:OP2	54:HD:27:LYS:NZ	2.28	0.63
5:JB:122:ASP:OD1	5:JB:122:ASP:N	2.31	0.63
17:VB:133:GLU:N	17:VB:133:GLU:OE2	2.31	0.63
1:A:723:U:O2'	1:A:724:G:O5'	2.15	0.63
28:GC:36:CYS:SG	28:GC:37:SER:N	2.70	0.63
38:RC:98:GLU:OE2	38:RC:103:ASN:ND2	2.31	0.63
1:A:1379:G:OP1	41:PA:6:ARG:NH1	2.31	0.62
47:AD:54:VAL:HA	47:AD:57:ARG:HH12	1.62	0.62
2:B:771:G:OP1	31:EA:10:ARG:NH1	2.30	0.62
2:GB:2210:G:H3'	2:GB:2211:G:N7	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:ID:2:GLY:O	55:ID:4:GLY:N	2.32	0.62
36:KA:69:LEU:HB3	36:KA:162:ILE:HG22	1.79	0.62
16:UB:67:ARG:NH1	16:UB:103:GLU:OE1	2.32	0.62
23:W:80:ARG:HB3	23:W:82:ARG:NH1	2.13	0.62
38:MA:79:PHE:O	38:MA:83:SER:OG	2.16	0.62
35:OC:262:SER:HB3	35:OC:265:LYS:HB2	1.79	0.62
1:A:1130:A:H2'	1:A:1131:G:H8	1.65	0.62
1:A:1412:C:H2'	1:A:1413:A:C8	2.34	0.62
1:A:820:U:H4'	1:A:821:G:OP2	1.97	0.62
51:ED:6:LEU:HD23	51:ED:23:VAL:HG11	1.81	0.62
13:M:85:LEU:HD13	13:M:120:ALA:HB2	1.80	0.62
2:B:1434:A:H61	2:B:1558:A:N6	1.96	0.62
2:B:2143:C:O2	2:B:2148:G:N2	2.28	0.62
2:GB:2784:C:H1'	6:KB:37:ARG:HH12	1.63	0.62
36:KA:124:SER:H	36:KA:125:PRO:HD2	1.64	0.62
15:O:18:LEU:HD21	15:O:22:ARG:NH1	2.15	0.62
14:SB:138:ASP:OD1	23:BC:81:ARG:NH1	2.33	0.62
39:NA:122:GLU:O	39:NA:126:ARG:NE	2.24	0.62
23:BC:79:ARG:HD2	23:BC:80:ARG:NH1	2.11	0.62
7:G:157:VAL:HB	7:G:194:MET:HG2	1.81	0.62
36:KA:23:ARG:HB2	36:KA:23:ARG:NH1	2.15	0.62
11:PB:46:VAL:HG23	11:PB:48:MET:HG2	1.80	0.62
2:B:1364:G:OP2	25:Y:3:LYS:HG3	1.99	0.62
55:DB:2:GLY:O	55:DB:4:GLY:N	2.33	0.62
13:M:99:LEU:HD23	13:M:102:ARG:HH21	1.65	0.62
37:QC:64:VAL:HG22	37:QC:99:VAL:HA	1.81	0.62
24:X:6:GLY:HA3	4:IA:1:C:H1'	1.80	0.62
38:MA:178:VAL:O	38:MA:180:GLY:N	2.32	0.62
23:W:127:LYS:HB2	23:W:162:GLU:HB2	1.82	0.62
1:A:1348:U:H4'	43:RA:120:ARG:HG3	1.80	0.62
2:B:1184:G:H5''	27:AA:29:ARG:HD3	1.81	0.62
1:FB:1379:G:OP1	41:UC:6:ARG:NH1	2.33	0.62
7:G:167:ALA:HB1	7:G:173:VAL:HG11	1.80	0.62
2:GB:2698:U:H2'	2:GB:2699:C:C6	2.34	0.62
2:B:2210:G:H3'	2:B:2211:G:N7	2.15	0.62
2:B:34:C:O2'	2:B:35:G:OP1	2.18	0.62
23:BC:157:LEU:HD23	23:BC:161:VAL:HG12	1.81	0.62
7:G:197:ASP:N	7:G:197:ASP:OD1	2.33	0.62
31:JC:34:ARG:HH11	31:JC:34:ARG:HG2	1.65	0.62
38:RC:9:CYS:HG	38:RC:31:CYS:HG	1.46	0.62
15:TB:67:LEU:HD22	15:TB:76:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:634:C:H2'	2:B:635:C:C6	2.35	0.61
7:G:12:LEU:HG	7:G:124:LEU:HD11	1.82	0.61
2:GB:1385:G:O2'	2:GB:1396:U:O2	2.16	0.61
8:MB:136:ARG:NE	8:MB:136:ARG:H	1.95	0.61
15:TB:97:VAL:HG22	15:TB:114:VAL:HG22	1.82	0.61
22:AC:44:ILE:H	22:AC:44:ILE:HD13	1.64	0.61
37:LA:16:ARG:NH2	37:LA:183:ASP:OD1	2.33	0.61
42:VC:89:PRO:HA	42:VC:92:ARG:NH1	2.15	0.61
23:W:157:LEU:HD23	23:W:161:VAL:HG12	1.83	0.61
1:FB:1348:U:H4'	43:WC:120:ARG:HG3	1.81	0.61
1:A:559:A:H4'	1:A:560:U:H3'	1.81	0.61
47:AD:24:GLY:HA3	47:AD:66:LEU:HD23	1.81	0.61
37:LA:31:HIS:HA	37:LA:34:LEU:HB3	1.82	0.61
17:VB:74:ARG:NH1	17:VB:74:ARG:HG2	2.14	0.61
1:FB:1531:A:OP2	1:FB:1532:U:H5	1.84	0.61
2:GB:1085:A:HO2'	2:GB:1104:C:HO2'	1.49	0.61
2:GB:1058:G:N2	2:GB:1087:G:OP2	2.32	0.61
4:IB:31:G:H1	4:IB:39:C:H42	1.46	0.61
10:J:91:SER:O	10:J:93:THR:N	2.33	0.61
36:KA:24:TRP:HD1	36:KA:24:TRP:H	1.49	0.61
38:RC:168:ARG:HG3	38:RC:168:ARG:HH11	1.65	0.61
22:V:50:ARG:HH11	22:V:50:ARG:HB2	1.66	0.61
6:F:48:GLN:HG2	6:F:78:LEU:HD12	1.81	0.61
2:GB:322:A:OP2	7:LB:169:ASN:HB2	2.01	0.61
44:SA:13:HIS:HA	44:SA:16:LEU:HB3	1.82	0.61
1:A:191(G):G:O2'	54:CB:101:GLY:O	2.19	0.61
1:FB:17:U:H2'	1:FB:18:C:C6	2.36	0.61
2:GB:2508:G:P	35:OC:228:ARG:HH22	2.24	0.61
16:P:67:ARG:NH1	16:P:103:GLU:OE1	2.32	0.61
42:QA:89:PRO:HA	42:QA:92:ARG:HH12	1.66	0.61
47:AD:34:LEU:HD13	47:AD:41:PRO:HA	1.82	0.61
2:B:1058:G:N2	2:B:1087:G:OP2	2.34	0.61
2:B:1252:G:N3	18:R:33:ARG:HD2	2.16	0.61
54:HD:43:LEU:O	54:HD:47:GLY:N	2.32	0.61
38:MA:98:GLU:OE2	38:MA:103:ASN:ND2	2.33	0.61
38:RC:103:ASN:OD1	38:RC:114:ARG:NH2	2.33	0.61
38:RC:26:CYS:HA	38:RC:31:CYS:HB2	1.81	0.61
40:TC:46:ARG:HH11	40:TC:46:ARG:CB	2.12	0.61
28:BA:36:CYS:SG	28:BA:37:SER:N	2.69	0.61
44:SA:34:VAL:HA	44:SA:74:ILE:HG22	1.82	0.61
2:B:270(Q):C:H6	2:B:270(Q):C:OP2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1184:G:H5''	27:FC:29:ARG:HD3	1.83	0.61
1:FB:1314:C:N4	53:GD:2:PRO:O	2.34	0.61
38:MA:168:ARG:HH11	38:MA:168:ARG:HG3	1.65	0.61
1:A:1022:G:C2	1:A:1023:G:H1'	2.36	0.60
2:GB:2168:G:O2'	2:GB:2170:A:N7	2.33	0.60
8:MB:136:ARG:HE	8:MB:136:ARG:N	1.98	0.60
36:PC:24:TRP:HD1	36:PC:24:TRP:H	1.48	0.60
2:B:819:A:OP2	2:B:1187:G:N2	2.21	0.60
54:CB:98:PRO:O	54:CB:100:ILE:N	2.33	0.60
49:CD:17:ARG:HD3	49:CD:26:GLU:OE2	2.01	0.60
1:FB:1022:G:C2	1:FB:1023:G:H1'	2.36	0.60
2:GB:645:C:H4'	2:GB:646:A:OP2	2.00	0.60
6:KB:105:THR:OG1	6:KB:199:ARG:NH2	2.34	0.60
45:YC:67:ASP:HA	45:YC:70:LYS:HE2	1.83	0.60
54:HD:98:PRO:O	54:HD:100:ILE:N	2.33	0.60
9:I:56:SER:HB3	9:I:61:HIS:ND1	2.16	0.60
15:O:97:VAL:HG22	15:O:114:VAL:HG22	1.83	0.60
37:QC:16:ARG:NH2	37:QC:183:ASP:OD1	2.35	0.60
14:SB:51:ARG:HG3	14:SB:66:ILE:HD11	1.84	0.60
21:U:60:ARG:NH1	31:EA:47:ARG:NH2	2.49	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.60
27:FC:3:ARG:HH11	27:FC:60:GLU:HB2	1.65	0.60
8:H:136:ARG:H	8:H:136:ARG:NE	1.97	0.60
36:PC:124:SER:H	36:PC:125:PRO:HD2	1.65	0.60
23:BC:127:LYS:HB2	23:BC:162:GLU:HB2	1.83	0.60
44:XC:62:HIS:HB3	48:BD:59:ALA:HB3	1.82	0.60
2:GB:634:C:H2'	2:GB:635:C:C6	2.36	0.60
37:QC:31:HIS:HA	37:QC:34:LEU:HB3	1.83	0.60
1:A:1367:C:H5'	44:SA:60:ARG:NH1	2.17	0.60
1:A:363:A:OP2	46:UA:34:ARG:HD3	2.02	0.60
17:VB:100:TYR:CD1	17:VB:103:ARG:NH1	2.69	0.60
1:A:17:U:H2'	1:A:18:C:C6	2.37	0.60
2:B:1094:U:H1'	2:B:1096:A:C8	2.37	0.60
2:B:1177:A:H2'	2:B:1178:C:O4'	2.02	0.60
2:B:2115:G:N2	2:B:2119:A:OP1	2.33	0.60
1:FB:184:G:H2'	1:FB:185:A:H8	1.65	0.60
14:N:43:THR:HA	14:N:94:VAL:HG12	1.83	0.60
10:OB:83:ALA:HA	10:OB:88:ILE:HG12	1.82	0.60
37:QC:59:ARG:NH1	37:QC:64:VAL:HG12	2.17	0.60
1:FB:1367:C:H5'	44:XC:60:ARG:NH1	2.16	0.60
22:AC:83:THR:OG1	22:AC:84:ARG:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:559:A:H4'	1:FB:560:U:H3'	1.81	0.60
2:GB:1252:G:N3	18:WB:33:ARG:HD2	2.16	0.60
2:GB:2023:G:H5'	2:GB:2617:C:H4'	1.82	0.60
42:QA:116:LYS:HD2	42:QA:129:VAL:HG11	1.84	0.60
1:A:1367:C:H4'	44:SA:48:THR:HG21	1.84	0.60
37:LA:58:GLU:HB3	44:SA:92:THR:HG21	1.83	0.60
1:A:116:A:H61	1:A:313:A:H1'	1.67	0.60
2:GB:1177:A:H2'	2:GB:1178:C:O4'	2.01	0.60
2:GB:330:A:H2	2:GB:1210:A:HO2'	1.49	0.60
36:PC:74:LYS:HZ2	36:PC:166:ASP:HB2	1.67	0.60
19:S:58:VAL:HG21	19:S:100:ARG:HH21	1.66	0.60
2:B:2168:G:O2'	2:B:2170:A:N7	2.33	0.60
3:HB:13:A:N1	3:HB:69:G:O2'	2.30	0.60
37:LA:52:LEU:HD13	37:LA:68:VAL:HG13	1.84	0.60
7:LB:119:ARG:NH1	7:LB:119:ARG:HB2	2.16	0.60
1:FB:1367:C:H4'	44:XC:48:THR:HG21	1.83	0.60
33:LC:11:CYS:HB3	33:LC:32:HIS:CE1	2.37	0.60
8:MB:11:TYR:HA	8:MB:15:VAL:HB	1.84	0.60
22:AC:23:ARG:NH2	22:AC:41:GLY:O	2.35	0.59
33:GA:11:CYS:HB3	33:GA:32:HIS:CE1	2.37	0.59
34:HA:14:A:H3'	34:HA:15:A:C8	2.37	0.59
36:KA:19:HIS:HD2	36:KA:189:ASP:OD2	1.85	0.59
13:M:118:GLY:O	13:M:137:LYS:NZ	2.31	0.59
13:M:91:PHE:O	13:M:121:LYS:NZ	2.33	0.59
37:LA:131:ARG:NH1	39:NA:50:GLU:HG3	2.17	0.59
49:CD:33:THR:HG21	49:CD:85:LEU:HD22	1.83	0.59
7:G:64:ILE:HD11	7:G:75:HIS:HB2	1.84	0.59
2:GB:507:A:O2'	2:GB:508:G:OP2	2.18	0.59
8:H:11:TYR:HA	8:H:15:VAL:HB	1.84	0.59
9:I:24:VAL:HG13	9:I:35:VAL:HB	1.83	0.59
10:J:93:THR:HG23	10:J:95:LYS:H	1.65	0.59
14:N:116:GLU:OE2	14:N:119:ARG:NE	2.32	0.59
1:A:1492:A:N6	46:UA:48:PRO:O	2.36	0.59
49:XA:33:THR:HG21	49:XA:85:LEU:HD22	1.83	0.59
1:A:1314:C:N4	53:BB:2:PRO:O	2.36	0.59
29:CA:16:ARG:NH1	29:CA:16:ARG:HG2	2.11	0.59
1:FB:164:U:H2'	1:FB:165:C:C6	2.36	0.59
2:GB:1364:G:OP2	25:DC:3:LYS:HG3	2.02	0.59
33:LC:25:VAL:HB	33:LC:34:GLN:HB2	1.83	0.59
10:OB:83:ALA:HA	10:OB:88:ILE:HG21	1.84	0.59
40:TC:33:TYR:HD1	40:TC:71:ARG:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1358:G:O2'	2:B:1373:A:N6	2.34	0.59
1:A:403:C:O2'	38:MA:122:ARG:NH2	2.35	0.59
8:MB:167:GLU:OE2	8:MB:167:GLU:N	2.35	0.59
15:TB:13:HIS:HD2	15:TB:16:HIS:H	1.49	0.59
42:VC:85:ARG:HD3	42:VC:87:SER:O	2.02	0.59
43:WC:105:ASP:OD2	43:WC:107:ARG:HG2	2.02	0.59
1:A:1531:A:OP2	1:A:1532:U:H5	1.84	0.59
1:A:184:G:H2'	1:A:185:A:H8	1.67	0.59
47:AD:108:ARG:NH1	47:AD:112:GLY:O	2.35	0.59
1:FB:116:A:H61	1:FB:313:A:H1'	1.66	0.59
1:FB:1498:UR3:OP2	34:MC:16:A:O2'	2.20	0.59
1:FB:1516:G:N1	1:FB:1519:MA6:OP2	2.36	0.59
2:GB:270(M):U:O2'	2:GB:270(O):G:N2	2.35	0.59
54:HD:10:LEU:HD12	54:HD:12:ALA:H	1.68	0.59
35:JA:262:SER:HB3	35:JA:265:LYS:HB2	1.84	0.59
2:GB:2393:A:H5''	13:RB:63:PRO:HB3	1.84	0.59
20:T:110:LYS:NZ	20:T:111:HIS:H	2.00	0.59
40:TC:46:ARG:HB2	40:TC:60:PHE:CE1	2.38	0.59
1:FB:692:U:O4	45:YC:26:ASN:ND2	2.35	0.59
2:B:2393:A:H5''	13:M:63:PRO:HB3	1.83	0.59
2:GB:1864:U:OP1	2:GB:2410:G:O2'	2.14	0.59
35:OC:182:HIS:HB3	35:OC:310:TYR:HE1	1.67	0.59
14:SB:43:THR:HA	14:SB:94:VAL:HG12	1.85	0.59
15:TB:100:LEU:HD11	15:TB:113:LEU:HD23	1.85	0.59
28:BA:44:THR:O	28:BA:46:GLN:N	2.35	0.59
28:BA:56:VAL:HG22	28:BA:61:ARG:HA	1.84	0.59
2:B:606:U:OP2	7:G:104:LYS:HE3	2.03	0.59
8:H:11:TYR:CZ	8:H:16:ARG:HD3	2.37	0.59
2:GB:1803:A:O2'	5:JB:259:THR:HG21	2.02	0.59
7:LB:107:LYS:NZ	7:LB:207:GLY:H	2.01	0.59
16:P:15:ARG:HG2	16:P:88:ASP:OD2	2.03	0.59
36:PC:19:HIS:HD2	36:PC:189:ASP:OD2	1.85	0.59
43:RA:95:LYS:H	43:RA:98:PRO:HG2	1.67	0.59
49:XA:3:ILE:HD13	49:XA:34:LEU:HD23	1.84	0.59
1:FB:1005:A:N6	1:FB:1024:G:O2'	2.36	0.59
33:GA:27:CYS:SG	33:GA:28:GLU:N	2.75	0.59
2:GB:1113:U:H2'	2:GB:1114:G:H8	1.66	0.59
37:QC:67:THR:HA	37:QC:102:ASN:HB3	1.83	0.59
13:RB:81:GLN:OE1	13:RB:107:LYS:N	2.32	0.59
18:WB:36:ARG:HD3	18:WB:40:PHE:CZ	2.38	0.59
1:FB:1320:C:N3	53:GD:36:ARG:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1022:G:O6	11:PB:66:LYS:NZ	2.36	0.59
31:JC:34:ARG:HG2	31:JC:34:ARG:NH1	2.18	0.59
14:N:82:ARG:NH1	24:X:4:LYS:HB2	2.18	0.59
13:RB:99:LEU:HD23	13:RB:102:ARG:HH21	1.68	0.59
12:QB:75:SER:HB2	17:VB:74:ARG:HH12	1.67	0.59
2:B:1022:G:O6	11:K:66:LYS:NZ	2.34	0.59
2:B:1091:G:N2	2:B:1100:C:O2'	2.36	0.59
2:B:270(M):U:O2'	2:B:270(O):G:N2	2.35	0.59
2:B:784:A:C5	5:E:229:VAL:HG21	2.38	0.59
35:JA:126:LEU:HG	35:JA:157:GLY:H	1.67	0.59
40:OA:33:TYR:HD1	40:OA:71:ARG:HG2	1.67	0.59
40:OA:68:PRO:HG2	40:OA:71:ARG:HH21	1.68	0.59
37:QC:85:ARG:HG2	37:QC:88:ARG:NH2	2.18	0.59
14:SB:82:ARG:NH1	24:CC:4:LYS:HB2	2.18	0.59
2:B:154(A):C:O2'	2:B:155:C:N3	2.36	0.58
25:DC:86:SER:N	25:DC:89:GLU:OE2	2.23	0.58
2:GB:1291:C:H2'	2:GB:1292:U:H6	1.68	0.58
10:J:83:ALA:HA	10:J:88:ILE:HG21	1.84	0.58
52:AB:33:ASP:OD2	52:AB:36:ASN:HB2	2.03	0.58
2:GB:140:A:H8	2:GB:1408:C:O2'	1.87	0.58
2:GB:1786:A:H1'	2:GB:1938:A:N6	2.17	0.58
37:LA:67:THR:HA	37:LA:102:ASN:HB3	1.85	0.58
2:B:2139:C:H3'	2:B:2140:C:C6	2.38	0.58
2:GB:2232:U:P	25:DC:40:ARG:HH22	2.26	0.58
1:FB:363:A:OP2	46:ZC:34:ARG:HD3	2.03	0.58
2:GB:2115:G:N2	2:GB:2119:A:OP1	2.35	0.58
2:GB:616:A:C4	7:LB:180:GLY:HA2	2.39	0.58
18:R:59:ARG:O	18:R:63:VAL:HG23	2.03	0.58
20:T:8:ARG:HB2	20:T:102:HIS:ND1	2.18	0.58
22:AC:50:ARG:HB2	22:AC:50:ARG:HH11	1.68	0.58
8:MB:115:ARG:NH1	47:AD:2:ALA:HB2	2.18	0.58
2:B:185:U:H4'	2:B:218:A:H4'	1.85	0.58
5:E:148:GLU:HB2	5:E:151:LYS:HD2	1.85	0.58
6:F:105:THR:OG1	6:F:199:ARG:NH2	2.36	0.58
1:FB:266:G:H3'	51:ED:67:LYS:HB2	1.85	0.58
2:GB:880:G:H1	2:GB:897:C:H42	1.49	0.58
28:GC:56:VAL:HG22	28:GC:61:ARG:HA	1.85	0.58
1:FB:191(G):G:O2'	54:HD:101:GLY:O	2.21	0.58
2:GB:2445:G:OP1	7:LB:74:ARG:NH2	2.37	0.58
43:RA:11:LYS:O	43:RA:13:ALA:N	2.32	0.58
43:RA:26:VAL:HB	43:RA:33:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AC:92:ASN:OD1	22:AC:93:GLY:N	2.37	0.58
2:B:1045:A:H1'	2:B:1047:G:H1'	1.85	0.58
2:B:2023:G:H5'	2:B:2617:C:H4'	1.85	0.58
2:B:2698:U:H2'	2:B:2699:C:C6	2.37	0.58
28:BA:62:ARG:NH1	28:BA:62:ARG:HA	2.18	0.58
1:FB:1124:G:N7	1:FB:1145:C:O2'	2.36	0.58
36:KA:48:MET:HA	36:KA:51:LEU:HB2	1.85	0.58
12:L:19:ILE:HG22	12:L:43:VAL:HA	1.86	0.58
37:LA:59:ARG:NH1	37:LA:64:VAL:HG12	2.18	0.58
14:N:65:PHE:HB2	14:N:105:GLU:HB2	1.85	0.58
40:OA:46:ARG:HH11	40:OA:46:ARG:CB	2.14	0.58
35:OC:126:LEU:HG	35:OC:157:GLY:H	1.69	0.58
36:PC:185:ILE:HG23	36:PC:199:TYR:HB2	1.86	0.58
44:XC:34:VAL:HA	44:XC:74:ILE:HG22	1.84	0.58
45:YC:31:THR:HG22	45:YC:42:TRP:HB2	1.86	0.58
47:AD:11:ARG:HA	47:AD:45:VAL:HB	1.84	0.58
2:B:2151:G:N2	2:B:2152:G:O6	2.37	0.58
2:B:2166:G:N7	2:B:2168:G:N2	2.51	0.58
33:GA:25:VAL:HB	33:GA:34:GLN:HB2	1.84	0.58
28:GC:44:THR:O	28:GC:46:GLN:N	2.37	0.58
8:MB:122:PRO:HG2	8:MB:182:LYS:HG2	1.86	0.58
12:QB:45:GLU:HA	12:QB:54:GLU:OE2	2.04	0.58
14:SB:47:ILE:HD12	14:SB:70:PRO:HG3	1.84	0.58
47:VA:11:ARG:HA	47:VA:45:VAL:HB	1.85	0.58
2:B:1653:G:H5''	15:O:2:ARG:HD3	1.86	0.58
2:B:885:C:N4	2:B:886:C:O2	2.36	0.58
28:BA:62:ARG:HA	28:BA:62:ARG:CZ	2.33	0.58
2:GB:885:C:N4	2:GB:886:C:O2	2.36	0.58
8:MB:50:ALA:HB1	8:MB:52:ILE:HG13	1.86	0.58
36:PC:74:LYS:HE3	36:PC:206:ASP:HA	1.86	0.58
19:XB:72:VAL:HG13	19:XB:85:LYS:HB3	1.84	0.58
1:FB:1368:G:H4'	44:XC:46:ARG:NH1	2.18	0.58
2:B:2792:G:H2'	2:B:2793:G:C8	2.39	0.58
2:B:896:A:H4'	2:B:896:A:OP2	2.04	0.58
1:FB:1353:G:OP1	55:ID:10:ARG:NH1	2.37	0.58
8:H:50:ALA:HB1	8:H:52:ILE:HG13	1.85	0.58
35:JA:226:THR:HG23	35:JA:241:ASP:HB3	1.86	0.58
8:MB:11:TYR:CZ	8:MB:16:ARG:HD3	2.38	0.58
14:N:76:LYS:HB3	14:N:91:GLU:HG3	1.85	0.58
36:PC:32:ILE:HD11	36:PC:40:HIS:HB3	1.86	0.58
37:QC:130:VAL:O	37:QC:134:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:WB:59:ARG:O	18:WB:63:VAL:HG23	2.04	0.58
1:FB:1343:G:O2'	43:WC:121:ARG:NH1	2.36	0.58
24:X:12:ASN:HA	24:X:14:ARG:NH2	2.19	0.58
2:B:2138:C:H42	2:B:2153:G:H1	1.50	0.58
2:GB:2139:C:H3'	2:GB:2140:C:C6	2.39	0.58
13:M:124:LYS:HE2	13:M:144:GLU:OE2	2.03	0.58
14:N:67:ARG:NH1	14:N:105:GLU:OE2	2.35	0.58
37:QC:65:ALA:HA	37:QC:100:ALA:HB3	1.86	0.58
39:SC:77:PRO:HG2	39:SC:78:HIS:CD2	2.38	0.58
16:UB:41:ASP:HB2	16:UB:48:LEU:HD21	1.86	0.58
2:B:1045:A:O2'	2:B:1047:G:N3	2.33	0.58
1:A:1320:C:N3	53:BB:36:ARG:HD3	2.18	0.58
31:EA:47:ARG:HB3	31:EA:47:ARG:HH11	1.67	0.58
1:FB:429:U:OP2	38:RC:36:ARG:NH2	2.37	0.58
2:GB:1060:U:H5''	2:GB:1061:U:H3'	1.86	0.58
2:GB:479:A:N3	2:GB:481:G:H5''	2.18	0.58
42:QA:89:PRO:HA	42:QA:92:ARG:NH1	2.19	0.58
2:GB:1532:C:H42	2:GB:1539:G:H1	1.52	0.57
38:MA:103:ASN:OD1	38:MA:114:ARG:NH2	2.36	0.57
42:QA:85:ARG:HD3	42:QA:87:SER:O	2.04	0.57
1:A:692:U:O4	45:TA:26:ASN:ND2	2.37	0.57
1:A:537:G:OP1	46:UA:113:ARG:NH2	2.30	0.57
1:A:740:U:OP1	49:XA:38:ARG:HD3	2.04	0.57
1:FB:1291:G:O2'	43:WC:38:GLN:OE1	2.22	0.57
2:GB:1025:G:C4	2:GB:1135:C:H1'	2.39	0.57
38:RC:9:CYS:HG	38:RC:18:LYS:NZ	2.00	0.57
2:B:1113:U:H2'	2:B:1114:G:H8	1.68	0.57
2:B:2317:C:H2'	2:B:2318:G:H5'	1.84	0.57
52:FD:33:ASP:OD2	52:FD:36:ASN:HB2	2.04	0.57
2:GB:2552:2MU:H2'	2:GB:2554:U:OP2	2.04	0.57
10:J:118:LYS:NZ	10:J:121:LYS:HG3	2.18	0.57
9:NB:56:SER:HB3	9:NB:61:HIS:ND1	2.19	0.57
1:FB:1493:A:N3	35:OC:119:THR:HG23	2.18	0.57
17:VB:129:ARG:HA	17:VB:132:LYS:HZ1	1.68	0.57
43:WC:83:ARG:HG2	43:WC:102:LEU:HD23	1.85	0.57
49:XA:25:THR:HG21	49:XA:70:LEU:HB2	1.87	0.57
1:A:1291:G:O2'	43:RA:38:GLN:OE1	2.22	0.57
1:FB:452:A:OP1	50:DD:43:LYS:NZ	2.37	0.57
51:ED:59:ILE:HG22	51:ED:73:VAL:HA	1.87	0.57
2:GB:185:U:H4'	2:GB:218:A:H4'	1.85	0.57
2:GB:2232:U:OP2	25:DC:40:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:774:A:H2'	2:GB:774:A:N3	2.19	0.57
37:LA:65:ALA:HA	37:LA:100:ALA:HB3	1.86	0.57
16:P:41:ASP:HB2	16:P:48:LEU:HD21	1.85	0.57
37:QC:52:LEU:HD13	37:QC:68:VAL:HG13	1.86	0.57
43:WC:26:VAL:HB	43:WC:33:PHE:HB2	1.86	0.57
2:B:784:A:H5'	2:B:785:G:OP1	2.05	0.57
1:FB:1323:G:H2'	1:FB:1324:A:C8	2.39	0.57
2:GB:1094:U:H1'	2:GB:1096:A:C8	2.40	0.57
2:GB:2317:C:H2'	2:GB:2318:G:H5'	1.87	0.57
2:GB:2494:G:O2'	14:SB:80:GLU:HA	2.03	0.57
35:JA:138:TYR:HE1	35:JA:338:ASP:OD2	1.86	0.57
8:MB:61:ALA:HB2	8:MB:68:PRO:HD3	1.87	0.57
39:NA:110:LEU:HD13	39:NA:118:ILE:HD13	1.85	0.57
40:OA:33:TYR:CE2	40:OA:78:GLU:HG3	2.39	0.57
17:Q:73:GLU:OE1	17:Q:103:ARG:NH2	2.37	0.57
17:Q:74:ARG:HG2	17:Q:74:ARG:NH1	2.20	0.57
43:RA:17:VAL:HG11	43:RA:81:ILE:HG12	1.85	0.57
39:SC:122:GLU:O	39:SC:126:ARG:NE	2.26	0.57
17:VB:91:ARG:HH11	17:VB:91:ARG:HG2	1.68	0.57
2:B:479:A:N3	2:B:481:G:H5''	2.20	0.57
2:GB:1339:G:H5''	21:ZB:16:LYS:HD3	1.87	0.57
8:H:67:LYS:H	28:BA:6:HIS:CE1	2.22	0.57
9:I:20:ALA:HB3	9:I:23:ARG:HG3	1.86	0.57
11:K:46:VAL:HG23	11:K:48:MET:HG2	1.85	0.57
2:GB:2680:C:H5'	6:KB:189:PRO:HA	1.87	0.57
15:O:100:LEU:HD11	15:O:113:LEU:HD23	1.87	0.57
2:B:1077:A:H3'	2:B:1078:U:H4'	1.85	0.57
2:B:2287:A:N6	2:B:2344:U:H3	1.99	0.57
2:B:2784:C:H1'	6:F:37:ARG:NH1	2.19	0.57
2:B:686:G:O5'	31:EA:11:LYS:NZ	2.38	0.57
6:F:61:ARG:HG2	6:F:61:ARG:NH1	2.20	0.57
17:Q:74:ARG:HD3	17:Q:76:PHE:CZ	2.39	0.57
1:A:1368:G:H4'	44:SA:46:ARG:NH1	2.19	0.57
16:UB:15:ARG:HG2	16:UB:88:ASP:OD2	2.04	0.57
23:BC:4:ARG:NH1	23:BC:60:GLU:HG2	2.20	0.57
49:CD:88:ARG:HB3	49:CD:88:ARG:NH2	2.20	0.57
2:GB:2166:G:N7	2:GB:2168:G:N2	2.52	0.57
36:KA:74:LYS:HZ2	36:KA:166:ASP:HB2	1.70	0.57
13:RB:2:LYS:HB3	13:RB:2:LYS:NZ	2.20	0.57
38:RC:9:CYS:SG	38:RC:26:CYS:SG	3.03	0.57
22:V:44:ILE:H	22:V:44:ILE:HD13	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:95:LEU:HD12	25:Y:98:LEU:HD12	1.86	0.57
45:YC:99:GLN:HE21	52:FD:88:LYS:NZ	2.03	0.57
1:A:1124:G:N7	1:A:1145:C:O2'	2.37	0.57
2:B:2021:C:OP1	29:CA:12:SER:OG	2.23	0.57
8:H:122:PRO:HG2	8:H:182:LYS:HG2	1.86	0.57
36:KA:74:LYS:HE3	36:KA:206:ASP:HA	1.86	0.57
36:KA:32:ILE:HD11	36:KA:40:HIS:HB3	1.87	0.57
10:OB:61:ARG:HD3	10:OB:64:GLU:OE2	2.04	0.57
1:FB:1158:C:O2'	36:PC:133:LYS:NZ	2.38	0.57
17:Q:129:ARG:HA	17:Q:132:LYS:HZ1	1.68	0.57
43:RA:83:ARG:HG2	43:RA:102:LEU:HD23	1.86	0.57
47:VA:22:ILE:HD12	47:VA:25:ILE:HD12	1.87	0.57
42:VC:112:LEU:HA	42:VC:134:ILE:HG12	1.87	0.57
43:WC:17:VAL:HG11	43:WC:81:ILE:HG12	1.85	0.57
1:A:452:A:OP1	50:YA:43:LYS:NZ	2.38	0.57
1:A:999:U:H3	1:A:1041:A:H62	1.52	0.57
2:GB:270(Q):C:OP2	2:GB:270(Q):C:H6	1.87	0.57
2:GB:796:C:H2'	2:GB:797:C:C6	2.40	0.57
5:JB:148:GLU:HB2	5:JB:151:LYS:HD2	1.87	0.57
37:LA:85:ARG:HG2	37:LA:88:ARG:NH2	2.20	0.57
13:M:71:VAL:HG22	13:M:72:PRO:HA	1.86	0.57
10:OB:57:ARG:HB3	10:OB:61:ARG:HH22	1.70	0.57
20:T:30:GLU:OE2	20:T:30:GLU:HA	2.04	0.57
47:VA:14:ARG:HE	47:VA:42:ALA:HA	1.69	0.57
23:W:4:ARG:NH1	23:W:60:GLU:HG2	2.19	0.57
24:X:2:ALA:HA	35:JA:236:HIS:CE1	2.39	0.57
1:FB:706:A:H5''	45:YC:22:HIS:CD2	2.39	0.57
1:A:1005:A:N6	1:A:1024:G:O2'	2.37	0.56
2:B:1291:C:H2'	2:B:1292:U:H6	1.70	0.56
2:B:2795:G:H1'	2:B:2802:G:N2	2.20	0.56
1:FB:539:A:H2'	1:FB:540:G:C8	2.40	0.56
2:GB:34:C:O2'	2:GB:35:G:OP1	2.22	0.56
2:GB:896:A:OP2	2:GB:896:A:H4'	2.04	0.56
8:H:61:ALA:HB2	8:H:68:PRO:HD3	1.87	0.56
36:KA:97:TRP:HH2	36:KA:176:GLU:OE2	1.87	0.56
8:MB:19:LEU:HD13	8:MB:32:PRO:HG2	1.86	0.56
9:NB:20:ALA:HB3	9:NB:23:ARG:HG3	1.86	0.56
41:PA:74:GLU:HG2	41:PA:91:VAL:HG22	1.87	0.56
36:PC:126:GLU:HA	36:PC:129:GLU:OE2	2.04	0.56
14:SB:60:ARG:NH2	23:BC:114:GLY:HA3	2.20	0.56
42:VC:116:LYS:HD2	42:VC:129:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2508:G:OP1	35:JA:228:ARG:NH2	2.36	0.56
2:B:1800:C:OP2	5:E:183:ARG:NH2	2.38	0.56
2:B:2680:C:H5'	6:F:189:PRO:HA	1.87	0.56
28:GC:62:ARG:CZ	28:GC:62:ARG:HA	2.35	0.56
4:IB:21:A:O4'	4:IB:48:C:N4	2.38	0.56
36:KA:46:LYS:HA	36:KA:49:GLU:HB3	1.87	0.56
17:Q:100:TYR:CD1	17:Q:103:ARG:NH1	2.73	0.56
38:RC:201:GLN:HE21	39:SC:99:GLY:HA2	1.70	0.56
2:GB:84:A:P	22:AC:8:LYS:HZ2	2.26	0.56
2:B:2552:2MU:O5'	2:B:2552:2MU:H6	2.06	0.56
1:FB:1004:A:N6	1:FB:1026:G:OP2	2.37	0.56
1:FB:222:U:H2'	1:FB:223:U:C6	2.40	0.56
2:GB:2792:G:H2'	2:GB:2793:G:C8	2.40	0.56
10:J:1:MET:N	10:J:21:VAL:O	2.38	0.56
10:J:61:ARG:HD3	10:J:64:GLU:OE2	2.05	0.56
34:MC:14:A:H3'	34:MC:15:A:C8	2.40	0.56
39:NA:139:LEU:HA	39:NA:142:LEU:HD22	1.87	0.56
18:R:69:CYS:HB3	18:R:74:LEU:O	2.05	0.56
4:D:43:A:H2'	4:D:44:A:C8	2.41	0.56
1:FB:537:G:OP1	46:ZC:113:ARG:NH2	2.29	0.56
5:JB:96:HIS:CD2	5:JB:102:LYS:HG2	2.40	0.56
36:KA:126:GLU:HA	36:KA:129:GLU:OE2	2.04	0.56
37:LA:191:THR:OG1	37:LA:194:GLY:O	2.22	0.56
36:PC:47:THR:HA	36:PC:202:PRO:HG2	1.88	0.56
1:A:1003:G:H2'	1:A:1004:A:H4'	1.87	0.56
54:CB:30:LYS:NZ	54:CB:30:LYS:HB2	2.19	0.56
2:GB:154:G:H2'	2:GB:155:C:O2	2.06	0.56
2:GB:2543:G:H2'	2:GB:2544:G:C8	2.40	0.56
2:GB:270(M):U:OP2	2:GB:270(M):U:H3'	2.05	0.56
54:HD:30:LYS:HB2	54:HD:30:LYS:NZ	2.21	0.56
39:NA:77:PRO:HG2	39:NA:78:HIS:CD2	2.41	0.56
15:TB:18:LEU:HD21	15:TB:22:ARG:NH1	2.19	0.56
49:XA:17:ARG:HD3	49:XA:26:GLU:OE2	2.06	0.56
4:D:21:A:O4'	4:D:48:C:N4	2.38	0.56
1:FB:1086:U:H3	1:FB:1099:G:H22	1.53	0.56
2:GB:2138:C:H42	2:GB:2153:G:H1	1.51	0.56
2:GB:882:G:O6	2:GB:894:C:N4	2.38	0.56
9:NB:60:ARG:HB3	9:NB:60:ARG:NH1	2.21	0.56
12:L:75:SER:HB2	17:Q:74:ARG:HH12	1.70	0.56
43:RA:50:LEU:HA	43:RA:53:VAL:HG22	1.88	0.56
39:SC:9:LYS:HB3	39:SC:33:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:12:ASN:HA	24:X:14:ARG:HH21	1.70	0.56
2:B:2139:C:H3'	2:B:2140:C:H6	1.70	0.56
1:FB:740:U:OP1	49:CD:38:ARG:HD3	2.04	0.56
2:GB:1077:A:H3'	2:GB:1078:U:H4'	1.86	0.56
2:GB:2795:G:H1'	2:GB:2802:G:N2	2.20	0.56
2:GB:784:A:H5'	2:GB:785:G:OP1	2.06	0.56
10:J:62:LYS:HD2	10:J:135:GLU:OE2	2.06	0.56
37:LA:130:VAL:O	37:LA:134:ILE:HG12	2.06	0.56
14:N:51:ARG:HG3	14:N:66:ILE:HD11	1.88	0.56
40:OA:15:ASP:OD1	40:OA:18:GLN:N	2.26	0.56
36:PC:46:LYS:HA	36:PC:49:GLU:HB3	1.87	0.56
39:SC:105:VAL:HB	39:SC:106:PRO:HD3	1.88	0.56
39:SC:31:LEU:HD22	39:SC:43:LEU:HD11	1.88	0.56
49:XA:82:ILE:HD12	49:XA:88:ARG:NH2	2.19	0.56
20:YB:8:ARG:HB2	20:YB:102:HIS:ND1	2.20	0.56
1:A:1422:G:O3'	12:L:49:ARG:NH1	2.37	0.56
2:B:2552:2MU:H2'	2:B:2554:U:OP2	2.05	0.56
1:FB:299:G:H2'	1:FB:300:A:C8	2.40	0.56
2:GB:1434:A:H61	2:GB:1558:A:N6	2.00	0.56
9:I:109:PHE:CE1	9:I:152:ARG:NH1	2.73	0.56
4:NC:23:C:H2'	4:NC:24:U:C6	2.41	0.56
36:PC:48:MET:HA	36:PC:51:LEU:HB2	1.86	0.56
13:RB:71:VAL:HG22	13:RB:72:PRO:HA	1.86	0.56
13:RB:91:PHE:O	13:RB:121:LYS:NZ	2.38	0.56
39:SC:110:LEU:HD13	39:SC:118:ILE:HD13	1.88	0.56
20:T:110:LYS:HZ2	20:T:111:HIS:H	1.54	0.56
2:B:84:A:P	22:V:8:LYS:HZ2	2.21	0.56
17:VB:73:GLU:OE1	17:VB:103:ARG:NH2	2.39	0.56
42:VC:28:ALA:HB3	42:VC:57:PRO:HB2	1.86	0.56
23:W:80:ARG:HG2	23:W:82:ARG:HH22	1.71	0.56
44:SA:62:HIS:HB3	48:WA:59:ALA:HB3	1.87	0.56
43:WC:50:LEU:HA	43:WC:53:VAL:HG22	1.88	0.56
2:B:1532:C:H42	2:B:1539:G:H1	1.53	0.56
2:B:880:G:H1	2:B:897:C:H42	1.54	0.56
49:CD:35:ARG:HG3	49:CD:35:ARG:NH1	2.21	0.56
1:FB:1118:C:H1'	1:FB:1179:A:C5	2.41	0.56
1:FB:1492:A:N6	46:ZC:48:PRO:O	2.38	0.56
1:FB:624:C:H2'	1:FB:625:G:H8	1.71	0.56
7:G:107:LYS:NZ	7:G:207:GLY:H	2.03	0.56
36:PC:97:TRP:HH2	36:PC:176:GLU:OE2	1.89	0.56
1:A:706:A:H4'	45:TA:22:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:TB:12:ARG:HG3	15:TB:12:ARG:NH1	2.20	0.56
22:AC:15:VAL:HG21	22:AC:42:VAL:HG11	1.88	0.56
1:FB:1005:A:H1'	1:FB:1026:G:H1	1.71	0.56
1:FB:1167:A:OP1	1:FB:1167:A:H8	1.88	0.56
1:FB:999:U:H3	1:FB:1041:A:H62	1.53	0.56
2:GB:1019:U:OP1	2:GB:1035:U:O2'	2.21	0.56
2:GB:2139:C:H3'	2:GB:2140:C:H6	1.71	0.56
2:GB:784:A:C5	5:JB:229:VAL:HG21	2.40	0.56
6:F:12:THR:HG21	17:Q:11:GLU:OE2	2.05	0.56
46:UA:117:ARG:HB3	46:UA:122:THR:HB	1.87	0.56
1:A:164:U:H2'	1:A:165:C:C6	2.41	0.56
1:A:973:G:OP1	44:SA:57:LYS:NZ	2.29	0.56
2:B:1025:G:C4	2:B:1135:C:H1'	2.41	0.56
2:B:882:G:O6	2:B:894:C:N4	2.38	0.56
51:ED:86:GLU:O	51:ED:90:ILE:HG22	2.06	0.56
36:KA:47:THR:HA	36:KA:202:PRO:HG2	1.87	0.56
2:GB:606:U:OP2	7:LB:104:LYS:HE3	2.06	0.56
8:MB:67:LYS:H	28:GC:6:HIS:CE1	2.23	0.56
9:NB:136:ILE:HD12	9:NB:136:ILE:H	1.71	0.56
11:PB:13:TRP:CE2	11:PB:133:GLN:HG2	2.41	0.56
23:W:4:ARG:HH11	23:W:60:GLU:HG2	1.69	0.56
20:YB:30:GLU:OE2	20:YB:30:GLU:HA	2.05	0.56
2:B:1786:A:H1'	2:B:1938:A:N6	2.21	0.55
2:B:2439:A:C8	2:B:2439:A:H5'	2.41	0.55
25:DC:95:LEU:HD12	25:DC:98:LEU:HD12	1.89	0.55
7:G:184:TYR:O	7:G:188:ARG:HG3	2.05	0.55
4:IB:17:C:OP2	4:IB:17(A):U:O2'	2.24	0.55
39:NA:9:LYS:HB3	39:NA:33:VAL:HG13	1.88	0.55
38:RC:18:LYS:CE	38:RC:26:CYS:SG	2.94	0.55
17:VB:77:PRO:HB2	17:VB:80:SER:HB2	1.87	0.55
2:B:857:C:H4'	24:X:23:VAL:HG21	1.88	0.55
1:A:982:U:OP2	48:WA:23:ARG:NH2	2.39	0.55
49:CD:3:ILE:HD13	49:CD:34:LEU:HD23	1.88	0.55
7:G:119:ARG:NH1	7:G:119:ARG:HB2	2.19	0.55
54:HD:13:LEU:O	54:HD:17:ARG:HG3	2.07	0.55
9:I:136:ILE:H	9:I:136:ILE:HD12	1.72	0.55
6:KB:61:ARG:HG2	6:KB:61:ARG:NH1	2.21	0.55
8:MB:98:ARG:HG3	8:MB:98:ARG:NH1	2.05	0.55
19:XB:58:VAL:HG21	19:XB:100:ARG:HH21	1.71	0.55
46:ZC:83:VAL:HG21	46:ZC:100:ILE:HD13	1.86	0.55
2:B:2543:G:H2'	2:B:2544:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BC:80:ARG:HG2	23:BC:82:ARG:HH22	1.72	0.55
1:A:108:G:N1	54:CB:15:ARG:HG2	2.21	0.55
49:CD:25:THR:HG21	49:CD:70:LEU:HB2	1.89	0.55
2:B:2347:C:OP1	30:DA:38:LYS:NZ	2.39	0.55
5:E:26:LYS:HD3	5:E:83:GLU:OE2	2.06	0.55
6:F:11:MET:HG2	6:F:24:THR:HB	1.88	0.55
42:QA:51:VAL:HG11	42:QA:60:ARG:HH12	1.70	0.55
22:V:15:VAL:HG21	22:V:42:VAL:HG11	1.87	0.55
22:V:92:ASN:OD1	22:V:93:GLY:N	2.39	0.55
2:B:2327:A:H2'	2:B:2328:A:C8	2.40	0.55
2:B:751:A:H5'	20:T:90:ARG:HA	1.89	0.55
1:FB:1005:A:H1'	1:FB:1026:G:N1	2.22	0.55
36:KA:161:ALA:HB1	36:KA:185:ILE:HD11	1.88	0.55
37:QC:148:GLY:HA3	37:QC:172:ARG:O	2.07	0.55
43:RA:10:ARG:HG3	43:RA:105:ASP:HB3	1.88	0.55
38:RC:12:CYS:SG	38:RC:18:LYS:HE3	2.46	0.55
38:RC:142:PRO:HA	38:RC:185:PHE:HD2	1.71	0.55
22:AC:46:LYS:HG2	22:AC:60:PHE:CD1	2.42	0.55
2:B:330:A:H2	2:B:1210:A:H2'	1.71	0.55
2:GB:2096:U:H2'	2:GB:2097:C:C6	2.41	0.55
39:NA:15:ARG:HD2	39:NA:26:PHE:CG	2.41	0.55
1:A:1080:A:OP1	39:NA:47:LYS:HD3	2.07	0.55
1:A:266:G:H3'	51:ZA:67:LYS:HB2	1.87	0.55
1:A:981:U:H5'	48:WA:21:TYR:CE2	2.42	0.55
2:B:1069:A:N7	2:B:1073:A:N6	2.49	0.55
49:CD:82:ILE:HD12	49:CD:88:ARG:NH2	2.22	0.55
1:FB:344:A:H4'	1:FB:345:C:OP2	2.06	0.55
2:B:320:A:OP2	7:G:137:LYS:HE2	2.07	0.55
2:GB:1021:A:H3'	2:GB:1021:A:C8	2.42	0.55
2:GB:1091:G:N2	2:GB:1100:C:O2'	2.40	0.55
10:J:27:ARG:HD2	25:Y:71:TYR:CE2	2.42	0.55
1:A:1423:G:P	12:L:49:ARG:HH12	2.29	0.55
14:N:60:ARG:NH2	23:W:114:GLY:HA3	2.21	0.55
15:TB:104:ARG:NH1	15:TB:107:ASP:OD2	2.38	0.55
40:TC:101:ALA:OXT	52:FD:28:GLU:HB2	2.07	0.55
17:VB:74:ARG:HD3	17:VB:76:PHE:CZ	2.40	0.55
42:VC:11:THR:HG23	42:VC:14:ARG:NH1	2.22	0.55
51:ZA:59:ILE:HG22	51:ZA:73:VAL:HA	1.88	0.55
1:A:1516:G:N1	1:A:1519:MA6:OP2	2.39	0.55
54:CB:10:LEU:HD12	54:CB:12:ALA:H	1.71	0.55
36:KA:84:GLU:HB3	36:KA:219:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2376:A:N6	16:UB:89:ARG:HD3	2.22	0.55
1:A:865:A:H5'	1:A:1078:U:C4	2.42	0.55
1:A:1269:A:N1	1:A:1312:G:O2'	2.37	0.55
2:B:363(F):U:H3'	2:B:363(G):A:C8	2.38	0.55
1:FB:7:G:H5'	1:FB:298:A:O4'	2.06	0.55
1:FB:706:A:H4'	45:YC:22:HIS:CD2	2.35	0.55
2:GB:330:A:H2	2:GB:1210:A:H2'	1.70	0.55
35:JA:116:ARG:HH11	35:JA:298:LEU:HD21	1.72	0.55
35:JA:248:HIS:HB3	35:JA:253:ILE:HG23	1.89	0.55
45:TA:31:THR:HG22	45:TA:42:TRP:HB2	1.88	0.55
18:WB:69:CYS:HB3	18:WB:74:LEU:O	2.07	0.55
43:WC:95:LYS:H	43:WC:98:PRO:HG2	1.72	0.55
1:A:1147:C:O2'	43:RA:16:ARG:HD2	2.06	0.55
2:B:1339:G:H5''	21:U:16:LYS:HD3	1.88	0.55
2:B:2171:A:O2'	2:B:2172:U:H5''	2.06	0.55
51:ED:52:LYS:NZ	51:ED:52:LYS:HB3	2.22	0.55
2:GB:1021:A:H8	2:GB:1022:G:H5''	1.72	0.55
2:GB:1045:A:H1'	2:GB:1047:G:H1'	1.88	0.55
2:GB:2313:C:H4'	8:MB:91:ARG:HG3	1.88	0.55
2:GB:2327:A:H2'	2:GB:2328:A:C8	2.42	0.55
54:HD:56:MET:HG3	54:HD:88:VAL:HG21	1.89	0.55
9:I:101:ARG:HH11	9:I:122:THR:HG23	1.71	0.55
11:K:13:TRP:CE2	11:K:133:GLN:HG2	2.42	0.55
36:KA:185:ILE:HG23	36:KA:199:TYR:HB2	1.88	0.55
24:CC:6:GLY:HA3	4:NC:1:C:O2	2.07	0.55
10:OB:91:SER:O	10:OB:93:THR:N	2.40	0.55
35:OC:248:HIS:HB2	35:OC:274:LEU:HD11	1.87	0.55
2:B:2376:A:N6	16:P:89:ARG:HD3	2.21	0.55
41:PA:28:ASN:OD1	41:PA:36:LYS:NZ	2.39	0.55
42:QA:11:THR:HG23	42:QA:14:ARG:NH1	2.22	0.55
2:B:154:G:H2'	2:B:155:C:O2	2.07	0.55
2:B:1939:5MU:OP1	2:B:2604:U:O2'	2.22	0.55
2:B:2304:G:H22	2:B:2312:U:H3	1.54	0.55
31:EA:34:ARG:HG2	31:EA:34:ARG:HH11	1.70	0.55
2:GB:2171:A:O2'	2:GB:2172:U:H5''	2.06	0.55
28:GC:24:THR:OG1	28:GC:25:TYR:N	2.39	0.55
28:GC:62:ARG:HA	28:GC:62:ARG:NH1	2.21	0.55
8:H:19:LEU:HD13	8:H:32:PRO:HG2	1.88	0.55
35:JA:247:THR:HG23	35:JA:254:VAL:HG22	1.89	0.55
42:QA:28:ALA:HB3	42:QA:57:PRO:HB2	1.89	0.55
13:RB:124:LYS:HE2	13:RB:144:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:RB:93:GLY:H	13:RB:123:LEU:HD22	1.72	0.55
45:TA:67:ASP:HA	45:TA:70:LYS:HE2	1.89	0.55
1:A:1005:A:H1'	1:A:1026:G:H1	1.71	0.54
1:A:59:A:H3'	1:A:331:G:H22	1.72	0.54
2:B:1060:U:H5''	2:B:1061:U:H3'	1.88	0.54
1:FB:474:G:OP2	50:DD:75:ARG:NH1	2.40	0.54
1:FB:646:U:H2'	1:FB:647:C:C6	2.43	0.54
14:N:116:GLU:OE2	14:N:119:ARG:NH2	2.40	0.54
10:OB:38:LEU:HB3	10:OB:40:THR:HG23	1.87	0.54
46:UA:24:VAL:HB	46:UA:27:LEU:HD22	1.89	0.54
6:KB:12:THR:HG21	17:VB:11:GLU:OE2	2.07	0.54
42:VC:51:VAL:HG11	42:VC:60:ARG:HH12	1.72	0.54
48:WA:21:TYR:HE1	48:WA:23:ARG:NH1	2.05	0.54
23:BC:4:ARG:HH11	23:BC:60:GLU:HG2	1.70	0.54
1:FB:1003:G:H2'	1:FB:1004:A:H4'	1.88	0.54
2:GB:154(A):C:O2'	2:GB:155:C:N3	2.40	0.54
10:OB:133:HIS:CE1	10:OB:135:GLU:HB3	2.42	0.54
10:OB:76:THR:HG22	10:OB:141:LYS:HD2	1.90	0.54
36:PC:23:ARG:HB2	36:PC:23:ARG:HH11	1.68	0.54
41:UC:74:GLU:HG2	41:UC:91:VAL:HG22	1.88	0.54
49:XA:21:ASP:OD2	49:XA:24:SER:HB3	2.08	0.54
2:B:1019:U:OP1	2:B:1035:U:O2'	2.23	0.54
14:SB:81:VAL:HG12	24:CC:5:LYS:HD2	1.89	0.54
49:CD:21:ASP:OD2	49:CD:24:SER:HB3	2.07	0.54
2:GB:2439:A:H5'	2:GB:2439:A:C8	2.42	0.54
4:IB:52:G:H1	4:IB:62:C:H42	1.55	0.54
35:JA:248:HIS:HB2	35:JA:274:LEU:HD11	1.89	0.54
13:M:81:GLN:OE1	13:M:107:LYS:N	2.32	0.54
15:O:12:ARG:NH1	15:O:12:ARG:HG3	2.20	0.54
1:FB:723:U:H1'	1:FB:724:G:OP1	2.08	0.54
2:GB:1796:U:H2'	2:GB:1797:C:C6	2.42	0.54
2:GB:2151:G:N2	2:GB:2152:G:O6	2.40	0.54
38:RC:43:HIS:CE1	38:RC:46:LYS:HZ2	2.25	0.54
1:A:1358:U:OP1	48:WA:35:ARG:HG2	2.07	0.54
1:A:222:U:H2'	1:A:223:U:C6	2.43	0.54
40:OA:101:ALA:OXT	52:AB:28:GLU:HB2	2.07	0.54
2:B:1358:G:O2'	2:B:1359:A:H5''	2.07	0.54
2:B:277:C:H4'	2:B:278:A:OP2	2.08	0.54
24:CC:12:ASN:HA	24:CC:14:ARG:NH2	2.23	0.54
31:EA:34:ARG:HG2	31:EA:34:ARG:NH1	2.22	0.54
1:FB:1347:G:C8	43:WC:107:ARG:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:179:A:H2'	1:FB:180:U:H6	1.72	0.54
1:FB:180:U:H2'	1:FB:181:G:H5'	1.90	0.54
2:GB:1045:A:O2'	2:GB:1047:G:N3	2.32	0.54
2:GB:1728:G:H8	2:GB:1732:A:H62	1.55	0.54
30:IC:34:LEU:H	30:IC:51:GLU:HB2	1.72	0.54
39:NA:105:VAL:HB	39:NA:106:PRO:HD3	1.88	0.54
13:RB:94:GLU:OE2	13:RB:124:LYS:HD2	2.07	0.54
39:SC:20:GLN:HG2	39:SC:25:ARG:HD2	1.89	0.54
1:A:109:A:C6	1:A:326:G:C6	2.96	0.54
31:EA:47:ARG:NH1	31:EA:47:ARG:HB3	2.22	0.54
1:FB:1358:U:OP1	48:BD:35:ARG:HG2	2.07	0.54
2:GB:207:A:H2'	2:GB:208:C:O4'	2.07	0.54
2:GB:2208:U:H2'	2:GB:2209:C:C6	2.43	0.54
37:LA:61:ALA:O	37:LA:63:ASN:ND2	2.40	0.54
38:MA:9:CYS:SG	38:MA:26:CYS:SG	3.06	0.54
14:SB:65:PHE:HB2	14:SB:105:GLU:HB2	1.90	0.54
22:V:46:LYS:HG2	22:V:60:PHE:CD1	2.42	0.54
21:ZB:90:GLU:HA	21:ZB:93:GLU:HG2	1.89	0.54
2:B:2115:G:H4'	2:B:2167:U:C2	2.43	0.54
1:FB:109:A:C6	1:FB:326:G:C6	2.95	0.54
1:FB:673:G:H2'	1:FB:674:G:C8	2.43	0.54
2:GB:1011:G:OP1	18:WB:77:SER:HB2	2.07	0.54
2:GB:2593:U:H2'	2:GB:2594:C:C6	2.42	0.54
9:I:3:ARG:NH1	9:I:3:ARG:HA	2.23	0.54
2:GB:1805:U:O2	5:JB:50:THR:HB	2.07	0.54
36:KA:131:PRO:HB2	36:KA:134:GLU:HG2	1.90	0.54
12:L:45:GLU:HA	12:L:54:GLU:OE2	2.06	0.54
9:NB:164:TYR:HB2	9:NB:167:GLU:HB2	1.89	0.54
43:RA:105:ASP:OD2	43:RA:107:ARG:HG2	2.07	0.54
22:V:38:ILE:HD11	22:V:66:PRO:HG3	1.88	0.54
23:W:185:GLU:HA	23:W:188:ALA:HB3	1.90	0.54
1:A:1118:C:H1'	1:A:1179:A:C5	2.43	0.54
1:A:224:C:H2'	1:A:225:C:C6	2.42	0.54
2:B:507:A:O2'	2:B:508:G:OP2	2.24	0.54
1:FB:108:G:N1	54:HD:15:ARG:HG2	2.23	0.54
9:I:28:GLY:HA3	9:I:79:VAL:HB	1.90	0.54
42:QA:112:LEU:HA	42:QA:134:ILE:HG12	1.89	0.54
43:RA:29:ASN:N	43:RA:63:ILE:O	2.32	0.54
19:S:72:VAL:HG13	19:S:85:LYS:HB3	1.88	0.54
44:XC:6:ILE:HD11	44:XC:72:VAL:HB	1.90	0.54
26:Z:2:LYS:H	26:Z:2:LYS:HD3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:ZC:28:LYS:NZ	46:ZC:64:TYR:HE2	2.05	0.54
1:A:646:U:H2'	1:A:647:C:C6	2.43	0.54
2:GB:1069:A:N7	2:GB:1073:A:N6	2.50	0.54
8:H:113:ARG:NH2	8:H:139:LEU:O	2.41	0.54
38:MA:196:LEU:O	38:MA:198:VAL:N	2.39	0.54
11:PB:35:ARG:HA	11:PB:116:LEU:HD13	1.90	0.54
13:RB:124:LYS:HG3	13:RB:144:GLU:OE2	2.08	0.54
2:GB:2875:C:O2'	17:VB:2:ASN:OD1	2.25	0.54
42:VC:11:THR:HG23	42:VC:14:ARG:HH12	1.71	0.54
44:XC:50:ILE:HB	48:BD:41:ARG:NH1	2.22	0.54
1:A:1005:A:H1'	1:A:1026:G:N1	2.22	0.54
1:A:1253:G:H1	1:A:1284:C:H42	1.55	0.54
1:A:7:G:H5'	1:A:298:A:O4'	2.07	0.54
47:AD:54:VAL:HG22	47:AD:57:ARG:HH12	1.73	0.54
2:B:2096:U:H2'	2:B:2097:C:C6	2.42	0.54
1:A:1226:C:H4'	53:BB:80:TYR:CZ	2.42	0.54
2:GB:848:G:O6	2:GB:929:G:H2'	2.07	0.54
3:HB:86:G:H1	3:HB:90:C:H42	1.55	0.54
36:KA:78:GLN:OE1	36:KA:94:ASN:ND2	2.41	0.54
37:LA:33:LEU:HD21	48:WA:53:LEU:HD22	1.90	0.54
1:A:1347:G:C8	43:RA:107:ARG:HG3	2.43	0.54
1:FB:1147:C:O2'	43:WC:16:ARG:HD2	2.07	0.54
49:XA:30:ALA:HA	49:XA:85:LEU:HD11	1.90	0.54
1:A:721:G:H4'	1:A:722:A:O4'	2.07	0.53
1:A:723:U:H1'	1:A:724:G:OP1	2.08	0.53
2:B:34:C:HO2'	2:B:35:G:P	2.30	0.53
1:FB:1133:G:H1	1:FB:1141:C:N4	2.07	0.53
2:GB:887:A:H1'	2:GB:890:A:H61	1.73	0.53
9:I:60:ARG:NH1	9:I:60:ARG:HB3	2.22	0.53
2:B:2494:G:O2'	14:N:80:GLU:HA	2.07	0.53
12:QB:98:VAL:HG22	12:QB:118:ALA:HA	1.91	0.53
13:RB:2:LYS:HZ3	13:RB:2:LYS:HB3	1.73	0.53
14:SB:1:MET:SD	14:SB:45:GLN:NE2	2.81	0.53
43:WC:29:ASN:N	43:WC:63:ILE:O	2.29	0.53
20:YB:110:LYS:HZ2	20:YB:111:HIS:H	1.56	0.53
1:A:624:C:H2'	1:A:625:G:H8	1.73	0.53
2:B:2208:U:H2'	2:B:2209:C:C6	2.42	0.53
2:B:443:A:H1'	2:B:1201:C:O4'	2.07	0.53
2:B:975:G:H1'	2:B:990:A:C2	2.43	0.53
23:BC:185:GLU:HA	23:BC:188:ALA:HB3	1.90	0.53
1:FB:59:A:H3'	1:FB:331:G:H22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:270(T):G:OP1	25:DC:76:ARG:NH1	2.40	0.53
2:GB:556:G:H2'	2:GB:557:U:C6	2.43	0.53
34:HA:19:PSU:N3	35:JA:120:GLY:O	2.41	0.53
11:K:138:LEU:HD13	11:K:139:GLU:H	1.73	0.53
38:RC:196:LEU:O	38:RC:198:VAL:N	2.39	0.53
14:SB:18:LYS:O	14:SB:98:LYS:NZ	2.39	0.53
43:WC:28:VAL:HG22	43:WC:63:ILE:HD12	1.89	0.53
2:B:1728:G:H8	2:B:1732:A:H62	1.54	0.53
51:ED:83:ASP:O	51:ED:86:GLU:HB2	2.08	0.53
1:FB:224:C:H2'	1:FB:225:C:C6	2.43	0.53
1:FB:666:G:H5'	1:FB:726:C:H1'	1.90	0.53
2:GB:1011:G:OP1	18:WB:75:ASN:HB2	2.09	0.53
4:IA:35:A:OP2	43:RA:128:ARG:NH1	2.42	0.53
36:KA:24:TRP:CZ3	36:KA:26:PRO:HA	2.43	0.53
33:LC:27:CYS:SG	33:LC:28:GLU:N	2.81	0.53
13:M:2:LYS:HB3	13:M:2:LYS:HZ3	1.73	0.53
38:MA:9:CYS:HG	38:MA:18:LYS:HZ2	1.54	0.53
42:QA:11:THR:HG23	42:QA:14:ARG:HH12	1.73	0.53
14:SB:67:ARG:NH1	14:SB:105:GLU:OE2	2.40	0.53
42:VC:4:ASP:OD2	42:VC:85:ARG:NE	2.41	0.53
25:Y:72:GLU:O	25:Y:76:ARG:HG3	2.08	0.53
2:B:2804:C:H2'	2:B:2805:G:O4'	2.07	0.53
2:B:289:A:H2'	2:B:290:G:O4'	2.08	0.53
28:BA:24:THR:OG1	28:BA:25:TYR:N	2.41	0.53
24:CC:6:GLY:HA3	4:NC:1:C:H1'	1.89	0.53
40:TC:99:ALA:O	52:FD:28:GLU:HG3	2.09	0.53
2:GB:1130:U:O2	6:KB:149:ARG:NH2	2.42	0.53
2:GB:277:C:H4'	2:GB:278:A:OP2	2.09	0.53
8:MB:55:LYS:O	8:MB:58:GLN:HG3	2.08	0.53
35:OC:248:HIS:HB3	35:OC:253:ILE:HG23	1.91	0.53
37:QC:177:THR:HG22	37:QC:180:ALA:H	1.74	0.53
46:ZC:117:ARG:HB3	46:ZC:122:THR:HB	1.90	0.53
1:A:1189:C:OP1	44:SA:51:ARG:NH2	2.39	0.53
2:B:2724:C:OP1	6:F:118:LYS:NZ	2.39	0.53
1:FB:981:U:H5'	48:BD:21:TYR:CE2	2.44	0.53
30:DA:34:LEU:H	30:DA:51:GLU:HB2	1.73	0.53
5:E:96:HIS:CD2	5:E:102:LYS:HG2	2.43	0.53
26:EC:37:PHE:O	26:EC:41:ILE:HG13	2.09	0.53
1:FB:706:A:C5'	45:YC:22:HIS:HD2	2.22	0.53
2:B:601:C:OP1	7:G:108:LYS:HE3	2.08	0.53
2:GB:1113:U:H2'	2:GB:1114:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:LEU:HB3	10:J:40:THR:HG23	1.91	0.53
17:Q:77:PRO:HB2	17:Q:80:SER:HB2	1.91	0.53
46:ZC:24:VAL:HB	46:ZC:27:LEU:HD22	1.91	0.53
1:A:474:G:OP2	50:YA:75:ARG:NH1	2.41	0.53
47:AD:22:ILE:HD12	47:AD:25:ILE:HD12	1.88	0.53
2:B:1113:U:H2'	2:B:1114:G:C8	2.44	0.53
2:B:2313:C:H4'	8:H:91:ARG:HG3	1.90	0.53
2:B:307:G:N2	2:B:309:G:H3'	2.24	0.53
49:CD:62:GLN:OE1	49:CD:65:ARG:NH1	2.41	0.53
52:FD:70:ILE:O	52:FD:74:ARG:HG3	2.09	0.53
2:GB:2784:C:H1'	6:KB:37:ARG:NH1	2.23	0.53
4:IB:43:A:H2'	4:IB:44:A:C8	2.43	0.53
35:JA:311:ASN:HB3	35:JA:316:ARG:HG2	1.91	0.53
36:KA:23:ARG:HB2	36:KA:23:ARG:HH11	1.73	0.53
34:MC:19:PSU:N3	35:OC:120:GLY:O	2.41	0.53
35:OC:311:ASN:HB3	35:OC:316:ARG:HG2	1.90	0.53
49:XA:88:ARG:NH2	49:XA:88:ARG:HB3	2.24	0.53
46:ZC:8:ASN:O	46:ZC:12:ARG:HG3	2.09	0.53
1:A:1167:A:OP1	1:A:1167:A:H8	1.91	0.53
1:A:1423:G:OP1	12:L:49:ARG:NH2	2.36	0.53
2:B:2232:U:OP2	25:Y:40:ARG:NH2	2.41	0.53
2:B:270(T):G:OP1	25:Y:76:ARG:NH1	2.41	0.53
1:FB:185:A:N3	54:HD:81:LYS:NZ	2.57	0.53
1:FB:519:C:OP1	35:OC:183:ARG:NH1	2.42	0.53
2:GB:289:A:H2'	2:GB:290:G:O4'	2.09	0.53
2:GB:83:G:N2	2:GB:102:G:H1'	2.24	0.53
10:J:118:LYS:NZ	10:J:119:PRO:O	2.42	0.53
36:KA:68:ILE:HG12	36:KA:161:ALA:HB3	1.90	0.53
13:M:94:GLU:OE2	13:M:124:LYS:HD2	2.09	0.53
13:M:124:LYS:HG3	13:M:144:GLU:OE2	2.09	0.53
35:OC:116:ARG:HH11	35:OC:298:LEU:HD21	1.74	0.53
43:RA:4:TYR:HB3	43:RA:88:TYR:HB2	1.90	0.53
14:SB:76:LYS:HB3	14:SB:91:GLU:HG3	1.91	0.53
23:W:29:TYR:HB3	23:W:34:ASN:HD22	1.73	0.53
20:YB:110:LYS:NZ	20:YB:111:HIS:H	2.06	0.53
2:B:1805:U:O2	5:E:50:THR:HB	2.08	0.53
2:B:887:A:H1'	2:B:890:A:H61	1.74	0.53
2:B:848:G:O6	2:B:929:G:H2'	2.09	0.53
8:H:3:LEU:HD13	8:H:5:LEU:HD21	1.90	0.53
36:PC:84:GLU:HB3	36:PC:219:VAL:HG21	1.90	0.53
4:IA:33:U:OP2	43:RA:128:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:C:H5''	43:RA:16:ARG:HH22	1.74	0.53
39:SC:15:ARG:HD2	39:SC:26:PHE:CG	2.44	0.53
25:Y:50:ARG:HD2	25:Y:57:GLU:OE2	2.07	0.53
26:Z:22:GLU:OE2	26:Z:68:ARG:NH2	2.41	0.53
1:A:1086:U:H3	1:A:1099:G:H22	1.57	0.53
2:B:2021:C:H4'	2:B:2022:U:OP2	2.09	0.53
1:FB:982:U:OP2	48:BD:23:ARG:NH2	2.42	0.53
10:J:133:HIS:CE1	10:J:135:GLU:HB3	2.44	0.53
38:MA:201:GLN:NE2	39:NA:116:THR:O	2.42	0.53
38:RC:71:SER:HB3	38:RC:74:GLN:HG3	1.91	0.53
44:SA:35:SER:HB3	44:SA:73:ASP:OD2	2.09	0.53
49:XA:35:ARG:NH1	49:XA:35:ARG:HG3	2.20	0.53
49:XA:62:GLN:OE1	49:XA:65:ARG:NH1	2.42	0.53
1:A:1133:G:H1	1:A:1141:C:N4	2.07	0.53
1:A:1460:A:OP2	54:CB:27:LYS:NZ	2.31	0.53
2:B:2648:C:H2'	2:B:2649:U:C6	2.44	0.53
2:B:556:G:H2'	2:B:557:U:C6	2.44	0.53
2:B:83:G:N2	2:B:102:G:H1'	2.24	0.53
2:GB:857:C:H4'	24:CC:23:VAL:HG21	1.90	0.53
2:GB:2347:C:OP1	30:IC:38:LYS:NZ	2.41	0.53
4:IB:16:C:H5'	4:IB:17:C:H5	1.73	0.53
35:OC:109:ARG:NH1	35:OC:210:PRO:HD3	2.24	0.53
42:QA:17:THR:HG22	42:QA:63:LEU:HG	1.91	0.53
39:SC:139:LEU:HA	39:SC:142:LEU:HD22	1.90	0.53
1:A:706:A:N3	45:TA:31:THR:HG21	2.24	0.53
40:TC:33:TYR:CE2	40:TC:78:GLU:HG3	2.44	0.53
46:UA:83:VAL:HG21	46:UA:100:ILE:HD13	1.90	0.53
17:VB:100:TYR:HD1	17:VB:103:ARG:NH1	2.06	0.53
44:XC:6:ILE:HG22	44:XC:98:ILE:HG22	1.91	0.53
51:ZA:6:LEU:HD23	51:ZA:23:VAL:HG11	1.91	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.91	0.52
2:B:2789:C:O3'	2:B:2790:A:H4'	2.09	0.52
2:B:848:G:H2'	2:B:849:A:C8	2.45	0.52
54:CB:13:LEU:O	54:CB:17:ARG:HG3	2.07	0.52
1:FB:269:C:H2'	1:FB:270:A:C8	2.44	0.52
1:FB:580:U:H2'	1:FB:581:G:O4'	2.09	0.52
2:GB:2370:G:C6	2:GB:2371:G:C6	2.97	0.52
2:GB:751:A:H5'	20:YB:90:ARG:HA	1.91	0.52
4:IB:19:G:H1	4:IB:56:C:H42	1.56	0.52
35:OC:326:LEU:HD13	35:OC:328:ARG:NH1	2.24	0.52
37:QC:61:ALA:O	37:QC:63:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2405:G:OP1	13:RB:77:ARG:NH2	2.41	0.52
1:FB:542:G:H5'	38:RC:41:GLY:HA3	1.91	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.44	0.52
2:B:363(G):A:H1'	2:B:364:C:H5	1.74	0.52
50:DD:53:VAL:HG12	50:DD:57:ARG:HH11	1.73	0.52
1:FB:614:A:H2'	1:FB:615:C:C6	2.45	0.52
2:GB:2552:2MU:O5'	2:GB:2552:2MU:H6	2.09	0.52
2:GB:300:A:H2'	2:GB:334:C:H1'	1.91	0.52
10:OB:118:LYS:HZ1	10:OB:121:LYS:HG3	1.74	0.52
42:QA:51:VAL:HG11	42:QA:60:ARG:NH1	2.25	0.52
43:RA:28:VAL:HG22	43:RA:63:ILE:HD12	1.90	0.52
38:RC:18:LYS:NZ	38:RC:31:CYS:HG	2.00	0.52
1:A:1118:C:H2'	1:A:1119:C:C6	2.45	0.52
5:E:26:LYS:HB3	5:E:83:GLU:HG2	1.92	0.52
10:J:57:ARG:HB3	10:J:61:ARG:HH22	1.73	0.52
12:L:98:VAL:HG22	12:L:118:ALA:HA	1.92	0.52
38:MA:155:LEU:HD13	38:MA:156:GLU:N	2.25	0.52
35:OC:226:THR:HG23	35:OC:241:ASP:HB3	1.91	0.52
37:QC:61:ALA:O	37:QC:63:ASN:N	2.39	0.52
45:TA:12:ARG:HG2	45:TA:13:GLN:HG2	1.92	0.52
1:FB:706:A:C4'	45:YC:22:HIS:HD2	2.20	0.52
1:A:344:A:H4'	1:A:345:C:OP2	2.10	0.52
1:A:642:A:H2'	1:A:643:C:C6	2.45	0.52
1:A:693:G:H2'	1:A:694:A:C8	2.45	0.52
1:FB:1391:U:H2'	1:FB:1392:G:C8	2.45	0.52
10:J:88:ILE:HD12	10:J:89:TYR:H	1.73	0.52
13:M:2:LYS:NZ	13:M:4:SER:OG	2.40	0.52
10:OB:93:THR:HG23	10:OB:95:LYS:H	1.74	0.52
17:Q:94:ALA:HB1	17:Q:99:LEU:HD21	1.91	0.52
42:QA:4:ASP:OD2	42:QA:85:ARG:NE	2.42	0.52
23:W:124:ILE:HD11	23:W:165:VAL:HG21	1.91	0.52
2:B:2079:U:OP1	25:Y:21:ARG:NH2	2.42	0.52
1:A:353:A:H5'	1:A:353:A:H8	1.75	0.52
1:A:383:A:C5	1:A:384:G:H1'	2.44	0.52
47:AD:14:ARG:HE	47:AD:42:ALA:HA	1.73	0.52
2:B:774:A:N3	2:B:774:A:H2'	2.24	0.52
24:CC:12:ASN:HA	24:CC:14:ARG:HH21	1.75	0.52
1:FB:1129:C:H5''	43:WC:16:ARG:HH22	1.74	0.52
7:G:53:THR:HG22	7:G:56:GLU:HG3	1.91	0.52
2:GB:307:G:N2	2:GB:309:G:H3'	2.25	0.52
14:N:47:ILE:HD12	14:N:70:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:PC:166:ASP:HB3	36:PC:169:LYS:HB3	1.91	0.52
2:B:2232:U:P	25:Y:40:ARG:HH22	2.32	0.52
2:B:1047:G:H2'	2:B:1110:G:N1	2.25	0.52
2:B:1657:C:H2'	2:B:1658:C:H6	1.75	0.52
2:B:545:G:H21	2:B:548:A:H62	1.58	0.52
27:FC:3:ARG:NH1	27:FC:60:GLU:OE1	2.43	0.52
7:G:127:GLU:HB3	7:G:196:LEU:HD12	1.91	0.52
2:GB:2648:C:H2'	2:GB:2649:U:C6	2.44	0.52
9:I:17:VAL:HG11	9:I:50:VAL:HG21	1.92	0.52
5:JB:26:LYS:HD3	5:JB:83:GLU:OE2	2.10	0.52
7:LB:107:LYS:HZ1	7:LB:207:GLY:H	1.58	0.52
36:PC:131:PRO:HB2	36:PC:134:GLU:HG2	1.90	0.52
1:A:180:U:H2'	1:A:181:G:H5'	1.92	0.52
2:B:1067:A:OP1	2:B:1068:G:N2	2.43	0.52
2:B:140:A:H8	2:B:1408:C:O2'	1.91	0.52
2:GB:2804:C:H2'	2:GB:2805:G:O4'	2.09	0.52
9:I:55:PRO:HG2	9:I:61:HIS:CE1	2.45	0.52
5:JB:62:TYR:HA	5:JB:87:ASN:ND2	2.24	0.52
4:NC:33:U:OP2	43:WC:128:ARG:NH2	2.43	0.52
38:RC:176:LEU:HD12	38:RC:182:LYS:O	2.09	0.52
39:SC:78:HIS:ND1	42:VC:104:ARG:HD2	2.19	0.52
51:ZA:86:GLU:O	51:ZA:90:ILE:HG22	2.09	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.52
2:B:270(M):U:H3'	2:B:270(M):U:OP2	2.10	0.52
2:GB:1709:U:H2'	2:GB:1710:C:C6	2.45	0.52
2:GB:320:A:H4'	2:GB:322:A:N7	2.25	0.52
8:H:136:ARG:N	8:H:136:ARG:HE	2.01	0.52
34:HA:14:A:H3'	34:HA:15:A:H8	1.74	0.52
36:PC:78:GLN:OE1	36:PC:94:ASN:ND2	2.42	0.52
37:QC:119:ARG:O	37:QC:123:GLN:HG3	2.09	0.52
13:RB:149:GLU:HA	13:RB:149:GLU:OE2	2.07	0.52
44:SA:5:ARG:HG3	44:SA:73:ASP:HB3	1.90	0.52
44:SA:8:LEU:HG	44:SA:96:ILE:HG23	1.91	0.52
14:SB:60:ARG:HA	23:BC:178:GLU:O	2.10	0.52
42:VC:17:THR:HG22	42:VC:63:LEU:HG	1.91	0.52
45:YC:12:ARG:HG2	45:YC:13:GLN:HG2	1.91	0.52
1:A:1397:C:O2'	1:A:1398:A:OP1	2.27	0.52
1:A:1496:C:H4'	2:B:1920:4OC:O2'	2.09	0.52
1:A:539:A:H2'	1:A:540:G:C8	2.44	0.52
2:B:1568:G:P	5:E:63:ARG:HH22	2.33	0.52
2:B:1796:U:H2'	2:B:1797:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:706:A:C5'	45:YC:22:HIS:CD2	2.93	0.52
2:GB:1047:G:H2'	2:GB:1110:G:N1	2.25	0.52
2:GB:2564:A:OP1	2:GB:2648:C:H4'	2.10	0.52
2:GB:1490:A:O2'	5:JB:99:ASP:OD1	2.22	0.52
38:MA:50:ARG:HD3	38:MA:51:PRO:HD2	1.92	0.52
36:PC:24:TRP:CZ3	36:PC:26:PRO:HA	2.45	0.52
42:QA:92:ARG:HG2	42:QA:92:ARG:HH11	1.75	0.52
18:R:36:ARG:HD3	18:R:40:PHE:CZ	2.45	0.52
40:TC:36:ARG:NH2	40:TC:66:GLU:OE1	2.41	0.52
21:U:90:GLU:HA	21:U:93:GLU:HG2	1.92	0.52
44:XC:35:SER:HB3	44:XC:73:ASP:OD2	2.10	0.52
1:A:179:A:H2'	1:A:180:U:H6	1.74	0.52
1:A:531:U:H2'	35:JA:314:GLN:NE2	2.24	0.52
2:B:26:G:C6	2:B:27:G:N1	2.78	0.52
48:BD:21:TYR:HE1	48:BD:23:ARG:NH1	2.08	0.52
4:D:17:C:OP2	4:D:17(A):U:O2'	2.26	0.52
2:GB:848:G:H2'	2:GB:849:A:C8	2.45	0.52
7:LB:127:GLU:HB3	7:LB:196:LEU:HD12	1.91	0.52
38:MA:71:SER:HB3	38:MA:74:GLN:HG3	1.92	0.52
9:NB:28:GLY:HA3	9:NB:79:VAL:HB	1.92	0.52
44:SA:50:ILE:HB	48:WA:41:ARG:NH1	2.25	0.52
44:XC:45:ARG:HG3	44:XC:47:PHE:HE2	1.75	0.52
1:A:731:G:OP1	1:A:766:A:H1'	2.09	0.51
3:C:16:G:N2	3:C:69:G:H1'	2.25	0.51
1:FB:1003:G:H1	1:FB:1038:C:H42	1.58	0.51
2:GB:1510:A:H2'	2:GB:1511:A:C8	2.45	0.51
2:GB:2115:G:H4'	2:GB:2167:U:C2	2.44	0.51
2:GB:2591:C:H2'	2:GB:2592:G:C8	2.45	0.51
8:H:113:ARG:NH1	8:H:142:PRO:HA	2.25	0.51
10:J:83:ALA:HA	10:J:88:ILE:HG12	1.92	0.51
35:JA:109:ARG:NH1	35:JA:210:PRO:HD3	2.25	0.51
37:LA:58:GLU:HB2	37:LA:65:ALA:HB3	1.92	0.51
14:N:18:LYS:O	14:N:98:LYS:NZ	2.39	0.51
35:OC:309:THR:HG1	35:OC:320:HIS:CE1	2.29	0.51
36:PC:161:ALA:HB1	36:PC:185:ILE:HD11	1.91	0.51
13:RB:118:GLY:O	13:RB:137:LYS:NZ	2.34	0.51
20:T:65:LEU:HD12	20:T:66:GLU:H	1.75	0.51
41:UC:115:ARG:O	41:UC:118:VAL:HB	2.11	0.51
1:A:509:A:N3	1:A:543:C:O2'	2.37	0.51
45:TA:99:GLN:HE21	52:AB:88:LYS:NZ	2.08	0.51
2:B:1405:U:H2'	2:B:1406:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:CD:88:ARG:HB3	49:CD:88:ARG:HH21	1.75	0.51
4:D:16:C:H5'	4:D:17:C:H5	1.74	0.51
54:HD:54:LYS:HA	54:HD:57:ARG:NH1	2.25	0.51
13:M:2:LYS:HB3	13:M:2:LYS:NZ	2.25	0.51
41:PA:57:GLU:H	41:PA:60:LYS:NZ	2.04	0.51
13:RB:81:GLN:HB2	13:RB:110:TYR:CD1	2.45	0.51
43:WC:10:ARG:HG3	43:WC:105:ASP:HB3	1.93	0.51
1:A:595:G:H1'	1:A:596:C:H5	1.76	0.51
1:A:614:A:H2'	1:A:615:C:C6	2.45	0.51
2:B:2168:G:H2'	2:B:2169:A:H3'	1.93	0.51
6:F:174:ASP:OD1	6:F:175:VAL:N	2.43	0.51
1:FB:1189:C:OP1	44:XC:51:ARG:NH2	2.40	0.51
2:GB:363(G):A:H1'	2:GB:364:C:H5	1.74	0.51
2:GB:911:A:H2'	14:SB:9:TYR:OH	2.10	0.51
1:FB:1226:C:H4'	53:GD:80:TYR:CZ	2.44	0.51
36:KA:74:LYS:HZ3	36:KA:166:ASP:HB2	1.73	0.51
37:LA:88:ARG:HD3	37:LA:101:LEU:HD22	1.91	0.51
37:LA:148:GLY:HA3	37:LA:172:ARG:O	2.10	0.51
38:MA:61:LYS:HD2	38:MA:207:TYR:OH	2.10	0.51
1:A:1343:G:O2'	43:RA:121:ARG:NH1	2.42	0.51
1:A:1368:G:H4'	44:SA:46:ARG:HH11	1.76	0.51
17:VB:18:ASP:N	17:VB:18:ASP:OD1	2.44	0.51
51:ZA:83:ASP:O	51:ZA:86:GLU:HB2	2.10	0.51
1:A:1128:C:H5''	43:RA:66:ARG:NH1	2.26	0.51
2:B:1021:A:H8	2:B:1022:G:H5''	1.75	0.51
2:B:1709:U:H2'	2:B:1710:C:C6	2.45	0.51
2:B:300:A:H2'	2:B:334:C:H1'	1.93	0.51
26:EC:1:MET:HG2	26:EC:5:GLU:HB3	1.91	0.51
1:FB:1517:G:H3'	1:FB:1518:MA6:H8	1.92	0.51
1:FB:323:U:H2'	1:FB:324:G:O4'	2.10	0.51
1:FB:679:C:H2'	1:FB:680:C:C6	2.46	0.51
7:G:53:THR:HG23	7:G:55:GLY:H	1.75	0.51
2:GB:1359:A:H2	2:GB:1372:U:N3	2.01	0.51
2:GB:1394:U:H4'	2:GB:1603:A:H4'	1.93	0.51
13:M:140:ALA:HA	2:GB:928:G:H5'	1.92	0.51
29:HC:16:ARG:HG2	29:HC:16:ARG:NH1	2.16	0.51
36:KA:211:ILE:O	36:KA:215:LEU:HB2	2.10	0.51
13:M:93:GLY:H	13:M:123:LEU:HD22	1.76	0.51
38:MA:142:PRO:HA	38:MA:185:PHE:HD2	1.75	0.51
14:N:37:LEU:HD21	14:N:130:LYS:HD3	1.92	0.51
35:OC:204:ALA:HB2	35:OC:298:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:NA:78:HIS:ND1	42:QA:104:ARG:HD2	2.21	0.51
37:QC:88:ARG:HD3	37:QC:101:LEU:HD22	1.91	0.51
45:TA:121:PRO:HG2	45:TA:126:ARG:HG3	1.92	0.51
26:EC:22:GLU:OE2	26:EC:68:ARG:NH2	2.44	0.51
1:FB:714:G:H2'	1:FB:715:A:C8	2.44	0.51
10:J:14:ASP:OD1	10:J:15:VAL:N	2.43	0.51
38:MA:28:SER:HB2	38:MA:29:PRO:HD2	1.93	0.51
8:MB:34:LEU:HD23	8:MB:161:THR:HG22	1.91	0.51
15:O:12:ARG:HD3	15:O:16:HIS:CD2	2.46	0.51
11:PB:99:LEU:O	11:PB:103:VAL:HG23	2.11	0.51
42:QA:85:ARG:NH1	42:QA:87:SER:O	2.43	0.51
43:RA:10:ARG:HD2	43:RA:75:ASP:HB2	1.93	0.51
1:A:108:G:C6	54:CB:15:ARG:HG2	2.46	0.51
1:A:1418:A:H5''	1:A:1419:G:OP2	2.11	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.11	0.51
2:B:1011:G:OP1	18:R:75:ASN:HB2	2.11	0.51
2:B:295:G:O5'	22:V:1:MET:HG3	2.11	0.51
1:FB:406:G:H1	1:FB:436:C:H42	1.59	0.51
1:FB:721:G:H4'	1:FB:722:A:O4'	2.10	0.51
7:G:33:LEU:HD11	7:G:112:MET:HB3	1.92	0.51
2:GB:2168:G:H2'	2:GB:2169:A:H3'	1.92	0.51
3:HB:43:C:H5''	28:GC:1:MET:HG3	1.93	0.51
35:JA:326:LEU:HD13	35:JA:328:ARG:NH1	2.25	0.51
11:K:99:LEU:O	11:K:103:VAL:HG23	2.09	0.51
6:KB:34:VAL:HG21	6:KB:78:LEU:HD11	1.92	0.51
7:LB:184:TYR:O	7:LB:188:ARG:HG3	2.10	0.51
13:M:149:GLU:HA	13:M:149:GLU:OE2	2.09	0.51
8:MB:3:LEU:HD13	8:MB:5:LEU:HD21	1.91	0.51
36:PC:68:ILE:HG12	36:PC:161:ALA:HB3	1.91	0.51
38:RC:79:PHE:O	38:RC:83:SER:OG	2.23	0.51
22:V:23:ARG:NH2	22:V:41:GLY:O	2.43	0.51
45:YC:91:ARG:HB3	45:YC:92:GLU:OE2	2.10	0.51
1:A:673:G:H2'	1:A:674:G:C8	2.46	0.51
40:OA:99:ALA:O	52:AB:28:GLU:HG3	2.11	0.51
2:B:370:G:H4'	2:B:371:A:OP2	2.10	0.51
4:D:52:G:H1	4:D:62:C:H42	1.58	0.51
4:D:53:G:N2	4:D:61:C:O2	2.42	0.51
8:H:55:LYS:O	8:H:58:GLN:HG3	2.11	0.51
9:I:12:PRO:O	9:I:15:VAL:HG22	2.11	0.51
31:JC:47:ARG:NH1	31:JC:47:ARG:HB3	2.26	0.51
36:KA:166:ASP:HB3	36:KA:169:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:34:LEU:O	11:PB:49:GLY:HA3	2.11	0.51
36:PC:211:ILE:O	36:PC:215:LEU:HB2	2.11	0.51
38:RC:168:ARG:HG3	38:RC:168:ARG:NH1	2.26	0.51
44:XC:8:LEU:HG	44:XC:96:ILE:HG23	1.91	0.51
45:YC:18:ARG:HH21	45:YC:36:ASP:C	2.14	0.51
2:B:1021:A:C8	2:B:1021:A:H3'	2.46	0.51
2:B:1364:G:P	25:Y:3:LYS:HG3	2.50	0.51
3:C:13:A:N1	3:C:69:G:O2'	2.30	0.51
26:EC:46:GLN:HB2	26:EC:49:LYS:HE3	1.93	0.51
1:FB:108:G:C6	54:HD:15:ARG:HG2	2.46	0.51
1:FB:595:G:H1'	1:FB:596:C:H5	1.75	0.51
40:TC:97:PHE:HB2	52:FD:32:ARG:NH1	2.25	0.51
2:GB:1783:A:H5'	2:GB:2608:G:H4'	1.93	0.51
2:GB:443:A:H1'	2:GB:1201:C:O4'	2.10	0.51
8:H:34:LEU:HD23	8:H:161:THR:HG22	1.93	0.51
4:IB:53:G:N2	4:IB:61:C:O2	2.43	0.51
38:MA:18:LYS:CE	38:MA:26:CYS:SG	2.96	0.51
9:NB:3:ARG:NH1	9:NB:3:ARG:HA	2.26	0.51
1:A:674:G:OP1	40:OA:87:ARG:NH2	2.42	0.51
10:OB:62:LYS:HD2	10:OB:135:GLU:OE2	2.11	0.51
10:OB:14:ASP:OD1	10:OB:15:VAL:N	2.43	0.51
39:NA:148:VAL:HG21	42:QA:107:LEU:HD22	1.93	0.51
16:UB:52:SER:O	16:UB:56:LEU:HB2	2.11	0.51
17:VB:127:ALA:O	17:VB:129:ARG:N	2.42	0.51
48:WA:40:CYS:SG	48:WA:43:CYS:SG	3.08	0.51
43:WC:4:TYR:HB3	43:WC:88:TYR:HB2	1.92	0.51
44:XC:5:ARG:HD3	44:XC:71:LEU:HD11	1.93	0.51
51:ZA:52:LYS:HB3	51:ZA:52:LYS:NZ	2.26	0.51
1:A:815:A:N3	1:A:1527:C:O2'	2.37	0.51
22:AC:38:ILE:HD11	22:AC:66:PRO:HG3	1.93	0.51
51:ED:14:LYS:N	51:ED:14:LYS:HE3	2.26	0.51
1:FB:1118:C:H2'	1:FB:1119:C:C6	2.46	0.51
1:FB:376:G:H5''	50:DD:5:ARG:HD2	1.93	0.51
1:FB:678:U:H2'	1:FB:679:C:C6	2.46	0.51
1:FB:987:G:H2'	1:FB:988:G:C8	2.46	0.51
2:GB:2021:C:H4'	2:GB:2022:U:OP2	2.10	0.51
9:I:164:TYR:HB2	9:I:167:GLU:HB2	1.91	0.51
2:GB:252:G:OP1	13:RB:50:ARG:NH1	2.43	0.51
38:RC:50:ARG:HD3	38:RC:51:PRO:HD2	1.92	0.51
2:B:857:C:H1'	24:X:26:TYR:HE1	1.75	0.51
26:Z:1:MET:HG2	26:Z:5:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:A:N3	54:CB:81:LYS:NZ	2.58	0.51
1:A:987:G:H2'	1:A:988:G:C8	2.46	0.51
2:B:271(C):G:O2'	2:B:421:U:OP2	2.19	0.51
54:CB:56:MET:HG3	54:CB:88:VAL:HG21	1.93	0.51
2:GB:1790:C:H5''	2:GB:1791:A:OP1	2.10	0.51
2:GB:34:C:HO2'	2:GB:35:G:P	2.34	0.51
4:IB:8:4SU:O2'	4:IB:46:G:N2	2.37	0.51
11:K:35:ARG:HA	11:K:116:LEU:HD13	1.92	0.51
9:NB:109:PHE:CE1	9:NB:152:ARG:NH1	2.78	0.51
36:PC:130:ARG:HG2	36:PC:131:PRO:HD2	1.93	0.51
1:FB:1057:G:H4'	37:QC:197:GLY:H	1.76	0.51
19:XB:44:LYS:NZ	19:XB:101:GLY:OXT	2.35	0.51
47:AD:3:ARG:NH1	47:AD:4:ILE:HG22	2.26	0.50
2:B:1171:G:N2	2:B:1178:C:N3	2.58	0.50
2:B:1394:U:H4'	2:B:1603:A:H4'	1.93	0.50
50:DD:40:ASP:HB3	50:DD:48:TRP:HB2	1.92	0.50
2:GB:1882:C:H2'	2:GB:1883:G:O4'	2.12	0.50
2:GB:2724:C:OP1	6:KB:118:LYS:NZ	2.39	0.50
2:GB:363(F):U:H3'	2:GB:363(G):A:C8	2.41	0.50
45:TA:77:MET:HG2	45:TA:103:LEU:HD21	1.94	0.50
40:TC:15:ASP:OD1	40:TC:18:GLN:N	2.26	0.50
48:WA:41:ARG:NH1	48:WA:42:ILE:HD11	2.26	0.50
1:A:983:A:H5'	1:A:984:C:OP2	2.11	0.50
2:B:2370:G:C6	2:B:2371:G:C6	2.99	0.50
2:B:998:C:OP2	18:R:58:ARG:NH2	2.37	0.50
1:FB:642:A:H2'	1:FB:643:C:C6	2.46	0.50
2:GB:1826:G:H4'	5:JB:242:ARG:HH21	1.75	0.50
2:GB:2892:A:H2'	2:GB:2893:G:O4'	2.11	0.50
2:GB:892:G:H2'	2:GB:893:C:H4'	1.93	0.50
4:IB:54:5MU:HN3	4:IB:58:A:H62	1.58	0.50
34:MC:13:A:H2'	34:MC:14:A:H4'	1.93	0.50
17:Q:18:ASP:OD1	17:Q:18:ASP:N	2.44	0.50
44:SA:6:ILE:HD11	44:SA:72:VAL:HB	1.92	0.50
51:ZA:14:LYS:HE3	51:ZA:14:LYS:N	2.26	0.50
1:A:28:G:O2'	1:A:296:U:OP1	2.25	0.50
2:B:2591:C:H2'	2:B:2592:G:C8	2.47	0.50
28:BA:48:ARG:HE	28:BA:52:THR:HA	1.76	0.50
2:GB:1171:G:N2	2:GB:1178:C:N3	2.57	0.50
2:GB:1495:A:H2'	2:GB:1496:A:C8	2.47	0.50
9:I:86:GLU:HG2	9:I:132:ARG:HG3	1.93	0.50
10:J:31:LEU:HD11	10:J:38:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:KA:19:HIS:CD2	36:KA:189:ASP:OD2	2.64	0.50
9:NB:55:PRO:HG2	9:NB:61:HIS:CE1	2.47	0.50
36:PC:163:PHE:CD2	36:PC:185:ILE:HB	2.47	0.50
1:A:430:A:OP2	38:MA:8:VAL:HG12	2.12	0.50
1:A:987:G:H1	1:A:1218:C:H42	1.59	0.50
2:B:1359:A:H2	2:B:1372:U:N3	2.00	0.50
2:B:1536:A:H5''	2:B:1537:C:C5	2.46	0.50
2:B:1592:C:H2'	2:B:1593:G:C8	2.46	0.50
2:B:2243:U:H2'	2:B:2244:U:C6	2.47	0.50
2:B:2312:U:H5'	8:H:88:ILE:HD11	1.93	0.50
23:BC:124:ILE:HD11	23:BC:165:VAL:HG21	1.94	0.50
6:F:116:VAL:HG13	6:F:122:PHE:HB2	1.93	0.50
1:FB:656:C:H4'	49:CD:62:GLN:NE2	2.20	0.50
2:GB:975:G:H1'	2:GB:990:A:C2	2.46	0.50
37:LA:180:ALA:HB1	37:LA:203:PHE:CE1	2.46	0.50
15:O:36:THR:HG22	15:O:37:THR:N	2.26	0.50
15:O:79:LEU:HA	15:O:83:ILE:HD12	1.94	0.50
44:SA:3:LYS:NZ	44:SA:75:ILE:O	2.42	0.50
45:TA:90:GLY:O	45:TA:92:GLU:N	2.44	0.50
40:TC:30:LEU:HB3	40:TC:35:ALA:HB3	1.93	0.50
1:FB:1128:C:H5''	43:WC:66:ARG:NH1	2.26	0.50
45:YC:87:THR:HA	45:YC:91:ARG:HD2	1.94	0.50
2:B:747:U:O2	2:B:2014:A:H1'	2.12	0.50
2:B:796:C:H2'	2:B:797:C:C6	2.46	0.50
1:FB:555:C:H2'	1:FB:556:C:C6	2.46	0.50
2:GB:1557:C:H5''	2:GB:1558:A:OP2	2.12	0.50
2:GB:609(B):G:N2	2:GB:619:G:H1'	2.26	0.50
5:JB:206:LEU:HD22	5:JB:211:ARG:HG2	1.93	0.50
12:L:36:GLY:HA3	12:L:109:LYS:HG3	1.94	0.50
38:MA:12:CYS:SG	38:MA:18:LYS:HE3	2.51	0.50
37:QC:58:GLU:HB2	37:QC:65:ALA:HB3	1.94	0.50
47:VA:54:VAL:HG22	47:VA:57:ARG:HH12	1.76	0.50
47:VA:70:LEU:O	47:VA:74:VAL:HG23	2.11	0.50
44:XC:5:ARG:HG3	44:XC:73:ASP:HB3	1.92	0.50
1:A:1104:G:O5'	36:KA:111:ARG:HD2	2.11	0.50
1:A:1414:U:H3	1:A:1486:G:H1	1.60	0.50
1:A:406:G:H1	1:A:436:C:H42	1.60	0.50
2:B:1570:A:H2'	2:B:1571:A:C8	2.47	0.50
2:B:2892:A:H2'	2:B:2893:G:O4'	2.12	0.50
2:B:540:G:H2'	2:B:541:C:C6	2.47	0.50
48:BD:41:ARG:NH1	48:BD:42:ILE:HD11	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:G:H1	4:D:56:C:H42	1.57	0.50
13:M:59:LEU:HD23	32:FA:58:ILE:HD13	1.93	0.50
1:FB:1253:G:H1	1:FB:1284:C:H42	1.57	0.50
1:FB:272:C:H2'	1:FB:273:A:H8	1.76	0.50
2:GB:1364:G:P	25:DC:3:LYS:HG3	2.52	0.50
2:GB:194:G:H2'	2:GB:195:A:O4'	2.11	0.50
6:KB:11:MET:HG2	6:KB:24:THR:HB	1.93	0.50
39:NA:20:GLN:HG2	39:NA:25:ARG:HD2	1.93	0.50
46:UA:38:THR:OG1	46:UA:57:LYS:HB3	2.11	0.50
8:H:115:ARG:NH1	47:VA:2:ALA:HB2	2.26	0.50
43:WC:86:VAL:HG11	43:WC:102:LEU:HD11	1.93	0.50
1:A:1124:G:H1	1:A:1149:C:H42	1.60	0.50
1:A:335:C:O2'	1:A:1433:A:N3	2.40	0.50
2:B:1495:A:H2'	2:B:1496:A:C8	2.45	0.50
25:DC:72:GLU:O	25:DC:76:ARG:HG3	2.12	0.50
26:EC:2:LYS:H	26:EC:2:LYS:HD3	1.76	0.50
1:FB:769:G:H4'	1:FB:1513:A:H4'	1.94	0.50
2:GB:1409:C:H2'	2:GB:1410:G:C8	2.46	0.50
2:GB:161:U:H2'	2:GB:163:U:OP2	2.11	0.50
2:GB:686:G:N2	2:GB:788:A:H61	2.10	0.50
2:GB:889:C:O2'	2:GB:890:A:O4'	2.30	0.50
2:B:2508:G:P	35:JA:228:ARG:HH22	2.34	0.50
16:P:52:SER:O	16:P:56:LEU:HB2	2.12	0.50
11:PB:9:VAL:HG21	11:PB:39:ARG:HH22	1.76	0.50
44:SA:44:VAL:HG22	44:SA:66:ARG:HG2	1.94	0.50
42:VC:20:TYR:HE2	42:VC:75:ARG:HD2	1.77	0.50
50:YA:53:VAL:HG12	50:YA:57:ARG:HH11	1.77	0.50
23:BC:52:SER:OG	23:BC:53:ILE:N	2.44	0.50
48:BD:40:CYS:SG	48:BD:43:CYS:SG	3.09	0.50
4:D:8:4SU:O2'	4:D:46:G:N2	2.36	0.50
1:FB:353:A:H8	1:FB:353:A:H5'	1.75	0.50
2:GB:958:U:H5'	14:SB:14:ARG:HD3	1.94	0.50
28:GC:48:ARG:HE	28:GC:52:THR:HA	1.77	0.50
10:J:76:THR:HG22	10:J:141:LYS:HD2	1.92	0.50
19:S:2:PHE:CZ	19:S:41:GLY:HA3	2.46	0.50
46:UA:8:ASN:O	46:UA:12:ARG:HG3	2.11	0.50
46:UA:28:LYS:NZ	46:UA:64:TYR:HE2	2.09	0.50
20:YB:82:LEU:HD22	20:YB:84:ARG:NH2	2.27	0.50
1:A:1004:A:N6	1:A:1026:G:OP2	2.40	0.50
1:A:1517:G:H3'	1:A:1518:MA6:H8	1.93	0.50
1:A:575:G:OP1	1:A:575:G:H4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AD:23:TYR:HB3	47:AD:67:GLU:HA	1.94	0.50
2:B:1292:U:H2'	2:B:1293:C:C6	2.47	0.50
2:B:2141:G:N2	2:B:2151:G:H1'	2.26	0.50
23:BC:29:TYR:HB3	23:BC:34:ASN:HD22	1.76	0.50
2:B:517:C:OP1	29:CA:16:ARG:NH2	2.44	0.50
2:B:2405:G:OP1	13:M:77:ARG:NH2	2.45	0.50
37:QC:180:ALA:HB1	37:QC:203:PHE:CE1	2.46	0.50
44:XC:3:LYS:NZ	44:XC:75:ILE:O	2.43	0.50
1:A:865:A:H5'	1:A:1078:U:O4	2.12	0.49
1:A:1132:C:H2'	1:A:1133:G:H8	1.76	0.49
2:B:969:U:H2'	2:B:970:C:C6	2.47	0.49
1:FB:1443:G:O6	2:GB:2863:C:H5''	2.11	0.49
1:FB:383:A:C5	1:FB:384:G:H1'	2.47	0.49
1:FB:706:A:N3	45:YC:31:THR:HG21	2.27	0.49
2:GB:270(G):U:H2'	2:GB:270(H):C:C6	2.47	0.49
6:KB:45:THR:O	6:KB:82:ARG:HD2	2.12	0.49
37:LA:119:ARG:O	37:LA:123:GLN:HG3	2.12	0.49
8:MB:113:ARG:NH1	8:MB:142:PRO:HA	2.25	0.49
9:NB:101:ARG:HH11	9:NB:122:THR:HG23	1.75	0.49
35:OC:165:LYS:NZ	35:OC:208:GLU:HG3	2.27	0.49
35:OC:247:THR:HG23	35:OC:254:VAL:HG22	1.93	0.49
36:PC:74:LYS:HZ3	36:PC:166:ASP:HB2	1.77	0.49
45:TA:91:ARG:HB3	45:TA:92:GLU:OE2	2.11	0.49
1:A:603:U:H2'	1:A:604:G:C8	2.48	0.49
1:A:679:C:H2'	1:A:680:C:C6	2.47	0.49
2:B:1510:A:H2'	2:B:1511:A:C8	2.46	0.49
2:B:1557:C:H5''	2:B:1558:A:OP2	2.12	0.49
2:B:2350:C:H2'	2:B:2351:G:O4'	2.13	0.49
2:B:2792:G:H2'	2:B:2793:G:H8	1.77	0.49
1:FB:1347:G:N2	1:FB:1373:G:H2'	2.27	0.49
1:FB:966:M2G:HM13	1:FB:967:5MC:H1'	1.94	0.49
2:GB:1800:C:OP2	5:JB:183:ARG:NH2	2.46	0.49
7:LB:53:THR:CG2	7:LB:55:GLY:H	2.24	0.49
8:MB:113:ARG:NH2	8:MB:139:LEU:O	2.45	0.49
40:OA:24:GLU:OE2	40:OA:24:GLU:HA	2.12	0.49
38:RC:61:LYS:HD2	38:RC:207:TYR:OH	2.11	0.49
14:SB:116:GLU:OE2	14:SB:119:ARG:NE	2.42	0.49
21:U:61:GLY:HA3	21:U:73:ARG:O	2.12	0.49
42:VC:51:VAL:HG11	42:VC:60:ARG:NH1	2.27	0.49
4:D:75:C:H5'	25:Y:30:VAL:HG21	1.93	0.49
1:A:1003:G:H1	1:A:1038:C:H42	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:H5'	46:UA:124:LYS:NZ	2.27	0.49
2:B:609(B):G:N2	2:B:619:G:H1'	2.27	0.49
2:GB:1358:G:O2'	2:GB:1359:A:H5''	2.13	0.49
2:GB:1692:U:H2'	2:GB:1694:C:C5	2.47	0.49
2:GB:2789:C:O3'	2:GB:2790:A:H4'	2.11	0.49
54:HD:30:LYS:HA	54:HD:33:ILE:HG12	1.94	0.49
6:KB:119:ARG:HG2	6:KB:120:TRP:CE2	2.48	0.49
13:M:65:ARG:HG3	13:M:66:GLY:N	2.26	0.49
9:NB:17:VAL:HG11	9:NB:50:VAL:HG21	1.94	0.49
40:OA:30:LEU:HB3	40:OA:35:ALA:HB3	1.94	0.49
35:OC:196:ILE:HD13	35:OC:313:PRO:HG2	1.95	0.49
3:C:7:G:H5'	16:P:29:PHE:CD2	2.48	0.49
42:QA:82:HIS:NE2	42:QA:84:ARG:HD2	2.27	0.49
2:GB:2563:U:H4'	12:QB:28:SER:HA	1.94	0.49
43:RA:86:VAL:HG11	43:RA:102:LEU:HD11	1.94	0.49
40:TC:68:PRO:HG2	40:TC:71:ARG:NH2	2.26	0.49
2:GB:1754:C:P	17:VB:96:ARG:HH12	2.35	0.49
42:VC:82:HIS:NE2	42:VC:84:ARG:HD2	2.27	0.49
23:W:155:LEU:O	23:W:157:LEU:HD12	2.11	0.49
44:XC:44:VAL:HG22	44:XC:66:ARG:HG2	1.93	0.49
20:YB:57:ASN:O	20:YB:61:ASN:HB2	2.13	0.49
46:ZC:11:VAL:HG13	51:ED:29:HIS:HD2	1.76	0.49
1:A:437:U:H5'	38:MA:155:LEU:HD11	1.93	0.49
2:B:889:C:O2'	2:B:890:A:O4'	2.31	0.49
1:FB:335:C:O2'	1:FB:1433:A:N3	2.41	0.49
2:GB:1059:G:N3	2:GB:1059:G:H2'	2.27	0.49
2:GB:1292:U:H2'	2:GB:1293:C:C6	2.47	0.49
2:GB:2564:A:C2	2:GB:2647:U:H4'	2.47	0.49
53:GD:31:ILE:HG13	53:GD:49:ILE:HG23	1.94	0.49
10:J:101:LEU:HG	10:J:107:ILE:HG12	1.95	0.49
35:JA:182:HIS:HB3	35:JA:310:TYR:HE1	1.77	0.49
36:KA:163:PHE:CD2	36:KA:185:ILE:HB	2.47	0.49
37:LA:33:LEU:HA	37:LA:36:ASP:HB2	1.94	0.49
36:PC:157:ARG:O	36:PC:158:LEU:HB3	2.11	0.49
12:QB:24:VAL:HB	12:QB:33:ALA:HB2	1.94	0.49
49:XA:54:ARG:O	49:XA:58:MET:HG3	2.11	0.49
19:XB:14:VAL:HG12	19:XB:18:LEU:HD23	1.93	0.49
50:YA:40:ASP:HB3	50:YA:48:TRP:HB2	1.93	0.49
1:A:1356:G:H2'	1:A:1357:A:H8	1.77	0.49
1:A:769:G:H4'	1:A:1513:A:H4'	1.94	0.49
2:B:1179:C:H2'	2:B:1180:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2794:C:H42	2:B:2802:G:H1	1.59	0.49
2:B:776:G:H4'	2:B:777:A:O5'	2.13	0.49
3:C:43:C:H5''	28:BA:1:MET:HG3	1.94	0.49
25:DC:40:ARG:HD3	25:DC:40:ARG:C	2.32	0.49
1:FB:272:C:H2'	1:FB:273:A:C8	2.47	0.49
1:FB:987:G:H1	1:FB:1218:C:H42	1.58	0.49
2:GB:1021:A:H8	2:GB:1021:A:H3'	1.77	0.49
30:IC:15:GLU:HG3	30:IC:47:THR:HG23	1.93	0.49
31:JC:5:TRP:NE1	31:JC:7:PRO:HG3	2.26	0.49
6:KB:174:ASP:OD1	6:KB:175:VAL:N	2.46	0.49
7:LB:181:LEU:HD11	7:LB:186:ILE:HD11	1.95	0.49
7:LB:195:ASP:HB3	7:LB:198:ALA:H	1.78	0.49
7:LB:33:LEU:HD11	7:LB:112:MET:HB3	1.93	0.49
36:PC:19:HIS:CD2	36:PC:189:ASP:OD2	2.65	0.49
36:PC:44:LEU:H	36:PC:44:LEU:HD12	1.76	0.49
42:QA:51:VAL:HG21	42:QA:60:ARG:HH11	1.77	0.49
47:VA:3:ARG:NH1	47:VA:3:ARG:CG	2.70	0.49
2:B:2334:G:O6	24:X:74:ARG:NH2	2.45	0.49
25:Y:2:SER:HB3	25:Y:46:LEU:HD12	1.94	0.49
1:A:1347:G:N2	1:A:1373:G:H2'	2.27	0.49
1:A:801:U:H2'	1:A:802:A:H8	1.77	0.49
2:B:1778:U:H2'	2:B:1784:A:N6	2.27	0.49
2:B:2055:C:H5'	2:B:2056:G:O5'	2.11	0.49
2:B:2564:A:C2	2:B:2647:U:H4'	2.47	0.49
3:C:7:G:H4'	16:P:29:PHE:HB2	1.94	0.49
1:FB:1412:C:H2'	1:FB:1413:A:H8	1.77	0.49
30:IC:6:ARG:NH1	30:IC:26:ASN:HB2	2.28	0.49
36:KA:7:VAL:HB	36:KA:8:LYS:HD2	1.95	0.49
2:B:2563:U:H4'	12:L:28:SER:HA	1.93	0.49
38:MA:168:ARG:NH1	38:MA:168:ARG:HG3	2.28	0.49
41:PA:115:ARG:O	41:PA:118:VAL:HB	2.12	0.49
15:TB:96:ARG:NH1	15:TB:115:GLU:OE2	2.46	0.49
41:UC:23:VAL:O	41:UC:27:ILE:HG13	2.13	0.49
47:VA:3:ARG:NH1	47:VA:4:ILE:HG22	2.26	0.49
43:WC:10:ARG:HD2	43:WC:75:ASP:HB2	1.92	0.49
1:A:1320:C:H2'	1:A:1321:C:O4'	2.13	0.49
2:B:14:A:H5''	2:B:15:G:OP2	2.13	0.49
2:B:2031:A:C6	2:B:2498:C:H1'	2.48	0.49
2:GB:857:C:H1'	24:CC:26:TYR:HE1	1.77	0.49
26:EC:18:PRO:O	26:EC:22:GLU:HG3	2.13	0.49
1:FB:1397:C:O2'	1:FB:1398:A:OP1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:977:A:H2'	1:FB:978:A:H5''	1.94	0.49
2:GB:1570:A:H2'	2:GB:1571:A:C8	2.48	0.49
2:GB:1778:U:H2'	2:GB:1784:A:N6	2.27	0.49
2:GB:271(C):G:H4'	2:GB:271(D):U:H5''	1.94	0.49
3:HB:7:G:H4'	16:UB:29:PHE:HB2	1.94	0.49
24:X:5:LYS:NZ	35:JA:262:SER:OG	2.45	0.49
31:JC:47:ARG:HH11	31:JC:47:ARG:HB3	1.76	0.49
36:KA:167:PRO:HG2	36:KA:188:ALA:HB2	1.95	0.49
38:MA:43:HIS:CE1	38:MA:46:LYS:HZ2	2.29	0.49
43:RA:50:LEU:HD12	43:RA:56:LEU:HD12	1.94	0.49
13:RB:2:LYS:NZ	13:RB:4:SER:OG	2.44	0.49
38:RC:111:ALA:HB2	38:RC:120:LEU:HD12	1.95	0.49
38:RC:155:LEU:HD13	38:RC:156:GLU:N	2.28	0.49
42:VC:122:ARG:HA	42:VC:125:ARG:HD2	1.94	0.49
2:GB:1187:G:H5''	19:XB:81:TYR:CE1	2.47	0.49
51:ZA:95:TYR:HA	51:ZA:98:LEU:HD12	1.94	0.49
46:ZC:38:THR:OG1	46:ZC:57:LYS:HB3	2.12	0.49
46:ZC:7:ILE:O	46:ZC:11:VAL:HG23	2.13	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.47	0.49
2:B:1359:A:H2'	2:B:1360:A:H5'	1.95	0.49
2:B:2082:A:H2'	2:B:2083:G:O4'	2.13	0.49
26:EC:35:LEU:HD12	26:EC:53:LEU:HD12	1.95	0.49
26:EC:64:LEU:O	26:EC:68:ARG:HG2	2.13	0.49
6:F:119:ARG:HG2	6:F:120:TRP:CE2	2.47	0.49
1:FB:801:U:H2'	1:FB:802:A:H8	1.78	0.49
7:G:95:ARG:HD3	7:G:97:TYR:CZ	2.47	0.49
2:GB:1667:G:O2'	2:GB:1991:U:O4	2.19	0.49
2:GB:2747:G:OP1	9:NB:138:LYS:NZ	2.42	0.49
2:GB:2622:C:O2'	2:GB:2825:G:N7	2.45	0.49
2:GB:857:C:N4	2:GB:858:U:O4	2.46	0.49
36:KA:177:ALA:HB1	36:KA:182:ILE:HB	1.95	0.49
37:LA:61:ALA:O	37:LA:63:ASN:N	2.43	0.49
38:RC:57:ARG:HB3	38:RC:206:PHE:HB2	1.94	0.49
20:T:20:VAL:O	20:T:23:LEU:HB2	2.12	0.49
20:T:82:LEU:HD22	20:T:84:ARG:NH2	2.28	0.49
2:B:1085:A:O2'	2:B:1104:C:O2'	2.27	0.49
2:B:1508:A:H3'	2:B:1509:A:C8	2.47	0.49
54:CB:54:LYS:HA	54:CB:57:ARG:NH1	2.28	0.49
5:E:112:GLN:O	5:E:115:GLN:HG2	2.12	0.49
1:FB:1025:U:H5'	1:FB:1026:G:H5'	1.95	0.49
1:FB:137:C:H2'	1:FB:138:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:983:A:H5'	1:FB:984:C:OP2	2.13	0.49
2:GB:1111:A:N3	2:GB:1112:G:H1'	2.27	0.49
2:GB:540:G:H2'	2:GB:541:C:C6	2.47	0.49
13:M:29:LYS:HB3	13:M:30:THR:H	1.47	0.49
2:B:1754:C:P	17:Q:96:ARG:HH12	2.36	0.49
18:R:14:HIS:O	18:R:18:LEU:HD12	2.13	0.49
44:SA:6:ILE:HG22	44:SA:98:ILE:HG22	1.94	0.49
2:GB:2849:U:OP2	17:VB:95:ARG:NH1	2.45	0.49
17:VB:94:ALA:HB1	17:VB:99:LEU:HD21	1.95	0.49
48:WA:2:ALA:HA	48:WA:6:LEU:HD13	1.94	0.49
46:ZC:60:LEU:HD21	46:ZC:66:VAL:HG22	1.95	0.49
1:A:323:U:H2'	1:A:324:G:O4'	2.12	0.49
2:B:1516:U:H2'	2:B:1517:G:H8	1.78	0.49
30:DA:15:GLU:HG3	30:DA:47:THR:HG23	1.94	0.49
1:FB:1062:U:H2'	1:FB:1063:C:C6	2.48	0.49
2:GB:1430:C:H2'	2:GB:1431:U:C6	2.48	0.49
2:GB:2779:U:OP1	2:GB:2780:G:H2'	2.12	0.49
55:ID:2:GLY:C	55:ID:4:GLY:H	2.15	0.49
35:JA:309:THR:HG1	35:JA:320:HIS:CE1	2.31	0.49
12:L:2:ILE:HD12	12:L:6:THR:HG21	1.93	0.49
37:LA:177:THR:HG22	37:LA:180:ALA:H	1.78	0.49
40:OA:97:PHE:HB2	52:AB:32:ARG:NH1	2.28	0.49
18:R:52:ARG:HA	18:R:55:ARG:HG3	1.94	0.49
1:FB:674:G:OP1	40:TC:87:ARG:NH2	2.45	0.49
45:YC:121:PRO:HG2	45:YC:126:ARG:HG3	1.94	0.49
46:ZC:69:TYR:HD2	46:ZC:99:HIS:CD2	2.30	0.49
1:A:773:G:O3'	5:E:202:LYS:NZ	2.38	0.48
47:AD:108:ARG:O	47:AD:112:GLY:N	2.46	0.48
2:B:1882:C:H2'	2:B:1883:G:O4'	2.13	0.48
4:D:51:C:H2'	4:D:52:G:C8	2.48	0.48
55:DB:2:GLY:C	55:DB:4:GLY:H	2.16	0.48
25:DC:95:LEU:O	25:DC:98:LEU:HB2	2.13	0.48
6:F:174:ASP:HB3	6:F:183:LEU:HD22	1.95	0.48
1:FB:1124:G:H1	1:FB:1149:C:H42	1.61	0.48
2:GB:2150:U:H2'	2:GB:2151:G:H8	1.78	0.48
1:A:1073:U:O2'	36:KA:104:ASN:OD1	2.27	0.48
12:L:24:VAL:HB	12:L:33:ALA:HB2	1.95	0.48
14:N:64:ILE:HG13	23:W:178:GLU:HG3	1.95	0.48
17:Q:109:GLU:HG2	17:Q:112:ARG:NH2	2.28	0.48
45:YC:90:GLY:O	45:YC:92:GLU:N	2.46	0.48
51:ZA:45:HIS:HB3	51:ZA:72:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:U:H5'	1:A:1026:G:H5'	1.94	0.48
1:A:38:G:H22	1:A:397:A:H5''	1.78	0.48
2:B:987:G:O2'	2:B:1000:A:N3	2.44	0.48
2:B:154(A):C:H2'	2:B:161:U:C5	2.48	0.48
2:B:2150:U:H2'	2:B:2151:G:H8	1.78	0.48
2:B:492:A:H2'	2:B:493:G:O4'	2.13	0.48
1:FB:1510:U:H2'	1:FB:1511:G:C8	2.48	0.48
2:GB:1067:A:OP1	2:GB:1068:G:N2	2.45	0.48
2:GB:1508:A:H3'	2:GB:1509:A:C8	2.48	0.48
2:GB:1532:C:H42	2:GB:1539:G:H22	1.62	0.48
2:GB:576:U:H2'	2:GB:577:G:C8	2.49	0.48
37:QC:180:ALA:HA	37:QC:206:GLU:HA	1.95	0.48
2:B:1187:G:H5''	19:S:81:TYR:CE1	2.49	0.48
44:SA:20:ALA:O	44:SA:23:ILE:HG22	2.13	0.48
44:SA:5:ARG:HD3	44:SA:71:LEU:HD11	1.95	0.48
40:TC:50:TYR:CE2	52:FD:77:GLY:HA2	2.48	0.48
43:WC:121:ARG:HH11	43:WC:121:ARG:HB2	1.78	0.48
1:A:1057:G:H4'	37:LA:197:GLY:H	1.77	0.48
1:A:1085:U:H3'	1:A:1086:U:C6	2.48	0.48
1:A:1412:C:H2'	1:A:1413:A:H8	1.78	0.48
1:A:1510:U:H2'	1:A:1511:G:C8	2.48	0.48
1:A:397:A:N3	1:A:397:A:H3'	2.28	0.48
1:A:437:U:OP1	38:MA:155:LEU:HD21	2.13	0.48
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.95	0.48
6:F:34:VAL:HG21	6:F:78:LEU:HD11	1.95	0.48
6:F:7:VAL:HG23	6:F:51:PHE:HE2	1.77	0.48
1:FB:1003:G:H1	1:FB:1038:C:N4	2.11	0.48
2:GB:2115:G:H2'	2:GB:2117:A:N7	2.29	0.48
2:GB:686:G:O5'	31:JC:11:LYS:NZ	2.46	0.48
35:JA:172:TYR:O	35:JA:176:LYS:HB2	2.13	0.48
39:NA:147:ASP:OD2	39:NA:150:ARG:NH2	2.46	0.48
39:NA:31:LEU:HD22	39:NA:43:LEU:HD11	1.95	0.48
15:O:70:LEU:O	15:O:72:ASP:N	2.45	0.48
10:OB:118:LYS:NZ	10:OB:119:PRO:O	2.46	0.48
16:P:60:GLY:O	16:P:61:ASN:HB3	2.14	0.48
37:QC:180:ALA:HB1	37:QC:203:PHE:HE1	1.78	0.48
19:S:14:VAL:HG12	19:S:18:LEU:HD23	1.96	0.48
39:SC:84:PHE:HB3	39:SC:134:ALA:HB2	1.95	0.48
45:TA:18:ARG:HH21	45:TA:36:ASP:C	2.16	0.48
18:WB:113:ALA:O	18:WB:117:GLN:HG2	2.12	0.48
44:XC:20:ALA:O	44:XC:23:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:H2'	1:A:978:A:H5'	1.94	0.48
53:BB:31:ILE:HG13	53:BB:49:ILE:HG23	1.94	0.48
2:B:1309:G:H4'	31:EA:7:PRO:HB2	1.95	0.48
2:GB:2208:U:H4'	5:JB:151:LYS:HG2	1.94	0.48
11:K:9:VAL:HG21	11:K:39:ARG:HH22	1.79	0.48
37:LA:180:ALA:HB1	37:LA:203:PHE:HE1	1.78	0.48
40:OA:80:ARG:HE	40:OA:88:VAL:HB	1.77	0.48
36:PC:167:PRO:HG2	36:PC:188:ALA:HB2	1.95	0.48
12:QB:36:GLY:HA3	12:QB:109:LYS:HG3	1.94	0.48
16:UB:4:LEU:HD23	16:UB:8:GLU:OE2	2.13	0.48
17:VB:132:LYS:HB2	17:VB:132:LYS:NZ	2.27	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.48	0.48
2:B:1467:C:OP2	2:B:1547:C:H5	1.96	0.48
2:B:309:G:N3	2:B:329:G:O2'	2.44	0.48
1:FB:191(D):U:H2'	1:FB:191(E):G:C8	2.49	0.48
1:FB:8:A:C6	38:RC:209:ARG:HB2	2.48	0.48
2:GB:1657:C:H2'	2:GB:1658:C:H6	1.78	0.48
2:GB:263:C:H2'	2:GB:264:C:O4'	2.13	0.48
2:GB:271(C):G:O2'	2:GB:421:U:OP2	2.18	0.48
2:GB:929:G:O5'	2:GB:929:G:H8	1.96	0.48
5:JB:246:PRO:O	5:JB:254:THR:HG22	2.12	0.48
13:M:77:ARG:HB2	13:M:77:ARG:HH11	1.76	0.48
13:M:83:VAL:HG12	13:M:112:LEU:HD21	1.96	0.48
17:Q:127:ALA:O	17:Q:129:ARG:N	2.43	0.48
14:SB:111:GLU:O	14:SB:115:MET:HG2	2.13	0.48
15:TB:36:THR:HG22	15:TB:37:THR:N	2.29	0.48
40:TC:27:GLN:HA	40:TC:30:LEU:HD12	1.95	0.48
3:HB:7:G:H5'	16:UB:29:PHE:CD2	2.49	0.48
45:YC:77:MET:HG2	45:YC:103:LEU:HD21	1.95	0.48
21:ZB:44:GLU:OE1	21:ZB:50:LYS:HD2	2.13	0.48
1:FB:500:G:H5'	46:ZC:124:LYS:HZ2	1.79	0.48
22:AC:15:VAL:HG11	22:AC:20:TYR:HB2	1.94	0.48
47:AD:29:ARG:NH1	47:AD:64:TRP:CG	2.81	0.48
2:B:1011:G:OP1	18:R:77:SER:HB2	2.13	0.48
2:B:1692:U:H2'	2:B:1694:C:C5	2.48	0.48
2:B:207:A:H2'	2:B:208:C:O4'	2.12	0.48
2:B:2345:G:OP2	30:DA:38:LYS:HD3	2.14	0.48
2:B:2693:A:H2'	2:B:2694:G:C8	2.48	0.48
2:B:540:G:H2'	2:B:541:C:H6	1.79	0.48
2:B:892:G:H2'	2:B:893:C:H4'	1.94	0.48
8:H:113:ARG:HD2	28:BA:33:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:TYR:HA	5:E:87:ASN:ND2	2.29	0.48
1:FB:1085:U:H3'	1:FB:1086:U:C6	2.48	0.48
1:FB:1414:U:H3	1:FB:1486:G:H1	1.62	0.48
1:FB:149:A:H2'	1:FB:150:C:C6	2.49	0.48
1:FB:500:G:H5'	46:ZC:124:LYS:NZ	2.29	0.48
2:GB:1060:U:C5'	2:GB:1061:U:H3'	2.43	0.48
2:GB:2211:G:H2'	2:GB:2212:A:C2	2.49	0.48
2:GB:295:G:O5'	22:AC:1:MET:HG3	2.14	0.48
2:GB:969:U:H2'	2:GB:970:C:C6	2.48	0.48
9:I:56:SER:OG	9:I:58:GLU:HG2	2.14	0.48
5:JB:112:GLN:O	5:JB:115:GLN:HG2	2.13	0.48
38:MA:176:LEU:HD12	38:MA:182:LYS:O	2.13	0.48
38:MA:9:CYS:HG	38:MA:18:LYS:NZ	2.05	0.48
9:NB:12:PRO:O	9:NB:15:VAL:HG22	2.14	0.48
15:O:33:ARG:HD2	15:O:113:LEU:HD13	1.94	0.48
10:OB:31:LEU:HD11	10:OB:38:LEU:HG	1.95	0.48
35:OC:172:TYR:O	35:OC:176:LYS:HB2	2.13	0.48
37:QC:191:THR:OG1	37:QC:194:GLY:O	2.22	0.48
20:T:57:ASN:O	20:T:61:ASN:HB2	2.13	0.48
20:T:82:LEU:HD22	20:T:84:ARG:HH22	1.79	0.48
41:UC:28:ASN:OD1	41:UC:36:LYS:NZ	2.43	0.48
42:VC:51:VAL:HG21	42:VC:60:ARG:HH11	1.77	0.48
26:Z:51:ARG:O	26:Z:55:ARG:HG2	2.14	0.48
51:ZA:78:GLU:OE2	51:ZA:81:ARG:HD3	2.13	0.48
1:A:1070:U:H2'	1:A:1071:C:C6	2.48	0.48
1:A:1241:G:H2'	1:A:1242:C:C6	2.49	0.48
1:A:192:U:H2'	1:A:193:C:C6	2.49	0.48
2:B:1059:G:N3	2:B:1059:G:H2'	2.29	0.48
2:B:1085:A:H8	2:B:1085:A:OP2	1.97	0.48
49:CD:30:ALA:HA	49:CD:85:LEU:HD11	1.95	0.48
6:F:4:ILE:HD13	6:F:28:ALA:HB1	1.95	0.48
1:FB:816:A:OP2	1:FB:1527:C:H5'	2.13	0.48
1:FB:603:U:H2'	1:FB:604:G:C8	2.48	0.48
2:GB:987:G:O2'	2:GB:1000:A:N3	2.44	0.48
2:GB:1441:G:H2'	2:GB:1442:G:H8	1.79	0.48
30:IC:13:CYS:SG	30:IC:47:THR:HG21	2.54	0.48
35:JA:337:LEU:O	35:JA:341:ILE:HG23	2.13	0.48
38:MA:57:ARG:HB3	38:MA:206:PHE:HB2	1.96	0.48
41:PA:38:LEU:O	41:PA:42:ILE:HG13	2.13	0.48
42:QA:20:TYR:HE2	42:QA:75:ARG:HD2	1.78	0.48
19:S:69:LYS:HA	19:S:88:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:ALA:HB3	20:T:106:ILE:HB	1.95	0.48
40:TC:75:LEU:O	40:TC:79:LEU:HG	2.14	0.48
42:VC:101:PRO:HG3	42:VC:133:LEU:HD11	1.96	0.48
1:A:1048:G:OP1	48:WA:3:ARG:HB3	2.14	0.48
52:AB:61:LYS:O	52:AB:65:ILE:HG13	2.14	0.48
2:B:1345:C:OP2	2:B:1346:G:OP2	2.32	0.48
2:B:1585:C:H4'	2:B:1586:A:OP2	2.14	0.48
2:B:270(G):U:H2'	2:B:270(H):C:C6	2.48	0.48
2:B:374:A:C2	2:B:401:A:C4	3.02	0.48
1:A:323:U:O3'	54:CB:22:ARG:HD3	2.14	0.48
4:D:54:5MU:HN3	4:D:58:A:H62	1.60	0.48
2:GB:1289:C:H2'	2:GB:1290:C:H6	1.79	0.48
2:GB:848:G:N9	2:GB:933:A:H8	2.12	0.48
6:KB:7:VAL:HG23	6:KB:51:PHE:HE2	1.77	0.48
7:LB:107:LYS:HD2	7:LB:206:ILE:HA	1.95	0.48
9:NB:86:GLU:HG2	9:NB:132:ARG:HG3	1.95	0.48
15:O:36:THR:HG22	15:O:37:THR:H	1.78	0.48
16:P:10:ARG:HG2	16:P:13:ARG:NH2	2.29	0.48
43:RA:76:ALA:O	43:RA:80:GLY:N	2.45	0.48
1:A:1054:C:N3	34:HA:22:A:N6	2.62	0.48
2:B:1130:U:O2	6:F:149:ARG:NH2	2.47	0.48
2:B:161:U:H2'	2:B:163:U:OP2	2.14	0.48
2:B:2646:C:H2'	2:B:2647:U:O4'	2.13	0.48
2:B:271(C):G:H4'	2:B:271(D):U:H5''	1.95	0.48
2:B:576:U:H2'	2:B:577:G:C8	2.48	0.48
1:FB:1031:G:H8	1:FB:1032(B):G:H1	1.62	0.48
1:FB:1070:U:H2'	1:FB:1071:C:C6	2.48	0.48
1:FB:270:A:H2'	1:FB:271:C:C6	2.49	0.48
2:GB:125:G:H4'	2:GB:126:A:OP2	2.13	0.48
24:X:2:ALA:HB3	4:IA:76:A:H62	1.78	0.48
10:J:110:ASP:OD1	10:J:112:LYS:HE3	2.14	0.48
7:LB:95:ARG:HD3	7:LB:97:TYR:CZ	2.49	0.48
38:MA:127:THR:HG23	38:MA:147:ALA:HB3	1.95	0.48
10:OB:6:LEU:HG	10:OB:36:ALA:HA	1.96	0.48
35:OC:214:LEU:O	35:OC:216:ASP:N	2.47	0.48
11:PB:30:ILE:HG22	11:PB:34:LEU:HD22	1.96	0.48
43:RA:121:ARG:HB2	43:RA:121:ARG:HH11	1.78	0.48
43:RA:42:ARG:HB2	43:RA:42:ARG:HE	1.57	0.48
13:RB:83:VAL:HG12	13:RB:112:LEU:HD21	1.94	0.48
17:VB:129:ARG:HA	17:VB:132:LYS:HZ3	1.76	0.48
14:N:60:ARG:HA	23:W:178:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2115:G:H2'	2:B:2117:A:N7	2.29	0.48
2:B:2114:A:H2	2:B:2171:A:H61	1.62	0.48
2:B:2593:U:H2'	2:B:2594:C:C6	2.49	0.48
2:B:900:A:H2'	2:B:901:A:O4'	2.14	0.48
5:E:136:ILE:HG22	5:E:140:THR:OG1	2.14	0.48
2:B:1902:C:H5'	5:E:246:PRO:HD3	1.96	0.48
1:FB:881:G:OP2	46:ZC:12:ARG:NH2	2.47	0.48
2:GB:1058:G:N2	2:GB:1080:C:H42	2.11	0.48
2:GB:1179:C:H2'	2:GB:1180:C:C6	2.48	0.48
2:GB:1448:G:H4'	2:GB:1543:A:OP1	2.14	0.48
2:GB:1798:U:H5'	5:JB:259:THR:CG2	2.34	0.48
2:GB:2114:A:H2	2:GB:2171:A:H61	1.62	0.48
2:GB:2243:U:H2'	2:GB:2244:U:C6	2.48	0.48
2:GB:370:G:H4'	2:GB:371:A:OP2	2.14	0.48
2:GB:607:U:OP1	7:LB:102:PRO:HA	2.14	0.48
8:MB:113:ARG:HD2	28:GC:33:VAL:HG13	1.94	0.48
8:H:7:LEU:HD22	8:H:176:LEU:HD22	1.96	0.48
32:KC:54:GLU:O	32:KC:58:ILE:HG13	2.14	0.48
13:M:81:GLN:HB2	13:M:110:TYR:CD1	2.49	0.48
2:B:2875:C:O2'	17:Q:2:ASN:OD1	2.26	0.48
21:U:53:LYS:HG2	21:U:82:GLN:HB3	1.96	0.48
1:A:1031:G:H8	1:A:1032(B):G:H1	1.62	0.47
1:A:137:C:H2'	1:A:138:G:H8	1.79	0.47
2:B:1587:A:H2'	2:B:1588:C:H6	1.79	0.47
1:FB:1314:C:H2'	1:FB:1315:U:C6	2.49	0.47
1:FB:59:A:H1'	1:FB:354:G:N2	2.30	0.47
1:FB:693:G:H2'	1:FB:694:A:C8	2.48	0.47
1:FB:938:A:C6	1:FB:939:G:C5	3.02	0.47
45:YC:108:ILE:HB	52:FD:87:ARG:HB3	1.96	0.47
2:GB:492:A:H2'	2:GB:493:G:O4'	2.13	0.47
28:GC:14:ILE:HG12	28:GC:31:ILE:HG13	1.96	0.47
3:HB:16:G:N2	3:HB:69:G:H1'	2.28	0.47
9:I:60:ARG:O	9:I:64:LEU:HG	2.14	0.47
5:JB:274:ARG:HG2	5:JB:274:ARG:HH11	1.79	0.47
39:NA:31:LEU:HD23	39:NA:31:LEU:HA	1.72	0.47
10:OB:118:LYS:HE2	10:OB:121:LYS:HE3	1.95	0.47
35:OC:138:TYR:HE1	35:OC:338:ASP:OD2	1.97	0.47
43:WC:11:LYS:O	43:WC:13:ALA:N	2.35	0.47
46:ZC:53:ARG:HG3	46:ZC:93:LEU:HD21	1.96	0.47
1:A:1158:C:O2'	36:KA:133:LYS:NZ	2.47	0.47
1:A:857:C:H2'	1:A:858:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:A:N3	2:B:1112:G:H1'	2.30	0.47
2:B:2564:A:OP1	2:B:2648:C:H4'	2.14	0.47
2:B:2646:C:OP2	2:B:2732:G:O2'	2.30	0.47
23:BC:54:HIS:CG	23:BC:101:PRO:HG3	2.49	0.47
23:BC:54:HIS:ND1	23:BC:101:PRO:HG3	2.29	0.47
30:DA:14:THR:O	30:DA:17:LYS:NZ	2.48	0.47
1:FB:1132:C:H2'	1:FB:1133:G:H8	1.78	0.47
2:GB:1007:C:OP1	11:PB:35:ARG:NH1	2.48	0.47
2:GB:1516:U:H2'	2:GB:1517:G:H8	1.79	0.47
2:GB:154(A):C:H2'	2:GB:161:U:C5	2.49	0.47
2:GB:2082:A:H2'	2:GB:2083:G:O4'	2.14	0.47
2:GB:2567:G:H2'	2:GB:2568:C:C6	2.49	0.47
2:GB:2850:A:OP2	2:GB:2866:U:H5	1.97	0.47
2:GB:674:G:P	7:LB:54:ARG:HH22	2.38	0.47
2:GB:998:C:OP2	18:WB:58:ARG:NH2	2.41	0.47
8:MB:166:ASP:O	8:MB:170:ARG:N	2.40	0.47
39:NA:84:PHE:HB3	39:NA:134:ALA:HB2	1.95	0.47
10:OB:110:ASP:HB3	10:OB:113:ARG:HG2	1.96	0.47
38:RC:26:CYS:SG	38:RC:31:CYS:SG	3.12	0.47
38:RC:53:ASP:O	38:RC:57:ARG:HD2	2.13	0.47
47:VA:23:TYR:HB3	47:VA:67:GLU:HA	1.95	0.47
47:VA:29:ARG:NH1	47:VA:64:TRP:CG	2.82	0.47
42:VC:64:LYS:HG3	42:VC:79:VAL:HG21	1.95	0.47
23:W:54:HIS:ND1	23:W:101:PRO:HG3	2.29	0.47
2:B:1430:C:H2'	2:B:1431:U:C6	2.49	0.47
3:C:42:C:O2	8:H:93:THR:N	2.39	0.47
1:FB:1241:G:H2'	1:FB:1242:C:C6	2.50	0.47
1:FB:1356:G:H2'	1:FB:1357:A:H8	1.75	0.47
2:GB:1939:5MU:OP1	2:GB:2604:U:O2'	2.28	0.47
10:J:69:LYS:NZ	10:J:73:GLU:OE2	2.44	0.47
2:GB:1309:G:H4'	31:JC:7:PRO:HB2	1.96	0.47
40:OA:36:ARG:NH2	40:OA:66:GLU:OE1	2.46	0.47
10:OB:1:MET:N	10:OB:21:VAL:O	2.43	0.47
37:QC:85:ARG:HG2	37:QC:88:ARG:HH21	1.79	0.47
13:RB:135:LEU:HD13	13:RB:139:LYS:HD2	1.95	0.47
38:RC:148:VAL:HG12	38:RC:181:MET:O	2.15	0.47
15:TB:12:ARG:HD3	15:TB:16:HIS:CD2	2.48	0.47
15:TB:70:LEU:O	15:TB:72:ASP:N	2.47	0.47
23:W:54:HIS:CG	23:W:101:PRO:HG3	2.50	0.47
25:Y:95:LEU:O	25:Y:98:LEU:HB2	2.14	0.47
26:Z:37:PHE:O	26:Z:40:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:C:H42	1:A:1022:G:H1	1.63	0.47
1:A:1278:U:H5''	1:A:1279:A:O4'	2.14	0.47
1:A:939:G:H2'	1:A:940:C:C6	2.49	0.47
2:B:2163:C:H5'	2:B:2164:C:OP2	2.15	0.47
2:B:2747:G:OP1	9:I:138:LYS:NZ	2.41	0.47
24:CC:2:ALA:HB3	4:NC:76:A:H62	1.80	0.47
4:D:32:5MC:H2'	4:D:33:U:O4'	2.13	0.47
25:DC:64:ALA:HA	25:DC:67:ILE:HG13	1.97	0.47
32:FA:54:GLU:O	32:FA:58:ILE:HG13	2.13	0.47
1:FB:1070:U:H2'	1:FB:1071:C:H6	1.79	0.47
1:FB:1278:U:H5''	1:FB:1279:A:O4'	2.14	0.47
1:FB:240:C:H42	1:FB:286:G:H1	1.63	0.47
1:FB:985:C:H2'	1:FB:986:A:C8	2.48	0.47
2:GB:2869:G:H2'	2:GB:2870:C:O4'	2.14	0.47
2:GB:880:G:H1	2:GB:897:C:N4	2.12	0.47
36:KA:130:ARG:HG2	36:KA:131:PRO:HD2	1.95	0.47
36:KA:44:LEU:H	36:KA:44:LEU:HD12	1.80	0.47
13:M:135:LEU:HD13	13:M:139:LYS:HD2	1.96	0.47
38:MA:201:GLN:HE21	39:NA:99:GLY:HA2	1.78	0.47
34:MC:20:A:N6	35:OC:190:THR:OG1	2.46	0.47
9:NB:126:PRO:HB2	9:NB:127:GLU:H	1.58	0.47
9:NB:60:ARG:O	9:NB:64:LEU:HG	2.15	0.47
36:PC:7:VAL:HB	36:PC:8:LYS:HD2	1.96	0.47
2:B:2849:U:OP2	17:Q:95:ARG:NH1	2.47	0.47
43:RA:48:GLU:N	43:RA:49:PRO:HD2	2.29	0.47
13:RB:84:ASN:HB2	13:RB:86:LYS:HG2	1.96	0.47
14:SB:110:THR:OG1	14:SB:113:GLN:HB2	2.15	0.47
23:W:158:PRO:O	23:W:161:VAL:HB	2.15	0.47
1:A:1070:U:H2'	1:A:1071:C:H6	1.79	0.47
1:A:974:A:H8	1:A:974:A:OP1	1.98	0.47
2:B:1058:G:N2	2:B:1080:C:H42	2.12	0.47
2:B:1550:C:H2'	2:B:1551:C:H6	1.79	0.47
2:B:2693:A:H2'	2:B:2694:G:H8	1.79	0.47
49:CD:26:GLU:HG3	49:CD:81:LEU:HD22	1.96	0.47
4:D:68:C:H2'	4:D:69:C:H6	1.79	0.47
30:DA:6:ARG:NH1	30:DA:26:ASN:HB2	2.28	0.47
2:GB:1313:U:H2'	2:GB:1610:A:C2	2.50	0.47
2:GB:2794:C:H42	2:GB:2802:G:H1	1.61	0.47
34:HA:13:A:H2'	34:HA:14:A:H4'	1.96	0.47
38:MA:111:ALA:HB2	38:MA:120:LEU:HD12	1.96	0.47
43:RA:34:ASN:O	43:RA:38:GLN:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RC:105:VAL:HG13	38:RC:110:PHE:HB2	1.95	0.47
38:RC:21:LEU:O	38:RC:22:LYS:HB2	2.13	0.47
44:SA:49:VAL:HG23	48:WA:41:ARG:HB2	1.96	0.47
41:UC:57:GLU:H	41:UC:60:LYS:NZ	2.05	0.47
43:WC:34:ASN:O	43:WC:38:GLN:HB3	2.13	0.47
44:XC:57:LYS:HG3	44:XC:60:ARG:HH21	1.79	0.47
25:Y:11:ARG:HB2	25:Y:12:PRO:HD2	1.95	0.47
1:A:1017:G:H2'	1:A:1018:C:C6	2.50	0.47
1:A:1003:G:H1	1:A:1038:C:N4	2.12	0.47
2:B:194:G:H2'	2:B:195:A:O4'	2.13	0.47
2:B:2798:C:H5''	2:B:2799:A:OP2	2.15	0.47
48:BD:2:ALA:HA	48:BD:6:LEU:HD13	1.95	0.47
46:ZC:11:VAL:HG13	51:ED:29:HIS:CD2	2.50	0.47
2:GB:540:G:H2'	2:GB:541:C:H6	1.80	0.47
34:HA:20:A:N6	35:JA:190:THR:OG1	2.46	0.47
3:HB:112:G:H2'	3:HB:113:C:C6	2.50	0.47
9:I:97:ARG:O	9:I:97:ARG:HD3	2.14	0.47
38:MA:8:VAL:HA	38:MA:11:LEU:HD13	1.97	0.47
16:P:68:GLN:HG2	16:P:71:ARG:HH21	1.79	0.47
17:Q:100:TYR:HD1	17:Q:103:ARG:NH1	2.12	0.47
37:QC:77:ILE:HG23	37:QC:84:ILE:HD12	1.96	0.47
46:UA:7:ILE:O	46:UA:11:VAL:HG23	2.14	0.47
42:VC:121:ASP:OD1	42:VC:121:ASP:N	2.47	0.47
2:B:1165:U:H2'	2:B:1166:C:C6	2.50	0.47
2:B:1826:G:H4'	5:E:242:ARG:HH21	1.79	0.47
2:B:2695:C:H2'	2:B:2696:U:C6	2.50	0.47
2:B:2850:A:OP2	2:B:2866:U:H5	1.98	0.47
51:ED:45:HIS:HB3	51:ED:72:ARG:HG2	1.95	0.47
1:FB:1418:A:H5''	1:FB:1419:G:OP2	2.14	0.47
1:FB:509:A:N3	1:FB:543:C:O2'	2.38	0.47
2:GB:1085:A:OP2	2:GB:1085:A:H8	1.98	0.47
2:GB:2792:G:H2'	2:GB:2793:G:H8	1.78	0.47
2:GB:2889:C:H2'	2:GB:2891:G:O4'	2.14	0.47
54:HD:23:ARG:NH1	54:HD:24:LEU:HD22	2.30	0.47
5:JB:228:PRO:HD3	5:JB:235:GLY:CA	2.45	0.47
36:KA:97:TRP:CH2	36:KA:176:GLU:OE2	2.68	0.47
38:MA:18:LYS:NZ	38:MA:31:CYS:HG	2.06	0.47
9:NB:140:LYS:HE2	9:NB:140:LYS:HB3	1.68	0.47
40:OA:27:GLN:HA	40:OA:30:LEU:HD12	1.95	0.47
17:Q:129:ARG:HA	17:Q:132:LYS:HZ3	1.78	0.47
14:SB:116:GLU:OE2	14:SB:119:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SB:60:ARG:HA	23:BC:179:ASP:HA	1.96	0.47
46:UA:28:LYS:HZ3	46:UA:64:TYR:HE2	1.61	0.47
42:VC:125:ARG:NH1	42:VC:125:ARG:HG2	2.30	0.47
26:Z:46:GLN:HB2	26:Z:49:LYS:HE3	1.97	0.47
46:UA:11:VAL:HG13	51:ZA:29:HIS:HD2	1.80	0.47
27:AA:29:ARG:HB2	27:AA:29:ARG:NH1	2.30	0.47
1:FB:1017:G:H2'	1:FB:1018:C:C6	2.50	0.47
2:GB:2021:C:OP1	29:HC:12:SER:OG	2.28	0.47
2:GB:2141:G:N2	2:GB:2151:G:H1'	2.30	0.47
2:GB:309:G:N3	2:GB:329:G:O2'	2.44	0.47
3:HB:42:C:O2	8:MB:93:THR:N	2.38	0.47
36:KA:157:ARG:O	36:KA:158:LEU:HB3	2.13	0.47
7:LB:53:THR:HG23	7:LB:55:GLY:H	1.79	0.47
38:MA:196:LEU:HD12	38:MA:196:LEU:HA	1.81	0.47
9:NB:102:ALA:HA	9:NB:117:PRO:HD3	1.97	0.47
4:NC:65:C:H2'	4:NC:66:C:H6	1.80	0.47
35:OC:314:GLN:HB2	35:OC:316:ARG:HD2	1.96	0.47
35:OC:134:MET:SD	35:OC:337:LEU:HD21	2.54	0.47
13:RB:65:ARG:HG3	13:RB:66:GLY:N	2.29	0.47
1:FB:1368:G:H4'	44:XC:46:ARG:HH11	1.77	0.47
20:YB:20:VAL:O	20:YB:23:LEU:HB2	2.15	0.47
1:A:149:A:H2'	1:A:150:C:C6	2.50	0.47
1:A:561:U:HO2'	1:A:562:C:P	2.37	0.47
1:A:620:C:C2	38:MA:135:LEU:HG	2.50	0.47
1:A:639:G:H2'	1:A:640:A:H8	1.79	0.47
52:AB:70:ILE:O	52:AB:74:ARG:HG3	2.15	0.47
1:FB:1226:C:N4	47:AD:104:ARG:HD2	2.30	0.47
2:B:1520:U:H2'	2:B:1521:G:O4'	2.15	0.47
2:B:1592:C:H2'	2:B:1593:G:H8	1.78	0.47
2:B:91:A:C4	2:B:92:G:C8	3.03	0.47
1:FB:1240:U:H4'	41:UC:38:LEU:HD21	1.95	0.47
2:GB:1550:C:H2'	2:GB:1551:C:H6	1.80	0.47
2:GB:1587:A:H2'	2:GB:1588:C:H6	1.79	0.47
2:GB:1587:A:H2'	2:GB:1588:C:C6	2.50	0.47
2:GB:1639:U:H4'	2:GB:2699:C:H4'	1.97	0.47
2:GB:2031:A:C6	2:GB:2498:C:H1'	2.50	0.47
54:HD:14:LYS:O	54:HD:18:GLN:HG3	2.15	0.47
4:IB:8:4SU:H2'	4:IB:13:C:H42	1.80	0.47
13:M:63:PRO:HB2	32:FA:30:ARG:HH21	1.79	0.47
38:MA:105:VAL:HG13	38:MA:110:PHE:HB2	1.95	0.47
9:NB:13:LYS:HA	9:NB:14:GLY:HA2	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:132:LYS:HG2	17:Q:136:GLN:HE21	1.80	0.47
37:QC:19:GLU:HG2	37:QC:54:ARG:CZ	2.45	0.47
19:XB:69:LYS:HA	19:XB:88:ARG:HG2	1.96	0.47
1:A:272:C:H2'	1:A:273:A:H8	1.79	0.47
2:B:911:A:H2'	14:N:9:TYR:OH	2.15	0.47
2:B:643:A:C8	30:DA:44:ARG:NH1	2.82	0.47
50:DD:1:MET:SD	50:DD:1:MET:N	2.80	0.47
5:E:206:LEU:HD22	5:E:211:ARG:HG2	1.97	0.47
6:F:45:THR:O	6:F:82:ARG:HD2	2.15	0.47
1:FB:432:A:H3'	1:FB:433:C:C6	2.50	0.47
2:GB:2055:C:H5'	2:GB:2056:G:O5'	2.14	0.47
2:GB:455:C:N3	2:GB:472:A:H2'	2.30	0.47
4:IB:51:C:H2'	4:IB:52:G:C8	2.50	0.47
5:JB:136:ILE:HG22	5:JB:140:THR:OG1	2.15	0.47
37:LA:180:ALA:HA	37:LA:206:GLU:HA	1.97	0.47
16:P:15:ARG:NH1	16:P:88:ASP:OD2	2.47	0.47
42:QA:121:ASP:N	42:QA:121:ASP:OD1	2.48	0.47
39:SC:31:LEU:HA	39:SC:31:LEU:HD23	1.71	0.47
45:TA:34:ASP:OD1	45:TA:38:ASN:HB2	2.15	0.47
15:TB:36:THR:HG22	15:TB:37:THR:H	1.80	0.47
16:UB:10:ARG:O	16:UB:14:VAL:HG12	2.15	0.47
42:VC:92:ARG:HH11	42:VC:92:ARG:HG2	1.79	0.47
1:A:756:C:H2'	1:A:757:U:O4'	2.14	0.47
47:AD:14:ARG:HG3	47:AD:44:ARG:CZ	2.45	0.47
1:A:1460:A:P	54:CB:27:LYS:HZ2	2.37	0.47
54:CB:30:LYS:HA	54:CB:33:ILE:HG12	1.96	0.47
5:E:8:PRO:HB3	5:E:14:ARG:HB2	1.96	0.47
1:FB:1314:C:OP2	53:GD:4:SER:OG	2.28	0.47
2:GB:1405:U:H2'	2:GB:1406:U:C6	2.49	0.47
2:GB:2114:A:H2	2:GB:2171:A:N6	2.13	0.47
2:GB:2557:G:H2'	2:GB:2558:C:C6	2.50	0.47
2:GB:2646:C:OP2	2:GB:2732:G:O2'	2.31	0.47
35:JA:115:VAL:HG12	35:JA:162:ILE:HG22	1.97	0.47
36:KA:21:ARG:O	36:KA:23:ARG:N	2.47	0.47
6:KB:4:ILE:HD13	6:KB:28:ALA:HB1	1.96	0.47
6:KB:78:LEU:HA	6:KB:78:LEU:HD13	1.81	0.47
37:LA:135:LYS:HA	37:LA:138:VAL:HG12	1.97	0.47
2:B:811:U:H2'	13:M:21:ARG:HA	1.97	0.47
38:MA:18:LYS:HG3	38:MA:20:TYR:H	1.79	0.47
8:MB:114:ILE:HG22	8:MB:140:ILE:HG12	1.96	0.47
2:GB:2306:C:N4	8:MB:42:GLY:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:34:LEU:HD21	11:PB:120:LEU:HB2	1.97	0.47
42:QA:101:PRO:HG3	42:QA:133:LEU:HD11	1.96	0.47
14:SB:79:LEU:HD13	14:SB:80:GLU:HG3	1.97	0.47
45:YC:86:GLY:O	45:YC:91:ARG:NH1	2.41	0.47
1:A:191(D):U:H2'	1:A:191(E):G:C8	2.50	0.46
1:A:474:G:H5'	50:YA:81:ARG:HG2	1.97	0.46
1:A:678:U:H2'	1:A:679:C:C6	2.50	0.46
27:AA:30:ARG:HG3	27:AA:30:ARG:HH11	1.79	0.46
2:B:1923:U:H2'	2:B:1924:C:C6	2.51	0.46
23:BC:155:LEU:O	23:BC:157:LEU:HD12	2.15	0.46
1:FB:192:U:H2'	1:FB:193:C:C6	2.50	0.46
1:FB:757:U:H2'	1:FB:758:G:O4'	2.15	0.46
2:GB:1070:A:N6	2:GB:1097:U:O2'	2.47	0.46
2:GB:1400:G:H2'	2:GB:1401:G:C8	2.50	0.46
2:GB:1653:G:H5''	15:TB:2:ARG:HD3	1.96	0.46
3:HB:1:U:C6	3:HB:1:U:OP2	2.67	0.46
1:A:519:C:OP2	35:JA:304:SER:HB3	2.15	0.46
5:JB:8:PRO:HB3	5:JB:14:ARG:HB2	1.97	0.46
2:GB:2758:A:C4	9:NB:67:LEU:HD21	2.50	0.46
36:PC:177:ALA:HB1	36:PC:182:ILE:HB	1.97	0.46
42:QA:123:GLU:O	42:QA:127:LEU:HD22	2.15	0.46
16:UB:60:GLY:O	16:UB:61:ASN:HB3	2.15	0.46
2:GB:583:G:OP2	18:WB:10:ARG:HD2	2.15	0.46
44:XC:67:THR:O	44:XC:67:THR:OG1	2.32	0.46
20:YB:73:ALA:HB3	20:YB:106:ILE:HB	1.97	0.46
45:YC:121:PRO:HB2	45:YC:125:PHE:HB2	1.97	0.46
1:A:1367:C:H5'	44:SA:60:ARG:HH12	1.79	0.46
2:B:1073:A:H5''	2:B:1074:G:C8	2.51	0.46
2:B:1409:C:H2'	2:B:1410:G:C8	2.50	0.46
2:B:1790:C:H5''	2:B:1791:A:OP1	2.14	0.46
2:B:278:A:H2'	2:B:279:C:O4'	2.16	0.46
2:B:280:C:C2	2:B:361:G:N2	2.83	0.46
2:B:2622:C:O2'	2:B:2825:G:N7	2.46	0.46
44:XC:49:VAL:HG23	48:BD:41:ARG:HB2	1.96	0.46
1:FB:1511:G:H2'	1:FB:1512:U:O4'	2.15	0.46
1:FB:731:G:OP1	1:FB:766:A:H1'	2.16	0.46
7:G:110:LEU:HD21	7:G:181:LEU:HG	1.96	0.46
2:GB:1291:C:H2'	2:GB:1292:U:C6	2.49	0.46
2:GB:1317:A:H2'	2:GB:1318:C:C6	2.50	0.46
54:HD:53:LEU:O	54:HD:57:ARG:HG3	2.14	0.46
35:JA:214:LEU:O	35:JA:216:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:30:ILE:HG22	11:K:34:LEU:HD22	1.97	0.46
9:NB:126:PRO:HG2	9:NB:130:ARG:CZ	2.45	0.46
44:SA:25:GLU:N	44:SA:25:GLU:OE2	2.46	0.46
49:XA:26:GLU:HG3	49:XA:81:LEU:HD22	1.96	0.46
1:A:174:C:H2'	1:A:175:C:C6	2.51	0.46
1:A:4:U:O4	42:QA:105:ARG:HG3	2.16	0.46
1:A:958:A:N3	1:A:985:C:O2'	2.43	0.46
2:B:1060:U:C5'	2:B:1061:U:H3'	2.45	0.46
2:B:1870:C:H2'	2:B:1871:A:O4'	2.16	0.46
2:B:2394:C:N3	4:D:76:A:O2'	2.39	0.46
23:BC:69:THR:HG22	23:BC:90:VAL:HA	1.97	0.46
4:IB:75:C:H5'	25:DC:30:VAL:HG21	1.97	0.46
1:FB:397:A:H5'	1:FB:398:C:OP1	2.15	0.46
1:FB:939:G:H2'	1:FB:940:C:C6	2.50	0.46
2:GB:1441:G:H2'	2:GB:1442:G:C8	2.51	0.46
2:GB:2350:C:H2'	2:GB:2351:G:O4'	2.15	0.46
2:GB:2863:C:OP1	17:VB:93:ARG:NH1	2.48	0.46
1:FB:1460:A:P	54:HD:27:LYS:NZ	2.88	0.46
54:HD:73:HIS:ND1	54:HD:75:ASN:OD1	2.47	0.46
6:KB:24:THR:HG22	6:KB:186:GLY:O	2.15	0.46
38:MA:177:ASP:OD1	38:MA:180:GLY:HA3	2.15	0.46
44:SA:45:ARG:HG3	44:SA:47:PHE:HE2	1.79	0.46
39:SC:147:ASP:OD2	39:SC:150:ARG:NH2	2.48	0.46
42:VC:87:SER:HA	42:VC:93:VAL:HG23	1.98	0.46
21:ZB:53:LYS:HG2	21:ZB:82:GLN:HB3	1.97	0.46
1:A:1277:C:H1'	1:A:1282:C:H1'	1.97	0.46
1:A:1452:C:O5'	1:A:1452:C:H6	1.98	0.46
1:A:272:C:H2'	1:A:273:A:C8	2.50	0.46
2:B:1313:U:H2'	2:B:1610:A:C2	2.50	0.46
2:B:1511:A:C8	2:B:1512:G:C8	3.02	0.46
2:B:270(A):A:H1'	2:B:370:G:C2	2.51	0.46
54:CB:53:LEU:O	54:CB:57:ARG:HG3	2.15	0.46
1:FB:1320:C:H2'	1:FB:1321:C:O4'	2.15	0.46
1:FB:1427:U:H2'	1:FB:1428:A:C8	2.50	0.46
7:G:107:LYS:HZ1	7:G:207:GLY:H	1.62	0.46
2:GB:1568:G:P	5:JB:63:ARG:HH22	2.38	0.46
2:GB:270(W):G:H2'	2:GB:270(X):G:H8	1.80	0.46
4:IA:23:C:H2'	4:IA:24:U:C6	2.50	0.46
4:IB:32:5MC:H2'	4:IB:33:U:O4'	2.15	0.46
35:JA:196:ILE:HD13	35:JA:313:PRO:HG2	1.96	0.46
5:JB:147:LEU:HD13	5:JB:155:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:72:TYR:HE2	11:K:87:LEU:HG	1.81	0.46
7:LB:53:THR:HG22	7:LB:56:GLU:HG3	1.98	0.46
13:M:86:LYS:HB3	13:M:118:GLY:HA3	1.98	0.46
34:MC:14:A:H3'	34:MC:15:A:H8	1.79	0.46
39:NA:107:ARG:HG3	39:NA:107:ARG:HH11	1.80	0.46
35:OC:156:HIS:HA	35:OC:157:GLY:HA2	1.73	0.46
42:QA:51:VAL:HG21	42:QA:60:ARG:NH1	2.30	0.46
37:QC:33:LEU:HA	37:QC:36:ASP:HB2	1.97	0.46
37:QC:35:GLU:O	37:QC:39:ILE:HG13	2.15	0.46
43:RA:127:LYS:HB3	43:RA:127:LYS:NZ	2.30	0.46
38:RC:8:VAL:HA	38:RC:11:LEU:HD13	1.98	0.46
39:SC:152:ARG:HB3	42:VC:43:GLY:HA3	1.97	0.46
46:UA:83:VAL:HG23	46:UA:107:ALA:HB2	1.96	0.46
24:X:65:GLY:HA2	24:X:84:LEU:HG	1.98	0.46
1:A:1513:A:H2'	1:A:1514:C:C6	2.50	0.46
1:A:8:A:N6	38:MA:209:ARG:HB2	2.30	0.46
2:B:2126:A:O3'	2:B:2127:G:H8	1.98	0.46
51:ED:95:TYR:HA	51:ED:98:LEU:HD12	1.97	0.46
1:FB:1314:C:H2'	1:FB:1315:U:H6	1.80	0.46
1:FB:45:U:H2'	1:FB:46:G:C8	2.50	0.46
1:FB:756:C:H2'	1:FB:757:U:O4'	2.16	0.46
1:FB:857:C:H2'	1:FB:858:G:O4'	2.14	0.46
40:TC:91:VAL:HG11	52:FD:72:ARG:NH1	2.31	0.46
2:GB:1213:A:N3	2:GB:1238:G:O2'	2.42	0.46
2:GB:1536:A:H5''	2:GB:1537:C:C5	2.51	0.46
2:GB:2163:C:H5'	2:GB:2164:C:OP2	2.15	0.46
2:GB:2646:C:H2'	2:GB:2647:U:O4'	2.15	0.46
4:IB:68:C:H2'	4:IB:69:C:H6	1.80	0.46
2:GB:601:C:OP1	7:LB:108:LYS:HE3	2.16	0.46
14:N:110:THR:OG1	14:N:113:GLN:HB2	2.15	0.46
15:O:72:ASP:HB3	15:O:75:LEU:HB3	1.98	0.46
42:QA:125:ARG:NH1	42:QA:125:ARG:HG2	2.31	0.46
38:RC:196:LEU:HA	38:RC:197:PRO:HD3	1.81	0.46
16:UB:10:ARG:HG2	16:UB:13:ARG:NH2	2.31	0.46
47:VA:50:GLU:HA	47:VA:53:VAL:HB	1.98	0.46
2:GB:2684:U:OP1	17:VB:53:ARG:HD3	2.15	0.46
1:A:1427:U:H2'	1:A:1428:A:C8	2.50	0.46
1:A:953:G:N7	47:VA:104:ARG:NH2	2.59	0.46
27:AA:23:LEU:HD13	27:AA:50:VAL:HG11	1.98	0.46
27:AA:7:LYS:HB2	27:AA:34:GLU:HG2	1.97	0.46
47:AD:70:LEU:O	47:AD:74:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1364:G:C8	25:Y:3:LYS:HD2	2.50	0.46
2:B:1490:A:H8	2:B:1490:A:O5'	1.99	0.46
2:B:1587:A:H2'	2:B:1588:C:C6	2.50	0.46
1:A:1418:A:H2	2:B:1948:G:N3	2.13	0.46
2:B:2275:C:O2	14:N:85:LYS:HG3	2.15	0.46
3:C:86:G:H1	3:C:90:C:H42	1.64	0.46
54:CB:30:LYS:NZ	54:CB:30:LYS:CB	2.78	0.46
24:CC:56:ASP:O	24:CC:57:PHE:HB2	2.16	0.46
25:DC:11:ARG:HB2	25:DC:12:PRO:HD2	1.98	0.46
1:FB:397:A:H3'	1:FB:397:A:N3	2.30	0.46
7:G:107:LYS:HD2	7:G:206:ILE:HA	1.98	0.46
2:GB:1057:A:H5''	2:GB:1086:A:H2	1.81	0.46
2:GB:1176:G:H3'	2:GB:1177:A:C8	2.51	0.46
2:GB:195:A:H61	2:GB:198:C:H3'	1.81	0.46
2:GB:2065:C:H2'	2:GB:2066:C:C6	2.50	0.46
4:IB:31:G:H1	4:IB:39:C:N4	2.13	0.46
5:JB:17:THR:O	5:JB:211:ARG:NH2	2.43	0.46
40:OA:46:ARG:HB2	40:OA:60:PHE:HE1	1.79	0.46
40:OA:78:GLU:O	40:OA:81:ILE:HG22	2.16	0.46
11:PB:72:TYR:HE2	11:PB:87:LEU:HG	1.81	0.46
42:QA:38:ILE:HD13	42:QA:120:THR:HG22	1.98	0.46
38:RC:127:THR:HG23	38:RC:147:ALA:HB3	1.96	0.46
40:TC:22:GLU:OE2	40:TC:84:ASN:HB2	2.16	0.46
41:UC:79:ARG:HD2	41:UC:80:VAL:N	2.30	0.46
6:KB:181:LEU:HD21	17:VB:6:LEU:HD12	1.97	0.46
48:WA:4:LYS:O	48:WA:7:ILE:HG22	2.16	0.46
1:A:1095:U:H2'	1:A:1096:C:C6	2.50	0.46
2:B:1187:G:O5'	2:B:1187:G:H8	1.98	0.46
2:B:1367:A:N7	2:B:1368:G:H1'	2.31	0.46
2:B:1532:C:H42	2:B:1539:G:H22	1.62	0.46
2:B:2114:A:H2	2:B:2171:A:N6	2.14	0.46
2:B:2889:C:H2'	2:B:2891:G:O4'	2.16	0.46
44:XC:51:ARG:O	48:BD:45:ARG:NH1	2.48	0.46
4:D:31:G:H1	4:D:39:C:N4	2.12	0.46
5:E:228:PRO:HD3	5:E:235:GLY:CA	2.46	0.46
6:F:119:ARG:HG2	6:F:120:TRP:NE1	2.30	0.46
1:FB:639:G:H2'	1:FB:640:A:H8	1.80	0.46
7:G:53:THR:CG2	7:G:55:GLY:H	2.28	0.46
2:B:674:G:O2'	7:G:74:ARG:HD3	2.16	0.46
2:GB:1520:U:H2'	2:GB:1521:G:O4'	2.15	0.46
2:GB:2660:A:H2'	2:GB:2661:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:247:G:H4'	2:GB:386:G:C5	2.51	0.46
8:H:177:GLY:O	8:H:179:PRO:HD3	2.16	0.46
4:IB:23:C:H2'	4:IB:24:U:C6	2.50	0.46
6:KB:116:VAL:HG13	6:KB:122:PHE:HB2	1.97	0.46
38:MA:21:LEU:O	38:MA:22:LYS:HB2	2.15	0.46
45:TA:99:GLN:HE21	52:AB:88:LYS:HZ1	1.64	0.46
41:UC:38:LEU:O	41:UC:42:ILE:HG13	2.15	0.46
50:YA:45:THR:O	50:YA:48:TRP:HD1	1.99	0.46
1:A:1201:A:H1'	1:A:1202:G:OP2	2.16	0.46
1:A:620:C:H2'	1:A:621:A:O4'	2.16	0.46
1:A:790:A:C6	1:A:791:G:C6	3.04	0.46
2:B:1021:A:H8	2:B:1021:A:H3'	1.81	0.46
2:B:235:U:H2'	2:B:236:C:C6	2.51	0.46
2:B:742:G:H2'	2:B:743:G:C8	2.51	0.46
26:EC:51:ARG:O	26:EC:55:ARG:HG2	2.16	0.46
1:FB:81:G:H2'	1:FB:82:U:C6	2.51	0.46
27:FC:30:ARG:HG3	27:FC:30:ARG:HH11	1.81	0.46
2:GB:1153:C:OP1	18:WB:92:ARG:NH2	2.47	0.46
10:J:7:GLU:HG3	10:J:8:PRO:HD2	1.98	0.46
10:J:83:ALA:HA	10:J:88:ILE:CG2	2.46	0.46
37:LA:92:ALA:HB2	37:LA:99:VAL:HG22	1.98	0.46
10:OB:130:TYR:CE2	10:OB:132:PRO:HB3	2.51	0.46
36:PC:10:LEU:HA	36:PC:12:GLU:HG3	1.98	0.46
38:RC:192:GLU:CD	38:RC:192:GLU:H	2.19	0.46
44:SA:57:LYS:HG3	44:SA:60:ARG:HH21	1.80	0.46
40:TC:80:ARG:HE	40:TC:88:VAL:HB	1.81	0.46
41:UC:23:VAL:HG13	41:UC:43:PHE:CE2	2.49	0.46
42:VC:51:VAL:HG21	42:VC:60:ARG:NH1	2.30	0.46
19:XB:2:PHE:CZ	19:XB:41:GLY:HA3	2.50	0.46
44:XC:24:VAL:HG13	44:XC:34:VAL:HG11	1.97	0.46
1:A:376:G:H5''	50:YA:5:ARG:HD2	1.97	0.46
21:ZB:61:GLY:HA3	21:ZB:73:ARG:O	2.16	0.46
1:A:1465:C:H2'	1:A:1466:C:O4'	2.16	0.46
1:A:382:A:H2'	1:A:383:A:H8	1.81	0.46
47:AD:3:ARG:NH1	47:AD:3:ARG:CG	2.73	0.46
2:B:263:C:H2'	2:B:264:C:O4'	2.15	0.46
2:B:857:C:N4	2:B:858:U:O4	2.49	0.46
54:CB:14:LYS:O	54:CB:18:GLN:HG3	2.16	0.46
54:CB:30:LYS:HZ1	54:CB:30:LYS:HB2	1.81	0.46
1:FB:1032(B):G:H2'	1:FB:1032(C):G:O4'	2.16	0.46
1:FB:444:C:H2'	1:FB:445:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:474:G:H5'	50:DD:81:ARG:HG2	1.96	0.46
27:FC:29:ARG:NH1	27:FC:29:ARG:HB2	2.31	0.46
7:G:195:ASP:HB3	7:G:198:ALA:H	1.81	0.46
54:HD:30:LYS:NZ	54:HD:30:LYS:CB	2.78	0.46
4:IA:66:C:H2'	4:IA:67:C:C6	2.51	0.46
2:GB:2312:U:H5'	8:MB:88:ILE:HD11	1.98	0.46
14:N:79:LEU:HD13	14:N:80:GLU:HG3	1.98	0.46
1:A:1350:A:O2'	41:PA:33:ASP:OD1	2.28	0.46
17:Q:54:ARG:HA	17:Q:59:THR:OG1	2.16	0.46
13:RB:86:LYS:HB3	13:RB:118:GLY:HA3	1.98	0.46
38:RC:28:SER:HB2	38:RC:29:PRO:HD2	1.97	0.46
22:V:51:VAL:HA	22:V:55:TYR:O	2.16	0.46
23:W:79:ARG:HB3	23:W:80:ARG:HD3	1.97	0.46
43:WC:48:GLU:N	43:WC:49:PRO:HD2	2.31	0.46
1:A:1032(B):G:H2'	1:A:1032(C):G:O4'	2.16	0.46
1:A:1314:C:H2'	1:A:1315:U:C6	2.51	0.46
1:A:1372:U:H2'	1:A:1373:G:O4'	2.16	0.46
2:B:550:G:O2'	2:B:1220:A:N3	2.39	0.46
2:B:2764:A:N7	2:B:2766:G:C6	2.84	0.46
28:BA:34:GLU:HB2	28:BA:35:VAL:H	1.53	0.46
48:BD:4:LYS:O	48:BD:7:ILE:HG22	2.16	0.46
54:CB:23:ARG:NH1	54:CB:24:LEU:HD22	2.31	0.46
30:DA:2:ALA:HB1	30:DA:6:ARG:O	2.16	0.46
1:FB:1452:C:O5'	1:FB:1452:C:H6	1.99	0.46
1:FB:382:A:H2'	1:FB:383:A:H8	1.81	0.46
27:FC:23:LEU:HD13	27:FC:50:VAL:HG11	1.99	0.46
2:GB:2649:U:H2'	2:GB:2650:U:C6	2.51	0.46
2:GB:2693:A:H2'	2:GB:2694:G:C8	2.51	0.46
2:GB:747:U:O2	2:GB:2014:A:H1'	2.16	0.46
2:GB:862:G:H2'	2:GB:863:A:O4'	2.16	0.46
36:KA:178:ARG:HD2	36:KA:196:LEU:O	2.16	0.46
36:KA:10:LEU:HG	36:KA:48:MET:SD	2.56	0.46
12:L:25:LEU:HA	12:L:25:LEU:HD23	1.70	0.46
7:LB:140:LEU:HA	7:LB:140:LEU:HD12	1.65	0.46
40:OA:75:LEU:O	40:OA:79:LEU:HG	2.16	0.46
10:OB:88:ILE:HD12	10:OB:89:TYR:H	1.80	0.46
11:PB:27:ALA:HB1	11:PB:103:VAL:HG22	1.97	0.46
12:QB:2:ILE:HD12	12:QB:6:THR:HG21	1.97	0.46
37:QC:33:LEU:HD21	48:BD:53:LEU:HD22	1.98	0.46
18:R:113:ALA:O	18:R:117:GLN:HG2	2.16	0.46
38:RC:177:ASP:OD2	38:RC:182:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:169:GLU:OE2	23:W:169:GLU:HA	2.16	0.46
43:WC:50:LEU:HD12	43:WC:56:LEU:HD12	1.97	0.46
51:ZA:43:LEU:HA	51:ZA:43:LEU:HD23	1.62	0.46
1:A:1097:C:H2'	1:A:1098:C:C6	2.51	0.45
1:A:816:A:OP2	1:A:1527:C:H5'	2.16	0.45
27:AA:10:LYS:HB3	27:AA:53:LEU:HA	1.98	0.45
2:B:1988:C:H2'	2:B:1989:G:O4'	2.16	0.45
2:B:270(W):G:H2'	2:B:270(X):G:H8	1.81	0.45
2:B:929:G:O5'	2:B:929:G:H8	1.99	0.45
2:B:974(B):C:H4'	2:B:974(B):C:OP2	2.16	0.45
28:BA:14:ILE:HG12	28:BA:31:ILE:HG13	1.97	0.45
4:D:8:4SU:H2'	4:D:13:C:H42	1.82	0.45
31:EA:5:TRP:NE1	31:EA:7:PRO:HG3	2.31	0.45
1:FB:1007:C:H42	1:FB:1022:G:H1	1.63	0.45
2:GB:1297:C:H2'	2:GB:1298:C:H6	1.82	0.45
2:GB:1478:G:O2'	2:GB:1558:A:C2	2.69	0.45
2:GB:1814:G:H4'	5:JB:51:VAL:HG21	1.98	0.45
2:GB:1988:C:H2'	2:GB:1989:G:O4'	2.16	0.45
2:GB:2798:C:H5''	2:GB:2799:A:OP2	2.16	0.45
2:GB:686:G:H21	2:GB:788:A:H61	1.62	0.45
2:GB:871:U:H2'	2:GB:872:A:C8	2.51	0.45
9:I:144:VAL:O	9:I:148:ILE:HG12	2.16	0.45
9:I:52:VAL:O	9:I:65:HIS:NE2	2.49	0.45
37:LA:85:ARG:HG2	37:LA:88:ARG:HH21	1.79	0.45
7:LB:129:PHE:HB2	7:LB:132:VAL:HG21	1.97	0.45
38:MA:177:ASP:OD2	38:MA:182:LYS:HG3	2.17	0.45
14:N:60:ARG:HA	23:W:179:ASP:HA	1.97	0.45
2:GB:2094:G:H5'	10:OB:25:TYR:CD1	2.51	0.45
10:OB:83:ALA:HA	10:OB:88:ILE:CG2	2.46	0.45
35:OC:115:VAL:HG12	35:OC:162:ILE:HG22	1.98	0.45
24:CC:2:ALA:N	35:OC:261:ARG:HD3	2.31	0.45
13:RB:77:ARG:HH11	13:RB:77:ARG:HB2	1.80	0.45
22:V:68:HIS:ND1	22:V:70:SER:HB3	2.31	0.45
1:A:1305:G:N2	1:A:1331:G:H1'	2.32	0.45
1:A:1312:G:N2	1:A:1325:C:O2	2.49	0.45
1:A:749:C:H2'	1:A:750:G:H8	1.81	0.45
2:B:1057:A:H5''	2:B:1086:A:H2	1.80	0.45
2:B:455:C:N3	2:B:472:A:H2'	2.31	0.45
4:D:68:C:H2'	4:D:69:C:C6	2.51	0.45
25:DC:14:VAL:HG11	25:DC:39:LYS:HZ2	1.81	0.45
1:FB:1053:G:N7	1:FB:1200:C:H5'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:1223:C:P	53:GD:78:ARG:HH21	2.40	0.45
2:GB:2304:G:H22	2:GB:2312:U:H3	1.61	0.45
2:GB:606:U:H4'	2:GB:658:C:H4'	1.98	0.45
2:GB:776:G:H4'	2:GB:777:A:O5'	2.16	0.45
28:GC:15:ILE:HG12	28:GC:21:VAL:HG22	1.98	0.45
5:JB:121:PRO:HB3	5:JB:135:PHE:CE2	2.52	0.45
40:TC:22:GLU:OE1	40:TC:82:ARG:NH2	2.48	0.45
1:A:1005:A:H2	1:A:1024:G:H21	1.63	0.45
1:A:500:G:H5'	46:UA:124:LYS:HZ2	1.82	0.45
1:A:819:A:H4'	1:A:820:U:OP2	2.16	0.45
2:B:1441:G:H2'	2:B:1442:G:C8	2.52	0.45
2:B:1441:G:H2'	2:B:1442:G:H8	1.81	0.45
2:B:17:G:H2'	2:B:18:C:C6	2.51	0.45
2:B:443:A:N7	7:G:45:ARG:HG2	2.32	0.45
28:BA:15:ILE:HG12	28:BA:21:VAL:HG13	1.99	0.45
3:C:112:G:H2'	3:C:113:C:C6	2.51	0.45
25:DC:2:SER:HB3	25:DC:46:LEU:HD12	1.97	0.45
1:FB:1312:G:N2	1:FB:1325:C:O2	2.49	0.45
1:FB:931:C:H42	1:FB:1386:G:H1	1.65	0.45
1:FB:620:C:H2'	1:FB:621:A:O4'	2.16	0.45
1:FB:997:U:H2'	1:FB:998(A):G:O4'	2.17	0.45
2:GB:2345:G:OP2	30:IC:38:LYS:HD3	2.17	0.45
2:GB:547:A:C3'	2:GB:548:A:C8	2.97	0.45
2:GB:879:G:H22	2:GB:899:A:H1'	1.81	0.45
10:J:8:PRO:HG3	10:J:15:VAL:HG12	1.98	0.45
35:JA:134:MET:SD	35:JA:337:LEU:HD21	2.56	0.45
31:JC:34:ARG:HH11	31:JC:34:ARG:CG	2.27	0.45
12:L:34:THR:OG1	12:L:35:VAL:N	2.46	0.45
40:OA:50:TYR:CE2	52:AB:77:GLY:HA2	2.51	0.45
10:OB:54:GLN:HA	10:OB:57:ARG:HH11	1.81	0.45
2:B:2319:G:O6	16:P:4:LEU:HD12	2.15	0.45
41:PA:79:ARG:HD2	41:PA:80:VAL:N	2.32	0.45
36:PC:178:ARG:HD2	36:PC:196:LEU:O	2.17	0.45
17:Q:132:LYS:NZ	17:Q:132:LYS:HB2	2.31	0.45
2:B:1754:C:P	17:Q:96:ARG:NH1	2.90	0.45
39:SC:107:ARG:HG3	39:SC:107:ARG:HH11	1.81	0.45
44:SA:65:LEU:HB2	48:WA:56:VAL:HG13	1.99	0.45
43:WC:108:VAL:HG12	43:WC:109:VAL:H	1.81	0.45
20:YB:65:LEU:HD12	20:YB:66:GLU:H	1.81	0.45
51:ZA:14:LYS:H	51:ZA:14:LYS:HE3	1.80	0.45
1:A:270:A:H2'	1:A:271:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:A:H1'	1:A:354:G:N2	2.32	0.45
47:AD:66:LEU:HA	47:AD:70:LEU:HD12	1.97	0.45
2:B:1007:C:OP1	11:K:35:ARG:NH1	2.50	0.45
2:B:1317:A:H2'	2:B:1318:C:C6	2.52	0.45
2:B:1639:U:H4'	2:B:2699:C:H4'	1.98	0.45
2:B:2649:U:H2'	2:B:2650:U:C6	2.51	0.45
2:B:320:A:H4'	2:B:322:A:N7	2.32	0.45
1:FB:1097:C:H2'	1:FB:1098:C:C6	2.52	0.45
7:G:64:ILE:H	7:G:64:ILE:HG13	1.46	0.45
2:GB:2064:C:H2'	2:GB:2065:C:C6	2.51	0.45
2:GB:270(A):A:H1'	2:GB:370:G:C2	2.52	0.45
9:I:3:ARG:NH2	9:I:5:GLY:H	2.13	0.45
36:KA:163:PHE:HD2	36:KA:163:PHE:HA	1.64	0.45
14:N:2:LEU:O	14:N:3:MET:HB3	2.16	0.45
16:P:10:ARG:O	16:P:14:VAL:HG12	2.17	0.45
41:PA:23:VAL:HG13	41:PA:43:PHE:CE2	2.52	0.45
36:PC:12:GLU:HA	36:PC:15:VAL:HG22	1.98	0.45
20:T:65:LEU:HD12	20:T:66:GLU:N	2.32	0.45
1:A:1492:A:H5'	46:UA:47:LYS:HD2	1.99	0.45
16:UB:68:GLN:HG2	16:UB:71:ARG:HH21	1.82	0.45
42:VC:38:ILE:HD13	42:VC:120:THR:HG22	1.98	0.45
20:YB:82:LEU:HD22	20:YB:84:ARG:HH22	1.82	0.45
1:A:555:C:H2'	1:A:556:C:C6	2.51	0.45
2:B:2869:G:H2'	2:B:2870:C:O4'	2.17	0.45
2:B:306:U:H2'	2:B:307:G:O4'	2.16	0.45
2:B:547:A:O5'	2:B:547:A:H8	1.99	0.45
2:B:648:G:H21	32:FA:46:ARG:NH1	2.07	0.45
2:B:725:G:C6	2:B:726:G:N1	2.85	0.45
53:BB:29:ARG:HA	53:BB:29:ARG:NH1	2.32	0.45
54:CB:23:ARG:HH11	54:CB:24:LEU:HD22	1.80	0.45
51:ED:78:GLU:OE2	51:ED:81:ARG:HD3	2.17	0.45
1:FB:174:C:H2'	1:FB:175:C:C6	2.52	0.45
2:GB:1999:C:H4'	2:GB:2723:C:O2	2.17	0.45
2:GB:742:G:H2'	2:GB:743:G:C8	2.50	0.45
54:HD:23:ARG:HH11	54:HD:24:LEU:HD22	1.81	0.45
9:I:126:PRO:HG2	9:I:130:ARG:CZ	2.46	0.45
8:MB:135:LEU:HD12	8:MB:136:ARG:HH21	1.81	0.45
41:PA:116:ALA:HA	41:PA:119:ARG:NH1	2.32	0.45
36:PC:97:TRP:CH2	36:PC:176:GLU:OE2	2.69	0.45
36:PC:19:HIS:NE2	36:PC:206:ASP:HB2	2.32	0.45
38:RC:18:LYS:HG3	38:RC:20:TYR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RC:4:TYR:HD2	38:RC:4:TYR:HA	1.70	0.45
25:Y:64:ALA:HA	25:Y:67:ILE:HG13	1.98	0.45
2:B:2208:U:H4'	5:E:151:LYS:HG2	1.97	0.45
2:B:2749:A:OP1	9:I:3:ARG:NH1	2.30	0.45
28:BA:15:ILE:HG12	28:BA:21:VAL:HG22	1.98	0.45
1:FB:1435:G:H2'	1:FB:1436:U:C6	2.51	0.45
1:FB:877:C:OP1	42:VC:88:LYS:NZ	2.41	0.45
2:GB:1056:G:H1'	2:GB:1103:A:N6	2.31	0.45
2:GB:1511:A:C8	2:GB:1512:G:C8	3.05	0.45
2:GB:330:A:H2	2:GB:1210:A:C2'	2.29	0.45
28:GC:15:ILE:HG12	28:GC:21:VAL:HG13	1.98	0.45
10:J:43:ASN:N	10:J:43:ASN:OD1	2.50	0.45
5:JB:169:GLU:OE2	5:JB:184:LYS:HE2	2.17	0.45
36:KA:10:LEU:HA	36:KA:12:GLU:HG3	1.97	0.45
8:MB:98:ARG:CG	8:MB:98:ARG:NH1	2.67	0.45
39:NA:144:THR:O	39:NA:148:VAL:HG23	2.17	0.45
4:NC:66:C:H2'	4:NC:67:C:C6	2.52	0.45
40:OA:22:GLU:OE2	40:OA:84:ASN:HB2	2.16	0.45
40:OA:40:VAL:HG22	40:OA:63:TYR:CD1	2.51	0.45
10:OB:64:GLU:HG3	10:OB:67:ARG:NH1	2.32	0.45
17:Q:91:ARG:HG2	17:Q:91:ARG:NH1	2.27	0.45
42:QA:37:ARG:O	42:QA:41:ARG:HG2	2.17	0.45
2:B:489:G:N7	20:T:49:LYS:NZ	2.65	0.45
15:TB:79:LEU:HA	15:TB:83:ILE:HD12	1.98	0.45
46:UA:53:ARG:HG3	46:UA:93:LEU:HD21	1.99	0.45
22:V:9:LYS:HA	22:V:10:GLY:HA2	1.58	0.45
17:VB:26:ASP:OD1	17:VB:120:ARG:NH2	2.46	0.45
1:FB:4:U:O4	42:VC:105:ARG:HG3	2.17	0.45
46:UA:11:VAL:HG13	51:ZA:29:HIS:CD2	2.52	0.45
1:A:229:U:H2'	1:A:230:G:O4'	2.17	0.45
1:A:432:A:H3'	1:A:433:C:C6	2.52	0.45
2:B:1448:G:H4'	2:B:1543:A:OP1	2.16	0.45
2:B:579:G:H2'	2:B:580:C:C6	2.52	0.45
23:BC:108:PRO:HG3	23:BC:141:VAL:HG22	1.98	0.45
49:CD:54:ARG:O	49:CD:58:MET:HG3	2.17	0.45
5:E:169:GLU:OE2	5:E:184:LYS:HE2	2.17	0.45
6:F:8:LYS:NZ	6:F:188:VAL:O	2.46	0.45
1:FB:1095:U:H2'	1:FB:1096:C:C6	2.51	0.45
1:FB:1277:C:H1'	1:FB:1282:C:H1'	1.98	0.45
2:GB:1009:A:OP2	11:PB:37:LYS:NZ	2.50	0.45
2:GB:1073:A:H5''	2:GB:1074:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1448:G:H5''	2:GB:1543:A:OP2	2.17	0.45
2:GB:2126:A:O3'	2:GB:2127:G:H8	1.98	0.45
2:GB:2334:G:O6	24:CC:74:ARG:NH2	2.49	0.45
13:M:80:TYR:CD1	13:M:111:ARG:HB2	2.52	0.45
8:MB:16:ARG:HB2	8:MB:17:PRO:HD3	1.99	0.45
8:MB:7:LEU:HD22	8:MB:176:LEU:HD22	1.98	0.45
14:N:1:MET:SD	14:N:45:GLN:NE2	2.90	0.45
10:OB:8:PRO:HG3	10:OB:15:VAL:HG12	1.99	0.45
41:PA:107:ALA:HA	41:PA:110:GLN:HG2	1.99	0.45
36:PC:70:PHE:CE1	36:PC:163:PHE:HD1	2.34	0.45
48:WA:21:TYR:CE1	48:WA:23:ARG:NH1	2.83	0.45
43:WC:76:ALA:O	43:WC:80:GLY:N	2.47	0.45
1:A:339:C:H2'	1:A:340:U:H6	1.82	0.45
1:A:563:A:N7	1:A:567:G:H1'	2.31	0.45
2:B:1899:G:H2'	2:B:1899:G:N3	2.32	0.45
2:B:607:U:OP1	7:G:102:PRO:HA	2.17	0.45
2:B:606:U:H4'	2:B:658:C:H4'	1.99	0.45
1:FB:819:A:H4'	1:FB:820:U:OP2	2.16	0.45
11:K:34:LEU:HD21	11:K:120:LEU:HB2	1.99	0.45
7:LB:129:PHE:HB2	7:LB:132:VAL:CG2	2.47	0.45
10:OB:29:TYR:CE1	10:OB:33:ARG:NH1	2.84	0.45
36:PC:127:ILE:HG23	36:PC:135:GLN:HB2	1.99	0.45
43:RA:7:THR:HB	43:RA:83:ARG:HH21	1.81	0.45
2:GB:252:G:P	13:RB:50:ARG:HH12	2.39	0.45
1:FB:429:U:OP1	38:RC:13:ARG:NH1	2.49	0.45
20:T:71:VAL:HA	20:T:107:LEU:HD12	1.99	0.45
45:TA:87:THR:HA	45:TA:91:ARG:HD2	1.99	0.45
47:VA:66:LEU:HA	47:VA:70:LEU:HD12	1.97	0.45
43:WC:127:LYS:NZ	43:WC:127:LYS:HB3	2.32	0.45
21:ZB:60:ARG:NH1	31:JC:47:ARG:NH2	2.59	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.45
2:B:1176:G:H3'	2:B:1177:A:C8	2.52	0.45
2:B:1478:G:O2'	2:B:1558:A:C2	2.70	0.45
2:B:1897:G:H2'	2:B:1898:U:O4'	2.17	0.45
2:B:2895:U:O5'	2:B:2895:U:H6	1.99	0.45
1:FB:1005:A:H2	1:FB:1024:G:H21	1.65	0.45
1:FB:624:C:H2'	1:FB:625:G:C8	2.52	0.45
7:G:108:LYS:O	7:G:112:MET:HB2	2.16	0.45
7:G:65:TRP:HB2	7:G:66:PRO:HD2	1.98	0.45
2:GB:1176:G:H8	2:GB:1177:A:C8	2.35	0.45
2:GB:637:A:OP1	13:RB:133:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2615:U:C2	29:HC:7:PRO:HA	2.52	0.45
30:IC:9:LEU:HA	30:IC:54:ILE:HB	1.98	0.45
35:JA:108:GLU:HB2	35:JA:170:GLY:HA2	1.99	0.45
5:JB:25:THR:HG21	5:JB:113:VAL:HG21	1.99	0.45
38:MA:98:GLU:OE1	38:MA:107:ARG:NH2	2.49	0.45
36:PC:229:VAL:HB	36:PC:231:GLU:OE2	2.17	0.45
37:QC:130:VAL:HG21	37:QC:157:ILE:HG23	1.99	0.45
44:SA:67:THR:O	44:SA:67:THR:OG1	2.34	0.45
17:VB:132:LYS:HG2	17:VB:136:GLN:HE21	1.81	0.45
42:VC:100:ILE:O	42:VC:125:ARG:NH2	2.50	0.45
23:W:108:PRO:HG3	23:W:141:VAL:HG22	1.98	0.45
46:ZC:59:ARG:HD3	46:ZC:65:GLU:HG2	1.98	0.45
1:A:1273:G:H2'	1:A:1274:G:O4'	2.17	0.45
1:A:162:A:C5	1:A:163:C:H1'	2.52	0.45
1:A:325:A:H2'	1:A:326:G:O4'	2.17	0.45
1:A:985:C:H2'	1:A:986:A:C8	2.52	0.45
2:B:1056:G:H1'	2:B:1103:A:N6	2.32	0.45
2:B:1173:G:O2'	2:B:1177:A:N6	2.50	0.45
2:B:1289:C:H2'	2:B:1290:C:H6	1.82	0.45
2:B:1783:A:H5'	2:B:2608:G:H4'	1.99	0.45
2:B:2660:A:H2'	2:B:2661:G:O4'	2.16	0.45
54:CB:89:ARG:O	54:CB:93:GLU:HG2	2.17	0.45
32:FA:28:GLY:O	32:FA:36:LYS:NZ	2.49	0.45
2:GB:2133:G:HO2'	2:GB:2157:G:N2	2.14	0.45
2:GB:2805:G:N2	2:GB:2807:G:O6	2.50	0.45
8:H:98:ARG:HG3	8:H:98:ARG:NH1	2.06	0.45
54:HD:66:ALA:HB3	54:HD:72:LEU:HD12	1.99	0.45
54:HD:89:ARG:O	54:HD:93:GLU:HG2	2.17	0.45
9:I:13:LYS:HA	9:I:14:GLY:HA2	1.62	0.45
35:JA:165:LYS:NZ	35:JA:208:GLU:HG3	2.31	0.45
37:LA:19:GLU:HG2	37:LA:54:ARG:CZ	2.46	0.45
7:LB:110:LEU:HD21	7:LB:181:LEU:HG	1.99	0.45
13:M:122:PRO:HB3	13:M:141:ALA:O	2.17	0.45
38:MA:53:ASP:O	38:MA:57:ARG:HD2	2.16	0.45
37:QC:135:LYS:HA	37:QC:138:VAL:HG12	1.98	0.45
44:SA:24:VAL:HG13	44:SA:34:VAL:HG11	1.99	0.45
15:TB:13:HIS:NE2	15:TB:16:HIS:HB2	2.31	0.45
26:Z:2:LYS:HE2	26:Z:5:GLU:HG3	1.99	0.45
46:ZC:84:LEU:HD22	46:ZC:104:VAL:HG11	1.99	0.45
1:A:1053:G:N7	1:A:1200:C:H5'	2.32	0.44
1:A:1240:U:H4'	41:PA:38:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:U:H2'	1:A:1392:G:C8	2.52	0.44
1:A:4:U:H4'	1:A:5:U:OP2	2.17	0.44
1:A:792:A:H4'	1:A:793:U:O5'	2.16	0.44
1:A:967:5MC:H2'	1:A:968:A:C8	2.52	0.44
2:B:1153:C:OP1	18:R:92:ARG:NH2	2.45	0.44
2:B:686:G:N2	2:B:788:A:H61	2.15	0.44
28:BA:62:ARG:HB3	28:BA:63:TYR:H	1.56	0.44
48:BD:21:TYR:CE1	48:BD:23:ARG:NH1	2.85	0.44
30:DA:9:LEU:HA	30:DA:54:ILE:HB	1.99	0.44
25:DC:50:ARG:HD2	25:DC:57:GLU:OE2	2.16	0.44
6:F:154:LYS:HD3	6:F:154:LYS:HA	1.83	0.44
7:G:188:ARG:HB3	13:M:3:LEU:HD22	1.98	0.44
2:GB:14:A:H5''	2:GB:15:G:OP2	2.18	0.44
2:GB:1532:C:N4	2:GB:1539:G:H22	2.15	0.44
2:GB:165:U:H2'	2:GB:171:G:O4'	2.17	0.44
8:H:15:VAL:HG21	8:H:176:LEU:HD23	1.99	0.44
4:IB:68:C:H2'	4:IB:69:C:C6	2.51	0.44
35:JA:137:ARG:NH1	35:JA:334:GLU:HG3	2.32	0.44
37:LA:125:GLU:HG2	37:LA:190:ARG:O	2.17	0.44
7:LB:108:LYS:O	7:LB:112:MET:HB2	2.17	0.44
9:NB:52:VAL:O	9:NB:65:HIS:NE2	2.50	0.44
4:NC:35:A:OP2	43:WC:128:ARG:NH1	2.49	0.44
10:OB:101:LEU:HG	10:OB:107:ILE:HG12	1.98	0.44
2:GB:1914:C:O2'	35:OC:294:ARG:HD2	2.17	0.44
18:R:89:GLU:OE2	19:S:50:PRO:HB3	2.17	0.44
46:UA:27:LEU:HD12	46:UA:27:LEU:HA	1.77	0.44
41:UC:88:PRO:HG2	41:UC:149:ARG:HA	1.98	0.44
25:Y:20:ARG:HG2	25:Y:20:ARG:HH11	1.82	0.44
1:A:1306:A:H1'	1:A:1332:A:C2	2.52	0.44
2:B:1176:G:H8	2:B:1177:A:C8	2.34	0.44
2:B:251:A:C5	2:B:252:G:H1'	2.52	0.44
2:B:969:U:O3'	27:AA:14:GLY:HA2	2.17	0.44
1:A:1460:A:P	54:CB:27:LYS:NZ	2.91	0.44
1:FB:1239:A:H62	1:FB:1299:A:H62	1.65	0.44
1:FB:162:A:C5	1:FB:163:C:H1'	2.51	0.44
1:FB:184:G:H2'	1:FB:185:A:C8	2.49	0.44
1:FB:325:A:H2'	1:FB:326:G:O4'	2.17	0.44
1:FB:546:G:P	38:RC:72:GLU:HB3	2.57	0.44
2:GB:1173:G:O2'	2:GB:1177:A:N6	2.50	0.44
2:GB:1614:A:C2	20:YB:93:ALA:HB2	2.52	0.44
2:GB:1897:G:H2'	2:GB:1898:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2378:A:H4'	16:UB:23:ARG:NH1	2.32	0.44
2:GB:305:U:H2'	2:GB:306:U:C6	2.52	0.44
2:GB:910:A:H62	14:SB:12:GLN:HA	1.82	0.44
30:IC:14:THR:O	30:IC:17:LYS:NZ	2.50	0.44
10:J:6:LEU:HG	10:J:36:ALA:HA	1.98	0.44
37:LA:43:LEU:HD11	37:LA:66:VAL:HG11	1.98	0.44
13:M:84:ASN:HB2	13:M:86:LYS:HG2	1.99	0.44
35:OC:337:LEU:O	35:OC:341:ILE:HG23	2.17	0.44
17:Q:100:TYR:HB3	17:Q:103:ARG:NH1	2.29	0.44
13:RB:85:LEU:HD12	13:RB:137:LYS:HD2	1.99	0.44
45:TA:32:ILE:HD12	45:TA:72:ALA:HB2	1.99	0.44
16:UB:66:ALA:O	16:UB:69:VAL:HG13	2.16	0.44
47:VA:79:LYS:HE3	47:VA:83:ASP:OD2	2.18	0.44
14:N:81:VAL:HG12	24:X:5:LYS:HD2	1.99	0.44
18:WB:89:GLU:OE2	19:XB:50:PRO:HB3	2.16	0.44
1:A:1314:C:H2'	1:A:1315:U:H6	1.82	0.44
1:A:409:G:OP1	38:MA:24:GLU:N	2.51	0.44
1:A:757:U:H2'	1:A:758:G:O4'	2.17	0.44
2:B:270(N):U:OP2	2:B:270(N):U:H6	2.00	0.44
2:B:1999:C:H4'	2:B:2723:C:O2	2.17	0.44
2:B:862:G:H2'	2:B:863:A:O4'	2.17	0.44
26:EC:2:LYS:HE2	26:EC:5:GLU:HG3	1.98	0.44
6:F:24:THR:HG22	6:F:186:GLY:O	2.17	0.44
2:GB:1359:A:H2'	2:GB:1360:A:H5'	1.98	0.44
2:GB:2236:C:H2'	2:GB:2237:G:O4'	2.18	0.44
2:GB:278:A:H2'	2:GB:279:C:O4'	2.17	0.44
2:GB:848:G:N3	2:GB:933:A:H1'	2.32	0.44
2:GB:952:G:C6	2:GB:953:A:N7	2.85	0.44
53:GD:15:LEU:O	53:GD:19:VAL:HG23	2.18	0.44
2:GB:517:C:OP1	29:HC:16:ARG:NH2	2.50	0.44
10:J:118:LYS:HE2	10:J:121:LYS:HE3	1.98	0.44
36:KA:16:HIS:O	36:KA:18:GLY:N	2.51	0.44
42:QA:6:ILE:HD11	42:QA:31:PHE:HD2	1.82	0.44
49:XA:88:ARG:HH21	49:XA:88:ARG:HB3	1.81	0.44
2:B:2064:C:H2'	2:B:2065:C:C6	2.53	0.44
2:B:252:G:OP1	13:M:50:ARG:NH1	2.49	0.44
2:B:270(S):G:H2'	2:B:270(T):G:C8	2.52	0.44
3:C:1:U:OP2	3:C:1:U:C6	2.71	0.44
4:D:23:C:H2'	4:D:24:U:C6	2.52	0.44
1:FB:1367:C:H5'	44:XC:60:ARG:HH12	1.79	0.44
2:GB:1467:C:OP2	2:GB:1547:C:H5	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1991:U:H2'	2:GB:1992:G:H5''	1.99	0.44
54:HD:100:ILE:HG12	54:HD:102:GLY:N	2.22	0.44
35:JA:204:ALA:HB2	35:JA:298:LEU:HD13	1.99	0.44
39:SC:148:VAL:HG21	42:VC:107:LEU:HD22	2.00	0.44
3:HB:116:G:H4'	16:UB:54:LEU:HG	1.99	0.44
1:A:59:A:H5''	1:A:60:A:H5''	2.00	0.44
1:A:926:G:C6	1:A:1505:G:C6	3.06	0.44
1:A:938:A:C6	1:A:939:G:C5	3.05	0.44
2:B:1009:A:OP2	11:K:37:LYS:NZ	2.51	0.44
2:B:768:G:O2'	2:B:1379:A:N1	2.46	0.44
2:B:2643:G:H2'	2:B:2644:G:O4'	2.18	0.44
2:B:270(R):C:HO2'	10:J:42:SER:HG	1.62	0.44
25:DC:7:ILE:HD13	25:DC:98:LEU:HD11	1.98	0.44
1:FB:1087:G:H2'	1:FB:1088:G:C8	2.52	0.44
1:FB:1306:A:H1'	1:FB:1332:A:C2	2.52	0.44
2:GB:1278:A:OP1	15:TB:36:THR:HG23	2.17	0.44
2:GB:1592:C:H2'	2:GB:1593:G:C8	2.52	0.44
2:GB:2123:G:N2	2:GB:2175:C:O2	2.45	0.44
2:GB:716:A:C2	2:GB:717:G:H1'	2.52	0.44
2:GB:882:G:H2'	2:GB:883:G:C8	2.52	0.44
53:GD:19:VAL:HA	53:GD:22:LEU:HD12	1.99	0.44
54:HD:83:ARG:HA	54:HD:86:ARG:HD3	1.99	0.44
30:IC:23:THR:OG1	30:IC:24:GLU:N	2.46	0.44
35:JA:312:PHE:CD1	35:JA:329:LEU:HD21	2.53	0.44
1:FB:1498:UR3:O2'	34:MC:17:U:OP1	2.27	0.44
40:OA:68:PRO:HG2	40:OA:71:ARG:NH2	2.31	0.44
10:OB:43:ASN:N	10:OB:43:ASN:OD1	2.51	0.44
35:OC:186:ARG:HA	35:OC:313:PRO:HD3	1.99	0.44
43:RA:108:VAL:HG12	43:RA:109:VAL:H	1.82	0.44
43:RA:13:ALA:HB2	43:RA:68:GLY:HA3	1.98	0.44
17:VB:6:LEU:HD13	17:VB:6:LEU:HA	1.87	0.44
18:WB:8:VAL:HG22	18:WB:12:ARG:HG3	2.00	0.44
1:A:353:A:H5'	1:A:353:A:C8	2.53	0.44
1:A:715:A:H2'	1:A:716:A:C8	2.52	0.44
47:AD:50:GLU:HA	47:AD:53:VAL:HB	2.00	0.44
2:B:2001:A:H4'	2:B:2689:U:O2'	2.16	0.44
2:B:2141:G:C2	2:B:2151:G:H1'	2.53	0.44
2:B:330:A:H2	2:B:1210:A:C2'	2.30	0.44
2:B:848:G:N3	2:B:933:A:H1'	2.32	0.44
51:ED:14:LYS:HE3	51:ED:14:LYS:H	1.82	0.44
6:F:111:ARG:HA	15:O:1:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:715:A:H2'	1:FB:716:A:C8	2.52	0.44
1:FB:88:C:H2'	1:FB:89:U:C6	2.52	0.44
1:FB:946:A:H2'	1:FB:947:G:C8	2.52	0.44
27:FC:10:LYS:HB3	27:FC:53:LEU:HA	2.00	0.44
2:GB:1005:C:H2'	2:GB:1006:C:C6	2.53	0.44
2:GB:374:A:C2	2:GB:401:A:C4	3.05	0.44
8:MB:109:VAL:HG13	28:GC:33:VAL:HG21	1.99	0.44
9:I:42:ARG:HB3	9:I:53:GLU:HB2	1.98	0.44
4:IA:65:C:H2'	4:IA:66:C:H6	1.82	0.44
11:K:27:ALA:HB1	11:K:103:VAL:HG22	1.99	0.44
38:MA:104:VAL:HG11	38:MA:146:ILE:HG13	1.98	0.44
46:UA:69:TYR:HD2	46:UA:99:HIS:CD2	2.36	0.44
42:VC:86:ILE:HG12	42:VC:135:CYS:HA	1.99	0.44
49:XA:63:ARG:HG2	49:XA:67:LEU:HD12	1.98	0.44
1:FB:1124:G:H5''	44:XC:35:SER:OG	2.17	0.44
45:TA:108:ILE:HB	52:AB:87:ARG:HB3	1.99	0.44
2:B:1070:A:N6	2:B:1097:U:O2'	2.48	0.44
2:B:38:A:H2'	2:B:39:C:C6	2.53	0.44
24:CC:29:GLN:HE21	24:CC:29:GLN:HB3	1.68	0.44
26:EC:17:SER:N	26:EC:20:GLU:OE1	2.30	0.44
1:FB:1272:G:C2	1:FB:1273:G:H1'	2.53	0.44
1:FB:1452:C:H2'	1:FB:1453:G:H5''	2.00	0.44
2:GB:2135:A:N6	2:GB:2155:G:H1	2.15	0.44
2:GB:900:A:H2'	2:GB:901:A:O4'	2.17	0.44
8:H:16:ARG:HB2	8:H:17:PRO:HD3	2.00	0.44
4:IB:67:C:H2'	4:IB:68:C:C6	2.53	0.44
4:IB:7:G:N2	4:IB:67:C:O2	2.51	0.44
2:GB:2667:C:H1'	9:NB:109:PHE:CD1	2.53	0.44
15:O:96:ARG:NH1	15:O:115:GLU:OE2	2.49	0.44
41:PA:79:ARG:CD	41:PA:80:VAL:H	2.31	0.44
36:PC:166:ASP:HA	36:PC:167:PRO:HD3	1.72	0.44
12:QB:64:ARG:O	12:QB:82:ASN:HA	2.18	0.44
37:QC:43:LEU:HD11	37:QC:66:VAL:HG11	1.99	0.44
43:RA:113:LYS:NZ	43:RA:119:ALA:O	2.51	0.44
46:UA:7:ILE:HA	46:UA:7:ILE:HD13	1.91	0.44
23:W:129:SER:HB3	23:W:132:ASN:HD21	1.83	0.44
48:WA:50:LYS:HD2	48:WA:50:LYS:HA	1.84	0.44
18:WB:102:GLU:HG3	19:XB:2:PHE:CE2	2.53	0.44
46:ZC:83:VAL:HG23	46:ZC:107:ALA:HB2	1.99	0.44
1:A:1062:U:H2'	1:A:1063:C:C6	2.53	0.44
1:A:114:U:H2'	1:A:115:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:U:O5'	1:A:84:U:H5''	2.18	0.44
2:B:1388:G:H2'	2:B:1389:G:H8	1.83	0.44
2:B:149:A:H2'	2:B:150:C:O4'	2.18	0.44
2:B:195:A:H61	2:B:198:C:H3'	1.83	0.44
2:B:2236:C:H2'	2:B:2237:G:O4'	2.17	0.44
2:B:307:G:H21	2:B:330:A:N6	2.10	0.44
2:B:547:A:C3'	2:B:548:A:C8	2.97	0.44
2:B:828:U:H4'	2:B:831:G:N1	2.33	0.44
4:D:17:C:H3'	4:D:17(A):U:H2'	1.99	0.44
1:FB:1273:G:H2'	1:FB:1274:G:O4'	2.17	0.44
1:FB:860:A:H2'	1:FB:861:G:O4'	2.18	0.44
2:GB:1870:C:H2'	2:GB:1871:A:O4'	2.18	0.44
2:B:2758:A:C4	9:I:67:LEU:HD21	2.53	0.44
10:J:110:ASP:HB3	10:J:113:ARG:HG2	1.99	0.44
10:J:4:ILE:HA	10:J:17:GLN:O	2.18	0.44
35:JA:314:GLN:HB2	35:JA:316:ARG:HD2	1.99	0.44
13:RB:50:ARG:HH21	32:KC:7:HIS:CD2	2.36	0.44
39:NA:80:ILE:HD11	39:NA:138:ALA:HB1	2.00	0.44
4:NC:35:A:H2'	4:NC:36:U:H6	1.83	0.44
16:P:4:LEU:HD23	16:P:8:GLU:OE2	2.18	0.44
36:PC:24:TRP:N	36:PC:24:TRP:CD1	2.84	0.44
37:QC:142:MET:HE1	37:QC:148:GLY:HA2	1.99	0.44
13:RB:59:LEU:HD23	32:KC:58:ILE:HD13	1.98	0.44
2:GB:489:G:N7	20:YB:49:LYS:NZ	2.65	0.44
1:A:1226:C:N4	47:VA:104:ARG:HD2	2.32	0.44
2:B:1291:C:H2'	2:B:1292:U:C6	2.52	0.44
2:B:1322:A:N1	2:B:1333:C:O2'	2.45	0.44
2:B:270(H):C:H2'	2:B:270(I):C:C6	2.53	0.44
2:B:861:A:O3'	14:N:18:LYS:NZ	2.51	0.44
23:BC:61:LEU:HB3	23:BC:63:ASP:OD1	2.18	0.44
24:CC:7:LEU:O	4:NC:1:C:O2'	2.34	0.44
49:CD:11:VAL:HG21	49:CD:34:LEU:HD13	2.00	0.44
21:ZB:5:TYR:CE1	26:EC:30:ARG:HG3	2.53	0.44
6:F:97:LYS:HG2	6:F:100:GLU:OE2	2.17	0.44
1:FB:749:C:H2'	1:FB:750:G:H8	1.82	0.44
2:GB:1408:C:H2'	2:GB:1409:C:C6	2.52	0.44
2:GB:2611:U:C4	29:HC:3:LYS:HG2	2.52	0.44
9:I:140:LYS:HE2	9:I:140:LYS:HB3	1.68	0.44
38:MA:5:ILE:H	38:MA:5:ILE:HG13	1.55	0.44
14:N:135:ASP:HB3	14:N:137:TYR:H	1.83	0.44
35:OC:316:ARG:HB3	35:OC:316:ARG:HE	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:138:LEU:HD13	11:PB:139:GLU:H	1.83	0.44
37:QC:112:SER:HB3	37:QC:115:LEU:HD12	2.00	0.44
13:RB:93:GLY:N	13:RB:123:LEU:HD22	2.33	0.44
1:A:1124:G:H5''	44:SA:35:SER:OG	2.18	0.44
20:T:6:ILE:HG12	20:T:104:THR:OG1	2.17	0.44
23:W:69:THR:HG22	23:W:90:VAL:HA	1.99	0.44
18:WB:52:ARG:HA	18:WB:55:ARG:HG3	2.00	0.44
1:FB:553:A:H5''	46:ZC:24:VAL:HG21	1.99	0.44
1:A:1508:G:H2'	1:A:1509:C:H6	1.84	0.43
1:A:343:U:H2'	1:A:345:C:C5	2.53	0.43
1:A:689:C:OP1	45:TA:27:ASN:ND2	2.48	0.43
1:A:997:U:H2'	1:A:998(A):G:O4'	2.18	0.43
22:AC:102:CYS:SG	22:AC:104:GLY:N	2.78	0.43
22:AC:9:LYS:HA	22:AC:10:GLY:HA2	1.61	0.43
2:B:305:U:H2'	2:B:306:U:C6	2.52	0.43
2:B:910:A:H62	14:N:12:GLN:HA	1.82	0.43
1:FB:1118:C:H2'	1:FB:1119:C:H6	1.83	0.43
1:FB:1201:A:H1'	1:FB:1202:G:OP2	2.18	0.43
1:FB:438:G:H4'	38:RC:123:HIS:CD2	2.53	0.43
1:FB:575:G:H4'	1:FB:575:G:OP1	2.18	0.43
2:GB:1842:G:H2'	2:GB:1843:C:C6	2.53	0.43
2:GB:235:U:H2'	2:GB:236:C:C6	2.52	0.43
2:GB:2451:A:H5'	24:CC:3:HIS:HE2	1.83	0.43
2:GB:664:C:H4'	2:GB:941:A:OP1	2.17	0.43
53:GD:22:LEU:HD23	53:GD:26:GLY:O	2.18	0.43
9:I:102:ALA:HA	9:I:117:PRO:HD3	2.00	0.43
55:ID:22:ARG:HA	55:ID:23:PRO:HD2	1.91	0.43
10:J:29:TYR:CE1	10:J:33:ARG:NH1	2.86	0.43
13:RB:63:PRO:HG2	32:KC:25:MET:HB2	2.00	0.43
14:N:111:GLU:O	14:N:115:MET:HG2	2.18	0.43
36:PC:64:ARG:HG3	36:PC:64:ARG:HH11	1.82	0.43
42:QA:100:ILE:O	42:QA:125:ARG:NH2	2.51	0.43
37:QC:86:VAL:O	37:QC:90:GLU:HG2	2.17	0.43
14:SB:69:PHE:HA	14:SB:70:PRO:HD3	1.75	0.43
1:FB:1350:A:O2'	41:UC:33:ASP:OD1	2.33	0.43
1:A:1144:G:N2	1:A:1146:A:H62	2.16	0.43
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.43
1:A:706:A:H5''	45:TA:22:HIS:CD2	2.53	0.43
2:B:1688:U:O2	2:B:1700:A:H5'	2.17	0.43
2:B:1790:C:H2'	2:B:1791:A:C5	2.52	0.43
53:BB:15:LEU:O	53:BB:19:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BD:53:LEU:O	48:BD:56:VAL:HG23	2.18	0.43
4:D:7:G:N2	4:D:67:C:O2	2.51	0.43
5:E:25:THR:HG21	5:E:113:VAL:HG21	2.00	0.43
1:FB:606:G:H2'	1:FB:631:G:N2	2.32	0.43
1:FB:689:C:OP1	45:YC:27:ASN:ND2	2.47	0.43
2:GB:969:U:O3'	27:FC:14:GLY:HA2	2.18	0.43
7:G:132:VAL:O	7:G:132:VAL:HG23	2.17	0.43
2:GB:1686:C:H2'	2:GB:1687:G:O4'	2.18	0.43
2:GB:2693:A:H2'	2:GB:2694:G:H8	1.82	0.43
2:GB:280:C:C2	2:GB:361:G:N2	2.86	0.43
2:GB:586:A:N1	2:GB:809:G:O2'	2.41	0.43
8:H:166:ASP:O	8:H:170:ARG:N	2.42	0.43
35:JA:248:HIS:CE1	35:JA:250:PRO:HD2	2.53	0.43
11:K:97:ARG:HA	11:K:100:GLU:HB2	2.01	0.43
36:KA:70:PHE:CE1	36:KA:163:PHE:HD1	2.36	0.43
6:KB:119:ARG:HG2	6:KB:120:TRP:NE1	2.33	0.43
37:LA:112:SER:HB3	37:LA:115:LEU:HD12	2.00	0.43
2:B:832:G:H5'	13:M:45:LEU:HD21	2.00	0.43
42:QA:87:SER:HA	42:QA:93:VAL:HG23	2.00	0.43
2:B:583:G:OP2	18:R:10:ARG:HD2	2.18	0.43
13:RB:59:LEU:HD21	32:KC:10:ALA:HA	2.00	0.43
15:TB:72:ASP:HB3	15:TB:75:LEU:HB3	2.00	0.43
17:VB:114:LEU:HA	17:VB:114:LEU:HD23	1.89	0.43
42:VC:97:VAL:HG21	42:VC:128:GLY:HA2	1.99	0.43
19:XB:97:LYS:HD2	19:XB:97:LYS:HA	1.80	0.43
1:A:375:U:O2	50:YA:28:ARG:NH2	2.51	0.43
45:YC:24:SER:HB2	45:YC:27:ASN:H	1.83	0.43
1:A:1272:G:C2	1:A:1273:G:H1'	2.53	0.43
47:AD:27:LYS:HE2	47:AD:27:LYS:HB2	1.86	0.43
47:AD:45:VAL:O	47:AD:48:LEU:HB2	2.18	0.43
47:AD:79:LYS:HE3	47:AD:83:ASP:OD2	2.18	0.43
2:B:2706:G:H2'	2:B:2707:G:O4'	2.19	0.43
2:B:2779:U:OP1	2:B:2780:G:H2'	2.18	0.43
2:B:2853:C:H2'	2:B:2854:G:C8	2.53	0.43
2:B:2863:C:OP1	17:Q:93:ARG:NH1	2.51	0.43
2:B:636:G:N7	13:M:113:LYS:HE2	2.34	0.43
14:SB:64:ILE:HG13	23:BC:178:GLU:HG3	2.00	0.43
1:FB:1054:C:OP2	1:FB:1197:G:OP2	2.36	0.43
1:FB:1451:A:H8	1:FB:1452:C:O4'	2.01	0.43
1:FB:801:U:H2'	1:FB:802:A:C8	2.52	0.43
1:FB:975:A:H5'	1:FB:975:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:FD:35:ARG:HH11	52:FD:35:ARG:HB2	1.84	0.43
2:GB:1165:U:H2'	2:GB:1166:C:C6	2.52	0.43
2:GB:550:G:O2'	2:GB:1220:A:N3	2.40	0.43
2:GB:1693:U:O2'	5:JB:14:ARG:NH2	2.51	0.43
2:GB:1754:C:P	17:VB:96:ARG:NH1	2.91	0.43
2:GB:2712(A):A:H5''	2:GB:2713:A:OP2	2.18	0.43
2:GB:306:U:H2'	2:GB:307:G:O4'	2.18	0.43
2:GB:448:U:O4	2:GB:583:G:H1'	2.17	0.43
8:H:103:LEU:HA	8:H:103:LEU:HD23	1.85	0.43
9:I:101:ARG:NH1	9:I:122:THR:HG23	2.31	0.43
35:JA:181:GLY:O	35:JA:307:ASN:HB2	2.18	0.43
35:JA:186:ARG:HA	35:JA:313:PRO:HD3	1.99	0.43
35:JA:251:THR:HB	35:JA:253:ILE:HG22	2.00	0.43
37:LA:77:ILE:HG23	37:LA:84:ILE:HD12	2.01	0.43
39:NA:92:LYS:HA	39:NA:93:PRO:HD3	1.89	0.43
9:NB:70:THR:HG22	9:NB:74:ASN:OD1	2.18	0.43
35:OC:108:GLU:HB2	35:OC:170:GLY:HA2	1.99	0.43
35:OC:317:VAL:HB	35:OC:329:LEU:HD13	1.99	0.43
42:QA:122:ARG:HA	42:QA:125:ARG:HD2	1.99	0.43
14:SB:2:LEU:HB2	14:SB:70:PRO:HG2	2.00	0.43
46:UA:60:LEU:HD21	46:UA:66:VAL:HG22	1.99	0.43
16:UB:15:ARG:NH1	16:UB:88:ASP:OD2	2.50	0.43
41:UC:79:ARG:CD	41:UC:80:VAL:H	2.30	0.43
26:Z:35:LEU:HD12	26:Z:53:LEU:HD12	2.01	0.43
1:A:919:A:O2'	1:A:1080:A:N1	2.44	0.43
1:A:1087:G:H2'	1:A:1088:G:C8	2.53	0.43
1:A:858:G:O6	1:A:869:G:H3'	2.18	0.43
2:B:1035:U:H2'	2:B:1036:G:C8	2.52	0.43
2:B:1429:G:H2'	2:B:1430:C:C6	2.53	0.43
2:B:2135:A:N6	2:B:2155:G:H1	2.16	0.43
2:B:2168:G:C8	2:B:2170:A:OP2	2.71	0.43
2:B:2123:G:N2	2:B:2175:C:O2	2.46	0.43
2:B:362:U:O2'	2:B:363(A):G:H5''	2.18	0.43
28:BA:5:ILE:HG13	28:BA:6:HIS:CD2	2.53	0.43
1:FB:375:U:O2	50:DD:28:ARG:NH2	2.50	0.43
6:F:24:THR:HG21	6:F:188:VAL:HG23	1.99	0.43
1:FB:114:U:H2'	1:FB:115:G:C8	2.54	0.43
1:FB:1465:C:H2'	1:FB:1466:C:O4'	2.19	0.43
52:FD:61:LYS:O	52:FD:65:ILE:HG13	2.17	0.43
2:GB:1429:G:H2'	2:GB:1430:C:C6	2.53	0.43
2:GB:1790:C:H2'	2:GB:1791:A:C5	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:270(M):U:P	2:GB:270(M):U:H3'	2.58	0.43
2:GB:2853:C:H2'	2:GB:2854:G:C8	2.53	0.43
2:GB:38:A:H2'	2:GB:39:C:C6	2.53	0.43
2:GB:545:G:H21	2:GB:548:A:H62	1.66	0.43
8:H:3:LEU:HB3	8:H:97:ASP:OD2	2.18	0.43
9:I:21:PRO:O	9:I:23:ARG:HG2	2.18	0.43
4:IB:17:C:H3'	4:IB:17(A):U:H2'	1.99	0.43
4:IB:63:G:H2'	4:IB:64:G:C8	2.52	0.43
5:JB:77:ALA:HB2	5:JB:97:TYR:CD1	2.54	0.43
36:KA:12:GLU:HA	36:KA:15:VAL:HG22	2.00	0.43
37:LA:86:VAL:O	37:LA:90:GLU:HG2	2.19	0.43
7:LB:132:VAL:O	7:LB:132:VAL:HG23	2.18	0.43
3:C:113:C:O2'	16:P:46:VAL:HG23	2.18	0.43
41:PA:88:PRO:HG2	41:PA:149:ARG:HA	1.99	0.43
41:PA:23:VAL:O	41:PA:27:ILE:HG13	2.18	0.43
36:PC:70:PHE:HE1	36:PC:163:PHE:HD1	1.67	0.43
39:NA:152:ARG:HB3	42:QA:43:GLY:HA3	1.99	0.43
37:QC:92:ALA:HB2	37:QC:99:VAL:HG22	2.01	0.43
43:RA:46:ALA:HB2	43:RA:74:ILE:HG23	2.00	0.43
14:SB:67:ARG:HH11	14:SB:67:ARG:HG3	1.83	0.43
2:B:84:A:P	22:V:8:LYS:NZ	2.87	0.43
47:VA:39:ILE:HG13	47:VA:56:LEU:HD22	1.99	0.43
42:VC:119:LEU:HD12	42:VC:123:GLU:HB2	1.99	0.43
42:VC:37:ARG:O	42:VC:41:ARG:HG2	2.19	0.43
23:W:30:ASN:O	23:W:32:HIS:N	2.51	0.43
48:WA:53:LEU:O	48:WA:56:VAL:HG23	2.18	0.43
43:WC:7:THR:HB	43:WC:83:ARG:HH21	1.83	0.43
19:XB:40:LEU:HA	19:XB:40:LEU:HD23	1.81	0.43
1:A:45:U:H2'	1:A:46:G:C8	2.54	0.43
1:A:546:G:P	38:MA:72:GLU:HB3	2.59	0.43
1:A:859:A:H2'	1:A:860:A:O4'	2.18	0.43
2:B:1093:G:H2'	2:B:1093:G:N3	2.33	0.43
2:B:2251:OMG:H1'	2:B:2251:OMG:HM23	1.65	0.43
2:B:882:G:H2'	2:B:883:G:C8	2.54	0.43
2:GB:2079:U:OP1	25:DC:21:ARG:NH2	2.52	0.43
50:DD:45:THR:O	50:DD:48:TRP:HD1	2.02	0.43
1:FB:1262:C:H2'	1:FB:1263:C:C6	2.54	0.43
7:G:116:ASP:OD2	13:M:1:MET:HB2	2.18	0.43
2:GB:1688:U:O2	2:GB:1700:A:H5'	2.18	0.43
2:GB:17:G:H2'	2:GB:18:C:C6	2.54	0.43
2:GB:1901:A:N3	2:GB:1901:A:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2010:G:H5''	20:YB:42:ARG:HB2	2.00	0.43
2:GB:2025:C:H2'	2:GB:2026:C:C6	2.53	0.43
2:GB:2805:G:N2	2:GB:2807:G:N7	2.66	0.43
2:GB:587:C:C6	2:GB:671:C:H1'	2.54	0.43
2:GB:760:G:H2'	2:GB:761:A:O4'	2.19	0.43
8:H:16:ARG:HD2	8:H:31:VAL:HG11	1.99	0.43
8:H:47:LYS:HG3	8:H:48:GLU:H	1.83	0.43
10:J:133:HIS:HA	10:J:134:PRO:HD3	1.81	0.43
37:LA:58:GLU:O	37:LA:65:ALA:N	2.51	0.43
8:MB:47:LYS:HG3	8:MB:48:GLU:H	1.83	0.43
41:PA:26:PHE:O	41:PA:30:ILE:HG13	2.19	0.43
40:TC:78:GLU:O	40:TC:81:ILE:HG22	2.19	0.43
16:UB:27:SER:HA	16:UB:88:ASP:HB3	2.00	0.43
47:VA:14:ARG:NE	47:VA:42:ALA:HA	2.32	0.43
47:VA:86:CYS:O	47:VA:90:LEU:HD22	2.19	0.43
43:WC:33:PHE:CE1	43:WC:37:PHE:HD2	2.36	0.43
1:FB:1147:C:HO2'	43:WC:5:TYR:HH	1.66	0.43
1:A:297:G:N2	1:A:300:A:OP2	2.45	0.43
2:B:1108:U:C4	2:B:1109:C:C4	3.07	0.43
2:B:189:G:OP2	25:Y:14:VAL:HG21	2.19	0.43
2:B:2320:A:N3	2:B:2320:A:H2'	2.32	0.43
2:B:448:U:O4	2:B:583:G:H1'	2.18	0.43
2:B:879:G:H22	2:B:899:A:H1'	1.83	0.43
3:C:73:A:C6	3:C:74:U:C2	3.06	0.43
5:E:246:PRO:O	5:E:254:THR:HG22	2.18	0.43
1:FB:875:C:O2'	42:VC:14:ARG:NH1	2.48	0.43
1:FB:974:A:H8	1:FB:974:A:OP1	2.01	0.43
27:FC:7:LYS:HB2	27:FC:34:GLU:HG2	2.01	0.43
2:GB:149:A:H2'	2:GB:150:C:O4'	2.18	0.43
2:GB:2514:U:H2'	2:GB:2515:C:C6	2.54	0.43
2:GB:275:G:H8	2:GB:275:G:O5'	2.01	0.43
2:GB:2895:U:O5'	2:GB:2895:U:H6	2.01	0.43
8:H:11:TYR:OH	8:H:16:ARG:HD3	2.18	0.43
35:JA:109:ARG:HD3	35:JA:208:GLU:O	2.18	0.43
2:GB:458:G:O2'	31:JC:39:ARG:HD3	2.17	0.43
37:LA:130:VAL:HG21	37:LA:157:ILE:HG23	2.01	0.43
38:MA:25:ARG:O	38:MA:28:SER:OG	2.21	0.43
8:MB:16:ARG:HD2	8:MB:31:VAL:HG11	1.99	0.43
8:MB:74:LYS:O	8:MB:84:LYS:HG3	2.18	0.43
40:OA:91:VAL:HG11	52:AB:72:ARG:NH1	2.33	0.43
35:OC:137:ARG:NH1	35:OC:334:GLU:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:PC:69:LEU:O	36:PC:163:PHE:N	2.46	0.43
17:Q:128:GLU:O	17:Q:132:LYS:NZ	2.51	0.43
18:R:112:ARG:NH1	19:S:47:VAL:HB	2.34	0.43
13:RB:107:LYS:O	13:RB:110:TYR:HB2	2.19	0.43
2:GB:811:U:H2'	13:RB:21:ARG:HA	2.01	0.43
41:UC:26:PHE:O	41:UC:30:ILE:HG13	2.19	0.43
17:VB:128:GLU:O	17:VB:132:LYS:NZ	2.50	0.43
20:YB:23:LEU:HA	20:YB:23:LEU:HD12	1.86	0.43
1:FB:695:A:OP2	45:YC:53:SER:HB2	2.18	0.43
1:A:1073:U:H3	1:A:1102:A:H61	1.66	0.43
52:AB:19:LYS:HB3	52:AB:20:ALA:H	1.66	0.43
47:AD:39:ILE:HG13	47:AD:56:LEU:HD22	2.01	0.43
2:B:2211:G:H2'	2:B:2212:A:C2	2.53	0.43
2:B:275:G:O5'	2:B:275:G:H8	2.01	0.43
2:B:464:U:H2'	2:B:465:G:O4'	2.19	0.43
8:H:109:VAL:HG13	28:BA:33:VAL:HG21	2.00	0.43
50:DD:53:VAL:CG1	50:DD:57:ARG:HH11	2.31	0.43
1:FB:790:A:C6	1:FB:791:G:C6	3.06	0.43
1:FB:82:U:O5'	1:FB:84:U:H5''	2.19	0.43
1:FB:949:A:H1'	1:FB:1364:U:H3	1.82	0.43
2:GB:1952:A:C6	2:GB:1953:A:N1	2.86	0.43
2:GB:2780:G:H4'	2:GB:2781:A:OP2	2.18	0.43
2:GB:464:U:H2'	2:GB:465:G:O4'	2.19	0.43
2:GB:579:G:H2'	2:GB:580:C:C6	2.54	0.43
2:GB:813:U:H2'	2:GB:814:C:C6	2.54	0.43
2:GB:876:C:H2'	2:GB:877:U:O4'	2.19	0.43
28:GC:34:GLU:HB2	28:GC:35:VAL:H	1.53	0.43
8:H:36:LYS:HD3	8:H:95:ARG:NH1	2.33	0.43
30:IC:34:LEU:HD23	30:IC:34:LEU:HA	1.76	0.43
9:NB:42:ARG:HB3	9:NB:53:GLU:HB2	2.01	0.43
10:OB:7:GLU:HG3	10:OB:8:PRO:HD2	2.00	0.43
36:PC:16:HIS:O	36:PC:18:GLY:N	2.52	0.43
13:RB:80:TYR:CD1	13:RB:111:ARG:HB2	2.53	0.43
40:TC:24:GLU:HA	40:TC:24:GLU:OE2	2.17	0.43
46:UA:124:LYS:HA	46:UA:125:PRO:HD3	1.73	0.43
18:WB:106:PHE:O	18:WB:110:VAL:HG23	2.19	0.43
1:A:1054:C:OP2	1:A:1197:G:OP2	2.36	0.43
1:A:1174:G:OP1	41:PA:5:ARG:NH2	2.52	0.43
2:B:1815:A:OP2	5:E:54:ARG:NH2	2.50	0.43
2:B:2514:U:H2'	2:B:2515:C:C6	2.54	0.43
2:B:589:C:H2'	2:B:590:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:G:H21	2:B:788:A:H61	1.66	0.43
2:B:700:G:O6	2:B:733:G:N2	2.52	0.43
48:BD:15:LYS:HB3	48:BD:15:LYS:NZ	2.34	0.43
51:ED:43:LEU:HA	51:ED:43:LEU:HD23	1.64	0.43
1:FB:99:C:H2'	1:FB:101:A:C8	2.53	0.43
1:FB:574:A:HO2'	1:FB:882:C:HO2'	1.66	0.43
1:FB:731:G:H5'	1:FB:766:A:H4'	2.00	0.43
2:GB:1093:G:N3	2:GB:1093:G:H2'	2.34	0.43
2:GB:1205:U:C4	7:LB:171:PRO:HA	2.53	0.43
2:GB:1357:U:H2'	2:GB:1358:G:O4'	2.18	0.43
2:GB:1693:U:OP2	2:GB:1694:C:H5	2.01	0.43
2:GB:2022:U:O2'	2:GB:2617:C:H5'	2.19	0.43
54:HD:30:LYS:HB2	54:HD:30:LYS:HZ1	1.84	0.43
12:L:68:GLU:HB3	12:L:78:ARG:NH1	2.34	0.43
13:M:63:PRO:HG2	32:FA:25:MET:HB2	1.99	0.43
35:OC:142:ARG:NH2	35:OC:174:ARG:NH1	2.63	0.43
3:C:116:G:H4'	16:P:54:LEU:HG	2.01	0.43
41:PA:76:ARG:HD3	41:PA:156:TRP:HZ2	1.83	0.43
17:Q:35:LYS:HE2	17:Q:37:GLY:O	2.18	0.43
42:QA:19:VAL:HG23	42:QA:21:LYS:HG2	2.01	0.43
37:QC:54:ARG:NE	37:QC:56:ASP:OD2	2.49	0.43
13:RB:29:LYS:HB3	13:RB:30:THR:H	1.41	0.43
47:VA:14:ARG:HG3	47:VA:44:ARG:CZ	2.49	0.43
37:LA:34:LEU:HD13	48:WA:25:VAL:HB	2.01	0.43
41:UC:150:ALA:HA	45:YC:59:TYR:HB3	2.00	0.43
45:YC:99:GLN:HE21	52:FD:88:LYS:HZ2	1.66	0.43
21:U:5:TYR:CE1	26:Z:30:ARG:HG3	2.54	0.43
26:Z:37:PHE:O	26:Z:41:ILE:HG13	2.18	0.43
1:A:1223:C:P	53:BB:78:ARG:HH21	2.42	0.43
1:A:801:U:H2'	1:A:802:A:C8	2.53	0.43
2:B:1060:U:H4'	2:B:1061:U:O5'	2.18	0.43
2:B:1532:C:N4	2:B:1539:G:H22	2.17	0.43
1:A:1408:A:HO2'	2:B:1916:A:H61	1.67	0.43
1:A:1517:G:H1'	2:B:1919:A:O3'	2.18	0.43
2:B:2344:U:O2'	30:DA:36:LEU:HD22	2.18	0.43
4:D:67:C:H2'	4:D:68:C:C6	2.53	0.43
32:FA:65:GLU:HA	32:FA:65:GLU:OE2	2.19	0.43
1:FB:1502:A:C8	1:FB:1505:G:N2	2.87	0.43
1:FB:229:U:H2'	1:FB:230:G:O4'	2.19	0.43
1:FB:815:A:N3	1:FB:1527:C:O2'	2.41	0.43
2:GB:2667:C:H1'	9:NB:109:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2706:G:H2'	2:GB:2707:G:O4'	2.18	0.43
2:GB:90:U:H1'	2:GB:91:A:C8	2.54	0.43
3:HB:73:A:C4	3:HB:104:A:C2	3.07	0.43
4:IA:47:U:H5''	4:IA:48:C:H5'	2.01	0.43
24:X:2:ALA:N	35:JA:261:ARG:HD3	2.34	0.43
8:MB:164:GLU:HB2	8:MB:168:GLU:OE2	2.19	0.43
9:NB:3:ARG:HA	9:NB:3:ARG:HH11	1.84	0.43
10:OB:110:ASP:HB3	10:OB:113:ARG:CG	2.49	0.43
16:P:3:ARG:NH1	16:P:4:LEU:H	2.16	0.43
11:PB:97:ARG:HA	11:PB:100:GLU:HB2	2.00	0.43
41:UC:79:ARG:HD2	41:UC:80:VAL:H	1.84	0.43
47:VA:108:ARG:O	47:VA:112:GLY:N	2.51	0.43
17:VB:100:TYR:HD1	17:VB:103:ARG:HH12	1.59	0.43
43:WC:13:ALA:HB2	43:WC:68:GLY:HA3	1.99	0.43
50:YA:49:LEU:HD12	50:YA:50:LYS:H	1.84	0.43
20:YB:11:ARG:HD3	20:YB:82:LEU:HD12	2.01	0.43
45:YC:48:ILE:HA	45:YC:48:ILE:HD12	1.71	0.43
1:A:1118:C:H2'	1:A:1119:C:H6	1.82	0.43
1:A:81:G:H2'	1:A:82:U:C6	2.54	0.43
2:B:1245:G:OP1	13:M:13:ASN:ND2	2.52	0.43
2:B:2783:G:H2'	2:B:2784:C:C6	2.54	0.43
23:BC:67:LEU:HA	23:BC:68:PRO:HD2	1.91	0.43
50:DD:25:ARG:H	50:DD:25:ARG:HG2	1.53	0.43
1:FB:265:G:H5'	51:ED:64:PRO:O	2.19	0.43
1:FB:946:A:O2'	1:FB:1333:A:N3	2.43	0.43
2:GB:1021:A:C8	2:GB:1022:G:H5''	2.54	0.43
2:GB:1367:A:N7	2:GB:1368:G:H1'	2.34	0.43
2:GB:1519:G:H2'	2:GB:1520:U:O4'	2.19	0.43
2:GB:1923:U:H2'	2:GB:1924:C:C6	2.54	0.43
2:GB:264:C:O2'	2:GB:265:A:H2'	2.19	0.43
2:GB:807:U:OP1	13:RB:36:LYS:NZ	2.40	0.43
2:GB:887:A:H1'	2:GB:890:A:N6	2.34	0.43
2:GB:974(B):C:OP2	2:GB:974(B):C:H4'	2.18	0.43
2:GB:994:C:OP1	18:WB:53:ARG:NH2	2.52	0.43
28:GC:5:ILE:HG13	28:GC:6:HIS:CD2	2.54	0.43
53:GD:69:HIS:HB3	53:GD:73:GLU:OE2	2.18	0.43
8:H:64:THR:HB	8:H:94:LEU:HD21	2.00	0.43
9:I:98:LEU:HG	9:I:125:VAL:HG23	2.00	0.43
9:I:87:LEU:HD23	9:I:164:TYR:HA	2.01	0.43
10:J:26:ALA:O	10:J:31:LEU:HB2	2.19	0.43
6:KB:24:THR:HG21	6:KB:188:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:64:ILE:HG13	7:LB:64:ILE:H	1.44	0.43
10:OB:101:LEU:HD23	10:OB:109:ILE:HG12	2.00	0.43
35:OC:312:PHE:CD1	35:OC:329:LEU:HD21	2.54	0.43
11:PB:7:LYS:HD3	11:PB:7:LYS:HA	1.75	0.43
36:PC:21:ARG:O	36:PC:23:ARG:N	2.52	0.43
41:PA:37:ASN:OD1	43:RA:41:VAL:HG22	2.18	0.43
17:VB:9:LEU:O	17:VB:12:SER:OG	2.26	0.43
43:WC:42:ARG:HB2	43:WC:42:ARG:HE	1.57	0.43
26:Z:18:PRO:O	26:Z:22:GLU:HG3	2.19	0.43
51:ZA:13:ASP:OD2	51:ZA:53:LEU:HB2	2.19	0.43
46:ZC:28:LYS:HZ3	46:ZC:64:TYR:HE2	1.67	0.43
1:A:1411:C:H2'	1:A:1412:C:C6	2.54	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.18	0.42
1:A:240:C:H42	1:A:286:G:H1	1.67	0.42
2:B:1641:A:H2'	2:B:1642:G:O4'	2.19	0.42
2:B:2611:U:C4	29:CA:3:LYS:HG2	2.53	0.42
54:CB:49:ALA:HB3	54:CB:99:LEU:HB2	2.00	0.42
7:G:112:MET:HB2	7:G:112:MET:HE3	1.88	0.42
2:GB:2093:G:C6	2:GB:2225:A:C8	3.07	0.42
2:GB:270(H):C:H2'	2:GB:270(I):C:C6	2.54	0.42
2:GB:26:G:C6	2:GB:27:G:N1	2.86	0.42
8:H:114:ILE:HG22	8:H:140:ILE:HG12	2.02	0.42
4:IB:67:C:H2'	4:IB:68:C:H6	1.84	0.42
13:M:19:VAL:HA	13:M:27:HIS:HB2	2.01	0.42
13:M:85:LEU:HD12	13:M:137:LYS:HD2	2.01	0.42
38:MA:192:GLU:N	38:MA:192:GLU:OE2	2.37	0.42
40:OA:4:TYR:CZ	40:OA:72:VAL:HG11	2.54	0.42
16:P:27:SER:HA	16:P:88:ASP:HB3	2.01	0.42
14:SB:68:ILE:HG23	14:SB:103:MET:HA	2.01	0.42
14:SB:38:GLU:HG3	14:SB:127:ILE:HB	2.02	0.42
39:SC:50:GLU:HB2	39:SC:53:LEU:HD13	2.00	0.42
45:TA:66:LEU:O	45:TA:70:LYS:HG3	2.19	0.42
18:WB:47:TYR:HA	18:WB:50:ARG:NH2	2.34	0.42
44:XC:38:ILE:HA	44:XC:39:PRO:HD3	1.82	0.42
1:A:262:A:C6	1:A:263:A:C6	3.07	0.42
2:B:1170:G:N2	2:B:1180:C:C2	2.87	0.42
2:B:165:U:H2'	2:B:171:G:O4'	2.19	0.42
2:B:2557:G:H2'	2:B:2558:C:C6	2.53	0.42
2:B:637:A:H4'	2:B:638:G:O5'	2.19	0.42
2:B:876:C:H2'	2:B:877:U:O4'	2.19	0.42
2:B:880:G:H1	2:B:897:C:N4	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:34:GLU:HG3	47:VA:3:ARG:HA	2.01	0.42
1:FB:433:C:H2'	1:FB:434:U:C6	2.53	0.42
1:FB:4:U:H4'	1:FB:5:U:OP2	2.19	0.42
1:FB:988:G:C2	1:FB:989:C:H1'	2.55	0.42
52:FD:76:LEU:HA	52:FD:76:LEU:HD13	1.80	0.42
7:G:140:LEU:HA	7:G:140:LEU:HD12	1.63	0.42
7:G:123:LEU:HD13	7:G:192:LEU:HB3	2.01	0.42
2:GB:1651:G:N7	15:TB:11:ASN:ND2	2.64	0.42
2:GB:2378:A:C5	2:GB:2379:G:H1'	2.54	0.42
2:GB:945:A:C4	2:GB:2448:A:C2	3.07	0.42
2:GB:2633:G:H2'	2:GB:2634:G:O4'	2.18	0.42
10:J:123:LEU:HD12	10:J:123:LEU:HA	1.93	0.42
10:J:54:GLN:HA	10:J:57:ARG:HH11	1.84	0.42
35:JA:328:ARG:NH1	35:JA:339:MET:HB3	2.34	0.42
5:JB:61:LEU:HA	5:JB:61:LEU:HD13	1.82	0.42
36:KA:19:HIS:NE2	36:KA:206:ASP:HB2	2.34	0.42
2:GB:592:G:H4'	32:KC:3:LYS:HB2	2.01	0.42
37:LA:6:HIS:HA	37:LA:7:PRO:HD3	1.93	0.42
13:M:47:ASP:HA	13:M:48:PRO:HD2	1.95	0.42
1:A:8:A:N6	38:MA:205:GLU:O	2.52	0.42
39:NA:79:GLU:H	39:NA:79:GLU:CD	2.22	0.42
9:NB:87:LEU:HD23	9:NB:164:TYR:HA	2.01	0.42
35:OC:251:THR:HB	35:OC:253:ILE:HG22	2.01	0.42
36:PC:47:THR:O	36:PC:51:LEU:N	2.52	0.42
38:RC:171:GLY:HA2	38:RC:172:PRO:HD3	1.88	0.42
38:RC:8:VAL:O	38:RC:11:LEU:HB2	2.18	0.42
44:SA:37:PRO:HA	44:SA:72:VAL:HG22	2.01	0.42
39:SC:78:HIS:CE1	42:VC:104:ARG:NH1	2.87	0.42
1:A:553:A:H5''	46:UA:24:VAL:HG21	2.01	0.42
44:XC:23:ILE:HD12	44:XC:23:ILE:HA	1.81	0.42
50:YA:1:MET:SD	50:YA:1:MET:N	2.81	0.42
20:YB:71:VAL:HA	20:YB:107:LEU:HD12	2.01	0.42
1:A:1262:C:H2'	1:A:1263:C:C6	2.54	0.42
1:A:843:U:C5	1:A:848:C:H1'	2.54	0.42
2:B:1651:G:N7	15:O:11:ASN:ND2	2.67	0.42
2:B:544:C:H2'	2:B:545:G:O4'	2.19	0.42
54:CB:66:ALA:HB3	54:CB:72:LEU:HD12	2.00	0.42
25:DC:20:ARG:HH11	25:DC:20:ARG:HG2	1.84	0.42
5:E:206:LEU:HD23	5:E:206:LEU:HA	1.73	0.42
1:FB:1513:A:H2'	1:FB:1514:C:C6	2.54	0.42
7:G:122:LYS:HB3	7:G:191:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1930:G:O2'	2:GB:1968:G:O6	2.28	0.42
2:GB:2196:C:O2'	2:GB:2197:U:H5'	2.18	0.42
2:GB:2262:U:H4'	2:GB:2328:A:C2	2.54	0.42
2:GB:392:C:H5''	2:GB:409:C:H5''	2.02	0.42
20:YB:34:ASN:ND2	29:HC:39:MET:HG3	2.35	0.42
35:JA:102:PRO:HB2	35:JA:103:LYS:H	1.64	0.42
5:JB:244:ARG:HB2	5:JB:245:PRO:HD2	2.02	0.42
2:GB:1902:C:H5'	5:JB:246:PRO:HD3	1.99	0.42
8:MB:119:GLY:HA3	8:MB:181:ARG:HA	2.01	0.42
39:NA:145:LYS:O	39:NA:149:GLU:HG3	2.20	0.42
39:NA:63:ARG:O	39:NA:66:MET:HG2	2.19	0.42
9:NB:60:ARG:HB3	9:NB:60:ARG:HH11	1.84	0.42
41:PA:114:ARG:H	41:PA:114:ARG:HG2	1.61	0.42
12:QB:119:PRO:HB2	17:VB:68:TYR:CD2	2.55	0.42
20:T:12:ILE:O	20:T:101:SER:OG	2.37	0.42
20:T:78:GLU:CD	20:T:99:ARG:HH11	2.22	0.42
45:TA:24:SER:HB2	45:TA:27:ASN:H	1.83	0.42
22:V:102:CYS:SG	22:V:104:GLY:N	2.77	0.42
22:V:13:VAL:HG12	22:V:74:PRO:HA	2.01	0.42
49:XA:2:PRO:HB2	49:XA:3:ILE:H	1.65	0.42
19:XB:68:LYS:HG2	19:XB:68:LYS:H	1.70	0.42
25:Y:40:ARG:C	25:Y:40:ARG:HD3	2.40	0.42
50:YA:6:LEU:HG	50:YA:17:TYR:HB3	2.00	0.42
1:A:134:A:N6	50:YA:25:ARG:NH1	2.68	0.42
2:B:155:C:H6	2:B:155:C:H2'	1.65	0.42
2:B:2747:G:O6	2:B:2755:C:H5''	2.20	0.42
2:B:952:G:C6	2:B:953:A:N7	2.87	0.42
1:FB:1125:U:O2'	1:FB:1126:U:O5'	2.33	0.42
1:FB:262:A:C6	1:FB:263:A:C6	3.07	0.42
52:FD:66:LEU:O	52:FD:70:ILE:HG13	2.20	0.42
2:GB:1585:C:H4'	2:GB:1586:A:OP2	2.20	0.42
2:GB:2074:U:H2'	2:GB:2075:U:C6	2.55	0.42
2:GB:2579:C:H4'	6:KB:134:ILE:HG12	2.00	0.42
4:IA:35:A:H2'	4:IA:36:U:H6	1.83	0.42
35:JA:138:TYR:CZ	35:JA:142:ARG:HD2	2.55	0.42
9:NB:118:PRO:HG2	9:NB:121:ILE:HG13	1.99	0.42
40:OA:5:GLU:HA	40:OA:63:TYR:O	2.19	0.42
35:OC:104:ASP:CG	35:OC:105:PRO:HD2	2.40	0.42
35:OC:181:GLY:O	35:OC:307:ASN:HB2	2.19	0.42
35:OC:109:ARG:HD3	35:OC:208:GLU:O	2.19	0.42
17:Q:50:ILE:HD13	17:Q:64:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RC:192:GLU:OE2	38:RC:192:GLU:N	2.39	0.42
14:SB:79:LEU:HD23	14:SB:79:LEU:HA	1.81	0.42
15:TB:33:ARG:HD2	15:TB:113:LEU:HD13	2.02	0.42
42:VC:4:ASP:HA	42:VC:5:PRO:HD2	1.92	0.42
23:W:152:ALA:C	23:W:154:ASP:H	2.23	0.42
45:YC:34:ASP:OD1	45:YC:38:ASN:HB2	2.19	0.42
45:YC:72:ALA:HB1	45:YC:77:MET:HE3	2.01	0.42
26:Z:64:LEU:O	26:Z:68:ARG:HG2	2.20	0.42
51:ZA:12:SER:HA	51:ZA:14:LYS:NZ	2.35	0.42
21:ZB:31:HIS:HA	21:ZB:32:PRO:HD3	1.89	0.42
1:A:186(A):C:H2'	1:A:186(B):C:C6	2.54	0.42
1:A:701:C:OP1	1:A:702:A:O2'	2.33	0.42
22:AC:13:VAL:HG12	22:AC:74:PRO:HA	2.00	0.42
2:B:1063:G:N1	2:B:1088:A:N1	2.68	0.42
2:B:1297:C:H2'	2:B:1298:C:H6	1.84	0.42
2:B:1539:G:H2'	2:B:1540:G:C8	2.53	0.42
2:B:1668:A:H4'	2:B:1669:A:O5'	2.20	0.42
2:B:1849:G:H2'	2:B:1850:G:H8	1.84	0.42
2:B:264:C:O2'	2:B:265:A:H2'	2.19	0.42
2:B:2690:C:N4	2:B:2713:A:H1'	2.34	0.42
2:B:2820:A:OP2	15:O:2:ARG:NH2	2.52	0.42
2:B:535:C:O3'	18:R:53:ARG:NH1	2.50	0.42
2:B:715:G:H2'	2:B:716:A:C8	2.53	0.42
2:B:879:G:H2'	2:B:880:G:H8	1.84	0.42
48:BD:50:LYS:HD2	48:BD:50:LYS:HA	1.82	0.42
3:C:3:C:C2	3:C:118:G:C2	3.07	0.42
24:CC:70:GLN:HG2	24:CC:72:ARG:HG3	2.00	0.42
30:DA:4:GLU:HG2	30:DA:4:GLU:H	1.72	0.42
1:FB:1133:G:H1	1:FB:1141:C:H42	1.68	0.42
1:FB:1291:G:C6	1:FB:1292:U:C4	3.07	0.42
1:FB:1411:C:H2'	1:FB:1412:C:C6	2.54	0.42
1:FB:160:A:H2'	1:FB:161:A:O4'	2.18	0.42
1:FB:343:U:H2'	1:FB:345:C:C5	2.55	0.42
1:FB:432:A:H3'	1:FB:433:C:H6	1.85	0.42
1:FB:563:A:N7	1:FB:567:G:H1'	2.35	0.42
1:FB:987:G:H2'	1:FB:988:G:H8	1.82	0.42
2:GB:1793:C:H2'	2:GB:1794:U:C6	2.55	0.42
2:GB:2141:G:C2	2:GB:2151:G:H1'	2.54	0.42
2:GB:2156:G:H2'	2:GB:2157:G:C5	2.55	0.42
2:GB:2479:G:H5''	2:GB:2537:U:O4'	2.19	0.42
2:GB:2850:A:OP2	2:GB:2866:U:C5	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:478:A:N1	2:GB:500:G:H4'	2.35	0.42
53:GD:62:ILE:HA	53:GD:66:MET:SD	2.60	0.42
47:AD:87:TYR:H	53:GD:73:GLU:HG2	1.85	0.42
3:C:42:C:OP1	8:H:67:LYS:HE2	2.20	0.42
54:HD:25:ARG:O	54:HD:29:LYS:HG3	2.19	0.42
55:ID:5:ASP:O	55:ID:7:ARG:N	2.47	0.42
10:J:14:ASP:OD1	10:J:15:VAL:HG12	2.19	0.42
35:JA:317:VAL:HB	35:JA:329:LEU:HD13	2.00	0.42
40:OA:86:ARG:O	40:OA:87:ARG:HG2	2.19	0.42
10:OB:40:THR:OG1	10:OB:43:ASN:OD1	2.36	0.42
36:PC:137:ARG:NH1	36:PC:138:LEU:HG	2.34	0.42
43:RA:28:VAL:HB	43:RA:36:TYR:HD2	1.84	0.42
38:RC:21:LEU:HG	38:RC:21:LEU:H	1.60	0.42
47:VA:3:ARG:NH1	47:VA:3:ARG:HB3	2.35	0.42
17:VB:35:LYS:HE2	17:VB:37:GLY:O	2.19	0.42
42:VC:86:ILE:HG13	42:VC:133:LEU:HD22	2.00	0.42
42:VC:46:LYS:HG3	42:VC:64:LYS:HB3	2.00	0.42
18:WB:76:TYR:CZ	18:WB:80:ILE:HG13	2.54	0.42
46:ZC:84:LEU:HD23	46:ZC:101:VAL:HG21	2.01	0.42
2:B:1471:A:C6	2:B:1522:G:C2	3.07	0.42
2:B:1693:U:O2'	5:E:14:ARG:NH2	2.53	0.42
2:B:2676:C:H2'	2:B:2677:G:H8	1.83	0.42
2:B:319:C:C2	2:B:333:G:N2	2.88	0.42
2:B:871:U:H2'	2:B:872:A:C8	2.54	0.42
2:B:910:A:C5	14:N:13:GLN:HG3	2.55	0.42
53:BB:58:VAL:HA	53:BB:59:PRO:HD3	1.77	0.42
23:BC:13:GLU:HB2	23:BC:18:LEU:HD11	2.01	0.42
3:C:78:A:C2	3:C:99:A:C4	3.07	0.42
5:E:61:LEU:HD13	5:E:61:LEU:HA	1.81	0.42
51:ED:84:LEU:HD23	51:ED:84:LEU:HA	1.82	0.42
1:FB:1004:A:H61	1:FB:1026:G:P	2.41	0.42
1:FB:1144:G:N2	1:FB:1146:A:H62	2.17	0.42
1:FB:1305:G:N2	1:FB:1331:G:H1'	2.34	0.42
1:FB:466:G:H4'	1:FB:467:G:OP2	2.19	0.42
1:FB:81:G:H2'	1:FB:82:U:C5	2.55	0.42
1:FB:968:A:H8	1:FB:968:A:OP1	2.03	0.42
40:TC:60:PHE:CZ	52:FD:78:LEU:HD21	2.54	0.42
2:GB:1187:G:H8	2:GB:1187:G:O5'	2.02	0.42
6:KB:68:ALA:O	6:KB:71:GLY:N	2.53	0.42
12:L:64:ARG:O	12:L:82:ASN:HA	2.20	0.42
40:OA:37:VAL:HA	40:OA:65:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:OA:19:LEU:HD21	40:OA:59:TYR:CE1	2.55	0.42
35:OC:248:HIS:CE1	35:OC:250:PRO:HD2	2.54	0.42
42:QA:119:LEU:HD12	42:QA:123:GLU:HB2	2.00	0.42
43:RA:33:PHE:CE1	43:RA:37:PHE:HD2	2.37	0.42
1:A:881:G:OP2	46:UA:12:ARG:NH2	2.53	0.42
8:H:115:ARG:NH2	47:VA:7:VAL:HG13	2.34	0.42
42:VC:123:GLU:O	42:VC:127:LEU:HD22	2.19	0.42
43:WC:113:LYS:HD3	43:WC:113:LYS:N	2.35	0.42
43:WC:113:LYS:NZ	43:WC:119:ALA:O	2.53	0.42
26:Z:16:LEU:O	26:Z:67:LYS:HE3	2.20	0.42
1:A:628:G:H2'	1:A:629:G:O4'	2.20	0.42
1:A:656:C:H4'	49:XA:62:GLN:NE2	2.24	0.42
2:B:2025:C:H2'	2:B:2026:C:C6	2.55	0.42
2:B:592:G:O2'	32:FA:4:MET:HB2	2.20	0.42
2:B:830:G:H4'	2:B:831:G:OP2	2.20	0.42
2:B:887:A:H1'	2:B:890:A:N6	2.35	0.42
23:BC:152:ALA:C	23:BC:154:ASP:H	2.23	0.42
1:FB:1137:C:H4'	1:FB:1138:G:C2	2.54	0.42
1:FB:353:A:H5'	1:FB:353:A:C8	2.54	0.42
1:FB:791:G:C6	1:FB:792:A:N7	2.88	0.42
2:GB:1060:U:H4'	2:GB:1061:U:O5'	2.20	0.42
2:GB:2037:G:C6	2:GB:2038:G:C6	3.08	0.42
2:GB:2319:G:O6	16:UB:4:LEU:HD12	2.20	0.42
2:GB:2320:A:H2'	2:GB:2320:A:N3	2.34	0.42
2:GB:2690:C:N4	2:GB:2713:A:H1'	2.35	0.42
10:J:101:LEU:HD23	10:J:109:ILE:HG12	2.02	0.42
36:KA:229:VAL:HB	36:KA:231:GLU:OE2	2.20	0.42
6:KB:181:LEU:HD12	6:KB:181:LEU:HA	1.79	0.42
6:KB:174:ASP:HB3	6:KB:183:LEU:HD22	2.01	0.42
37:LA:131:ARG:NH1	37:LA:135:LYS:HE2	2.34	0.42
8:MB:166:ASP:O	8:MB:170:ARG:HB2	2.20	0.42
8:MB:54:GLU:HA	8:MB:57:ALA:HB3	2.01	0.42
14:N:109:VAL:HG22	14:N:113:GLN:OE1	2.19	0.42
24:CC:2:ALA:HA	35:OC:236:HIS:CE1	2.54	0.42
36:PC:106:LYS:HE2	36:PC:106:LYS:HB3	1.92	0.42
17:Q:26:ASP:OD1	17:Q:120:ARG:NH2	2.47	0.42
39:NA:78:HIS:CE1	42:QA:104:ARG:NH1	2.88	0.42
42:QA:64:LYS:HG3	42:QA:79:VAL:HG21	2.01	0.42
37:QC:30:ARG:NH1	37:QC:31:HIS:CD2	2.88	0.42
38:RC:104:VAL:HG11	38:RC:146:ILE:HG13	2.01	0.42
16:UB:3:ARG:NH1	16:UB:4:LEU:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:UC:37:ASN:OD1	43:WC:41:VAL:HG22	2.19	0.42
14:N:82:ARG:HH11	24:X:4:LYS:HB2	1.83	0.42
50:YA:25:ARG:H	50:YA:25:ARG:HG2	1.54	0.42
1:A:14:U:H2'	1:A:16:A:OP2	2.20	0.42
1:A:184:G:H2'	1:A:185:A:C8	2.51	0.42
1:A:601:C:H2'	1:A:602:A:C8	2.54	0.42
2:B:1510:A:C8	2:B:1511:A:C8	3.07	0.42
2:B:1541:U:H2'	2:B:1542:G:O4'	2.19	0.42
5:E:77:ALA:HB2	5:E:97:TYR:CD1	2.54	0.42
1:FB:377:G:H1	1:FB:386:C:H42	1.68	0.42
7:G:129:PHE:HB2	7:G:132:VAL:HG21	2.01	0.42
2:GB:1409:C:H2'	2:GB:1410:G:H8	1.84	0.42
2:GB:1541:U:H2'	2:GB:1542:G:O4'	2.19	0.42
2:GB:1592:C:H2'	2:GB:1593:G:H8	1.83	0.42
2:GB:2168:G:C8	2:GB:2170:A:OP2	2.73	0.42
2:GB:2747:G:O6	2:GB:2755:C:H5''	2.19	0.42
2:GB:307:G:H21	2:GB:330:A:N6	2.12	0.42
2:GB:507:A:HO2'	2:GB:508:G:P	2.42	0.42
2:GB:875:G:H2'	2:GB:876:C:O4'	2.20	0.42
2:GB:980:A:C4	2:GB:1136:G:O4'	2.73	0.42
8:H:165:THR:OG1	8:H:166:ASP:N	2.53	0.42
10:J:64:GLU:HG3	10:J:67:ARG:NH1	2.34	0.42
10:J:67:ARG:HG3	10:J:68:LEU:HD12	2.01	0.42
7:LB:185:ASP:OD1	7:LB:188:ARG:NH1	2.53	0.42
38:MA:148:VAL:HG12	38:MA:181:MET:O	2.20	0.42
8:MB:64:THR:HB	8:MB:94:LEU:HD21	2.01	0.42
16:P:26:LEU:HD22	16:P:87:PHE:CE1	2.55	0.42
36:PC:10:LEU:HG	36:PC:48:MET:SD	2.59	0.42
36:PC:219:VAL:HA	36:PC:222:ILE:HB	2.01	0.42
40:TC:100:ASN:OD1	52:FD:23:LYS:HG2	2.19	0.42
40:TC:5:GLU:HA	40:TC:63:TYR:O	2.20	0.42
17:VB:109:GLU:HG2	17:VB:112:ARG:NH2	2.34	0.42
42:VC:23:SER:OG	42:VC:60:ARG:HG3	2.20	0.42
42:VC:31:PHE:O	42:VC:35:ILE:HG13	2.19	0.42
1:A:1277:C:O2'	1:A:1279:A:H1'	2.19	0.42
1:A:1452:C:H2'	1:A:1453:G:H5''	2.01	0.42
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.42
1:A:433:C:H2'	1:A:434:U:C6	2.55	0.42
1:A:882:C:O2'	1:A:883:C:H5'	2.20	0.42
2:GB:296:C:O3'	22:AC:95:LYS:NZ	2.53	0.42
2:B:1657:C:H2'	2:B:1658:C:C6	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2317:C:C2'	2:B:2318:G:H5'	2.48	0.42
2:B:609(B):G:H2'	2:B:610:C:C6	2.55	0.42
2:B:813:U:H2'	2:B:814:C:C6	2.54	0.42
54:CB:83:ARG:HA	54:CB:86:ARG:HD3	2.02	0.42
4:D:63:G:H2'	4:D:64:G:C8	2.55	0.42
4:D:7:G:H5''	4:D:8:4SU:H5	2.01	0.42
1:FB:381:C:H2'	1:FB:382:A:O4'	2.20	0.42
2:GB:1490:A:O5'	2:GB:1490:A:H8	2.03	0.42
2:GB:1510:A:C8	2:GB:1511:A:C8	3.08	0.42
2:GB:1575:C:H2'	2:GB:1576:U:O4'	2.20	0.42
8:H:50:ALA:C	8:H:52:ILE:H	2.23	0.42
9:I:155:SER:HB3	9:I:158:HIS:O	2.19	0.42
4:IB:10:G:H2'	4:IB:11:A:H8	1.84	0.42
10:J:109:ILE:H	10:J:109:ILE:HG13	1.80	0.42
11:K:99:LEU:HA	11:K:99:LEU:HD23	1.87	0.42
36:KA:69:LEU:O	36:KA:163:PHE:N	2.45	0.42
32:KC:52:LYS:HB3	32:KC:53:PRO:HD3	2.02	0.42
4:NC:35:A:H2'	4:NC:36:U:C6	2.55	0.42
10:OB:67:ARG:HG3	10:OB:68:LEU:HD12	2.01	0.42
16:P:26:LEU:HD22	16:P:87:PHE:HE1	1.85	0.42
42:QA:4:ASP:HA	42:QA:5:PRO:HD2	1.88	0.42
18:R:95:LEU:HD13	18:R:95:LEU:HA	1.80	0.42
44:SA:38:ILE:HA	44:SA:39:PRO:HD3	1.82	0.42
2:GB:2275:C:O2	14:SB:85:LYS:HG3	2.19	0.42
39:SC:69:VAL:HG11	39:SC:113:ALA:HB1	2.02	0.42
46:UA:84:LEU:HD22	46:UA:104:VAL:HG11	2.02	0.42
47:VA:97:PRO:HA	47:VA:110:ARG:HG3	2.01	0.42
36:PC:178:ARG:NH2	42:VC:74:PRO:HB3	2.34	0.42
18:WB:80:ILE:HD13	18:WB:80:ILE:HA	1.76	0.42
1:A:236:G:H2'	1:A:237:C:O4'	2.20	0.42
1:A:38:G:N1	1:A:397:A:OP1	2.51	0.42
1:A:452:A:O2'	1:A:453:A:H8	2.03	0.42
47:AD:66:LEU:C	47:AD:70:LEU:HB2	2.40	0.42
2:B:1252:G:C2	2:B:1253:A:C2	3.08	0.42
2:B:1901:A:N3	2:B:1901:A:H2'	2.35	0.42
2:B:2287:A:C4	2:B:2289:G:C8	3.08	0.42
2:B:573:G:O2'	2:B:574:C:H3'	2.20	0.42
2:B:616:A:C4	7:G:180:GLY:HA2	2.55	0.42
48:BD:14:PRO:HB2	48:BD:15:LYS:H	1.56	0.42
54:CB:25:ARG:O	54:CB:29:LYS:HG3	2.19	0.42
49:CD:63:ARG:HG2	49:CD:67:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:1350:A:C6	1:FB:1351:U:C4	3.08	0.42
1:FB:603:U:H2'	1:FB:604:G:H8	1.85	0.42
1:FB:967:5MC:H2'	1:FB:968:A:C8	2.54	0.42
2:GB:330:A:C2	2:GB:1210:A:H2'	2.53	0.42
2:GB:2159:G:H2'	2:GB:2160:G:C8	2.55	0.42
2:GB:2298:A:N6	2:GB:2318:G:H8	1.94	0.42
2:GB:643:A:C8	30:IC:44:ARG:NH1	2.88	0.42
53:GD:36:ARG:HB2	53:GD:72:GLY:HA3	2.01	0.42
54:HD:88:VAL:O	54:HD:92:LEU:HB2	2.20	0.42
4:IA:47:U:H6	4:IA:47:U:OP2	2.02	0.42
37:LA:138:VAL:O	37:LA:142:MET:HB2	2.20	0.42
8:MB:121:ASN:ND2	8:MB:181:ARG:HH22	2.17	0.42
8:MB:121:ASN:HA	8:MB:122:PRO:HD3	1.91	0.42
39:NA:20:GLN:O	39:NA:23:GLY:N	2.43	0.42
10:OB:48:GLU:O	10:OB:52:ARG:HB2	2.20	0.42
2:GB:1141:U:H2'	11:PB:63:THR:HG21	2.01	0.42
36:PC:25:ASN:O	36:PC:27:LYS:N	2.53	0.42
42:QA:97:VAL:HG21	42:QA:128:GLY:HA2	2.02	0.42
14:SB:2:LEU:O	14:SB:3:MET:HB3	2.20	0.42
39:SC:79:GLU:H	39:SC:79:GLU:CD	2.23	0.42
46:UA:59:ARG:HD3	46:UA:65:GLU:HG2	2.02	0.42
49:XA:11:VAL:HG21	49:XA:34:LEU:HD13	2.01	0.42
19:XB:8:GLY:HA3	19:XB:23:GLU:HB2	2.01	0.42
25:Y:50:ARG:HG2	25:Y:59:THR:HB	2.02	0.42
1:A:1226:C:H4'	53:BB:80:TYR:OH	2.19	0.41
1:A:444:C:H2'	1:A:445:G:H8	1.85	0.41
1:A:583:A:H61	1:A:758:G:H1'	1.85	0.41
1:A:624:C:H2'	1:A:625:G:C8	2.54	0.41
1:A:828:A:H2'	1:A:829:G:O4'	2.19	0.41
27:AA:3:ARG:NH1	27:AA:60:GLU:OE1	2.53	0.41
2:B:1005:C:H2'	2:B:1006:C:C6	2.54	0.41
2:B:2325:G:H5''	2:B:2326:C:OP2	2.20	0.41
2:B:2712:U:H1'	2:B:2712(A):A:C8	2.55	0.41
2:B:2773:C:H2'	2:B:2774:C:H6	1.85	0.41
53:BB:22:LEU:HD23	53:BB:26:GLY:O	2.20	0.41
44:XC:61:GLU:HG3	48:BD:58:LYS:HE3	2.01	0.41
4:D:67:C:H2'	4:D:68:C:H6	1.84	0.41
26:EC:41:ILE:HG13	26:EC:41:ILE:H	1.57	0.41
6:F:78:LEU:HA	6:F:78:LEU:HD13	1.79	0.41
1:FB:1048:G:OP1	48:BD:3:ARG:HB3	2.19	0.41
1:FB:1372:U:H2'	1:FB:1373:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:14:U:H2'	1:FB:16:A:OP2	2.20	0.41
1:FB:628:G:H2'	1:FB:629:G:O4'	2.19	0.41
2:GB:1063:G:N1	2:GB:1088:A:N1	2.68	0.41
2:GB:1388:G:H2'	2:GB:1389:G:H8	1.85	0.41
1:FB:784:C:H4'	2:GB:1837:C:OP1	2.20	0.41
8:H:135:LEU:HD12	8:H:136:ARG:HH21	1.84	0.41
8:H:164:GLU:HB2	8:H:168:GLU:OE2	2.20	0.41
4:IA:35:A:H2'	4:IA:36:U:C6	2.55	0.41
38:MA:4:TYR:HA	38:MA:4:TYR:HD2	1.70	0.41
39:NA:69:VAL:HG11	39:NA:113:ALA:HB1	2.02	0.41
9:NB:11:VAL:HG13	9:NB:15:VAL:HG23	2.02	0.41
35:OC:182:HIS:HB3	35:OC:310:TYR:CE1	2.50	0.41
2:B:2378:A:H4'	16:P:23:ARG:NH1	2.35	0.41
36:PC:220:ASP:C	36:PC:222:ILE:H	2.23	0.41
19:S:29:PRO:HA	19:S:61:VAL:HG22	2.02	0.41
39:SC:80:ILE:HD11	39:SC:138:ALA:HB1	2.00	0.41
2:B:1614:A:C2	20:T:93:ALA:HB2	2.55	0.41
45:TA:121:PRO:HB2	45:TA:125:PHE:HB2	2.01	0.41
45:TA:86:GLY:O	45:TA:91:ARG:NH1	2.47	0.41
40:TC:37:VAL:HA	40:TC:65:VAL:HG12	2.01	0.41
41:UC:107:ALA:HA	41:UC:110:GLN:HG2	2.01	0.41
22:V:15:VAL:HG11	22:V:20:TYR:HB2	2.01	0.41
23:W:61:LEU:HB3	23:W:63:ASP:OD1	2.20	0.41
18:WB:14:HIS:O	18:WB:18:LEU:HD12	2.19	0.41
43:WC:53:VAL:HG11	43:WC:85:LEU:HD13	2.01	0.41
25:Y:85:LEU:HD23	25:Y:89:GLU:HB3	2.02	0.41
20:YB:13:SER:HA	20:YB:14:PRO:HD3	1.90	0.41
1:A:1291:G:C6	1:A:1292:U:C4	3.09	0.41
1:A:1293:G:H2'	1:A:1294:G:C8	2.56	0.41
1:A:332:G:OP2	54:CB:10:LEU:HG	2.21	0.41
1:A:603:U:H2'	1:A:604:G:H8	1.84	0.41
1:A:88:C:H2'	1:A:89:U:C6	2.54	0.41
47:AD:14:ARG:NE	47:AD:42:ALA:HA	2.35	0.41
47:AD:97:PRO:HA	47:AD:110:ARG:HG3	2.01	0.41
2:B:1519:G:H2'	2:B:1520:U:O4'	2.20	0.41
2:B:1798:U:H5'	5:E:259:THR:CG2	2.38	0.41
2:B:1850:G:H1	2:B:1892:C:H42	1.68	0.41
2:B:2088:G:C6	2:B:2089:U:C4	3.08	0.41
2:B:2364:C:H2'	2:B:2365:G:O4'	2.20	0.41
2:B:352:G:H4'	2:B:353:G:OP2	2.20	0.41
2:B:958:U:H5'	14:N:14:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BC:150:LEU:HD12	23:BC:171:ILE:HB	2.02	0.41
55:DB:2:GLY:N	55:DB:5:ASP:HB2	2.35	0.41
31:EA:3:ARG:HA	31:EA:3:ARG:HD3	1.74	0.41
1:FB:562:C:H4'	1:FB:563:A:O5'	2.20	0.41
2:GB:186:G:H2'	2:GB:187:G:H8	1.85	0.41
2:GB:2162:G:H1'	2:GB:2173:A:H1'	2.02	0.41
2:GB:742:G:H2'	2:GB:743:G:H8	1.85	0.41
9:I:70:THR:HG22	9:I:74:ASN:OD1	2.20	0.41
10:J:110:ASP:HA	10:J:111:PRO:HD2	1.86	0.41
10:J:57:ARG:HG3	10:J:57:ARG:H	1.71	0.41
2:GB:784:A:C6	5:JB:229:VAL:HG21	2.55	0.41
36:KA:59:GLU:HG3	36:KA:225:ALA:HB2	2.01	0.41
2:B:411:G:C5	13:M:72:PRO:HB3	2.56	0.41
8:MB:103:LEU:HD23	8:MB:103:LEU:HA	1.88	0.41
1:A:864:A:H5'	39:NA:86:ALA:HB2	2.02	0.41
15:O:74:LYS:HE2	15:O:74:LYS:HB2	1.90	0.41
42:QA:50:ARG:H	42:QA:50:ARG:HG2	1.54	0.41
39:SC:40:ARG:CZ	39:SC:68:GLU:HB2	2.49	0.41
39:SC:92:LYS:HA	39:SC:93:PRO:HD3	1.88	0.41
40:TC:46:ARG:HB2	40:TC:60:PHE:HE1	1.82	0.41
41:UC:46:ALA:O	41:UC:50:ILE:HG13	2.20	0.41
43:WC:28:VAL:HB	43:WC:36:TYR:HD2	1.85	0.41
1:A:1350:A:C6	1:A:1351:U:C4	3.09	0.41
27:AA:26:LEU:HA	27:AA:26:LEU:HD23	1.85	0.41
2:B:1773:A:C5	2:B:1829:A:H1'	2.55	0.41
2:B:1842:G:H2'	2:B:1843:C:C6	2.55	0.41
2:B:2567:G:H2'	2:B:2568:C:C6	2.56	0.41
2:B:2615:U:C2	29:CA:7:PRO:HA	2.55	0.41
2:B:2780:G:H4'	2:B:2781:A:OP2	2.19	0.41
2:B:392:C:H5''	2:B:409:C:H5''	2.02	0.41
2:B:587:C:C6	2:B:671:C:H1'	2.56	0.41
2:B:716:A:C2	2:B:717:G:H1'	2.55	0.41
26:EC:37:PHE:O	26:EC:40:SER:HB3	2.19	0.41
32:FA:36:LYS:HD3	32:FA:40:GLU:OE2	2.21	0.41
1:FB:623:C:O5'	1:FB:623:C:H6	2.03	0.41
27:FC:1:MET:HA	27:FC:2:PRO:HD2	1.92	0.41
2:GB:1613:G:C2	2:GB:1619:G:C5	3.08	0.41
2:GB:1800:C:OP1	5:JB:260:ARG:NH2	2.53	0.41
2:GB:270(S):G:H2'	2:GB:270(T):G:C8	2.54	0.41
54:HD:49:ALA:HB3	54:HD:99:LEU:HB2	2.02	0.41
36:KA:166:ASP:HA	36:KA:167:PRO:HD3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:KA:97:TRP:HH2	36:KA:176:GLU:CD	2.24	0.41
36:KA:215:LEU:O	36:KA:219:VAL:HG23	2.20	0.41
13:M:119:GLU:HB2	27:FC:1:MET:N	2.35	0.41
14:N:69:PHE:HA	14:N:70:PRO:HD3	1.76	0.41
9:NB:3:ARG:NH2	9:NB:5:GLY:H	2.18	0.41
10:OB:110:ASP:OD1	10:OB:112:LYS:HE3	2.20	0.41
16:P:41:ASP:OD2	16:P:44:LYS:HG3	2.19	0.41
42:QA:125:ARG:HH11	42:QA:125:ARG:HG2	1.85	0.41
12:QB:25:LEU:HD23	12:QB:25:LEU:HA	1.71	0.41
37:QC:125:GLU:HG2	37:QC:190:ARG:O	2.19	0.41
44:SA:25:GLU:O	44:SA:29:ARG:HG3	2.20	0.41
16:UB:26:LEU:HD22	16:UB:87:PHE:HE1	1.85	0.41
4:IB:30:G:H21	41:UC:144:MET:CE	2.33	0.41
17:VB:126:ALA:HA	17:VB:129:ARG:CZ	2.49	0.41
42:VC:53:VAL:HB	42:VC:58:TYR:CD2	2.56	0.41
1:A:432:A:H2'	1:A:433:C:O4'	2.20	0.41
27:AA:3:ARG:HB2	27:AA:60:GLU:HB2	2.03	0.41
22:AC:68:HIS:ND1	22:AC:70:SER:HB3	2.35	0.41
2:B:330:A:C2	2:B:1210:A:H2'	2.54	0.41
2:B:1406:U:H2'	2:B:1407:C:C6	2.55	0.41
2:B:1800:C:OP1	5:E:260:ARG:NH2	2.52	0.41
2:B:2101:G:C5	2:B:2102:U:C4	3.09	0.41
2:B:2216:G:H2'	2:B:2217:G:H8	1.85	0.41
2:B:2331:G:O2'	2:B:2336:A:N1	2.42	0.41
2:B:2695:C:H2'	2:B:2696:U:H6	1.85	0.41
2:B:2818:G:O2'	2:B:2837:G:H5'	2.20	0.41
23:BC:129:SER:HB3	23:BC:132:ASN:HD21	1.85	0.41
23:BC:61:LEU:HB2	23:BC:65:GLN:HB2	2.02	0.41
4:D:10:G:H2'	4:D:11:A:H8	1.85	0.41
4:D:51:C:O2	4:D:64:G:N2	2.53	0.41
1:FB:149:A:H2'	1:FB:150:C:H6	1.85	0.41
1:FB:339:C:H2'	1:FB:340:U:H6	1.84	0.41
1:FB:487:A:H5''	1:FB:488:C:OP2	2.20	0.41
1:FB:59:A:H5''	1:FB:60:A:H5''	2.03	0.41
1:FB:78:G:H2'	1:FB:79:G:O4'	2.21	0.41
1:FB:828:A:H2'	1:FB:829:G:O4'	2.19	0.41
2:GB:1297:C:H2'	2:GB:1298:C:C6	2.55	0.41
2:GB:1470:G:H8	2:GB:1470:G:O5'	2.03	0.41
2:GB:2251:OMG:HM23	2:GB:2251:OMG:H1'	1.72	0.41
2:GB:2319:G:OP1	2:GB:2319:G:H3'	2.20	0.41
28:GC:40:HIS:HA	28:GC:41:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:60:ARG:HB3	9:I:60:ARG:HH11	1.86	0.41
9:I:52:VAL:HG23	9:I:65:HIS:CD2	2.56	0.41
35:JA:131:LEU:HA	35:JA:134:MET:HG2	2.03	0.41
35:JA:131:LEU:O	35:JA:134:MET:HG3	2.20	0.41
35:JA:278:ILE:HG13	35:JA:279:HIS:N	2.35	0.41
5:JB:26:LYS:HB3	5:JB:83:GLU:HG2	2.03	0.41
1:A:1055:A:H2'	37:LA:156:ARG:HD2	2.02	0.41
38:MA:8:VAL:O	38:MA:11:LEU:HB2	2.20	0.41
38:MA:8:VAL:HB	38:MA:115:ARG:NH1	2.35	0.41
39:NA:113:ALA:HB3	39:NA:115:VAL:HG23	2.03	0.41
9:NB:101:ARG:HG3	9:NB:117:PRO:HG3	2.02	0.41
38:RC:12:CYS:SG	38:RC:18:LYS:CE	3.08	0.41
14:SB:72:LYS:HA	14:SB:73:PRO:HD3	1.87	0.41
1:A:695:A:OP2	45:TA:53:SER:HB2	2.20	0.41
41:UC:53:LYS:O	41:UC:54:THR:OG1	2.37	0.41
23:W:31:ARG:H	23:W:31:ARG:HG2	1.68	0.41
1:A:1239:A:H62	1:A:1299:A:H62	1.68	0.41
1:A:339:C:H2'	1:A:340:U:C6	2.55	0.41
1:A:375:U:H4'	50:YA:17:TYR:CE1	2.56	0.41
1:A:606:G:H2'	1:A:631:G:N2	2.35	0.41
1:A:778:G:H8	1:A:778:G:O5'	2.04	0.41
47:AD:37:THR:O	47:AD:55:ARG:NH1	2.48	0.41
2:B:1952:A:C6	2:B:1953:A:N1	2.89	0.41
2:B:2479:G:H5''	2:B:2537:U:O4'	2.20	0.41
2:B:2633:G:H2'	2:B:2634:G:O4'	2.20	0.41
23:BC:169:GLU:HA	23:BC:169:GLU:OE2	2.20	0.41
31:EA:26:GLY:O	31:EA:30:VAL:HG23	2.20	0.41
6:F:68:ALA:O	6:F:71:GLY:N	2.53	0.41
1:FB:253:U:H2'	1:FB:254:G:C8	2.56	0.41
1:FB:428:G:O4'	1:FB:430:A:C8	2.73	0.41
2:GB:1289:C:H2'	2:GB:1290:C:C6	2.55	0.41
2:GB:1373:A:H2'	2:GB:1374:G:O4'	2.21	0.41
2:GB:1773:A:C5	2:GB:1829:A:H1'	2.55	0.41
2:GB:251:A:C5	2:GB:252:G:H1'	2.55	0.41
2:GB:637:A:H4'	2:GB:638:G:O5'	2.21	0.41
53:GD:29:ARG:NH1	53:GD:29:ARG:HA	2.35	0.41
3:HB:30:C:H2'	3:HB:31:C:H5'	2.03	0.41
4:IB:8:4SU:H1'	4:IB:48:C:O2	2.21	0.41
35:JA:103:LYS:O	35:JA:104:ASP:HB2	2.20	0.41
5:JB:227:ASN:HB3	5:JB:228:PRO:HD2	2.03	0.41
36:KA:178:ARG:NH2	42:QA:74:PRO:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:NB:101:ARG:NH1	9:NB:122:THR:HG23	2.35	0.41
16:P:56:LEU:HA	16:P:56:LEU:HD22	1.88	0.41
11:PB:35:ARG:HH11	11:PB:35:ARG:HG2	1.86	0.41
17:Q:6:LEU:HD13	17:Q:6:LEU:HA	1.82	0.41
38:RC:177:ASP:OD1	38:RC:180:GLY:HA3	2.20	0.41
40:TC:40:VAL:HG22	40:TC:63:TYR:CD1	2.55	0.41
42:VC:85:ARG:NH1	42:VC:87:SER:O	2.53	0.41
46:ZC:59:ARG:HH11	46:ZC:65:GLU:HG3	1.84	0.41
1:A:253:U:H2'	1:A:254:G:C8	2.56	0.41
1:A:382:A:H2'	1:A:383:A:C8	2.55	0.41
1:A:373:A:O2'	1:A:451:A:N7	2.54	0.41
2:B:1935:G:H1'	2:B:1964:G:N2	2.36	0.41
2:B:2005:A:H5''	2:B:2006:C:OP2	2.20	0.41
2:B:481:G:C2	2:B:507:A:C4	3.08	0.41
2:B:57:C:H2'	2:B:58:G:O4'	2.20	0.41
2:B:751:A:C6	2:B:789:A:C5	3.09	0.41
2:B:807:U:OP2	13:M:41:ARG:NH2	2.54	0.41
2:B:848:G:N9	2:B:933:A:H8	2.17	0.41
2:B:895:U:H5'	2:B:896:A:OP1	2.21	0.41
53:BB:19:VAL:HA	53:BB:22:LEU:HD12	2.02	0.41
53:BB:3:ARG:NH1	53:BB:7:LYS:HD3	2.36	0.41
25:DC:73:LEU:HB3	25:DC:94:LEU:HD22	2.02	0.41
1:FB:617:G:H4'	50:DD:44:THR:O	2.21	0.41
1:FB:1277:C:O2'	1:FB:1279:A:H1'	2.20	0.41
1:FB:382:A:H2'	1:FB:383:A:C8	2.56	0.41
1:FB:630:G:H3'	1:FB:631:G:H8	1.85	0.41
52:FD:73:ALA:HB3	52:FD:79:LEU:HD12	2.02	0.41
2:GB:117:G:C6	2:GB:119:A:C6	3.08	0.41
2:GB:2321:G:H5'	2:GB:2322:A:OP2	2.20	0.41
2:GB:2643:G:H2'	2:GB:2644:G:O4'	2.20	0.41
2:GB:2712:U:H1'	2:GB:2712(A):A:C8	2.56	0.41
2:GB:544:C:H2'	2:GB:545:G:O4'	2.21	0.41
2:GB:7:G:H4'	11:PB:13:TRP:CH2	2.56	0.41
2:GB:828:U:H4'	2:GB:831:G:N1	2.35	0.41
4:IA:35:A:P	43:RA:128:ARG:HH11	2.43	0.41
4:IA:47:U:H6	4:IA:47:U:P	2.44	0.41
4:IB:40:C:H2'	4:IB:41:C:H6	1.85	0.41
10:J:31:LEU:HD21	10:J:37:VAL:HA	2.03	0.41
4:IA:76:A:O2'	35:JA:235:GLN:HB2	2.20	0.41
37:LA:35:GLU:O	37:LA:39:ILE:HG13	2.21	0.41
8:MB:11:TYR:OH	8:MB:16:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:OA:60:PHE:CZ	52:AB:78:LEU:HD21	2.54	0.41
10:OB:26:ALA:O	10:OB:31:LEU:HB2	2.20	0.41
10:OB:6:LEU:HD11	10:OB:37:VAL:HB	2.03	0.41
12:QB:64:ARG:NH1	12:QB:81:ASP:OD1	2.54	0.41
2:GB:637:A:H8	13:RB:117:GLU:HG3	1.86	0.41
19:S:31:ALA:O	19:S:61:VAL:HG12	2.21	0.41
40:TC:8:ILE:HB	40:TC:61:LEU:HB2	2.03	0.41
41:UC:116:ALA:HA	41:UC:119:ARG:NH1	2.36	0.41
17:VB:100:TYR:HB3	17:VB:103:ARG:NH1	2.29	0.41
44:XC:25:GLU:N	44:XC:25:GLU:OE2	2.51	0.41
1:A:987:G:H2'	1:A:988:G:H8	1.82	0.41
52:AB:66:LEU:O	52:AB:70:ILE:HG13	2.21	0.41
2:B:1472:A:H61	2:B:1521:G:H1'	1.85	0.41
2:B:221:A:H61	2:B:265:A:H8	1.69	0.41
2:B:2483:C:H2'	2:B:2484:G:O4'	2.21	0.41
24:CC:65:GLY:HA2	24:CC:84:LEU:HG	2.02	0.41
1:FB:375:U:H4'	50:DD:17:TYR:CE1	2.56	0.41
50:DD:4:ILE:HG23	50:DD:36:ILE:HD11	2.02	0.41
50:DD:55:ARG:HD2	50:DD:55:ARG:HA	1.83	0.41
5:E:121:PRO:HB3	5:E:135:PHE:CE2	2.56	0.41
1:FB:191(E):G:H2'	1:FB:191(F):U:C6	2.56	0.41
1:FB:378:G:C6	1:FB:379:C:C4	3.08	0.41
2:GB:1454:U:OP1	15:TB:77:ARG:NH1	2.53	0.41
2:GB:2451:A:H5'	24:CC:3:HIS:NE2	2.36	0.41
2:GB:2893:G:O5'	2:GB:2893:G:H8	2.04	0.41
2:GB:385:C:O2'	2:GB:388:G:N2	2.53	0.41
2:GB:656:G:H2'	2:GB:657:U:C6	2.55	0.41
2:GB:879:G:H2'	2:GB:880:G:H8	1.85	0.41
5:JB:108:PRO:HB3	5:JB:143:HIS:HE1	1.85	0.41
5:JB:213:ARG:HD2	5:JB:217:ARG:O	2.20	0.41
5:JB:273:ARG:HH11	5:JB:273:ARG:HB3	1.85	0.41
36:KA:70:PHE:HE1	36:KA:163:PHE:HD1	1.68	0.41
37:LA:30:ARG:NH1	37:LA:31:HIS:CD2	2.89	0.41
9:NB:9:ILE:HA	9:NB:10:PRO:HD2	1.91	0.41
40:OA:22:GLU:OE1	40:OA:82:ARG:NH2	2.54	0.41
40:OA:6:VAL:HG12	40:OA:8:ILE:HD11	2.03	0.41
41:PA:87:VAL:HA	41:PA:88:PRO:HD3	1.86	0.41
17:Q:126:ALA:HA	17:Q:129:ARG:CZ	2.51	0.41
43:RA:22:GLY:HA3	43:RA:60:ASP:CG	2.41	0.41
14:SB:118:LEU:HD23	14:SB:118:LEU:HA	1.92	0.41
20:T:11:ARG:HD3	20:T:82:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:45:VAL:O	22:V:62:GLU:HA	2.20	0.41
1:A:1216:G:OP1	48:WA:2:ALA:N	2.53	0.41
43:WC:40:LEU:HB2	43:WC:43:ALA:HB2	2.02	0.41
45:YC:79:SER:HA	45:YC:104:GLN:CB	2.46	0.41
1:A:1004:A:H61	1:A:1026:G:P	2.43	0.41
1:A:1128:C:H4'	1:A:1148:U:O2	2.20	0.41
1:A:1417:G:O2'	1:A:1483:A:N6	2.53	0.41
1:A:1504:G:OP1	1:A:1507:A:H4'	2.20	0.41
1:A:706:A:C5'	45:TA:22:HIS:CD2	3.03	0.41
27:AA:35:ARG:HH21	27:AA:37:LEU:HD21	1.86	0.41
2:B:1289:C:H2'	2:B:1290:C:C6	2.56	0.41
2:B:1586:A:C2'	2:B:1587:A:H5'	2.50	0.41
2:B:1686:C:H2'	2:B:1687:G:O4'	2.21	0.41
2:B:221:A:N6	2:B:265:A:H8	2.18	0.41
28:BA:40:HIS:HA	28:BA:41:PRO:HD2	1.87	0.41
53:BB:29:ARG:HA	53:BB:29:ARG:HH11	1.86	0.41
23:BC:4:ARG:HD3	23:BC:60:GLU:OE2	2.21	0.41
31:EA:34:ARG:CG	31:EA:34:ARG:HH11	2.31	0.41
1:FB:1101:A:H4'	1:FB:1102:A:O5'	2.21	0.41
1:FB:335:C:H2'	1:FB:336:C:C6	2.55	0.41
2:GB:479:A:H1'	2:GB:480:A:H5''	2.02	0.41
53:GD:3:ARG:NH1	53:GD:7:LYS:HD3	2.35	0.41
8:H:119:GLY:HA3	8:H:181:ARG:HA	2.03	0.41
36:KA:217:ARG:HA	36:KA:217:ARG:HD3	1.90	0.41
7:LB:123:LEU:HD13	7:LB:192:LEU:HB3	2.03	0.41
13:M:83:VAL:CG1	13:M:112:LEU:HD21	2.51	0.41
8:MB:106:LEU:HA	8:MB:110:ALA:HB3	2.03	0.41
14:N:2:LEU:HB2	14:N:70:PRO:HG2	2.01	0.41
9:NB:144:VAL:O	9:NB:148:ILE:HG12	2.20	0.41
35:OC:271:LEU:HA	35:OC:271:LEU:HD23	1.95	0.41
36:PC:163:PHE:HD2	36:PC:163:PHE:HA	1.63	0.41
36:PC:87:ARG:CZ	36:PC:233:SER:HB2	2.51	0.41
12:QB:105:GLU:N	12:QB:105:GLU:OE1	2.50	0.41
37:QC:38:ARG:HD2	37:QC:94:LEU:HD11	2.02	0.41
18:R:76:TYR:CZ	18:R:80:ILE:HG13	2.56	0.41
47:VA:84:ILE:HB	53:BB:74:PHE:HE1	1.86	0.41
44:XC:15:THR:HB	44:XC:91:PRO:HG3	2.03	0.41
20:YB:45:TYR:CZ	20:YB:49:LYS:HE3	2.55	0.41
26:Z:1:MET:HE2	26:Z:9:GLN:HB2	2.02	0.41
1:A:1031:G:C8	1:A:1032(B):G:N1	2.88	0.41
1:A:1296:C:H4'	1:A:1302:U:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:A:H2'	1:A:1361:G:O4'	2.21	0.41
1:A:1502:A:C8	1:A:1505:G:N2	2.88	0.41
1:A:335:C:H2'	1:A:336:C:C6	2.55	0.41
1:A:860:A:H2'	1:A:861:G:O4'	2.21	0.41
52:AB:53:ARG:HA	52:AB:56:THR:OG1	2.21	0.41
2:B:2022:U:O2'	2:B:2617:C:H5'	2.21	0.41
2:B:270(W):G:C4	2:B:270(X):G:C8	3.09	0.41
2:B:2850:A:OP2	2:B:2866:U:C5	2.74	0.41
23:BC:97:GLU:HB3	23:BC:125:LEU:HD11	2.03	0.41
5:E:147:LEU:HD13	5:E:155:LEU:HD11	2.02	0.41
1:FB:1296:C:H4'	1:FB:1302:U:C5	2.56	0.41
1:FB:433:C:H2'	1:FB:434:U:H6	1.86	0.41
1:FB:778:G:H2'	1:FB:779:C:O4'	2.21	0.41
7:G:120:GLU:HB3	7:G:122:LYS:HG2	2.03	0.41
2:GB:1021:A:C3'	2:GB:1021:A:C8	3.02	0.41
2:GB:2652:C:H2'	2:GB:2653:U:O4'	2.21	0.41
2:GB:57:C:H2'	2:GB:58:G:O4'	2.21	0.41
2:GB:733:G:O6	2:GB:761:A:C8	2.73	0.41
1:FB:323:U:O3'	54:HD:22:ARG:HD3	2.21	0.41
13:M:50:ARG:HH21	32:FA:7:HIS:CD2	2.39	0.41
14:N:68:ILE:HG23	14:N:103:MET:HA	2.03	0.41
2:B:1454:U:OP1	15:O:77:ARG:NH1	2.50	0.41
35:OC:103:LYS:O	35:OC:104:ASP:HB2	2.20	0.41
41:PA:53:LYS:O	41:PA:54:THR:OG1	2.34	0.41
37:QC:191:THR:HB	37:QC:193:TYR:CE2	2.56	0.41
39:SC:127:ASN:HA	39:SC:128:PRO:HD2	1.93	0.41
20:T:9:TYR:H	20:T:102:HIS:CE1	2.39	0.41
20:T:45:TYR:CZ	20:T:49:LYS:HE3	2.56	0.41
45:TA:34:ASP:OD2	45:TA:36:ASP:HB2	2.21	0.41
46:UA:59:ARG:HH11	46:UA:65:GLU:HG3	1.85	0.41
47:VA:60:VAL:HG13	47:VA:64:TRP:CE3	2.56	0.41
17:VB:132:LYS:NZ	17:VB:132:LYS:CB	2.84	0.41
23:W:44:PHE:CE1	23:W:86:VAL:HG11	2.55	0.41
51:ZA:83:ASP:N	51:ZA:83:ASP:OD1	2.54	0.41
1:A:1137:C:H4'	1:A:1138:G:C2	2.56	0.41
1:A:381:C:H2'	1:A:382:A:O4'	2.21	0.41
1:A:570:G:H1'	1:A:820:U:C4	2.55	0.41
2:B:125:G:H4'	2:B:126:A:OP2	2.21	0.41
2:B:247:G:H4'	2:B:386:G:C5	2.55	0.41
2:B:483:A:O2'	22:V:59:GLY:N	2.53	0.41
2:B:656:G:H2'	2:B:657:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:U:H1'	2:B:91:A:C8	2.56	0.41
23:BC:158:PRO:O	23:BC:161:VAL:HB	2.20	0.41
23:BC:79:ARG:HB3	23:BC:80:ARG:HD3	2.02	0.41
6:F:56:PRO:C	6:F:58:ARG:H	2.25	0.41
1:FB:1009:G:N2	1:FB:1020:U:O2	2.41	0.41
1:FB:1191:A:OP1	37:QC:4:LYS:HG3	2.20	0.41
1:FB:1293:G:H2'	1:FB:1294:G:C8	2.56	0.41
52:FD:41:LYS:HB3	52:FD:41:LYS:HE2	1.82	0.41
2:GB:2344:U:O2'	30:IC:36:LEU:HD22	2.21	0.41
2:GB:2853:C:H2'	2:GB:2854:G:H8	1.86	0.41
36:KA:126:GLU:CD	36:KA:130:ARG:HB2	2.41	0.41
12:L:63:VAL:HG12	12:L:106:LEU:HD11	2.03	0.41
2:B:637:A:H8	13:M:117:GLU:HG3	1.86	0.41
38:MA:144:ASP:OD1	38:MA:144:ASP:N	2.54	0.41
8:MB:177:GLY:O	8:MB:179:PRO:HD3	2.20	0.41
15:O:104:ARG:HG2	15:O:111:LEU:HD21	2.02	0.41
15:O:45:ARG:HE	15:O:45:ARG:HB3	1.52	0.41
41:PA:46:ALA:O	41:PA:50:ILE:HG13	2.21	0.41
2:B:2684:U:OP1	17:Q:53:ARG:HD3	2.21	0.41
42:QA:46:LYS:HG3	42:QA:64:LYS:HB3	2.03	0.41
37:QC:138:VAL:O	37:QC:142:MET:HB2	2.21	0.41
43:RA:53:VAL:HG11	43:RA:85:LEU:HD13	2.01	0.41
13:RB:106:LEU:HD13	13:RB:112:LEU:HD23	2.03	0.41
38:RC:101:LEU:HB2	38:RC:138:TYR:HB3	2.03	0.41
19:S:8:GLY:HA3	19:S:23:GLU:HB2	2.03	0.41
22:V:29:GLU:HG2	22:V:30:VAL:N	2.36	0.41
17:VB:132:LYS:HZ2	17:VB:132:LYS:HB2	1.85	0.41
17:VB:50:ILE:HD13	17:VB:64:ARG:HB2	2.03	0.41
24:X:2:ALA:HB3	4:IA:76:A:N6	2.36	0.41
19:XB:31:ALA:O	19:XB:61:VAL:HG12	2.21	0.41
45:YC:101:SER:OG	45:YC:103:LEU:HB2	2.21	0.41
1:A:265:G:H5'	51:ZA:64:PRO:O	2.21	0.41
1:A:1418:A:N6	1:A:1482:G:O2'	2.53	0.41
47:AD:84:ILE:HB	53:GD:74:PHE:HE1	1.86	0.41
2:B:1235:G:C2	2:B:1236:G:N2	2.89	0.41
2:B:2065:C:H2'	2:B:2066:C:C6	2.55	0.41
2:B:457:A:N6	2:B:470:A:H5''	2.36	0.41
3:C:48:A:H2'	3:C:49:C:C6	2.56	0.41
25:DC:65:SER:OG	25:DC:66:HIS:ND1	2.41	0.41
50:DD:52:ASP:OD2	50:DD:55:ARG:HG2	2.20	0.41
1:FB:186(A):C:H2'	1:FB:186(B):C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:332:G:OP2	54:HD:10:LEU:HG	2.21	0.41
1:FB:949:A:H1'	1:FB:1364:U:N3	2.36	0.41
1:FB:954:G:H2'	1:FB:955:U:C6	2.56	0.41
7:G:196:LEU:HA	7:G:196:LEU:HD23	1.83	0.41
2:GB:1239:G:H2'	2:GB:1240:U:O4'	2.21	0.41
2:GB:1814:G:C4'	5:JB:51:VAL:HG21	2.51	0.41
2:GB:794:G:H2'	2:GB:795:C:C6	2.56	0.41
10:J:72:LEU:HD21	10:J:107:ILE:CD1	2.51	0.41
35:JA:125:ALA:O	35:JA:158:GLY:HA3	2.21	0.41
13:M:93:GLY:N	13:M:123:LEU:HD22	2.35	0.41
13:M:59:LEU:HD21	32:FA:10:ALA:HA	2.03	0.41
13:M:95:VAL:O	13:M:126:VAL:HG23	2.21	0.41
40:OA:100:ASN:OD1	52:AB:23:LYS:HG2	2.21	0.41
35:OC:138:TYR:CZ	35:OC:142:ARG:HD2	2.56	0.41
36:PC:134:GLU:HA	36:PC:134:GLU:OE2	2.21	0.41
12:QB:68:GLU:HB3	12:QB:78:ARG:NH1	2.36	0.41
38:RC:60:GLU:HG3	38:RC:198:VAL:HG23	2.03	0.41
42:VC:19:VAL:HG23	42:VC:21:LYS:HG2	2.03	0.41
45:YC:32:ILE:HD12	45:YC:72:ALA:HB2	2.02	0.41
51:ZA:90:ILE:O	51:ZA:93:GLN:HG2	2.22	0.41
1:A:1134:G:OP2	1:A:1134:G:H8	2.04	0.40
1:A:1262:C:H42	1:A:1273:G:H1	1.69	0.40
1:A:174:C:H2'	1:A:175:C:H6	1.85	0.40
1:A:411:A:H2'	1:A:412:A:H4'	2.03	0.40
1:A:433:C:H2'	1:A:434:U:H6	1.86	0.40
1:A:778:G:H2'	1:A:779:C:O4'	2.21	0.40
1:A:875:C:O2'	42:QA:14:ARG:NH1	2.49	0.40
2:B:1490:A:H4'	2:B:1491:G:OP2	2.21	0.40
2:B:2319:G:OP1	2:B:2319:G:H3'	2.21	0.40
2:B:249:C:O2	32:FA:12:LYS:NZ	2.45	0.40
2:B:2516:G:C6	2:B:2517:C:C4	3.09	0.40
2:B:2667:C:H1'	9:I:109:PHE:CD1	2.55	0.40
3:C:65:C:O2'	3:C:66:A:OP1	2.39	0.40
6:F:37:ARG:HA	6:F:42:ASP:OD2	2.21	0.40
1:FB:792:A:H4'	1:FB:793:U:O5'	2.21	0.40
7:G:185:ASP:OD1	7:G:188:ARG:NH1	2.55	0.40
33:GA:27:CYS:HB3	33:GA:32:HIS:HB2	2.03	0.40
2:GB:1035:U:H2'	2:GB:1036:G:C8	2.55	0.40
2:GB:1849:G:H2'	2:GB:1850:G:H8	1.86	0.40
2:GB:191:A:H2'	2:GB:192:C:C6	2.57	0.40
2:GB:262:A:H2'	2:GB:263:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:2001:A:H4'	2:GB:2689:U:O2'	2.21	0.40
2:GB:2783:G:H2'	2:GB:2784:C:C6	2.55	0.40
4:IA:21:A:HO2'	4:IA:22:G:H8	1.67	0.40
35:JA:354:ALA:HA	35:JA:358:GLU:HB3	2.03	0.40
5:JB:273:ARG:HB3	5:JB:273:ARG:NH1	2.36	0.40
11:K:10:GLU:CD	11:K:11:PRO:HD2	2.41	0.40
36:KA:47:THR:O	36:KA:51:LEU:N	2.53	0.40
12:L:111:PHE:O	12:L:115:VAL:HG23	2.20	0.40
12:L:118:ALA:HA	12:L:119:PRO:HD3	1.80	0.40
38:MA:155:LEU:HD13	38:MA:157:LEU:H	1.86	0.40
38:MA:190:ASP:O	38:MA:193:ASP:HB2	2.21	0.40
14:N:38:GLU:HG3	14:N:127:ILE:HB	2.02	0.40
10:OB:57:ARG:HA	10:OB:60:GLU:HB3	2.03	0.40
10:OB:72:LEU:HD21	10:OB:107:ILE:CD1	2.52	0.40
42:QA:86:ILE:HG12	42:QA:135:CYS:HA	2.03	0.40
37:QC:88:ARG:HD3	37:QC:101:LEU:HB3	2.03	0.40
43:RA:40:LEU:HB2	43:RA:43:ALA:HB2	2.03	0.40
13:RB:100:LEU:HD23	13:RB:100:LEU:HA	1.86	0.40
38:RC:121:VAL:O	38:RC:134:ASP:HA	2.21	0.40
15:TB:74:LYS:HB2	15:TB:74:LYS:HE2	1.91	0.40
21:U:47:PHE:O	21:U:49:VAL:HG13	2.21	0.40
1:A:110:C:H2'	1:A:111:G:O4'	2.21	0.40
1:A:1307:U:H2'	1:A:1308:U:O4'	2.21	0.40
1:A:1422:G:H2'	1:A:1423:G:C8	2.56	0.40
1:A:394:G:H2'	1:A:395:C:C6	2.56	0.40
2:B:1693:U:OP2	2:B:1694:C:H5	2.05	0.40
2:B:1923:U:H2'	2:B:1924:C:H6	1.86	0.40
2:B:2162:G:H1'	2:B:2173:A:H1'	2.02	0.40
2:B:2262:U:H4'	2:B:2328:A:C2	2.56	0.40
2:B:2377:A:H2'	2:B:2378:A:C8	2.56	0.40
2:B:270(Q):C:H2'	2:B:270(R):C:H6	1.85	0.40
2:B:2881:C:H2'	2:B:2882:A:O4'	2.21	0.40
2:B:674:G:H1'	7:G:74:ARG:HD3	2.03	0.40
2:B:92:G:H2'	2:B:93:C:C6	2.56	0.40
23:BC:91:LEU:HD12	23:BC:96:VAL:HG11	2.02	0.40
4:D:58:A:N6	4:D:61:C:C2	2.90	0.40
31:EA:35:ARG:HG3	31:EA:42:LEU:HD21	2.04	0.40
51:ED:84:LEU:O	51:ED:87:LYS:HG3	2.21	0.40
1:FB:1285:A:H4'	1:FB:1286:A:O5'	2.22	0.40
1:FB:1519:MA6:H5''	1:FB:1520:G:OP2	2.22	0.40
1:FB:432:A:H2'	1:FB:433:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:528:C:H41	46:ZC:49:ASN:CG	2.24	0.40
2:GB:2257:U:O2'	2:GB:2258:C:H5'	2.21	0.40
2:GB:2336:A:H3'	2:GB:2337:G:H8	1.86	0.40
2:GB:242:G:H5''	32:KC:64:TYR:CE2	2.56	0.40
2:GB:2477:C:O2	33:LC:4:ARG:NH2	2.39	0.40
2:GB:221:A:N6	2:GB:265:A:H8	2.19	0.40
2:GB:320:A:H4'	2:GB:322:A:C8	2.56	0.40
2:GB:895:U:H5'	2:GB:896:A:OP1	2.21	0.40
2:GB:91:A:C4	2:GB:92:G:C8	3.09	0.40
9:I:163:TYR:CE1	9:I:169:VAL:HG13	2.56	0.40
9:I:3:ARG:HH11	9:I:3:ARG:HA	1.84	0.40
4:IB:30:G:H21	41:UC:144:MET:HE1	1.87	0.40
5:JB:62:TYR:HA	5:JB:87:ASN:HD21	1.84	0.40
36:KA:127:ILE:HG23	36:KA:135:GLN:HB2	2.02	0.40
6:KB:8:LYS:NZ	6:KB:188:VAL:O	2.47	0.40
7:LB:29:ASN:HA	7:LB:30:PRO:HD2	1.99	0.40
8:MB:36:LYS:HD3	8:MB:95:ARG:NH1	2.36	0.40
9:NB:155:SER:HB3	9:NB:158:HIS:O	2.20	0.40
10:OB:4:ILE:HA	10:OB:17:GLN:O	2.22	0.40
16:P:28:VAL:HG11	16:P:98:VAL:HG13	2.04	0.40
36:PC:20:GLU:O	36:PC:39:ILE:HG22	2.21	0.40
12:QB:75:SER:HB2	17:VB:74:ARG:NH1	2.34	0.40
37:QC:58:GLU:O	37:QC:65:ALA:N	2.53	0.40
13:RB:83:VAL:CG1	13:RB:112:LEU:HD21	2.50	0.40
45:TA:48:ILE:HD12	45:TA:48:ILE:HA	1.71	0.40
41:UC:114:ARG:HG2	41:UC:114:ARG:H	1.63	0.40
1:FB:1240:U:C2	41:UC:32:ARG:HD2	2.56	0.40
18:WB:85:LYS:HB3	18:WB:85:LYS:HE3	1.92	0.40
43:WC:46:ALA:HB2	43:WC:74:ILE:HG23	2.01	0.40
2:B:2451:A:H5'	24:X:3:HIS:HE2	1.86	0.40
45:YC:59:TYR:CZ	45:YC:63:LEU:HD11	2.56	0.40
46:ZC:32:PHE:CD1	46:ZC:86:ARG:HB3	2.56	0.40
1:A:1191:A:OP1	37:LA:4:LYS:HG3	2.21	0.40
1:A:931:C:H42	1:A:1386:G:H1	1.70	0.40
1:A:973:G:H3'	1:A:974:A:H5''	2.03	0.40
27:AA:59:VAL:HB	27:AA:60:GLU:H	1.66	0.40
2:B:1575:C:H2'	2:B:1576:U:O4'	2.20	0.40
2:B:1800:C:OP1	5:E:264:LYS:NZ	2.44	0.40
2:B:2321:G:H5'	2:B:2322:A:OP2	2.21	0.40
2:B:2471:C:N4	2:B:2476:A:O2'	2.53	0.40
2:B:2582:G:H2'	2:B:2582:G:N3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:A:H2'	3:C:79:C:O4'	2.21	0.40
54:CB:88:VAL:O	54:CB:92:LEU:HB2	2.20	0.40
30:DA:47:THR:HG22	30:DA:48:VAL:O	2.20	0.40
2:B:784:A:C6	5:E:229:VAL:HG21	2.56	0.40
5:E:70:TRP:CH2	5:E:150:LYS:HG3	2.55	0.40
2:B:592:G:H4'	32:FA:3:LYS:HB2	2.03	0.40
1:FB:1031:G:C8	1:FB:1032(B):G:N1	2.89	0.40
1:FB:652:U:O4	1:FB:752:G:O2'	2.21	0.40
1:FB:690:G:H2'	1:FB:691:G:O4'	2.21	0.40
1:FB:826:C:H5'	42:VC:12:ARG:NH2	2.36	0.40
1:FB:926:G:C6	1:FB:1505:G:C6	3.09	0.40
2:GB:2323:G:H2'	2:GB:2324:C:O4'	2.21	0.40
2:GB:265:A:H1'	2:GB:266:G:O4'	2.21	0.40
2:GB:725:G:C6	2:GB:726:G:N1	2.90	0.40
3:HB:3:C:C2	3:HB:118:G:C2	3.09	0.40
3:HB:73:A:C6	3:HB:74:U:C2	3.10	0.40
54:HD:64:ASP:OD2	54:HD:81:LYS:HD3	2.20	0.40
10:J:80:PRO:HA	10:J:145:VAL:HG23	2.02	0.40
35:JA:351:ASP:O	35:JA:355:ALA:HB2	2.21	0.40
41:PA:79:ARG:HD2	41:PA:80:VAL:H	1.86	0.40
36:PC:215:LEU:O	36:PC:219:VAL:HG23	2.21	0.40
17:Q:55:ASN:H	17:Q:59:THR:HB	1.86	0.40
6:F:181:LEU:HD21	17:Q:6:LEU:HD12	2.03	0.40
18:R:8:VAL:HG22	18:R:12:ARG:HG3	2.04	0.40
19:S:24:LYS:HA	19:S:92:THR:OG1	2.21	0.40
44:SA:77:PRO:HB2	44:SA:78:ASN:H	1.71	0.40
45:TA:66:LEU:HD22	45:TA:66:LEU:HA	1.80	0.40
47:VA:19:LEU:HD13	47:VA:19:LEU:HA	1.80	0.40
47:VA:45:VAL:O	47:VA:48:LEU:HB2	2.20	0.40
42:VC:120:THR:HG23	42:VC:123:GLU:OE2	2.21	0.40
23:W:162:GLU:O	23:W:164:ALA:N	2.54	0.40
51:ZA:84:LEU:HD23	51:ZA:84:LEU:HA	1.87	0.40
1:A:292:G:N7	1:A:293:G:H1'	2.36	0.40
1:A:338:A:C6	1:A:339:C:C4	3.10	0.40
1:A:560:U:H5'	1:A:566:G:N2	2.36	0.40
1:A:988:G:C2	1:A:989:C:H1'	2.56	0.40
1:A:9:G:H2'	1:A:10:A:C8	2.56	0.40
22:AC:51:VAL:HA	22:AC:55:TYR:O	2.21	0.40
22:AC:76:CYS:HA	22:AC:77:PRO:HD2	1.84	0.40
47:AD:60:VAL:HG13	47:AD:64:TRP:CE3	2.57	0.40
2:B:1400:G:H2'	2:B:1401:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1448:G:H5''	2:B:1543:A:OP2	2.22	0.40
2:B:2723:C:OP2	6:F:109:LYS:NZ	2.55	0.40
53:BB:36:ARG:HB2	53:BB:72:GLY:HA3	2.04	0.40
50:DD:49:LEU:HD12	50:DD:50:LYS:H	1.86	0.40
50:DD:6:LEU:HG	50:DD:17:TYR:HB3	2.03	0.40
5:E:227:ASN:HB3	5:E:228:PRO:HD2	2.03	0.40
1:FB:1128:C:H4'	1:FB:1148:U:O2	2.21	0.40
1:FB:843:U:C5	1:FB:848:C:H1'	2.55	0.40
27:FC:26:LEU:HA	27:FC:26:LEU:HD23	1.93	0.40
27:FC:59:VAL:O	27:FC:60:GLU:HB3	2.21	0.40
2:GB:101:G:H4'	2:GB:102:G:OP2	2.21	0.40
2:GB:273(G):C:H2'	2:GB:274:G:O4'	2.21	0.40
2:GB:2773:C:H2'	2:GB:2774:C:H6	1.87	0.40
2:GB:2820:A:OP2	15:TB:2:ARG:NH2	2.54	0.40
2:GB:352:G:H4'	2:GB:353:G:OP2	2.21	0.40
2:GB:613:U:H2'	2:GB:614:U:O4'	2.21	0.40
2:GB:715:G:H2'	2:GB:716:A:C8	2.57	0.40
2:GB:830:G:H4'	2:GB:831:G:OP2	2.22	0.40
3:HB:48:A:H2'	3:HB:49:C:C6	2.57	0.40
9:I:46:GLU:OE1	9:I:51:ARG:NE	2.53	0.40
4:IA:24:U:H2'	4:IA:25:C:O4'	2.22	0.40
10:J:88:ILE:HD12	10:J:89:TYR:N	2.36	0.40
2:GB:1655:A:H1'	6:KB:113:PHE:CD2	2.57	0.40
37:LA:108:ASN:HB3	37:LA:111:LEU:HD12	2.04	0.40
1:A:438:G:H4'	38:MA:123:HIS:CD2	2.57	0.40
8:MB:126:ASP:HB2	8:MB:130:ASN:O	2.22	0.40
14:N:112:GLU:HG2	14:N:113:GLN:N	2.37	0.40
35:OC:227:PHE:HA	35:OC:241:ASP:OD2	2.22	0.40
16:P:66:ALA:O	16:P:69:VAL:HG13	2.22	0.40
11:PB:67:LEU:HA	11:PB:67:LEU:HD13	1.90	0.40
37:QC:139:GLN:HG3	37:QC:140:ARG:HH12	1.86	0.40
37:QC:28:GLN:HA	37:QC:31:HIS:CE1	2.56	0.40
44:SA:23:ILE:HD12	44:SA:23:ILE:HA	1.79	0.40
16:UB:105:ALA:O	16:UB:110:LEU:HB2	2.21	0.40
47:VA:66:LEU:C	47:VA:70:LEU:HB2	2.42	0.40
23:W:52:SER:OG	23:W:53:ILE:N	2.53	0.40
26:Z:39:ALA:HA	26:Z:44:LEU:HB3	2.03	0.40
1:A:191(E):G:H2'	1:A:191(F):U:C6	2.57	0.40
1:A:528:C:H41	46:UA:49:ASN:CG	2.23	0.40
1:A:767:A:H2'	1:A:768:A:O4'	2.22	0.40
1:A:975:A:H5'	1:A:975:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1357:U:H2'	2:B:1358:G:O4'	2.21	0.40
2:B:17:G:H2'	2:B:18:C:H6	1.85	0.40
2:B:2893:G:O5'	2:B:2893:G:H8	2.05	0.40
3:HB:75:G:H22	23:BC:73:GLN:HE21	1.70	0.40
23:BC:44:PHE:CE1	23:BC:86:VAL:HG11	2.56	0.40
26:EC:29:LYS:HG2	26:EC:57:ILE:HD13	2.04	0.40
1:FB:1410:G:C2	1:FB:1491:G:C2	3.09	0.40
1:FB:173:U:H5	1:FB:198:G:HO2'	1.69	0.40
1:FB:297:G:N2	1:FB:300:A:OP2	2.44	0.40
1:FB:583:A:H61	1:FB:758:G:H1'	1.87	0.40
7:G:60:SER:OG	7:G:61:GLY:N	2.54	0.40
2:GB:1817:G:OP1	5:JB:88:ARG:NH2	2.47	0.40
2:GB:189:G:OP2	25:DC:14:VAL:HG21	2.22	0.40
2:GB:2101:G:C5	2:GB:2102:U:C4	3.09	0.40
2:GB:2109:U:H5'	2:GB:2149:G:H21	1.87	0.40
2:GB:2152:G:H3'	2:GB:2153:G:H8	1.87	0.40
2:GB:2584:U:H2'	2:GB:2585:U:H2'	2.03	0.40
2:GB:2627:G:N2	2:GB:2777:G:OP2	2.55	0.40
2:GB:547:A:N7	2:GB:548:A:C6	2.90	0.40
2:GB:609(B):G:H2'	2:GB:610:C:C6	2.56	0.40
2:GB:879:G:N2	2:GB:899:A:H1'	2.36	0.40
35:JA:146:VAL:HG23	35:JA:164:ALA:HB1	2.03	0.40
36:KA:106:LYS:HE2	36:KA:106:LYS:HB3	1.93	0.40
38:MA:76:ARG:HD2	38:MA:76:ARG:HA	1.83	0.40
15:O:59:ASP:OD2	15:O:61:HIS:HB3	2.21	0.40
35:OC:278:ILE:HG13	35:OC:279:HIS:N	2.36	0.40
11:PB:35:ARG:NH1	11:PB:35:ARG:HG2	2.37	0.40
17:Q:56:GLY:O	17:Q:59:THR:HG22	2.22	0.40
42:QA:86:ILE:HG13	42:QA:133:LEU:HD22	2.04	0.40
1:A:1128:C:C5'	43:RA:66:ARG:HH12	2.35	0.40
39:SC:144:THR:O	39:SC:148:VAL:HG23	2.22	0.40
20:T:12:ILE:HD13	20:T:17:VAL:HG22	2.03	0.40
20:T:69:LEU:HA	20:T:69:LEU:HD23	1.83	0.40
16:UB:41:ASP:OD2	16:UB:44:LYS:HG3	2.21	0.40
1:A:1308:U:H3'	47:VA:99:ARG:NH1	2.36	0.40
23:W:136:PHE:O	23:W:137:ILE:HD13	2.21	0.40
1:FB:1128:C:C5'	43:WC:66:ARG:HH12	2.35	0.40
44:XC:55:LYS:HB3	44:XC:56:HIS:H	1.74	0.40
26:Z:56:GLN:HA	26:Z:59:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	252 (92%)	20 (7%)	1 (0%)	39	75
5	JB	273/275 (99%)	250 (92%)	22 (8%)	1 (0%)	39	75
6	F	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	19	58
6	KB	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	19	58
7	G	200/205 (98%)	184 (92%)	14 (7%)	2 (1%)	19	58
7	LB	200/205 (98%)	182 (91%)	16 (8%)	2 (1%)	19	58
8	H	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	8	36
8	MB	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	8	36
9	I	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	30	68
9	NB	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	30	68
10	J	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	6	30
10	OB	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	6	30
11	K	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
11	PB	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
12	L	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	43
12	QB	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	24	63
13	M	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	26	65
13	RB	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	26	65
14	N	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	65
14	SB	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	65
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	43
15	TB	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	11	43
16	P	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	10	40
16	UB	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	10	40
17	Q	135/146 (92%)	122 (90%)	10 (7%)	3 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	VB	135/146 (92%)	122 (90%)	11 (8%)	2 (2%)	13	46
18	R	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
18	WB	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
19	S	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	9	38
19	XB	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	19	58
20	T	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	YB	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
21	U	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
21	ZB	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
22	AC	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
22	V	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
23	BC	187/206 (91%)	167 (89%)	16 (9%)	4 (2%)	9	37
23	W	187/206 (91%)	167 (89%)	16 (9%)	4 (2%)	9	37
24	CC	82/85 (96%)	75 (92%)	4 (5%)	3 (4%)	4	23
24	X	82/85 (96%)	75 (92%)	4 (5%)	3 (4%)	4	23
25	DC	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	17	55
25	Y	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	9	37
26	EC	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
26	Z	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
27	AA	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	11	43
27	FC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	11	43
28	BA	67/71 (94%)	45 (67%)	16 (24%)	6 (9%)	1	5
28	GC	67/71 (94%)	45 (67%)	16 (24%)	6 (9%)	1	5
29	CA	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	HC	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	DA	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	IC	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	JC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	KC	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	GA	35/37 (95%)	32 (91%)	1 (3%)	2 (6%)	2	12
33	LC	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	6	29
35	JA	256/368 (70%)	215 (84%)	32 (12%)	9 (4%)	4	24
35	OC	256/368 (70%)	218 (85%)	28 (11%)	10 (4%)	4	22
36	KA	232/256 (91%)	191 (82%)	24 (10%)	17 (7%)	1	7
36	PC	232/256 (91%)	190 (82%)	25 (11%)	17 (7%)	1	7
37	LA	204/239 (85%)	181 (89%)	18 (9%)	5 (2%)	7	32
37	QC	204/239 (85%)	179 (88%)	20 (10%)	5 (2%)	7	32
38	MA	206/209 (99%)	184 (89%)	17 (8%)	5 (2%)	7	33
38	RC	206/209 (99%)	182 (88%)	19 (9%)	5 (2%)	7	33
39	NA	149/162 (92%)	132 (89%)	14 (9%)	3 (2%)	9	38
39	SC	149/162 (92%)	132 (89%)	14 (9%)	3 (2%)	9	38
40	OA	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
40	TC	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
41	PA	153/156 (98%)	139 (91%)	9 (6%)	5 (3%)	5	26
41	UC	153/156 (98%)	137 (90%)	11 (7%)	5 (3%)	5	26
42	QA	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
42	VC	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
43	RA	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	12	44
43	WC	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	24	63
44	SA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	5	27
44	XC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	5	27
45	TA	114/129 (88%)	103 (90%)	8 (7%)	3 (3%)	7	32
45	YC	114/129 (88%)	104 (91%)	7 (6%)	3 (3%)	7	32
46	UA	119/132 (90%)	104 (87%)	13 (11%)	2 (2%)	11	43
46	ZC	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	11	43
47	AD	115/126 (91%)	101 (88%)	13 (11%)	1 (1%)	21	61
47	VA	115/126 (91%)	100 (87%)	14 (12%)	1 (1%)	21	61
48	BD	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	5	25
48	WA	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	5	25
49	CD	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	XA	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	16	52
50	DD	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
50	YA	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
51	ED	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	9	37
51	ZA	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	9	37
52	AB	68/88 (77%)	60 (88%)	7 (10%)	1 (2%)	13	46
52	FD	68/88 (77%)	61 (90%)	5 (7%)	2 (3%)	6	29
53	BB	81/93 (87%)	70 (86%)	7 (9%)	4 (5%)	3	16
53	GD	81/93 (87%)	70 (86%)	7 (9%)	4 (5%)	3	16
54	CB	97/106 (92%)	83 (86%)	9 (9%)	5 (5%)	2	15
54	HD	97/106 (92%)	82 (84%)	10 (10%)	5 (5%)	2	15
55	DB	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	3	17
55	ID	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	3	17
All	All	11996/12852 (93%)	10786 (90%)	982 (8%)	228 (2%)	10	40

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	47	LYS
9	I	126	PRO
10	J	92	VAL
14	N	60	ARG
15	O	2	ARG
24	X	4	LYS
25	Y	3	LYS
28	BA	45	GLY
28	BA	50	VAL
35	JA	104	ASP
36	KA	17	PHE
36	KA	36	ARG
36	KA	125	PRO
36	KA	128	GLU
38	MA	4	TYR
38	MA	5	ILE
44	SA	77	PRO
45	TA	91	ARG
54	CB	99	LEU

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Mol	Chain	Res	Type
55	DB	3	LYS
8	MB	43	LEU
8	MB	47	LYS
9	NB	126	PRO
10	OB	89	TYR
10	OB	92	VAL
14	SB	60	ARG
15	TB	2	ARG
24	CC	4	LYS
25	DC	3	LYS
28	GC	45	GLY
28	GC	50	VAL
35	OC	104	ASP
36	PC	17	PHE
36	PC	36	ARG
36	PC	125	PRO
36	PC	128	GLU
38	RC	4	TYR
38	RC	5	ILE
44	XC	77	PRO
45	YC	91	ARG
54	HD	99	LEU
55	ID	3	LYS
6	F	58	ARG
8	H	43	LEU
10	J	88	ILE
10	J	89	TYR
23	W	163	LEU
28	BA	47	GLN
35	JA	102	PRO
35	JA	159	TYR
35	JA	193	GLN
36	KA	22	LYS
36	KA	78	GLN
36	KA	124	SER
36	KA	126	GLU
36	KA	226	ARG
37	LA	26	LYS
37	LA	156	ARG
39	NA	65	ASN
41	PA	4	ARG
41	PA	17	VAL

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Mol	Chain	Res	Type
46	UA	22	SER
46	UA	125	PRO
47	VA	100	GLY
48	WA	3	ARG
48	WA	14	PRO
6	KB	58	ARG
10	OB	88	ILE
23	BC	163	LEU
28	GC	47	GLN
35	OC	102	PRO
35	OC	159	TYR
35	OC	193	GLN
36	PC	22	LYS
36	PC	78	GLN
36	PC	124	SER
36	PC	204	ASN
36	PC	226	ARG
37	QC	26	LYS
37	QC	156	ARG
39	SC	65	ASN
41	UC	4	ARG
41	UC	17	VAL
46	ZC	125	PRO
47	AD	100	GLY
48	BD	3	ARG
48	BD	14	PRO
6	F	52	LEU
7	G	21	ALA
7	G	22	ALA
10	J	85	GLU
13	M	103	ALA
15	O	71	GLN
17	Q	12	SER
17	Q	37	GLY
19	S	79	VAL
23	W	153	SER
28	BA	34	GLU
33	GA	11	CYS
35	JA	299	GLY
36	KA	204	ASN
36	KA	207	ALA
36	KA	237	ALA

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Mol	Chain	Res	Type
39	NA	74	GLY
41	PA	54	THR
41	PA	85	TYR
43	RA	96	LEU
44	SA	33	GLN
44	SA	78	ASN
51	ZA	77	VAL
53	BB	81	ARG
54	CB	11	SER
6	KB	52	LEU
7	LB	22	ALA
10	OB	85	GLU
13	RB	103	ALA
15	TB	71	GLN
17	VB	12	SER
17	VB	37	GLY
23	BC	153	SER
28	GC	34	GLU
35	OC	218	ASN
35	OC	299	GLY
36	PC	23	ARG
36	PC	126	GLU
36	PC	237	ALA
37	QC	62	ASP
39	SC	6	PHE
39	SC	74	GLY
41	UC	54	THR
41	UC	85	TYR
43	WC	96	LEU
44	XC	33	GLN
44	XC	78	ASN
46	ZC	22	SER
53	GD	81	ARG
16	P	60	GLY
23	W	157	LEU
35	JA	144	TRP
35	JA	218	ASN
36	KA	23	ARG
36	KA	26	PRO
36	KA	158	LEU
37	LA	3	ASN
37	LA	62	ASP

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Mol	Chain	Res	Type
39	NA	6	PHE
52	AB	41	LYS
53	BB	45	VAL
54	CB	10	LEU
54	CB	47	GLY
54	CB	97	ALA
7	LB	21	ALA
12	QB	111	PHE
16	UB	60	GLY
19	XB	79	VAL
23	BC	157	LEU
33	LC	11	CYS
35	OC	144	TRP
36	PC	158	LEU
36	PC	207	ALA
37	QC	3	ASN
51	ED	77	VAL
54	HD	11	SER
54	HD	97	ALA
8	H	52	ILE
8	H	124	SER
12	L	5	GLN
16	P	61	ASN
19	S	53	GLU
28	BA	53	GLU
33	GA	12	ASP
35	JA	143	ARG
35	JA	215	PRO
38	MA	22	LYS
38	MA	23	GLY
43	RA	12	GLU
45	TA	90	GLY
49	XA	14	GLU
51	ZA	31	LEU
8	MB	52	ILE
8	MB	124	SER
16	UB	61	ASN
23	BC	135	GLU
24	CC	13	GLY
28	GC	53	GLU
35	OC	143	ARG
35	OC	215	PRO

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Mol	Chain	Res	Type
36	PC	26	PRO
38	RC	22	LYS
45	YC	90	GLY
51	ED	31	LEU
52	FD	41	LYS
52	FD	59	SER
53	GD	27	GLU
53	GD	45	VAL
54	HD	10	LEU
54	HD	47	GLY
23	W	135	GLU
24	X	13	GLY
36	KA	239	VAL
41	PA	80	VAL
45	TA	105	VAL
53	BB	27	GLU
35	OC	355	ALA
36	PC	239	VAL
38	RC	23	GLY
41	UC	80	VAL
45	YC	105	VAL
49	CD	88	ARG
5	E	236	GLY
12	L	27	GLY
24	X	6	GLY
28	BA	5	ILE
36	KA	15	VAL
38	MA	197	PRO
36	PC	15	VAL
27	AA	59	VAL
37	LA	25	GLY
5	JB	236	GLY
27	FC	59	VAL
28	GC	5	ILE
53	BB	67	VAL
24	CC	6	GLY
37	QC	25	GLY
38	RC	197	PRO
53	GD	67	VAL
17	Q	135	VAL
25	Y	55	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	196 (90%)	21 (10%)	10	36
5	JB	217/217 (100%)	193 (89%)	24 (11%)	8	29
6	F	165/166 (99%)	150 (91%)	15 (9%)	12	40
6	KB	165/166 (99%)	149 (90%)	16 (10%)	10	36
7	G	161/162 (99%)	137 (85%)	24 (15%)	4	15
7	LB	161/162 (99%)	138 (86%)	23 (14%)	4	17
8	H	154/156 (99%)	132 (86%)	22 (14%)	4	17
8	MB	154/156 (99%)	132 (86%)	22 (14%)	4	17
9	I	144/148 (97%)	130 (90%)	14 (10%)	10	36
9	NB	144/148 (97%)	130 (90%)	14 (10%)	10	36
10	J	122/124 (98%)	95 (78%)	27 (22%)	1	5
10	OB	122/124 (98%)	96 (79%)	26 (21%)	1	6
11	K	119/119 (100%)	103 (87%)	16 (13%)	5	20
11	PB	119/119 (100%)	103 (87%)	16 (13%)	5	20
12	L	100/100 (100%)	90 (90%)	10 (10%)	9	34
12	QB	100/100 (100%)	89 (89%)	11 (11%)	8	30
13	M	116/116 (100%)	103 (89%)	13 (11%)	7	29
13	RB	116/116 (100%)	104 (90%)	12 (10%)	9	32
14	N	111/111 (100%)	100 (90%)	11 (10%)	10	34
14	SB	111/111 (100%)	101 (91%)	10 (9%)	12	41
15	O	101/101 (100%)	89 (88%)	12 (12%)	6	25
15	TB	101/101 (100%)	88 (87%)	13 (13%)	5	21
16	P	87/88 (99%)	73 (84%)	14 (16%)	3	13
16	UB	87/88 (99%)	73 (84%)	14 (16%)	3	13
17	Q	121/128 (94%)	111 (92%)	10 (8%)	14	46
17	VB	121/128 (94%)	112 (93%)	9 (7%)	17	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	93/94 (99%)	84 (90%)	9 (10%)	10	36
18	WB	93/94 (99%)	84 (90%)	9 (10%)	10	36
19	S	82/82 (100%)	69 (84%)	13 (16%)	3	13
19	XB	82/82 (100%)	69 (84%)	13 (16%)	3	13
20	T	91/92 (99%)	84 (92%)	7 (8%)	16	50
20	YB	91/92 (99%)	84 (92%)	7 (8%)	16	50
21	U	77/78 (99%)	69 (90%)	8 (10%)	9	32
21	ZB	77/78 (99%)	70 (91%)	7 (9%)	12	40
22	AC	87/91 (96%)	77 (88%)	10 (12%)	7	27
22	V	87/91 (96%)	79 (91%)	8 (9%)	11	40
23	BC	163/179 (91%)	144 (88%)	19 (12%)	7	26
23	W	163/179 (91%)	144 (88%)	19 (12%)	7	26
24	CC	66/67 (98%)	60 (91%)	6 (9%)	12	40
24	X	66/67 (98%)	60 (91%)	6 (9%)	12	40
25	DC	81/83 (98%)	72 (89%)	9 (11%)	8	29
25	Y	81/83 (98%)	72 (89%)	9 (11%)	8	29
26	EC	66/67 (98%)	60 (91%)	6 (9%)	12	40
26	Z	66/67 (98%)	60 (91%)	6 (9%)	12	40
27	AA	52/52 (100%)	47 (90%)	5 (10%)	10	37
27	FC	52/52 (100%)	47 (90%)	5 (10%)	10	37
28	BA	59/63 (94%)	52 (88%)	7 (12%)	6	25
28	GC	59/63 (94%)	52 (88%)	7 (12%)	6	25
29	CA	51/52 (98%)	46 (90%)	5 (10%)	10	36
29	HC	51/52 (98%)	46 (90%)	5 (10%)	10	36
30	DA	51/52 (98%)	46 (90%)	5 (10%)	10	36
30	IC	51/52 (98%)	46 (90%)	5 (10%)	10	36
31	EA	41/42 (98%)	35 (85%)	6 (15%)	4	16
31	JC	41/42 (98%)	37 (90%)	4 (10%)	10	36
32	FA	54/55 (98%)	48 (89%)	6 (11%)	8	29
32	KC	54/55 (98%)	50 (93%)	4 (7%)	17	51
33	GA	34/34 (100%)	33 (97%)	1 (3%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	LC	34/34 (100%)	34 (100%)	0	100	100
35	JA	209/308 (68%)	178 (85%)	31 (15%)	4	16
35	OC	209/308 (68%)	177 (85%)	32 (15%)	3	14
36	KA	202/220 (92%)	172 (85%)	30 (15%)	4	15
36	PC	202/220 (92%)	172 (85%)	30 (15%)	4	15
37	LA	160/188 (85%)	141 (88%)	19 (12%)	6	25
37	QC	160/188 (85%)	142 (89%)	18 (11%)	7	28
38	MA	180/181 (99%)	153 (85%)	27 (15%)	3	15
38	RC	180/181 (99%)	152 (84%)	28 (16%)	3	14
39	NA	116/123 (94%)	100 (86%)	16 (14%)	4	19
39	SC	116/123 (94%)	98 (84%)	18 (16%)	3	14
40	OA	90/90 (100%)	81 (90%)	9 (10%)	9	34
40	TC	90/90 (100%)	81 (90%)	9 (10%)	9	34
41	PA	126/127 (99%)	113 (90%)	13 (10%)	9	32
41	UC	126/127 (99%)	112 (89%)	14 (11%)	8	29
42	QA	119/119 (100%)	106 (89%)	13 (11%)	8	30
42	VC	119/119 (100%)	106 (89%)	13 (11%)	8	30
43	RA	98/99 (99%)	81 (83%)	17 (17%)	2	11
43	WC	98/99 (99%)	82 (84%)	16 (16%)	3	12
44	SA	88/92 (96%)	81 (92%)	7 (8%)	15	48
44	XC	88/92 (96%)	81 (92%)	7 (8%)	15	48
45	TA	88/99 (89%)	80 (91%)	8 (9%)	12	40
45	YC	88/99 (89%)	79 (90%)	9 (10%)	9	33
46	UA	102/108 (94%)	90 (88%)	12 (12%)	6	25
46	ZC	102/108 (94%)	91 (89%)	11 (11%)	8	30
47	AD	94/101 (93%)	79 (84%)	15 (16%)	3	13
47	VA	94/101 (93%)	79 (84%)	15 (16%)	3	13
48	BD	49/50 (98%)	41 (84%)	8 (16%)	3	12
48	WA	49/50 (98%)	41 (84%)	8 (16%)	3	12
49	CD	79/80 (99%)	75 (95%)	4 (5%)	29	66
49	XA	79/80 (99%)	75 (95%)	4 (5%)	29	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	DD	72/74 (97%)	63 (88%)	9 (12%)	6	22
50	YA	72/74 (97%)	63 (88%)	9 (12%)	6	22
51	ED	94/97 (97%)	86 (92%)	8 (8%)	13	45
51	ZA	94/97 (97%)	85 (90%)	9 (10%)	10	37
52	AB	61/77 (79%)	56 (92%)	5 (8%)	14	47
52	FD	61/77 (79%)	56 (92%)	5 (8%)	14	47
53	BB	72/80 (90%)	63 (88%)	9 (12%)	6	22
53	GD	72/80 (90%)	65 (90%)	7 (10%)	10	36
54	CB	76/82 (93%)	67 (88%)	9 (12%)	6	25
54	HD	76/82 (93%)	68 (90%)	8 (10%)	8	31
55	DB	19/22 (86%)	18 (95%)	1 (5%)	28	64
55	ID	19/22 (86%)	18 (95%)	1 (5%)	28	64
All	All	10120/10672 (95%)	8924 (88%)	1196 (12%)	6	25

All (1196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	28	GLU
5	E	61	LEU
5	E	71	ASP
5	E	91	ARG
5	E	94	LEU
5	E	98	VAL
5	E	99	ASP
5	E	127	VAL
5	E	140	THR
5	E	150	LYS
5	E	171	ASP
5	E	193	VAL
5	E	200	ASP
5	E	211	ARG
5	E	221	VAL
5	E	229	VAL
5	E	242	ARG
5	E	259	THR
5	E	273	ARG
5	E	274	ARG
5	E	275	LYS

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Mol	Chain	Res	Type
6	F	9	VAL
6	F	13	ARG
6	F	21	VAL
6	F	24	THR
6	F	75	VAL
6	F	92	THR
6	F	93	VAL
6	F	116	VAL
6	F	119	ARG
6	F	128	SER
6	F	154	LYS
6	F	175	VAL
6	F	181	LEU
6	F	182	LEU
6	F	192	ASN
7	G	6	MET
7	G	15	SER
7	G	18	ARG
7	G	53	THR
7	G	57	VAL
7	G	62	ARG
7	G	64	ILE
7	G	70	THR
7	G	74	ARG
7	G	110	LEU
7	G	119	ARG
7	G	126	VAL
7	G	129	PHE
7	G	140	LEU
7	G	158	THR
7	G	170	LEU
7	G	175	THR
7	G	188	ARG
7	G	190	GLU
7	G	191	ARG
7	G	192	LEU
7	G	197	ASP
7	G	200	GLU
7	G	205	ARG
8	H	3	LEU
8	H	7	LEU
8	H	22	ARG

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Mol	Chain	Res	Type
8	H	33	ARG
8	H	38	VAL
8	H	43	LEU
8	H	49	ASP
8	H	53	LEU
8	H	60	LEU
8	H	62	LEU
8	H	67	LYS
8	H	70	VAL
8	H	82	LEU
8	H	91	ARG
8	H	98	ARG
8	H	115	ARG
8	H	118	ARG
8	H	136	ARG
8	H	140	ILE
8	H	143	GLU
8	H	167	GLU
8	H	170	ARG
9	I	3	ARG
9	I	16	SER
9	I	24	VAL
9	I	37	VAL
9	I	43	VAL
9	I	57	ASP
9	I	71	LEU
9	I	84	SER
9	I	97	ARG
9	I	104	GLU
9	I	106	THR
9	I	127	GLU
9	I	136	ILE
9	I	169	VAL
10	J	1	MET
10	J	9	LEU
10	J	19	VAL
10	J	21	VAL
10	J	43	ASN
10	J	44	LEU
10	J	57	ARG
10	J	61	ARG
10	J	74	ASN

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Mol	Chain	Res	Type
10	J	77	LEU
10	J	82	ARG
10	J	86	THR
10	J	88	ILE
10	J	89	TYR
10	J	96	ASP
10	J	99	GLU
10	J	107	ILE
10	J	108	THR
10	J	112	LYS
10	J	118	LYS
10	J	122	GLU
10	J	125	GLU
10	J	129	THR
10	J	131	LYS
10	J	140	LEU
10	J	144	VAL
10	J	145	VAL
11	K	9	VAL
11	K	14	VAL
11	K	19	GLU
11	K	28	THR
11	K	34	LEU
11	K	48	MET
11	K	67	LEU
11	K	68	GLU
11	K	76	SER
11	K	83	LYS
11	K	84	LYS
11	K	87	LEU
11	K	93	THR
11	K	96	GLU
11	K	99	LEU
11	K	138	LEU
12	L	10	VAL
12	L	24	VAL
12	L	31	LYS
12	L	32	TYR
12	L	45	GLU
12	L	53	LYS
12	L	70	LYS
12	L	78	ARG

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Mol	Chain	Res	Type
12	L	98	VAL
12	L	116	SER
13	M	3	LEU
13	M	29	LYS
13	M	42	SER
13	M	58	THR
13	M	68	GLN
13	M	71	VAL
13	M	90	ARG
13	M	112	LEU
13	M	117	GLU
13	M	126	VAL
13	M	135	LEU
13	M	147	LEU
13	M	149	GLU
14	N	16	ARG
14	N	31	ASP
14	N	59	ARG
14	N	75	THR
14	N	76	LYS
14	N	79	LEU
14	N	81	VAL
14	N	98	LYS
14	N	106	VAL
14	N	109	VAL
14	N	141	GLN
15	O	1	MET
15	O	15	SER
15	O	18	LEU
15	O	28	LEU
15	O	29	LEU
15	O	67	LEU
15	O	73	VAL
15	O	91	GLN
15	O	100	LEU
15	O	102	GLU
15	O	105	ARG
15	O	111	LEU
16	P	3	ARG
16	P	5	THR
16	P	23	ARG
16	P	36	TYR

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Mol	Chain	Res	Type
16	P	48	LEU
16	P	50	SER
16	P	56	LEU
16	P	59	LYS
16	P	69	VAL
16	P	85	VAL
16	P	98	VAL
16	P	107	GLU
16	P	110	LEU
16	P	111	GLU
17	Q	1	MET
17	Q	6	LEU
17	Q	19	LEU
17	Q	28	VAL
17	Q	31	SER
17	Q	39	ARG
17	Q	65	LYS
17	Q	74	ARG
17	Q	118	ARG
17	Q	128	GLU
18	R	17	ILE
18	R	27	LEU
18	R	30	LYS
18	R	55	ARG
18	R	74	LEU
18	R	77	SER
18	R	83	LEU
18	R	89	GLU
18	R	95	LEU
19	S	7	THR
19	S	19	LYS
19	S	32	THR
19	S	38	LEU
19	S	51	VAL
19	S	53	GLU
19	S	61	VAL
19	S	62	LEU
19	S	68	LYS
19	S	72	VAL
19	S	73	SER
19	S	79	VAL
19	S	82	ARG

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Mol	Chain	Res	Type
20	T	11	ARG
20	T	19	LEU
20	T	23	LEU
20	T	30	GLU
20	T	63	ASP
20	T	92	ARG
20	T	107	LEU
21	U	13	LEU
21	U	15	GLU
21	U	45	THR
21	U	57	LEU
21	U	70	LEU
21	U	81	VAL
21	U	82	GLN
21	U	90	GLU
22	V	2	ARG
22	V	21	LYS
22	V	44	ILE
22	V	50	ARG
22	V	61	ILE
22	V	90	LEU
22	V	97	ARG
22	V	107	ASP
23	W	1	MET
23	W	18	LEU
23	W	31	ARG
23	W	42	VAL
23	W	53	ILE
23	W	72	ARG
23	W	80	ARG
23	W	86	VAL
23	W	91	LEU
23	W	103	ARG
23	W	116	VAL
23	W	132	ASN
23	W	136	PHE
23	W	144	LEU
23	W	157	LEU
23	W	163	LEU
23	W	169	GLU
23	W	175	VAL
23	W	180	VAL

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Mol	Chain	Res	Type
24	X	5	LYS
24	X	7	LEU
24	X	10	THR
24	X	12	ASN
24	X	82	ARG
24	X	84	LEU
25	Y	13	ILE
25	Y	21	ARG
25	Y	30	VAL
25	Y	40	ARG
25	Y	51	VAL
25	Y	59	THR
25	Y	61	ARG
25	Y	95	LEU
25	Y	98	LEU
26	Z	2	LYS
26	Z	3	LEU
26	Z	31	GLU
26	Z	41	ILE
26	Z	53	LEU
26	Z	70	GLN
27	AA	3	ARG
27	AA	18	ASP
27	AA	23	LEU
27	AA	54	VAL
27	AA	56	VAL
28	BA	3	GLU
28	BA	10	VAL
28	BA	31	ILE
28	BA	34	GLU
28	BA	46	GLN
28	BA	61	ARG
28	BA	62	ARG
29	CA	6	VAL
29	CA	26	THR
29	CA	29	ILE
29	CA	48	GLU
29	CA	55	ARG
30	DA	6	ARG
30	DA	13	CYS
30	DA	14	THR
30	DA	19	ARG

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Mol	Chain	Res	Type
30	DA	30	THR
31	EA	1	MET
31	EA	4	THR
31	EA	10	ARG
31	EA	11	LYS
31	EA	24	THR
31	EA	41	ARG
32	FA	4	MET
32	FA	14	VAL
32	FA	19	SER
32	FA	26	LYS
32	FA	31	HIS
32	FA	32	LEU
33	GA	26	ILE
35	JA	119	THR
35	JA	134	MET
35	JA	146	VAL
35	JA	149	MET
35	JA	150	SER
35	JA	155	GLU
35	JA	156	HIS
35	JA	162	ILE
35	JA	167	SER
35	JA	169	ASP
35	JA	176	LYS
35	JA	196	ILE
35	JA	197	HIS
35	JA	208	GLU
35	JA	209	LEU
35	JA	226	THR
35	JA	228	ARG
35	JA	229	SER
35	JA	247	THR
35	JA	251	THR
35	JA	253	ILE
35	JA	260	GLU
35	JA	306	ARG
35	JA	316	ARG
35	JA	318	THR
35	JA	326	LEU
35	JA	327	TYR
35	JA	328	ARG

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Mol	Chain	Res	Type
35	JA	332	VAL
35	JA	340	LEU
35	JA	347	GLU
36	KA	10	LEU
36	KA	11	LEU
36	KA	12	GLU
36	KA	16	HIS
36	KA	21	ARG
36	KA	22	LYS
36	KA	23	ARG
36	KA	24	TRP
36	KA	39	ILE
36	KA	51	LEU
36	KA	75	LYS
36	KA	83	MET
36	KA	94	ASN
36	KA	119	GLU
36	KA	137	ARG
36	KA	142	LEU
36	KA	153	ARG
36	KA	160	ASP
36	KA	163	PHE
36	KA	168	THR
36	KA	169	LYS
36	KA	170	GLU
36	KA	172	ILE
36	KA	179	LYS
36	KA	185	ILE
36	KA	190	THR
36	KA	213	LEU
36	KA	215	LEU
36	KA	229	VAL
36	KA	239	VAL
37	LA	3	ASN
37	LA	17	ASP
37	LA	28	GLN
37	LA	30	ARG
37	LA	31	HIS
37	LA	32	LEU
37	LA	36	ASP
37	LA	63	ASN
37	LA	77	ILE

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Mol	Chain	Res	Type
37	LA	79	ARG
37	LA	87	LEU
37	LA	91	LEU
37	LA	105	GLU
37	LA	131	ARG
37	LA	140	ARG
37	LA	164	ARG
37	LA	165	THR
37	LA	173	VAL
37	LA	190	ARG
38	MA	3	ARG
38	MA	4	TYR
38	MA	9	CYS
38	MA	17	VAL
38	MA	49	ARG
38	MA	50	ARG
38	MA	57	ARG
38	MA	80	GLU
38	MA	83	SER
38	MA	96	LEU
38	MA	114	ARG
38	MA	115	ARG
38	MA	119	GLN
38	MA	127	THR
38	MA	131	ARG
38	MA	135	LEU
38	MA	141	ARG
38	MA	153	ARG
38	MA	154	ASN
38	MA	155	LEU
38	MA	162	LEU
38	MA	163	GLU
38	MA	173	TRP
38	MA	182	LYS
38	MA	190	ASP
38	MA	194	LEU
38	MA	202	LEU
39	NA	10	MET
39	NA	12	LEU
39	NA	41	VAL
39	NA	51	VAL
39	NA	56	GLN

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Mol	Chain	Res	Type
39	NA	64	ARG
39	NA	69	VAL
39	NA	72	GLN
39	NA	73	ASN
39	NA	78	HIS
39	NA	91	LEU
39	NA	126	ARG
39	NA	135	THR
39	NA	140	ARG
39	NA	142	LEU
39	NA	151	LEU
40	OA	19	LEU
40	OA	24	GLU
40	OA	25	ILE
40	OA	43	LEU
40	OA	46	ARG
40	OA	55	ASP
40	OA	71	ARG
40	OA	83	ASP
40	OA	98	LEU
41	PA	5	ARG
41	PA	8	GLU
41	PA	24	THR
41	PA	56	GLN
41	PA	57	GLU
41	PA	59	LEU
41	PA	78	ARG
41	PA	84	ASN
41	PA	89	MET
41	PA	104	LEU
41	PA	114	ARG
41	PA	125	MET
41	PA	155	ARG
42	QA	1	MET
42	QA	18	ARG
42	QA	26	VAL
42	QA	29	SER
42	QA	50	ARG
42	QA	63	LEU
42	QA	85	ARG
42	QA	102	ARG
42	QA	112	LEU

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Mol	Chain	Res	Type
42	QA	119	LEU
42	QA	120	THR
42	QA	127	LEU
42	QA	133	LEU
43	RA	10	ARG
43	RA	23	ASN
43	RA	26	VAL
43	RA	31	GLN
43	RA	38	GLN
43	RA	41	VAL
43	RA	42	ARG
43	RA	44	VAL
43	RA	54	ASP
43	RA	58	ARG
43	RA	65	VAL
43	RA	88	TYR
43	RA	108	VAL
43	RA	109	VAL
43	RA	113	LYS
43	RA	121	ARG
43	RA	128	ARG
44	SA	6	ILE
44	SA	9	ARG
44	SA	29	ARG
44	SA	45	ARG
44	SA	67	THR
44	SA	95	GLU
44	SA	96	ILE
45	TA	14	VAL
45	TA	22	HIS
45	TA	33	THR
45	TA	40	ILE
45	TA	48	ILE
45	TA	66	LEU
45	TA	73	MET
45	TA	103	LEU
46	UA	18	VAL
46	UA	20	LYS
46	UA	27	LEU
46	UA	33	ARG
46	UA	34	ARG
46	UA	36	VAL

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Mol	Chain	Res	Type
46	UA	41	ARG
46	UA	44	THR
46	UA	65	GLU
46	UA	86	ARG
46	UA	97	ARG
46	UA	126	LYS
47	VA	3	ARG
47	VA	4	ILE
47	VA	7	VAL
47	VA	11	ARG
47	VA	19	LEU
47	VA	27	LYS
47	VA	37	THR
47	VA	50	GLU
47	VA	70	LEU
47	VA	77	ASN
47	VA	80	ARG
47	VA	90	LEU
47	VA	105	THR
47	VA	108	ARG
47	VA	117	VAL
48	WA	7	ILE
48	WA	8	GLU
48	WA	13	THR
48	WA	18	VAL
48	WA	23	ARG
48	WA	32	SER
48	WA	33	VAL
48	WA	56	VAL
49	XA	34	LEU
49	XA	38	ARG
49	XA	66	LEU
49	XA	84	LYS
50	YA	1	MET
50	YA	2	VAL
50	YA	25	ARG
50	YA	31	LYS
50	YA	45	THR
50	YA	60	LEU
50	YA	67	THR
50	YA	69	THR
50	YA	82	GLN

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Mol	Chain	Res	Type
51	ZA	9	VAL
51	ZA	14	LYS
51	ZA	35	VAL
51	ZA	63	ARG
51	ZA	75	ARG
51	ZA	87	LYS
51	ZA	92	ARG
51	ZA	93	GLN
51	ZA	96	GLN
52	AB	26	LEU
52	AB	31	LEU
52	AB	42	ARG
52	AB	76	LEU
52	AB	82	THR
53	BB	22	LEU
53	BB	25	LYS
53	BB	28	LYS
53	BB	31	ILE
53	BB	37	ARG
53	BB	51	VAL
53	BB	62	ILE
53	BB	67	VAL
53	BB	83	HIS
54	CB	10	LEU
54	CB	13	LEU
54	CB	15	ARG
54	CB	30	LYS
54	CB	31	SER
54	CB	41	VAL
54	CB	62	LEU
54	CB	71	THR
54	CB	91	LEU
55	DB	10	ARG
5	JB	5	LYS
5	JB	28	GLU
5	JB	61	LEU
5	JB	71	ASP
5	JB	89	SER
5	JB	91	ARG
5	JB	94	LEU
5	JB	98	VAL
5	JB	99	ASP

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Mol	Chain	Res	Type
5	JB	127	VAL
5	JB	140	THR
5	JB	150	LYS
5	JB	171	ASP
5	JB	193	VAL
5	JB	200	ASP
5	JB	211	ARG
5	JB	221	VAL
5	JB	229	VAL
5	JB	242	ARG
5	JB	259	THR
5	JB	266	SER
5	JB	273	ARG
5	JB	274	ARG
5	JB	275	LYS
6	KB	9	VAL
6	KB	13	ARG
6	KB	21	VAL
6	KB	24	THR
6	KB	75	VAL
6	KB	92	THR
6	KB	93	VAL
6	KB	116	VAL
6	KB	119	ARG
6	KB	128	SER
6	KB	154	LYS
6	KB	175	VAL
6	KB	178	GLU
6	KB	181	LEU
6	KB	182	LEU
6	KB	192	ASN
7	LB	6	MET
7	LB	15	SER
7	LB	18	ARG
7	LB	53	THR
7	LB	62	ARG
7	LB	64	ILE
7	LB	70	THR
7	LB	74	ARG
7	LB	110	LEU
7	LB	119	ARG
7	LB	126	VAL

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Mol	Chain	Res	Type
7	LB	129	PHE
7	LB	140	LEU
7	LB	158	THR
7	LB	170	LEU
7	LB	175	THR
7	LB	188	ARG
7	LB	190	GLU
7	LB	191	ARG
7	LB	192	LEU
7	LB	197	ASP
7	LB	200	GLU
7	LB	205	ARG
8	MB	3	LEU
8	MB	7	LEU
8	MB	22	ARG
8	MB	33	ARG
8	MB	38	VAL
8	MB	43	LEU
8	MB	49	ASP
8	MB	53	LEU
8	MB	60	LEU
8	MB	62	LEU
8	MB	67	LYS
8	MB	70	VAL
8	MB	82	LEU
8	MB	91	ARG
8	MB	98	ARG
8	MB	115	ARG
8	MB	118	ARG
8	MB	136	ARG
8	MB	140	ILE
8	MB	143	GLU
8	MB	167	GLU
8	MB	170	ARG
9	NB	3	ARG
9	NB	16	SER
9	NB	24	VAL
9	NB	37	VAL
9	NB	43	VAL
9	NB	57	ASP
9	NB	71	LEU
9	NB	84	SER

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Mol	Chain	Res	Type
9	NB	97	ARG
9	NB	104	GLU
9	NB	106	THR
9	NB	127	GLU
9	NB	136	ILE
9	NB	169	VAL
10	OB	1	MET
10	OB	9	LEU
10	OB	19	VAL
10	OB	43	ASN
10	OB	44	LEU
10	OB	57	ARG
10	OB	61	ARG
10	OB	74	ASN
10	OB	77	LEU
10	OB	82	ARG
10	OB	86	THR
10	OB	88	ILE
10	OB	89	TYR
10	OB	96	ASP
10	OB	99	GLU
10	OB	107	ILE
10	OB	108	THR
10	OB	112	LYS
10	OB	118	LYS
10	OB	122	GLU
10	OB	125	GLU
10	OB	129	THR
10	OB	131	LYS
10	OB	140	LEU
10	OB	144	VAL
10	OB	145	VAL
11	PB	9	VAL
11	PB	14	VAL
11	PB	19	GLU
11	PB	28	THR
11	PB	34	LEU
11	PB	48	MET
11	PB	67	LEU
11	PB	68	GLU
11	PB	76	SER
11	PB	83	LYS

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Mol	Chain	Res	Type
11	PB	84	LYS
11	PB	87	LEU
11	PB	93	THR
11	PB	96	GLU
11	PB	99	LEU
11	PB	138	LEU
12	QB	10	VAL
12	QB	21	CYS
12	QB	24	VAL
12	QB	31	LYS
12	QB	32	TYR
12	QB	45	GLU
12	QB	53	LYS
12	QB	70	LYS
12	QB	78	ARG
12	QB	98	VAL
12	QB	116	SER
13	RB	3	LEU
13	RB	29	LYS
13	RB	42	SER
13	RB	58	THR
13	RB	71	VAL
13	RB	90	ARG
13	RB	112	LEU
13	RB	117	GLU
13	RB	126	VAL
13	RB	135	LEU
13	RB	147	LEU
13	RB	149	GLU
14	SB	16	ARG
14	SB	59	ARG
14	SB	75	THR
14	SB	76	LYS
14	SB	79	LEU
14	SB	81	VAL
14	SB	98	LYS
14	SB	106	VAL
14	SB	109	VAL
14	SB	141	GLN
15	TB	13	HIS
15	TB	15	SER
15	TB	18	LEU

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Mol	Chain	Res	Type
15	TB	28	LEU
15	TB	29	LEU
15	TB	67	LEU
15	TB	73	VAL
15	TB	91	GLN
15	TB	100	LEU
15	TB	102	GLU
15	TB	104	ARG
15	TB	105	ARG
15	TB	111	LEU
16	UB	3	ARG
16	UB	5	THR
16	UB	23	ARG
16	UB	36	TYR
16	UB	48	LEU
16	UB	50	SER
16	UB	56	LEU
16	UB	59	LYS
16	UB	69	VAL
16	UB	85	VAL
16	UB	98	VAL
16	UB	107	GLU
16	UB	110	LEU
16	UB	111	GLU
17	VB	1	MET
17	VB	6	LEU
17	VB	19	LEU
17	VB	28	VAL
17	VB	31	SER
17	VB	39	ARG
17	VB	65	LYS
17	VB	74	ARG
17	VB	128	GLU
18	WB	17	ILE
18	WB	27	LEU
18	WB	30	LYS
18	WB	55	ARG
18	WB	74	LEU
18	WB	77	SER
18	WB	83	LEU
18	WB	89	GLU
18	WB	95	LEU

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Mol	Chain	Res	Type
19	XB	7	THR
19	XB	19	LYS
19	XB	32	THR
19	XB	38	LEU
19	XB	46	VAL
19	XB	51	VAL
19	XB	53	GLU
19	XB	61	VAL
19	XB	62	LEU
19	XB	72	VAL
19	XB	73	SER
19	XB	79	VAL
19	XB	82	ARG
20	YB	11	ARG
20	YB	19	LEU
20	YB	23	LEU
20	YB	30	GLU
20	YB	63	ASP
20	YB	92	ARG
20	YB	107	LEU
21	ZB	15	GLU
21	ZB	45	THR
21	ZB	57	LEU
21	ZB	70	LEU
21	ZB	81	VAL
21	ZB	82	GLN
21	ZB	90	GLU
22	AC	2	ARG
22	AC	21	LYS
22	AC	44	ILE
22	AC	50	ARG
22	AC	61	ILE
22	AC	64	GLU
22	AC	90	LEU
22	AC	97	ARG
22	AC	102	CYS
22	AC	107	ASP
23	BC	1	MET
23	BC	18	LEU
23	BC	31	ARG
23	BC	42	VAL
23	BC	53	ILE

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Mol	Chain	Res	Type
23	BC	72	ARG
23	BC	80	ARG
23	BC	86	VAL
23	BC	91	LEU
23	BC	103	ARG
23	BC	116	VAL
23	BC	132	ASN
23	BC	136	PHE
23	BC	144	LEU
23	BC	157	LEU
23	BC	163	LEU
23	BC	169	GLU
23	BC	175	VAL
23	BC	180	VAL
24	CC	5	LYS
24	CC	7	LEU
24	CC	10	THR
24	CC	12	ASN
24	CC	82	ARG
24	CC	84	LEU
25	DC	13	ILE
25	DC	21	ARG
25	DC	30	VAL
25	DC	40	ARG
25	DC	51	VAL
25	DC	59	THR
25	DC	61	ARG
25	DC	95	LEU
25	DC	98	LEU
26	EC	2	LYS
26	EC	3	LEU
26	EC	31	GLU
26	EC	41	ILE
26	EC	53	LEU
26	EC	70	GLN
27	FC	3	ARG
27	FC	18	ASP
27	FC	23	LEU
27	FC	54	VAL
27	FC	56	VAL
28	GC	3	GLU
28	GC	10	VAL

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Mol	Chain	Res	Type
28	GC	31	ILE
28	GC	34	GLU
28	GC	46	GLN
28	GC	61	ARG
28	GC	62	ARG
29	HC	6	VAL
29	HC	26	THR
29	HC	29	ILE
29	HC	48	GLU
29	HC	55	ARG
30	IC	6	ARG
30	IC	13	CYS
30	IC	14	THR
30	IC	19	ARG
30	IC	30	THR
31	JC	1	MET
31	JC	4	THR
31	JC	11	LYS
31	JC	24	THR
32	KC	14	VAL
32	KC	26	LYS
32	KC	31	HIS
32	KC	32	LEU
35	OC	119	THR
35	OC	134	MET
35	OC	146	VAL
35	OC	149	MET
35	OC	150	SER
35	OC	155	GLU
35	OC	156	HIS
35	OC	162	ILE
35	OC	167	SER
35	OC	169	ASP
35	OC	176	LYS
35	OC	196	ILE
35	OC	197	HIS
35	OC	208	GLU
35	OC	209	LEU
35	OC	226	THR
35	OC	228	ARG
35	OC	229	SER
35	OC	247	THR

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Mol	Chain	Res	Type
35	OC	251	THR
35	OC	253	ILE
35	OC	260	GLU
35	OC	306	ARG
35	OC	316	ARG
35	OC	318	THR
35	OC	326	LEU
35	OC	327	TYR
35	OC	328	ARG
35	OC	332	VAL
35	OC	336	LYS
35	OC	340	LEU
35	OC	347	GLU
36	PC	10	LEU
36	PC	11	LEU
36	PC	12	GLU
36	PC	16	HIS
36	PC	21	ARG
36	PC	22	LYS
36	PC	23	ARG
36	PC	24	TRP
36	PC	39	ILE
36	PC	51	LEU
36	PC	75	LYS
36	PC	83	MET
36	PC	94	ASN
36	PC	119	GLU
36	PC	137	ARG
36	PC	142	LEU
36	PC	153	ARG
36	PC	160	ASP
36	PC	163	PHE
36	PC	168	THR
36	PC	169	LYS
36	PC	170	GLU
36	PC	172	ILE
36	PC	179	LYS
36	PC	185	ILE
36	PC	190	THR
36	PC	213	LEU
36	PC	215	LEU
36	PC	229	VAL

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Mol	Chain	Res	Type
36	PC	239	VAL
37	QC	3	ASN
37	QC	17	ASP
37	QC	28	GLN
37	QC	31	HIS
37	QC	32	LEU
37	QC	36	ASP
37	QC	63	ASN
37	QC	77	ILE
37	QC	79	ARG
37	QC	87	LEU
37	QC	91	LEU
37	QC	105	GLU
37	QC	131	ARG
37	QC	140	ARG
37	QC	164	ARG
37	QC	165	THR
37	QC	173	VAL
37	QC	190	ARG
38	RC	3	ARG
38	RC	4	TYR
38	RC	9	CYS
38	RC	21	LEU
38	RC	49	ARG
38	RC	50	ARG
38	RC	57	ARG
38	RC	80	GLU
38	RC	83	SER
38	RC	96	LEU
38	RC	114	ARG
38	RC	115	ARG
38	RC	119	GLN
38	RC	127	THR
38	RC	131	ARG
38	RC	135	LEU
38	RC	141	ARG
38	RC	153	ARG
38	RC	154	ASN
38	RC	155	LEU
38	RC	157	LEU
38	RC	162	LEU
38	RC	163	GLU

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Mol	Chain	Res	Type
38	RC	173	TRP
38	RC	182	LYS
38	RC	190	ASP
38	RC	194	LEU
38	RC	202	LEU
39	SC	5	ASP
39	SC	10	MET
39	SC	12	LEU
39	SC	41	VAL
39	SC	51	VAL
39	SC	56	GLN
39	SC	64	ARG
39	SC	69	VAL
39	SC	72	GLN
39	SC	73	ASN
39	SC	78	HIS
39	SC	87	SER
39	SC	91	LEU
39	SC	126	ARG
39	SC	135	THR
39	SC	140	ARG
39	SC	142	LEU
39	SC	151	LEU
40	TC	19	LEU
40	TC	24	GLU
40	TC	25	ILE
40	TC	43	LEU
40	TC	46	ARG
40	TC	55	ASP
40	TC	71	ARG
40	TC	83	ASP
40	TC	98	LEU
41	UC	5	ARG
41	UC	8	GLU
41	UC	24	THR
41	UC	56	GLN
41	UC	57	GLU
41	UC	59	LEU
41	UC	78	ARG
41	UC	84	ASN
41	UC	89	MET
41	UC	104	LEU

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Mol	Chain	Res	Type
41	UC	114	ARG
41	UC	122	HIS
41	UC	125	MET
41	UC	155	ARG
42	VC	1	MET
42	VC	18	ARG
42	VC	26	VAL
42	VC	29	SER
42	VC	50	ARG
42	VC	63	LEU
42	VC	85	ARG
42	VC	102	ARG
42	VC	112	LEU
42	VC	119	LEU
42	VC	120	THR
42	VC	127	LEU
42	VC	133	LEU
43	WC	10	ARG
43	WC	26	VAL
43	WC	31	GLN
43	WC	38	GLN
43	WC	41	VAL
43	WC	42	ARG
43	WC	44	VAL
43	WC	54	ASP
43	WC	58	ARG
43	WC	65	VAL
43	WC	88	TYR
43	WC	108	VAL
43	WC	109	VAL
43	WC	113	LYS
43	WC	121	ARG
43	WC	128	ARG
44	XC	6	ILE
44	XC	9	ARG
44	XC	29	ARG
44	XC	45	ARG
44	XC	67	THR
44	XC	95	GLU
44	XC	96	ILE
45	YC	14	VAL
45	YC	22	HIS

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Mol	Chain	Res	Type
45	YC	33	THR
45	YC	40	ILE
45	YC	48	ILE
45	YC	66	LEU
45	YC	73	MET
45	YC	103	LEU
45	YC	109	VAL
46	ZC	18	VAL
46	ZC	20	LYS
46	ZC	27	LEU
46	ZC	33	ARG
46	ZC	36	VAL
46	ZC	41	ARG
46	ZC	44	THR
46	ZC	65	GLU
46	ZC	86	ARG
46	ZC	97	ARG
46	ZC	126	LYS
47	AD	3	ARG
47	AD	4	ILE
47	AD	7	VAL
47	AD	11	ARG
47	AD	19	LEU
47	AD	27	LYS
47	AD	37	THR
47	AD	50	GLU
47	AD	70	LEU
47	AD	77	ASN
47	AD	80	ARG
47	AD	90	LEU
47	AD	105	THR
47	AD	108	ARG
47	AD	117	VAL
48	BD	7	ILE
48	BD	8	GLU
48	BD	13	THR
48	BD	18	VAL
48	BD	23	ARG
48	BD	32	SER
48	BD	33	VAL
48	BD	56	VAL
49	CD	34	LEU

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Mol	Chain	Res	Type
49	CD	38	ARG
49	CD	66	LEU
49	CD	84	LYS
50	DD	1	MET
50	DD	2	VAL
50	DD	25	ARG
50	DD	31	LYS
50	DD	45	THR
50	DD	60	LEU
50	DD	67	THR
50	DD	69	THR
50	DD	82	GLN
51	ED	9	VAL
51	ED	14	LYS
51	ED	35	VAL
51	ED	63	ARG
51	ED	75	ARG
51	ED	87	LYS
51	ED	93	GLN
51	ED	96	GLN
52	FD	26	LEU
52	FD	31	LEU
52	FD	42	ARG
52	FD	76	LEU
52	FD	82	THR
53	GD	28	LYS
53	GD	31	ILE
53	GD	37	ARG
53	GD	51	VAL
53	GD	62	ILE
53	GD	67	VAL
53	GD	83	HIS
54	HD	10	LEU
54	HD	13	LEU
54	HD	15	ARG
54	HD	31	SER
54	HD	41	VAL
54	HD	62	LEU
54	HD	71	THR
54	HD	91	LEU
55	ID	10	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
15	O	13	HIS
23	W	73	GLN
36	KA	19	HIS
36	KA	78	GLN
36	KA	94	ASN
37	LA	31	HIS
43	RA	3	GLN
45	TA	22	HIS
45	TA	99	GLN
6	KB	192	ASN
15	TB	13	HIS
23	BC	73	GLN
36	PC	19	HIS
36	PC	78	GLN
36	PC	94	ASN
37	QC	31	HIS
43	WC	3	GLN
45	YC	22	HIS
45	YC	99	GLN
46	ZC	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	227 (15%)	11 (0%)
1	FB	1502/1507 (99%)	229 (15%)	11 (0%)
2	B	2876/2880 (99%)	476 (16%)	24 (0%)
2	GB	2876/2880 (99%)	476 (16%)	21 (0%)
3	C	119/120 (99%)	16 (13%)	1 (0%)
3	HB	119/120 (99%)	16 (13%)	1 (0%)
34	HA	9/27 (33%)	4 (44%)	0
34	MC	9/27 (33%)	4 (44%)	0
4	D	76/77 (98%)	15 (19%)	0
4	IA	76/77 (98%)	7 (9%)	1 (1%)
4	IB	76/77 (98%)	15 (19%)	0
4	NC	76/77 (98%)	7 (9%)	1 (1%)
All	All	9316/9376 (99%)	1492 (16%)	71 (0%)

All (1492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	59	A
1	A	61	G
1	A	65	U
1	A	66	G
1	A	77	C
1	A	79	G
1	A	80	G
1	A	84	U
1	A	85	U
1	A	86	U
1	A	87	A
1	A	88	C
1	A	89	U
1	A	101	A
1	A	105	G
1	A	116	A
1	A	121	C
1	A	131	C
1	A	163	C
1	A	182	U
1	A	188	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	209	U
1	A	210	U
1	A	216	G
1	A	231	G
1	A	240	C
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	328	C
1	A	332	G
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	397	A
1	A	398	C
1	A	402	G
1	A	406	G
1	A	412	A
1	A	413	G
1	A	422	C
1	A	429	U
1	A	439	A
1	A	452	A
1	A	465	A
1	A	482	A
1	A	485	G
1	A	487	A
1	A	496	A
1	A	497	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	532	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	596	C

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Mol	Chain	Res	Type
1	A	607	A
1	A	618	C
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	694	A
1	A	695	A
1	A	703	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	725	G
1	A	731	G
1	A	734	G
1	A	748	C
1	A	749	C
1	A	755	G
1	A	764	C
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	816	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	836	G
1	A	842	C
1	A	843	U
1	A	859	A
1	A	870	U
1	A	872	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	M2G
1	A	969	A

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Mol	Chain	Res	Type
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	992	U
1	A	993	G
1	A	997	U
1	A	998(A)	G
1	A	999	U
1	A	1002	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1028(C)	C
1	A	1029	G
1	A	1030	C
1	A	1031	G
1	A	1032(A)	A
1	A	1032(B)	G
1	A	1032(C)	G
1	A	1033	G
1	A	1035	A
1	A	1042	G
1	A	1045	C
1	A	1050	G
1	A	1054	C
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1129	C
1	A	1134	G
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1146	A

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Mol	Chain	Res	Type
1	A	1151	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1171	G
1	A	1184	G
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1199	U
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1240	U
1	A	1257	U
1	A	1258	G
1	A	1263	C
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1287	A
1	A	1297	C
1	A	1299	A
1	A	1302	U
1	A	1305	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1362(B)	C
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1397	C

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Mol	Chain	Res	Type
1	A	1398	A
1	A	1419	G
1	A	1442	G
1	A	1453	G
1	A	1454	G
1	A	1460	A
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1532	U
2	B	14	A
2	B	15	G
2	B	34	C
2	B	35	G
2	B	46	C
2	B	58	G
2	B	71	A
2	B	74	A
2	B	75	G
2	B	93	C
2	B	118	A
2	B	119	A
2	B	120	U
2	B	125	G
2	B	135	G
2	B	149	A
2	B	154(A)	C
2	B	155	C
2	B	161	U
2	B	163	U
2	B	164	U
2	B	181	A
2	B	188	G
2	B	196	A
2	B	199	A
2	B	205	G

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Mol	Chain	Res	Type
2	B	214	G
2	B	215	G
2	B	216	A
2	B	221	A
2	B	222	A
2	B	228	A
2	B	229	A
2	B	233	A
2	B	248	G
2	B	249	C
2	B	250	G
2	B	266	G
2	B	269	U
2	B	270(L)	C
2	B	270(M)	U
2	B	270(N)	U
2	B	270(O)	G
2	B	270(P)	U
2	B	270(Q)	C
2	B	271(C)	G
2	B	271(D)	U
2	B	271	G
2	B	273(G)	C
2	B	278	A
2	B	283	A
2	B	311	A
2	B	317	G
2	B	324	A
2	B	329	G
2	B	330	A
2	B	352	G
2	B	353	G
2	B	363(A)	G
2	B	363(G)	A
2	B	372	G
2	B	386	G
2	B	396	G
2	B	405	U
2	B	407	G
2	B	411	G
2	B	412	A
2	B	442	G

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Mol	Chain	Res	Type
2	B	443	A
2	B	444	C
2	B	455	C
2	B	456	C
2	B	457	A
2	B	479	A
2	B	481	G
2	B	494	G
2	B	504	U
2	B	505	A
2	B	508	G
2	B	509	C
2	B	510	C
2	B	529	A
2	B	531	C
2	B	532	A
2	B	533	G
2	B	549	G
2	B	550	G
2	B	563	G
2	B	571	A
2	B	573	G
2	B	575	A
2	B	603	A
2	B	604	G
2	B	607	U
2	B	615	G
2	B	616	A
2	B	617	G
2	B	627	A
2	B	637	A
2	B	645	C
2	B	646	A
2	B	654	U
2	B	655	A
2	B	664	C
2	B	686	G
2	B	717	G
2	B	730	C
2	B	765	G
2	B	775	G
2	B	776	G

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Mol	Chain	Res	Type
2	B	782	A
2	B	784	A
2	B	785	G
2	B	792	G
2	B	805	G
2	B	812	C
2	B	819	A
2	B	827	U
2	B	828	U
2	B	855	G
2	B	859	G
2	B	869	G
2	B	878	A
2	B	879	G
2	B	886	C
2	B	887	A
2	B	888	C
2	B	890	A
2	B	893	C
2	B	894	C
2	B	895	U
2	B	896	A
2	B	907	U
2	B	910	A
2	B	917	A
2	B	932	G
2	B	941	A
2	B	945	A
2	B	946	G
2	B	959	A
2	B	961	C
2	B	974(A)	G
2	B	974(B)	C
2	B	983	A
2	B	989	G
2	B	990	A
2	B	996	A
2	B	1012	U
2	B	1013	C
2	B	1022	G
2	B	1025	G
2	B	1026	U

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Mol	Chain	Res	Type
2	B	1033	U
2	B	1039	G
2	B	1042	G
2	B	1044	G
2	B	1045	A
2	B	1046	A
2	B	1047	G
2	B	1054	A
2	B	1057	A
2	B	1058	G
2	B	1059	G
2	B	1060	U
2	B	1061	U
2	B	1062	G
2	B	1066	U
2	B	1068	G
2	B	1069	A
2	B	1070	A
2	B	1071	G
2	B	1072	C
2	B	1073	A
2	B	1075	C
2	B	1076	C
2	B	1077	A
2	B	1078	U
2	B	1079	C
2	B	1081	U
2	B	1082	U
2	B	1083	U
2	B	1085	A
2	B	1086	A
2	B	1088	A
2	B	1089	G
2	B	1090	U
2	B	1091	G
2	B	1094	U
2	B	1097	U
2	B	1098	A
2	B	1101	U
2	B	1107	G
2	B	1111	A
2	B	1112	G

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Mol	Chain	Res	Type
2	B	1122	G
2	B	1126	A
2	B	1129	A
2	B	1130	U
2	B	1135	C
2	B	1136	G
2	B	1139	G
2	B	1142(B)	A
2	B	1143	A
2	B	1155	A
2	B	1174	A
2	B	1175	U
2	B	1177	A
2	B	1205	U
2	B	1210	A
2	B	1211	U
2	B	1218	C
2	B	1220	A
2	B	1253	A
2	B	1256	G
2	B	1271	G
2	B	1272	A
2	B	1273	U
2	B	1300	U
2	B	1301	A
2	B	1313	U
2	B	1359	A
2	B	1360	A
2	B	1365	A
2	B	1380	G
2	B	1385	G
2	B	1395	A
2	B	1416	G
2	B	1417	C
2	B	1419	A
2	B	1420	U
2	B	1421	G
2	B	1428	C
2	B	1444(B)	A
2	B	1449(B)	A
2	B	1459	G
2	B	1460	A

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Mol	Chain	Res	Type
2	B	1461	G
2	B	1467	C
2	B	1471	A
2	B	1483	G
2	B	1493	C
2	B	1494	A
2	B	1497	U
2	B	1508	A
2	B	1510	A
2	B	1511	A
2	B	1512	G
2	B	1513	C
2	B	1532	C
2	B	1534	G
2	B	1535	U
2	B	1537	C
2	B	1538	G
2	B	1544	C
2	B	1547	C
2	B	1558	A
2	B	1559	G
2	B	1566	A
2	B	1569	A
2	B	1578	U
2	B	1585	C
2	B	1587	A
2	B	1595	G
2	B	1608	A
2	B	1609	A
2	B	1610	A
2	B	1631	A
2	B	1647	G
2	B	1648	C
2	B	1654	A
2	B	1667	G
2	B	1674	G
2	B	1693	U
2	B	1700	A
2	B	1701	A
2	B	1729	A
2	B	1730	U
2	B	1731	G

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Mol	Chain	Res	Type
2	B	1743	G
2	B	1762	A
2	B	1763	G
2	B	1764	G
2	B	1773	A
2	B	1776	G
2	B	1781	C
2	B	1791	A
2	B	1800	C
2	B	1801	G
2	B	1811	G
2	B	1816	G
2	B	1829	A
2	B	1835	G
2	B	1839	G
2	B	1847	A
2	B	1859	A
2	B	1872	A
2	B	1878	G
2	B	1900	A
2	B	1903	G
2	B	1905	C
2	B	1906	G
2	B	1913	A
2	B	1914	C
2	B	1921	G
2	B	1929	G
2	B	1930	G
2	B	1936	A
2	B	1940	U
2	B	1955	U
2	B	1963	U
2	B	1965	C
2	B	1967	C
2	B	1970	A
2	B	1971	A
2	B	1972	A
2	B	1984	G
2	B	1992	G
2	B	1993	U
2	B	1997	G
2	B	2020	A

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Mol	Chain	Res	Type
2	B	2023	G
2	B	2031	A
2	B	2032	G
2	B	2033	A
2	B	2043	C
2	B	2055	C
2	B	2056	G
2	B	2060	A
2	B	2061	G
2	B	2062	A
2	B	2069	G
2	B	2100	G
2	B	2110	G
2	B	2113	U
2	B	2116	G
2	B	2117	A
2	B	2118	U
2	B	2119	A
2	B	2122	U
2	B	2125	G
2	B	2126	A
2	B	2127	G
2	B	2130	U
2	B	2131	G
2	B	2132	U
2	B	2133	G
2	B	2134	A
2	B	2136	C
2	B	2137	C
2	B	2138	C
2	B	2142	C
2	B	2145	C
2	B	2146	C
2	B	2147	G
2	B	2148	G
2	B	2152	G
2	B	2162	G
2	B	2164	C
2	B	2165	G
2	B	2166	G
2	B	2167	U
2	B	2169	A

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Mol	Chain	Res	Type
2	B	2171	A
2	B	2172	U
2	B	2173	A
2	B	2176	A
2	B	2187	G
2	B	2189	U
2	B	2198	A
2	B	2210	G
2	B	2211	G
2	B	2212	A
2	B	2213	U
2	B	2225	A
2	B	2226	C
2	B	2238	G
2	B	2239	G
2	B	2243	U
2	B	2269	A
2	B	2275	C
2	B	2278	A
2	B	2279	G
2	B	2283	C
2	B	2287	A
2	B	2288	A
2	B	2305	A
2	B	2308	G
2	B	2309	A
2	B	2311	A
2	B	2312	U
2	B	2319	G
2	B	2320	A
2	B	2321	G
2	B	2322	A
2	B	2325	G
2	B	2327	A
2	B	2336	A
2	B	2347	C
2	B	2383	G
2	B	2385	C
2	B	2396	G
2	B	2401	U
2	B	2406	U
2	B	2424	C

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Mol	Chain	Res	Type
2	B	2425	A
2	B	2429	G
2	B	2430	A
2	B	2435	A
2	B	2439	A
2	B	2440	C
2	B	2441	C
2	B	2448	A
2	B	2476	A
2	B	2477	C
2	B	2502	G
2	B	2504	U
2	B	2505	G
2	B	2506	U
2	B	2518	A
2	B	2525	G
2	B	2529	G
2	B	2534	A
2	B	2554	U
2	B	2566	A
2	B	2567	G
2	B	2573	C
2	B	2574	G
2	B	2596	U
2	B	2602	A
2	B	2609	U
2	B	2611	U
2	B	2612	C
2	B	2615	U
2	B	2630	G
2	B	2663	G
2	B	2682	U
2	B	2683	C
2	B	2689	U
2	B	2690	C
2	B	2691	C
2	B	2703	C
2	B	2712(A)	A
2	B	2713	A
2	B	2714	G
2	B	2718	G
2	B	2726	U

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Mol	Chain	Res	Type
2	B	2733	A
2	B	2751	G
2	B	2757	A
2	B	2758	A
2	B	2764	A
2	B	2765	A
2	B	2766	G
2	B	2778	A
2	B	2789	C
2	B	2790	A
2	B	2791	C
2	B	2793	G
2	B	2794	C
2	B	2797	U
2	B	2798	C
2	B	2799	A
2	B	2801	A
2	B	2802	G
2	B	2805	G
2	B	2807	G
2	B	2818	G
2	B	2820	A
2	B	2821	A
2	B	2835	A
2	B	2836	U
2	B	2872	G
2	B	2879	C
2	B	2880	C
2	B	2892	A
2	B	2894	G
3	C	2	C
3	C	9	G
3	C	12	C
3	C	25	A
3	C	30	C
3	C	35	U
3	C	45	A
3	C	56	G
3	C	66	A
3	C	73	A
3	C	74	U
3	C	89(B)	A

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Mol	Chain	Res	Type
3	C	90	C
3	C	109	G
3	C	111	U
3	C	119	A
4	D	7	G
4	D	8	4SU
4	D	16	C
4	D	17(A)	U
4	D	19	G
4	D	20	U
4	D	22	G
4	D	35	A
4	D	36	U
4	D	37	A
4	D	46	G
4	D	47	U
4	D	48	C
4	D	58	A
4	D	61	C
34	HA	14	A
34	HA	16	A
34	HA	21	A
34	HA	22	A
4	IA	10	G
4	IA	18	G
4	IA	20	U
4	IA	47	U
4	IA	48	C
4	IA	52	G
4	IA	76	A
1	FB	9	G
1	FB	22	G
1	FB	32	A
1	FB	39	G
1	FB	47	C
1	FB	48	C
1	FB	50	A
1	FB	51	A
1	FB	54	C
1	FB	59	A
1	FB	61	G
1	FB	65	U

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Mol	Chain	Res	Type
1	FB	66	G
1	FB	77	C
1	FB	79	G
1	FB	80	G
1	FB	84	U
1	FB	85	U
1	FB	86	U
1	FB	87	A
1	FB	88	C
1	FB	89	U
1	FB	101	A
1	FB	105	G
1	FB	116	A
1	FB	121	C
1	FB	131	C
1	FB	163	C
1	FB	182	U
1	FB	188	U
1	FB	195	A
1	FB	197	A
1	FB	201	C
1	FB	209	U
1	FB	210	U
1	FB	216	G
1	FB	231	G
1	FB	240	C
1	FB	247	G
1	FB	251	G
1	FB	266	G
1	FB	267	C
1	FB	289	G
1	FB	319	G
1	FB	321	A
1	FB	328	C
1	FB	332	G
1	FB	346	G
1	FB	352	C
1	FB	353	A
1	FB	354	G
1	FB	367	U
1	FB	372	C
1	FB	373	A

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Mol	Chain	Res	Type
1	FB	384	G
1	FB	397	A
1	FB	398	C
1	FB	402	G
1	FB	406	G
1	FB	412	A
1	FB	413	G
1	FB	422	C
1	FB	429	U
1	FB	439	A
1	FB	452	A
1	FB	465	A
1	FB	482	A
1	FB	485	G
1	FB	487	A
1	FB	496	A
1	FB	497	U
1	FB	509	A
1	FB	510	A
1	FB	511	C
1	FB	518	C
1	FB	521	G
1	FB	532	A
1	FB	547	A
1	FB	559	A
1	FB	560	U
1	FB	561	U
1	FB	572	A
1	FB	573	A
1	FB	575	G
1	FB	576	G
1	FB	577	G
1	FB	607	A
1	FB	618	C
1	FB	653	A
1	FB	665	A
1	FB	687	A
1	FB	688	G
1	FB	695	A
1	FB	722	A
1	FB	723	U
1	FB	724	G

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Mol	Chain	Res	Type
1	FB	725	G
1	FB	731	G
1	FB	734	G
1	FB	748	C
1	FB	749	C
1	FB	755	G
1	FB	764	C
1	FB	774	G
1	FB	777	A
1	FB	793	U
1	FB	794	A
1	FB	815	A
1	FB	816	A
1	FB	817	C
1	FB	819	A
1	FB	828	A
1	FB	836	G
1	FB	842	C
1	FB	843	U
1	FB	859	A
1	FB	870	U
1	FB	872	A
1	FB	902	G
1	FB	914	A
1	FB	926	G
1	FB	927	G
1	FB	931	C
1	FB	934	C
1	FB	935	A
1	FB	960	U
1	FB	966	M2G
1	FB	969	A
1	FB	971	G
1	FB	974	A
1	FB	975	A
1	FB	976	G
1	FB	977	A
1	FB	982	U
1	FB	984	C
1	FB	992	U
1	FB	993	G
1	FB	997	U

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Mol	Chain	Res	Type
1	FB	998(A)	G
1	FB	999	U
1	FB	1002	G
1	FB	1003	G
1	FB	1004	A
1	FB	1005	A
1	FB	1025	U
1	FB	1027	C
1	FB	1028(C)	C
1	FB	1029	G
1	FB	1030	C
1	FB	1031	G
1	FB	1032(A)	A
1	FB	1032(B)	G
1	FB	1032(C)	G
1	FB	1033	G
1	FB	1035	A
1	FB	1042	G
1	FB	1045	C
1	FB	1050	G
1	FB	1054	C
1	FB	1081	G
1	FB	1094	G
1	FB	1095	U
1	FB	1101	A
1	FB	1108	G
1	FB	1129	C
1	FB	1134	G
1	FB	1136	U
1	FB	1137	C
1	FB	1139	G
1	FB	1140	C
1	FB	1146	A
1	FB	1151	A
1	FB	1152	A
1	FB	1157	A
1	FB	1159	U
1	FB	1171	G
1	FB	1184	G
1	FB	1193	G
1	FB	1196	U
1	FB	1197	G

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Mol	Chain	Res	Type
1	FB	1199	U
1	FB	1202	G
1	FB	1212	U
1	FB	1213	A
1	FB	1225	A
1	FB	1227	A
1	FB	1236	A
1	FB	1238	A
1	FB	1240	U
1	FB	1257	U
1	FB	1258	G
1	FB	1263	C
1	FB	1270	C
1	FB	1280	A
1	FB	1281	U
1	FB	1282	C
1	FB	1287	A
1	FB	1297	C
1	FB	1299	A
1	FB	1302	U
1	FB	1305	G
1	FB	1317	C
1	FB	1319	A
1	FB	1320	C
1	FB	1322	C
1	FB	1346	A
1	FB	1347	G
1	FB	1353	G
1	FB	1362(B)	C
1	FB	1364	U
1	FB	1368	G
1	FB	1370	G
1	FB	1397	C
1	FB	1398	A
1	FB	1419	G
1	FB	1442	G
1	FB	1453	G
1	FB	1454	G
1	FB	1460	A
1	FB	1487	G
1	FB	1492	A
1	FB	1497	G

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Mol	Chain	Res	Type
1	FB	1504	G
1	FB	1506	U
1	FB	1517	G
1	FB	1520	G
1	FB	1529	G
1	FB	1530	G
1	FB	1532	U
2	GB	14	A
2	GB	15	G
2	GB	34	C
2	GB	35	G
2	GB	46	C
2	GB	58	G
2	GB	71	A
2	GB	74	A
2	GB	75	G
2	GB	93	C
2	GB	118	A
2	GB	119	A
2	GB	120	U
2	GB	125	G
2	GB	135	G
2	GB	140	A
2	GB	149	A
2	GB	154(A)	C
2	GB	155	C
2	GB	161	U
2	GB	163	U
2	GB	164	U
2	GB	181	A
2	GB	188	G
2	GB	196	A
2	GB	199	A
2	GB	205	G
2	GB	214	G
2	GB	215	G
2	GB	216	A
2	GB	221	A
2	GB	222	A
2	GB	228	A
2	GB	229	A
2	GB	233	A

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Mol	Chain	Res	Type
2	GB	248	G
2	GB	249	C
2	GB	250	G
2	GB	266	G
2	GB	269	U
2	GB	270(L)	C
2	GB	270(M)	U
2	GB	270(N)	U
2	GB	270(O)	G
2	GB	270(P)	U
2	GB	270(Q)	C
2	GB	271(C)	G
2	GB	271(D)	U
2	GB	271	G
2	GB	273(G)	C
2	GB	278	A
2	GB	283	A
2	GB	311	A
2	GB	312	G
2	GB	317	G
2	GB	324	A
2	GB	329	G
2	GB	330	A
2	GB	352	G
2	GB	353	G
2	GB	363(A)	G
2	GB	363(G)	A
2	GB	372	G
2	GB	386	G
2	GB	396	G
2	GB	405	U
2	GB	407	G
2	GB	411	G
2	GB	412	A
2	GB	442	G
2	GB	443	A
2	GB	444	C
2	GB	455	C
2	GB	456	C
2	GB	457	A
2	GB	479	A
2	GB	481	G

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Mol	Chain	Res	Type
2	GB	494	G
2	GB	504	U
2	GB	505	A
2	GB	508	G
2	GB	509	C
2	GB	510	C
2	GB	529	A
2	GB	531	C
2	GB	532	A
2	GB	533	G
2	GB	563	G
2	GB	571	A
2	GB	573	G
2	GB	575	A
2	GB	603	A
2	GB	604	G
2	GB	607	U
2	GB	615	G
2	GB	616	A
2	GB	617	G
2	GB	627	A
2	GB	637	A
2	GB	645	C
2	GB	646	A
2	GB	654	U
2	GB	664	C
2	GB	686	G
2	GB	717	G
2	GB	730	C
2	GB	765	G
2	GB	775	G
2	GB	776	G
2	GB	782	A
2	GB	784	A
2	GB	785	G
2	GB	792	G
2	GB	805	G
2	GB	812	C
2	GB	819	A
2	GB	827	U
2	GB	828	U
2	GB	855	G

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Mol	Chain	Res	Type
2	GB	859	G
2	GB	869	G
2	GB	878	A
2	GB	879	G
2	GB	886	C
2	GB	887	A
2	GB	888	C
2	GB	890	A
2	GB	893	C
2	GB	894	C
2	GB	895	U
2	GB	896	A
2	GB	907	U
2	GB	910	A
2	GB	917	A
2	GB	932	G
2	GB	941	A
2	GB	945	A
2	GB	946	G
2	GB	959	A
2	GB	961	C
2	GB	974(A)	G
2	GB	974(B)	C
2	GB	983	A
2	GB	989	G
2	GB	996	A
2	GB	1012	U
2	GB	1013	C
2	GB	1022	G
2	GB	1025	G
2	GB	1026	U
2	GB	1033	U
2	GB	1042	G
2	GB	1044	G
2	GB	1045	A
2	GB	1046	A
2	GB	1047	G
2	GB	1054	A
2	GB	1057	A
2	GB	1058	G
2	GB	1059	G
2	GB	1060	U

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Mol	Chain	Res	Type
2	GB	1061	U
2	GB	1062	G
2	GB	1066	U
2	GB	1068	G
2	GB	1069	A
2	GB	1070	A
2	GB	1071	G
2	GB	1072	C
2	GB	1073	A
2	GB	1075	C
2	GB	1076	C
2	GB	1077	A
2	GB	1078	U
2	GB	1079	C
2	GB	1081	U
2	GB	1082	U
2	GB	1083	U
2	GB	1085	A
2	GB	1086	A
2	GB	1088	A
2	GB	1089	G
2	GB	1090	U
2	GB	1091	G
2	GB	1094	U
2	GB	1097	U
2	GB	1098	A
2	GB	1101	U
2	GB	1107	G
2	GB	1111	A
2	GB	1112	G
2	GB	1122	G
2	GB	1126	A
2	GB	1129	A
2	GB	1130	U
2	GB	1135	C
2	GB	1136	G
2	GB	1139	G
2	GB	1142(B)	A
2	GB	1143	A
2	GB	1155	A
2	GB	1174	A
2	GB	1175	U

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Mol	Chain	Res	Type
2	GB	1177	A
2	GB	1205	U
2	GB	1210	A
2	GB	1211	U
2	GB	1218	C
2	GB	1220	A
2	GB	1253	A
2	GB	1256	G
2	GB	1271	G
2	GB	1272	A
2	GB	1273	U
2	GB	1300	U
2	GB	1301	A
2	GB	1313	U
2	GB	1359	A
2	GB	1360	A
2	GB	1365	A
2	GB	1380	G
2	GB	1385	G
2	GB	1395	A
2	GB	1416	G
2	GB	1417	C
2	GB	1419	A
2	GB	1420	U
2	GB	1421	G
2	GB	1428	C
2	GB	1444(B)	A
2	GB	1449(B)	A
2	GB	1459	G
2	GB	1460	A
2	GB	1461	G
2	GB	1467	C
2	GB	1471	A
2	GB	1483	G
2	GB	1493	C
2	GB	1494	A
2	GB	1497	U
2	GB	1508	A
2	GB	1510	A
2	GB	1511	A
2	GB	1512	G
2	GB	1513	C

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Mol	Chain	Res	Type
2	GB	1532	C
2	GB	1534	G
2	GB	1535	U
2	GB	1537	C
2	GB	1538	G
2	GB	1544	C
2	GB	1547	C
2	GB	1558	A
2	GB	1559	G
2	GB	1566	A
2	GB	1569	A
2	GB	1578	U
2	GB	1580	A
2	GB	1585	C
2	GB	1587	A
2	GB	1595	G
2	GB	1608	A
2	GB	1609	A
2	GB	1610	A
2	GB	1631	A
2	GB	1647	G
2	GB	1648	C
2	GB	1649	G
2	GB	1654	A
2	GB	1667	G
2	GB	1674	G
2	GB	1700	A
2	GB	1701	A
2	GB	1729	A
2	GB	1730	U
2	GB	1731	G
2	GB	1743	G
2	GB	1762	A
2	GB	1763	G
2	GB	1764	G
2	GB	1773	A
2	GB	1776	G
2	GB	1781	C
2	GB	1791	A
2	GB	1800	C
2	GB	1801	G
2	GB	1811	G

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Mol	Chain	Res	Type
2	GB	1816	G
2	GB	1829	A
2	GB	1835	G
2	GB	1839	G
2	GB	1847	A
2	GB	1859	A
2	GB	1872	A
2	GB	1878	G
2	GB	1900	A
2	GB	1903	G
2	GB	1905	C
2	GB	1906	G
2	GB	1913	A
2	GB	1914	C
2	GB	1921	G
2	GB	1929	G
2	GB	1930	G
2	GB	1936	A
2	GB	1940	U
2	GB	1955	U
2	GB	1963	U
2	GB	1965	C
2	GB	1967	C
2	GB	1970	A
2	GB	1971	A
2	GB	1972	A
2	GB	1984	G
2	GB	1992	G
2	GB	1993	U
2	GB	1997	G
2	GB	2020	A
2	GB	2023	G
2	GB	2031	A
2	GB	2032	G
2	GB	2033	A
2	GB	2043	C
2	GB	2055	C
2	GB	2056	G
2	GB	2060	A
2	GB	2061	G
2	GB	2062	A
2	GB	2069	G

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Mol	Chain	Res	Type
2	GB	2093	G
2	GB	2100	G
2	GB	2110	G
2	GB	2113	U
2	GB	2116	G
2	GB	2117	A
2	GB	2118	U
2	GB	2119	A
2	GB	2122	U
2	GB	2125	G
2	GB	2126	A
2	GB	2127	G
2	GB	2130	U
2	GB	2131	G
2	GB	2132	U
2	GB	2133	G
2	GB	2134	A
2	GB	2136	C
2	GB	2137	C
2	GB	2138	C
2	GB	2142	C
2	GB	2145	C
2	GB	2146	C
2	GB	2147	G
2	GB	2148	G
2	GB	2152	G
2	GB	2162	G
2	GB	2164	C
2	GB	2165	G
2	GB	2166	G
2	GB	2167	U
2	GB	2169	A
2	GB	2171	A
2	GB	2172	U
2	GB	2173	A
2	GB	2176	A
2	GB	2187	G
2	GB	2189	U
2	GB	2198	A
2	GB	2210	G
2	GB	2211	G
2	GB	2212	A

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Mol	Chain	Res	Type
2	GB	2213	U
2	GB	2225	A
2	GB	2226	C
2	GB	2238	G
2	GB	2239	G
2	GB	2243	U
2	GB	2269	A
2	GB	2275	C
2	GB	2278	A
2	GB	2279	G
2	GB	2283	C
2	GB	2287	A
2	GB	2288	A
2	GB	2305	A
2	GB	2308	G
2	GB	2309	A
2	GB	2311	A
2	GB	2312	U
2	GB	2319	G
2	GB	2320	A
2	GB	2321	G
2	GB	2322	A
2	GB	2325	G
2	GB	2327	A
2	GB	2334	G
2	GB	2336	A
2	GB	2347	C
2	GB	2383	G
2	GB	2385	C
2	GB	2396	G
2	GB	2401	U
2	GB	2406	U
2	GB	2422	A
2	GB	2424	C
2	GB	2425	A
2	GB	2429	G
2	GB	2430	A
2	GB	2435	A
2	GB	2439	A
2	GB	2440	C
2	GB	2441	C
2	GB	2448	A

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Mol	Chain	Res	Type
2	GB	2476	A
2	GB	2477	C
2	GB	2502	G
2	GB	2504	U
2	GB	2505	G
2	GB	2506	U
2	GB	2518	A
2	GB	2525	G
2	GB	2529	G
2	GB	2554	U
2	GB	2566	A
2	GB	2567	G
2	GB	2573	C
2	GB	2574	G
2	GB	2596	U
2	GB	2602	A
2	GB	2609	U
2	GB	2611	U
2	GB	2612	C
2	GB	2615	U
2	GB	2630	G
2	GB	2663	G
2	GB	2682	U
2	GB	2683	C
2	GB	2689	U
2	GB	2690	C
2	GB	2691	C
2	GB	2703	C
2	GB	2712(A)	A
2	GB	2713	A
2	GB	2714	G
2	GB	2718	G
2	GB	2726	U
2	GB	2733	A
2	GB	2751	G
2	GB	2757	A
2	GB	2758	A
2	GB	2764	A
2	GB	2765	A
2	GB	2766	G
2	GB	2778	A
2	GB	2789	C

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Mol	Chain	Res	Type
2	GB	2790	A
2	GB	2791	C
2	GB	2793	G
2	GB	2794	C
2	GB	2797	U
2	GB	2798	C
2	GB	2799	A
2	GB	2801	A
2	GB	2802	G
2	GB	2805	G
2	GB	2807	G
2	GB	2818	G
2	GB	2820	A
2	GB	2821	A
2	GB	2835	A
2	GB	2836	U
2	GB	2872	G
2	GB	2879	C
2	GB	2880	C
2	GB	2892	A
2	GB	2894	G
3	HB	2	C
3	HB	9	G
3	HB	12	C
3	HB	25	A
3	HB	30	C
3	HB	35	U
3	HB	45	A
3	HB	56	G
3	HB	66	A
3	HB	73	A
3	HB	74	U
3	HB	89(B)	A
3	HB	90	C
3	HB	109	G
3	HB	111	U
3	HB	119	A
4	IB	7	G
4	IB	8	4SU
4	IB	16	C
4	IB	17(A)	U
4	IB	19	G

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Mol	Chain	Res	Type
4	IB	20	U
4	IB	22	G
4	IB	35	A
4	IB	36	U
4	IB	37	A
4	IB	46	G
4	IB	47	U
4	IB	48	C
4	IB	58	A
4	IB	61	C
34	MC	14	A
34	MC	16	A
34	MC	21	A
34	MC	22	A
4	NC	10	G
4	NC	18	G
4	NC	20	U
4	NC	47	U
4	NC	48	C
4	NC	52	G
4	NC	76	A

All (71) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	509	A
1	A	560	U
1	A	687	A
1	A	723	U
1	A	748	C
1	A	793	U
1	A	842	C
1	A	913	A
1	A	1201	A
1	A	1491	G
2	B	34	C
2	B	196	A
2	B	277	C
2	B	507	A
2	B	528	A
2	B	645	C

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Mol	Chain	Res	Type
2	B	774	A
2	B	784	A
2	B	893	C
2	B	974(A)	G
2	B	1060	U
2	B	1210	A
2	B	1379	A
2	B	1396	U
2	B	1420	U
2	B	1531	C
2	B	1608	A
2	B	1992	G
2	B	2062	A
2	B	2136	C
2	B	2439	A
2	B	2518	A
2	B	2611	U
2	B	2756	U
3	C	65	C
4	IA	19	G
1	FB	115	G
1	FB	509	A
1	FB	560	U
1	FB	687	A
1	FB	723	U
1	FB	748	C
1	FB	793	U
1	FB	842	C
1	FB	913	A
1	FB	1201	A
1	FB	1491	G
2	GB	34	C
2	GB	277	C
2	GB	507	A
2	GB	528	A
2	GB	645	C
2	GB	784	A
2	GB	893	C
2	GB	974(A)	G
2	GB	1060	U
2	GB	1210	A
2	GB	1379	A

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Mol	Chain	Res	Type
2	GB	1396	U
2	GB	1420	U
2	GB	1531	C
2	GB	1608	A
2	GB	1992	G
2	GB	2062	A
2	GB	2136	C
2	GB	2439	A
2	GB	2611	U
2	GB	2756	U
3	HB	65	C
4	NC	19	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

66 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	A	1207	1	18,26,27	2.25	3 (16%)	21,38,41	2.01	6 (28%)
1	5MC	A	1400	1	14,22,23	1.34	2 (14%)	17,32,35	0.94	1 (5%)
1	4OC	A	1402	1	15,23,24	0.64	0	21,32,35	1.79	3 (14%)
1	5MC	A	1404	1	14,22,23	1.42	2 (14%)	17,32,35	1.40	2 (11%)
1	5MC	A	1407	1	14,22,23	1.26	2 (14%)	17,32,35	1.02	1 (5%)
1	UR3	A	1498	1,56	13,22,23	1.59	1 (7%)	18,32,35	0.66	0
1	MA6	A	1518	1	18,26,27	1.37	2 (11%)	15,38,41	3.36	3 (20%)
1	MA6	A	1519	1	18,26,27	1.37	3 (16%)	15,38,41	2.64	3 (20%)
1	PSU	A	516	1	15,21,22	1.53	3 (20%)	16,30,33	2.08	3 (18%)
1	7MG	A	527	1,56	20,26,27	2.17	4 (20%)	23,39,42	2.44	9 (39%)
1	M2G	A	966	1	18,27,28	2.26	3 (16%)	22,40,43	1.67	5 (22%)
1	5MC	A	967	1	14,22,23	1.41	2 (14%)	17,32,35	1.06	1 (5%)
2	PSU	B	1911	2	15,21,22	1.48	3 (20%)	16,30,33	2.33	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5MU	B	1915	2	13,22,23	1.41	2 (15%)	16,32,35	1.83	2 (12%)
2	PSU	B	1917	2	15,21,22	1.57	3 (20%)	16,30,33	2.24	3 (18%)
2	4OC	B	1920	56,2	15,22,24	0.84	1 (6%)	20,31,35	1.41	3 (15%)
2	5MU	B	1939	56,2	13,22,23	1.64	2 (15%)	16,32,35	2.13	2 (12%)
2	5MC	B	1942	56,2	14,22,23	1.34	2 (14%)	17,32,35	0.95	1 (5%)
2	5MC	B	1962	56,2	14,22,23	1.39	2 (14%)	17,32,35	0.77	0
2	OMG	B	2251	2,4	18,26,27	1.79	2 (11%)	21,38,41	1.61	3 (14%)
2	2MA	B	2503	2	17,25,26	1.94	3 (17%)	18,37,40	2.85	1 (5%)
2	2MU	B	2552	56,2	14,22,24	2.61	6 (42%)	19,31,36	1.72	3 (15%)
2	PSU	B	2605	2	15,21,22	1.53	3 (20%)	16,30,33	2.08	3 (18%)
4	5MC	D	32	4	14,22,23	1.41	2 (14%)	17,32,35	1.14	2 (11%)
4	5MU	D	54	4	13,22,23	1.66	2 (15%)	16,32,35	2.57	2 (12%)
4	PSU	D	55	4	15,21,22	1.76	4 (26%)	16,30,33	2.09	3 (18%)
4	4SU	D	8	4	12,21,22	1.33	1 (8%)	15,30,33	2.51	1 (6%)
1	2MG	FB	1207	1	18,26,27	2.18	2 (11%)	21,38,41	1.89	7 (33%)
1	5MC	FB	1400	1	14,22,23	1.28	2 (14%)	17,32,35	0.69	0
1	4OC	FB	1402	1,56	15,23,24	0.63	0	21,32,35	1.89	3 (14%)
1	5MC	FB	1404	1	14,22,23	1.43	2 (14%)	17,32,35	1.30	2 (11%)
1	5MC	FB	1407	1	14,22,23	1.31	2 (14%)	17,32,35	0.91	0
1	UR3	FB	1498	1,56	13,22,23	1.55	1 (7%)	18,32,35	0.61	0
1	MA6	FB	1518	1	18,26,27	1.31	2 (11%)	15,38,41	3.12	3 (20%)
1	MA6	FB	1519	1	18,26,27	1.29	3 (16%)	15,38,41	2.20	3 (20%)
1	PSU	FB	516	1	15,21,22	1.54	4 (26%)	16,30,33	2.21	3 (18%)
1	7MG	FB	527	1	20,26,27	2.10	4 (20%)	23,39,42	2.31	8 (34%)
1	M2G	FB	966	1	18,27,28	2.16	3 (16%)	22,40,43	1.67	5 (22%)
1	5MC	FB	967	1	14,22,23	1.34	1 (7%)	17,32,35	0.79	1 (5%)
2	PSU	GB	1911	2	15,21,22	1.44	3 (20%)	16,30,33	2.03	3 (18%)
2	5MU	GB	1915	2	13,22,23	1.53	2 (15%)	16,32,35	2.36	2 (12%)
2	PSU	GB	1917	2	15,21,22	1.60	3 (20%)	16,30,33	2.16	3 (18%)
2	4OC	GB	1920	2	15,22,24	0.87	1 (6%)	20,31,35	1.45	3 (15%)
2	5MU	GB	1939	56,2	13,22,23	1.62	2 (15%)	16,32,35	2.15	2 (12%)
2	5MC	GB	1942	2	14,22,23	1.35	2 (14%)	17,32,35	0.95	1 (5%)
2	5MC	GB	1962	2	14,22,23	1.39	2 (14%)	17,32,35	1.04	2 (11%)
2	OMG	GB	2251	2,4	18,26,27	1.72	2 (11%)	21,38,41	1.60	4 (19%)
2	2MA	GB	2503	2	17,25,26	2.15	3 (17%)	18,37,40	1.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MU	GB	2552	56,2	14,22,24	2.45	3 (21%)	19,31,36	1.72	3 (15%)
2	PSU	GB	2605	2	15,21,22	1.63	3 (20%)	16,30,33	2.16	3 (18%)
34	PSU	HA	19	34	15,21,22	1.53	4 (26%)	16,30,33	2.19	3 (18%)
4	5MC	IA	32	4	14,22,23	1.37	1 (7%)	17,32,35	1.15	1 (5%)
4	5MU	IA	54	56,4	13,22,23	1.67	2 (15%)	16,32,35	2.73	2 (12%)
4	PSU	IA	55	4	15,21,22	1.61	4 (26%)	16,30,33	2.09	2 (12%)
4	4SU	IA	8	4	12,21,22	1.36	1 (8%)	15,30,33	2.64	1 (6%)
4	5MC	IB	32	4	14,22,23	1.38	2 (14%)	17,32,35	1.11	2 (11%)
4	5MU	IB	54	4	13,22,23	1.61	2 (15%)	16,32,35	2.59	2 (12%)
4	PSU	IB	55	4	15,21,22	1.72	4 (26%)	16,30,33	2.11	3 (18%)
4	4SU	IB	8	4	12,21,22	1.27	1 (8%)	15,30,33	2.45	1 (6%)
34	PSU	MC	19	56,34	15,21,22	1.57	4 (26%)	16,30,33	2.15	3 (18%)
4	5MC	NC	32	4	14,22,23	1.35	2 (14%)	17,32,35	1.10	1 (5%)
4	5MU	NC	54	4	13,22,23	1.83	2 (15%)	16,32,35	2.75	2 (12%)
4	PSU	NC	55	4	15,21,22	1.69	4 (26%)	16,30,33	2.13	3 (18%)
4	4SU	NC	8	4	12,21,22	1.29	2 (16%)	15,30,33	2.68	1 (6%)
46	0TD	UA	92	46	4,9,10	1.49	1 (25%)	4,11,13	2.95	1 (25%)
46	0TD	ZC	92	46	4,9,10	1.54	1 (25%)	4,11,13	2.97	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1,56	-	0/3/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1,56	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	B	1915	2	-	0/3/25/26	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
2	4OC	B	1920	56,2	-	0/5/27/30	0/2/2/2
2	5MU	B	1939	56,2	-	0/3/25/26	0/2/2/2
2	5MC	B	1942	56,2	-	0/3/25/26	0/2/2/2
2	5MC	B	1962	56,2	-	0/3/25/26	0/2/2/2
2	OMG	B	2251	2,4	-	0/5/27/28	0/3/3/3
2	2MA	B	2503	2	-	0/3/25/26	0/3/3/3
2	2MU	B	2552	56,2	-	0/5/27/28	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/3/25/26	0/2/2/2
4	5MU	D	54	4	-	0/3/25/26	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	0/3/25/26	0/2/2/2
1	2MG	FB	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	FB	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	FB	1402	1,56	-	0/7/29/30	0/2/2/2
1	5MC	FB	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	FB	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	FB	1498	1,56	-	0/3/25/26	0/2/2/2
1	MA6	FB	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	FB	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	FB	516	1	-	0/7/25/26	0/2/2/2
1	7MG	FB	527	1	-	0/7/37/38	0/3/3/3
1	M2G	FB	966	1	-	0/7/29/30	0/3/3/3
1	5MC	FB	967	1	-	0/3/25/26	0/2/2/2
2	PSU	GB	1911	2	-	0/7/25/26	0/2/2/2
2	5MU	GB	1915	2	-	0/3/25/26	0/2/2/2
2	PSU	GB	1917	2	-	0/7/25/26	0/2/2/2
2	4OC	GB	1920	2	-	0/5/27/30	0/2/2/2
2	5MU	GB	1939	56,2	-	0/3/25/26	0/2/2/2
2	5MC	GB	1942	2	-	0/3/25/26	0/2/2/2
2	5MC	GB	1962	2	-	0/3/25/26	0/2/2/2
2	OMG	GB	2251	2,4	-	0/5/27/28	0/3/3/3
2	2MA	GB	2503	2	-	0/3/25/26	0/3/3/3
2	2MU	GB	2552	56,2	-	0/5/27/28	0/2/2/2
2	PSU	GB	2605	2	-	0/7/25/26	0/2/2/2
34	PSU	HA	19	34	-	0/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/3/25/26	0/2/2/2
4	5MU	IA	54	56,4	-	0/3/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MC	IB	32	4	-	0/3/25/26	0/2/2/2
4	5MU	IB	54	4	-	0/3/25/26	0/2/2/2
4	PSU	IB	55	4	-	0/7/25/26	0/2/2/2
4	4SU	IB	8	4	-	0/3/25/26	0/2/2/2
34	PSU	MC	19	56,34	-	0/7/25/26	0/2/2/2
4	5MC	NC	32	4	-	0/3/25/26	0/2/2/2
4	5MU	NC	54	4	-	0/3/25/26	0/2/2/2
4	PSU	NC	55	4	-	0/7/25/26	0/2/2/2
4	4SU	NC	8	4	-	0/3/25/26	0/2/2/2
46	0TD	UA	92	46	-	0/2/12/14	0/0/0/0
46	0TD	ZC	92	46	-	0/2/12/14	0/0/0/0

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2552	2MU	C3'-C2'	-4.97	1.41	1.53
2	GB	2552	2MU	C3'-C2'	-4.81	1.42	1.53
1	FB	1404	5MC	C5-C4	-3.36	1.35	1.41
2	B	1962	5MC	C5-C4	-3.13	1.36	1.41
2	B	1942	5MC	C5-C4	-3.08	1.36	1.41
2	B	2552	2MU	O3'-C3'	-3.04	1.35	1.43
1	FB	1407	5MC	C5-C4	-2.98	1.36	1.41
2	GB	1962	5MC	C5-C4	-2.94	1.36	1.41
1	FB	527	7MG	CM7-N7	-2.91	1.41	1.46
1	A	527	7MG	CM7-N7	-2.83	1.41	1.46
1	A	967	5MC	C5-C4	-2.80	1.36	1.41
2	GB	1942	5MC	C5-C4	-2.67	1.37	1.41
1	A	1404	5MC	C5-C4	-2.64	1.37	1.41
4	D	32	5MC	C5-C4	-2.63	1.37	1.41
2	GB	2552	2MU	O3'-C3'	-2.60	1.36	1.43
1	A	1407	5MC	C5-C4	-2.59	1.37	1.41
46	ZC	92	0TD	CB-SB	-2.48	1.78	1.84
4	IB	32	5MC	C5-C4	-2.48	1.37	1.41
1	A	1400	5MC	C5-C4	-2.40	1.37	1.41
2	B	2552	2MU	O4'-C4'	-2.39	1.39	1.45
2	B	2552	2MU	C3'-C4'	-2.38	1.46	1.53
4	NC	32	5MC	C5-C4	-2.37	1.37	1.41
1	FB	1400	5MC	C5-C4	-2.37	1.37	1.41
46	UA	92	0TD	CB-SB	-2.30	1.78	1.84
2	B	1911	PSU	O4'-C1'	-2.16	1.41	1.44
2	B	2552	2MU	C5'-C4'	-2.15	1.44	1.51
2	GB	1911	PSU	O4'-C1'	-2.15	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2605	PSU	O4'-C1'	-2.13	1.41	1.44
4	NC	8	4SU	C6-C5	-2.13	1.33	1.38
2	B	1917	PSU	O4'-C1'	-2.07	1.41	1.44
34	MC	19	PSU	O4'-C1'	-2.04	1.41	1.44
34	HA	19	PSU	O4'-C1'	-2.03	1.41	1.44
1	FB	516	PSU	O4'-C1'	-2.02	1.41	1.44
34	MC	19	PSU	C6-C5	2.02	1.41	1.38
1	A	1519	MA6	C2-N1	2.04	1.37	1.33
4	IA	55	PSU	C6-C5	2.08	1.41	1.38
1	A	1207	2MG	C6-N1	2.11	1.36	1.33
1	FB	516	PSU	C5-C1'	2.13	1.54	1.52
2	GB	1917	PSU	C6-C5	2.15	1.41	1.38
4	NC	55	PSU	C5-C1'	2.16	1.54	1.52
4	IB	55	PSU	C6-C5	2.17	1.41	1.38
4	D	55	PSU	C6-C5	2.21	1.41	1.38
4	IA	55	PSU	C5-C1'	2.32	1.54	1.52
34	HA	19	PSU	C5-C1'	2.33	1.54	1.52
4	NC	55	PSU	C6-C5	2.33	1.41	1.38
1	FB	1519	MA6	C2-N1	2.37	1.38	1.33
2	B	1920	4OC	C4-N4	2.40	1.42	1.35
1	FB	1519	MA6	C6-N1	2.44	1.37	1.34
2	GB	1920	4OC	C4-N4	2.54	1.42	1.35
1	A	516	PSU	C5-C1'	2.66	1.54	1.52
1	A	966	M2G	C4-N3	2.68	1.40	1.35
34	HA	19	PSU	C6-N1	2.69	1.40	1.34
1	FB	966	M2G	C4-N3	2.78	1.40	1.35
1	FB	516	PSU	C6-N1	2.83	1.40	1.34
2	B	1911	PSU	C6-N1	2.90	1.40	1.34
1	A	527	7MG	C6-C5	2.91	1.45	1.41
1	FB	527	7MG	C6-C5	2.91	1.45	1.41
1	A	516	PSU	C6-N1	2.94	1.40	1.34
4	IA	55	PSU	C6-N1	2.95	1.40	1.34
2	B	1917	PSU	C6-N1	2.96	1.40	1.34
1	FB	1518	MA6	C6-N1	2.96	1.38	1.34
1	A	1519	MA6	C6-N1	3.04	1.38	1.34
2	B	1915	5MU	C4-N3	3.05	1.38	1.33
34	MC	19	PSU	C6-N1	3.06	1.40	1.34
2	GB	1917	PSU	C6-N1	3.11	1.41	1.34
2	GB	2605	PSU	C6-N1	3.12	1.41	1.34
2	GB	1911	PSU	C6-N1	3.12	1.41	1.34
2	GB	1915	5MU	C4-N3	3.15	1.38	1.33
2	GB	1939	5MU	C4-N3	3.17	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1939	5MU	C4-N3	3.18	1.38	1.33
1	A	1518	MA6	C6-N1	3.18	1.38	1.34
4	IB	55	PSU	C6-N1	3.19	1.41	1.34
4	NC	55	PSU	C6-N1	3.28	1.41	1.34
4	D	55	PSU	C5-C1'	3.30	1.55	1.52
4	IA	54	5MU	C4-N3	3.31	1.39	1.33
4	D	55	PSU	C6-N1	3.34	1.41	1.34
2	GB	1911	PSU	C4-N3	3.34	1.39	1.33
2	GB	2605	PSU	C4-N3	3.34	1.39	1.33
4	IB	54	5MU	C4-N3	3.38	1.39	1.33
2	B	2605	PSU	C6-N1	3.41	1.41	1.34
2	B	2605	PSU	C4-N3	3.44	1.39	1.33
2	B	1915	5MU	O4-C4	3.47	1.33	1.24
2	B	1911	PSU	C4-N3	3.48	1.39	1.33
4	IB	55	PSU	C5-C1'	3.50	1.55	1.52
4	D	54	5MU	C4-N3	3.52	1.39	1.33
1	FB	1407	5MC	C4-N4	3.55	1.43	1.34
1	A	1407	5MC	C4-N4	3.56	1.43	1.34
1	A	516	PSU	C4-N3	3.58	1.39	1.33
34	HA	19	PSU	C4-N3	3.58	1.39	1.33
1	FB	527	7MG	C2-N2	3.58	1.41	1.34
2	GB	2503	2MA	C2-N1	3.59	1.40	1.34
4	NC	8	4SU	C5-C4	3.60	1.43	1.38
2	B	1942	5MC	C4-N4	3.60	1.43	1.34
2	GB	2605	PSU	C5-C1'	3.66	1.55	1.52
4	IB	8	4SU	C5-C4	3.67	1.43	1.38
2	B	1917	PSU	C4-N3	3.68	1.39	1.33
1	FB	1404	5MC	C4-N4	3.74	1.44	1.34
1	FB	1400	5MC	C4-N4	3.75	1.44	1.34
4	IB	55	PSU	C4-N3	3.76	1.39	1.33
2	GB	1942	5MC	C4-N4	3.77	1.44	1.34
2	B	2503	2MA	C2-N1	3.77	1.41	1.34
4	IA	55	PSU	C4-N3	3.78	1.39	1.33
2	B	1962	5MC	C4-N4	3.79	1.44	1.34
2	GB	1962	5MC	C4-N4	3.83	1.44	1.34
2	GB	1917	PSU	C4-N3	3.84	1.40	1.33
2	GB	2503	2MA	C8-N7	3.85	1.42	1.34
4	NC	54	5MU	C4-N3	3.85	1.40	1.33
34	MC	19	PSU	C4-N3	3.85	1.40	1.33
1	A	967	5MC	C4-N4	3.86	1.44	1.34
2	B	2503	2MA	C8-N7	3.86	1.42	1.34
1	A	1400	5MC	C4-N4	3.86	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FB	1519	MA6	C4-N3	3.87	1.41	1.35
4	D	8	4SU	C5-C4	3.90	1.43	1.38
4	D	55	PSU	C4-N3	3.97	1.40	1.33
4	IB	32	5MC	C4-N4	3.99	1.44	1.34
1	FB	516	PSU	C4-N3	4.01	1.40	1.33
4	IA	8	4SU	C5-C4	4.02	1.43	1.38
4	D	32	5MC	C4-N4	4.05	1.45	1.34
1	A	527	7MG	C2-N2	4.05	1.42	1.34
2	GB	1915	5MU	O4-C4	4.06	1.34	1.24
4	NC	55	PSU	C4-N3	4.06	1.40	1.33
1	FB	1518	MA6	C4-N3	4.08	1.41	1.35
1	FB	967	5MC	C4-N4	4.08	1.45	1.34
2	B	1939	5MU	O4-C4	4.12	1.35	1.24
1	A	1519	MA6	C4-N3	4.14	1.41	1.35
4	NC	32	5MC	C4-N4	4.14	1.45	1.34
2	B	2251	OMG	C2-N2	4.15	1.42	1.34
2	GB	2251	OMG	C2-N2	4.16	1.42	1.34
1	A	1518	MA6	C4-N3	4.19	1.41	1.35
1	A	1404	5MC	C4-N4	4.21	1.45	1.34
2	GB	1939	5MU	O4-C4	4.21	1.35	1.24
4	IB	54	5MU	O4-C4	4.21	1.35	1.24
4	IA	32	5MC	C4-N4	4.23	1.45	1.34
4	D	54	5MU	O4-C4	4.33	1.35	1.24
4	IA	54	5MU	O4-C4	4.57	1.36	1.24
4	NC	54	5MU	O4-C4	4.86	1.36	1.24
1	FB	966	M2G	C2-N2	5.31	1.43	1.34
1	A	1498	UR3	O4-C4	5.34	1.38	1.24
1	FB	1498	UR3	O4-C4	5.38	1.38	1.24
2	B	2503	2MA	C6-N6	5.41	1.38	1.29
2	GB	2251	OMG	O6-C6	5.46	1.38	1.24
2	B	2251	OMG	O6-C6	5.54	1.38	1.24
1	A	966	M2G	C2-N2	5.72	1.44	1.34
1	FB	966	M2G	O6-C6	6.18	1.40	1.24
1	FB	1207	2MG	C2-N2	6.23	1.41	1.34
2	B	2552	2MU	O4-C4	6.24	1.40	1.24
1	FB	1207	2MG	O6-C6	6.25	1.40	1.24
2	GB	2552	2MU	O4-C4	6.29	1.40	1.24
1	A	966	M2G	O6-C6	6.37	1.40	1.24
1	A	1207	2MG	O6-C6	6.39	1.40	1.24
1	A	1207	2MG	C2-N2	6.41	1.41	1.34
2	GB	2503	2MA	C6-N6	6.53	1.40	1.29
1	FB	527	7MG	O6-C6	7.12	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	O6-C6	7.22	1.42	1.24

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	N3-C2-N1	-11.59	119.77	128.87
1	FB	1518	MA6	N3-C2-N1	-10.55	120.58	128.87
4	NC	8	4SU	C5-C4-N3	-9.98	112.97	123.56
4	IA	8	4SU	C5-C4-N3	-9.83	113.13	123.56
4	D	8	4SU	C5-C4-N3	-9.52	113.46	123.56
4	IB	8	4SU	C5-C4-N3	-9.25	113.75	123.56
1	A	1519	MA6	N3-C2-N1	-8.71	122.03	128.87
4	IA	54	5MU	C5-C4-N3	-8.18	118.48	125.35
4	NC	54	5MU	C5-C4-N3	-7.88	118.73	125.35
4	IB	54	5MU	C5-C4-N3	-7.05	119.43	125.35
4	D	54	5MU	C5-C4-N3	-6.98	119.49	125.35
1	FB	1519	MA6	N3-C2-N1	-6.90	123.45	128.87
2	GB	1939	5MU	C5-C4-N3	-6.72	119.71	125.35
2	B	1939	5MU	C5-C4-N3	-6.37	120.00	125.35
2	GB	1915	5MU	C5-C4-N3	-6.25	120.11	125.35
1	A	527	7MG	C5-C4-N3	-5.17	121.47	126.74
1	FB	527	7MG	C5-C4-N3	-4.84	121.81	126.74
1	A	527	7MG	N1-C2-N3	-4.31	118.47	125.51
2	B	1915	5MU	C5-C4-N3	-4.29	121.75	125.35
2	B	2605	PSU	C5-C6-N1	-4.18	118.54	124.38
2	B	2251	OMG	N3-C2-N1	-4.07	122.03	127.56
2	GB	2251	OMG	N3-C2-N1	-3.99	122.13	127.56
1	FB	527	7MG	N1-C2-N3	-3.86	119.20	125.51
2	GB	1917	PSU	C5-C6-N1	-3.82	119.05	124.38
1	A	516	PSU	C5-C6-N1	-3.75	119.15	124.38
1	A	1207	2MG	C5-C6-N1	-3.70	118.69	123.52
1	FB	966	M2G	CM2-N2-C2	-3.64	117.68	121.34
2	B	2251	OMG	C5-C6-N1	-3.63	118.77	123.52
2	GB	2605	PSU	C5-C6-N1	-3.63	119.32	124.38
1	FB	1207	2MG	C5-C6-N1	-3.62	118.79	123.52
34	MC	19	PSU	C5-C6-N1	-3.61	119.34	124.38
34	HA	19	PSU	C5-C6-N1	-3.52	119.48	124.38
4	IA	55	PSU	C5-C6-N1	-3.49	119.51	124.38
2	B	1917	PSU	C5-C6-N1	-3.43	119.59	124.38
1	FB	516	PSU	C5-C6-N1	-3.43	119.60	124.38
4	NC	55	PSU	C5-C6-N1	-3.42	119.61	124.38
1	FB	966	M2G	C5-C6-N1	-3.39	119.09	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	M2G	C5-C6-N1	-3.39	119.10	123.52
2	GB	1911	PSU	C5-C6-N1	-3.38	119.67	124.38
4	D	55	PSU	C5-C6-N1	-3.36	119.69	124.38
1	A	1404	5MC	CM5-C5-C4	-3.34	117.93	121.47
1	A	527	7MG	C8-N9-C1'	-3.31	112.50	122.43
2	GB	2251	OMG	C5-C6-N1	-3.31	119.20	123.52
1	FB	527	7MG	C8-N9-C1'	-3.27	112.62	122.43
4	IB	55	PSU	C5-C6-N1	-3.23	119.87	124.38
1	A	1518	MA6	C1'-N9-C4	-3.15	123.29	126.81
1	FB	1402	4OC	CM4-N4-C4	-3.15	120.22	122.87
1	FB	1404	5MC	CM5-C5-C4	-3.11	118.18	121.47
1	FB	1518	MA6	C1'-N9-C4	-3.09	123.36	126.81
1	A	1207	2MG	N3-C2-N1	-3.06	121.61	126.19
4	IA	32	5MC	CM5-C5-C4	-3.04	118.25	121.47
1	A	966	M2G	CM2-N2-C2	-3.03	118.30	121.34
1	A	527	7MG	C5-C6-N1	-3.02	118.90	123.39
2	B	1911	PSU	C5-C6-N1	-2.89	120.35	124.38
4	NC	32	5MC	CM5-C5-C4	-2.75	118.56	121.47
1	FB	527	7MG	C5-C6-N1	-2.73	119.32	123.39
1	FB	1207	2MG	N3-C2-N1	-2.72	122.11	126.19
1	A	966	M2G	C1'-N9-C4	-2.72	123.77	126.81
1	A	1402	4OC	CM4-N4-C4	-2.68	120.61	122.87
1	A	1207	2MG	CM2-N2-C2	-2.66	120.04	123.03
1	FB	966	M2G	C1'-N9-C4	-2.48	124.04	126.81
4	IB	32	5MC	CM5-C5-C4	-2.28	119.06	121.47
4	D	32	5MC	CM5-C5-C4	-2.27	119.07	121.47
2	B	2552	2MU	C2'-C1'-N1	-2.25	107.04	113.48
1	A	1407	5MC	CM5-C5-C4	-2.20	119.13	121.47
1	FB	1207	2MG	CM2-N2-C2	-2.19	120.57	123.03
1	A	1400	5MC	CM5-C5-C4	-2.18	119.15	121.47
1	FB	1519	MA6	C1'-N9-C4	-2.17	124.38	126.81
1	A	1519	MA6	C1'-N9-C4	-2.16	124.39	126.81
2	GB	1962	5MC	CM5-C5-C4	-2.14	119.20	121.47
2	GB	2552	2MU	C2'-C1'-N1	-2.05	107.61	113.48
1	FB	1207	2MG	C6-C5-C4	-2.01	118.56	120.86
1	FB	967	5MC	N4-C4-N3	2.03	119.90	116.92
1	FB	527	7MG	C2-N3-C4	2.10	120.47	114.50
2	GB	2251	OMG	CM2-O2'-C2'	2.12	120.54	114.58
4	NC	55	PSU	O4'-C1'-C2'	2.14	107.00	104.69
1	A	527	7MG	C4-N9-C1'	2.14	131.73	126.65
4	IB	55	PSU	O4'-C1'-C2'	2.22	107.09	104.69
2	GB	2552	2MU	C6'-O2'-C2'	2.24	120.87	114.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	55	PSU	O4'-C1'-C2'	2.25	107.12	104.69
2	B	2605	PSU	O4'-C1'-C2'	2.25	107.12	104.69
2	GB	2605	PSU	O4'-C1'-C2'	2.26	107.13	104.69
2	B	1942	5MC	N4-C4-N3	2.29	120.28	116.92
2	GB	1942	5MC	N4-C4-N3	2.33	120.33	116.92
1	FB	966	M2G	N3-C2-N2	2.33	119.70	117.14
2	GB	1920	4OC	N4-C4-N3	2.34	120.58	116.50
1	A	527	7MG	C2-N3-C4	2.37	121.24	114.50
2	GB	1962	5MC	N4-C4-N3	2.45	120.51	116.92
2	B	1917	PSU	O4'-C1'-C2'	2.50	107.40	104.69
1	FB	1207	2MG	N2-C2-N1	2.51	119.85	116.94
2	B	2552	2MU	C6'-O2'-C2'	2.53	121.66	114.58
1	A	966	M2G	N3-C2-N2	2.60	120.00	117.14
1	A	1207	2MG	N2-C2-N1	2.62	119.98	116.94
2	GB	1917	PSU	O4'-C1'-C2'	2.67	107.58	104.69
4	IB	32	5MC	N4-C4-N3	2.74	120.93	116.92
1	FB	1402	4OC	C2-N3-C4	2.75	118.92	115.43
2	B	1920	4OC	N4-C4-N3	2.83	121.44	116.50
4	D	32	5MC	N4-C4-N3	2.86	121.11	116.92
1	A	967	5MC	N4-C4-N3	2.89	121.15	116.92
1	A	1402	4OC	C2-N3-C4	2.90	119.12	115.43
1	A	527	7MG	N3-C4-N9	2.98	130.83	126.98
2	GB	1911	PSU	O4'-C1'-C2'	2.98	107.91	104.69
2	GB	1920	4OC	CM2-O2'-C2'	3.01	123.01	114.58
34	MC	19	PSU	O4'-C1'-C2'	3.02	107.96	104.69
34	HA	19	PSU	O4'-C1'-C2'	3.03	107.97	104.69
2	B	1920	4OC	CM2-O2'-C2'	3.10	123.27	114.58
1	FB	1404	5MC	N4-C4-N3	3.11	121.48	116.92
2	B	1911	PSU	O4'-C1'-C2'	3.12	108.06	104.69
1	A	516	PSU	O4'-C1'-C2'	3.20	108.15	104.69
1	FB	516	PSU	O4'-C1'-C2'	3.24	108.19	104.69
1	FB	527	7MG	N3-C4-N9	3.26	131.20	126.98
1	A	527	7MG	N2-C2-N1	3.32	122.68	117.20
1	FB	527	7MG	N2-C2-N1	3.36	122.75	117.20
2	B	1920	4OC	C6-C5-C4	3.42	118.78	117.44
1	FB	1519	MA6	C2-N1-C6	3.44	119.74	111.64
1	FB	966	M2G	C2-N3-C4	3.50	118.83	114.99
1	A	1404	5MC	N4-C4-N3	3.54	122.11	116.92
1	A	966	M2G	C2-N3-C4	3.75	119.10	114.99
2	GB	2251	OMG	C6-N1-C2	3.79	120.32	115.88
1	FB	1207	2MG	C2-N3-C4	3.89	119.26	114.99
1	FB	1207	2MG	C6-N1-C2	3.93	120.87	115.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C2-N3-C4	3.98	119.35	114.99
1	A	1519	MA6	C2-N1-C6	4.02	121.11	111.64
2	B	2251	OMG	C6-N1-C2	4.05	120.63	115.88
2	GB	1920	4OC	C6-C5-C4	4.10	119.04	117.44
1	A	1207	2MG	C6-N1-C2	4.21	121.27	115.24
1	A	1518	MA6	C2-N1-C6	4.45	122.14	111.64
1	FB	1518	MA6	C2-N1-C6	4.47	122.19	111.64
2	GB	1939	5MU	C4-N3-C2	4.68	119.06	115.16
2	B	2552	2MU	C4-N3-C2	5.03	119.51	114.21
46	ZC	92	0TD	CSB-SB-CB	5.04	110.86	101.44
46	UA	92	0TD	CSB-SB-CB	5.04	110.86	101.44
2	B	1939	5MU	C4-N3-C2	5.13	119.44	115.16
2	B	1915	5MU	C4-N3-C2	5.21	119.50	115.16
2	GB	2552	2MU	C4-N3-C2	5.55	120.06	114.21
1	FB	527	7MG	C6-N1-C2	5.80	122.68	115.88
2	B	2605	PSU	C4-N3-C2	6.02	120.18	115.16
1	A	527	7MG	C6-N1-C2	6.11	123.04	115.88
1	A	1402	4OC	C6-C5-C4	6.28	119.89	117.42
2	GB	1911	PSU	C4-N3-C2	6.29	120.40	115.16
1	A	516	PSU	C4-N3-C2	6.40	120.50	115.16
2	GB	1917	PSU	C4-N3-C2	6.58	120.65	115.16
4	IA	55	PSU	C4-N3-C2	6.60	120.67	115.16
2	GB	1915	5MU	C4-N3-C2	6.61	120.67	115.16
34	MC	19	PSU	C4-N3-C2	6.70	120.74	115.16
1	FB	1402	4OC	C6-C5-C4	6.74	120.07	117.42
4	D	55	PSU	C4-N3-C2	6.75	120.79	115.16
4	IA	54	5MU	C4-N3-C2	6.78	120.81	115.16
2	GB	2605	PSU	C4-N3-C2	6.78	120.82	115.16
4	NC	55	PSU	C4-N3-C2	6.80	120.83	115.16
4	IB	55	PSU	C4-N3-C2	6.92	120.93	115.16
34	HA	19	PSU	C4-N3-C2	7.02	121.01	115.16
1	FB	516	PSU	C4-N3-C2	7.10	121.08	115.16
4	IB	54	5MU	C4-N3-C2	7.21	121.17	115.16
4	D	54	5MU	C4-N3-C2	7.22	121.18	115.16
4	NC	54	5MU	C4-N3-C2	7.24	121.20	115.16
2	GB	2503	2MA	C2-N3-C4	7.26	118.79	115.29
2	B	1917	PSU	C4-N3-C2	7.35	121.29	115.16
2	B	1911	PSU	C4-N3-C2	7.85	121.70	115.16
2	B	2503	2MA	C2-N3-C4	11.61	120.88	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	1	0
1	A	1518	MA6	1	0
1	A	1519	MA6	1	0
1	A	966	M2G	1	0
1	A	967	5MC	2	0
2	B	1920	4OC	1	0
2	B	1939	5MU	1	0
2	B	2251	OMG	1	0
2	B	2552	2MU	2	0
4	D	32	5MC	1	0
4	D	54	5MU	1	0
4	D	8	4SU	3	0
1	FB	1498	UR3	2	0
1	FB	1518	MA6	1	0
1	FB	1519	MA6	2	0
1	FB	966	M2G	1	0
1	FB	967	5MC	2	0
2	GB	1939	5MU	1	0
2	GB	2251	OMG	1	0
2	GB	2552	2MU	2	0
34	HA	19	PSU	1	0
4	IB	32	5MC	1	0
4	IB	54	5MU	1	0
4	IB	8	4SU	3	0
34	MC	19	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2903 ligands modelled in this entry, 2903 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1495/1507 (99%)	0.42	99 (6%) 22 8	52, 100, 166, 256	0
1	FB	1495/1507 (99%)	0.44	87 (5%) 26 11	57, 88, 151, 209	0
2	B	2869/2880 (99%)	0.35	135 (4%) 35 16	36, 55, 145, 201	0
2	GB	2869/2880 (99%)	0.52	187 (6%) 22 8	47, 73, 172, 242	0
3	C	120/120 (100%)	0.24	4 (3%) 50 26	63, 83, 96, 117	0
3	HB	120/120 (100%)	0.31	6 (5%) 32 13	80, 111, 128, 144	0
4	D	73/77 (94%)	1.00	18 (24%) 1 0	67, 157, 172, 174	0
4	IA	73/77 (94%)	-0.09	0 100 100	52, 84, 91, 100	0
4	IB	73/77 (94%)	1.19	20 (27%) 1 0	79, 164, 182, 186	0
4	NC	73/77 (94%)	-0.15	0 100 100	61, 89, 100, 105	0
5	E	275/275 (100%)	-0.08	1 (0%) 93 85	36, 50, 58, 66	0
5	JB	275/275 (100%)	0.04	6 (2%) 65 42	45, 65, 74, 85	0
6	F	204/206 (99%)	0.10	6 (2%) 55 31	39, 60, 79, 86	0
6	KB	204/206 (99%)	0.22	2 (0%) 84 69	53, 77, 97, 107	0
7	G	202/205 (98%)	0.33	3 (1%) 76 58	34, 59, 78, 86	0
7	LB	202/205 (98%)	0.14	2 (0%) 84 69	50, 78, 91, 101	0
8	H	181/182 (99%)	0.45	19 (10%) 8 3	85, 91, 111, 119	0
8	MB	181/182 (99%)	0.88	30 (16%) 2 1	99, 119, 132, 135	0
9	I	174/180 (96%)	-0.19	1 (0%) 90 80	64, 72, 78, 91	0
9	NB	174/180 (96%)	1.38	50 (28%) 1 0	109, 147, 163, 169	0
10	J	146/148 (98%)	0.25	3 (2%) 67 44	64, 96, 111, 113	0
10	OB	146/148 (98%)	0.78	22 (15%) 3 1	86, 120, 129, 130	0
11	K	140/140 (100%)	-0.26	0 100 100	44, 56, 75, 77	0
11	PB	140/140 (100%)	0.05	3 (2%) 67 44	64, 82, 99, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	L	122/122 (100%)	-0.30	0 100 100	50, 59, 68, 71	0
12	QB	122/122 (100%)	-0.18	0 100 100	59, 69, 75, 79	0
13	M	150/150 (100%)	0.51	20 (13%) 4 2	36, 64, 87, 90	0
13	RB	150/150 (100%)	0.94	28 (18%) 2 1	50, 79, 105, 107	0
14	N	141/141 (100%)	-0.19	1 (0%) 89 78	48, 59, 72, 80	0
14	SB	141/141 (100%)	0.07	2 (1%) 78 60	63, 82, 97, 103	0
15	O	118/118 (100%)	0.19	0 100 100	47, 60, 73, 78	0
15	TB	118/118 (100%)	0.48	9 (7%) 17 6	62, 76, 83, 87	0
16	P	110/112 (98%)	0.36	9 (8%) 14 5	72, 80, 87, 89	0
16	UB	110/112 (98%)	1.34	35 (31%) 1 0	91, 106, 113, 116	0
17	Q	137/146 (93%)	-0.01	5 (3%) 46 23	59, 68, 119, 142	0
17	VB	137/146 (93%)	0.02	1 (0%) 89 78	69, 79, 108, 117	0
18	R	117/118 (99%)	0.01	1 (0%) 85 72	39, 52, 63, 67	0
18	WB	117/118 (99%)	0.75	18 (15%) 3 1	55, 77, 90, 93	0
19	S	101/101 (100%)	-0.28	0 100 100	40, 60, 67, 71	0
19	XB	101/101 (100%)	0.02	1 (0%) 84 69	56, 84, 94, 99	0
20	T	112/113 (99%)	-0.20	0 100 100	39, 49, 66, 80	0
20	YB	112/113 (99%)	-0.18	0 100 100	54, 68, 87, 100	0
21	U	95/96 (98%)	-0.02	2 (2%) 67 44	49, 56, 66, 74	0
21	ZB	95/96 (98%)	0.27	6 (6%) 23 9	71, 84, 95, 97	0
22	AC	107/110 (97%)	0.78	19 (17%) 2 1	82, 90, 101, 103	0
22	V	107/110 (97%)	0.24	5 (4%) 35 16	55, 63, 76, 82	0
23	BC	189/206 (91%)	1.11	50 (26%) 1 0	89, 108, 118, 121	0
23	W	189/206 (91%)	0.26	16 (8%) 13 4	65, 83, 93, 96	0
24	CC	84/85 (98%)	0.38	7 (8%) 14 5	72, 78, 89, 93	0
24	X	84/85 (98%)	0.28	7 (8%) 14 5	52, 59, 72, 77	0
25	DC	97/98 (98%)	0.13	0 100 100	56, 73, 108, 115	0
25	Y	97/98 (98%)	0.05	1 (1%) 84 69	43, 56, 88, 95	0
26	EC	70/72 (97%)	1.21	20 (28%) 1 0	89, 95, 103, 107	0
26	Z	70/72 (97%)	0.17	0 100 100	57, 63, 68, 77	0
27	AA	60/60 (100%)	-0.12	1 (1%) 73 52	47, 58, 74, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	FC	60/60 (100%)	0.04	0 100 100	69, 78, 88, 92	0
28	BA	69/71 (97%)	1.80	29 (42%) 0 0	119, 124, 142, 145	0
28	GC	69/71 (97%)	1.75	28 (40%) 0 0	135, 143, 153, 154	0
29	CA	59/60 (98%)	-0.32	0 100 100	36, 58, 68, 71	0
29	HC	59/60 (98%)	-0.11	0 100 100	53, 77, 85, 87	0
30	DA	53/54 (98%)	0.71	9 (16%) 2 1	61, 66, 69, 70	0
30	IC	53/54 (98%)	1.30	19 (35%) 0 0	74, 82, 85, 87	0
31	EA	48/49 (97%)	0.03	0 100 100	38, 40, 47, 52	0
31	JC	48/49 (97%)	0.07	0 100 100	53, 57, 64, 71	0
32	FA	64/65 (98%)	0.34	2 (3%) 52 28	43, 49, 58, 59	0
32	KC	64/65 (98%)	0.48	11 (17%) 2 1	58, 65, 74, 74	0
33	GA	37/37 (100%)	0.82	3 (8%) 15 5	55, 61, 67, 69	0
33	LC	37/37 (100%)	1.96	20 (54%) 0 0	85, 96, 105, 112	0
34	HA	10/27 (37%)	1.40	4 (40%) 0 0	81, 92, 108, 109	0
34	MC	10/27 (37%)	1.36	3 (30%) 1 0	89, 94, 109, 110	0
35	JA	258/368 (70%)	0.26	21 (8%) 15 5	61, 96, 121, 135	0
35	OC	258/368 (70%)	0.64	39 (15%) 3 1	88, 105, 134, 141	0
36	KA	234/256 (91%)	1.35	65 (27%) 1 0	109, 125, 145, 157	0
36	PC	234/256 (91%)	1.11	52 (22%) 1 0	101, 123, 139, 163	0
37	LA	206/239 (86%)	0.14	2 (0%) 84 69	104, 117, 133, 134	0
37	QC	206/239 (86%)	0.08	3 (1%) 76 58	100, 115, 131, 132	0
38	MA	208/209 (99%)	0.65	27 (12%) 5 2	89, 104, 113, 118	0
38	RC	208/209 (99%)	0.24	10 (4%) 34 15	74, 81, 88, 92	0
39	NA	151/162 (93%)	0.13	0 100 100	82, 95, 103, 111	0
39	SC	151/162 (93%)	-0.00	3 (1%) 68 46	73, 85, 92, 105	0
40	OA	101/101 (100%)	0.02	1 (0%) 84 69	75, 83, 91, 103	0
40	TC	101/101 (100%)	0.25	8 (7%) 15 5	87, 95, 100, 110	0
41	PA	155/156 (99%)	0.28	11 (7%) 19 7	103, 113, 119, 122	0
41	UC	155/156 (99%)	0.34	11 (7%) 19 7	102, 111, 118, 120	0
42	QA	138/138 (100%)	0.29	8 (5%) 26 11	83, 97, 104, 109	0
42	VC	138/138 (100%)	0.16	7 (5%) 32 13	73, 87, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RA	127/128 (99%)	1.76	39 (30%) 1 0	90, 141, 148, 151	0
43	WC	127/128 (99%)	1.49	36 (28%) 1 0	88, 135, 144, 148	0
44	SA	98/105 (93%)	1.84	34 (34%) 0 0	101, 144, 156, 156	0
44	XC	98/105 (93%)	1.78	29 (29%) 1 0	103, 139, 151, 153	0
45	TA	116/129 (89%)	0.21	5 (4%) 39 18	66, 84, 93, 97	0
45	YC	116/129 (89%)	0.46	10 (8%) 13 4	69, 90, 96, 103	0
46	UA	121/132 (91%)	0.43	7 (5%) 26 11	74, 79, 88, 93	0
46	ZC	121/132 (91%)	0.28	4 (3%) 50 26	67, 73, 80, 84	0
47	AD	117/126 (92%)	1.11	27 (23%) 1 0	98, 137, 141, 143	0
47	VA	117/126 (92%)	0.81	16 (13%) 4 2	94, 125, 130, 131	0
48	BD	60/61 (98%)	0.91	9 (15%) 3 1	108, 116, 133, 134	0
48	WA	60/61 (98%)	0.69	4 (6%) 21 7	110, 119, 127, 128	0
49	CD	88/89 (98%)	0.67	7 (7%) 15 5	70, 86, 94, 96	0
49	XA	88/89 (98%)	0.62	6 (6%) 20 7	66, 85, 94, 96	0
50	DD	83/88 (94%)	1.10	18 (21%) 1 0	73, 80, 94, 111	0
50	YA	83/88 (94%)	1.87	38 (45%) 0 0	96, 109, 126, 143	0
51	ED	99/105 (94%)	0.42	4 (4%) 42 20	69, 81, 87, 90	0
51	ZA	99/105 (94%)	0.18	3 (3%) 54 29	72, 88, 93, 94	0
52	AB	70/88 (79%)	0.56	3 (4%) 39 18	77, 88, 98, 101	0
52	FD	70/88 (79%)	1.05	16 (22%) 1 0	84, 94, 104, 109	0
53	BB	83/93 (89%)	0.95	20 (24%) 1 0	104, 130, 136, 138	0
53	GD	83/93 (89%)	1.59	28 (33%) 0 0	111, 139, 144, 146	0
54	CB	99/106 (93%)	1.70	39 (39%) 0 0	97, 111, 126, 128	0
54	HD	99/106 (93%)	0.96	23 (23%) 1 0	79, 97, 112, 114	0
55	DB	24/27 (88%)	4.15	20 (83%) 0 0	113, 123, 127, 132	0
55	ID	24/27 (88%)	5.33	23 (95%) 0 0	118, 127, 133, 138	0
All	All	21476/22228 (96%)	0.46	1832 (8%) 13 4	34, 82, 143, 256	0

All (1832) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	GB	2799	A	14.7
1	FB	1001	G	13.7

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Mol	Chain	Res	Type	RSRZ
1	FB	1002	G	13.6
2	GB	1057	A	12.2
2	GB	1084	A	11.7
26	EC	1	MET	11.7
2	GB	1093	G	11.6
43	WC	7	THR	11.5
2	B	2799	A	11.3
2	GB	2798	C	11.2
2	GB	1064	C	11.1
44	XC	73	ASP	11.0
55	DB	17	THR	10.9
2	GB	2161	C	10.6
2	GB	1060	U	10.5
2	GB	1058	G	10.1
2	GB	1070	A	10.0
4	D	17	C	10.0
2	B	1058	G	10.0
2	GB	2160	G	9.8
1	FB	84	U	9.8
2	B	2160	G	9.7
1	A	1001	G	9.7
43	RA	8	GLY	9.6
2	GB	1083	U	9.6
44	SA	38	ILE	9.6
48	BD	2	ALA	9.6
43	RA	14	VAL	9.5
43	RA	7	THR	9.4
2	GB	2173	A	9.3
4	IB	16	C	9.1
44	XC	34	VAL	9.1
55	ID	2	GLY	9.0
48	WA	2	ALA	9.0
9	NB	68	THR	8.9
2	B	2136	C	8.9
2	GB	2802	G	8.8
10	OB	83	ALA	8.8
2	GB	2116	G	8.5
44	SA	72	VAL	8.5
2	GB	1085	A	8.5
2	GB	1059	G	8.4
44	XC	72	VAL	8.4
44	SA	69	ASN	8.4

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Mol	Chain	Res	Type	RSRZ
2	GB	1054	A	8.4
36	PC	239	VAL	8.3
2	GB	2136	C	8.3
2	GB	1068	G	8.3
55	ID	9	ARG	8.3
2	GB	2174	C	8.3
47	AD	2	ALA	8.2
2	GB	1089	G	8.2
55	DB	18	TYR	8.2
43	RA	15	ALA	8.1
1	A	1002	G	8.1
2	B	1537	C	8.0
2	B	2801	A	8.0
2	B	2798	C	8.0
55	ID	18	TYR	8.0
2	B	1070	A	8.0
16	UB	52	SER	7.9
2	B	276	A	7.8
43	RA	9	ARG	7.8
44	XC	35	SER	7.7
43	RA	5	TYR	7.7
55	ID	24	ARG	7.7
2	B	2161	C	7.7
2	GB	2801	A	7.6
2	GB	1094	U	7.6
36	PC	240	GLN	7.6
44	SA	39	PRO	7.4
44	SA	71	LEU	7.4
4	IB	17	C	7.4
2	B	277	C	7.4
43	RA	17	VAL	7.4
2	B	1065	U	7.4
2	B	2116	G	7.4
43	RA	6	GLY	7.4
1	FB	1000	A	7.4
2	B	1536	A	7.4
2	GB	1063	G	7.3
4	D	16	C	7.3
50	YA	8	ARG	7.3
55	ID	6	ARG	7.3
44	SA	70	ARG	7.2
2	B	1064	C	7.2

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Mol	Chain	Res	Type	RSRZ
38	MA	4	TYR	7.2
16	UB	34	HIS	7.2
44	XC	38	ILE	7.1
36	PC	238	LEU	7.1
44	SA	8	LEU	7.0
55	ID	8	THR	7.0
4	IB	17(A)	U	7.0
4	D	18	G	6.9
38	RC	4	TYR	6.9
53	GD	33	THR	6.9
2	B	1067	A	6.9
24	CC	3	HIS	6.9
55	ID	21	TYR	6.9
2	GB	2805	G	6.9
2	GB	1065	U	6.8
43	WC	66	ARG	6.8
43	RA	66	ARG	6.8
43	WC	18	PHE	6.8
16	UB	36	TYR	6.7
44	XC	71	LEU	6.7
2	GB	1067	A	6.7
2	B	2803	C	6.6
1	A	1025	U	6.6
2	GB	1066	U	6.6
44	XC	36	GLY	6.6
4	D	17(A)	U	6.6
2	GB	11	G	6.6
2	GB	1055	G	6.6
1	FB	1003	G	6.5
2	B	1069	A	6.5
2	GB	1069	A	6.4
8	MB	69	ALA	6.4
53	GD	34	TRP	6.4
2	B	1068	G	6.4
2	B	2173	A	6.4
43	WC	16	ARG	6.4
2	B	1061	U	6.3
2	GB	1061	U	6.3
2	B	2159	G	6.3
13	M	110	TYR	6.3
43	RA	18	PHE	6.3
4	IB	47	U	6.3

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Mol	Chain	Res	Type	RSRZ
2	B	2802	G	6.3
2	B	1057	A	6.2
50	YA	13	HIS	6.2
2	GB	2797	U	6.2
4	IB	20	U	6.2
54	CB	80	ARG	6.2
2	GB	1536	A	6.2
2	B	2797	U	6.2
54	CB	64	ASP	6.2
2	B	1095	A	6.2
55	DB	7	ARG	6.2
24	X	3	HIS	6.1
9	NB	52	VAL	6.1
2	B	1083	U	6.0
2	B	2896	C	6.0
48	WA	6	LEU	6.0
55	DB	21	TYR	6.0
50	YA	7	ALA	6.0
53	GD	71	LEU	6.0
2	GB	1062	G	6.0
1	A	1000	A	6.0
44	SA	7	LYS	6.0
44	XC	37	PRO	6.0
2	B	2895	U	5.9
33	LC	37	GLY	5.9
55	ID	5	ASP	5.9
30	IC	39	TYR	5.9
38	RC	2	GLY	5.9
2	B	1055	G	5.9
2	GB	2162	G	5.9
2	B	2125	G	5.8
54	CB	60	GLU	5.8
50	YA	17	TYR	5.8
35	OC	326	LEU	5.8
1	A	82	U	5.7
9	NB	61	HIS	5.7
4	D	20	U	5.7
55	DB	2	GLY	5.7
2	GB	2125	G	5.7
36	PC	140	HIS	5.7
55	DB	8	THR	5.7
43	WC	19	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
28	GC	28	LYS	5.7
2	GB	2803	C	5.6
2	B	2135	A	5.6
36	KA	133	LYS	5.6
2	B	1059	G	5.6
54	CB	70	SER	5.6
44	SA	93	GLY	5.6
53	GD	32	LYS	5.6
2	GB	1049	C	5.6
2	GB	1075	C	5.6
2	B	2162	G	5.5
1	FB	1034	G	5.5
1	A	1149	C	5.5
43	WC	3	GLN	5.5
9	NB	64	LEU	5.4
44	SA	99	LYS	5.4
2	GB	2795	G	5.4
2	GB	1088	A	5.4
28	GC	68	ARG	5.4
2	GB	1080	C	5.4
36	KA	165	VAL	5.4
2	B	1056	G	5.4
16	UB	29	PHE	5.4
47	AD	27	LYS	5.4
53	GD	77	THR	5.4
16	UB	53	SER	5.4
2	GB	10	G	5.4
2	B	2174	C	5.4
55	ID	15	ARG	5.3
35	OC	300	SER	5.3
53	GD	75	ALA	5.3
49	XA	69	TYR	5.3
2	GB	2121	G	5.3
9	NB	67	LEU	5.3
8	MB	12	TYR	5.3
50	YA	39	TYR	5.3
55	ID	7	ARG	5.3
2	B	2894	G	5.3
43	RA	65	VAL	5.3
44	SA	35	SER	5.3
54	HD	74	LYS	5.3
53	GD	35	SER	5.3

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Mol	Chain	Res	Type	RSRZ
55	DB	5	ASP	5.2
34	MC	13	A	5.2
2	B	1084	A	5.2
2	GB	2135	A	5.2
30	IC	20	ASN	5.2
2	GB	1087	G	5.2
9	NB	4	ILE	5.2
55	ID	14	TRP	5.2
2	GB	1095	A	5.2
42	QA	1	MET	5.2
47	AD	87	TYR	5.2
16	UB	37	ALA	5.2
43	RA	102	LEU	5.1
54	CB	65	LYS	5.1
1	A	1024	G	5.1
36	PC	215	LEU	5.1
54	CB	68	LYS	5.1
2	GB	2895	U	5.1
24	X	4	LYS	5.1
44	XC	39	PRO	5.1
55	DB	6	ARG	5.1
54	CB	77	ALA	5.1
36	KA	215	LEU	5.1
50	YA	6	LEU	5.1
2	B	2892	A	5.1
52	FD	31	LEU	5.1
8	MB	35	GLU	5.0
2	B	1066	U	5.0
2	B	2795	G	5.0
2	GB	1071	G	5.0
55	ID	25	LYS	5.0
55	ID	16	GLY	5.0
2	GB	1103	A	5.0
36	KA	239	VAL	5.0
47	AD	102	ARG	5.0
9	NB	16	SER	5.0
42	VC	1	MET	5.0
52	FD	22	VAL	5.0
2	B	10	G	5.0
55	ID	10	ARG	5.0
44	XC	5	ARG	4.9
26	EC	5	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
9	NB	43	VAL	4.9
1	A	1003	G	4.9
2	GB	2175	C	4.9
1	FB	1025	U	4.9
9	NB	17	VAL	4.9
9	NB	60	ARG	4.9
47	AD	19	LEU	4.9
2	B	11	G	4.9
2	GB	2894	G	4.9
28	BA	69	LYS	4.9
55	ID	20	LYS	4.9
9	NB	2	SER	4.9
1	FB	1138	G	4.9
2	GB	1106	G	4.9
2	GB	1104	C	4.8
1	A	466	G	4.8
48	BD	6	LEU	4.8
2	B	2175	C	4.8
43	RA	62	TYR	4.8
50	YA	9	PHE	4.8
43	WC	62	TYR	4.8
23	BC	97	GLU	4.8
44	XC	40	LEU	4.8
53	GD	52	TYR	4.8
2	GB	1086	A	4.8
8	MB	93	THR	4.7
13	RB	76	LYS	4.7
2	GB	1107	G	4.7
23	BC	87	ASP	4.7
1	FB	81	G	4.7
13	RB	81	GLN	4.7
2	GB	1099	G	4.7
43	RA	16	ARG	4.7
2	GB	1096	A	4.7
1	FB	1033	G	4.7
2	B	1098	A	4.7
42	VC	2	LEU	4.7
54	CB	9	ASN	4.7
54	CB	74	LYS	4.7
43	RA	3	GLN	4.7
44	XC	33	GLN	4.6
13	M	105	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	GB	1056	G	4.6
2	GB	2804	C	4.6
2	GB	1174	A	4.6
44	SA	6	ILE	4.6
55	ID	22	ARG	4.6
4	IB	18	G	4.6
36	KA	96	ARG	4.6
2	GB	12	U	4.6
43	WC	9	ARG	4.6
53	BB	71	LEU	4.6
1	A	1127	G	4.6
22	AC	59	GLY	4.6
2	B	2117	A	4.6
23	BC	75	ASN	4.6
44	XC	99	LYS	4.6
1	FB	82	U	4.6
1	A	1033	G	4.6
36	PC	12	GLU	4.6
43	RA	63	ILE	4.6
4	IB	59	A	4.6
2	GB	1052	C	4.6
43	WC	83	ARG	4.6
2	GB	2629	A	4.5
1	FB	1221	G	4.5
2	GB	2119	A	4.5
35	OC	152	SER	4.5
55	DB	10	ARG	4.5
2	B	2129	C	4.5
21	ZB	1	MET	4.5
55	ID	3	LYS	4.5
43	RA	83	ARG	4.5
16	UB	51	ALA	4.5
28	BA	32	TYR	4.5
55	ID	13	ILE	4.5
35	JA	182	HIS	4.5
26	EC	2	LYS	4.5
2	GB	1082	U	4.5
2	B	2119	A	4.5
48	BD	19	ARG	4.4
2	GB	2117	A	4.4
9	NB	65	HIS	4.4
35	OC	327	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
33	LC	22	ARG	4.4
54	CB	104	LEU	4.4
1	FB	1027	C	4.4
2	GB	363(G)	A	4.4
8	H	39	ILE	4.4
2	B	1085	A	4.4
44	XC	8	LEU	4.4
36	PC	133	LYS	4.4
26	EC	56	GLN	4.4
55	DB	15	ARG	4.4
2	GB	1081	U	4.4
34	HA	13	A	4.4
44	XC	70	ARG	4.4
50	YA	15	PRO	4.4
23	BC	91	LEU	4.4
2	GB	1105	U	4.3
2	B	1053	C	4.3
16	P	31	SER	4.3
4	D	61	C	4.3
4	D	47	U	4.3
44	SA	40	LEU	4.3
28	BA	67	TYR	4.3
16	UB	58	LEU	4.3
36	PC	72	GLY	4.3
55	DB	9	ARG	4.3
30	IC	2	ALA	4.3
28	BA	31	ILE	4.3
24	X	2	ALA	4.3
50	YA	12	LYS	4.3
9	NB	55	PRO	4.3
1	A	1280	A	4.3
28	BA	55	ARG	4.3
8	MB	157	ILE	4.3
48	BD	5	ALA	4.3
50	YA	73	LEU	4.3
2	B	2121	G	4.3
8	MB	68	PRO	4.3
13	RB	105	LEU	4.3
1	FB	1041	A	4.3
9	NB	9	ILE	4.3
4	IB	61	C	4.3
41	UC	33	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
23	BC	74	VAL	4.3
54	CB	69	GLY	4.2
2	B	1099	G	4.2
8	H	66	GLN	4.2
44	XC	7	LYS	4.2
47	AD	31	LYS	4.2
8	H	35	GLU	4.2
43	RA	19	LEU	4.2
2	B	12	U	4.2
36	KA	211	ILE	4.2
44	SA	37	PRO	4.2
53	GD	50	ALA	4.2
38	RC	42	GLN	4.2
38	MA	70	ILE	4.2
54	CB	83	ARG	4.2
2	GB	1079	C	4.2
30	IC	21	TYR	4.2
43	WC	65	VAL	4.2
55	ID	23	PRO	4.2
41	UC	5	ARG	4.2
1	FB	87	A	4.1
36	KA	152	PHE	4.1
1	FB	1039	C	4.1
41	UC	85	TYR	4.1
44	SA	19	SER	4.1
50	DD	12	LYS	4.1
4	IB	15	G	4.1
8	H	133	LEU	4.1
1	A	1129	C	4.1
43	WC	64	THR	4.1
2	B	1062	G	4.1
13	RB	79	ARG	4.1
13	M	106	LEU	4.1
2	B	1535	U	4.1
36	KA	218	ALA	4.1
1	A	87	A	4.1
36	KA	101	MET	4.1
9	NB	108	GLY	4.1
50	YA	18	ARG	4.1
23	BC	99	TYR	4.1
23	BC	72	ARG	4.0
54	CB	63	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
36	KA	222	ILE	4.0
36	KA	134	GLU	4.0
1	A	84	U	4.0
54	CB	56	MET	4.0
50	DD	6	LEU	4.0
9	NB	26	VAL	4.0
55	DB	20	LYS	4.0
36	KA	187	LEU	4.0
36	PC	9	GLU	4.0
9	I	2	SER	4.0
36	KA	196	LEU	4.0
8	MB	102	PHE	4.0
10	J	89	TYR	4.0
1	A	1026	G	4.0
2	GB	2159	G	4.0
36	KA	238	LEU	4.0
2	GB	1100	C	4.0
54	CB	81	LYS	4.0
2	B	1054	A	4.0
23	BC	39	VAL	4.0
2	B	2805	G	4.0
23	BC	73	GLN	4.0
50	YA	19	ILE	4.0
1	FB	1032(C)	G	3.9
2	GB	1102	C	3.9
4	D	19	G	3.9
2	B	2172	U	3.9
35	JA	104	ASP	3.9
38	MA	112	VAL	3.9
36	KA	102	LEU	3.9
28	BA	33	VAL	3.9
36	PC	39	ILE	3.9
24	X	5	LYS	3.9
2	B	1100	C	3.9
13	RB	107	LYS	3.9
28	GC	10	VAL	3.9
30	DA	21	TYR	3.9
53	GD	12	ASP	3.9
10	OB	40	THR	3.9
36	PC	214	ILE	3.9
50	DD	17	TYR	3.9
13	RB	104	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	FB	994	A	3.9
2	GB	2892	A	3.9
36	PC	237	ALA	3.9
36	PC	232	PRO	3.9
53	GD	15	LEU	3.9
55	ID	4	GLY	3.9
4	D	21	A	3.9
1	FB	1224	G	3.9
13	RB	87	ASP	3.9
1	FB	1267	C	3.9
9	NB	27	LYS	3.9
54	CB	66	ALA	3.9
44	SA	74	ILE	3.9
9	NB	54	ARG	3.8
16	P	29	PHE	3.8
13	RB	84	ASN	3.8
43	WC	82	ALA	3.8
47	VA	19	LEU	3.8
53	GD	53	ASN	3.8
54	CB	71	THR	3.8
55	DB	23	PRO	3.8
43	WC	4	TYR	3.8
16	UB	30	ARG	3.8
55	DB	22	ARG	3.8
35	JA	200	ALA	3.8
1	FB	1004	A	3.8
2	B	1063	G	3.8
4	IB	19	G	3.8
22	AC	60	PHE	3.8
1	A	1170	A	3.8
9	NB	72	ILE	3.8
13	M	104	GLY	3.8
36	KA	163	PHE	3.8
38	MA	42	GLN	3.8
43	RA	64	THR	3.8
2	B	9	U	3.8
2	GB	9	U	3.8
4	IB	60	U	3.8
1	A	1041	A	3.8
13	RB	88	LEU	3.8
30	IC	44	ARG	3.8
2	B	363(G)	A	3.8

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Mol	Chain	Res	Type	RSRZ
40	TC	99	ALA	3.8
43	WC	14	VAL	3.8
44	SA	24	VAL	3.8
33	LC	17	ILE	3.8
2	GB	2108	C	3.8
22	V	2	ARG	3.7
1	FB	466	G	3.7
47	AD	98	VAL	3.7
26	EC	55	ARG	3.7
1	FB	86	U	3.7
1	FB	977	A	3.7
13	RB	118	GLY	3.7
28	BA	68	ARG	3.7
50	DD	68	ASP	3.7
30	DA	20	ASN	3.7
54	CB	75	ASN	3.7
44	SA	95	GLU	3.7
50	YA	16	HIS	3.7
54	CB	62	LEU	3.7
3	HB	5	C	3.7
36	KA	28	PHE	3.7
9	NB	53	GLU	3.7
36	PC	132	LYS	3.7
13	RB	106	LEU	3.7
44	SA	96	ILE	3.7
36	KA	137	ARG	3.7
44	SA	94	VAL	3.7
2	B	2630	G	3.7
26	EC	7	ARG	3.7
53	BB	78	ARG	3.7
53	GD	51	VAL	3.7
2	GB	546	C	3.7
8	MB	92	VAL	3.7
28	BA	65	ASP	3.7
32	KC	46	ARG	3.7
54	CB	57	ARG	3.7
13	RB	108	LYS	3.7
46	UA	93	LEU	3.7
1	A	89	U	3.7
1	FB	1040	U	3.7
44	SA	9	ARG	3.7
13	RB	110	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
15	TB	7	GLY	3.7
47	AD	13	LYS	3.7
13	RB	150	ALA	3.7
24	CC	2	ALA	3.7
47	VA	10	PRO	3.6
43	WC	61	ALA	3.6
1	FB	983	A	3.6
36	KA	71	VAL	3.6
54	HD	81	LYS	3.6
1	A	1138	G	3.6
50	YA	71	ARG	3.6
16	UB	35	ILE	3.6
2	GB	2793	G	3.6
4	IB	21	A	3.6
28	BA	1	MET	3.6
8	MB	34	LEU	3.6
22	AC	57	GLN	3.6
2	GB	2122	U	3.6
36	KA	144	ARG	3.6
41	PA	32	ARG	3.6
35	OC	325	THR	3.6
42	QA	2	LEU	3.6
23	BC	169	GLU	3.6
16	UB	97	ARG	3.6
35	OC	104	ASP	3.6
1	FB	1222	G	3.6
2	B	2120	G	3.6
4	IB	22	G	3.6
30	DA	39	TYR	3.6
49	CD	57	LEU	3.6
17	Q	136	GLN	3.6
28	BA	49	PHE	3.6
2	B	1105	U	3.6
2	B	1089	G	3.6
43	RA	29	ASN	3.6
47	AD	12	ASN	3.6
36	KA	230	VAL	3.6
2	B	2629	A	3.6
34	HA	15	A	3.6
1	FB	1032(B)	G	3.6
8	H	36	LYS	3.6
10	OB	41	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
35	JA	103	LYS	3.6
35	OC	153	GLU	3.6
32	KC	38	GLY	3.6
23	BC	127	LYS	3.5
41	PA	22	LEU	3.5
50	YA	10	GLY	3.5
1	FB	993	G	3.5
2	GB	273(A)	G	3.5
36	KA	229	VAL	3.5
38	RC	5	ILE	3.5
26	EC	10	LEU	3.5
43	WC	102	LEU	3.5
54	CB	84	LEU	3.5
36	KA	81	VAL	3.5
36	KA	164	VAL	3.5
42	QA	129	VAL	3.5
2	B	1082	U	3.5
35	OC	102	PRO	3.5
42	VC	116	LYS	3.5
1	A	1126	U	3.5
35	OC	316	ARG	3.5
44	SA	17	ASP	3.5
44	XC	17	ASP	3.5
13	M	107	LYS	3.5
35	JA	357	SER	3.5
2	B	2804	C	3.5
38	MA	109	GLY	3.5
2	B	270(M)	U	3.5
8	MB	36	LYS	3.5
28	BA	56	VAL	3.5
35	OC	115	VAL	3.5
36	PC	230	VAL	3.5
51	ED	45	HIS	3.5
2	GB	2176	A	3.5
16	UB	55	ALA	3.5
2	B	1538	G	3.5
2	GB	2751	G	3.5
4	D	34	C	3.5
47	VA	98	VAL	3.5
22	AC	89	PHE	3.5
9	NB	50	VAL	3.5
30	DA	44	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
30	IC	49	HIS	3.5
43	WC	93	ARG	3.5
13	M	103	ALA	3.5
22	AC	56	PRO	3.5
28	GC	25	TYR	3.5
42	VC	129	VAL	3.5
13	M	79	ARG	3.5
8	H	160	VAL	3.4
44	XC	41	PRO	3.4
28	GC	14	ILE	3.4
9	NB	5	GLY	3.4
54	HD	101	GLY	3.4
1	A	91	C	3.4
4	IB	48	C	3.4
32	KC	41	ILE	3.4
43	RA	127	LYS	3.4
1	FB	1220	G	3.4
2	B	1534	G	3.4
22	AC	1	MET	3.4
43	RA	30	GLY	3.4
47	VA	2	ALA	3.4
36	KA	132	LYS	3.4
16	P	30	ARG	3.4
23	BC	152	ALA	3.4
43	WC	2	GLU	3.4
13	RB	91	PHE	3.4
55	ID	12	LYS	3.4
16	UB	31	SER	3.4
2	GB	1097	U	3.4
23	BC	53	ILE	3.4
13	RB	77	ARG	3.4
43	RA	13	ALA	3.4
2	B	1087	G	3.4
50	DD	39	TYR	3.4
52	FD	66	LEU	3.4
45	YC	29	ILE	3.4
50	DD	42	ARG	3.4
30	IC	41	PRO	3.4
36	KA	98	LEU	3.4
40	OA	101	ALA	3.4
43	RA	84	ALA	3.4
23	BC	29	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	2151	G	3.4
14	N	141	GLN	3.4
1	FB	1024	G	3.4
23	BC	174	VAL	3.4
28	GC	26	SER	3.4
23	BC	125	LEU	3.4
36	PC	137	ARG	3.4
47	AD	94	ARG	3.4
36	PC	165	VAL	3.4
18	WB	80	ILE	3.4
44	XC	69	ASN	3.4
1	FB	1140	C	3.4
53	GD	78	ARG	3.4
23	BC	86	VAL	3.3
28	GC	54	GLY	3.3
44	XC	10	GLY	3.3
54	CB	79	ARG	3.3
1	A	1027	C	3.3
8	MB	39	ILE	3.3
2	GB	2126	A	3.3
50	YA	35	LYS	3.3
1	FB	1326	C	3.3
2	B	1075	C	3.3
53	GD	49	ILE	3.3
38	MA	2	GLY	3.3
49	XA	25	THR	3.3
36	KA	232	PRO	3.3
13	M	81	GLN	3.3
1	A	1148	U	3.3
2	B	2631	G	3.3
54	CB	106	ALA	3.3
28	BA	9	LEU	3.3
53	BB	38	SER	3.3
1	A	1128	C	3.3
2	GB	1053	C	3.3
8	MB	63	ILE	3.3
33	LC	24	TYR	3.3
9	NB	59	ARG	3.3
9	NB	71	LEU	3.3
13	M	100	LEU	3.3
28	BA	27	THR	3.3
28	GC	9	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	GB	271(C)	G	3.3
2	GB	1215	G	3.3
53	GD	13	ASP	3.3
47	AD	28	ALA	3.3
2	GB	1589	C	3.3
13	M	115	LEU	3.3
30	IC	36	LEU	3.3
2	GB	2169	A	3.3
25	Y	26	ARG	3.3
38	RC	10	ARG	3.3
50	YA	69	THR	3.3
9	NB	58	GLU	3.3
50	YA	42	ARG	3.3
1	FB	1218	C	3.3
36	KA	73	THR	3.3
43	RA	82	ALA	3.3
22	AC	95	LYS	3.3
50	YA	14	ASN	3.2
9	NB	110	SER	3.2
1	A	90	C	3.2
2	GB	2129	C	3.2
43	WC	17	VAL	3.2
17	Q	1	MET	3.2
44	SA	41	PRO	3.2
2	B	1174	A	3.2
54	CB	103	GLY	3.2
10	OB	45	LYS	3.2
30	IC	38	LYS	3.2
28	GC	35	VAL	3.2
42	VC	95	VAL	3.2
47	AD	15	VAL	3.2
54	HD	79	ARG	3.2
1	FB	1131	G	3.2
16	UB	7	TYR	3.2
28	GC	32	TYR	3.2
38	RC	3	ARG	3.2
49	CD	25	THR	3.2
46	UA	110	VAL	3.2
48	BD	8	GLU	3.2
22	AC	4	LYS	3.2
50	YA	4	ILE	3.2
6	F	60	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
47	AD	34	LEU	3.2
50	YA	28	ARG	3.2
2	B	6	A	3.2
2	GB	2170	A	3.2
15	TB	69	ASP	3.2
23	W	1	MET	3.2
44	XC	75	ILE	3.2
1	A	88	C	3.2
23	BC	7	ALA	3.2
28	GC	56	VAL	3.2
1	A	1032(C)	G	3.2
1	A	1222	G	3.2
2	B	1060	U	3.2
13	RB	85	LEU	3.2
44	XC	68	HIS	3.2
1	FB	1223	C	3.2
44	SA	5	ARG	3.2
2	GB	2109	U	3.2
2	GB	2120	G	3.2
36	PC	40	HIS	3.2
13	RB	83	VAL	3.2
23	BC	88	PHE	3.2
16	UB	57	LYS	3.2
28	BA	63	TYR	3.2
1	FB	1125	U	3.2
2	GB	1576	U	3.2
52	FD	23	LYS	3.2
54	HD	83	ARG	3.2
2	B	2126	A	3.2
15	TB	6	SER	3.2
8	MB	64	THR	3.2
22	V	1	MET	3.2
24	X	9	SER	3.2
35	OC	302	ASP	3.2
43	WC	87	GLN	3.2
1	A	1125	U	3.2
16	UB	92	TYR	3.2
16	P	33	LYS	3.2
22	AC	85	VAL	3.2
23	BC	165	VAL	3.2
35	JA	352	GLN	3.2
36	PC	218	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
26	EC	59	ARG	3.2
36	KA	93	VAL	3.2
47	AD	30	ALA	3.2
1	FB	220	G	3.2
52	FD	62	GLU	3.2
4	D	48	C	3.1
4	IB	56	C	3.1
52	FD	67	ALA	3.1
14	SB	137	TYR	3.1
1	A	64	G	3.1
1	A	1096	C	3.1
1	FB	1139	G	3.1
43	WC	6	GLY	3.1
53	GD	38	SER	3.1
43	WC	49	PRO	3.1
2	B	1528	A	3.1
24	CC	4	LYS	3.1
1	A	1034	G	3.1
4	IB	34	C	3.1
10	OB	61	ARG	3.1
41	PA	5	ARG	3.1
21	ZB	6	ASP	3.1
16	UB	87	PHE	3.1
2	B	1097	U	3.1
36	KA	148	TYR	3.1
2	GB	1044	G	3.1
54	CB	102	GLY	3.1
47	AD	43	THR	3.1
44	SA	97	GLU	3.1
45	TA	25	TYR	3.1
1	A	1039	C	3.1
28	GC	3	GLU	3.1
36	PC	71	VAL	3.1
55	DB	14	TRP	3.1
26	EC	9	GLN	3.1
2	GB	2172	U	3.1
23	BC	98	MET	3.1
35	OC	317	VAL	3.1
43	WC	29	ASN	3.1
23	BC	69	THR	3.1
26	EC	58	ALA	3.1
40	TC	101	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
10	OB	82	ARG	3.1
2	GB	654	U	3.1
50	YA	29	ASP	3.1
50	DD	7	ALA	3.1
54	HD	99	LEU	3.1
14	SB	141	GLN	3.1
47	VA	102	ARG	3.1
26	EC	6	VAL	3.1
1	A	1124	G	3.1
2	GB	1101	U	3.1
2	GB	2123	G	3.1
8	MB	135	LEU	3.1
16	P	92	TYR	3.1
18	WB	78	THR	3.1
43	RA	103	THR	3.1
53	GD	36	ARG	3.1
2	GB	1092	C	3.1
5	JB	276	LYS	3.1
35	JA	300	SER	3.1
35	OC	354	ALA	3.1
2	GB	1051	G	3.1
36	KA	72	GLY	3.1
53	GD	11	VAL	3.1
55	DB	3	LYS	3.1
32	KC	42	ARG	3.1
47	VA	5	ALA	3.1
23	BC	171	ILE	3.0
2	GB	1074	G	3.0
38	MA	66	ARG	3.0
43	RA	79	LEU	3.0
1	FB	196	A	3.0
2	GB	1098	A	3.0
22	AC	58	GLY	3.0
53	BB	35	SER	3.0
1	A	86	U	3.0
35	JA	306	ARG	3.0
45	YC	87	THR	3.0
54	HD	68	LYS	3.0
2	B	2166	G	3.0
51	ED	8	GLY	3.0
53	BB	49	ILE	3.0
36	KA	212	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
36	KA	233	SER	3.0
2	B	1094	U	3.0
23	BC	70	LEU	3.0
49	CD	56	LEU	3.0
16	UB	33	LYS	3.0
36	PC	88	ALA	3.0
43	RA	4	TYR	3.0
54	CB	72	LEU	3.0
2	B	2170	A	3.0
1	A	93	U	3.0
23	W	88	PHE	3.0
36	PC	201	ILE	3.0
28	BA	16	CYS	3.0
36	KA	234	PRO	3.0
36	PC	37	ASN	3.0
6	F	63	LEU	3.0
30	DA	42	TRP	3.0
35	OC	201	CYS	3.0
23	W	72	ARG	3.0
43	WC	5	TYR	3.0
44	SA	20	ALA	3.0
1	A	65	U	3.0
4	IB	14	A	3.0
4	IB	58	A	3.0
9	NB	7	LEU	3.0
54	HD	64	ASP	3.0
36	KA	188	ALA	3.0
43	WC	86	VAL	3.0
23	BC	163	LEU	3.0
50	DD	60	LEU	3.0
1	A	990	C	3.0
1	A	1150	U	3.0
9	NB	41	MET	3.0
36	PC	152	PHE	3.0
54	CB	76	ALA	3.0
23	BC	24	LEU	3.0
36	PC	19	HIS	3.0
52	FD	43	PHE	3.0
22	AC	93	GLY	3.0
28	BA	34	GLU	3.0
33	LC	9	ARG	3.0
28	BA	28	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
32	KC	36	LYS	3.0
1	A	1035	A	3.0
35	OC	307	ASN	3.0
45	YC	117	ASN	3.0
50	DD	69	THR	3.0
9	NB	40	GLU	3.0
1	FB	1216	G	2.9
2	GB	1444	G	2.9
35	OC	344	ILE	2.9
36	PC	211	ILE	2.9
23	BC	96	VAL	2.9
1	A	984	C	2.9
2	GB	2128	C	2.9
47	AD	25	ILE	2.9
2	B	271(D)	U	2.9
2	GB	2349	G	2.9
13	RB	128	HIS	2.9
8	MB	60	LEU	2.9
28	GC	16	CYS	2.9
36	PC	95	GLN	2.9
8	MB	103	LEU	2.9
23	BC	5	LEU	2.9
35	OC	337	LEU	2.9
47	AD	60	VAL	2.9
1	A	186(A)	C	2.9
8	MB	91	ARG	2.9
22	V	94	LYS	2.9
46	ZC	72	GLY	2.9
35	OC	150	SER	2.9
43	RA	81	ILE	2.9
18	WB	76	TYR	2.9
1	FB	197	A	2.9
1	A	1040	U	2.9
42	VC	97	VAL	2.9
55	ID	17	THR	2.9
23	BC	71	VAL	2.9
1	FB	1035	A	2.9
34	MC	14	A	2.9
30	IC	42	TRP	2.9
32	KC	40	GLU	2.9
44	SA	4	ILE	2.9
2	B	2164	C	2.9

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Mol	Chain	Res	Type	RSRZ
33	LC	15	LYS	2.9
53	GD	74	PHE	2.9
2	GB	2150	U	2.9
35	JA	301	GLY	2.9
53	GD	72	GLY	2.9
54	CB	101	GLY	2.9
23	W	27	VAL	2.9
43	RA	86	VAL	2.9
43	WC	79	LEU	2.9
54	HD	65	LYS	2.9
53	BB	50	ALA	2.9
2	B	2382	G	2.9
54	CB	58	LYS	2.9
28	GC	31	ILE	2.9
47	VA	25	ILE	2.9
46	ZC	119	LYS	2.9
2	GB	1076	C	2.9
1	A	1139	G	2.9
1	FB	1286	A	2.9
34	MC	15	A	2.9
43	RA	104	ARG	2.9
36	PC	46	LYS	2.9
55	ID	11	GLY	2.9
8	MB	41	GLN	2.8
16	UB	11	LYS	2.8
53	BB	52	TYR	2.8
1	FB	1036	G	2.8
52	FD	85	LEU	2.8
36	KA	147	LYS	2.8
9	NB	174	GLY	2.8
54	HD	84	LEU	2.8
43	WC	63	ILE	2.8
54	CB	16	HIS	2.8
35	OC	301	GLY	2.8
4	D	56	C	2.8
23	BC	126	VAL	2.8
35	OC	105	PRO	2.8
16	P	34	HIS	2.8
9	NB	94	TYR	2.8
32	KC	43	GLN	2.8
45	YC	25	TYR	2.8
50	YA	38	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
8	MB	89	GLY	2.8
26	EC	54	LYS	2.8
2	GB	1534	G	2.8
3	C	61	G	2.8
43	RA	75	ASP	2.8
8	MB	158	ALA	2.8
44	SA	34	VAL	2.8
40	TC	89	MET	2.8
2	B	2122	U	2.8
10	OB	131	LYS	2.8
8	H	135	LEU	2.8
24	X	8	GLY	2.8
23	BC	168	GLU	2.8
30	IC	45	LYS	2.8
41	UC	115	ARG	2.8
1	A	1281	U	2.8
2	GB	895	U	2.8
44	SA	90	LEU	2.8
23	W	174	VAL	2.8
33	LC	1	MET	2.8
16	P	36	TYR	2.8
23	W	70	LEU	2.8
38	MA	43	HIS	2.8
50	YA	77	ALA	2.8
50	DD	13	HIS	2.8
28	BA	2	LYS	2.8
23	W	29	TYR	2.8
23	BC	164	ALA	2.8
2	B	1238	G	2.8
2	B	2891	G	2.8
52	FD	34	TYR	2.8
53	GD	80	TYR	2.8
5	JB	262	ARG	2.8
33	LC	16	VAL	2.8
36	PC	163	PHE	2.8
2	B	2347	C	2.8
40	TC	90	VAL	2.8
41	UC	80	VAL	2.8
43	WC	21	PRO	2.8
53	GD	37	ARG	2.8
33	LC	36	GLN	2.7
1	FB	1127	G	2.7

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Mol	Chain	Res	Type	RSRZ
24	CC	7	LEU	2.7
1	FB	1280	A	2.7
2	B	2134	A	2.7
18	WB	84	LYS	2.7
18	WB	116	ALA	2.7
33	LC	5	ALA	2.7
26	EC	24	LEU	2.7
47	VA	27	LYS	2.7
52	FD	58	LEU	2.7
53	BB	3	ARG	2.7
2	GB	2110	G	2.7
2	GB	2149	G	2.7
2	GB	2893	G	2.7
9	NB	109	PHE	2.7
50	YA	37	GLY	2.7
2	GB	2134	A	2.7
9	NB	111	HIS	2.7
35	OC	314	GLN	2.7
8	MB	133	LEU	2.7
2	B	362	U	2.7
4	D	60	U	2.7
8	MB	38	VAL	2.7
35	JA	355	ALA	2.7
8	H	157	ILE	2.7
35	JA	199	SER	2.7
2	B	7	G	2.7
2	GB	1047	G	2.7
8	MB	66	GLN	2.7
16	UB	32	LEU	2.7
2	B	2179	C	2.7
2	GB	366	C	2.7
35	JA	159	TYR	2.7
35	OC	162	ILE	2.7
50	YA	5	ARG	2.7
28	GC	27	THR	2.7
36	PC	51	LEU	2.7
2	B	2158	A	2.7
2	GB	1527	G	2.7
41	PA	43	PHE	2.7
17	VB	94	ALA	2.7
33	LC	2	LYS	2.7
35	OC	103	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	FB	1219	U	2.7
46	ZC	116	SER	2.7
47	AD	103	THR	2.7
5	JB	275	LYS	2.7
36	PC	77	ALA	2.7
2	B	1096	A	2.7
2	GB	1046	A	2.7
1	A	1023	G	2.7
2	B	2127	G	2.7
30	IC	11	LEU	2.7
35	OC	242	SER	2.7
41	PA	101	LEU	2.7
2	B	2130	U	2.7
2	GB	2692	C	2.7
46	UA	109	GLY	2.7
28	GC	30	GLU	2.7
16	UB	56	LEU	2.7
54	CB	18	GLN	2.7
1	A	1220	G	2.7
2	GB	2807	G	2.7
4	D	22	G	2.7
55	DB	16	GLY	2.7
1	A	985	C	2.7
50	DD	36	ILE	2.7
51	ZA	6	LEU	2.7
9	NB	6	ARG	2.7
13	M	70	GLN	2.7
42	QA	131	GLY	2.7
38	RC	9	CYS	2.7
2	GB	2808	U	2.7
36	KA	207	ALA	2.7
43	WC	81	ILE	2.7
1	A	181	G	2.7
1	A	388	G	2.7
2	B	2345	G	2.7
10	OB	38	LEU	2.7
36	KA	69	LEU	2.7
50	YA	41	PRO	2.7
9	NB	162	ILE	2.7
1	A	185	A	2.7
2	B	1081	U	2.7
2	GB	1535	U	2.7

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Mol	Chain	Res	Type	RSRZ
2	GB	2171	A	2.7
2	GB	2693	A	2.7
5	JB	102	LYS	2.7
50	YA	68	ASP	2.7
44	XC	28	ARG	2.7
28	GC	29	PRO	2.7
36	PC	7	VAL	2.7
16	UB	95	HIS	2.7
36	KA	237	ALA	2.7
50	YA	36	ILE	2.7
1	A	389	A	2.6
1	FB	1148	U	2.6
36	KA	70	PHE	2.6
2	B	2114	A	2.6
2	GB	2790	A	2.6
1	FB	1129	C	2.6
2	GB	1091	G	2.6
33	LC	8	LYS	2.6
43	RA	28	VAL	2.6
10	OB	31	LEU	2.6
2	GB	1531	C	2.6
1	A	92	G	2.6
4	IB	46	G	2.6
24	CC	8	GLY	2.6
52	AB	34	TYR	2.6
28	BA	66	SER	2.6
55	DB	4	GLY	2.6
24	X	7	LEU	2.6
44	XC	87	THR	2.6
50	YA	74	LEU	2.6
2	GB	273(B)	G	2.6
50	DD	16	HIS	2.6
9	NB	3	ARG	2.6
33	LC	35	ARG	2.6
51	ZA	8	GLY	2.6
10	OB	116	LEU	2.6
36	KA	208	ILE	2.6
2	GB	1590	U	2.6
38	RC	115	ARG	2.6
28	BA	57	GLU	2.6
35	OC	118	GLY	2.6
41	PA	80	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
18	WB	77	SER	2.6
1	FB	1005	A	2.6
53	GD	55	LYS	2.6
53	BB	2	PRO	2.6
26	EC	4	SER	2.6
47	AD	46	LYS	2.6
18	WB	59	ARG	2.6
41	UC	41	ARG	2.6
49	CD	17	ARG	2.6
2	GB	1762	A	2.6
23	BC	30	ASN	2.6
2	B	2128	C	2.6
3	C	6	C	2.6
38	MA	156	GLU	2.6
55	DB	12	LYS	2.6
54	CB	23	ARG	2.6
54	CB	25	ARG	2.6
53	BB	53	ASN	2.6
1	A	81	G	2.6
2	B	2124	G	2.6
2	GB	352	G	2.6
36	KA	80	ILE	2.6
47	VA	4	ILE	2.6
33	LC	34	GLN	2.6
36	PC	188	ALA	2.6
35	OC	305	ASP	2.6
18	WB	74	LEU	2.6
47	VA	103	THR	2.6
1	A	1005	A	2.6
2	GB	2370	G	2.6
1	FB	999	U	2.6
2	GB	271(B)	C	2.6
23	BC	89	PHE	2.6
36	KA	77	ALA	2.6
36	PC	31	TYR	2.6
35	JA	305	ASP	2.6
38	MA	65	ARG	2.6
48	BD	12	ARG	2.6
6	F	55	ASN	2.6
36	PC	194	PRO	2.6
36	KA	141	GLU	2.5
1	A	191(G)	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	221	C	2.5
1	FB	744	C	2.5
2	GB	1467	C	2.5
55	DB	24	ARG	2.5
11	PB	37	LYS	2.5
22	AC	94	LYS	2.5
32	KC	39	LYS	2.5
9	NB	152	ARG	2.5
36	KA	76	GLN	2.5
17	Q	135	VAL	2.5
42	VC	130	GLY	2.5
7	LB	171	PRO	2.5
22	AC	5	MET	2.5
2	B	2168	G	2.5
53	GD	2	PRO	2.5
49	XA	51	HIS	2.5
9	NB	87	LEU	2.5
2	B	2169	A	2.5
54	HD	86	ARG	2.5
35	OC	159	TYR	2.5
1	A	391	G	2.5
2	GB	1110	G	2.5
6	F	9	VAL	2.5
53	BB	34	TRP	2.5
22	AC	90	LEU	2.5
30	IC	9	LEU	2.5
2	B	2113	U	2.5
36	KA	231	GLU	2.5
28	GC	6	HIS	2.5
1	FB	979	C	2.5
53	BB	15	LEU	2.5
1	A	1171	G	2.5
2	B	2893	G	2.5
36	PC	48	MET	2.5
8	H	2	PRO	2.5
24	CC	9	SER	2.5
1	A	999	U	2.5
28	GC	60	GLN	2.5
33	LC	23	VAL	2.5
41	UC	109	ASN	2.5
32	FA	42	ARG	2.5
2	B	1103	A	2.5

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Mol	Chain	Res	Type	RSRZ
2	GB	31	C	2.5
2	GB	1111	A	2.5
2	GB	2163	C	2.5
2	GB	2164	C	2.5
3	HB	28	C	2.5
4	D	59	A	2.5
47	VA	9	ILE	2.5
1	A	79	G	2.5
2	GB	2124	G	2.5
37	QC	2	GLY	2.5
28	GC	55	ARG	2.5
32	KC	29	LYS	2.5
54	CB	85	MET	2.5
1	A	374	A	2.5
2	GB	1486	A	2.5
16	UB	49	VAL	2.5
9	NB	56	SER	2.5
22	AC	2	ARG	2.5
36	KA	217	ARG	2.5
44	SA	73	ASP	2.5
2	GB	271(D)	U	2.5
23	W	89	PHE	2.5
2	GB	30	G	2.5
2	GB	272	G	2.5
43	RA	77	ILE	2.5
52	FD	68	LYS	2.5
1	FB	219	C	2.5
38	MA	135	LEU	2.5
2	GB	896	A	2.5
18	WB	79	PHE	2.5
38	MA	9	CYS	2.5
28	GC	5	ILE	2.5
16	UB	54	LEU	2.5
45	YC	86	GLY	2.5
1	A	1028(A)	C	2.5
16	UB	27	SER	2.5
16	UB	39	ILE	2.5
38	MA	146	ILE	2.5
38	MA	158	ILE	2.5
47	AD	4	ILE	2.5
50	DD	11	SER	2.5
35	OC	154	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
10	J	121	LYS	2.5
47	VA	13	LYS	2.5
38	MA	102	ASP	2.5
43	RA	87	GLN	2.5
2	GB	2872	G	2.5
47	AD	88	ARG	2.5
1	A	219	C	2.4
2	GB	2666	C	2.4
8	MB	155	MET	2.4
1	FB	1092	A	2.4
1	FB	1288	A	2.4
35	JA	154	GLY	2.4
46	UA	42	THR	2.4
35	OC	306	ARG	2.4
49	XA	73	GLU	2.4
9	NB	105	LEU	2.4
45	YC	84	VAL	2.4
1	A	1362(B)	C	2.4
51	ED	44	ALA	2.4
16	UB	68	GLN	2.4
36	PC	231	GLU	2.4
45	TA	121	PRO	2.4
32	KC	34	TRP	2.4
15	TB	68	ARG	2.4
38	MA	3	ARG	2.4
1	FB	174	C	2.4
2	B	1466	G	2.4
2	B	2123	G	2.4
2	GB	1485	G	2.4
3	HB	116	G	2.4
4	D	57	A	2.4
15	TB	5	LYS	2.4
8	MB	29	TRP	2.4
28	GC	63	TYR	2.4
43	RA	61	ALA	2.4
13	M	86	LYS	2.4
21	U	33	LYS	2.4
36	KA	146	GLN	2.4
44	SA	98	ILE	2.4
1	A	186(B)	C	2.4
1	A	1223	C	2.4
23	W	175	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
32	FA	39	LYS	2.4
44	XC	26	ALA	2.4
23	BC	133	ILE	2.4
43	RA	73	GLN	2.4
8	MB	145	THR	2.4
10	OB	92	VAL	2.4
27	AA	1	MET	2.4
36	KA	54	THR	2.4
36	PC	87	ARG	2.4
48	WA	19	ARG	2.4
2	B	2145	C	2.4
2	GB	267	C	2.4
2	GB	2178	C	2.4
26	EC	52	ASP	2.4
1	FB	1123	A	2.4
3	HB	7	G	2.4
16	UB	69	VAL	2.4
54	HD	85	MET	2.4
16	UB	72	ALA	2.4
1	A	63	C	2.4
1	A	1092	A	2.4
8	H	38	VAL	2.4
10	OB	58	LEU	2.4
16	UB	73	LEU	2.4
34	HA	22	A	2.4
47	AD	26	GLY	2.4
30	IC	23	THR	2.4
38	MA	110	PHE	2.4
35	OC	151	ALA	2.4
41	PA	4	ARG	2.4
54	CB	59	ALA	2.4
10	OB	68	LEU	2.4
10	OB	140	LEU	2.4
16	UB	38	GLN	2.4
17	Q	137	LYS	2.4
35	JA	356	LEU	2.4
1	A	1093	A	2.4
1	A	1130	A	2.4
36	PC	217	ARG	2.4
1	A	1036	G	2.4
2	B	1465	G	2.4
36	PC	8	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
44	XC	6	ILE	2.4
53	BB	32	LYS	2.4
23	BC	90	VAL	2.4
1	FB	218	C	2.4
38	MA	26	CYS	2.4
1	A	994	A	2.4
1	FB	978	A	2.4
43	WC	88	TYR	2.4
45	YC	123	LYS	2.4
50	DD	19	ILE	2.4
35	OC	211	ASP	2.4
7	G	163	VAL	2.4
13	M	71	VAL	2.4
43	RA	80	GLY	2.4
33	GA	18	ARG	2.4
47	AD	101	GLN	2.4
33	LC	28	GLU	2.4
18	WB	92	ARG	2.3
36	PC	99	GLY	2.3
36	PC	76	GLN	2.3
10	OB	44	LEU	2.3
30	IC	34	LEU	2.3
1	FB	1038	C	2.3
2	GB	645	C	2.3
3	HB	27	C	2.3
35	OC	233	GLY	2.3
13	M	108	LYS	2.3
2	GB	311	A	2.3
10	OB	72	LEU	2.3
30	DA	11	LEU	2.3
43	WC	15	ALA	2.3
22	AC	54	LYS	2.3
53	BB	33	THR	2.3
2	B	8	A	2.3
2	GB	1077	A	2.3
9	NB	63	SER	2.3
28	GC	12	ALA	2.3
1	A	208	U	2.3
2	B	2167	U	2.3
23	BC	25	PRO	2.3
8	H	37	VAL	2.3
28	GC	24	THR	2.3

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Mol	Chain	Res	Type	RSRZ
38	MA	165	MET	2.3
8	H	41	GLN	2.3
36	KA	193	ASP	2.3
1	A	1221	G	2.3
50	DD	18	ARG	2.3
54	HD	57	ARG	2.3
18	WB	65	ILE	2.3
22	V	3	VAL	2.3
45	TA	122	LYS	2.3
2	B	1213	A	2.3
2	GB	1214	A	2.3
34	HA	14	A	2.3
42	QA	128	GLY	2.3
23	W	33	LEU	2.3
23	BC	155	LEU	2.3
54	HD	78	ALA	2.3
2	B	1104	C	2.3
41	PA	23	VAL	2.3
1	A	112	G	2.3
23	BC	114	GLY	2.3
35	OC	357	SER	2.3
44	SA	36	GLY	2.3
2	B	2897	U	2.3
2	GB	270(P)	U	2.3
3	C	29	A	2.3
10	OB	90	GLY	2.3
36	KA	91	PRO	2.3
50	YA	30	GLY	2.3
50	DD	8	ARG	2.3
2	B	1071	G	2.3
1	FB	172	A	2.3
1	FB	185	A	2.3
8	H	159	VAL	2.3
9	NB	24	VAL	2.3
13	M	150	ALA	2.3
36	KA	214	ILE	2.3
13	RB	71	VAL	2.3
36	PC	193	ASP	2.3
8	H	142	PRO	2.3
1	FB	186(A)	C	2.3
21	ZB	31	HIS	2.3
2	GB	2348	U	2.3

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Mol	Chain	Res	Type	RSRZ
8	H	95	ARG	2.3
1	A	191(E)	G	2.3
1	FB	1026	G	2.3
2	B	2131	G	2.3
10	OB	84	GLY	2.3
13	RB	82	GLY	2.3
48	WA	29	ARG	2.3
53	BB	37	ARG	2.3
54	CB	8	ARG	2.3
10	J	140	LEU	2.3
35	JA	152	SER	2.3
50	YA	11	SER	2.3
33	LC	20	HIS	2.3
53	GD	57	HIS	2.3
1	FB	998(B)	C	2.3
3	HB	6	C	2.3
37	LA	185	GLY	2.3
8	H	94	LEU	2.3
35	JA	339	MET	2.3
38	MA	120	LEU	2.3
13	RB	75	ILE	2.3
54	HD	100	ILE	2.3
16	P	7	TYR	2.3
21	ZB	33	LYS	2.3
33	LC	33	LYS	2.3
43	WC	59	PHE	2.3
2	GB	2179	C	2.3
28	BA	52	THR	2.3
36	PC	220	ASP	2.3
47	VA	12	ASN	2.3
8	H	34	LEU	2.3
13	RB	122	PRO	2.3
26	EC	3	LEU	2.3
2	B	1086	A	2.3
23	BC	51	ALA	2.3
4	D	15	G	2.2
36	PC	35	GLU	2.2
18	WB	55	ARG	2.2
51	ZA	7	THR	2.2
1	A	390	C	2.2
28	BA	29	PRO	2.2
38	RC	40	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
53	GD	58	VAL	2.2
9	NB	14	GLY	2.2
35	OC	331	GLU	2.2
1	A	195	A	2.2
1	A	1014	A	2.2
7	G	124	LEU	2.2
26	EC	61	LEU	2.2
54	HD	72	LEU	2.2
1	A	184	G	2.2
2	GB	615	G	2.2
2	GB	1487	G	2.2
8	MB	97	ASP	2.2
41	UC	28	ASN	2.2
23	BC	57	ILE	2.2
23	BC	108	PRO	2.2
23	BC	146	ILE	2.2
28	BA	14	ILE	2.2
43	RA	36	TYR	2.2
1	A	172	A	2.2
1	FB	143	A	2.2
37	LA	191	THR	2.2
44	XC	4	ILE	2.2
45	YC	119	CYS	2.2
1	FB	654	G	2.2
33	GA	9	ARG	2.2
30	IC	46	HIS	2.2
45	TA	123	LYS	2.2
1	FB	1137	C	2.2
2	GB	1505	C	2.2
49	CD	51	HIS	2.2
13	RB	112	LEU	2.2
50	DD	9	PHE	2.2
16	UB	5	THR	2.2
38	MA	62	GLN	2.2
47	VA	61	GLU	2.2
49	XA	62	GLN	2.2
1	A	1095	U	2.2
1	FB	1302	U	2.2
2	B	546	C	2.2
2	B	2111	C	2.2
8	MB	148	MET	2.2
23	BC	100	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
28	BA	10	VAL	2.2
39	SC	18	ARG	2.2
50	YA	40	ASP	2.2
13	RB	120	ALA	2.2
36	PC	47	THR	2.2
53	BB	76	PRO	2.2
1	A	1032(A)	A	2.2
2	B	1509	A	2.2
2	GB	504	U	2.2
45	YC	125	PHE	2.2
28	GC	33	VAL	2.2
46	UA	53	ARG	2.2
47	AD	3	ARG	2.2
52	FD	32	ARG	2.2
10	OB	89	TYR	2.2
44	SA	10	GLY	2.2
54	HD	77	ALA	2.2
13	RB	90	ARG	2.2
4	D	58	A	2.2
53	BB	51	VAL	2.2
36	PC	148	TYR	2.2
1	A	1030	C	2.2
1	A	1325	C	2.2
41	PA	33	ASP	2.2
1	A	1032(B)	G	2.2
1	FB	1042	G	2.2
2	B	2115	G	2.2
2	GB	266	G	2.2
2	GB	271	G	2.2
2	GB	2792	G	2.2
7	G	129	PHE	2.2
11	PB	43	THR	2.2
35	OC	202	THR	2.2
40	TC	7	ASN	2.2
43	WC	20	ARG	2.2
52	FD	56	THR	2.2
53	GD	70	LYS	2.2
54	HD	9	ASN	2.2
42	QA	95	VAL	2.2
45	YC	22	HIS	2.2
1	FB	223	U	2.2
6	KB	186	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
9	NB	31	GLY	2.2
8	H	139	LEU	2.2
50	YA	70	ALA	2.2
36	KA	95	GLN	2.2
39	SC	88	LYS	2.2
53	BB	55	LYS	2.2
1	FB	984	C	2.2
2	GB	2347	C	2.2
3	C	28	C	2.2
18	WB	90	VAL	2.2
2	GB	101	G	2.2
2	GB	1488	G	2.2
13	M	80	TYR	2.2
15	TB	14	SER	2.2
26	EC	8	LYS	2.2
36	PC	147	LYS	2.2
38	MA	115	ARG	2.2
48	BD	4	LYS	2.2
36	KA	42	ILE	2.2
2	GB	1537	C	2.2
2	GB	2145	C	2.2
8	MB	61	ALA	2.2
16	UB	4	LEU	2.2
46	UA	111	LYS	2.2
54	CB	105	SER	2.2
1	A	988	G	2.2
1	FB	538	G	2.2
13	M	72	PRO	2.2
23	BC	130	PRO	2.2
40	TC	97	PHE	2.2
50	YA	80	PHE	2.2
50	DD	15	PRO	2.2
18	WB	88	ILE	2.2
36	PC	219	VAL	2.2
2	GB	1528	A	2.2
43	WC	30	GLY	2.2
26	EC	60	LEU	2.1
36	KA	78	GLN	2.1
38	RC	71	SER	2.1
52	AB	81	PHE	2.1
9	NB	104	GLU	2.1
9	NB	169	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
23	W	97	GLU	2.1
44	XC	74	ILE	2.1
2	B	2112	G	2.1
2	GB	2382	G	2.1
1	FB	1451	A	2.1
2	GB	1045	A	2.1
36	KA	213	LEU	2.1
43	WC	27	THR	2.1
53	BB	77	THR	2.1
54	HD	104	LEU	2.1
16	P	52	SER	2.1
38	MA	119	GLN	2.1
9	NB	8	PRO	2.1
10	OB	134	PRO	2.1
28	GC	50	VAL	2.1
43	WC	12	GLU	2.1
48	BD	9	LYS	2.1
23	W	28	MET	2.1
28	BA	17	GLY	2.1
41	PA	82	GLY	2.1
53	BB	16	LEU	2.1
13	RB	127	ALA	2.1
22	AC	84	ARG	2.1
30	DA	38	LYS	2.1
47	AD	11	ARG	2.1
13	M	83	VAL	2.1
28	BA	35	VAL	2.1
5	JB	256	GLY	2.1
15	TB	39	PRO	2.1
1	FB	1321	C	2.1
1	FB	1327	C	2.1
35	OC	299	GLY	2.1
37	QC	196	LEU	2.1
52	FD	51	LEU	2.1
35	OC	320	HIS	2.1
38	MA	122	ARG	2.1
47	AD	99	ARG	2.1
6	F	77	ILE	2.1
2	GB	1444(B)	A	2.1
5	JB	100	GLY	2.1
9	NB	112	PRO	2.1
36	KA	18	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
36	PC	213	LEU	2.1
5	E	262	ARG	2.1
8	MB	37	VAL	2.1
23	W	74	VAL	2.1
10	OB	34	GLY	2.1
36	KA	90	MET	2.1
42	QA	130	GLY	2.1
35	JA	304	SER	2.1
2	B	2176	A	2.1
4	IB	57	A	2.1
1	A	1029	G	2.1
1	A	1094	G	2.1
1	FB	988	G	2.1
1	FB	1094	G	2.1
2	B	407	G	2.1
2	GB	2112	G	2.1
30	IC	51	GLU	2.1
36	KA	15	VAL	2.1
7	LB	33	LEU	2.1
44	XC	66	ARG	2.1
54	CB	14	LYS	2.1
42	QA	31	PHE	2.1
1	A	1049	U	2.1
2	B	1237	A	2.1
2	B	2171	A	2.1
16	UB	28	VAL	2.1
1	A	174	C	2.1
1	A	224	C	2.1
2	GB	327	G	2.1
18	WB	60	LEU	2.1
22	AC	88	LYS	2.1
41	UC	32	ARG	2.1
48	BD	15	LYS	2.1
36	KA	122	PHE	2.1
44	SA	11	PHE	2.1
21	U	34	ALA	2.1
38	MA	24	GLU	2.1
10	OB	138	ILE	2.1
15	TB	9	LYS	2.1
21	ZB	8	ILE	2.1
26	EC	25	VAL	2.1
35	JA	148	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
54	CB	22	ARG	2.1
2	GB	270(Z)	G	2.1
2	GB	1238	G	2.1
22	V	36	ALA	2.1
13	M	114	ILE	2.1
22	AC	50	ARG	2.1
33	LC	3	VAL	2.1
13	RB	138	LEU	2.1
30	IC	10	LEU	2.1
6	KB	1	MET	2.1
1	A	843	U	2.1
1	A	393	A	2.1
23	W	99	TYR	2.1
35	JA	153	GLU	2.1
1	FB	1325	C	2.1
2	GB	1072	C	2.1
33	GA	17	ILE	2.1
16	UB	88	ASP	2.1
28	BA	54	GLY	2.1
28	GC	45	GLY	2.1
33	LC	12	ASP	2.1
47	VA	56	LEU	2.1
39	SC	20	GLN	2.1
41	UC	26	PHE	2.1
50	YA	76	GLN	2.1
30	DA	23	THR	2.1
35	OC	238	ASN	2.1
40	TC	100	ASN	2.1
50	YA	72	ARG	2.1
54	HD	21	LYS	2.1
6	F	151	TYR	2.1
36	KA	197	VAL	2.1
41	UC	7	ALA	2.1
47	VA	17	VAL	2.1
15	TB	4	LEU	2.1
23	BC	144	LEU	2.1
36	PC	149	LEU	2.1
2	GB	1468	C	2.1
2	GB	1546(B)	C	2.1
52	FD	87	ARG	2.0
1	FB	1124	G	2.0
2	GB	281	G	2.0

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Mol	Chain	Res	Type	RSRZ
2	GB	326	G	2.0
19	XB	12	TYR	2.0
45	TA	117	ASN	2.0
23	W	171	ILE	2.0
28	BA	45	GLY	2.0
30	DA	36	LEU	2.0
50	YA	66	PRO	2.0
41	PA	81	GLY	2.0
47	AD	100	GLY	2.0
24	CC	74	ARG	2.0
18	WB	68	ALA	2.0
21	ZB	5	TYR	2.0
35	OC	243	ALA	2.0
36	PC	207	ALA	2.0
38	MA	31	CYS	2.0
13	M	112	LEU	2.0
36	KA	75	LYS	2.0
9	NB	51	ARG	2.0
17	Q	3	ARG	2.0
30	IC	37	ARG	2.0
23	W	73	GLN	2.0
49	XA	49	ASP	2.0
54	HD	90	GLN	2.0
1	FB	728	A	2.0
1	FB	974	A	2.0
2	GB	2114	A	2.0
23	BC	8	TYR	2.0
1	A	754	C	2.0
2	B	1052	C	2.0
18	WB	83	LEU	2.0
23	BC	113	ALA	2.0
38	MA	23	GLY	2.0
52	AB	56	THR	2.0
2	GB	271(A)	U	2.0
1	FB	198	G	2.0
9	NB	101	ARG	2.0
23	BC	76	LEU	2.0
51	ED	74	LEU	2.0
54	HD	76	ALA	2.0
37	QC	190	ARG	2.0
49	CD	54	ARG	2.0
1	FB	221	C	2.0

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Mol	Chain	Res	Type	RSRZ
28	GC	7	PRO	2.0
54	HD	98	PRO	2.0
32	KC	35	GLN	2.0
36	KA	240	GLN	2.0
23	BC	85	HIS	2.0
28	BA	25	TYR	2.0
36	KA	97	TRP	2.0
40	TC	72	VAL	2.0
46	UA	115	LYS	2.0
46	ZC	115	LYS	2.0
52	FD	88	LYS	2.0
8	H	158	ALA	2.0
36	KA	221	LEU	2.0
1	FB	1031	G	2.0
49	CD	2	PRO	2.0
1	A	1151	A	2.0
2	B	1762	A	2.0
2	B	2810	A	2.0
1	A	1282	C	2.0
2	B	1499	C	2.0
18	WB	75	ASN	2.0
18	R	117	GLN	2.0
11	PB	115	ARG	2.0
35	JA	201	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	2MU	GB	2552	21/23	0.96	0.21	-	56,57,58,58	0
1	5MC	FB	1407	21/22	0.96	0.21	-	69,70,71,71	0
2	5MU	GB	1915	21/22	0.96	0.12	-	88,89,91,92	0
1	5MC	A	967	21/22	0.96	0.20	-	90,91,93,93	0
1	M2G	A	966	25/26	0.95	0.25	-	88,90,91,92	0
4	5MC	IA	32	21/22	0.94	0.18	-	84,84,85,85	0
2	2MU	B	2552	21/23	0.98	0.25	-	45,46,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
46	0TD	ZC	92	10/11	0.93	0.46	-	77,78,78,78	0
4	4SU	D	8	20/21	0.66	0.37	-	163,164,165,165	0
2	5MU	B	1915	21/22	0.93	0.16	-	75,77,79,79	0
4	PSU	D	55	20/21	0.81	0.41	-	168,169,171,171	0
4	5MU	IA	54	21/22	0.96	0.27	-	86,88,90,90	0
34	PSU	HA	19	20/21	0.89	0.22	-	87,87,88,88	0
2	4OC	B	1920	21/23	0.95	0.23	-	61,63,64,65	0
1	2MG	A	1207	24/25	0.91	0.17	-	107,110,114,115	0
2	4OC	GB	1920	21/23	0.95	0.23	-	70,72,73,74	0
2	PSU	GB	1917	20/21	0.95	0.17	-	77,79,81,82	0
4	5MC	IB	32	21/22	0.86	0.22	-	147,147,148,148	0
1	MA6	FB	1519	24/25	0.96	0.22	-	63,65,66,66	0
4	5MU	IB	54	21/22	0.85	0.50	-	180,181,182,183	0
1	5MC	FB	1400	21/22	0.97	0.19	-	78,80,82,83	0
1	MA6	FB	1518	24/25	0.97	0.21	-	63,64,66,66	0
2	2MA	GB	2503	23/24	0.93	0.28	-	51,52,53,53	0
2	5MC	B	1942	21/22	0.96	0.19	-	49,50,51,51	0
4	5MC	D	32	21/22	0.91	0.17	-	139,139,139,139	0
1	5MC	FB	967	21/22	0.93	0.27	-	88,89,91,92	0
2	PSU	B	1911	20/21	0.95	0.22	-	63,65,67,67	0
2	5MU	GB	1939	21/22	0.97	0.29	-	53,54,54,55	0
2	PSU	B	1917	20/21	0.96	0.18	-	64,66,68,69	0
4	4SU	IA	8	20/21	0.93	0.17	-	84,86,86,87	0
4	PSU	IA	55	20/21	0.91	0.19	-	87,88,90,90	0
2	OMG	GB	2251	24/25	0.96	0.22	-	57,58,60,60	0
2	PSU	B	2605	20/21	0.97	0.22	-	41,42,43,43	0
4	5MU	NC	54	21/22	0.92	0.27	-	97,98,100,100	0
46	0TD	UA	92	10/11	0.88	0.41	-	81,81,81,81	0
2	5MU	B	1939	21/22	0.96	0.32	-	44,45,46,46	0
4	PSU	NC	55	20/21	0.93	0.18	-	97,98,99,99	0
1	2MG	FB	1207	24/25	0.91	0.19	-	108,110,113,114	0
4	5MU	D	54	21/22	0.89	0.38	-	167,167,169,169	0
1	UR3	A	1498	21/22	0.97	0.21	-	67,68,69,69	0
1	PSU	FB	516	20/21	0.90	0.20	-	83,84,87,87	0
1	7MG	A	527	24/25	0.93	0.24	-	79,81,83,84	0
4	5MC	NC	32	21/22	0.94	0.20	-	85,86,86,86	0
1	7MG	FB	527	24/25	0.93	0.21	-	74,75,76,77	0
2	5MC	B	1962	21/22	0.97	0.20	-	50,52,53,54	0
1	MA6	A	1519	24/25	0.97	0.26	-	60,63,64,64	0
4	PSU	IB	55	20/21	0.65	0.56	-	182,183,184,184	0
1	PSU	A	516	20/21	0.91	0.20	-	90,92,95,95	0
1	5MC	A	1400	21/22	0.94	0.20	-	80,82,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	M2G	FB	966	25/26	0.94	0.26	-	86,88,90,91	0
2	2MA	B	2503	23/24	0.97	0.27	-	37,38,38,38	0
1	4OC	FB	1402	22/23	0.95	0.21	-	73,74,75,75	0
4	4SU	IB	8	20/21	0.69	0.33	-	169,170,170,170	0
2	OMG	B	2251	24/25	0.96	0.24	-	44,44,45,45	0
34	PSU	MC	19	20/21	0.93	0.16	-	91,91,91,91	0
1	5MC	FB	1404	21/22	0.96	0.25	-	65,66,66,66	0
2	5MC	GB	1962	21/22	0.95	0.20	-	58,59,60,61	0
2	5MC	GB	1942	21/22	0.95	0.18	-	59,60,61,62	0
4	4SU	NC	8	20/21	0.96	0.12	-	89,91,92,92	0
2	PSU	GB	1911	20/21	0.95	0.21	-	72,75,76,77	0
1	UR3	FB	1498	21/22	0.96	0.27	-	70,70,71,71	0
1	5MC	A	1404	21/22	0.94	0.22	-	64,66,67,67	0
2	PSU	GB	2605	20/21	0.96	0.20	-	51,52,52,53	0
1	MA6	A	1518	24/25	0.97	0.26	-	59,62,63,63	0
1	4OC	A	1402	22/23	0.91	0.26	-	72,73,75,75	0
1	5MC	A	1407	21/22	0.93	0.22	-	64,65,67,68	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1869	1/1	0.94	1.02	64.98	79,79,79,79	0
56	MG	GB	3304	1/1	0.96	0.90	62.46	58,58,58,58	0
56	MG	FB	1603	1/1	0.87	0.87	56.39	60,60,60,60	0
56	MG	B	3631	1/1	0.98	0.60	47.31	50,50,50,50	0
56	MG	B	3499	1/1	0.57	0.82	46.50	48,48,48,48	0
56	MG	FB	1787	1/1	0.80	1.62	40.07	77,77,77,77	0
56	MG	B	3270	1/1	0.95	0.85	39.93	56,56,56,56	0
56	MG	GB	2963	1/1	0.84	1.11	37.14	59,59,59,59	0
56	MG	GB	2902	1/1	0.91	0.83	36.57	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3822	1/1	0.82	0.65	33.68	44,44,44,44	0
56	MG	F	313	1/1	0.94	0.93	32.81	49,49,49,49	0
56	MG	GB	3604	1/1	0.82	0.66	32.70	64,64,64,64	0
56	MG	B	3519	1/1	0.89	1.07	30.98	50,50,50,50	0
56	MG	B	2921	1/1	0.96	0.75	29.92	42,42,42,42	0
56	MG	B	3775	1/1	0.92	0.39	29.58	42,42,42,42	0
56	MG	B	3694	1/1	0.95	1.12	29.31	54,54,54,54	0
56	MG	GB	3052	1/1	0.87	0.74	28.48	55,55,55,55	0
56	MG	FB	1755	1/1	0.65	0.64	27.60	70,70,70,70	0
56	MG	B	2920	1/1	0.91	0.43	27.23	44,44,44,44	0
56	MG	GB	2909	1/1	0.97	0.64	26.65	38,38,38,38	0
56	MG	GB	3503	1/1	0.97	0.55	26.10	52,52,52,52	0
56	MG	A	1743	1/1	0.73	1.02	25.86	80,80,80,80	0
56	MG	GB	2918	1/1	0.74	0.58	25.49	56,56,56,56	0
56	MG	GB	3626	1/1	0.70	1.14	24.61	81,81,81,81	0
56	MG	B	2931	1/1	0.90	0.67	24.51	39,39,39,39	0
56	MG	GB	2989	1/1	0.95	0.81	24.41	59,59,59,59	0
56	MG	A	1610	1/1	0.80	0.85	23.56	78,78,78,78	0
56	MG	GB	3678	1/1	0.93	0.67	23.49	87,87,87,87	0
56	MG	B	2924	1/1	0.96	0.42	21.50	35,35,35,35	0
56	MG	SA	203	1/1	0.82	1.04	21.49	109,109,109,109	0
56	MG	B	2990	1/1	0.94	0.47	21.07	41,41,41,41	0
56	MG	B	2980	1/1	0.96	0.49	20.89	54,54,54,54	0
56	MG	B	3815	1/1	0.76	0.74	20.65	61,61,61,61	0
56	MG	GB	2934	1/1	0.91	0.48	20.64	60,60,60,60	0
56	MG	FB	1750	1/1	0.84	0.61	20.61	70,70,70,70	0
56	MG	B	3324	1/1	0.95	0.50	20.10	44,44,44,44	0
56	MG	GB	2954	1/1	0.94	0.57	19.87	50,50,50,50	0
56	MG	B	3814	1/1	0.94	0.41	19.80	38,38,38,38	0
56	MG	FB	1949	1/1	0.93	0.67	19.54	82,82,82,82	0
56	MG	B	3410	1/1	0.95	0.66	19.26	49,49,49,49	0
56	MG	GB	2976	1/1	0.89	0.48	19.10	52,52,52,52	0
56	MG	B	2923	1/1	0.95	0.39	18.57	40,40,40,40	0
56	MG	B	3092	1/1	0.93	0.31	18.13	44,44,44,44	0
56	MG	GB	2933	1/1	0.84	0.72	18.01	63,63,63,63	0
56	MG	B	3810	1/1	0.88	0.41	17.66	59,59,59,59	0
56	MG	GB	3242	1/1	0.85	0.59	17.62	65,65,65,65	0
56	MG	GB	3090	1/1	0.89	0.53	17.60	67,67,67,67	0
56	MG	A	1662	1/1	0.96	0.64	17.44	95,95,95,95	0
56	MG	B	3027	1/1	0.88	0.59	17.44	42,42,42,42	0
56	MG	B	3603	1/1	0.96	0.54	17.35	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1727	1/1	0.54	0.70	17.10	92,92,92,92	0
56	MG	GB	2922	1/1	0.79	0.55	17.02	63,63,63,63	0
56	MG	GB	2911	1/1	0.94	0.66	16.92	45,45,45,45	0
56	MG	B	3666	1/1	0.92	0.71	16.68	41,41,41,41	0
56	MG	GB	3039	1/1	0.86	0.53	16.60	52,52,52,52	0
56	MG	B	2927	1/1	0.97	0.42	16.56	50,50,50,50	0
56	MG	GB	3600	1/1	0.92	0.56	16.50	52,52,52,52	0
56	MG	B	3473	1/1	0.91	0.53	16.37	51,51,51,51	0
56	MG	GB	3368	1/1	0.92	0.68	16.35	70,70,70,70	0
56	MG	GB	2974	1/1	0.86	0.51	16.35	49,49,49,49	0
56	MG	B	3197	1/1	0.93	0.42	16.28	53,53,53,53	0
56	MG	GB	3362	1/1	0.77	0.41	16.20	76,76,76,76	0
56	MG	A	1643	1/1	0.72	0.49	16.05	70,70,70,70	0
56	MG	B	3001	1/1	0.88	0.45	16.04	37,37,37,37	0
56	MG	LB	303	1/1	0.97	0.66	15.84	53,53,53,53	0
56	MG	A	1604	1/1	0.94	0.45	15.84	73,73,73,73	0
56	MG	B	3526	1/1	0.97	0.63	15.83	49,49,49,49	0
56	MG	GB	3686	1/1	0.93	0.50	15.71	65,65,65,65	0
56	MG	GB	2904	1/1	0.95	0.61	15.60	57,57,57,57	0
56	MG	F	308	1/1	0.84	1.57	15.21	58,58,58,58	0
56	MG	FB	1937	1/1	0.98	0.93	14.93	65,65,65,65	0
56	MG	GB	3491	1/1	0.88	0.48	14.73	55,55,55,55	0
56	MG	B	2999	1/1	0.94	0.51	14.43	35,35,35,35	0
56	MG	GB	3141	1/1	0.91	0.38	14.41	49,49,49,49	0
56	MG	B	3226	1/1	0.85	0.39	14.41	64,64,64,64	0
56	MG	FB	1607	1/1	0.94	0.37	14.38	58,58,58,58	0
56	MG	GB	3177	1/1	0.91	0.72	14.37	58,58,58,58	0
56	MG	GB	3049	1/1	0.97	0.50	14.01	61,61,61,61	0
56	MG	GB	3069	1/1	0.86	0.51	13.83	59,59,59,59	0
56	MG	FB	1642	1/1	0.88	0.64	13.63	104,104,104,104	0
56	MG	FB	1627	1/1	0.90	0.43	13.57	75,75,75,75	0
56	MG	B	2979	1/1	0.93	0.29	13.37	43,43,43,43	0
56	MG	GB	3011	1/1	0.83	0.53	13.22	54,54,54,54	0
56	MG	B	3416	1/1	0.90	0.40	13.14	37,37,37,37	0
56	MG	A	1606	1/1	0.90	0.56	13.09	95,95,95,95	0
56	MG	B	2970	1/1	0.97	0.60	13.07	36,36,36,36	0
56	MG	GB	3601	1/1	0.73	0.86	12.81	58,58,58,58	0
56	MG	GB	3349	1/1	0.87	0.52	12.78	51,51,51,51	0
56	MG	B	2993	1/1	0.94	0.43	12.78	47,47,47,47	0
56	MG	R	202	1/1	0.78	0.82	12.75	49,49,49,49	0
56	MG	B	3144	1/1	0.97	0.48	12.66	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3031	1/1	0.94	0.36	12.60	54,54,54,54	0
56	MG	B	3070	1/1	0.81	0.48	12.42	47,47,47,47	0
56	MG	FB	1845	1/1	0.98	0.84	12.19	74,74,74,74	0
56	MG	B	3025	1/1	0.94	0.31	12.09	47,47,47,47	0
56	MG	B	3278	1/1	0.92	0.32	12.08	54,54,54,54	0
56	MG	FB	1681	1/1	0.85	0.51	11.94	99,99,99,99	0
56	MG	B	2991	1/1	0.74	0.29	11.88	56,56,56,56	0
56	MG	B	2953	1/1	0.92	0.39	11.84	37,37,37,37	0
56	MG	FB	1601	1/1	0.86	0.34	11.82	88,88,88,88	0
56	MG	B	3229	1/1	0.94	0.54	11.73	45,45,45,45	0
56	MG	FB	1740	1/1	0.88	0.38	11.71	96,96,96,96	0
56	MG	FB	1697	1/1	0.94	0.50	11.55	94,94,94,94	0
56	MG	B	2904	1/1	0.97	0.40	11.52	46,46,46,46	0
56	MG	B	2961	1/1	0.88	0.38	11.49	38,38,38,38	0
56	MG	GB	3021	1/1	0.84	0.59	11.49	56,56,56,56	0
56	MG	FB	1690	1/1	0.59	0.44	11.46	69,69,69,69	0
56	MG	GB	2917	1/1	0.90	0.56	11.44	46,46,46,46	0
56	MG	A	1786	1/1	0.92	0.72	11.26	59,59,59,59	0
56	MG	GB	3650	1/1	0.82	0.38	11.10	57,57,57,57	0
56	MG	B	2911	1/1	0.93	0.33	11.06	48,48,48,48	0
56	MG	F	305	1/1	0.91	0.68	11.04	58,58,58,58	0
56	MG	GB	3016	1/1	0.87	0.49	11.01	76,76,76,76	0
56	MG	FB	1713	1/1	0.91	0.43	11.00	75,75,75,75	0
56	MG	B	3039	1/1	0.75	0.47	10.85	50,50,50,50	0
56	MG	GB	3015	1/1	0.93	0.36	10.66	54,54,54,54	0
56	MG	K	204	1/1	0.95	0.71	10.57	65,65,65,65	0
56	MG	GB	3500	1/1	0.91	0.62	10.33	57,57,57,57	0
56	MG	GB	3000	1/1	0.91	0.38	10.22	67,67,67,67	0
56	MG	GB	3098	1/1	0.77	0.35	10.19	68,68,68,68	0
56	MG	X	105	1/1	0.80	0.81	10.13	55,55,55,55	0
56	MG	B	2988	1/1	0.95	0.41	10.13	38,38,38,38	0
56	MG	A	1676	1/1	0.95	0.59	10.05	80,80,80,80	0
56	MG	GB	3228	1/1	0.78	0.46	9.96	62,62,62,62	0
56	MG	GB	2907	1/1	0.91	0.35	9.85	60,60,60,60	0
56	MG	B	3833	1/1	0.98	0.56	9.81	48,48,48,48	0
56	MG	B	3134	1/1	0.71	0.38	9.77	56,56,56,56	0
56	MG	B	2914	1/1	0.96	0.28	9.74	47,47,47,47	0
56	MG	B	2912	1/1	0.80	0.38	9.65	59,59,59,59	0
56	MG	FB	1657	1/1	0.92	0.45	9.65	62,62,62,62	0
56	MG	B	2937	1/1	0.94	0.31	9.57	50,50,50,50	0
56	MG	B	3206	1/1	0.90	0.39	9.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3071	1/1	0.93	0.36	9.28	56,56,56,56	0
56	MG	B	2928	1/1	0.95	0.35	9.24	39,39,39,39	0
56	MG	B	3301	1/1	0.82	0.40	9.23	49,49,49,49	0
56	MG	A	1709	1/1	0.85	0.50	9.23	83,83,83,83	0
56	MG	A	1656	1/1	0.73	0.79	9.12	100,100,100,100	0
56	MG	GB	3103	1/1	0.91	0.42	9.11	70,70,70,70	0
56	MG	A	1613	1/1	0.51	0.45	9.09	79,79,79,79	0
56	MG	B	3339	1/1	0.82	0.29	9.06	60,60,60,60	0
56	MG	B	2992	1/1	0.78	0.41	9.06	38,38,38,38	0
56	MG	FB	1620	1/1	0.80	0.34	8.97	67,67,67,67	0
56	MG	GB	2935	1/1	0.82	0.43	8.95	50,50,50,50	0
56	MG	GB	3297	1/1	0.88	0.32	8.89	67,67,67,67	0
56	MG	B	2916	1/1	0.98	0.44	8.87	36,36,36,36	0
56	MG	FB	1738	1/1	0.92	0.42	8.83	69,69,69,69	0
56	MG	GB	2906	1/1	0.97	0.54	8.82	53,53,53,53	0
56	MG	GB	3149	1/1	0.89	0.46	8.81	58,58,58,58	0
56	MG	B	3334	1/1	0.79	0.34	8.76	46,46,46,46	0
56	MG	GB	2948	1/1	0.97	0.34	8.65	51,51,51,51	0
56	MG	B	3255	1/1	0.90	0.41	8.59	48,48,48,48	0
56	MG	CB	201	1/1	0.90	1.37	8.54	94,94,94,94	0
56	MG	GB	3108	1/1	0.91	0.37	8.51	54,54,54,54	0
56	MG	L	201	1/1	0.84	0.72	8.25	54,54,54,54	0
56	MG	B	2930	1/1	0.94	0.42	8.24	34,34,34,34	0
56	MG	B	3208	1/1	0.98	0.29	8.18	47,47,47,47	0
56	MG	GB	2982	1/1	0.86	0.31	8.18	67,67,67,67	0
56	MG	GB	3051	1/1	0.93	0.34	8.17	67,67,67,67	0
56	MG	B	3430	1/1	0.91	0.28	8.16	46,46,46,46	0
56	MG	A	1637	1/1	0.85	0.35	8.16	67,67,67,67	0
56	MG	B	3841	1/1	0.90	1.27	8.11	73,73,73,73	0
56	MG	GB	2956	1/1	0.90	0.42	8.10	47,47,47,47	0
56	MG	GB	2969	1/1	0.93	0.27	7.98	53,53,53,53	0
56	MG	A	1603	1/1	0.91	0.50	7.97	78,78,78,78	0
56	MG	B	2951	1/1	0.97	0.47	7.96	43,43,43,43	0
56	MG	FB	1827	1/1	0.79	0.39	7.95	71,71,71,71	0
56	MG	FB	1834	1/1	0.80	0.34	7.88	68,68,68,68	0
56	MG	GB	3660	1/1	0.95	0.61	7.87	46,46,46,46	0
56	MG	B	3507	1/1	0.93	0.28	7.86	42,42,42,42	0
56	MG	B	2950	1/1	0.83	0.35	7.80	62,62,62,62	0
56	MG	B	3757	1/1	0.83	0.36	7.73	53,53,53,53	0
56	MG	FB	1623	1/1	0.95	0.29	7.65	53,53,53,53	0
56	MG	B	2922	1/1	0.95	0.35	7.52	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	C	206	1/1	0.94	0.28	7.50	54,54,54,54	0
56	MG	B	3635	1/1	0.92	0.64	7.50	56,56,56,56	0
56	MG	B	2996	1/1	0.98	0.32	7.47	38,38,38,38	0
56	MG	WA	101	1/1	0.57	0.65	7.40	109,109,109,109	0
56	MG	B	3523	1/1	0.82	0.37	7.39	54,54,54,54	0
56	MG	GB	3710	1/1	0.98	0.39	7.31	61,61,61,61	0
56	MG	B	3816	1/1	0.94	0.62	7.26	60,60,60,60	0
56	MG	GB	3305	1/1	0.99	0.42	7.25	49,49,49,49	0
56	MG	GB	3234	1/1	0.94	0.40	7.12	57,57,57,57	0
56	MG	GB	3268	1/1	0.97	0.47	7.10	42,42,42,42	0
56	MG	GB	3043	1/1	0.91	0.24	7.10	52,52,52,52	0
56	MG	FB	1765	1/1	0.85	0.44	7.08	77,77,77,77	0
56	MG	B	3100	1/1	0.94	0.29	7.06	46,46,46,46	0
56	MG	G	3202	1/1	0.97	0.52	7.02	34,34,34,34	0
56	MG	GB	3056	1/1	0.79	0.47	7.00	57,57,57,57	0
56	MG	VB	207	1/1	0.88	0.61	6.98	83,83,83,83	0
56	MG	GB	3169	1/1	0.60	0.38	6.95	54,54,54,54	0
56	MG	RC	306	1/1	0.92	0.39	6.94	81,81,81,81	0
56	MG	GB	3489	1/1	0.65	0.26	6.91	65,65,65,65	0
56	MG	FB	1790	1/1	0.77	0.48	6.90	63,63,63,63	0
56	MG	B	3047	1/1	0.94	0.31	6.87	42,42,42,42	0
56	MG	FB	1614	1/1	0.92	0.31	6.82	70,70,70,70	0
56	MG	GB	3061	1/1	0.80	0.29	6.70	62,62,62,62	0
56	MG	GB	3512	1/1	0.93	0.35	6.61	67,67,67,67	0
56	MG	GB	3064	1/1	0.67	0.31	6.53	72,72,72,72	0
56	MG	FB	1847	1/1	0.90	0.83	6.53	67,67,67,67	0
56	MG	O	202	1/1	0.82	0.45	6.51	70,70,70,70	0
56	MG	GB	3009	1/1	0.86	0.28	6.48	62,62,62,62	0
56	MG	GB	3711	1/1	0.93	0.77	6.45	77,77,77,77	0
56	MG	B	3161	1/1	0.95	0.32	6.41	38,38,38,38	0
56	MG	B	3322	1/1	0.85	0.30	6.38	46,46,46,46	0
56	MG	B	3344	1/1	0.91	0.29	6.33	49,49,49,49	0
56	MG	GB	3128	1/1	0.95	0.55	6.30	58,58,58,58	0
56	MG	FB	1680	1/1	0.94	0.50	6.28	87,87,87,87	0
56	MG	B	3084	1/1	0.96	0.35	6.27	42,42,42,42	0
56	MG	B	3019	1/1	0.87	0.33	6.18	51,51,51,51	0
56	MG	HD	201	1/1	0.97	0.78	6.13	79,79,79,79	0
56	MG	B	3829	1/1	0.92	0.24	6.10	46,46,46,46	0
56	MG	GB	3309	1/1	0.88	0.40	6.10	57,57,57,57	0
56	MG	F	304	1/1	0.92	0.36	6.09	49,49,49,49	0
56	MG	GB	3697	1/1	0.97	0.46	6.08	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3105	1/1	0.88	0.32	6.08	73,73,73,73	0
56	MG	SC	201	1/1	0.87	0.55	6.06	70,70,70,70	0
56	MG	B	3346	1/1	0.91	0.55	6.05	45,45,45,45	0
56	MG	B	2909	1/1	0.92	0.33	5.97	33,33,33,33	0
56	MG	GB	3224	1/1	0.94	0.29	5.90	61,61,61,61	0
56	MG	B	3062	1/1	0.87	0.28	5.85	40,40,40,40	0
56	MG	FB	1889	1/1	0.77	0.78	5.76	69,69,69,69	0
56	MG	B	3706	1/1	0.92	0.31	5.75	50,50,50,50	0
56	MG	M	207	1/1	0.95	0.93	5.74	51,51,51,51	0
56	MG	B	3236	1/1	0.97	0.34	5.73	44,44,44,44	0
56	MG	B	3075	1/1	0.95	0.40	5.71	42,42,42,42	0
56	MG	B	3046	1/1	0.95	0.31	5.71	34,34,34,34	0
56	MG	FB	1609	1/1	0.92	0.30	5.69	64,64,64,64	0
56	MG	GB	3275	1/1	0.92	0.75	5.64	61,61,61,61	0
56	MG	FB	1636	1/1	0.85	0.58	5.49	98,98,98,98	0
56	MG	B	3531	1/1	0.90	0.35	5.47	42,42,42,42	0
56	MG	M	203	1/1	0.92	0.34	5.25	43,43,43,43	0
56	MG	B	3556	1/1	0.99	0.34	5.19	45,45,45,45	0
56	MG	RB	206	1/1	0.96	0.45	5.15	59,59,59,59	0
56	MG	GB	3220	1/1	0.51	0.32	5.08	121,121,121,121	0
56	MG	B	2965	1/1	0.77	0.29	5.01	45,45,45,45	0
56	MG	B	2995	1/1	0.68	0.26	4.97	49,49,49,49	0
56	MG	B	3002	1/1	0.97	0.28	4.96	38,38,38,38	0
56	MG	FB	1707	1/1	0.93	0.28	4.94	69,69,69,69	0
56	MG	B	3345	1/1	0.89	0.93	4.94	72,72,72,72	0
56	MG	B	3784	1/1	0.98	0.41	4.93	44,44,44,44	0
56	MG	B	3544	1/1	0.82	0.22	4.91	85,85,85,85	0
56	MG	B	2964	1/1	0.75	0.22	4.89	55,55,55,55	0
56	MG	HB	202	1/1	0.72	0.26	4.85	79,79,79,79	0
56	MG	FB	1911	1/1	0.59	0.52	4.82	110,110,110,110	0
56	MG	GB	3384	1/1	0.94	0.57	4.81	63,63,63,63	0
56	MG	GB	3176	1/1	0.94	0.32	4.81	51,51,51,51	0
56	MG	C	233	1/1	0.58	0.20	4.80	84,84,84,84	0
56	MG	C	244	1/1	0.88	0.41	4.72	65,65,65,65	0
56	MG	GB	3707	1/1	0.96	0.41	4.71	42,42,42,42	0
56	MG	GB	3081	1/1	0.75	0.30	4.68	51,51,51,51	0
56	MG	B	3422	1/1	0.93	0.28	4.67	66,66,66,66	0
56	MG	A	1875	1/1	0.11	1.37	4.67	126,126,126,126	0
56	MG	FB	1927	1/1	0.94	0.31	4.61	69,69,69,69	0
56	MG	QB	205	1/1	0.90	0.52	4.60	68,68,68,68	0
56	MG	A	1620	1/1	0.90	0.27	4.59	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3352	1/1	0.82	0.26	4.58	67,67,67,67	0
56	MG	LA	301	1/1	0.86	0.66	4.53	109,109,109,109	0
56	MG	B	2929	1/1	0.94	0.29	4.48	47,47,47,47	0
56	MG	B	3445	1/1	0.38	0.24	4.40	116,116,116,116	0
56	MG	YB	206	1/1	0.91	0.22	4.38	70,70,70,70	0
56	MG	GB	3593	1/1	0.94	0.38	4.37	53,53,53,53	0
56	MG	B	3717	1/1	0.94	0.49	4.26	52,52,52,52	0
56	MG	GB	3643	1/1	0.90	0.29	4.23	55,55,55,55	0
56	MG	A	1814	1/1	0.78	0.30	4.21	92,92,92,92	0
56	MG	A	1809	1/1	0.79	0.49	4.21	97,97,97,97	0
56	MG	FB	1688	1/1	0.83	0.33	4.19	64,64,64,64	0
56	MG	Q	202	1/1	0.82	0.59	4.17	74,74,74,74	0
56	MG	B	3330	1/1	0.93	0.33	4.12	41,41,41,41	0
56	MG	GB	3540	1/1	0.90	0.30	4.11	115,115,115,115	0
56	MG	GB	3668	1/1	0.96	0.37	4.05	68,68,68,68	0
56	MG	GB	3074	1/1	0.92	0.27	4.02	59,59,59,59	0
56	MG	IA	102	1/1	0.83	0.22	3.97	81,81,81,81	0
56	MG	GB	3332	1/1	0.72	0.34	3.97	64,64,64,64	0
56	MG	JA	403	1/1	0.86	0.38	3.95	47,47,47,47	0
56	MG	B	3458	1/1	0.93	0.29	3.91	41,41,41,41	0
56	MG	AA	101	1/1	0.90	0.45	3.89	59,59,59,59	0
56	MG	B	3453	1/1	0.82	0.40	3.86	44,44,44,44	0
56	MG	MB	201	1/1	0.86	0.31	3.83	111,111,111,111	0
56	MG	B	3840	1/1	0.97	0.27	3.77	48,48,48,48	0
56	MG	AA	102	1/1	0.93	0.41	3.71	59,59,59,59	0
56	MG	A	1794	1/1	0.80	0.43	3.70	73,73,73,73	0
56	MG	N	201	1/1	0.94	0.34	3.70	51,51,51,51	0
56	MG	IA	116	1/1	0.82	0.20	3.69	84,84,84,84	0
56	MG	A	1601	1/1	0.91	0.25	3.68	56,56,56,56	0
56	MG	KB	301	1/1	0.76	0.37	3.68	62,62,62,62	0
56	MG	GB	2978	1/1	0.92	0.30	3.67	58,58,58,58	0
56	MG	XB	201	1/1	0.89	0.36	3.67	55,55,55,55	0
56	MG	GB	3673	1/1	0.97	0.33	3.66	50,50,50,50	0
56	MG	FB	1908	1/1	0.93	0.28	3.65	65,65,65,65	0
56	MG	G	3201	1/1	0.92	0.32	3.62	36,36,36,36	0
56	MG	GB	2983	1/1	0.88	0.31	3.61	69,69,69,69	0
56	MG	VB	205	1/1	0.88	0.49	3.59	70,70,70,70	0
56	MG	FB	1932	1/1	0.81	0.82	3.58	89,89,89,89	0
56	MG	RB	205	1/1	0.95	0.35	3.58	55,55,55,55	0
56	MG	TB	202	1/1	0.95	0.41	3.57	72,72,72,72	0
56	MG	FB	1800	1/1	0.87	0.39	3.53	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3108	1/1	0.94	0.27	3.53	35,35,35,35	0
56	MG	GB	2938	1/1	0.97	0.26	3.51	45,45,45,45	0
56	MG	GB	3695	1/1	0.86	0.39	3.46	75,75,75,75	0
56	MG	LB	302	1/1	0.85	0.31	3.43	61,61,61,61	0
56	MG	B	3029	1/1	0.97	0.26	3.40	41,41,41,41	0
56	MG	H	202	1/1	0.87	0.35	3.36	89,89,89,89	0
56	MG	GB	3645	1/1	0.86	0.27	3.36	71,71,71,71	0
56	MG	B	3040	1/1	0.92	0.35	3.31	41,41,41,41	0
56	MG	GB	3606	1/1	0.57	0.59	3.29	75,75,75,75	0
56	MG	B	3406	1/1	0.89	0.30	3.27	55,55,55,55	0
56	MG	B	3741	1/1	0.90	0.22	3.23	47,47,47,47	0
56	MG	B	3479	1/1	0.93	0.25	3.20	39,39,39,39	0
56	MG	GB	3313	1/1	0.88	0.30	3.19	56,56,56,56	0
56	MG	GB	3174	1/1	0.74	0.24	3.17	64,64,64,64	0
56	MG	FB	1731	1/1	0.82	0.29	3.09	70,70,70,70	0
56	MG	B	3262	1/1	0.84	0.24	3.05	45,45,45,45	0
56	MG	GB	3204	1/1	0.88	0.28	3.04	53,53,53,53	0
56	MG	GB	3435	1/1	0.87	0.35	3.00	53,53,53,53	0
56	MG	B	3579	1/1	0.91	0.30	2.98	47,47,47,47	0
56	MG	GB	3359	1/1	0.88	0.45	2.95	77,77,77,77	0
56	MG	A	1715	1/1	0.68	0.29	2.95	102,102,102,102	0
56	MG	GB	3194	1/1	0.79	0.32	2.92	62,62,62,62	0
56	MG	MA	301	1/1	0.73	0.42	2.91	97,97,97,97	0
56	MG	E	307	1/1	0.96	0.37	2.91	55,55,55,55	0
56	MG	FB	1608	1/1	0.96	0.29	2.89	72,72,72,72	0
56	MG	WB	202	1/1	0.93	0.78	2.89	80,80,80,80	0
56	MG	B	3043	1/1	0.95	0.24	2.89	54,54,54,54	0
56	MG	GB	3057	1/1	0.93	0.29	2.88	44,44,44,44	0
56	MG	KC	102	1/1	0.87	0.37	2.87	61,61,61,61	0
56	MG	B	3128	1/1	0.94	0.24	2.87	33,33,33,33	0
56	MG	GB	3455	1/1	0.91	0.32	2.85	64,64,64,64	0
56	MG	SB	203	1/1	0.81	0.37	2.85	73,73,73,73	0
56	MG	GB	3624	1/1	0.91	0.24	2.80	65,65,65,65	0
56	MG	HB	205	1/1	0.86	0.28	2.79	74,74,74,74	0
56	MG	B	3528	1/1	0.90	0.26	2.72	43,43,43,43	0
56	MG	FB	1878	1/1	0.51	0.49	2.70	75,75,75,75	0
56	MG	B	3779	1/1	0.97	0.23	2.69	58,58,58,58	0
56	MG	C	209	1/1	0.81	0.27	2.60	62,62,62,62	0
56	MG	GB	3222	1/1	0.70	0.35	2.60	60,60,60,60	0
56	MG	GB	3230	1/1	0.31	0.22	2.59	110,110,110,110	0
56	MG	FB	1746	1/1	0.84	0.29	2.47	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	I	202	1/1	0.86	0.21	2.46	70,70,70,70	0
56	MG	B	3567	1/1	0.58	0.30	2.44	106,106,106,106	0
56	MG	F	301	1/1	0.82	0.26	2.44	46,46,46,46	0
56	MG	YC	204	1/1	0.73	0.25	2.43	94,94,94,94	0
56	MG	FB	1722	1/1	0.75	0.35	2.42	101,101,101,101	0
56	MG	RC	311	1/1	0.96	0.29	2.32	78,78,78,78	0
56	MG	OC	404	1/1	0.72	0.34	2.32	97,97,97,97	0
56	MG	FA	103	1/1	0.92	0.35	2.29	48,48,48,48	0
56	MG	RA	202	1/1	0.59	0.49	2.26	117,117,117,117	0
56	MG	A	1645	1/1	0.92	0.26	2.26	75,75,75,75	0
56	MG	B	3013	1/1	0.98	0.25	2.24	50,50,50,50	0
56	MG	BC	306	1/1	0.56	0.39	2.23	108,108,108,108	0
56	MG	GB	3171	1/1	0.93	0.33	2.23	63,63,63,63	0
56	MG	B	2975	1/1	0.95	0.24	2.23	49,49,49,49	0
56	MG	GB	3203	1/1	0.94	0.27	2.21	60,60,60,60	0
56	MG	PB	203	1/1	0.92	0.45	2.21	91,91,91,91	0
56	MG	LB	305	1/1	0.94	0.27	2.14	55,55,55,55	0
56	MG	GB	3421	1/1	0.96	0.28	2.11	77,77,77,77	0
56	MG	GB	3047	1/1	0.87	0.24	2.08	59,59,59,59	0
56	MG	A	1886	1/1	0.85	0.37	2.07	78,78,78,78	0
56	MG	RC	303	1/1	0.95	0.32	2.06	75,75,75,75	0
56	MG	GB	3060	1/1	0.93	0.32	1.96	61,61,61,61	0
56	MG	B	3672	1/1	0.97	0.20	1.90	52,52,52,52	0
56	MG	FB	1710	1/1	0.89	0.25	1.88	67,67,67,67	0
56	MG	N	204	1/1	0.95	0.35	1.87	61,61,61,61	0
56	MG	FB	1920	1/1	0.81	0.22	1.87	70,70,70,70	0
57	ZN	CA	101	1/1	0.99	0.20	1.84	62,62,62,62	0
56	MG	F	314	1/1	0.97	0.28	1.77	39,39,39,39	0
56	MG	B	3444	1/1	0.89	0.22	1.77	52,52,52,52	0
56	MG	YC	201	1/1	0.85	0.53	1.74	68,68,68,68	0
56	MG	A	1677	1/1	0.82	0.29	1.73	105,105,105,105	0
56	MG	B	3249	1/1	0.95	0.27	1.73	43,43,43,43	0
56	MG	VC	201	1/1	0.97	0.34	1.73	77,77,77,77	0
56	MG	SB	201	1/1	0.86	0.30	1.72	77,77,77,77	0
56	MG	GB	3005	1/1	0.86	0.23	1.71	61,61,61,61	0
56	MG	A	1669	1/1	0.73	0.35	1.66	114,114,114,114	0
56	MG	B	3258	1/1	0.94	0.24	1.64	49,49,49,49	0
56	MG	B	3511	1/1	0.82	0.33	1.63	65,65,65,65	0
56	MG	A	1681	1/1	0.87	0.24	1.62	69,69,69,69	0
56	MG	FB	1907	1/1	0.57	0.32	1.59	115,115,115,115	0
56	MG	B	3760	1/1	0.92	0.35	1.58	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	M	208	1/1	0.91	0.27	1.57	44,44,44,44	0
56	MG	B	3719	1/1	0.87	0.21	1.57	79,79,79,79	0
56	MG	JB	312	1/1	0.89	0.27	1.56	62,62,62,62	0
56	MG	OA	201	1/1	0.96	0.26	1.53	72,72,72,72	0
56	MG	FB	1860	1/1	0.94	0.37	1.45	89,89,89,89	0
56	MG	B	3317	1/1	0.71	0.32	1.44	55,55,55,55	0
56	MG	GB	3062	1/1	0.90	0.24	1.44	61,61,61,61	0
56	MG	G	3208	1/1	0.87	0.39	1.42	58,58,58,58	0
56	MG	A	1630	1/1	0.85	0.21	1.38	88,88,88,88	0
56	MG	GB	3137	1/1	0.93	0.25	1.32	66,66,66,66	0
56	MG	E	309	1/1	0.97	0.26	1.29	53,53,53,53	0
56	MG	B	3041	1/1	0.87	0.22	1.28	39,39,39,39	0
56	MG	FB	1647	1/1	0.80	0.17	1.28	143,143,143,143	0
56	MG	GB	3070	1/1	0.93	0.27	1.27	63,63,63,63	0
56	MG	JA	406	1/1	0.77	0.23	1.26	87,87,87,87	0
56	MG	B	3352	1/1	0.90	0.29	1.26	53,53,53,53	0
56	MG	GB	3311	1/1	0.82	0.20	1.22	64,64,64,64	0
56	MG	B	3535	1/1	0.90	0.23	1.19	60,60,60,60	0
56	MG	B	3575	1/1	0.83	0.20	1.18	69,69,69,69	0
56	MG	GB	3031	1/1	0.79	0.27	1.18	60,60,60,60	0
56	MG	GB	3513	1/1	0.85	0.28	1.15	49,49,49,49	0
56	MG	A	1759	1/1	0.81	0.25	1.14	62,62,62,62	0
56	MG	QB	204	1/1	0.92	0.23	1.07	65,65,65,65	0
56	MG	B	2973	1/1	0.87	0.18	1.07	41,41,41,41	0
56	MG	GB	3398	1/1	0.90	0.35	1.06	63,63,63,63	0
56	MG	A	1687	1/1	0.87	0.19	1.06	84,84,84,84	0
56	MG	GB	3289	1/1	0.75	0.21	1.05	63,63,63,63	0
56	MG	G	3207	1/1	0.91	0.30	1.01	36,36,36,36	0
56	MG	B	3529	1/1	0.88	0.33	0.98	43,43,43,43	0
56	MG	B	3045	1/1	0.95	0.21	0.94	43,43,43,43	0
56	MG	FB	1897	1/1	0.88	0.22	0.91	67,67,67,67	0
56	MG	FB	1678	1/1	0.88	0.19	0.90	70,70,70,70	0
56	MG	GB	3506	1/1	0.93	0.36	0.88	71,71,71,71	0
56	MG	GB	2962	1/1	0.98	0.28	0.87	61,61,61,61	0
56	MG	GB	3670	1/1	0.93	0.23	0.87	52,52,52,52	0
56	MG	FB	1761	1/1	0.86	0.23	0.86	72,72,72,72	0
56	MG	B	3089	1/1	0.84	0.17	0.85	67,67,67,67	0
56	MG	GB	3050	1/1	0.78	0.20	0.85	70,70,70,70	0
56	MG	GB	3175	1/1	0.98	0.26	0.81	52,52,52,52	0
56	MG	B	3246	1/1	0.90	0.21	0.78	47,47,47,47	0
56	MG	B	3315	1/1	0.77	0.31	0.75	43,43,43,43	0
56	MG	GB	2997	1/1	0.97	0.24	0.75	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3192	1/1	0.86	0.22	0.74	49,49,49,49	0
56	MG	JB	302	1/1	0.91	0.29	0.73	63,63,63,63	0
56	MG	B	3329	1/1	0.96	0.21	0.69	47,47,47,47	0
56	MG	GB	3308	1/1	0.78	0.21	0.69	61,61,61,61	0
56	MG	GB	2926	1/1	0.87	0.23	0.69	69,69,69,69	0
56	MG	B	3632	1/1	0.92	0.33	0.63	64,64,64,64	0
56	MG	B	3141	1/1	0.96	0.22	0.57	44,44,44,44	0
56	MG	HB	221	1/1	0.65	0.31	0.55	114,114,114,114	0
56	MG	VC	202	1/1	0.87	0.27	0.54	75,75,75,75	0
56	MG	GB	3392	1/1	0.90	0.33	0.53	56,56,56,56	0
56	MG	B	3318	1/1	0.94	0.23	0.47	49,49,49,49	0
56	MG	GB	2947	1/1	0.77	0.33	0.45	109,109,109,109	0
56	MG	E	305	1/1	0.91	0.19	0.39	50,50,50,50	0
56	MG	GB	2923	1/1	0.82	0.28	0.38	62,62,62,62	0
56	MG	XC	202	1/1	0.85	0.32	0.35	113,113,113,113	0
56	MG	A	1887	1/1	0.82	0.24	0.35	87,87,87,87	0
56	MG	HB	223	1/1	0.92	0.28	0.33	85,85,85,85	0
56	MG	B	2938	1/1	0.97	0.21	0.33	55,55,55,55	0
56	MG	GB	3541	1/1	0.86	0.21	0.32	64,64,64,64	0
56	MG	SB	204	1/1	0.86	0.30	0.31	81,81,81,81	0
56	MG	GB	3546	1/1	0.78	0.23	0.28	63,63,63,63	0
56	MG	GB	2944	1/1	0.68	0.23	0.27	90,90,90,90	0
56	MG	GB	3075	1/1	0.95	0.20	0.25	65,65,65,65	0
56	MG	C	203	1/1	0.87	0.16	0.24	79,79,79,79	0
56	MG	ZA	203	1/1	0.90	0.23	0.22	91,91,91,91	0
56	MG	FB	1948	1/1	0.80	0.33	0.21	116,116,116,116	0
56	MG	ZA	201	1/1	0.76	0.22	0.20	85,85,85,85	0
56	MG	KB	304	1/1	0.86	0.26	0.20	82,82,82,82	0
56	MG	FB	1645	1/1	0.94	0.19	0.18	56,56,56,56	0
56	MG	B	3771	1/1	0.93	0.24	0.17	47,47,47,47	0
56	MG	FB	1748	1/1	0.73	0.20	0.17	116,116,116,116	0
56	MG	GB	3208	1/1	0.83	0.20	0.17	53,53,53,53	0
56	MG	KC	103	1/1	0.78	0.26	0.15	64,64,64,64	0
56	MG	FB	1616	1/1	0.48	0.15	0.15	87,87,87,87	0
56	MG	B	3060	1/1	0.70	0.21	0.14	53,53,53,53	0
56	MG	B	3724	1/1	0.91	0.19	0.08	48,48,48,48	0
56	MG	GB	3179	1/1	0.87	0.24	0.06	69,69,69,69	0
56	MG	GB	3712	1/1	0.93	0.29	0.06	66,66,66,66	0
56	MG	GB	3480	1/1	0.89	0.39	0.06	70,70,70,70	0
56	MG	B	3364	1/1	0.92	0.21	0.05	37,37,37,37	0
56	MG	B	3000	1/1	0.90	0.17	0.03	70,70,70,70	0
56	MG	G	3203	1/1	0.94	0.21	0.02	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	JB	301	1/1	0.94	0.26	0.01	45,45,45,45	0
56	MG	B	3641	1/1	0.96	0.18	-0.03	50,50,50,50	0
57	ZN	HC	101	1/1	0.95	0.18	-0.03	86,86,86,86	0
56	MG	ED	201	1/1	0.84	0.20	-0.03	83,83,83,83	0
56	MG	A	1631	1/1	0.92	0.26	-0.05	98,98,98,98	0
56	MG	YB	202	1/1	0.79	0.19	-0.08	71,71,71,71	0
56	MG	GB	3460	1/1	0.92	0.29	-0.10	63,63,63,63	0
56	MG	A	1654	1/1	0.94	0.18	-0.10	83,83,83,83	0
56	MG	GB	3231	1/1	0.90	0.17	-0.14	60,60,60,60	0
56	MG	B	3222	1/1	0.84	0.22	-0.15	50,50,50,50	0
56	MG	B	3831	1/1	0.96	0.22	-0.19	43,43,43,43	0
56	MG	GB	3354	1/1	0.90	0.30	-0.20	81,81,81,81	0
56	MG	X	108	1/1	0.90	0.34	-0.21	53,53,53,53	0
56	MG	HB	206	1/1	0.88	0.20	-0.23	118,118,118,118	0
56	MG	GB	3431	1/1	0.88	0.24	-0.26	76,76,76,76	0
56	MG	B	3021	1/1	0.98	0.21	-0.26	43,43,43,43	0
56	MG	GB	2931	1/1	0.98	0.22	-0.30	47,47,47,47	0
56	MG	B	3213	1/1	0.99	0.18	-0.33	48,48,48,48	0
56	MG	JA	402	1/1	0.90	0.20	-0.33	54,54,54,54	0
56	MG	B	3138	1/1	0.85	0.19	-0.35	63,63,63,63	0
56	MG	B	3428	1/1	0.96	0.18	-0.37	48,48,48,48	0
56	MG	RC	305	1/1	0.95	0.16	-0.38	75,75,75,75	0
56	MG	GB	2998	1/1	0.96	0.17	-0.40	55,55,55,55	0
56	MG	B	3725	1/1	0.82	0.18	-0.40	53,53,53,53	0
57	ZN	BA	101	1/1	0.90	0.31	-0.41	131,131,131,131	0
56	MG	B	3126	1/1	0.95	0.20	-0.43	43,43,43,43	0
56	MG	NC	112	1/1	0.59	0.32	-0.44	76,76,76,76	0
56	MG	TB	204	1/1	0.92	0.24	-0.45	73,73,73,73	0
56	MG	FB	1749	1/1	0.93	0.25	-0.47	111,111,111,111	0
56	MG	IA	114	1/1	0.56	0.29	-0.47	71,71,71,71	0
56	MG	JA	409	1/1	0.98	0.23	-0.48	89,89,89,89	0
56	MG	C	235	1/1	0.97	0.14	-0.51	73,73,73,73	0
56	MG	GB	3390	1/1	0.96	0.19	-0.57	47,47,47,47	0
56	MG	GB	3378	1/1	0.89	0.22	-0.57	74,74,74,74	0
56	MG	FB	1854	1/1	0.85	0.15	-0.58	86,86,86,86	0
56	MG	B	3061	1/1	0.94	0.19	-0.58	58,58,58,58	0
56	MG	B	3397	1/1	0.92	0.18	-0.60	52,52,52,52	0
56	MG	JA	405	1/1	0.90	0.32	-0.61	91,91,91,91	0
56	MG	RC	310	1/1	0.66	0.22	-0.63	83,83,83,83	0
56	MG	L	203	1/1	0.91	0.16	-0.65	71,71,71,71	0
56	MG	GB	3168	1/1	0.94	0.20	-0.67	61,61,61,61	0
56	MG	B	2932	1/1	0.99	0.20	-0.67	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3295	1/1	0.84	0.15	-0.67	65,65,65,65	0
56	MG	GB	3150	1/1	0.88	0.20	-0.68	46,46,46,46	0
56	MG	B	3216	1/1	0.95	0.17	-0.73	51,51,51,51	0
56	MG	B	3370	1/1	0.83	0.18	-0.74	64,64,64,64	0
56	MG	B	3272	1/1	0.92	0.23	-0.78	63,63,63,63	0
56	MG	GB	3644	1/1	0.94	0.17	-0.78	77,77,77,77	0
56	MG	GB	3496	1/1	0.96	0.17	-0.80	70,70,70,70	0
56	MG	C	216	1/1	0.85	0.18	-0.80	80,80,80,80	0
56	MG	FB	1929	1/1	0.61	0.17	-0.81	94,94,94,94	0
57	ZN	GC	101	1/1	0.88	0.22	-0.82	149,149,149,149	0
56	MG	B	3723	1/1	0.83	0.18	-0.82	67,67,67,67	0
56	MG	B	2919	1/1	0.78	0.19	-0.83	52,52,52,52	0
57	ZN	V	501	1/1	0.99	0.09	-0.87	72,72,72,72	0
56	MG	J	203	1/1	0.99	0.15	-0.87	80,80,80,80	0
56	MG	C	208	1/1	0.85	0.12	-0.88	81,81,81,81	0
56	MG	B	3068	1/1	0.92	0.17	-0.91	43,43,43,43	0
56	MG	FA	104	1/1	0.84	0.20	-0.93	49,49,49,49	0
56	MG	JB	307	1/1	0.75	0.15	-0.95	63,63,63,63	0
56	MG	B	3088	1/1	0.94	0.18	-0.98	50,50,50,50	0
56	MG	JA	413	1/1	0.86	0.20	-1.03	97,97,97,97	0
56	MG	FB	1747	1/1	0.96	0.16	-1.04	101,101,101,101	0
56	MG	GB	3154	1/1	0.84	0.14	-1.04	61,61,61,61	0
56	MG	GB	3343	1/1	0.94	0.20	-1.08	57,57,57,57	0
57	ZN	GA	101	1/1	0.99	0.13	-1.12	70,70,70,70	0
56	MG	A	1611	1/1	0.89	0.16	-1.14	96,96,96,96	0
57	ZN	DA	101	1/1	0.97	0.10	-1.16	71,71,71,71	0
56	MG	GB	3669	1/1	0.95	0.15	-1.18	57,57,57,57	0
56	MG	GB	3483	1/1	0.72	0.16	-1.25	78,78,78,78	0
56	MG	WC	201	1/1	0.85	0.21	-1.26	121,121,121,121	0
56	MG	B	3159	1/1	0.90	0.20	-1.26	47,47,47,47	0
56	MG	B	3057	1/1	0.97	0.13	-1.30	61,61,61,61	0
56	MG	GB	3428	1/1	0.94	0.23	-1.32	59,59,59,59	0
56	MG	B	3722	1/1	0.91	0.20	-1.36	44,44,44,44	0
56	MG	GB	3331	1/1	0.76	0.17	-1.36	61,61,61,61	0
56	MG	FB	1944	1/1	0.89	0.17	-1.37	78,78,78,78	0
56	MG	BC	309	1/1	0.79	0.15	-1.38	98,98,98,98	0
56	MG	FB	1938	1/1	0.90	0.19	-1.38	104,104,104,104	0
56	MG	BC	301	1/1	0.89	0.23	-1.39	85,85,85,85	0
56	MG	RC	307	1/1	0.95	0.12	-1.39	85,85,85,85	0
56	MG	B	3035	1/1	0.89	0.14	-1.40	63,63,63,63	0
56	MG	B	3652	1/1	0.97	0.18	-1.46	56,56,56,56	0
57	ZN	LC	101	1/1	0.99	0.11	-1.49	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	ZN	IC	101	1/1	0.99	0.06	-1.53	91,91,91,91	0
56	MG	FB	1666	1/1	0.94	0.17	-1.53	66,66,66,66	0
56	MG	BB	101	1/1	0.96	0.32	-1.60	127,127,127,127	0
56	MG	B	3337	1/1	0.91	0.17	-1.63	46,46,46,46	0
56	MG	GB	3026	1/1	0.90	0.15	-1.67	54,54,54,54	0
56	MG	FA	102	1/1	0.94	0.19	-1.67	58,58,58,58	0
56	MG	E	302	1/1	0.95	0.14	-1.70	52,52,52,52	0
56	MG	FB	1818	1/1	0.98	0.11	-1.73	83,83,83,83	0
56	MG	M	201	1/1	0.82	0.14	-1.78	44,44,44,44	0
56	MG	A	1682	1/1	0.89	0.10	-1.82	98,98,98,98	0
56	MG	B	3536	1/1	0.90	0.26	-1.82	38,38,38,38	0
56	MG	GB	3239	1/1	0.96	0.17	-1.82	54,54,54,54	0
56	MG	B	2968	1/1	0.93	0.12	-1.85	53,53,53,53	0
56	MG	B	3207	1/1	0.91	0.18	-1.86	41,41,41,41	0
56	MG	GB	3260	1/1	0.88	0.18	-1.87	59,59,59,59	0
56	MG	GB	3157	1/1	0.92	0.14	-1.92	68,68,68,68	0
56	MG	GB	3035	1/1	0.91	0.16	-1.93	65,65,65,65	0
56	MG	T	204	1/1	0.93	0.15	-1.93	56,56,56,56	0
56	MG	GB	3437	1/1	0.86	0.16	-1.94	70,70,70,70	0
56	MG	B	2901	1/1	0.91	0.15	-2.06	49,49,49,49	0
56	MG	FB	1873	1/1	0.82	0.15	-2.09	107,107,107,107	0
56	MG	GB	3283	1/1	0.72	0.13	-2.10	73,73,73,73	0
56	MG	OB	201	1/1	0.88	0.10	-2.11	102,102,102,102	0
56	MG	E	306	1/1	0.96	0.08	-2.11	51,51,51,51	0
56	MG	B	3297	1/1	0.84	0.13	-2.13	50,50,50,50	0
56	MG	FB	1621	1/1	0.93	0.17	-2.14	74,74,74,74	0
57	ZN	AC	201	1/1	0.91	0.09	-2.16	100,100,100,100	0
56	MG	A	1635	1/1	0.77	0.12	-2.19	104,104,104,104	0
56	MG	FB	1658	1/1	0.92	0.13	-2.25	72,72,72,72	0
56	MG	B	3350	1/1	0.96	0.14	-2.25	40,40,40,40	0
56	MG	B	3072	1/1	0.94	0.18	-2.26	46,46,46,46	0
56	MG	B	3147	1/1	0.91	0.14	-2.27	52,52,52,52	0
56	MG	GB	3709	1/1	0.90	0.12	-2.36	74,74,74,74	0
56	MG	B	3037	1/1	0.96	0.13	-2.38	52,52,52,52	0
56	MG	GB	3032	1/1	0.92	0.16	-2.40	54,54,54,54	0
56	MG	A	1702	1/1	0.64	0.14	-2.50	147,147,147,147	0
56	MG	O	201	1/1	0.98	0.12	-2.53	76,76,76,76	0
56	MG	B	3015	1/1	0.88	0.16	-2.54	49,49,49,49	0
56	MG	B	3713	1/1	0.98	0.15	-2.55	46,46,46,46	0
56	MG	B	3094	1/1	0.84	0.10	-2.55	51,51,51,51	0
56	MG	B	3480	1/1	0.97	0.12	-2.61	44,44,44,44	0
56	MG	GB	3112	1/1	0.77	0.13	-2.64	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	2960	1/1	0.88	0.18	-2.65	47,47,47,47	0
56	MG	B	3354	1/1	0.89	0.14	-2.65	48,48,48,48	0
56	MG	GB	3018	1/1	0.92	0.20	-2.73	73,73,73,73	0
56	MG	B	3165	1/1	0.85	0.15	-2.74	46,46,46,46	0
56	MG	C	215	1/1	0.95	0.15	-2.79	58,58,58,58	0
56	MG	GB	3614	1/1	0.92	0.25	-2.82	139,139,139,139	0
56	MG	B	3442	1/1	0.93	0.09	-2.84	58,58,58,58	0
56	MG	B	2982	1/1	0.98	0.15	-2.98	42,42,42,42	0
56	MG	GB	2993	1/1	0.92	0.14	-2.99	71,71,71,71	0
56	MG	BC	308	1/1	0.93	0.07	-3.01	104,104,104,104	0
56	MG	FB	1692	1/1	0.94	0.14	-3.04	67,67,67,67	0
56	MG	GB	3315	1/1	0.95	0.13	-3.18	51,51,51,51	0
56	MG	B	3486	1/1	0.88	0.10	-3.45	51,51,51,51	0
56	MG	B	2949	1/1	0.88	0.11	-3.53	45,45,45,45	0
56	MG	B	3838	1/1	0.88	0.09	-3.66	54,54,54,54	0
56	MG	B	3646	1/1	0.91	0.12	-3.68	54,54,54,54	0
56	MG	FB	1663	1/1	0.73	0.11	-3.76	156,156,156,156	0
56	MG	GB	3127	1/1	0.86	0.12	-3.82	68,68,68,68	0
56	MG	B	3729	1/1	0.95	0.10	-4.04	93,93,93,93	0
56	MG	B	3142	1/1	0.90	0.11	-4.05	46,46,46,46	0
56	MG	GB	3037	1/1	0.97	0.17	-4.07	52,52,52,52	0
56	MG	B	2974	1/1	0.98	0.11	-4.85	39,39,39,39	0
56	MG	GB	3143	1/1	0.95	0.06	-5.12	78,78,78,78	0
56	MG	B	3500	1/1	0.83	0.11	-5.17	52,52,52,52	0
56	MG	B	3201	1/1	0.93	0.11	-5.37	59,59,59,59	0
56	MG	GB	3153	1/1	0.92	0.15	-5.61	59,59,59,59	0
56	MG	GB	3521	1/1	0.94	0.11	-5.69	76,76,76,76	0
56	MG	B	3647	1/1	0.97	0.15	-6.93	48,48,48,48	0
56	MG	B	3085	1/1	0.97	0.11	-7.26	38,38,38,38	0
56	MG	B	3080	1/1	0.95	0.10	-7.45	66,66,66,66	0
56	MG	GB	3402	1/1	0.95	0.09	-7.94	66,66,66,66	0
56	MG	GB	3158	1/1	0.96	0.13	-8.04	52,52,52,52	0
56	MG	B	3256	1/1	0.95	0.16	-8.89	38,38,38,38	0
56	MG	A	1622	1/1	0.92	0.47	-	73,73,73,73	0
56	MG	GB	3088	1/1	0.74	0.76	-	60,60,60,60	0
56	MG	FB	1851	1/1	0.91	0.26	-	70,70,70,70	0
56	MG	GB	3086	1/1	0.61	0.11	-	107,107,107,107	0
56	MG	B	3494	1/1	0.85	0.20	-	70,70,70,70	0
56	MG	B	2905	1/1	0.96	0.29	-	45,45,45,45	0
56	MG	B	3310	1/1	0.68	0.28	-	56,56,56,56	0
56	MG	HB	222	1/1	0.91	0.07	-	108,108,108,108	0
56	MG	GB	3135	1/1	0.88	0.30	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3102	1/1	0.93	0.65	-	50,50,50,50	0
56	MG	GB	3522	1/1	0.94	0.47	-	71,71,71,71	0
56	MG	GB	2932	1/1	0.84	0.45	-	68,68,68,68	0
56	MG	GB	3594	1/1	0.71	0.26	-	68,68,68,68	0
56	MG	FB	1882	1/1	0.93	0.31	-	77,77,77,77	0
56	MG	B	3572	1/1	0.81	0.52	-	66,66,66,66	0
56	MG	B	3300	1/1	0.98	0.09	-	50,50,50,50	0
56	MG	B	3582	1/1	0.96	0.16	-	46,46,46,46	0
56	MG	GB	3259	1/1	0.79	0.40	-	70,70,70,70	0
56	MG	B	3067	1/1	0.95	0.23	-	50,50,50,50	0
56	MG	F	307	1/1	0.92	0.18	-	70,70,70,70	0
56	MG	FB	1888	1/1	0.67	0.48	-	82,82,82,82	0
56	MG	B	3653	1/1	0.91	0.28	-	56,56,56,56	0
56	MG	C	237	1/1	0.79	0.36	-	83,83,83,83	0
56	MG	KA	304	1/1	0.66	0.42	-	109,109,109,109	0
56	MG	B	3521	1/1	0.64	0.19	-	73,73,73,73	0
56	MG	B	3052	1/1	0.91	0.18	-	47,47,47,47	0
56	MG	B	3730	1/1	0.95	0.13	-	55,55,55,55	0
56	MG	FB	1721	1/1	0.76	0.54	-	76,76,76,76	0
56	MG	B	3512	1/1	0.79	0.57	-	71,71,71,71	0
56	MG	A	1784	1/1	0.95	0.45	-	85,85,85,85	0
56	MG	GB	3328	1/1	0.77	0.17	-	75,75,75,75	0
56	MG	GB	3433	1/1	0.92	0.26	-	65,65,65,65	0
56	MG	FB	1622	1/1	0.79	0.51	-	74,74,74,74	0
56	MG	GB	3058	1/1	0.86	0.24	-	49,49,49,49	0
56	MG	GB	2925	1/1	0.90	0.46	-	54,54,54,54	0
56	MG	GB	3579	1/1	0.65	0.34	-	65,65,65,65	0
56	MG	GB	3671	1/1	0.92	0.21	-	82,82,82,82	0
56	MG	GB	3099	1/1	0.97	0.49	-	48,48,48,48	0
56	MG	WB	203	1/1	0.69	0.10	-	87,87,87,87	0
56	MG	GB	3563	1/1	0.67	0.41	-	72,72,72,72	0
56	MG	Y	103	1/1	0.83	0.23	-	74,74,74,74	0
56	MG	B	3093	1/1	0.82	0.22	-	54,54,54,54	0
56	MG	B	3705	1/1	0.92	0.19	-	49,49,49,49	0
56	MG	GB	3079	1/1	0.97	0.36	-	62,62,62,62	0
56	MG	A	1805	1/1	0.90	0.17	-	87,87,87,87	0
56	MG	A	1876	1/1	0.81	0.32	-	83,83,83,83	0
56	MG	FB	1791	1/1	0.75	0.27	-	105,105,105,105	0
56	MG	GB	3498	1/1	0.94	0.38	-	74,74,74,74	0
56	MG	B	3036	1/1	0.89	0.62	-	45,45,45,45	0
56	MG	B	3475	1/1	0.97	0.51	-	46,46,46,46	0
56	MG	GB	3502	1/1	0.86	0.44	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RC	308	1/1	0.54	0.41	-	83,83,83,83	0
56	MG	P	202	1/1	0.85	0.19	-	94,94,94,94	0
56	MG	B	3231	1/1	0.88	0.46	-	47,47,47,47	0
56	MG	GB	3355	1/1	0.96	0.32	-	69,69,69,69	0
56	MG	B	3101	1/1	0.90	0.30	-	47,47,47,47	0
56	MG	B	3637	1/1	0.77	0.66	-	62,62,62,62	0
56	MG	B	3175	1/1	0.80	0.29	-	60,60,60,60	0
56	MG	A	1795	1/1	0.94	0.30	-	110,110,110,110	0
56	MG	A	1840	1/1	0.79	0.31	-	65,65,65,65	0
56	MG	B	3189	1/1	0.90	0.28	-	59,59,59,59	0
56	MG	B	3539	1/1	0.81	0.34	-	51,51,51,51	0
56	MG	F	310	1/1	0.90	0.41	-	69,69,69,69	0
56	MG	A	1742	1/1	0.96	0.51	-	66,66,66,66	0
56	MG	B	3401	1/1	0.64	0.35	-	46,46,46,46	0
56	MG	B	3484	1/1	0.89	0.45	-	50,50,50,50	0
56	MG	K	208	1/1	0.86	0.23	-	71,71,71,71	0
56	MG	A	1711	1/1	0.81	0.51	-	95,95,95,95	0
56	MG	A	1659	1/1	0.87	0.21	-	87,87,87,87	0
56	MG	B	3487	1/1	0.89	0.47	-	81,81,81,81	0
56	MG	B	3202	1/1	0.80	0.21	-	64,64,64,64	0
56	MG	B	3533	1/1	0.87	0.23	-	60,60,60,60	0
56	MG	B	3266	1/1	0.88	0.21	-	54,54,54,54	0
56	MG	GB	3073	1/1	0.93	0.12	-	64,64,64,64	0
56	MG	FB	1925	1/1	0.83	0.21	-	147,147,147,147	0
56	MG	GB	3492	1/1	0.94	0.34	-	70,70,70,70	0
56	MG	GB	3706	1/1	0.79	0.42	-	83,83,83,83	0
56	MG	NC	113	1/1	0.86	0.33	-	80,80,80,80	0
56	MG	GB	3388	1/1	0.97	0.32	-	64,64,64,64	0
56	MG	GB	2984	1/1	0.93	0.25	-	66,66,66,66	0
56	MG	GB	3200	1/1	0.93	0.78	-	63,63,63,63	0
56	MG	B	3122	1/1	0.95	0.37	-	46,46,46,46	0
56	MG	B	3082	1/1	0.93	0.39	-	44,44,44,44	0
56	MG	B	3817	1/1	0.88	0.21	-	46,46,46,46	0
56	MG	OC	401	1/1	0.68	0.20	-	68,68,68,68	0
56	MG	GB	3466	1/1	0.98	0.17	-	80,80,80,80	0
56	MG	GB	3530	1/1	0.92	0.23	-	85,85,85,85	0
56	MG	B	3769	1/1	0.84	0.36	-	69,69,69,69	0
56	MG	GB	3584	1/1	0.87	0.08	-	71,71,71,71	0
56	MG	GB	3076	1/1	0.90	0.34	-	59,59,59,59	0
56	MG	B	3016	1/1	0.95	0.09	-	76,76,76,76	0
56	MG	FB	1637	1/1	0.68	0.18	-	64,64,64,64	0
56	MG	GB	3608	1/1	0.85	0.22	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	2918	1/1	0.92	0.49	-	43,43,43,43	0
56	MG	Y	102	1/1	0.78	0.26	-	54,54,54,54	0
56	MG	B	3644	1/1	0.86	0.17	-	146,146,146,146	0
56	MG	GB	3481	1/1	0.91	0.27	-	64,64,64,64	0
56	MG	GB	3564	1/1	0.90	0.23	-	70,70,70,70	0
56	MG	B	3115	1/1	0.93	0.23	-	39,39,39,39	0
56	MG	GB	3173	1/1	0.88	0.26	-	80,80,80,80	0
56	MG	A	1718	1/1	0.80	0.54	-	64,64,64,64	0
56	MG	FB	1654	1/1	0.83	0.50	-	56,56,56,56	0
56	MG	GB	3038	1/1	0.67	0.18	-	71,71,71,71	0
56	MG	FB	1671	1/1	0.89	0.58	-	87,87,87,87	0
56	MG	B	3819	1/1	0.91	0.17	-	56,56,56,56	0
56	MG	GB	3085	1/1	0.81	0.44	-	60,60,60,60	0
56	MG	GB	3087	1/1	0.85	0.22	-	75,75,75,75	0
56	MG	A	1797	1/1	0.67	0.20	-	90,90,90,90	0
56	MG	B	3048	1/1	0.88	0.34	-	45,45,45,45	0
56	MG	GB	3202	1/1	0.86	0.39	-	101,101,101,101	0
56	MG	FB	1631	1/1	0.83	0.87	-	96,96,96,96	0
56	MG	B	3553	1/1	0.87	0.13	-	59,59,59,59	0
56	MG	GB	3225	1/1	0.93	0.17	-	65,65,65,65	0
56	MG	B	3605	1/1	0.85	0.93	-	57,57,57,57	0
56	MG	B	3761	1/1	0.83	0.38	-	53,53,53,53	0
56	MG	Y	105	1/1	0.91	0.17	-	52,52,52,52	0
56	MG	B	3498	1/1	0.91	0.34	-	60,60,60,60	0
56	MG	GB	2991	1/1	0.71	0.62	-	63,63,63,63	0
56	MG	GB	3524	1/1	0.65	0.22	-	83,83,83,83	0
56	MG	B	3569	1/1	0.95	0.20	-	61,61,61,61	0
56	MG	GB	3195	1/1	0.86	0.38	-	52,52,52,52	0
56	MG	FB	1659	1/1	0.93	0.24	-	69,69,69,69	0
56	MG	A	1772	1/1	0.90	0.29	-	143,143,143,143	0
56	MG	B	3293	1/1	0.86	0.11	-	82,82,82,82	0
56	MG	GB	3586	1/1	0.57	0.38	-	187,187,187,187	0
56	MG	B	3565	1/1	0.94	0.27	-	49,49,49,49	0
56	MG	GB	3113	1/1	0.97	0.28	-	69,69,69,69	0
56	MG	FB	1942	1/1	0.78	0.30	-	72,72,72,72	0
56	MG	B	3171	1/1	0.96	0.19	-	48,48,48,48	0
56	MG	B	3736	1/1	0.79	0.44	-	52,52,52,52	0
56	MG	GB	3548	1/1	0.68	0.58	-	68,68,68,68	0
56	MG	FB	1675	1/1	0.85	0.17	-	72,72,72,72	0
56	MG	B	3820	1/1	0.97	0.12	-	54,54,54,54	0
56	MG	GB	3235	1/1	0.83	0.33	-	57,57,57,57	0
56	MG	FB	1838	1/1	0.87	0.37	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1625	1/1	0.79	0.77	-	66,66,66,66	0
56	MG	FB	1701	1/1	0.87	0.31	-	68,68,68,68	0
56	MG	M	204	1/1	0.89	0.11	-	69,69,69,69	0
56	MG	B	3685	1/1	0.65	0.59	-	117,117,117,117	0
56	MG	B	3615	1/1	0.70	0.23	-	159,159,159,159	0
56	MG	FB	1672	1/1	0.87	0.35	-	60,60,60,60	0
56	MG	A	1641	1/1	0.94	0.43	-	79,79,79,79	0
56	MG	B	3177	1/1	0.93	0.30	-	47,47,47,47	0
56	MG	B	3576	1/1	0.90	0.12	-	69,69,69,69	0
56	MG	GB	3238	1/1	0.58	0.38	-	76,76,76,76	0
56	MG	B	3247	1/1	0.62	0.38	-	62,62,62,62	0
56	MG	GB	3034	1/1	0.91	0.52	-	63,63,63,63	0
56	MG	FB	1655	1/1	0.89	0.36	-	63,63,63,63	0
56	MG	B	3621	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	B	3050	1/1	0.87	0.22	-	42,42,42,42	0
56	MG	A	1688	1/1	0.64	0.42	-	82,82,82,82	0
56	MG	B	3376	1/1	0.95	0.07	-	133,133,133,133	0
56	MG	B	2971	1/1	0.91	0.42	-	51,51,51,51	0
56	MG	IA	117	1/1	0.66	0.23	-	81,81,81,81	0
56	MG	B	3447	1/1	0.96	0.12	-	63,63,63,63	0
56	MG	B	3439	1/1	0.92	0.18	-	49,49,49,49	0
56	MG	GB	3229	1/1	0.65	0.40	-	120,120,120,120	0
56	MG	B	3336	1/1	0.82	0.21	-	60,60,60,60	0
56	MG	B	3599	1/1	0.90	0.47	-	69,69,69,69	0
56	MG	GB	3256	1/1	0.93	0.37	-	72,72,72,72	0
56	MG	GB	3262	1/1	0.81	0.67	-	50,50,50,50	0
56	MG	HC	102	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	GB	3629	1/1	0.89	0.42	-	57,57,57,57	0
56	MG	FB	1832	1/1	0.83	0.63	-	76,76,76,76	0
56	MG	GB	3317	1/1	0.81	0.24	-	70,70,70,70	0
56	MG	FB	1830	1/1	0.95	0.50	-	69,69,69,69	0
56	MG	GB	3187	1/1	0.81	0.49	-	55,55,55,55	0
56	MG	B	3098	1/1	0.76	0.37	-	46,46,46,46	0
56	MG	SA	201	1/1	0.64	0.43	-	120,120,120,120	0
56	MG	A	1714	1/1	0.77	0.68	-	97,97,97,97	0
56	MG	B	3600	1/1	0.90	0.28	-	54,54,54,54	0
56	MG	GB	3013	1/1	0.95	0.53	-	56,56,56,56	0
56	MG	B	3607	1/1	0.89	0.13	-	59,59,59,59	0
56	MG	GB	2977	1/1	0.96	0.51	-	52,52,52,52	0
56	MG	GB	3191	1/1	0.76	0.54	-	68,68,68,68	0
56	MG	GB	3129	1/1	0.87	0.27	-	65,65,65,65	0
56	MG	W	308	1/1	0.69	0.24	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	2912	1/1	0.96	0.73	-	57,57,57,57	0
56	MG	GB	3213	1/1	0.95	0.22	-	59,59,59,59	0
56	MG	FB	1822	1/1	0.66	0.23	-	73,73,73,73	0
56	MG	Y	101	1/1	0.97	0.14	-	49,49,49,49	0
56	MG	L	204	1/1	0.91	0.09	-	60,60,60,60	0
56	MG	GB	3529	1/1	0.88	0.20	-	107,107,107,107	0
56	MG	B	3659	1/1	0.85	0.28	-	52,52,52,52	0
56	MG	FB	1781	1/1	0.92	0.36	-	90,90,90,90	0
56	MG	B	3628	1/1	0.85	0.35	-	61,61,61,61	0
56	MG	B	3400	1/1	0.83	0.19	-	43,43,43,43	0
56	MG	FB	1719	1/1	0.87	0.34	-	67,67,67,67	0
56	MG	FB	1644	1/1	0.72	0.12	-	81,81,81,81	0
56	MG	GB	3001	1/1	0.68	0.37	-	111,111,111,111	0
56	MG	B	3449	1/1	0.87	0.34	-	46,46,46,46	0
56	MG	F	302	1/1	0.70	0.28	-	79,79,79,79	0
56	MG	GB	3583	1/1	0.89	0.33	-	68,68,68,68	0
56	MG	B	3826	1/1	0.79	0.23	-	97,97,97,97	0
56	MG	B	3525	1/1	0.84	0.17	-	64,64,64,64	0
56	MG	YC	206	1/1	0.91	0.11	-	88,88,88,88	0
56	MG	B	3174	1/1	0.92	0.37	-	42,42,42,42	0
56	MG	GB	3504	1/1	0.66	0.16	-	195,195,195,195	0
56	MG	OC	402	1/1	0.30	0.38	-	110,110,110,110	0
56	MG	FB	1837	1/1	0.80	0.63	-	91,91,91,91	0
56	MG	B	2966	1/1	0.95	0.25	-	60,60,60,60	0
56	MG	GB	3132	1/1	0.91	0.27	-	65,65,65,65	0
56	MG	B	3398	1/1	0.84	0.12	-	64,64,64,64	0
56	MG	B	3172	1/1	0.89	0.16	-	59,59,59,59	0
56	MG	FB	1605	1/1	0.93	0.80	-	70,70,70,70	0
56	MG	FB	1843	1/1	0.81	0.22	-	85,85,85,85	0
56	MG	GB	3476	1/1	0.19	0.57	-	130,130,130,130	0
56	MG	GB	3675	1/1	0.68	0.19	-	134,134,134,134	0
56	MG	B	3096	1/1	0.97	0.36	-	54,54,54,54	0
56	MG	GB	3633	1/1	0.89	0.16	-	74,74,74,74	0
56	MG	FB	1923	1/1	0.70	0.25	-	67,67,67,67	0
56	MG	GB	3680	1/1	0.95	0.35	-	60,60,60,60	0
56	MG	FB	1833	1/1	0.79	0.20	-	62,62,62,62	0
56	MG	NB	203	1/1	0.85	0.40	-	92,92,92,92	0
56	MG	B	2985	1/1	0.94	0.33	-	46,46,46,46	0
56	MG	GB	3189	1/1	0.90	0.41	-	64,64,64,64	0
56	MG	B	3081	1/1	0.93	0.37	-	44,44,44,44	0
56	MG	B	3651	1/1	0.84	0.13	-	74,74,74,74	0
56	MG	B	3412	1/1	0.73	0.18	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3361	1/1	0.52	0.89	-	91,91,91,91	0
56	MG	B	3261	1/1	0.91	0.19	-	50,50,50,50	0
56	MG	B	3751	1/1	0.96	0.20	-	48,48,48,48	0
56	MG	B	3541	1/1	0.90	0.40	-	120,120,120,120	0
56	MG	GB	3413	1/1	0.87	0.62	-	58,58,58,58	0
56	MG	B	3391	1/1	0.76	0.34	-	56,56,56,56	0
56	MG	FB	1798	1/1	0.92	0.34	-	79,79,79,79	0
56	MG	GB	3207	1/1	0.41	0.33	-	126,126,126,126	0
56	MG	EA	102	1/1	0.95	0.36	-	44,44,44,44	0
56	MG	FB	1941	1/1	0.68	0.37	-	89,89,89,89	0
56	MG	B	3673	1/1	0.81	0.33	-	50,50,50,50	0
56	MG	A	1788	1/1	0.72	0.53	-	76,76,76,76	0
56	MG	IA	107	1/1	0.94	0.17	-	76,76,76,76	0
56	MG	GB	3628	1/1	0.90	0.30	-	73,73,73,73	0
56	MG	B	3563	1/1	0.81	0.20	-	47,47,47,47	0
56	MG	FB	1918	1/1	0.59	0.31	-	92,92,92,92	0
56	MG	A	1706	1/1	0.92	0.72	-	88,88,88,88	0
56	MG	FB	1669	1/1	0.72	0.15	-	67,67,67,67	0
56	MG	PA	203	1/1	0.78	0.24	-	92,92,92,92	0
56	MG	A	1691	1/1	0.88	0.37	-	61,61,61,61	0
56	MG	A	1802	1/1	0.56	0.27	-	73,73,73,73	0
56	MG	GB	2913	1/1	0.92	0.44	-	63,63,63,63	0
56	MG	B	3232	1/1	0.78	0.33	-	57,57,57,57	0
56	MG	GB	3267	1/1	0.89	0.23	-	74,74,74,74	0
56	MG	GB	3172	1/1	0.96	0.14	-	57,57,57,57	0
56	MG	GB	3420	1/1	0.83	0.28	-	99,99,99,99	0
56	MG	A	1829	1/1	0.90	0.36	-	109,109,109,109	0
56	MG	B	3592	1/1	0.74	0.24	-	73,73,73,73	0
56	MG	B	3693	1/1	0.81	0.21	-	51,51,51,51	0
56	MG	VB	206	1/1	0.91	0.30	-	69,69,69,69	0
56	MG	FB	1809	1/1	0.90	0.34	-	63,63,63,63	0
56	MG	B	3373	1/1	0.91	0.17	-	50,50,50,50	0
56	MG	B	3792	1/1	0.80	0.16	-	100,100,100,100	0
56	MG	GB	3622	1/1	0.75	0.30	-	105,105,105,105	0
56	MG	B	3030	1/1	0.90	0.50	-	59,59,59,59	0
56	MG	FB	1814	1/1	0.86	0.26	-	78,78,78,78	0
56	MG	GB	3303	1/1	0.84	0.34	-	61,61,61,61	0
56	MG	GB	2936	1/1	0.87	0.45	-	54,54,54,54	0
56	MG	B	3327	1/1	0.87	0.15	-	43,43,43,43	0
56	MG	A	1608	1/1	0.95	0.76	-	55,55,55,55	0
56	MG	HC	103	1/1	0.89	0.33	-	90,90,90,90	0
56	MG	B	3384	1/1	0.91	0.54	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	FB	1704	1/1	0.61	0.76	-	93,93,93,93	0
56	MG	M	206	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	IA	119	1/1	0.77	0.18	-	73,73,73,73	0
56	MG	B	3382	1/1	0.85	0.22	-	54,54,54,54	0
56	MG	B	3434	1/1	0.42	0.26	-	75,75,75,75	0
56	MG	FB	1784	1/1	0.88	0.23	-	60,60,60,60	0
56	MG	B	3657	1/1	0.88	0.34	-	45,45,45,45	0
56	MG	B	3143	1/1	0.93	0.62	-	39,39,39,39	0
56	MG	B	2942	1/1	0.95	0.80	-	58,58,58,58	0
56	MG	B	3737	1/1	0.84	0.18	-	62,62,62,62	0
56	MG	FB	1895	1/1	0.90	0.29	-	73,73,73,73	0
56	MG	GB	3241	1/1	0.83	0.40	-	74,74,74,74	0
56	MG	GB	3703	1/1	0.85	0.23	-	70,70,70,70	0
56	MG	GB	2967	1/1	0.70	0.57	-	61,61,61,61	0
56	MG	GB	3501	1/1	0.90	0.32	-	77,77,77,77	0
56	MG	GB	3247	1/1	0.77	0.59	-	62,62,62,62	0
56	MG	GB	3636	1/1	0.86	0.49	-	75,75,75,75	0
56	MG	C	204	1/1	0.96	0.21	-	54,54,54,54	0
56	MG	FB	1767	1/1	0.59	0.48	-	121,121,121,121	0
56	MG	B	3752	1/1	0.93	0.34	-	53,53,53,53	0
56	MG	B	3299	1/1	0.93	0.23	-	45,45,45,45	0
56	MG	GB	3416	1/1	0.74	0.57	-	61,61,61,61	0
56	MG	GB	3324	1/1	0.68	0.29	-	105,105,105,105	0
56	MG	FB	1683	1/1	0.93	0.78	-	75,75,75,75	0
56	MG	GB	3104	1/1	0.89	0.24	-	65,65,65,65	0
56	MG	B	3340	1/1	0.82	0.36	-	62,62,62,62	0
56	MG	GB	3562	1/1	0.71	0.13	-	57,57,57,57	0
56	MG	GB	3055	1/1	0.92	0.20	-	64,64,64,64	0
56	MG	G	3204	1/1	0.80	0.72	-	49,49,49,49	0
56	MG	B	3111	1/1	0.98	0.47	-	33,33,33,33	0
56	MG	B	3018	1/1	0.81	0.18	-	50,50,50,50	0
56	MG	B	3338	1/1	0.80	0.39	-	47,47,47,47	0
56	MG	B	3369	1/1	0.46	0.14	-	69,69,69,69	0
56	MG	B	2946	1/1	0.93	0.16	-	72,72,72,72	0
56	MG	GB	3201	1/1	0.93	0.63	-	57,57,57,57	0
56	MG	A	1673	1/1	0.82	0.25	-	75,75,75,75	0
56	MG	B	3264	1/1	0.85	0.10	-	70,70,70,70	0
56	MG	GB	3648	1/1	0.77	0.21	-	88,88,88,88	0
56	MG	B	3518	1/1	0.88	0.21	-	56,56,56,56	0
56	MG	FB	1884	1/1	0.91	0.13	-	87,87,87,87	0
56	MG	NC	109	1/1	0.95	0.44	-	89,89,89,89	0
56	MG	GB	3196	1/1	0.85	0.26	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	F	315	1/1	0.71	0.16	-	67,67,67,67	0
56	MG	A	1878	1/1	0.79	0.99	-	101,101,101,101	0
56	MG	QC	302	1/1	0.75	0.40	-	103,103,103,103	0
56	MG	FB	1816	1/1	0.95	0.37	-	75,75,75,75	0
56	MG	GB	3537	1/1	0.83	0.16	-	93,93,93,93	0
56	MG	A	1722	1/1	0.75	0.10	-	98,98,98,98	0
56	MG	B	3034	1/1	0.87	0.42	-	55,55,55,55	0
56	MG	B	3186	1/1	0.81	0.29	-	48,48,48,48	0
56	MG	B	3773	1/1	0.77	0.21	-	99,99,99,99	0
56	MG	B	3132	1/1	0.83	0.46	-	46,46,46,46	0
56	MG	FB	1703	1/1	0.92	0.38	-	86,86,86,86	0
56	MG	A	1708	1/1	0.93	0.47	-	79,79,79,79	0
56	MG	GB	3017	1/1	0.90	0.34	-	56,56,56,56	0
56	MG	GB	3581	1/1	0.95	0.15	-	69,69,69,69	0
56	MG	B	3505	1/1	0.84	0.23	-	51,51,51,51	0
56	MG	B	3485	1/1	0.71	0.12	-	117,117,117,117	0
56	MG	B	3371	1/1	0.93	0.13	-	133,133,133,133	0
56	MG	B	2976	1/1	0.90	0.28	-	44,44,44,44	0
56	MG	FB	1947	1/1	0.87	0.77	-	73,73,73,73	0
56	MG	B	3758	1/1	0.78	0.15	-	80,80,80,80	0
56	MG	GB	3507	1/1	0.94	0.09	-	109,109,109,109	0
56	MG	GB	3066	1/1	0.82	0.53	-	55,55,55,55	0
56	MG	B	3707	1/1	0.36	0.51	-	113,113,113,113	0
56	MG	FB	1877	1/1	0.96	0.29	-	80,80,80,80	0
56	MG	GB	2903	1/1	0.95	0.39	-	36,36,36,36	0
56	MG	GB	2914	1/1	0.88	0.49	-	58,58,58,58	0
56	MG	A	1658	1/1	0.96	0.16	-	87,87,87,87	0
56	MG	GB	2995	1/1	0.90	0.44	-	58,58,58,58	0
56	MG	FB	1766	1/1	0.90	0.17	-	84,84,84,84	0
56	MG	FB	1811	1/1	0.87	0.16	-	143,143,143,143	0
56	MG	MA	304	1/1	0.62	0.22	-	96,96,96,96	0
56	MG	BA	104	1/1	0.38	0.28	-	105,105,105,105	0
56	MG	B	2967	1/1	0.87	0.36	-	53,53,53,53	0
56	MG	A	1737	1/1	0.82	0.21	-	106,106,106,106	0
56	MG	A	1871	1/1	0.89	0.26	-	85,85,85,85	0
56	MG	B	3194	1/1	0.75	0.15	-	53,53,53,53	0
56	MG	B	3663	1/1	0.89	0.21	-	51,51,51,51	0
56	MG	C	231	1/1	0.77	0.17	-	89,89,89,89	0
56	MG	B	3801	1/1	0.87	0.16	-	74,74,74,74	0
56	MG	AD	201	1/1	0.68	0.12	-	80,80,80,80	0
56	MG	B	3515	1/1	0.14	0.21	-	167,167,167,167	0
56	MG	SC	207	1/1	0.86	0.36	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3437	1/1	0.92	0.15	-	39,39,39,39	0
56	MG	A	1865	1/1	0.93	0.68	-	77,77,77,77	0
56	MG	GB	3598	1/1	0.68	0.59	-	78,78,78,78	0
56	MG	B	3636	1/1	0.82	0.45	-	171,171,171,171	0
56	MG	FB	1754	1/1	0.92	0.16	-	86,86,86,86	0
56	MG	MB	205	1/1	0.48	0.47	-	122,122,122,122	0
56	MG	GB	3151	1/1	0.85	0.14	-	70,70,70,70	0
56	MG	FB	1933	1/1	0.82	0.43	-	126,126,126,126	0
56	MG	B	3325	1/1	0.92	0.20	-	53,53,53,53	0
56	MG	FB	1653	1/1	0.94	0.38	-	65,65,65,65	0
56	MG	FB	1862	1/1	0.62	0.48	-	118,118,118,118	0
56	MG	B	3688	1/1	0.79	0.26	-	60,60,60,60	0
56	MG	GB	3121	1/1	0.89	0.48	-	62,62,62,62	0
56	MG	B	3557	1/1	0.87	0.26	-	47,47,47,47	0
56	MG	MB	204	1/1	0.45	0.25	-	115,115,115,115	0
56	MG	GB	3595	1/1	0.70	0.84	-	74,74,74,74	0
56	MG	GB	3387	1/1	0.76	0.55	-	66,66,66,66	0
56	MG	FB	1702	1/1	0.60	0.22	-	81,81,81,81	0
56	MG	B	3028	1/1	0.83	0.41	-	50,50,50,50	0
56	MG	P	203	1/1	0.81	0.20	-	75,75,75,75	0
56	MG	B	3681	1/1	0.82	0.17	-	71,71,71,71	0
56	MG	C	218	1/1	0.69	0.38	-	66,66,66,66	0
56	MG	A	1852	1/1	0.60	0.70	-	96,96,96,96	0
56	MG	GB	3118	1/1	0.94	0.34	-	56,56,56,56	0
56	MG	FB	1676	1/1	0.94	0.10	-	74,74,74,74	0
56	MG	HB	224	1/1	0.92	0.32	-	118,118,118,118	0
56	MG	B	2956	1/1	0.91	0.49	-	49,49,49,49	0
56	MG	GB	3569	1/1	0.93	0.16	-	55,55,55,55	0
56	MG	B	3225	1/1	0.92	0.38	-	46,46,46,46	0
56	MG	F	311	1/1	0.82	0.14	-	59,59,59,59	0
56	MG	YC	205	1/1	0.84	0.77	-	66,66,66,66	0
56	MG	FB	1764	1/1	0.90	0.40	-	82,82,82,82	0
56	MG	QB	202	1/1	0.66	0.33	-	66,66,66,66	0
56	MG	GB	3082	1/1	0.81	0.51	-	53,53,53,53	0
56	MG	B	2944	1/1	0.93	0.50	-	44,44,44,44	0
56	MG	P	204	1/1	0.92	0.08	-	77,77,77,77	0
56	MG	A	1680	1/1	0.78	0.33	-	75,75,75,75	0
56	MG	GB	3493	1/1	0.64	0.74	-	62,62,62,62	0
56	MG	FB	1745	1/1	0.93	0.25	-	67,67,67,67	0
56	MG	GB	2943	1/1	0.43	0.51	-	92,92,92,92	0
56	MG	C	227	1/1	0.95	0.22	-	64,64,64,64	0
56	MG	B	3077	1/1	0.72	0.82	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1738	1/1	0.72	0.44	-	86,86,86,86	0
56	MG	FB	1839	1/1	0.86	0.35	-	78,78,78,78	0
56	MG	FB	1919	1/1	0.56	0.71	-	126,126,126,126	0
56	MG	A	1693	1/1	0.86	0.46	-	79,79,79,79	0
56	MG	A	1731	1/1	0.20	0.41	-	134,134,134,134	0
56	MG	GB	3139	1/1	0.16	0.35	-	125,125,125,125	0
56	MG	GB	3611	1/1	0.72	0.32	-	77,77,77,77	0
56	MG	A	1678	1/1	0.61	0.48	-	97,97,97,97	0
56	MG	B	3463	1/1	0.66	0.17	-	65,65,65,65	0
56	MG	FB	1824	1/1	0.68	0.60	-	70,70,70,70	0
56	MG	FB	1872	1/1	0.96	0.14	-	87,87,87,87	0
56	MG	CC	102	1/1	0.75	0.22	-	77,77,77,77	0
56	MG	B	3550	1/1	0.75	0.31	-	147,147,147,147	0
56	MG	GB	3578	1/1	0.90	0.10	-	92,92,92,92	0
56	MG	GB	3377	1/1	0.81	0.31	-	72,72,72,72	0
56	MG	GB	3472	1/1	0.66	0.42	-	189,189,189,189	0
56	MG	GB	3126	1/1	0.82	0.15	-	53,53,53,53	0
56	MG	B	3387	1/1	0.79	0.32	-	60,60,60,60	0
56	MG	B	3091	1/1	0.92	0.39	-	36,36,36,36	0
56	MG	B	3408	1/1	0.95	0.34	-	55,55,55,55	0
56	MG	B	3753	1/1	0.48	2.06	-	75,75,75,75	0
56	MG	B	2959	1/1	0.92	0.10	-	84,84,84,84	0
56	MG	OA	203	1/1	0.85	0.20	-	62,62,62,62	0
56	MG	B	3313	1/1	0.91	0.19	-	49,49,49,49	0
56	MG	B	3683	1/1	0.88	0.25	-	52,52,52,52	0
56	MG	GB	3642	1/1	0.56	0.72	-	76,76,76,76	0
56	MG	HB	227	1/1	0.68	0.17	-	99,99,99,99	0
56	MG	B	3813	1/1	0.83	0.35	-	52,52,52,52	0
56	MG	B	3821	1/1	0.91	0.24	-	53,53,53,53	0
56	MG	B	3418	1/1	0.81	0.23	-	76,76,76,76	0
56	MG	B	3158	1/1	0.94	0.31	-	50,50,50,50	0
56	MG	VB	208	1/1	0.74	0.57	-	74,74,74,74	0
56	MG	FB	1775	1/1	0.75	0.31	-	83,83,83,83	0
56	MG	B	3763	1/1	0.92	0.92	-	56,56,56,56	0
56	MG	B	3691	1/1	0.86	0.27	-	92,92,92,92	0
56	MG	A	1700	1/1	0.61	0.34	-	82,82,82,82	0
56	MG	A	1845	1/1	0.64	0.23	-	107,107,107,107	0
56	MG	GB	3605	1/1	0.87	0.37	-	61,61,61,61	0
56	MG	B	3160	1/1	0.87	0.36	-	60,60,60,60	0
56	MG	B	3617	1/1	0.90	0.81	-	54,54,54,54	0
56	MG	B	3178	1/1	0.92	0.41	-	43,43,43,43	0
56	MG	B	3669	1/1	0.66	0.47	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3003	1/1	0.87	0.33	-	55,55,55,55	0
56	MG	B	3649	1/1	0.93	0.15	-	104,104,104,104	0
56	MG	GB	3367	1/1	0.83	0.16	-	76,76,76,76	0
56	MG	GB	2996	1/1	0.93	0.51	-	57,57,57,57	0
56	MG	A	1808	1/1	0.90	0.79	-	94,94,94,94	0
56	MG	GB	3430	1/1	0.68	0.28	-	75,75,75,75	0
56	MG	FB	1842	1/1	0.86	0.33	-	73,73,73,73	0
56	MG	A	1820	1/1	0.83	0.27	-	93,93,93,93	0
56	MG	GB	2929	1/1	0.96	0.47	-	46,46,46,46	0
56	MG	B	3642	1/1	0.89	0.45	-	52,52,52,52	0
56	MG	GB	3365	1/1	0.94	0.42	-	60,60,60,60	0
56	MG	NC	114	1/1	0.82	0.42	-	64,64,64,64	0
56	MG	GB	3414	1/1	0.90	0.11	-	75,75,75,75	0
56	MG	B	3396	1/1	0.86	0.37	-	49,49,49,49	0
56	MG	GB	3271	1/1	0.83	0.59	-	84,84,84,84	0
56	MG	GB	3380	1/1	0.70	0.36	-	57,57,57,57	0
56	MG	B	3675	1/1	0.81	0.30	-	60,60,60,60	0
56	MG	B	3090	1/1	0.71	0.25	-	53,53,53,53	0
56	MG	GB	3651	1/1	0.84	0.22	-	130,130,130,130	0
56	MG	HB	210	1/1	0.80	0.15	-	114,114,114,114	0
56	MG	B	3259	1/1	0.95	0.36	-	38,38,38,38	0
56	MG	E	301	1/1	0.83	0.35	-	52,52,52,52	0
56	MG	GB	3566	1/1	0.84	0.21	-	66,66,66,66	0
56	MG	NC	106	1/1	0.78	0.66	-	77,77,77,77	0
56	MG	B	3734	1/1	0.84	0.28	-	69,69,69,69	0
56	MG	FB	1902	1/1	0.92	0.15	-	132,132,132,132	0
56	MG	GB	3045	1/1	0.98	0.39	-	51,51,51,51	0
56	MG	A	1850	1/1	0.89	0.25	-	117,117,117,117	0
56	MG	B	3168	1/1	0.98	0.48	-	35,35,35,35	0
56	MG	B	3012	1/1	0.93	0.20	-	51,51,51,51	0
56	MG	B	3414	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	B	3366	1/1	0.84	0.24	-	50,50,50,50	0
56	MG	B	3218	1/1	0.79	0.10	-	61,61,61,61	0
56	MG	GB	3381	1/1	0.78	0.15	-	66,66,66,66	0
56	MG	B	2948	1/1	0.98	0.61	-	43,43,43,43	0
56	MG	B	3762	1/1	0.89	0.36	-	71,71,71,71	0
56	MG	B	3298	1/1	0.91	0.23	-	168,168,168,168	0
56	MG	JA	412	1/1	0.50	0.16	-	107,107,107,107	0
56	MG	HB	219	1/1	0.61	0.74	-	94,94,94,94	0
56	MG	GB	3115	1/1	0.87	0.48	-	61,61,61,61	0
56	MG	C	225	1/1	0.72	0.23	-	83,83,83,83	0
56	MG	GB	3487	1/1	0.69	0.23	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3263	1/1	0.87	0.23	-	77,77,77,77	0
56	MG	CA	102	1/1	0.89	0.31	-	52,52,52,52	0
56	MG	GB	3014	1/1	0.92	0.30	-	64,64,64,64	0
56	MG	B	3238	1/1	0.87	0.19	-	44,44,44,44	0
56	MG	W	304	1/1	0.68	0.24	-	82,82,82,82	0
56	MG	B	2984	1/1	0.93	0.34	-	58,58,58,58	0
56	MG	B	2908	1/1	0.97	0.36	-	42,42,42,42	0
56	MG	B	3145	1/1	0.93	0.18	-	43,43,43,43	0
56	MG	NC	102	1/1	0.92	0.18	-	65,65,65,65	0
56	MG	B	3774	1/1	0.78	0.43	-	46,46,46,46	0
56	MG	GB	2950	1/1	0.89	0.44	-	60,60,60,60	0
56	MG	B	3260	1/1	0.96	0.39	-	47,47,47,47	0
56	MG	A	1843	1/1	0.68	0.45	-	89,89,89,89	0
56	MG	GB	3063	1/1	0.94	0.16	-	53,53,53,53	0
56	MG	GB	3067	1/1	0.83	0.34	-	57,57,57,57	0
56	MG	B	3620	1/1	0.90	0.22	-	50,50,50,50	0
56	MG	B	3209	1/1	0.95	0.26	-	51,51,51,51	0
56	MG	GB	3661	1/1	0.81	0.22	-	66,66,66,66	0
56	MG	PB	202	1/1	0.73	0.59	-	89,89,89,89	0
56	MG	A	1844	1/1	0.91	0.19	-	89,89,89,89	0
56	MG	FB	1857	1/1	0.66	0.47	-	82,82,82,82	0
56	MG	B	3311	1/1	0.91	0.27	-	46,46,46,46	0
56	MG	B	3796	1/1	0.93	0.41	-	113,113,113,113	0
56	MG	GB	3166	1/1	0.86	0.60	-	52,52,52,52	0
56	MG	OA	202	1/1	0.89	0.12	-	78,78,78,78	0
56	MG	FB	1720	1/1	0.83	0.18	-	81,81,81,81	0
56	MG	B	2994	1/1	0.89	0.42	-	58,58,58,58	0
56	MG	FB	1770	1/1	0.64	0.61	-	93,93,93,93	0
56	MG	GB	3475	1/1	0.95	0.15	-	79,79,79,79	0
56	MG	GB	3470	1/1	0.98	0.40	-	73,73,73,73	0
56	MG	B	3123	1/1	0.96	0.58	-	33,33,33,33	0
56	MG	F	303	1/1	0.89	0.09	-	71,71,71,71	0
56	MG	B	3676	1/1	0.90	0.12	-	55,55,55,55	0
56	MG	JA	401	1/1	0.87	0.28	-	52,52,52,52	0
56	MG	B	3828	1/1	0.89	0.41	-	66,66,66,66	0
56	MG	A	1881	1/1	0.90	0.36	-	128,128,128,128	0
56	MG	GB	2930	1/1	0.91	0.61	-	64,64,64,64	0
56	MG	GB	3319	1/1	0.79	0.20	-	84,84,84,84	0
56	MG	B	3341	1/1	0.80	0.25	-	58,58,58,58	0
56	MG	B	3243	1/1	0.90	0.71	-	43,43,43,43	0
56	MG	A	1859	1/1	0.64	0.38	-	90,90,90,90	0
56	MG	GB	3080	1/1	0.87	0.38	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3551	1/1	0.90	0.27	-	96,96,96,96	0
56	MG	X	107	1/1	0.91	0.24	-	72,72,72,72	0
56	MG	B	3638	1/1	0.85	0.21	-	61,61,61,61	0
56	MG	MB	202	1/1	0.71	0.47	-	110,110,110,110	0
56	MG	GB	3116	1/1	0.92	0.32	-	66,66,66,66	0
56	MG	B	3789	1/1	0.92	0.24	-	46,46,46,46	0
56	MG	FB	1670	1/1	0.87	0.53	-	74,74,74,74	0
56	MG	FB	1737	1/1	0.88	0.47	-	61,61,61,61	0
56	MG	GB	3681	1/1	0.89	0.21	-	60,60,60,60	0
56	MG	A	1634	1/1	0.60	0.47	-	72,72,72,72	0
56	MG	I	207	1/1	0.78	0.20	-	70,70,70,70	0
56	MG	GB	3310	1/1	0.85	0.39	-	69,69,69,69	0
56	MG	B	3251	1/1	0.97	0.54	-	53,53,53,53	0
56	MG	GB	3464	1/1	0.97	0.14	-	83,83,83,83	0
56	MG	GB	3573	1/1	0.88	0.16	-	69,69,69,69	0
56	MG	B	3547	1/1	0.89	0.14	-	90,90,90,90	0
56	MG	RB	204	1/1	0.84	0.67	-	98,98,98,98	0
56	MG	B	3643	1/1	0.94	0.17	-	56,56,56,56	0
56	MG	GB	3156	1/1	0.92	0.48	-	46,46,46,46	0
56	MG	H	203	1/1	0.63	0.42	-	89,89,89,89	0
56	MG	GB	2980	1/1	0.90	0.68	-	43,43,43,43	0
56	MG	GB	3237	1/1	0.74	0.83	-	93,93,93,93	0
56	MG	GB	3484	1/1	0.94	0.21	-	60,60,60,60	0
56	MG	GB	3457	1/1	0.82	0.15	-	80,80,80,80	0
56	MG	B	3520	1/1	0.75	0.33	-	64,64,64,64	0
56	MG	GB	3298	1/1	0.61	0.32	-	80,80,80,80	0
56	MG	A	1707	1/1	0.86	0.34	-	79,79,79,79	0
56	MG	FB	1855	1/1	0.87	0.28	-	68,68,68,68	0
56	MG	B	3772	1/1	0.82	0.40	-	57,57,57,57	0
56	MG	B	3073	1/1	0.81	0.19	-	62,62,62,62	0
56	MG	B	3832	1/1	0.88	0.16	-	59,59,59,59	0
56	MG	A	1775	1/1	0.78	0.40	-	96,96,96,96	0
56	MG	GB	3672	1/1	0.90	0.20	-	68,68,68,68	0
56	MG	A	1672	1/1	0.83	0.73	-	105,105,105,105	0
56	MG	GB	3335	1/1	0.93	0.39	-	54,54,54,54	0
56	MG	B	3427	1/1	0.97	0.34	-	47,47,47,47	0
56	MG	A	1741	1/1	0.81	0.20	-	73,73,73,73	0
56	MG	A	1724	1/1	0.80	0.45	-	68,68,68,68	0
56	MG	GB	2927	1/1	0.89	0.35	-	62,62,62,62	0
56	MG	B	3640	1/1	0.81	0.47	-	53,53,53,53	0
56	MG	FB	1840	1/1	0.85	0.10	-	110,110,110,110	0
56	MG	B	3493	1/1	0.04	0.36	-	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3812	1/1	0.83	0.15	-	62,62,62,62	0
56	MG	FB	1726	1/1	0.76	0.49	-	94,94,94,94	0
56	MG	FB	1611	1/1	0.80	0.18	-	63,63,63,63	0
56	MG	GB	2986	1/1	0.87	0.73	-	49,49,49,49	0
56	MG	GB	3023	1/1	0.89	0.31	-	51,51,51,51	0
56	MG	B	3450	1/1	0.92	0.12	-	63,63,63,63	0
56	MG	FB	1876	1/1	0.77	0.16	-	170,170,170,170	0
56	MG	GB	3180	1/1	0.94	0.33	-	68,68,68,68	0
56	MG	C	234	1/1	0.82	0.16	-	65,65,65,65	0
56	MG	B	3129	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	A	1618	1/1	0.85	0.34	-	80,80,80,80	0
56	MG	B	3423	1/1	0.85	0.31	-	43,43,43,43	0
56	MG	B	3497	1/1	0.79	0.47	-	52,52,52,52	0
56	MG	FB	1846	1/1	0.80	0.14	-	73,73,73,73	0
56	MG	A	1621	1/1	0.82	0.26	-	85,85,85,85	0
56	MG	GB	3233	1/1	0.93	0.16	-	65,65,65,65	0
56	MG	N	202	1/1	0.83	0.20	-	71,71,71,71	0
56	MG	B	3601	1/1	0.93	0.28	-	53,53,53,53	0
56	MG	HB	226	1/1	0.50	0.38	-	105,105,105,105	0
56	MG	FB	1626	1/1	0.77	0.16	-	72,72,72,72	0
56	MG	RB	202	1/1	0.78	0.57	-	77,77,77,77	0
56	MG	B	3419	1/1	0.79	0.32	-	54,54,54,54	0
56	MG	A	1830	1/1	0.78	0.40	-	67,67,67,67	0
56	MG	GB	3474	1/1	0.69	0.44	-	69,69,69,69	0
56	MG	S	206	1/1	0.94	0.23	-	57,57,57,57	0
56	MG	GB	3318	1/1	0.92	0.68	-	54,54,54,54	0
56	MG	B	3610	1/1	0.92	0.14	-	73,73,73,73	0
56	MG	A	1855	1/1	0.95	0.42	-	89,89,89,89	0
56	MG	GB	3656	1/1	0.75	0.24	-	93,93,93,93	0
56	MG	GB	3531	1/1	0.25	0.18	-	106,106,106,106	0
56	MG	FC	101	1/1	0.90	0.15	-	87,87,87,87	0
56	MG	FB	1774	1/1	0.94	0.53	-	67,67,67,67	0
56	MG	B	3491	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	GB	3599	1/1	0.60	0.24	-	101,101,101,101	0
56	MG	WB	201	1/1	0.91	0.12	-	80,80,80,80	0
56	MG	B	3112	1/1	0.83	0.26	-	49,49,49,49	0
56	MG	IA	118	1/1	0.82	0.29	-	67,67,67,67	0
56	MG	GB	3341	1/1	0.92	0.44	-	54,54,54,54	0
56	MG	YB	203	1/1	0.90	0.14	-	86,86,86,86	0
56	MG	B	3314	1/1	0.90	0.17	-	44,44,44,44	0
56	MG	HB	211	1/1	0.70	0.67	-	87,87,87,87	0
56	MG	B	3157	1/1	0.86	0.32	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3366	1/1	0.95	0.20	-	65,65,65,65	0
56	MG	IA	110	1/1	0.91	0.27	-	83,83,83,83	0
56	MG	GB	2966	1/1	0.94	0.48	-	56,56,56,56	0
56	MG	A	1861	1/1	0.81	0.34	-	92,92,92,92	0
56	MG	GB	3588	1/1	0.54	0.51	-	69,69,69,69	0
56	MG	GB	3640	1/1	0.93	0.12	-	96,96,96,96	0
56	MG	GB	2970	1/1	0.73	0.18	-	52,52,52,52	0
56	MG	C	202	1/1	0.93	0.38	-	59,59,59,59	0
56	MG	GB	2924	1/1	0.97	0.53	-	51,51,51,51	0
56	MG	DB	101	1/1	0.84	0.67	-	119,119,119,119	0
56	MG	B	3492	1/1	0.86	0.17	-	75,75,75,75	0
56	MG	B	3435	1/1	0.78	0.47	-	63,63,63,63	0
56	MG	B	3377	1/1	0.93	0.24	-	44,44,44,44	0
56	MG	B	3127	1/1	0.87	0.14	-	55,55,55,55	0
56	MG	SC	203	1/1	0.80	0.35	-	85,85,85,85	0
56	MG	B	3616	1/1	0.94	0.08	-	95,95,95,95	0
56	MG	MB	203	1/1	0.48	0.31	-	116,116,116,116	0
56	MG	GB	3357	1/1	0.96	0.18	-	152,152,152,152	0
56	MG	GB	2958	1/1	0.71	0.80	-	65,65,65,65	0
56	MG	GB	3205	1/1	0.88	0.15	-	71,71,71,71	0
56	MG	FB	1744	1/1	0.97	0.26	-	55,55,55,55	0
56	MG	B	3254	1/1	0.90	0.35	-	61,61,61,61	0
56	MG	B	2913	1/1	0.95	0.36	-	38,38,38,38	0
56	MG	C	214	1/1	0.82	0.24	-	79,79,79,79	0
56	MG	GB	3451	1/1	0.88	0.24	-	79,79,79,79	0
56	MG	B	3252	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	GB	3340	1/1	0.94	0.18	-	66,66,66,66	0
56	MG	B	3283	1/1	0.85	0.37	-	92,92,92,92	0
56	MG	B	3205	1/1	0.87	0.73	-	68,68,68,68	0
56	MG	B	3765	1/1	0.91	0.34	-	50,50,50,50	0
56	MG	A	1679	1/1	0.82	0.27	-	95,95,95,95	0
56	MG	IA	101	1/1	0.85	0.08	-	67,67,67,67	0
56	MG	NC	110	1/1	0.90	0.16	-	69,69,69,69	0
56	MG	GB	3096	1/1	0.89	0.34	-	56,56,56,56	0
56	MG	GB	3693	1/1	0.81	0.20	-	69,69,69,69	0
56	MG	GB	3412	1/1	0.93	0.09	-	75,75,75,75	0
56	MG	FB	1819	1/1	0.89	0.31	-	71,71,71,71	0
56	MG	A	1705	1/1	0.93	0.14	-	66,66,66,66	0
56	MG	IB	102	1/1	0.91	0.23	-	112,112,112,112	0
56	MG	GB	3270	1/1	0.59	0.24	-	97,97,97,97	0
56	MG	GB	3042	1/1	0.87	0.25	-	54,54,54,54	0
56	MG	B	3287	1/1	0.75	0.88	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3684	1/1	0.96	0.08	-	61,61,61,61	0
56	MG	B	3658	1/1	0.94	0.29	-	54,54,54,54	0
56	MG	B	3680	1/1	0.91	0.21	-	52,52,52,52	0
56	MG	A	1873	1/1	0.86	0.61	-	80,80,80,80	0
56	MG	B	3235	1/1	0.61	0.43	-	72,72,72,72	0
56	MG	RB	201	1/1	0.82	0.20	-	71,71,71,71	0
56	MG	FB	1772	1/1	0.77	0.26	-	68,68,68,68	0
56	MG	B	3481	1/1	0.89	0.22	-	54,54,54,54	0
56	MG	PA	201	1/1	0.60	0.25	-	99,99,99,99	0
56	MG	C	226	1/1	0.97	0.10	-	89,89,89,89	0
56	MG	B	3421	1/1	0.96	0.10	-	80,80,80,80	0
56	MG	GB	3452	1/1	0.30	0.68	-	74,74,74,74	0
56	MG	GB	2940	1/1	0.69	0.44	-	79,79,79,79	0
56	MG	FB	1724	1/1	0.82	0.13	-	142,142,142,142	0
56	MG	J	201	1/1	0.89	0.15	-	84,84,84,84	0
56	MG	B	3750	1/1	0.93	0.31	-	57,57,57,57	0
56	MG	IA	121	1/1	0.95	0.14	-	79,79,79,79	0
56	MG	B	3167	1/1	0.92	0.25	-	44,44,44,44	0
56	MG	B	3508	1/1	0.88	0.12	-	65,65,65,65	0
56	MG	GB	3094	1/1	0.90	0.38	-	54,54,54,54	0
56	MG	B	3163	1/1	0.89	0.28	-	49,49,49,49	0
56	MG	B	3166	1/1	0.41	0.25	-	93,93,93,93	0
56	MG	A	1623	1/1	0.85	0.52	-	67,67,67,67	0
56	MG	RA	204	1/1	0.75	0.20	-	137,137,137,137	0
56	MG	UA	201	1/1	0.80	0.13	-	75,75,75,75	0
56	MG	FB	1705	1/1	0.94	0.12	-	60,60,60,60	0
56	MG	A	1793	1/1	0.97	0.11	-	116,116,116,116	0
56	MG	GB	3635	1/1	0.72	0.49	-	78,78,78,78	0
56	MG	FB	1664	1/1	0.93	0.32	-	85,85,85,85	0
56	MG	B	3787	1/1	0.83	0.10	-	132,132,132,132	0
56	MG	GB	3138	1/1	0.96	0.30	-	67,67,67,67	0
56	MG	B	3432	1/1	0.81	0.22	-	68,68,68,68	0
56	MG	NB	201	1/1	0.72	0.43	-	130,130,130,130	0
56	MG	B	3465	1/1	0.83	0.13	-	91,91,91,91	0
56	MG	B	3538	1/1	0.93	0.24	-	57,57,57,57	0
56	MG	B	3454	1/1	0.83	0.87	-	67,67,67,67	0
56	MG	FB	1915	1/1	0.60	0.42	-	87,87,87,87	0
56	MG	FB	1940	1/1	0.80	0.16	-	94,94,94,94	0
56	MG	B	3708	1/1	0.69	0.13	-	71,71,71,71	0
56	MG	B	3540	1/1	0.88	0.09	-	85,85,85,85	0
56	MG	B	3596	1/1	0.69	0.44	-	55,55,55,55	0
56	MG	FB	1685	1/1	0.68	0.28	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3586	1/1	0.86	0.14	-	116,116,116,116	0
56	MG	B	3269	1/1	0.91	0.49	-	52,52,52,52	0
56	MG	B	3351	1/1	0.65	0.19	-	77,77,77,77	0
56	MG	GB	3246	1/1	0.86	0.10	-	79,79,79,79	0
56	MG	C	229	1/1	0.84	0.57	-	80,80,80,80	0
56	MG	FB	1910	1/1	0.57	0.52	-	78,78,78,78	0
56	MG	XC	201	1/1	0.55	0.53	-	112,112,112,112	0
56	MG	GB	3585	1/1	0.47	0.17	-	158,158,158,158	0
56	MG	B	3316	1/1	0.87	0.36	-	35,35,35,35	0
56	MG	A	1849	1/1	0.70	0.53	-	88,88,88,88	0
56	MG	B	3546	1/1	0.69	0.57	-	47,47,47,47	0
56	MG	B	3307	1/1	0.80	0.20	-	81,81,81,81	0
56	MG	GB	3273	1/1	0.84	0.26	-	54,54,54,54	0
56	MG	B	2962	1/1	0.74	0.62	-	43,43,43,43	0
56	MG	B	3348	1/1	0.94	0.80	-	55,55,55,55	0
56	MG	C	201	1/1	0.89	0.34	-	67,67,67,67	0
56	MG	FB	1890	1/1	0.92	0.26	-	60,60,60,60	0
56	MG	B	3604	1/1	0.79	0.34	-	60,60,60,60	0
56	MG	GB	3440	1/1	0.65	0.60	-	80,80,80,80	0
56	MG	C	239	1/1	0.86	0.16	-	87,87,87,87	0
56	MG	GB	3140	1/1	0.83	0.13	-	74,74,74,74	0
56	MG	B	3807	1/1	0.74	0.33	-	92,92,92,92	0
56	MG	OC	406	1/1	0.89	0.13	-	70,70,70,70	0
56	MG	FB	1795	1/1	0.85	0.17	-	61,61,61,61	0
56	MG	B	3148	1/1	0.95	0.06	-	67,67,67,67	0
56	MG	A	1879	1/1	0.90	0.40	-	65,65,65,65	0
56	MG	B	3155	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	B	3426	1/1	0.70	0.85	-	57,57,57,57	0
56	MG	B	3360	1/1	0.93	0.22	-	43,43,43,43	0
56	MG	A	1653	1/1	0.96	0.71	-	74,74,74,74	0
56	MG	GB	2921	1/1	0.73	0.57	-	72,72,72,72	0
56	MG	DD	101	1/1	0.89	0.67	-	71,71,71,71	0
56	MG	B	3151	1/1	0.82	0.11	-	55,55,55,55	0
56	MG	HB	232	1/1	0.91	0.23	-	84,84,84,84	0
56	MG	B	3560	1/1	0.89	0.20	-	114,114,114,114	0
56	MG	U	102	1/1	0.89	0.41	-	55,55,55,55	0
56	MG	B	3670	1/1	0.93	0.44	-	52,52,52,52	0
56	MG	EA	101	1/1	0.85	0.57	-	45,45,45,45	0
56	MG	B	3204	1/1	0.84	0.28	-	40,40,40,40	0
56	MG	GB	3253	1/1	0.87	0.10	-	76,76,76,76	0
56	MG	A	1721	1/1	0.83	0.40	-	97,97,97,97	0
56	MG	FB	1813	1/1	0.88	0.16	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	K	201	1/1	0.91	0.22	-	58,58,58,58	0
56	MG	A	1648	1/1	0.83	0.38	-	100,100,100,100	0
56	MG	B	3721	1/1	0.36	0.77	-	147,147,147,147	0
56	MG	B	3244	1/1	0.94	0.39	-	53,53,53,53	0
56	MG	A	1740	1/1	0.90	0.17	-	80,80,80,80	0
56	MG	FB	1777	1/1	0.86	0.29	-	97,97,97,97	0
56	MG	O	203	1/1	0.86	0.19	-	65,65,65,65	0
56	MG	GB	3276	1/1	0.94	0.12	-	79,79,79,79	0
56	MG	B	3032	1/1	0.95	0.34	-	43,43,43,43	0
56	MG	GB	3040	1/1	0.92	0.72	-	48,48,48,48	0
56	MG	B	3195	1/1	0.93	0.34	-	52,52,52,52	0
56	MG	PA	202	1/1	0.94	0.38	-	102,102,102,102	0
56	MG	B	3580	1/1	0.80	0.27	-	58,58,58,58	0
56	MG	HB	208	1/1	0.14	0.32	-	126,126,126,126	0
56	MG	B	3215	1/1	0.93	0.37	-	47,47,47,47	0
56	MG	B	3650	1/1	0.91	0.66	-	58,58,58,58	0
56	MG	FB	1758	1/1	0.88	0.35	-	129,129,129,129	0
56	MG	A	1796	1/1	0.88	0.61	-	61,61,61,61	0
56	MG	SC	205	1/1	0.69	0.14	-	99,99,99,99	0
56	MG	A	1818	1/1	0.91	0.33	-	65,65,65,65	0
56	MG	A	1885	1/1	0.74	0.20	-	135,135,135,135	0
56	MG	B	3367	1/1	0.93	0.15	-	63,63,63,63	0
56	MG	GB	3425	1/1	0.84	0.41	-	58,58,58,58	0
56	MG	A	1812	1/1	0.52	0.32	-	128,128,128,128	0
56	MG	B	3117	1/1	0.95	0.45	-	48,48,48,48	0
56	MG	A	1748	1/1	0.89	0.76	-	76,76,76,76	0
56	MG	B	3007	1/1	0.83	0.34	-	51,51,51,51	0
56	MG	B	3099	1/1	0.90	0.38	-	37,37,37,37	0
56	MG	A	1642	1/1	0.73	0.20	-	125,125,125,125	0
56	MG	B	3328	1/1	0.72	0.17	-	72,72,72,72	0
56	MG	B	3697	1/1	0.91	0.49	-	56,56,56,56	0
56	MG	GB	3423	1/1	0.64	0.32	-	75,75,75,75	0
56	MG	A	1671	1/1	0.72	0.73	-	94,94,94,94	0
56	MG	GB	2908	1/1	0.86	0.76	-	44,44,44,44	0
56	MG	BC	305	1/1	0.82	0.06	-	110,110,110,110	0
56	MG	GB	2901	1/1	0.94	0.19	-	58,58,58,58	0
56	MG	FB	1792	1/1	0.65	0.42	-	165,165,165,165	0
56	MG	GB	3004	1/1	0.71	0.49	-	60,60,60,60	0
56	MG	A	1629	1/1	0.85	0.53	-	67,67,67,67	0
56	MG	G	3206	1/1	0.97	0.21	-	58,58,58,58	0
56	MG	A	1757	1/1	0.87	0.10	-	118,118,118,118	0
56	MG	GB	3274	1/1	0.84	0.22	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3780	1/1	0.92	0.09	-	70,70,70,70	0
56	MG	A	1874	1/1	0.68	0.45	-	126,126,126,126	0
56	MG	GB	3089	1/1	0.94	0.13	-	66,66,66,66	0
56	MG	B	3656	1/1	0.93	0.52	-	59,59,59,59	0
56	MG	GB	2985	1/1	0.82	0.44	-	58,58,58,58	0
56	MG	FB	1733	1/1	0.94	0.13	-	62,62,62,62	0
56	MG	EC	101	1/1	0.88	0.10	-	95,95,95,95	0
56	MG	FB	1836	1/1	0.81	0.19	-	66,66,66,66	0
56	MG	GB	3558	1/1	0.86	0.33	-	98,98,98,98	0
56	MG	B	3263	1/1	0.83	0.16	-	69,69,69,69	0
56	MG	B	3395	1/1	0.88	0.58	-	58,58,58,58	0
56	MG	B	3710	1/1	0.86	0.55	-	69,69,69,69	0
56	MG	FB	1709	1/1	0.76	0.22	-	130,130,130,130	0
56	MG	B	3591	1/1	0.91	0.25	-	61,61,61,61	0
56	MG	N	206	1/1	0.94	0.35	-	69,69,69,69	0
56	MG	B	3489	1/1	0.96	0.75	-	40,40,40,40	0
56	MG	FB	1682	1/1	0.91	0.24	-	64,64,64,64	0
56	MG	GB	3692	1/1	0.78	0.65	-	81,81,81,81	0
56	MG	A	1767	1/1	0.95	0.11	-	77,77,77,77	0
56	MG	GB	3582	1/1	0.80	0.21	-	68,68,68,68	0
56	MG	FB	1874	1/1	0.70	0.42	-	69,69,69,69	0
56	MG	GB	3254	1/1	0.89	0.15	-	62,62,62,62	0
56	MG	B	3733	1/1	0.83	0.30	-	54,54,54,54	0
56	MG	KA	302	1/1	0.80	0.25	-	123,123,123,123	0
56	MG	FB	1945	1/1	0.93	0.14	-	68,68,68,68	0
56	MG	GB	3690	1/1	0.79	0.33	-	64,64,64,64	0
56	MG	A	1860	1/1	0.81	0.70	-	81,81,81,81	0
56	MG	B	2969	1/1	0.94	0.37	-	57,57,57,57	0
56	MG	GB	3114	1/1	0.90	0.20	-	69,69,69,69	0
56	MG	A	1646	1/1	0.93	0.17	-	74,74,74,74	0
56	MG	B	3241	1/1	0.89	0.12	-	77,77,77,77	0
56	MG	GB	3330	1/1	0.57	0.24	-	79,79,79,79	0
56	MG	I	205	1/1	0.75	0.24	-	69,69,69,69	0
56	MG	JB	305	1/1	0.71	0.33	-	76,76,76,76	0
56	MG	GB	3708	1/1	0.96	0.30	-	71,71,71,71	0
56	MG	FB	1632	1/1	0.89	0.31	-	69,69,69,69	0
56	MG	B	3625	1/1	0.85	0.19	-	58,58,58,58	0
56	MG	B	3543	1/1	0.97	0.15	-	44,44,44,44	0
56	MG	B	3542	1/1	0.96	0.30	-	66,66,66,66	0
56	MG	A	1730	1/1	0.87	0.21	-	81,81,81,81	0
56	MG	FB	1863	1/1	0.84	0.76	-	72,72,72,72	0
56	MG	A	1765	1/1	0.80	0.12	-	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3720	1/1	0.79	0.30	-	59,59,59,59	0
56	MG	FB	1718	1/1	0.90	0.21	-	66,66,66,66	0
56	MG	A	1807	1/1	0.95	0.42	-	87,87,87,87	0
56	MG	FB	1756	1/1	0.73	0.28	-	68,68,68,68	0
56	MG	GB	3209	1/1	-0.26	0.50	-	133,133,133,133	0
56	MG	B	3608	1/1	0.79	0.43	-	63,63,63,63	0
56	MG	GB	2979	1/1	0.73	0.83	-	52,52,52,52	0
56	MG	S	204	1/1	0.79	0.19	-	60,60,60,60	0
56	MG	GB	3552	1/1	0.90	0.17	-	68,68,68,68	0
56	MG	GB	3459	1/1	0.64	0.16	-	140,140,140,140	0
56	MG	GB	3054	1/1	0.92	0.10	-	56,56,56,56	0
56	MG	GB	3190	1/1	0.53	0.42	-	71,71,71,71	0
56	MG	FB	1896	1/1	0.26	0.32	-	82,82,82,82	0
56	MG	FB	1921	1/1	0.90	0.28	-	78,78,78,78	0
56	MG	UA	202	1/1	0.64	0.27	-	79,79,79,79	0
56	MG	CC	101	1/1	0.93	0.31	-	66,66,66,66	0
56	MG	GB	3226	1/1	0.81	0.56	-	67,67,67,67	0
56	MG	JA	408	1/1	0.80	0.28	-	97,97,97,97	0
56	MG	B	3613	1/1	0.86	0.13	-	55,55,55,55	0
56	MG	KA	303	1/1	0.79	0.11	-	130,130,130,130	0
56	MG	A	1848	1/1	0.83	0.34	-	70,70,70,70	0
56	MG	GB	3538	1/1	0.94	0.31	-	58,58,58,58	0
56	MG	A	1685	1/1	0.55	0.60	-	76,76,76,76	0
56	MG	B	3842	1/1	0.83	0.52	-	60,60,60,60	0
56	MG	B	3756	1/1	0.90	0.22	-	59,59,59,59	0
56	MG	FB	1694	1/1	0.91	0.41	-	81,81,81,81	0
56	MG	B	3193	1/1	0.84	0.12	-	54,54,54,54	0
56	MG	FB	1885	1/1	0.68	0.48	-	115,115,115,115	0
56	MG	HB	218	1/1	0.92	0.23	-	116,116,116,116	0
56	MG	B	3524	1/1	0.96	0.23	-	48,48,48,48	0
56	MG	GB	3535	1/1	0.86	0.21	-	83,83,83,83	0
56	MG	HA	102	1/1	0.77	0.45	-	69,69,69,69	0
56	MG	GB	3155	1/1	0.84	0.18	-	89,89,89,89	0
56	MG	FB	1684	1/1	0.73	0.73	-	79,79,79,79	0
56	MG	GB	2965	1/1	0.93	0.26	-	54,54,54,54	0
56	MG	B	3257	1/1	0.96	0.24	-	54,54,54,54	0
56	MG	MA	303	1/1	0.66	0.17	-	101,101,101,101	0
56	MG	B	3667	1/1	0.37	0.21	-	145,145,145,145	0
56	MG	GB	3227	1/1	0.69	0.11	-	95,95,95,95	0
56	MG	B	3033	1/1	0.93	0.30	-	50,50,50,50	0
56	MG	GB	3170	1/1	0.70	0.28	-	77,77,77,77	0
56	MG	A	1675	1/1	0.66	0.42	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	102	1/1	0.61	0.26	-	83,83,83,83	0
56	MG	A	1827	1/1	0.82	0.60	-	85,85,85,85	0
56	MG	B	2958	1/1	0.91	0.43	-	49,49,49,49	0
56	MG	GB	3705	1/1	0.25	0.18	-	104,104,104,104	0
56	MG	I	206	1/1	0.83	0.20	-	74,74,74,74	0
56	MG	GB	3426	1/1	0.72	0.21	-	117,117,117,117	0
56	MG	B	3623	1/1	0.85	0.19	-	64,64,64,64	0
56	MG	FB	1859	1/1	0.86	1.02	-	83,83,83,83	0
56	MG	NC	108	1/1	0.86	0.67	-	81,81,81,81	0
56	MG	GB	3389	1/1	0.80	0.12	-	74,74,74,74	0
56	MG	B	3353	1/1	0.90	0.06	-	173,173,173,173	0
56	MG	B	2978	1/1	0.96	0.31	-	44,44,44,44	0
56	MG	FB	1802	1/1	0.84	0.13	-	64,64,64,64	0
56	MG	FB	1778	1/1	0.83	0.64	-	83,83,83,83	0
56	MG	A	1657	1/1	0.88	0.58	-	90,90,90,90	0
56	MG	B	3190	1/1	0.89	0.33	-	57,57,57,57	0
56	MG	B	3748	1/1	0.87	1.34	-	65,65,65,65	0
56	MG	A	1862	1/1	0.83	0.44	-	60,60,60,60	0
56	MG	FB	1805	1/1	0.43	0.60	-	74,74,74,74	0
56	MG	A	1756	1/1	0.90	0.11	-	66,66,66,66	0
56	MG	GB	3120	1/1	0.95	0.27	-	79,79,79,79	0
56	MG	UC	202	1/1	0.86	0.20	-	105,105,105,105	0
56	MG	B	3548	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	GB	3514	1/1	0.86	0.34	-	67,67,67,67	0
56	MG	A	1787	1/1	0.92	0.43	-	77,77,77,77	0
56	MG	FB	1804	1/1	0.90	0.17	-	81,81,81,81	0
56	MG	B	3630	1/1	0.82	0.46	-	39,39,39,39	0
56	MG	GB	3616	1/1	0.87	0.27	-	81,81,81,81	0
56	MG	GB	3360	1/1	0.47	0.23	-	84,84,84,84	0
56	MG	Z	103	1/1	0.87	0.08	-	74,74,74,74	0
56	MG	GB	3159	1/1	0.87	0.38	-	81,81,81,81	0
56	MG	A	1667	1/1	0.85	0.63	-	82,82,82,82	0
56	MG	A	1769	1/1	0.84	0.26	-	85,85,85,85	0
56	MG	A	1749	1/1	0.73	0.33	-	110,110,110,110	0
56	MG	GB	2928	1/1	0.96	0.46	-	77,77,77,77	0
56	MG	B	2925	1/1	0.90	0.35	-	52,52,52,52	0
56	MG	B	3570	1/1	0.94	0.18	-	65,65,65,65	0
56	MG	GB	3351	1/1	0.79	0.25	-	83,83,83,83	0
56	MG	K	209	1/1	0.91	0.14	-	67,67,67,67	0
56	MG	A	1716	1/1	0.85	0.20	-	78,78,78,78	0
56	MG	B	3562	1/1	0.81	0.18	-	73,73,73,73	0
56	MG	FB	1865	1/1	0.94	0.38	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	C	217	1/1	0.88	0.42	-	60,60,60,60	0
56	MG	A	1674	1/1	0.73	0.34	-	65,65,65,65	0
56	MG	GB	3662	1/1	0.75	0.10	-	117,117,117,117	0
56	MG	NC	107	1/1	0.93	0.14	-	96,96,96,96	0
56	MG	GB	3091	1/1	0.97	0.22	-	57,57,57,57	0
56	MG	JB	306	1/1	0.80	0.20	-	69,69,69,69	0
56	MG	B	3380	1/1	0.89	0.16	-	51,51,51,51	0
56	MG	HB	220	1/1	0.87	0.28	-	92,92,92,92	0
56	MG	B	3059	1/1	0.97	0.27	-	43,43,43,43	0
56	MG	B	3692	1/1	0.98	0.20	-	51,51,51,51	0
56	MG	B	3655	1/1	0.91	0.34	-	46,46,46,46	0
56	MG	HB	212	1/1	0.76	0.29	-	85,85,85,85	0
56	MG	A	1699	1/1	0.83	0.17	-	92,92,92,92	0
56	MG	B	3766	1/1	0.91	0.33	-	42,42,42,42	0
56	MG	HB	209	1/1	0.86	0.32	-	81,81,81,81	0
56	MG	B	3304	1/1	0.96	0.60	-	43,43,43,43	0
56	MG	B	3076	1/1	0.94	0.33	-	45,45,45,45	0
56	MG	GB	3443	1/1	0.73	0.39	-	69,69,69,69	0
56	MG	A	1692	1/1	0.93	0.61	-	63,63,63,63	0
56	MG	A	1615	1/1	0.66	0.31	-	89,89,89,89	0
56	MG	PC	303	1/1	0.45	0.18	-	133,133,133,133	0
56	MG	A	1883	1/1	0.93	0.38	-	79,79,79,79	0
56	MG	LB	301	1/1	0.86	0.23	-	60,60,60,60	0
56	MG	C	205	1/1	0.91	0.85	-	68,68,68,68	0
56	MG	A	1832	1/1	0.91	0.31	-	67,67,67,67	0
56	MG	FB	1871	1/1	0.23	0.91	-	114,114,114,114	0
56	MG	GB	3407	1/1	0.88	0.24	-	54,54,54,54	0
56	MG	GB	3095	1/1	0.82	0.61	-	63,63,63,63	0
56	MG	GB	2915	1/1	0.91	0.55	-	52,52,52,52	0
56	MG	C	230	1/1	0.82	0.17	-	69,69,69,69	0
56	MG	B	3809	1/1	0.80	0.25	-	66,66,66,66	0
56	MG	GB	3348	1/1	0.93	0.20	-	59,59,59,59	0
56	MG	B	3561	1/1	0.94	0.99	-	52,52,52,52	0
56	MG	GB	3561	1/1	0.82	0.38	-	68,68,68,68	0
56	MG	B	3665	1/1	0.86	0.15	-	56,56,56,56	0
56	MG	FB	1633	1/1	0.79	0.76	-	68,68,68,68	0
56	MG	GB	3339	1/1	0.43	0.47	-	67,67,67,67	0
56	MG	GB	3258	1/1	0.81	0.31	-	74,74,74,74	0
56	MG	B	3662	1/1	0.87	0.35	-	65,65,65,65	0
56	MG	B	3726	1/1	0.98	0.33	-	50,50,50,50	0
56	MG	GB	3486	1/1	0.87	0.19	-	68,68,68,68	0
56	MG	FB	1648	1/1	0.92	0.32	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	FB	1643	1/1	0.61	0.70	-	94,94,94,94	0
56	MG	B	3133	1/1	0.93	0.21	-	50,50,50,50	0
56	MG	JB	313	1/1	0.85	0.60	-	68,68,68,68	0
56	MG	B	3440	1/1	0.79	0.55	-	59,59,59,59	0
56	MG	B	3478	1/1	0.86	0.22	-	50,50,50,50	0
56	MG	B	3182	1/1	0.91	0.37	-	50,50,50,50	0
56	MG	A	1817	1/1	0.83	0.40	-	66,66,66,66	0
56	MG	B	2981	1/1	0.90	0.50	-	41,41,41,41	0
56	MG	B	3466	1/1	0.89	0.18	-	51,51,51,51	0
56	MG	GB	3658	1/1	0.83	0.40	-	95,95,95,95	0
56	MG	A	1824	1/1	0.75	0.55	-	111,111,111,111	0
56	MG	B	3534	1/1	0.95	0.40	-	45,45,45,45	0
56	MG	KA	301	1/1	0.62	0.23	-	118,118,118,118	0
56	MG	A	1633	1/1	0.82	0.41	-	86,86,86,86	0
56	MG	B	3728	1/1	0.93	0.41	-	50,50,50,50	0
56	MG	FB	1619	1/1	0.98	0.28	-	58,58,58,58	0
56	MG	B	3095	1/1	0.91	0.16	-	56,56,56,56	0
56	MG	A	1668	1/1	0.82	0.36	-	80,80,80,80	0
56	MG	A	1867	1/1	0.77	0.20	-	64,64,64,64	0
56	MG	JA	411	1/1	0.60	0.28	-	100,100,100,100	0
56	MG	GB	3379	1/1	0.84	0.48	-	64,64,64,64	0
56	MG	A	1697	1/1	0.53	0.87	-	78,78,78,78	0
56	MG	GB	3511	1/1	0.82	0.22	-	82,82,82,82	0
56	MG	B	3588	1/1	0.90	0.52	-	46,46,46,46	0
56	MG	FB	1651	1/1	0.75	1.15	-	90,90,90,90	0
56	MG	FB	1698	1/1	0.94	0.17	-	82,82,82,82	0
56	MG	B	3744	1/1	0.81	0.29	-	48,48,48,48	0
56	MG	CD	101	1/1	0.89	0.34	-	77,77,77,77	0
56	MG	FB	1628	1/1	0.83	0.26	-	81,81,81,81	0
56	MG	GB	3294	1/1	0.84	0.28	-	64,64,64,64	0
56	MG	B	3767	1/1	0.89	0.14	-	60,60,60,60	0
56	MG	FB	1875	1/1	0.88	0.21	-	72,72,72,72	0
56	MG	Z	101	1/1	0.80	0.17	-	76,76,76,76	0
56	MG	YA	101	1/1	0.90	0.31	-	98,98,98,98	0
56	MG	DA	104	1/1	0.73	0.22	-	71,71,71,71	0
56	MG	FB	1858	1/1	0.92	0.20	-	97,97,97,97	0
56	MG	B	3679	1/1	0.93	0.08	-	66,66,66,66	0
56	MG	K	206	1/1	0.80	0.18	-	73,73,73,73	0
56	MG	GB	3704	1/1	0.87	1.01	-	86,86,86,86	0
56	MG	FB	1868	1/1	0.48	1.02	-	87,87,87,87	0
56	MG	GB	3647	1/1	0.78	0.75	-	77,77,77,77	0
56	MG	B	3055	1/1	0.98	0.37	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3785	1/1	0.77	0.33	-	61,61,61,61	0
56	MG	GB	3432	1/1	0.88	0.91	-	49,49,49,49	0
56	MG	B	3005	1/1	0.92	0.54	-	45,45,45,45	0
56	MG	GB	3036	1/1	0.84	0.15	-	58,58,58,58	0
56	MG	B	3448	1/1	0.88	0.27	-	58,58,58,58	0
56	MG	A	1760	1/1	0.43	0.24	-	136,136,136,136	0
56	MG	B	3120	1/1	0.69	0.55	-	56,56,56,56	0
56	MG	B	3504	1/1	0.88	0.23	-	45,45,45,45	0
56	MG	QB	206	1/1	0.94	0.43	-	63,63,63,63	0
56	MG	C	238	1/1	0.93	0.09	-	91,91,91,91	0
56	MG	A	1842	1/1	0.96	0.15	-	67,67,67,67	0
56	MG	CD	102	1/1	0.69	0.19	-	75,75,75,75	0
56	MG	FB	1926	1/1	0.89	0.33	-	85,85,85,85	0
56	MG	FB	1928	1/1	0.85	0.22	-	62,62,62,62	0
56	MG	GB	3291	1/1	0.84	0.16	-	73,73,73,73	0
56	MG	A	1882	1/1	0.68	0.27	-	104,104,104,104	0
56	MG	A	1728	1/1	0.87	0.18	-	61,61,61,61	0
56	MG	B	3331	1/1	0.87	0.40	-	49,49,49,49	0
56	MG	GB	3248	1/1	0.86	0.34	-	60,60,60,60	0
56	MG	A	1828	1/1	0.86	0.19	-	106,106,106,106	0
56	MG	B	3490	1/1	0.85	0.29	-	44,44,44,44	0
56	MG	GB	3325	1/1	0.85	0.40	-	54,54,54,54	0
56	MG	B	3211	1/1	0.66	0.21	-	65,65,65,65	0
56	MG	FB	1610	1/1	0.95	0.19	-	68,68,68,68	0
56	MG	B	2954	1/1	0.96	0.56	-	42,42,42,42	0
56	MG	A	1624	1/1	0.89	0.34	-	63,63,63,63	0
56	MG	FB	1673	1/1	0.95	0.67	-	113,113,113,113	0
56	MG	GB	3490	1/1	0.74	0.58	-	63,63,63,63	0
56	MG	B	3280	1/1	0.86	0.42	-	87,87,87,87	0
56	MG	GB	3044	1/1	0.93	0.63	-	57,57,57,57	0
56	MG	B	3227	1/1	0.88	0.25	-	44,44,44,44	0
56	MG	GB	3434	1/1	0.92	0.11	-	63,63,63,63	0
56	MG	IA	115	1/1	0.88	0.19	-	73,73,73,73	0
56	MG	B	3162	1/1	0.86	0.68	-	43,43,43,43	0
56	MG	HB	216	1/1	0.90	0.56	-	136,136,136,136	0
56	MG	A	1762	1/1	0.89	0.42	-	93,93,93,93	0
56	MG	GB	3679	1/1	0.93	0.72	-	72,72,72,72	0
56	MG	B	3645	1/1	0.88	0.32	-	70,70,70,70	0
56	MG	GB	3623	1/1	0.78	0.24	-	63,63,63,63	0
56	MG	B	3695	1/1	0.66	0.81	-	71,71,71,71	0
56	MG	GB	3131	1/1	0.95	0.21	-	71,71,71,71	0
56	MG	GB	3022	1/1	0.89	0.56	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3436	1/1	0.78	0.20	-	81,81,81,81	0
56	MG	B	3634	1/1	0.31	0.19	-	106,106,106,106	0
56	MG	A	1758	1/1	0.95	0.39	-	77,77,77,77	0
56	MG	B	2963	1/1	0.91	0.37	-	49,49,49,49	0
56	MG	GB	2957	1/1	0.86	0.59	-	51,51,51,51	0
56	MG	GB	2952	1/1	0.73	0.41	-	63,63,63,63	0
56	MG	GB	2972	1/1	0.90	0.62	-	51,51,51,51	0
56	MG	B	3502	1/1	0.94	0.13	-	48,48,48,48	0
56	MG	GB	3215	1/1	0.88	0.44	-	55,55,55,55	0
56	MG	GB	3186	1/1	0.70	0.27	-	63,63,63,63	0
56	MG	B	3624	1/1	0.89	0.66	-	66,66,66,66	0
56	MG	B	3574	1/1	0.88	0.29	-	117,117,117,117	0
56	MG	C	222	1/1	0.96	0.09	-	105,105,105,105	0
56	MG	GB	3462	1/1	0.45	0.80	-	101,101,101,101	0
56	MG	GB	3277	1/1	0.87	0.24	-	54,54,54,54	0
56	MG	B	3648	1/1	0.51	0.53	-	146,146,146,146	0
56	MG	ED	202	1/1	0.89	0.38	-	72,72,72,72	0
56	MG	A	1651	1/1	0.86	0.37	-	97,97,97,97	0
56	MG	B	3393	1/1	0.90	0.18	-	46,46,46,46	0
56	MG	B	3106	1/1	0.75	0.25	-	58,58,58,58	0
56	MG	B	3083	1/1	0.98	0.15	-	40,40,40,40	0
56	MG	FB	1930	1/1	0.73	0.51	-	68,68,68,68	0
56	MG	W	306	1/1	0.87	0.19	-	77,77,77,77	0
56	MG	FB	1634	1/1	0.52	0.20	-	80,80,80,80	0
56	MG	A	1776	1/1	0.76	1.04	-	78,78,78,78	0
56	MG	GB	3406	1/1	0.85	0.33	-	59,59,59,59	0
56	MG	A	1822	1/1	0.81	0.78	-	72,72,72,72	0
56	MG	B	3611	1/1	0.93	0.21	-	48,48,48,48	0
56	MG	HB	213	1/1	0.92	0.27	-	122,122,122,122	0
56	MG	B	3559	1/1	0.80	0.11	-	63,63,63,63	0
56	MG	GB	3545	1/1	0.91	0.29	-	77,77,77,77	0
56	MG	GB	3278	1/1	0.61	0.43	-	75,75,75,75	0
56	MG	B	3253	1/1	0.90	0.28	-	53,53,53,53	0
56	MG	CD	103	1/1	0.81	0.29	-	84,84,84,84	0
56	MG	A	1854	1/1	0.90	0.18	-	75,75,75,75	0
56	MG	FB	1674	1/1	0.91	0.11	-	69,69,69,69	0
56	MG	B	3626	1/1	0.88	0.23	-	54,54,54,54	0
56	MG	A	1798	1/1	0.58	0.54	-	70,70,70,70	0
56	MG	GB	3694	1/1	0.86	0.47	-	61,61,61,61	0
56	MG	A	1838	1/1	0.94	0.25	-	106,106,106,106	0
56	MG	HB	204	1/1	0.52	0.32	-	91,91,91,91	0
56	MG	GB	2937	1/1	0.93	0.19	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	FB	1826	1/1	0.92	0.11	-	143,143,143,143	0
56	MG	B	3286	1/1	0.94	0.27	-	41,41,41,41	0
56	MG	B	3361	1/1	0.79	0.33	-	72,72,72,72	0
56	MG	GB	3609	1/1	0.96	0.19	-	73,73,73,73	0
56	MG	A	1638	1/1	0.89	0.43	-	61,61,61,61	0
56	MG	GB	3084	1/1	0.83	0.28	-	79,79,79,79	0
56	MG	FB	1886	1/1	0.94	0.15	-	82,82,82,82	0
56	MG	GB	3344	1/1	0.91	0.35	-	77,77,77,77	0
56	MG	GB	3557	1/1	0.81	0.24	-	76,76,76,76	0
56	MG	B	3585	1/1	0.94	0.26	-	49,49,49,49	0
56	MG	DC	102	1/1	0.86	0.25	-	78,78,78,78	0
56	MG	GB	3560	1/1	0.94	0.30	-	60,60,60,60	0
56	MG	Q	201	1/1	0.95	0.31	-	62,62,62,62	0
56	MG	GB	3117	1/1	0.49	0.36	-	82,82,82,82	0
56	MG	FB	1725	1/1	0.92	0.44	-	68,68,68,68	0
56	MG	GB	3375	1/1	0.82	0.19	-	76,76,76,76	0
56	MG	GB	3539	1/1	0.88	0.20	-	68,68,68,68	0
56	MG	FB	1807	1/1	0.79	0.72	-	97,97,97,97	0
56	MG	GB	3471	1/1	0.92	0.32	-	64,64,64,64	0
56	MG	B	3629	1/1	0.20	0.20	-	125,125,125,125	0
56	MG	FB	1646	1/1	0.80	0.35	-	81,81,81,81	0
56	MG	X	103	1/1	0.91	0.17	-	64,64,64,64	0
56	MG	GB	3666	1/1	0.67	0.14	-	125,125,125,125	0
56	MG	FB	1771	1/1	0.77	0.54	-	83,83,83,83	0
56	MG	FB	1776	1/1	0.84	0.30	-	67,67,67,67	0
56	MG	GB	3391	1/1	0.92	0.23	-	60,60,60,60	0
56	MG	T	203	1/1	0.82	0.18	-	58,58,58,58	0
56	MG	R	201	1/1	0.70	0.43	-	54,54,54,54	0
56	MG	FB	1894	1/1	0.80	0.43	-	70,70,70,70	0
56	MG	E	304	1/1	0.88	0.21	-	55,55,55,55	0
56	MG	A	1801	1/1	0.47	0.24	-	97,97,97,97	0
56	MG	A	1710	1/1	0.51	0.89	-	135,135,135,135	0
56	MG	E	303	1/1	0.81	0.26	-	62,62,62,62	0
56	MG	GB	3272	1/1	0.89	0.30	-	62,62,62,62	0
56	MG	B	3268	1/1	0.93	0.22	-	70,70,70,70	0
56	MG	GB	3382	1/1	0.81	0.25	-	72,72,72,72	0
56	MG	GB	3587	1/1	0.82	0.27	-	101,101,101,101	0
56	MG	GB	2964	1/1	0.96	0.32	-	59,59,59,59	0
56	MG	B	2997	1/1	0.97	0.45	-	42,42,42,42	0
56	MG	B	3074	1/1	0.89	0.36	-	36,36,36,36	0
56	MG	GB	3306	1/1	0.78	0.61	-	57,57,57,57	0
56	MG	FB	1667	1/1	0.88	0.51	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3221	1/1	0.87	0.24	-	53,53,53,53	0
56	MG	B	3718	1/1	0.83	0.53	-	54,54,54,54	0
56	MG	B	3597	1/1	0.75	0.32	-	49,49,49,49	0
56	MG	D	102	1/1	0.91	0.31	-	153,153,153,153	0
56	MG	GB	2905	1/1	0.92	0.86	-	62,62,62,62	0
56	MG	B	3309	1/1	0.81	0.14	-	56,56,56,56	0
56	MG	F	306	1/1	0.77	0.19	-	60,60,60,60	0
56	MG	IB	103	1/1	0.72	0.20	-	146,146,146,146	0
56	MG	A	1768	1/1	0.73	0.56	-	84,84,84,84	0
56	MG	GB	3072	1/1	0.95	0.59	-	49,49,49,49	0
56	MG	GB	3702	1/1	0.77	0.21	-	53,53,53,53	0
56	MG	GB	3290	1/1	0.96	0.18	-	48,48,48,48	0
56	MG	PC	304	1/1	0.51	0.27	-	135,135,135,135	0
56	MG	FB	1753	1/1	0.43	0.83	-	92,92,92,92	0
56	MG	FB	1904	1/1	0.90	0.48	-	60,60,60,60	0
56	MG	HB	217	1/1	0.50	0.16	-	111,111,111,111	0
56	MG	GB	3523	1/1	0.85	0.42	-	61,61,61,61	0
56	MG	GB	3338	1/1	0.52	0.26	-	71,71,71,71	0
56	MG	GB	3597	1/1	0.69	0.18	-	80,80,80,80	0
56	MG	FB	1689	1/1	0.89	0.61	-	66,66,66,66	0
56	MG	FB	1656	1/1	0.84	0.54	-	70,70,70,70	0
56	MG	B	2972	1/1	0.92	0.41	-	45,45,45,45	0
56	MG	GB	3618	1/1	0.95	0.20	-	109,109,109,109	0
56	MG	KC	105	1/1	0.74	0.80	-	73,73,73,73	0
56	MG	B	3431	1/1	0.96	0.62	-	47,47,47,47	0
56	MG	SC	206	1/1	0.50	0.18	-	93,93,93,93	0
56	MG	FB	1779	1/1	0.90	0.40	-	88,88,88,88	0
56	MG	GB	2945	1/1	0.83	0.09	-	92,92,92,92	0
56	MG	FB	1844	1/1	0.85	0.55	-	81,81,81,81	0
56	MG	IA	104	1/1	0.93	0.26	-	44,44,44,44	0
56	MG	GB	3316	1/1	0.88	0.29	-	73,73,73,73	0
56	MG	GC	102	1/1	0.80	0.21	-	127,127,127,127	0
56	MG	B	3627	1/1	0.61	0.56	-	56,56,56,56	0
56	MG	B	3392	1/1	0.86	0.07	-	78,78,78,78	0
56	MG	S	201	1/1	0.88	0.21	-	63,63,63,63	0
56	MG	B	3438	1/1	0.63	0.35	-	63,63,63,63	0
56	MG	B	3056	1/1	0.89	0.21	-	49,49,49,49	0
56	MG	GB	3286	1/1	0.81	0.34	-	125,125,125,125	0
56	MG	GB	2988	1/1	0.92	0.31	-	50,50,50,50	0
56	MG	GB	3654	1/1	0.78	0.23	-	72,72,72,72	0
56	MG	GB	2999	1/1	0.93	0.23	-	67,67,67,67	0
56	MG	A	1729	1/1	0.89	0.44	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1780	1/1	0.48	0.59	-	83,83,83,83	0
56	MG	RB	203	1/1	0.79	0.56	-	57,57,57,57	0
56	MG	GB	3257	1/1	0.85	0.08	-	86,86,86,86	0
56	MG	B	3237	1/1	0.93	0.25	-	45,45,45,45	0
56	MG	HB	207	1/1	0.92	0.51	-	107,107,107,107	0
56	MG	FB	1639	1/1	0.92	0.19	-	72,72,72,72	0
56	MG	A	1806	1/1	0.85	0.44	-	56,56,56,56	0
56	MG	B	3078	1/1	0.88	0.44	-	43,43,43,43	0
56	MG	W	303	1/1	0.69	0.13	-	87,87,87,87	0
56	MG	A	1639	1/1	0.95	0.38	-	61,61,61,61	0
56	MG	Q	204	1/1	0.86	0.17	-	74,74,74,74	0
56	MG	B	2917	1/1	0.86	0.65	-	46,46,46,46	0
56	MG	A	1665	1/1	0.86	0.35	-	66,66,66,66	0
56	MG	A	1736	1/1	0.99	0.12	-	53,53,53,53	0
56	MG	B	3793	1/1	0.90	0.15	-	81,81,81,81	0
56	MG	A	1725	1/1	0.72	0.20	-	114,114,114,114	0
56	MG	FB	1913	1/1	0.93	0.25	-	72,72,72,72	0
56	MG	B	3011	1/1	0.84	0.22	-	55,55,55,55	0
56	MG	GB	3326	1/1	0.72	0.39	-	60,60,60,60	0
56	MG	A	1821	1/1	0.77	0.29	-	77,77,77,77	0
56	MG	YC	203	1/1	0.83	0.18	-	82,82,82,82	0
56	MG	B	3839	1/1	0.78	0.27	-	50,50,50,50	0
56	MG	GB	3424	1/1	0.84	0.18	-	128,128,128,128	0
56	MG	GB	3547	1/1	0.88	0.54	-	67,67,67,67	0
56	MG	B	3830	1/1	0.93	0.15	-	60,60,60,60	0
56	MG	B	3671	1/1	0.74	0.53	-	46,46,46,46	0
56	MG	GB	3321	1/1	0.79	0.32	-	61,61,61,61	0
56	MG	HB	225	1/1	0.85	0.38	-	96,96,96,96	0
56	MG	B	3065	1/1	0.98	0.15	-	63,63,63,63	0
56	MG	FB	1881	1/1	0.91	0.26	-	68,68,68,68	0
56	MG	GB	2920	1/1	0.95	0.61	-	57,57,57,57	0
56	MG	GB	3456	1/1	0.94	0.19	-	68,68,68,68	0
56	MG	A	1750	1/1	0.94	0.29	-	80,80,80,80	0
56	MG	J	202	1/1	0.63	0.26	-	79,79,79,79	0
56	MG	B	3069	1/1	0.94	0.26	-	40,40,40,40	0
56	MG	FB	1808	1/1	0.89	0.20	-	66,66,66,66	0
56	MG	B	3248	1/1	0.79	0.27	-	84,84,84,84	0
56	MG	FB	1893	1/1	0.88	0.54	-	86,86,86,86	0
56	MG	B	3250	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	FB	1613	1/1	0.65	0.46	-	80,80,80,80	0
56	MG	FB	1835	1/1	0.70	0.23	-	104,104,104,104	0
56	MG	FB	1751	1/1	0.93	0.44	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3182	1/1	0.90	0.14	-	88,88,88,88	0
56	MG	GB	3232	1/1	0.84	0.42	-	61,61,61,61	0
56	MG	FB	1898	1/1	0.89	0.14	-	70,70,70,70	0
56	MG	K	202	1/1	0.87	0.07	-	63,63,63,63	0
56	MG	A	1880	1/1	0.76	0.43	-	77,77,77,77	0
56	MG	GB	3509	1/1	0.87	0.40	-	75,75,75,75	0
56	MG	QB	201	1/1	0.85	0.34	-	73,73,73,73	0
56	MG	FB	1635	1/1	0.69	0.46	-	78,78,78,78	0
56	MG	JA	407	1/1	0.91	0.27	-	61,61,61,61	0
56	MG	GB	3663	1/1	-0.05	0.26	-	206,206,206,206	0
56	MG	B	3754	1/1	0.92	0.09	-	57,57,57,57	0
56	MG	B	3224	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	B	3738	1/1	0.76	0.27	-	55,55,55,55	0
56	MG	A	1701	1/1	0.96	0.32	-	56,56,56,56	0
56	MG	B	3009	1/1	0.97	0.21	-	72,72,72,72	0
56	MG	A	1689	1/1	0.80	0.18	-	56,56,56,56	0
56	MG	GB	3698	1/1	0.95	0.10	-	68,68,68,68	0
56	MG	RC	301	1/1	0.94	0.66	-	69,69,69,69	0
56	MG	DA	102	1/1	0.88	0.12	-	62,62,62,62	0
56	MG	VB	202	1/1	0.69	0.36	-	80,80,80,80	0
56	MG	B	3417	1/1	0.98	0.61	-	57,57,57,57	0
56	MG	IB	101	1/1	0.92	0.44	-	89,89,89,89	0
56	MG	GB	3526	1/1	0.84	0.52	-	80,80,80,80	0
56	MG	FB	1641	1/1	0.71	0.70	-	61,61,61,61	0
56	MG	GB	3249	1/1	0.75	0.25	-	68,68,68,68	0
56	MG	GB	3193	1/1	0.19	0.35	-	141,141,141,141	0
56	MG	A	1837	1/1	0.77	0.19	-	124,124,124,124	0
56	MG	GB	3613	1/1	0.88	0.35	-	57,57,57,57	0
56	MG	A	1789	1/1	0.65	0.22	-	87,87,87,87	0
56	MG	B	3835	1/1	0.89	0.15	-	80,80,80,80	0
56	MG	B	3323	1/1	0.77	0.24	-	83,83,83,83	0
56	MG	B	3125	1/1	0.88	0.19	-	60,60,60,60	0
56	MG	YC	202	1/1	0.94	0.31	-	81,81,81,81	0
56	MG	A	1683	1/1	0.88	0.81	-	80,80,80,80	0
56	MG	GB	3255	1/1	0.90	0.39	-	100,100,100,100	0
56	MG	GA	102	1/1	0.82	0.24	-	67,67,67,67	0
56	MG	IA	108	1/1	0.55	0.42	-	82,82,82,82	0
56	MG	ZC	201	1/1	0.83	0.26	-	70,70,70,70	0
56	MG	VB	203	1/1	0.72	0.28	-	79,79,79,79	0
56	MG	B	3042	1/1	0.90	0.21	-	53,53,53,53	0
56	MG	B	2903	1/1	0.97	0.50	-	35,35,35,35	0
56	MG	GB	3048	1/1	0.55	0.29	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	A	1774	1/1	0.95	0.28	-	106,106,106,106	0
56	MG	B	3296	1/1	0.84	0.21	-	55,55,55,55	0
56	MG	A	1754	1/1	0.89	0.35	-	90,90,90,90	0
56	MG	B	3808	1/1	0.89	0.19	-	50,50,50,50	0
56	MG	GB	3185	1/1	0.91	0.23	-	67,67,67,67	0
56	MG	B	3709	1/1	0.78	0.43	-	64,64,64,64	0
56	MG	B	3358	1/1	0.58	0.39	-	96,96,96,96	0
56	MG	A	1627	1/1	0.94	0.38	-	73,73,73,73	0
56	MG	A	1819	1/1	0.74	1.89	-	82,82,82,82	0
56	MG	A	1698	1/1	0.82	0.77	-	77,77,77,77	0
56	MG	GB	3252	1/1	0.84	0.28	-	59,59,59,59	0
56	MG	B	3824	1/1	0.57	0.41	-	68,68,68,68	0
56	MG	GB	3630	1/1	0.55	1.21	-	75,75,75,75	0
56	MG	B	3053	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	GB	2942	1/1	0.89	0.60	-	54,54,54,54	0
56	MG	B	3578	1/1	0.73	0.19	-	54,54,54,54	0
56	MG	GB	2975	1/1	0.95	0.25	-	61,61,61,61	0
56	MG	FB	1736	1/1	0.84	0.24	-	58,58,58,58	0
56	MG	B	3281	1/1	0.86	0.28	-	53,53,53,53	0
56	MG	A	1751	1/1	0.91	0.37	-	86,86,86,86	0
56	MG	B	3404	1/1	0.91	0.13	-	47,47,47,47	0
56	MG	B	3700	1/1	0.94	0.15	-	46,46,46,46	0
56	MG	C	219	1/1	0.65	0.31	-	81,81,81,81	0
56	MG	B	2986	1/1	0.87	0.41	-	37,37,37,37	0
56	MG	GB	3124	1/1	0.97	0.12	-	79,79,79,79	0
56	MG	B	3568	1/1	0.91	0.21	-	53,53,53,53	0
56	MG	GB	3683	1/1	0.94	0.19	-	64,64,64,64	0
56	MG	B	2998	1/1	0.89	0.33	-	47,47,47,47	0
56	MG	FB	1742	1/1	0.94	0.42	-	67,67,67,67	0
56	MG	B	3843	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	GB	3572	1/1	0.92	0.30	-	67,67,67,67	0
56	MG	EC	103	1/1	0.88	0.09	-	90,90,90,90	0
56	MG	B	3677	1/1	0.40	0.23	-	149,149,149,149	0
56	MG	ZC	202	1/1	0.74	0.17	-	75,75,75,75	0
56	MG	C	224	1/1	0.87	0.16	-	74,74,74,74	0
56	MG	FB	1934	1/1	0.72	0.88	-	82,82,82,82	0
56	MG	B	3192	1/1	0.87	0.21	-	58,58,58,58	0
56	MG	YB	204	1/1	0.88	0.14	-	78,78,78,78	0
56	MG	RA	201	1/1	0.82	0.24	-	123,123,123,123	0
56	MG	C	210	1/1	0.79	0.35	-	75,75,75,75	0
56	MG	GB	3109	1/1	0.55	0.35	-	63,63,63,63	0
56	MG	GB	3025	1/1	0.81	0.42	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	FB	1899	1/1	0.50	0.26	-	86,86,86,86	0
56	MG	B	3471	1/1	0.94	0.15	-	49,49,49,49	0
56	MG	GB	2953	1/1	0.93	0.32	-	56,56,56,56	0
56	MG	HB	231	1/1	0.77	0.24	-	79,79,79,79	0
56	MG	GB	3479	1/1	0.80	0.40	-	66,66,66,66	0
56	MG	GB	3327	1/1	0.90	0.44	-	76,76,76,76	0
56	MG	FB	1852	1/1	0.86	0.98	-	76,76,76,76	0
56	MG	GB	3517	1/1	-0.20	0.26	-	219,219,219,219	0
56	MG	FB	1810	1/1	0.93	0.71	-	71,71,71,71	0
56	MG	N	205	1/1	0.90	0.12	-	65,65,65,65	0
56	MG	AA	103	1/1	0.73	0.21	-	59,59,59,59	0
56	MG	GB	3519	1/1	0.73	0.34	-	85,85,85,85	0
56	MG	K	205	1/1	0.89	0.25	-	56,56,56,56	0
56	MG	GB	3299	1/1	0.79	0.18	-	134,134,134,134	0
56	MG	B	3282	1/1	0.89	0.24	-	50,50,50,50	0
56	MG	W	301	1/1	0.73	0.22	-	73,73,73,73	0
56	MG	FB	1708	1/1	0.87	0.21	-	73,73,73,73	0
56	MG	B	3049	1/1	0.90	0.57	-	40,40,40,40	0
56	MG	A	1735	1/1	0.85	0.44	-	69,69,69,69	0
56	MG	FB	1730	1/1	0.89	0.20	-	78,78,78,78	0
56	MG	A	1666	1/1	0.90	1.15	-	80,80,80,80	0
56	MG	B	3501	1/1	0.80	0.31	-	48,48,48,48	0
56	MG	B	3284	1/1	0.76	0.53	-	72,72,72,72	0
56	MG	FB	1848	1/1	0.79	0.33	-	76,76,76,76	0
56	MG	TB	203	1/1	0.88	0.33	-	66,66,66,66	0
56	MG	GB	3461	1/1	0.85	0.34	-	76,76,76,76	0
56	MG	B	3010	1/1	0.86	0.42	-	77,77,77,77	0
56	MG	OB	202	1/1	0.74	0.33	-	115,115,115,115	0
56	MG	GB	2919	1/1	0.93	0.54	-	66,66,66,66	0
56	MG	GB	3279	1/1	0.90	0.25	-	69,69,69,69	0
56	MG	A	1684	1/1	0.78	0.22	-	67,67,67,67	0
56	MG	PC	301	1/1	0.78	0.28	-	115,115,115,115	0
56	MG	GB	3567	1/1	0.82	0.50	-	52,52,52,52	0
56	MG	FB	1803	1/1	0.94	0.10	-	84,84,84,84	0
56	MG	GB	3399	1/1	0.92	0.15	-	54,54,54,54	0
56	MG	GB	3534	1/1	0.76	0.42	-	59,59,59,59	0
56	MG	FB	1943	1/1	0.47	0.66	-	105,105,105,105	0
56	MG	A	1753	1/1	0.91	0.17	-	84,84,84,84	0
56	MG	B	3461	1/1	0.77	0.33	-	56,56,56,56	0
56	MG	GB	3617	1/1	0.94	0.32	-	67,67,67,67	0
56	MG	B	3654	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	GB	3376	1/1	0.66	0.23	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1640	1/1	0.84	0.25	-	76,76,76,76	0
56	MG	B	3374	1/1	0.71	0.26	-	61,61,61,61	0
56	MG	GB	3269	1/1	0.90	0.14	-	77,77,77,77	0
56	MG	B	3023	1/1	0.70	0.41	-	75,75,75,75	0
56	MG	RC	304	1/1	0.90	0.13	-	80,80,80,80	0
56	MG	B	3668	1/1	0.62	0.27	-	63,63,63,63	0
56	MG	B	3105	1/1	0.86	0.28	-	78,78,78,78	0
56	MG	FB	1946	1/1	0.76	0.32	-	70,70,70,70	0
56	MG	B	3390	1/1	0.92	0.09	-	72,72,72,72	0
56	MG	GB	3415	1/1	0.93	0.39	-	55,55,55,55	0
56	MG	IB	104	1/1	0.58	0.28	-	163,163,163,163	0
56	MG	GB	3592	1/1	0.82	0.15	-	116,116,116,116	0
56	MG	GB	3199	1/1	0.90	0.19	-	67,67,67,67	0
56	MG	B	3066	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	KC	101	1/1	0.89	0.28	-	58,58,58,58	0
56	MG	B	3477	1/1	0.95	0.09	-	43,43,43,43	0
56	MG	HB	201	1/1	0.94	0.46	-	78,78,78,78	0
56	MG	GB	3250	1/1	0.81	0.16	-	77,77,77,77	0
56	MG	GB	3119	1/1	0.69	0.28	-	59,59,59,59	0
56	MG	FB	1916	1/1	0.86	0.54	-	73,73,73,73	0
56	MG	A	1704	1/1	0.66	0.19	-	65,65,65,65	0
56	MG	GB	3607	1/1	0.33	0.37	-	111,111,111,111	0
56	MG	A	1713	1/1	0.67	0.75	-	88,88,88,88	0
56	MG	GB	3655	1/1	0.64	0.40	-	59,59,59,59	0
56	MG	B	2936	1/1	0.97	0.74	-	34,34,34,34	0
56	MG	FB	1821	1/1	0.72	0.12	-	135,135,135,135	0
56	MG	B	3749	1/1	0.85	0.34	-	130,130,130,130	0
56	MG	B	3696	1/1	0.86	0.21	-	52,52,52,52	0
56	MG	B	3476	1/1	0.74	0.30	-	67,67,67,67	0
56	MG	QA	201	1/1	0.91	0.17	-	106,106,106,106	0
56	MG	B	3277	1/1	0.86	0.29	-	51,51,51,51	0
56	MG	GB	3515	1/1	0.94	0.17	-	76,76,76,76	0
56	MG	B	3660	1/1	0.83	0.21	-	54,54,54,54	0
56	MG	B	3152	1/1	0.91	0.24	-	56,56,56,56	0
56	MG	GB	3243	1/1	0.67	0.12	-	93,93,93,93	0
56	MG	C	223	1/1	0.89	0.23	-	56,56,56,56	0
56	MG	B	3581	1/1	0.83	0.45	-	46,46,46,46	0
56	MG	B	3275	1/1	0.93	0.33	-	49,49,49,49	0
56	MG	GB	3580	1/1	0.85	0.72	-	74,74,74,74	0
56	MG	GB	2971	1/1	0.85	0.25	-	93,93,93,93	0
56	MG	B	3389	1/1	0.26	0.33	-	124,124,124,124	0
56	MG	FB	1780	1/1	0.56	0.74	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	2945	1/1	0.88	0.17	-	47,47,47,47	0
56	MG	KC	104	1/1	0.88	0.39	-	60,60,60,60	0
56	MG	DA	103	1/1	0.90	0.32	-	68,68,68,68	0
56	MG	GB	3665	1/1	0.91	0.28	-	61,61,61,61	0
56	MG	B	3305	1/1	0.95	0.23	-	49,49,49,49	0
56	MG	B	3790	1/1	0.59	1.01	-	62,62,62,62	0
56	MG	GB	3164	1/1	0.89	0.59	-	46,46,46,46	0
56	MG	B	3103	1/1	0.93	0.18	-	51,51,51,51	0
56	MG	Q	203	1/1	0.88	0.08	-	78,78,78,78	0
56	MG	B	3806	1/1	0.84	0.35	-	58,58,58,58	0
56	MG	GD	101	1/1	-0.02	0.56	-	99,99,99,99	0
56	MG	GB	3059	1/1	0.84	0.33	-	91,91,91,91	0
56	MG	GB	3320	1/1	0.81	0.26	-	60,60,60,60	0
56	MG	B	3185	1/1	0.92	0.08	-	45,45,45,45	0
56	MG	A	1752	1/1	0.88	0.14	-	67,67,67,67	0
56	MG	B	3698	1/1	0.95	0.51	-	77,77,77,77	0
56	MG	GB	3146	1/1	0.83	0.34	-	67,67,67,67	0
56	MG	GB	3145	1/1	0.81	0.30	-	65,65,65,65	0
56	MG	GB	3436	1/1	0.95	0.12	-	71,71,71,71	0
56	MG	GB	3160	1/1	0.91	0.08	-	89,89,89,89	0
56	MG	E	308	1/1	0.78	1.00	-	52,52,52,52	0
56	MG	B	3131	1/1	0.85	0.30	-	57,57,57,57	0
56	MG	B	3024	1/1	0.95	0.50	-	40,40,40,40	0
56	MG	A	1779	1/1	0.82	0.40	-	82,82,82,82	0
56	MG	B	3590	1/1	0.69	0.14	-	95,95,95,95	0
56	MG	LA	302	1/1	0.71	0.21	-	119,119,119,119	0
56	MG	B	3176	1/1	0.98	0.24	-	53,53,53,53	0
56	MG	B	3368	1/1	0.83	0.22	-	57,57,57,57	0
56	MG	A	1841	1/1	0.88	0.18	-	67,67,67,67	0
56	MG	B	3064	1/1	0.86	0.14	-	52,52,52,52	0
56	MG	FB	1936	1/1	0.79	0.37	-	87,87,87,87	0
56	MG	B	3379	1/1	0.74	0.34	-	52,52,52,52	0
56	MG	A	1617	1/1	0.90	0.12	-	59,59,59,59	0
56	MG	A	1660	1/1	0.89	0.49	-	60,60,60,60	0
56	MG	C	221	1/1	0.95	0.39	-	70,70,70,70	0
56	MG	B	3139	1/1	0.81	0.18	-	47,47,47,47	0
56	MG	B	3219	1/1	0.94	0.54	-	43,43,43,43	0
56	MG	XA	101	1/1	0.58	0.30	-	86,86,86,86	0
56	MG	GB	3528	1/1	0.45	0.79	-	79,79,79,79	0
56	MG	FB	1696	1/1	0.71	0.33	-	85,85,85,85	0
56	MG	B	2941	1/1	0.95	0.42	-	49,49,49,49	0
56	MG	B	3844	1/1	0.88	0.31	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3699	1/1	0.69	0.33	-	57,57,57,57	0
56	MG	XB	203	1/1	0.86	0.15	-	79,79,79,79	0
56	MG	CA	104	1/1	0.92	0.21	-	65,65,65,65	0
56	MG	GB	3211	1/1	0.85	0.22	-	61,61,61,61	0
56	MG	B	3026	1/1	0.95	0.33	-	40,40,40,40	0
56	MG	FB	1785	1/1	0.69	0.12	-	87,87,87,87	0
56	MG	MA	305	1/1	0.66	0.27	-	103,103,103,103	0
56	MG	B	3462	1/1	0.93	0.20	-	41,41,41,41	0
56	MG	B	3827	1/1	0.82	0.20	-	64,64,64,64	0
56	MG	B	3551	1/1	0.76	0.34	-	51,51,51,51	0
56	MG	S	207	1/1	0.89	0.86	-	49,49,49,49	0
56	MG	JB	304	1/1	0.64	0.46	-	76,76,76,76	0
56	MG	PC	305	1/1	0.69	0.33	-	96,96,96,96	0
56	MG	FB	1624	1/1	0.93	0.36	-	66,66,66,66	0
56	MG	K	207	1/1	0.82	0.15	-	67,67,67,67	0
56	MG	B	3058	1/1	0.97	0.44	-	48,48,48,48	0
56	MG	A	1825	1/1	0.89	0.21	-	56,56,56,56	0
56	MG	A	1831	1/1	0.79	0.58	-	96,96,96,96	0
56	MG	HB	230	1/1	0.85	0.29	-	131,131,131,131	0
56	MG	A	1799	1/1	0.71	0.49	-	118,118,118,118	0
56	MG	FB	1714	1/1	0.88	0.20	-	66,66,66,66	0
56	MG	A	1663	1/1	0.80	0.33	-	63,63,63,63	0
56	MG	G	3209	1/1	0.89	0.60	-	48,48,48,48	0
56	MG	GB	3674	1/1	0.75	1.16	-	84,84,84,84	0
56	MG	B	3468	1/1	0.84	0.33	-	57,57,57,57	0
56	MG	M	202	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	B	3121	1/1	0.93	0.18	-	43,43,43,43	0
56	MG	GB	2987	1/1	0.89	0.57	-	48,48,48,48	0
56	MG	GB	3136	1/1	0.67	0.36	-	71,71,71,71	0
56	MG	FB	1729	1/1	0.81	0.21	-	72,72,72,72	0
56	MG	GB	2981	1/1	0.94	0.62	-	50,50,50,50	0
56	MG	B	3513	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	B	3682	1/1	0.92	0.65	-	67,67,67,67	0
56	MG	FB	1796	1/1	0.84	0.27	-	79,79,79,79	0
56	MG	B	3701	1/1	0.72	0.17	-	115,115,115,115	0
56	MG	B	3602	1/1	0.96	0.15	-	54,54,54,54	0
56	MG	GB	3603	1/1	0.66	0.12	-	101,101,101,101	0
56	MG	C	213	1/1	0.65	0.28	-	72,72,72,72	0
56	MG	GB	3589	1/1	0.90	0.53	-	94,94,94,94	0
56	MG	B	3079	1/1	0.66	0.32	-	48,48,48,48	0
56	MG	GB	3450	1/1	0.79	0.19	-	77,77,77,77	0
56	MG	B	3054	1/1	0.88	0.19	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	F	312	1/1	0.85	0.08	-	77,77,77,77	0
56	MG	FB	1815	1/1	0.74	0.34	-	79,79,79,79	0
56	MG	NC	111	1/1	0.85	0.19	-	87,87,87,87	0
56	MG	GB	3445	1/1	0.77	0.36	-	122,122,122,122	0
56	MG	T	201	1/1	0.95	0.22	-	42,42,42,42	0
56	MG	C	212	1/1	0.53	0.28	-	62,62,62,62	0
56	MG	B	2906	1/1	0.93	0.60	-	29,29,29,29	0
56	MG	BC	303	1/1	0.61	0.32	-	106,106,106,106	0
56	MG	GB	3312	1/1	0.90	0.11	-	73,73,73,73	0
56	MG	B	3114	1/1	0.94	0.53	-	49,49,49,49	0
56	MG	UB	201	1/1	0.65	0.30	-	99,99,99,99	0
56	MG	B	3239	1/1	0.82	0.11	-	64,64,64,64	0
56	MG	GB	3148	1/1	0.94	0.27	-	59,59,59,59	0
56	MG	GB	3422	1/1	0.93	0.25	-	64,64,64,64	0
56	MG	GB	3627	1/1	0.96	0.43	-	60,60,60,60	0
56	MG	B	3279	1/1	0.85	0.20	-	75,75,75,75	0
56	MG	GB	3347	1/1	0.59	0.59	-	66,66,66,66	0
56	MG	GB	3010	1/1	0.89	0.27	-	67,67,67,67	0
56	MG	VB	204	1/1	0.75	0.18	-	74,74,74,74	0
56	MG	B	3320	1/1	0.81	0.19	-	64,64,64,64	0
56	MG	FB	1615	1/1	0.78	0.80	-	87,87,87,87	0
56	MG	B	3549	1/1	0.90	0.20	-	51,51,51,51	0
56	MG	GB	3101	1/1	0.68	0.61	-	115,115,115,115	0
56	MG	VA	202	1/1	0.71	0.52	-	100,100,100,100	0
56	MG	T	205	1/1	0.85	0.17	-	58,58,58,58	0
56	MG	B	3690	1/1	0.96	0.13	-	59,59,59,59	0
56	MG	FB	1687	1/1	0.86	0.28	-	109,109,109,109	0
56	MG	GB	3216	1/1	0.96	0.47	-	60,60,60,60	0
56	MG	FB	1905	1/1	0.78	0.59	-	70,70,70,70	0
56	MG	B	3506	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	FB	1630	1/1	0.91	0.18	-	64,64,64,64	0
56	MG	GB	3147	1/1	0.86	0.61	-	54,54,54,54	0
56	MG	B	3614	1/1	0.82	0.61	-	50,50,50,50	0
56	MG	A	1686	1/1	0.79	0.51	-	87,87,87,87	0
56	MG	B	3409	1/1	0.95	0.20	-	105,105,105,105	0
56	MG	GB	3123	1/1	0.71	0.21	-	62,62,62,62	0
56	MG	A	1864	1/1	0.43	0.25	-	138,138,138,138	0
56	MG	XA	102	1/1	0.85	0.12	-	88,88,88,88	0
56	MG	B	3716	1/1	0.91	0.16	-	65,65,65,65	0
56	MG	GB	3482	1/1	0.78	0.32	-	77,77,77,77	0
56	MG	B	3552	1/1	0.97	0.21	-	46,46,46,46	0
56	MG	FB	1602	1/1	0.87	0.41	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3542	1/1	0.87	0.20	-	112,112,112,112	0
56	MG	A	1719	1/1	0.75	0.17	-	101,101,101,101	0
56	MG	GB	3024	1/1	0.88	0.33	-	57,57,57,57	0
56	MG	A	1851	1/1	0.70	0.34	-	117,117,117,117	0
56	MG	GB	3301	1/1	0.86	0.45	-	55,55,55,55	0
56	MG	S	208	1/1	0.92	0.71	-	53,53,53,53	0
56	MG	B	3587	1/1	0.72	0.18	-	62,62,62,62	0
56	MG	B	3285	1/1	0.81	0.37	-	42,42,42,42	0
56	MG	B	3004	1/1	0.85	0.45	-	43,43,43,43	0
56	MG	A	1616	1/1	0.75	0.39	-	74,74,74,74	0
56	MG	B	3271	1/1	0.88	0.12	-	68,68,68,68	0
56	MG	A	1857	1/1	0.83	0.36	-	69,69,69,69	0
56	MG	B	3118	1/1	0.90	0.16	-	96,96,96,96	0
56	MG	GB	3478	1/1	0.77	0.14	-	187,187,187,187	0
56	MG	B	3363	1/1	0.87	0.42	-	44,44,44,44	0
56	MG	B	3319	1/1	0.91	0.57	-	47,47,47,47	0
56	MG	GB	3556	1/1	0.76	0.62	-	77,77,77,77	0
56	MG	B	3811	1/1	0.91	0.31	-	48,48,48,48	0
56	MG	B	3110	1/1	0.86	0.45	-	48,48,48,48	0
56	MG	B	3564	1/1	0.90	0.10	-	52,52,52,52	0
56	MG	B	3343	1/1	0.89	0.15	-	56,56,56,56	0
56	MG	B	3288	1/1	0.81	0.58	-	59,59,59,59	0
56	MG	HB	203	1/1	0.39	0.30	-	101,101,101,101	0
56	MG	B	3359	1/1	0.80	0.23	-	63,63,63,63	0
56	MG	GB	3689	1/1	0.75	0.60	-	67,67,67,67	0
56	MG	GB	3142	1/1	0.78	0.44	-	50,50,50,50	0
56	MG	FB	1799	1/1	0.94	0.26	-	71,71,71,71	0
56	MG	GB	3053	1/1	0.89	0.22	-	53,53,53,53	0
56	MG	GB	3333	1/1	0.92	0.34	-	66,66,66,66	0
56	MG	A	1747	1/1	0.66	0.82	-	104,104,104,104	0
56	MG	OC	407	1/1	0.50	0.24	-	109,109,109,109	0
56	MG	YB	205	1/1	0.75	0.36	-	57,57,57,57	0
56	MG	SA	202	1/1	0.90	0.23	-	125,125,125,125	0
56	MG	B	3573	1/1	0.74	0.32	-	57,57,57,57	0
56	MG	GB	3544	1/1	0.55	0.43	-	70,70,70,70	0
56	MG	GB	3372	1/1	0.84	0.44	-	81,81,81,81	0
56	MG	B	3242	1/1	0.89	0.26	-	49,49,49,49	0
56	MG	P	201	1/1	0.85	0.13	-	82,82,82,82	0
56	MG	B	3109	1/1	0.95	0.20	-	53,53,53,53	0
56	MG	GB	3700	1/1	0.72	0.45	-	61,61,61,61	0
56	MG	B	3119	1/1	0.89	0.20	-	69,69,69,69	0
56	MG	GB	3083	1/1	0.91	0.33	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3046	1/1	0.94	0.43	-	55,55,55,55	0
56	MG	B	2915	1/1	0.90	0.34	-	57,57,57,57	0
56	MG	FB	1939	1/1	0.48	2.08	-	98,98,98,98	0
56	MG	B	3537	1/1	0.94	0.19	-	46,46,46,46	0
56	MG	G	3205	1/1	0.92	0.19	-	40,40,40,40	0
56	MG	GB	3068	1/1	0.96	0.30	-	66,66,66,66	0
56	MG	B	3678	1/1	0.95	0.16	-	57,57,57,57	0
56	MG	FB	1695	1/1	0.82	0.13	-	156,156,156,156	0
56	MG	B	3732	1/1	0.80	0.38	-	57,57,57,57	0
56	MG	G	3211	1/1	0.77	0.45	-	60,60,60,60	0
56	MG	GB	3410	1/1	0.85	0.20	-	76,76,76,76	0
56	MG	B	3837	1/1	0.94	0.50	-	50,50,50,50	0
56	MG	C	241	1/1	0.88	0.12	-	81,81,81,81	0
56	MG	GB	2973	1/1	0.97	0.25	-	50,50,50,50	0
56	MG	I	204	1/1	0.88	0.44	-	68,68,68,68	0
56	MG	B	3764	1/1	0.89	0.22	-	48,48,48,48	0
56	MG	C	242	1/1	0.95	0.42	-	86,86,86,86	0
56	MG	A	1720	1/1	0.84	0.94	-	72,72,72,72	0
56	MG	B	3759	1/1	0.78	0.36	-	47,47,47,47	0
56	MG	EC	102	1/1	0.88	0.38	-	91,91,91,91	0
56	MG	ZB	101	1/1	0.51	0.39	-	78,78,78,78	0
56	MG	B	3527	1/1	0.67	0.81	-	52,52,52,52	0
56	MG	B	3372	1/1	0.86	0.34	-	40,40,40,40	0
56	MG	B	3137	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	GB	3555	1/1	0.56	0.51	-	72,72,72,72	0
56	MG	B	3425	1/1	0.81	0.14	-	47,47,47,47	0
56	MG	IA	111	1/1	0.92	0.42	-	49,49,49,49	0
56	MG	S	202	1/1	0.88	0.14	-	63,63,63,63	0
56	MG	A	1782	1/1	0.92	0.16	-	130,130,130,130	0
56	MG	B	3743	1/1	0.91	0.50	-	52,52,52,52	0
56	MG	RA	203	1/1	0.78	0.38	-	119,119,119,119	0
56	MG	GB	3322	1/1	0.83	0.68	-	56,56,56,56	0
56	MG	FB	1762	1/1	0.82	0.38	-	69,69,69,69	0
56	MG	B	3116	1/1	0.85	0.39	-	49,49,49,49	0
56	MG	B	3711	1/1	0.82	0.73	-	64,64,64,64	0
56	MG	GB	3463	1/1	0.76	0.42	-	66,66,66,66	0
56	MG	GB	3565	1/1	0.92	0.25	-	60,60,60,60	0
56	MG	B	3805	1/1	0.89	0.34	-	54,54,54,54	0
56	MG	A	1723	1/1	0.86	0.59	-	79,79,79,79	0
56	MG	B	3321	1/1	0.80	0.16	-	60,60,60,60	0
56	MG	GB	3374	1/1	0.79	0.25	-	62,62,62,62	0
56	MG	UA	203	1/1	0.81	0.65	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3337	1/1	0.95	0.22	-	58,58,58,58	0
56	MG	B	3661	1/1	0.92	0.43	-	51,51,51,51	0
56	MG	B	3488	1/1	0.93	0.43	-	57,57,57,57	0
56	MG	B	3446	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	CA	103	1/1	0.96	0.29	-	49,49,49,49	0
56	MG	B	3836	1/1	0.86	0.26	-	46,46,46,46	0
56	MG	FB	1760	1/1	0.92	0.17	-	68,68,68,68	0
56	MG	B	3240	1/1	0.92	0.18	-	51,51,51,51	0
56	MG	IA	113	1/1	0.93	0.28	-	71,71,71,71	0
56	MG	GB	3453	1/1	0.94	0.11	-	85,85,85,85	0
56	MG	GB	3266	1/1	0.78	0.57	-	57,57,57,57	0
56	MG	B	3496	1/1	0.09	0.22	-	167,167,167,167	0
56	MG	GB	3505	1/1	0.90	0.37	-	81,81,81,81	0
56	MG	F	309	1/1	0.81	0.28	-	38,38,38,38	0
56	MG	GB	3417	1/1	0.91	0.24	-	66,66,66,66	0
56	MG	A	1833	1/1	0.74	0.43	-	116,116,116,116	0
56	MG	A	1690	1/1	0.21	0.21	-	94,94,94,94	0
56	MG	B	3273	1/1	0.84	0.16	-	76,76,76,76	0
56	MG	B	3164	1/1	0.95	0.21	-	46,46,46,46	0
56	MG	BC	304	1/1	0.87	0.22	-	91,91,91,91	0
56	MG	BA	103	1/1	0.71	0.33	-	107,107,107,107	0
56	MG	GB	3631	1/1	0.84	0.20	-	60,60,60,60	0
56	MG	GB	3394	1/1	0.69	0.32	-	77,77,77,77	0
56	MG	GB	3465	1/1	0.21	0.26	-	114,114,114,114	0
56	MG	FB	1861	1/1	0.18	0.59	-	119,119,119,119	0
56	MG	B	2952	1/1	0.91	0.33	-	46,46,46,46	0
56	MG	B	3276	1/1	0.83	0.18	-	68,68,68,68	0
56	MG	B	3455	1/1	0.91	0.27	-	47,47,47,47	0
56	MG	A	1800	1/1	0.83	0.20	-	132,132,132,132	0
56	MG	B	3770	1/1	0.94	0.40	-	65,65,65,65	0
56	MG	A	1763	1/1	0.91	0.14	-	109,109,109,109	0
56	MG	B	3383	1/1	0.81	0.23	-	47,47,47,47	0
56	MG	B	3169	1/1	0.91	0.25	-	47,47,47,47	0
56	MG	FB	1864	1/1	0.96	0.29	-	103,103,103,103	0
56	MG	FB	1741	1/1	0.66	0.65	-	127,127,127,127	0
56	MG	B	3230	1/1	0.85	0.35	-	59,59,59,59	0
56	MG	B	3385	1/1	0.95	0.36	-	59,59,59,59	0
56	MG	GB	3508	1/1	0.86	0.49	-	78,78,78,78	0
56	MG	GB	3559	1/1	0.84	0.17	-	72,72,72,72	0
56	MG	GB	3264	1/1	0.86	0.13	-	71,71,71,71	0
56	MG	FB	1617	1/1	0.90	0.38	-	59,59,59,59	0
56	MG	GB	3688	1/1	0.70	0.54	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3306	1/1	0.93	0.49	-	44,44,44,44	0
56	MG	A	1771	1/1	0.93	0.32	-	80,80,80,80	0
56	MG	FB	1783	1/1	0.76	0.24	-	79,79,79,79	0
56	MG	I	203	1/1	0.90	0.12	-	68,68,68,68	0
56	MG	A	1872	1/1	0.89	0.28	-	111,111,111,111	0
56	MG	VA	203	1/1	0.65	0.50	-	102,102,102,102	0
56	MG	GB	3244	1/1	0.93	0.22	-	52,52,52,52	0
56	MG	GB	3358	1/1	0.96	0.21	-	87,87,87,87	0
56	MG	FB	1612	1/1	0.95	0.53	-	63,63,63,63	0
56	MG	GB	2916	1/1	0.94	0.14	-	51,51,51,51	0
56	MG	NA	201	1/1	0.68	0.51	-	100,100,100,100	0
56	MG	GB	3107	1/1	0.78	0.22	-	81,81,81,81	0
56	MG	C	243	1/1	0.92	0.29	-	57,57,57,57	0
56	MG	GB	3280	1/1	0.88	0.16	-	84,84,84,84	0
56	MG	B	3495	1/1	0.88	0.22	-	46,46,46,46	0
56	MG	GB	3411	1/1	0.60	0.43	-	67,67,67,67	0
56	MG	GB	3369	1/1	0.81	0.36	-	90,90,90,90	0
56	MG	A	1605	1/1	0.86	0.32	-	67,67,67,67	0
56	MG	FB	1693	1/1	0.84	0.50	-	66,66,66,66	0
56	MG	B	3589	1/1	0.78	0.38	-	60,60,60,60	0
56	MG	FB	1812	1/1	0.90	0.35	-	70,70,70,70	0
56	MG	A	1781	1/1	0.98	0.18	-	95,95,95,95	0
56	MG	B	3107	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	GB	3345	1/1	0.72	0.36	-	68,68,68,68	0
56	MG	A	1839	1/1	0.98	0.22	-	85,85,85,85	0
56	MG	B	2957	1/1	0.96	0.11	-	45,45,45,45	0
56	MG	GB	3577	1/1	0.86	0.18	-	91,91,91,91	0
56	MG	B	3051	1/1	0.80	0.75	-	40,40,40,40	0
56	MG	B	3609	1/1	0.88	0.20	-	44,44,44,44	0
56	MG	B	3571	1/1	0.78	0.16	-	66,66,66,66	0
56	MG	GB	3449	1/1	0.17	0.21	-	197,197,197,197	0
56	MG	RC	302	1/1	0.92	0.26	-	77,77,77,77	0
56	MG	XB	202	1/1	0.88	0.06	-	76,76,76,76	0
56	MG	B	3554	1/1	0.49	0.29	-	60,60,60,60	0
56	MG	GB	3401	1/1	0.53	0.29	-	68,68,68,68	0
56	MG	B	3388	1/1	0.88	0.27	-	55,55,55,55	0
56	MG	W	305	1/1	0.84	0.11	-	67,67,67,67	0
56	MG	FB	1763	1/1	0.86	0.22	-	67,67,67,67	0
56	MG	GB	3370	1/1	0.92	0.29	-	65,65,65,65	0
56	MG	GB	3641	1/1	0.72	0.32	-	64,64,64,64	0
56	MG	GB	3444	1/1	0.76	0.39	-	78,78,78,78	0
56	MG	B	2977	1/1	0.92	0.25	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3403	1/1	0.84	0.66	-	65,65,65,65	0
56	MG	FB	1711	1/1	0.85	0.34	-	69,69,69,69	0
56	MG	FB	1866	1/1	0.88	0.13	-	94,94,94,94	0
56	MG	A	1650	1/1	0.93	0.45	-	86,86,86,86	0
56	MG	B	3583	1/1	0.83	0.32	-	73,73,73,73	0
56	MG	S	205	1/1	0.91	0.19	-	54,54,54,54	0
56	MG	B	3618	1/1	0.88	0.59	-	43,43,43,43	0
56	MG	A	1777	1/1	0.73	0.24	-	91,91,91,91	0
56	MG	B	3740	1/1	0.95	0.69	-	70,70,70,70	0
56	MG	B	3228	1/1	0.81	0.25	-	58,58,58,58	0
56	MG	A	1783	1/1	0.86	0.09	-	111,111,111,111	0
56	MG	GB	3197	1/1	0.74	0.29	-	100,100,100,100	0
56	MG	FB	1686	1/1	0.62	0.56	-	124,124,124,124	0
56	MG	JB	308	1/1	0.86	0.48	-	73,73,73,73	0
56	MG	GB	3527	1/1	0.82	0.90	-	81,81,81,81	0
56	MG	B	3063	1/1	0.90	0.50	-	44,44,44,44	0
56	MG	B	3220	1/1	0.95	0.17	-	46,46,46,46	0
56	MG	B	3441	1/1	0.87	0.23	-	49,49,49,49	0
56	MG	B	3245	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	FB	1665	1/1	0.88	0.73	-	70,70,70,70	0
56	MG	B	3702	1/1	0.83	1.70	-	86,86,86,86	0
56	MG	B	3265	1/1	0.84	0.54	-	62,62,62,62	0
56	MG	A	1858	1/1	0.82	0.42	-	100,100,100,100	0
56	MG	GB	3346	1/1	0.83	0.42	-	66,66,66,66	0
56	MG	JA	410	1/1	0.87	0.10	-	96,96,96,96	0
56	MG	FB	1699	1/1	0.92	0.13	-	86,86,86,86	0
56	MG	VA	201	1/1	0.80	0.51	-	123,123,123,123	0
56	MG	B	3777	1/1	0.89	0.23	-	50,50,50,50	0
56	MG	B	3312	1/1	0.83	0.37	-	53,53,53,53	0
56	MG	JB	311	1/1	0.89	0.74	-	63,63,63,63	0
56	MG	GB	3438	1/1	0.90	0.37	-	52,52,52,52	0
56	MG	GB	3620	1/1	0.87	0.44	-	69,69,69,69	0
56	MG	B	2989	1/1	0.93	0.26	-	53,53,53,53	0
56	MG	IA	112	1/1	0.96	0.28	-	83,83,83,83	0
56	MG	PC	302	1/1	0.49	0.25	-	104,104,104,104	0
56	MG	B	3823	1/1	0.64	0.28	-	92,92,92,92	0
56	MG	GB	3027	1/1	0.82	0.13	-	74,74,74,74	0
56	MG	B	3739	1/1	0.91	0.19	-	53,53,53,53	0
56	MG	B	2910	1/1	0.96	0.30	-	34,34,34,34	0
56	MG	FB	1912	1/1	0.91	0.26	-	73,73,73,73	0
56	MG	A	1811	1/1	0.90	0.51	-	76,76,76,76	0
56	MG	B	3411	1/1	0.36	0.36	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3454	1/1	0.81	0.31	-	77,77,77,77	0
56	MG	A	1670	1/1	0.88	0.24	-	122,122,122,122	0
56	MG	B	3135	1/1	0.94	0.17	-	48,48,48,48	0
56	MG	QA	202	1/1	0.16	0.61	-	100,100,100,100	0
56	MG	GB	3568	1/1	0.85	0.17	-	66,66,66,66	0
56	MG	A	1733	1/1	0.71	0.13	-	100,100,100,100	0
56	MG	GB	3019	1/1	0.87	0.93	-	49,49,49,49	0
56	MG	FB	1900	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	GB	3296	1/1	0.91	0.35	-	65,65,65,65	0
56	MG	I	201	1/1	0.92	0.14	-	77,77,77,77	0
56	MG	GB	3097	1/1	0.69	0.41	-	57,57,57,57	0
56	MG	B	3689	1/1	0.81	0.29	-	50,50,50,50	0
56	MG	NA	202	1/1	0.71	0.20	-	101,101,101,101	0
56	MG	B	3594	1/1	0.91	0.20	-	56,56,56,56	0
56	MG	B	3735	1/1	0.88	0.25	-	71,71,71,71	0
56	MG	B	3407	1/1	0.90	0.28	-	72,72,72,72	0
56	MG	FB	1806	1/1	0.81	0.24	-	135,135,135,135	0
56	MG	GB	3664	1/1	0.81	0.41	-	58,58,58,58	0
56	MG	B	3342	1/1	0.83	0.22	-	115,115,115,115	0
56	MG	OC	405	1/1	0.85	0.25	-	91,91,91,91	0
56	MG	B	3214	1/1	0.94	0.47	-	83,83,83,83	0
56	MG	A	1766	1/1	0.95	0.17	-	103,103,103,103	0
56	MG	FB	1752	1/1	0.72	0.55	-	96,96,96,96	0
56	MG	GB	3292	1/1	0.93	0.21	-	86,86,86,86	0
56	MG	FB	1906	1/1	0.59	0.33	-	136,136,136,136	0
56	MG	FB	1768	1/1	0.82	0.22	-	80,80,80,80	0
56	MG	GB	3008	1/1	0.94	0.22	-	62,62,62,62	0
56	MG	GB	3029	1/1	0.89	0.29	-	75,75,75,75	0
56	MG	B	3191	1/1	0.85	0.12	-	59,59,59,59	0
56	MG	GB	3167	1/1	0.70	0.23	-	82,82,82,82	0
56	MG	T	202	1/1	0.94	0.61	-	45,45,45,45	0
56	MG	FB	1829	1/1	0.96	0.29	-	69,69,69,69	0
56	MG	GB	2939	1/1	0.86	0.47	-	64,64,64,64	0
56	MG	FB	1649	1/1	0.93	0.29	-	62,62,62,62	0
56	MG	GB	3638	1/1	0.64	0.51	-	66,66,66,66	0
56	MG	FB	1831	1/1	0.89	0.28	-	81,81,81,81	0
56	MG	A	1614	1/1	0.97	0.52	-	52,52,52,52	0
56	MG	B	2926	1/1	0.97	0.52	-	36,36,36,36	0
56	MG	FB	1759	1/1	0.88	0.29	-	66,66,66,66	0
56	MG	FB	1786	1/1	0.54	0.23	-	119,119,119,119	0
56	MG	XA	103	1/1	0.84	0.10	-	72,72,72,72	0
56	MG	B	3451	1/1	0.95	0.28	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3467	1/1	0.65	0.17	-	120,120,120,120	0
56	MG	B	3470	1/1	0.90	0.11	-	71,71,71,71	0
56	MG	B	3804	1/1	0.92	0.16	-	51,51,51,51	0
56	MG	B	3799	1/1	0.86	0.36	-	89,89,89,89	0
56	MG	GB	2910	1/1	0.94	0.48	-	48,48,48,48	0
56	MG	B	3291	1/1	0.78	0.24	-	109,109,109,109	0
56	MG	B	3294	1/1	0.88	0.32	-	75,75,75,75	0
56	MG	JB	303	1/1	0.77	0.18	-	71,71,71,71	0
56	MG	A	1764	1/1	0.66	0.17	-	85,85,85,85	0
56	MG	B	3355	1/1	0.85	0.21	-	55,55,55,55	0
56	MG	A	1649	1/1	0.88	0.42	-	101,101,101,101	0
56	MG	FB	1828	1/1	0.78	0.29	-	70,70,70,70	0
56	MG	B	3394	1/1	0.94	0.48	-	52,52,52,52	0
56	MG	FB	1892	1/1	0.93	0.32	-	68,68,68,68	0
56	MG	FB	1931	1/1	0.79	0.17	-	144,144,144,144	0
56	MG	FB	1606	1/1	0.96	0.45	-	57,57,57,57	0
56	MG	B	3022	1/1	0.96	0.24	-	45,45,45,45	0
56	MG	B	3778	1/1	0.88	0.15	-	67,67,67,67	0
56	MG	GB	3485	1/1	0.98	0.15	-	68,68,68,68	0
56	MG	C	240	1/1	0.56	0.19	-	75,75,75,75	0
56	MG	GB	3223	1/1	0.79	0.37	-	81,81,81,81	0
56	MG	SB	202	1/1	0.93	0.43	-	80,80,80,80	0
56	MG	GB	3020	1/1	0.70	0.38	-	60,60,60,60	0
56	MG	B	3474	1/1	0.82	0.30	-	41,41,41,41	0
56	MG	C	232	1/1	0.88	0.27	-	82,82,82,82	0
56	MG	ZA	202	1/1	0.69	0.21	-	87,87,87,87	0
56	MG	B	3020	1/1	0.94	0.32	-	37,37,37,37	0
56	MG	IB	105	1/1	0.83	0.33	-	117,117,117,117	0
56	MG	B	3196	1/1	0.93	0.42	-	80,80,80,80	0
56	MG	K	203	1/1	0.80	0.12	-	73,73,73,73	0
56	MG	GB	3396	1/1	0.90	0.24	-	71,71,71,71	0
56	MG	A	1647	1/1	0.96	0.20	-	82,82,82,82	0
56	MG	NB	202	1/1	0.79	0.33	-	120,120,120,120	0
56	MG	FB	1849	1/1	0.87	0.35	-	65,65,65,65	0
56	MG	GB	3093	1/1	0.88	0.31	-	58,58,58,58	0
56	MG	JB	309	1/1	0.85	0.15	-	69,69,69,69	0
56	MG	GB	3161	1/1	0.88	0.56	-	73,73,73,73	0
56	MG	DC	103	1/1	0.93	0.47	-	76,76,76,76	0
56	MG	B	3530	1/1	0.82	0.38	-	58,58,58,58	0
56	MG	B	3146	1/1	0.88	0.29	-	48,48,48,48	0
56	MG	GB	3429	1/1	0.78	0.23	-	49,49,49,49	0
56	MG	N	203	1/1	0.92	0.28	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	A	1791	1/1	0.93	0.11	-	59,59,59,59	0
56	MG	PB	201	1/1	0.88	0.17	-	93,93,93,93	0
56	MG	FB	1870	1/1	0.29	0.22	-	127,127,127,127	0
56	MG	A	1870	1/1	0.39	0.19	-	123,123,123,123	0
56	MG	FB	1914	1/1	0.93	0.28	-	63,63,63,63	0
56	MG	GB	3287	1/1	0.82	0.23	-	62,62,62,62	0
56	MG	A	1661	1/1	0.89	0.24	-	64,64,64,64	0
56	MG	GB	3439	1/1	0.84	0.28	-	74,74,74,74	0
56	MG	X	101	1/1	0.94	0.28	-	58,58,58,58	0
56	MG	B	3517	1/1	0.90	0.12	-	53,53,53,53	0
56	MG	GB	2992	1/1	0.89	0.27	-	64,64,64,64	0
56	MG	GB	2960	1/1	0.96	0.26	-	63,63,63,63	0
56	MG	GB	3383	1/1	0.51	0.41	-	191,191,191,191	0
56	MG	GB	3441	1/1	0.42	0.33	-	155,155,155,155	0
56	MG	GB	3639	1/1	0.73	0.37	-	71,71,71,71	0
56	MG	KB	303	1/1	0.83	0.20	-	79,79,79,79	0
56	MG	IA	120	1/1	0.82	0.14	-	85,85,85,85	0
56	MG	A	1695	1/1	0.71	0.29	-	71,71,71,71	0
56	MG	GB	3553	1/1	0.80	0.29	-	86,86,86,86	0
56	MG	A	1655	1/1	0.86	0.19	-	66,66,66,66	0
56	MG	B	2983	1/1	0.74	0.28	-	50,50,50,50	0
56	MG	GB	3385	1/1	0.63	0.71	-	98,98,98,98	0
56	MG	B	3086	1/1	0.95	0.23	-	43,43,43,43	0
56	MG	B	3014	1/1	0.85	0.26	-	56,56,56,56	0
56	MG	B	3776	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	FB	1728	1/1	0.93	0.12	-	81,81,81,81	0
56	MG	GB	3251	1/1	0.85	0.44	-	55,55,55,55	0
56	MG	BC	307	1/1	0.73	0.12	-	104,104,104,104	0
56	MG	B	3381	1/1	0.76	0.27	-	77,77,77,77	0
56	MG	YB	201	1/1	0.85	0.41	-	72,72,72,72	0
56	MG	FB	1917	1/1	0.68	0.58	-	110,110,110,110	0
56	MG	B	3699	1/1	0.82	0.48	-	49,49,49,49	0
56	MG	A	1863	1/1	0.96	0.23	-	93,93,93,93	0
56	MG	GB	3532	1/1	0.79	0.28	-	70,70,70,70	0
56	MG	B	2939	1/1	0.94	0.45	-	48,48,48,48	0
56	MG	B	3173	1/1	0.92	0.24	-	40,40,40,40	0
56	MG	GB	3077	1/1	0.91	0.40	-	68,68,68,68	0
56	MG	FB	1723	1/1	0.88	0.29	-	86,86,86,86	0
56	MG	GB	3240	1/1	0.91	0.10	-	106,106,106,106	0
56	MG	A	1703	1/1	0.80	0.37	-	61,61,61,61	0
56	MG	B	3365	1/1	0.95	0.36	-	73,73,73,73	0
56	MG	B	3210	1/1	0.97	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3782	1/1	0.37	0.22	-	175,175,175,175	0
56	MG	GB	3033	1/1	0.84	0.10	-	79,79,79,79	0
56	MG	B	3006	1/1	0.87	0.22	-	53,53,53,53	0
56	MG	B	3595	1/1	0.99	0.44	-	75,75,75,75	0
56	MG	B	3044	1/1	0.99	0.57	-	40,40,40,40	0
56	MG	NA	203	1/1	0.70	0.38	-	98,98,98,98	0
56	MG	A	1717	1/1	0.60	0.68	-	86,86,86,86	0
56	MG	UC	201	1/1	0.51	0.39	-	105,105,105,105	0
56	MG	FB	1887	1/1	0.71	0.28	-	65,65,65,65	0
56	MG	FB	1773	1/1	0.83	0.37	-	78,78,78,78	0
56	MG	GB	3646	1/1	0.88	0.14	-	75,75,75,75	0
56	MG	X	102	1/1	0.85	0.17	-	50,50,50,50	0
56	MG	B	3584	1/1	0.90	0.51	-	46,46,46,46	0
56	MG	GB	2951	1/1	0.91	0.26	-	71,71,71,71	0
56	MG	FB	1841	1/1	0.92	0.62	-	85,85,85,85	0
56	MG	GB	3314	1/1	0.79	0.20	-	140,140,140,140	0
56	MG	GB	2994	1/1	0.86	0.53	-	74,74,74,74	0
56	MG	Y	104	1/1	0.73	0.23	-	71,71,71,71	0
56	MG	B	3509	1/1	0.95	0.09	-	52,52,52,52	0
56	MG	B	3459	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	HB	214	1/1	0.84	0.45	-	107,107,107,107	0
56	MG	FB	1879	1/1	0.90	0.29	-	78,78,78,78	0
56	MG	B	3187	1/1	0.81	0.19	-	59,59,59,59	0
56	MG	FB	1734	1/1	0.77	0.57	-	65,65,65,65	0
56	MG	Z	102	1/1	0.84	0.13	-	67,67,67,67	0
56	MG	FB	1679	1/1	0.71	0.67	-	81,81,81,81	0
56	MG	GB	3210	1/1	0.88	0.15	-	77,77,77,77	0
56	MG	GB	3525	1/1	0.83	0.18	-	79,79,79,79	0
56	MG	A	1761	1/1	0.74	0.21	-	74,74,74,74	0
56	MG	A	1694	1/1	0.88	0.36	-	90,90,90,90	0
56	MG	FB	1903	1/1	0.92	0.42	-	76,76,76,76	0
56	MG	FB	1769	1/1	0.75	0.28	-	91,91,91,91	0
56	MG	B	3212	1/1	0.89	0.26	-	52,52,52,52	0
56	MG	TB	201	1/1	0.82	0.21	-	66,66,66,66	0
56	MG	H	201	1/1	0.88	0.20	-	79,79,79,79	0
56	MG	B	3746	1/1	0.64	0.16	-	68,68,68,68	0
56	MG	B	2907	1/1	0.93	0.68	-	41,41,41,41	0
56	MG	GB	3677	1/1	0.92	0.27	-	60,60,60,60	0
56	MG	GB	3543	1/1	0.89	0.44	-	55,55,55,55	0
56	MG	GB	3134	1/1	0.86	0.97	-	61,61,61,61	0
56	MG	GB	3419	1/1	0.50	0.28	-	74,74,74,74	0
56	MG	AA	104	1/1	0.80	0.17	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3149	1/1	0.79	0.28	-	42,42,42,42	0
56	MG	GB	3302	1/1	0.92	0.42	-	47,47,47,47	0
56	MG	GB	3030	1/1	0.90	0.41	-	88,88,88,88	0
56	MG	A	1773	1/1	0.89	0.39	-	88,88,88,88	0
56	MG	GB	3696	1/1	0.60	0.47	-	72,72,72,72	0
56	MG	B	3274	1/1	0.89	0.29	-	54,54,54,54	0
56	MG	GB	3212	1/1	0.95	0.56	-	55,55,55,55	0
56	MG	B	3183	1/1	0.90	0.11	-	57,57,57,57	0
56	MG	B	2947	1/1	0.87	1.02	-	40,40,40,40	0
56	MG	GB	3409	1/1	0.83	0.22	-	70,70,70,70	0
56	MG	B	3333	1/1	0.98	0.10	-	78,78,78,78	0
56	MG	KB	302	1/1	0.68	0.11	-	75,75,75,75	0
56	MG	GB	3188	1/1	0.60	0.35	-	179,179,179,179	0
56	MG	A	1619	1/1	0.91	0.52	-	61,61,61,61	0
56	MG	LB	304	1/1	0.85	0.15	-	83,83,83,83	0
56	MG	GB	3495	1/1	0.76	0.16	-	72,72,72,72	0
56	MG	B	2940	1/1	0.89	0.51	-	33,33,33,33	0
56	MG	GB	3684	1/1	0.86	0.26	-	66,66,66,66	0
56	MG	B	3795	1/1	0.05	0.65	-	151,151,151,151	0
56	MG	B	3154	1/1	0.84	0.16	-	58,58,58,58	0
56	MG	FB	1853	1/1	0.97	0.34	-	126,126,126,126	0
56	MG	FB	1668	1/1	0.82	0.39	-	82,82,82,82	0
56	MG	B	3071	1/1	0.85	0.14	-	58,58,58,58	0
56	MG	B	3742	1/1	0.88	0.70	-	54,54,54,54	0
56	MG	FB	1717	1/1	0.58	0.30	-	74,74,74,74	0
56	MG	GB	3356	1/1	0.94	0.09	-	134,134,134,134	0
56	MG	A	1696	1/1	0.31	1.49	-	157,157,157,157	0
56	MG	DC	101	1/1	0.96	0.35	-	60,60,60,60	0
56	MG	B	3452	1/1	0.87	0.44	-	82,82,82,82	0
56	MG	GB	3659	1/1	0.77	0.22	-	80,80,80,80	0
56	MG	B	3200	1/1	0.96	0.26	-	66,66,66,66	0
56	MG	FB	1715	1/1	0.79	0.22	-	82,82,82,82	0
56	MG	B	3405	1/1	0.69	0.14	-	124,124,124,124	0
56	MG	GB	3520	1/1	0.89	0.38	-	73,73,73,73	0
56	MG	MA	302	1/1	0.92	0.30	-	105,105,105,105	0
56	MG	HA	101	1/1	0.91	0.74	-	77,77,77,77	0
56	MG	NC	101	1/1	0.84	0.14	-	85,85,85,85	0
56	MG	GB	3285	1/1	0.94	0.64	-	52,52,52,52	0
56	MG	A	1846	1/1	0.91	0.22	-	57,57,57,57	0
56	MG	JA	404	1/1	0.55	0.37	-	83,83,83,83	0
56	MG	B	3802	1/1	0.94	0.22	-	77,77,77,77	0
56	MG	B	3745	1/1	0.85	0.42	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	L	205	1/1	0.94	0.24	-	61,61,61,61	0
56	MG	A	1853	1/1	0.79	0.30	-	99,99,99,99	0
56	MG	B	3003	1/1	0.74	0.43	-	53,53,53,53	0
56	MG	GB	3446	1/1	0.89	0.43	-	75,75,75,75	0
56	MG	B	3399	1/1	0.89	0.25	-	53,53,53,53	0
56	MG	GB	3405	1/1	0.77	0.26	-	70,70,70,70	0
56	MG	FB	1604	1/1	0.83	0.27	-	67,67,67,67	0
56	MG	B	3102	1/1	0.84	0.20	-	46,46,46,46	0
56	MG	A	1628	1/1	0.78	0.73	-	77,77,77,77	0
56	MG	B	3402	1/1	0.89	0.20	-	179,179,179,179	0
56	MG	GB	3499	1/1	0.80	0.55	-	61,61,61,61	0
56	MG	GB	3610	1/1	0.97	0.35	-	78,78,78,78	0
56	MG	GB	3336	1/1	0.93	0.24	-	68,68,68,68	0
56	MG	B	3566	1/1	0.92	0.89	-	60,60,60,60	0
56	MG	B	3731	1/1	0.94	0.11	-	46,46,46,46	0
56	MG	HB	229	1/1	0.98	0.13	-	100,100,100,100	0
56	MG	A	1835	1/1	0.91	0.21	-	70,70,70,70	0
56	MG	GB	3393	1/1	0.70	0.19	-	192,192,192,192	0
56	MG	GB	3477	1/1	0.90	0.22	-	60,60,60,60	0
56	MG	B	3825	1/1	0.93	0.27	-	55,55,55,55	0
56	MG	GB	3221	1/1	0.80	0.59	-	164,164,164,164	0
56	MG	B	3545	1/1	0.94	0.12	-	74,74,74,74	0
56	MG	A	1866	1/1	0.82	0.12	-	95,95,95,95	0
56	MG	FB	1891	1/1	0.93	0.17	-	132,132,132,132	0
56	MG	JB	310	1/1	0.94	0.12	-	64,64,64,64	0
56	MG	NC	104	1/1	0.86	0.16	-	93,93,93,93	0
56	MG	B	3180	1/1	0.95	0.17	-	58,58,58,58	0
56	MG	FB	1901	1/1	0.80	0.30	-	75,75,75,75	0
56	MG	GB	3549	1/1	0.77	0.27	-	86,86,86,86	0
56	MG	A	1745	1/1	0.76	0.31	-	78,78,78,78	0
56	MG	B	3781	1/1	0.79	0.12	-	69,69,69,69	0
56	MG	A	1868	1/1	0.64	0.82	-	71,71,71,71	0
56	MG	GB	3265	1/1	0.72	0.16	-	100,100,100,100	0
56	MG	B	3457	1/1	0.80	0.31	-	66,66,66,66	0
56	MG	NC	105	1/1	0.87	0.19	-	94,94,94,94	0
56	MG	B	3483	1/1	0.95	0.15	-	48,48,48,48	0
56	MG	GB	3300	1/1	0.79	0.70	-	90,90,90,90	0
56	MG	B	3140	1/1	0.89	0.25	-	54,54,54,54	0
56	MG	B	3087	1/1	0.91	0.20	-	53,53,53,53	0
56	MG	FB	1789	1/1	0.95	0.21	-	69,69,69,69	0
56	MG	GB	3363	1/1	0.93	0.49	-	75,75,75,75	0
56	MG	GB	3621	1/1	0.92	0.15	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	HB	215	1/1	0.41	0.19	-	109,109,109,109	0
56	MG	GB	3178	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	B	3375	1/1	0.90	0.21	-	79,79,79,79	0
56	MG	GB	3687	1/1	0.81	0.14	-	72,72,72,72	0
56	MG	FB	1661	1/1	0.77	0.15	-	66,66,66,66	0
56	MG	B	2955	1/1	0.95	0.12	-	46,46,46,46	0
56	MG	B	3308	1/1	0.77	0.43	-	50,50,50,50	0
56	MG	A	1804	1/1	0.24	0.35	-	136,136,136,136	0
56	MG	B	2935	1/1	0.87	0.55	-	44,44,44,44	0
56	MG	FB	1739	1/1	0.88	0.65	-	70,70,70,70	0
56	MG	FB	1794	1/1	0.82	0.74	-	85,85,85,85	0
56	MG	GB	3570	1/1	0.90	0.34	-	82,82,82,82	0
56	MG	GB	3028	1/1	0.80	0.25	-	71,71,71,71	0
56	MG	A	1836	1/1	0.87	0.34	-	105,105,105,105	0
56	MG	GB	3701	1/1	0.72	0.66	-	70,70,70,70	0
56	MG	GB	3122	1/1	0.81	0.14	-	76,76,76,76	0
56	MG	B	3420	1/1	0.83	0.34	-	43,43,43,43	0
56	MG	GB	3448	1/1	0.84	0.79	-	48,48,48,48	0
56	MG	B	3460	1/1	0.92	0.24	-	43,43,43,43	0
56	MG	FB	1825	1/1	0.83	0.75	-	86,86,86,86	0
56	MG	GB	3615	1/1	0.88	0.45	-	76,76,76,76	0
56	MG	XB	204	1/1	0.84	0.28	-	97,97,97,97	0
56	MG	C	220	1/1	0.96	0.16	-	83,83,83,83	0
56	MG	GB	3284	1/1	0.94	0.40	-	64,64,64,64	0
56	MG	GB	3281	1/1	0.92	0.50	-	72,72,72,72	0
56	MG	A	1816	1/1	0.14	0.20	-	108,108,108,108	0
56	MG	GB	3612	1/1	0.65	0.79	-	71,71,71,71	0
56	MG	FB	1801	1/1	0.83	0.20	-	75,75,75,75	0
56	MG	YB	207	1/1	0.66	0.72	-	79,79,79,79	0
56	MG	GB	3554	1/1	0.74	0.49	-	71,71,71,71	0
56	MG	E	310	1/1	0.69	0.24	-	57,57,57,57	0
56	MG	A	1712	1/1	0.84	0.22	-	76,76,76,76	0
56	MG	GB	3152	1/1	0.77	0.27	-	74,74,74,74	0
56	MG	GB	3497	1/1	0.83	0.26	-	59,59,59,59	0
56	MG	B	3295	1/1	0.86	0.27	-	55,55,55,55	0
56	MG	GB	3571	1/1	0.55	0.37	-	66,66,66,66	0
56	MG	FB	1883	1/1	0.85	0.18	-	70,70,70,70	0
56	MG	A	1877	1/1	0.76	0.17	-	167,167,167,167	0
56	MG	B	3332	1/1	0.96	0.18	-	65,65,65,65	0
56	MG	GB	3634	1/1	0.88	0.33	-	63,63,63,63	0
56	MG	B	3289	1/1	0.93	0.46	-	38,38,38,38	0
56	MG	GB	3371	1/1	0.86	0.25	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3236	1/1	0.82	0.50	-	74,74,74,74	0
56	MG	A	1626	1/1	0.82	0.27	-	63,63,63,63	0
56	MG	GB	3632	1/1	0.83	0.15	-	130,130,130,130	0
56	MG	A	1609	1/1	0.72	0.35	-	55,55,55,55	0
56	MG	GB	3165	1/1	0.87	0.22	-	66,66,66,66	0
56	MG	GB	3652	1/1	0.80	0.12	-	73,73,73,73	0
56	MG	GB	2949	1/1	0.92	0.28	-	52,52,52,52	0
56	MG	FB	1652	1/1	0.85	0.80	-	70,70,70,70	0
56	MG	GB	3163	1/1	0.82	0.24	-	74,74,74,74	0
56	MG	B	3803	1/1	0.89	0.18	-	58,58,58,58	0
56	MG	GB	3397	1/1	0.77	0.44	-	60,60,60,60	0
56	MG	FB	1650	1/1	0.85	0.62	-	66,66,66,66	0
56	MG	B	3612	1/1	0.86	0.38	-	59,59,59,59	0
56	MG	B	3622	1/1	0.84	0.27	-	55,55,55,55	0
56	MG	B	3326	1/1	0.95	0.31	-	44,44,44,44	0
56	MG	B	3456	1/1	0.86	0.28	-	50,50,50,50	0
56	MG	FB	1743	1/1	0.85	0.26	-	84,84,84,84	0
56	MG	A	1826	1/1	0.90	0.21	-	58,58,58,58	0
56	MG	TA	201	1/1	0.49	0.26	-	92,92,92,92	0
56	MG	GB	3468	1/1	0.78	0.47	-	86,86,86,86	0
56	MG	B	3514	1/1	0.81	0.31	-	55,55,55,55	0
56	MG	OC	403	1/1	0.71	0.32	-	112,112,112,112	0
56	MG	C	228	1/1	0.92	0.11	-	76,76,76,76	0
56	MG	GB	3516	1/1	0.80	0.26	-	63,63,63,63	0
56	MG	B	3674	1/1	0.65	0.20	-	131,131,131,131	0
56	MG	B	3153	1/1	0.92	0.68	-	42,42,42,42	0
56	MG	GB	3574	1/1	0.85	0.16	-	83,83,83,83	0
56	MG	GB	3408	1/1	0.81	0.39	-	55,55,55,55	0
56	MG	GB	3110	1/1	0.92	0.29	-	72,72,72,72	0
56	MG	A	1823	1/1	0.90	0.33	-	54,54,54,54	0
56	MG	B	3577	1/1	0.87	0.32	-	66,66,66,66	0
56	MG	W	307	1/1	0.88	0.16	-	87,87,87,87	0
56	MG	X	104	1/1	0.90	0.27	-	51,51,51,51	0
56	MG	FB	1735	1/1	0.95	0.08	-	85,85,85,85	0
56	MG	A	1652	1/1	0.87	0.14	-	70,70,70,70	0
56	MG	B	3639	1/1	0.97	0.14	-	46,46,46,46	0
56	MG	GB	3536	1/1	0.90	0.31	-	67,67,67,67	0
56	MG	B	3714	1/1	0.90	0.17	-	52,52,52,52	0
56	MG	B	3150	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	A	1636	1/1	0.81	0.22	-	82,82,82,82	0
56	MG	FB	1716	1/1	0.90	0.16	-	82,82,82,82	0
56	MG	GB	3012	1/1	0.91	0.40	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3633	1/1	0.93	0.14	-	63,63,63,63	0
56	MG	GB	2946	1/1	0.95	0.45	-	52,52,52,52	0
56	MG	B	3357	1/1	0.90	0.15	-	54,54,54,54	0
56	MG	OA	204	1/1	0.73	0.35	-	82,82,82,82	0
56	MG	QC	301	1/1	0.61	0.91	-	97,97,97,97	0
56	MG	FB	1817	1/1	0.79	0.73	-	62,62,62,62	0
56	MG	A	1744	1/1	0.87	0.21	-	87,87,87,87	0
56	MG	GB	3041	1/1	0.74	0.17	-	93,93,93,93	0
56	MG	HB	228	1/1	0.74	0.34	-	81,81,81,81	0
56	MG	B	3199	1/1	0.83	0.45	-	55,55,55,55	0
56	MG	B	3184	1/1	0.97	0.25	-	46,46,46,46	0
56	MG	GB	3676	1/1	0.95	0.31	-	88,88,88,88	0
56	MG	FB	1869	1/1	0.85	0.30	-	109,109,109,109	0
56	MG	FB	1638	1/1	0.70	0.42	-	60,60,60,60	0
56	MG	B	3349	1/1	-0.01	0.33	-	132,132,132,132	0
56	MG	GB	3353	1/1	0.77	0.40	-	68,68,68,68	0
56	MG	B	3124	1/1	0.87	0.19	-	44,44,44,44	0
56	MG	MC	101	1/1	0.85	0.36	-	94,94,94,94	0
56	MG	B	3017	1/1	0.73	0.63	-	51,51,51,51	0
56	MG	FB	1625	1/1	0.82	0.45	-	78,78,78,78	0
56	MG	GB	3111	1/1	0.76	0.37	-	66,66,66,66	0
56	MG	GB	3364	1/1	0.92	0.11	-	70,70,70,70	0
56	MG	B	3097	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	A	1813	1/1	0.62	0.34	-	89,89,89,89	0
56	MG	GB	3442	1/1	0.84	0.18	-	194,194,194,194	0
56	MG	GB	3518	1/1	0.83	0.16	-	96,96,96,96	0
56	MG	B	3593	1/1	0.43	0.45	-	78,78,78,78	0
56	MG	A	1815	1/1	0.76	0.19	-	108,108,108,108	0
56	MG	GB	3550	1/1	0.93	0.26	-	61,61,61,61	0
56	MG	A	1734	1/1	0.82	1.07	-	72,72,72,72	0
56	MG	A	1612	1/1	0.85	0.37	-	54,54,54,54	0
56	MG	GB	3619	1/1	0.82	0.25	-	75,75,75,75	0
56	MG	A	1746	1/1	0.81	0.21	-	141,141,141,141	0
56	MG	M	205	1/1	0.81	0.32	-	45,45,45,45	0
56	MG	SC	204	1/1	0.64	0.27	-	81,81,81,81	0
56	MG	GB	3576	1/1	0.71	0.20	-	70,70,70,70	0
56	MG	B	3335	1/1	0.77	0.15	-	78,78,78,78	0
56	MG	B	3686	1/1	0.96	0.26	-	43,43,43,43	0
56	MG	B	3403	1/1	0.98	0.16	-	50,50,50,50	0
56	MG	B	3223	1/1	0.94	0.13	-	65,65,65,65	0
56	MG	B	2934	1/1	0.82	0.36	-	62,62,62,62	0
56	MG	FB	1793	1/1	0.91	0.76	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3458	1/1	0.87	0.20	-	95,95,95,95	0
56	MG	L	202	1/1	0.90	0.24	-	58,58,58,58	0
56	MG	GB	3691	1/1	0.85	0.43	-	71,71,71,71	0
56	MG	GB	3065	1/1	0.80	0.31	-	95,95,95,95	0
56	MG	FB	1662	1/1	0.90	0.19	-	66,66,66,66	0
56	MG	NC	103	1/1	0.91	0.27	-	84,84,84,84	0
56	MG	FB	1757	1/1	0.74	0.15	-	101,101,101,101	0
56	MG	GB	3184	1/1	0.84	0.31	-	61,61,61,61	0
56	MG	D	101	1/1	0.73	0.52	-	100,100,100,100	0
56	MG	B	3768	1/1	0.90	0.22	-	41,41,41,41	0
56	MG	C	207	1/1	0.86	0.40	-	57,57,57,57	0
56	MG	B	3788	1/1	0.91	0.21	-	56,56,56,56	0
56	MG	FB	1660	1/1	0.93	0.24	-	70,70,70,70	0
56	MG	MB	206	1/1	0.85	0.22	-	127,127,127,127	0
56	MG	B	3156	1/1	0.89	0.21	-	50,50,50,50	0
56	MG	FB	1788	1/1	0.79	0.18	-	76,76,76,76	0
56	MG	B	3619	1/1	0.90	0.12	-	70,70,70,70	0
56	MG	BC	302	1/1	0.55	0.13	-	109,109,109,109	0
56	MG	GB	3590	1/1	0.67	0.24	-	76,76,76,76	0
56	MG	B	3467	1/1	0.81	0.32	-	50,50,50,50	0
56	MG	GB	3625	1/1	0.82	0.27	-	78,78,78,78	0
56	MG	GB	3130	1/1	0.89	0.26	-	60,60,60,60	0
56	MG	B	3008	1/1	0.95	0.13	-	80,80,80,80	0
56	MG	GB	2961	1/1	0.74	0.34	-	64,64,64,64	0
56	MG	GB	3657	1/1	0.83	0.29	-	101,101,101,101	0
56	MG	RC	309	1/1	0.90	0.24	-	77,77,77,77	0
56	MG	A	1847	1/1	0.78	0.58	-	93,93,93,93	0
56	MG	A	1755	1/1	0.83	0.20	-	71,71,71,71	0
56	MG	X	106	1/1	0.92	0.42	-	63,63,63,63	0
56	MG	GB	2968	1/1	0.92	0.49	-	69,69,69,69	0
56	MG	FB	1935	1/1	0.75	0.65	-	71,71,71,71	0
56	MG	QC	304	1/1	0.84	0.33	-	104,104,104,104	0
56	MG	B	3783	1/1	0.91	0.82	-	50,50,50,50	0
56	MG	A	1644	1/1	0.95	0.12	-	62,62,62,62	0
56	MG	GB	3261	1/1	0.82	0.19	-	134,134,134,134	0
56	MG	B	3233	1/1	0.97	0.10	-	51,51,51,51	0
56	MG	FB	1732	1/1	0.79	0.55	-	105,105,105,105	0
56	MG	G	3210	1/1	0.76	0.46	-	62,62,62,62	0
56	MG	B	2987	1/1	0.92	0.52	-	34,34,34,34	0
56	MG	A	1664	1/1	0.76	0.81	-	73,73,73,73	0
56	MG	GB	3473	1/1	0.89	0.67	-	76,76,76,76	0
56	MG	GB	3494	1/1	0.97	0.50	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	PB	204	1/1	0.94	0.10	-	95,95,95,95	0
56	MG	B	3104	1/1	0.91	0.12	-	70,70,70,70	0
56	MG	GB	3092	1/1	0.92	0.34	-	87,87,87,87	0
56	MG	B	3443	1/1	0.74	0.12	-	176,176,176,176	0
56	MG	B	3386	1/1	0.92	0.26	-	101,101,101,101	0
56	MG	B	3356	1/1	0.87	0.20	-	50,50,50,50	0
56	MG	GB	3533	1/1	0.77	0.30	-	93,93,93,93	0
56	MG	GB	3206	1/1	0.90	0.46	-	64,64,64,64	0
56	MG	GB	3183	1/1	0.80	0.51	-	61,61,61,61	0
56	MG	TC	201	1/1	0.73	0.42	-	79,79,79,79	0
56	MG	GB	3307	1/1	0.87	0.38	-	51,51,51,51	0
56	MG	C	236	1/1	0.71	0.17	-	77,77,77,77	0
56	MG	GB	3218	1/1	0.76	0.73	-	61,61,61,61	0
56	MG	B	3302	1/1	0.85	0.48	-	54,54,54,54	0
56	MG	GB	3181	1/1	0.92	0.20	-	64,64,64,64	0
56	MG	GB	3342	1/1	0.93	0.41	-	45,45,45,45	0
56	MG	B	3170	1/1	0.90	0.16	-	62,62,62,62	0
56	MG	GB	3293	1/1	0.50	0.18	-	190,190,190,190	0
56	MG	B	3482	1/1	0.93	0.25	-	47,47,47,47	0
56	MG	B	3130	1/1	0.80	0.17	-	80,80,80,80	0
56	MG	GB	3427	1/1	0.77	0.42	-	61,61,61,61	0
56	MG	B	3755	1/1	0.92	0.28	-	61,61,61,61	0
56	MG	FB	1820	1/1	0.71	0.21	-	85,85,85,85	0
56	MG	B	3362	1/1	0.82	0.13	-	66,66,66,66	0
56	MG	A	1602	1/1	0.90	0.41	-	69,69,69,69	0
56	MG	B	3188	1/1	0.65	0.30	-	74,74,74,74	0
56	MG	GC	103	1/1	0.49	0.16	-	135,135,135,135	0
56	MG	A	1785	1/1	0.45	0.26	-	107,107,107,107	0
56	MG	B	3303	1/1	0.87	0.23	-	41,41,41,41	0
56	MG	B	2943	1/1	0.96	0.31	-	37,37,37,37	0
56	MG	B	3292	1/1	0.87	0.22	-	50,50,50,50	0
56	MG	B	3179	1/1	0.96	0.38	-	47,47,47,47	0
56	MG	GB	3653	1/1	0.91	0.37	-	78,78,78,78	0
56	MG	FB	1640	1/1	0.96	0.54	-	64,64,64,64	0
56	MG	GB	3596	1/1	0.79	0.31	-	90,90,90,90	0
56	MG	FB	1867	1/1	0.84	0.15	-	82,82,82,82	0
56	MG	B	3794	1/1	0.80	0.46	-	60,60,60,60	0
56	MG	B	3715	1/1	0.76	0.37	-	64,64,64,64	0
56	MG	GB	3323	1/1	0.63	0.57	-	71,71,71,71	0
56	MG	GB	3386	1/1	0.86	0.46	-	76,76,76,76	0
56	MG	GB	3350	1/1	0.90	0.25	-	61,61,61,61	0
56	MG	B	3234	1/1	0.88	0.38	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B	3532	1/1	0.45	0.24	-	95,95,95,95	0
56	MG	GB	3100	1/1	0.95	0.38	-	58,58,58,58	0
56	MG	A	1726	1/1	0.92	0.25	-	73,73,73,73	0
56	MG	B	3203	1/1	0.90	0.14	-	57,57,57,57	0
56	MG	B	2902	1/1	0.97	0.50	-	35,35,35,35	0
56	MG	A	1803	1/1	0.67	0.40	-	103,103,103,103	0
56	MG	B	3522	1/1	0.95	0.17	-	49,49,49,49	0
56	MG	B	3433	1/1	0.64	0.19	-	101,101,101,101	0
56	MG	FB	1909	1/1	0.82	0.34	-	72,72,72,72	0
56	MG	B	3181	1/1	0.74	0.35	-	57,57,57,57	0
56	MG	GB	3133	1/1	0.75	0.16	-	69,69,69,69	0
56	MG	GB	3106	1/1	0.75	0.38	-	66,66,66,66	0
56	MG	GB	3329	1/1	0.79	0.44	-	85,85,85,85	0
56	MG	FB	1922	1/1	0.92	0.36	-	83,83,83,83	0
56	MG	B	3798	1/1	0.87	0.47	-	157,157,157,157	0
56	MG	FB	1706	1/1	0.81	0.20	-	69,69,69,69	0
56	MG	FB	1691	1/1	0.88	0.54	-	74,74,74,74	0
56	MG	IA	109	1/1	0.92	0.11	-	79,79,79,79	0
56	MG	GB	3162	1/1	0.62	0.29	-	101,101,101,101	0
56	MG	GB	3288	1/1	0.82	0.29	-	73,73,73,73	0
56	MG	FB	1880	1/1	0.79	0.30	-	74,74,74,74	0
56	MG	A	1792	1/1	0.48	0.45	-	132,132,132,132	0
56	MG	QB	203	1/1	0.98	0.12	-	69,69,69,69	0
56	MG	GB	2959	1/1	0.88	0.70	-	56,56,56,56	0
56	MG	B	3786	1/1	0.81	0.15	-	68,68,68,68	0
56	MG	GB	3682	1/1	0.82	0.53	-	77,77,77,77	0
56	MG	GB	3219	1/1	0.59	0.21	-	85,85,85,85	0
56	MG	C	211	1/1	0.89	0.27	-	83,83,83,83	0
56	MG	FB	1629	1/1	0.91	0.49	-	66,66,66,66	0
56	MG	GB	3373	1/1	0.83	0.33	-	85,85,85,85	0
56	MG	B	2933	1/1	0.93	0.20	-	52,52,52,52	0
56	MG	FB	1700	1/1	0.91	0.31	-	73,73,73,73	0
56	MG	GB	3282	1/1	0.93	0.23	-	70,70,70,70	0
56	MG	FA	101	1/1	0.91	0.33	-	54,54,54,54	0
56	MG	GB	3637	1/1	0.92	0.61	-	49,49,49,49	0
56	MG	B	3429	1/1	0.83	0.53	-	46,46,46,46	0
56	MG	GB	3447	1/1	0.78	0.19	-	199,199,199,199	0
56	MG	B	3464	1/1	0.91	0.33	-	48,48,48,48	0
56	MG	B	3267	1/1	0.81	0.19	-	61,61,61,61	0
56	MG	GB	3469	1/1	0.74	0.58	-	65,65,65,65	0
56	MG	B	3747	1/1	0.69	0.25	-	74,74,74,74	0
56	MG	EC	104	1/1	0.89	0.17	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	GB	3591	1/1	0.88	0.24	-	71,71,71,71	0
56	MG	GB	2941	1/1	0.89	0.61	-	53,53,53,53	0
56	MG	B	3424	1/1	0.76	0.54	-	57,57,57,57	0
56	MG	B	3510	1/1	0.94	0.19	-	45,45,45,45	0
56	MG	A	1607	1/1	0.88	0.29	-	76,76,76,76	0
56	MG	FB	1850	1/1	0.93	0.18	-	89,89,89,89	0
56	MG	IA	103	1/1	0.77	0.31	-	76,76,76,76	0
56	MG	B	3687	1/1	0.76	0.24	-	52,52,52,52	0
56	MG	GB	3125	1/1	0.71	0.30	-	62,62,62,62	0
56	MG	B	3834	1/1	0.21	2.04	-	165,165,165,165	0
56	MG	A	1778	1/1	0.80	0.70	-	104,104,104,104	0
56	MG	VB	201	1/1	0.63	0.23	-	74,74,74,74	0
56	MG	GB	3006	1/1	0.69	0.19	-	83,83,83,83	0
56	MG	A	1834	1/1	0.82	0.55	-	82,82,82,82	0
56	MG	B	3347	1/1	0.85	0.19	-	54,54,54,54	0
56	MG	B	3413	1/1	0.37	0.77	-	140,140,140,140	0
56	MG	QC	303	1/1	0.60	0.56	-	120,120,120,120	0
56	MG	GB	3404	1/1	0.86	0.37	-	64,64,64,64	0
56	MG	B	3664	1/1	0.71	0.36	-	54,54,54,54	0
56	MG	B	3712	1/1	0.95	0.36	-	59,59,59,59	0
56	MG	GB	3488	1/1	0.67	0.38	-	78,78,78,78	0
56	MG	GB	3667	1/1	0.92	0.35	-	54,54,54,54	0
56	MG	GB	3078	1/1	0.91	0.28	-	64,64,64,64	0
56	MG	B	3503	1/1	0.51	0.17	-	77,77,77,77	0
56	MG	A	1884	1/1	0.90	0.26	-	60,60,60,60	0
56	MG	W	302	1/1	0.86	0.08	-	70,70,70,70	0
56	MG	B	3791	1/1	-0.07	0.44	-	139,139,139,139	0
56	MG	A	1810	1/1	0.79	0.62	-	75,75,75,75	0
56	MG	FB	1712	1/1	0.49	0.52	-	78,78,78,78	0
56	MG	GB	3685	1/1	0.74	0.25	-	70,70,70,70	0
56	MG	GB	3217	1/1	0.70	0.55	-	65,65,65,65	0
56	MG	B	3797	1/1	0.88	0.23	-	60,60,60,60	0
56	MG	B	3472	1/1	0.86	0.21	-	55,55,55,55	0
56	MG	GB	3400	1/1	0.89	0.25	-	71,71,71,71	0
56	MG	GB	3144	1/1	0.95	0.26	-	57,57,57,57	0
56	MG	B	3598	1/1	0.81	0.26	-	62,62,62,62	0
56	MG	GB	3602	1/1	0.84	0.33	-	75,75,75,75	0
56	MG	IA	106	1/1	0.88	0.14	-	82,82,82,82	0
56	MG	GB	3002	1/1	0.76	0.59	-	88,88,88,88	0
56	MG	GB	3510	1/1	0.57	0.20	-	73,73,73,73	0
56	MG	GB	3245	1/1	0.85	0.18	-	76,76,76,76	0
56	MG	B	3038	1/1	0.93	0.45	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	FB	1797	1/1	0.86	0.38	-	81,81,81,81	0
56	MG	FB	1727	1/1	0.72	0.44	-	141,141,141,141	0
56	MG	B	3818	1/1	0.71	0.96	-	177,177,177,177	0
56	MG	B	3136	1/1	0.91	0.28	-	43,43,43,43	0
56	MG	A	1732	1/1	0.93	0.25	-	56,56,56,56	0
56	MG	FB	1856	1/1	0.92	0.22	-	100,100,100,100	0
56	MG	MB	207	1/1	0.80	0.34	-	105,105,105,105	0
56	MG	GB	3198	1/1	0.78	0.64	-	59,59,59,59	0
56	MG	B	3469	1/1	0.91	0.30	-	60,60,60,60	0
56	MG	A	1739	1/1	0.96	0.24	-	59,59,59,59	0
56	MG	B	3704	1/1	0.89	0.32	-	69,69,69,69	0
56	MG	FB	1823	1/1	0.84	0.12	-	87,87,87,87	0
56	MG	FB	1924	1/1	0.82	0.28	-	71,71,71,71	0
56	MG	GB	3575	1/1	0.89	0.20	-	72,72,72,72	0
56	MG	GB	3418	1/1	0.84	0.22	-	58,58,58,58	0
56	MG	B	3800	1/1	0.90	0.45	-	52,52,52,52	0
56	MG	U	101	1/1	0.89	0.16	-	56,56,56,56	0
56	MG	GB	3395	1/1	0.60	1.18	-	81,81,81,81	0
56	MG	A	1856	1/1	0.83	0.57	-	87,87,87,87	0
56	MG	A	1790	1/1	0.89	0.26	-	65,65,65,65	0
56	MG	FB	1618	1/1	0.96	0.29	-	67,67,67,67	0
56	MG	B	3290	1/1	0.89	0.27	-	51,51,51,51	0
56	MG	GB	3214	1/1	0.81	0.35	-	64,64,64,64	0
56	MG	GB	3007	1/1	0.74	0.33	-	73,73,73,73	0
56	MG	B	3555	1/1	0.85	0.28	-	54,54,54,54	0
56	MG	B	3703	1/1	0.82	0.57	-	59,59,59,59	0
56	MG	S	203	1/1	0.94	0.40	-	57,57,57,57	0
56	MG	GB	3334	1/1	0.83	0.23	-	109,109,109,109	0
56	MG	B	3217	1/1	0.89	0.29	-	54,54,54,54	0
56	MG	GB	3649	1/1	0.93	0.43	-	70,70,70,70	0
56	MG	B	3516	1/1	0.87	0.17	-	57,57,57,57	0
56	MG	B	3198	1/1	0.93	0.34	-	47,47,47,47	0
56	MG	A	1770	1/1	0.72	0.54	-	139,139,139,139	0
56	MG	B	3606	1/1	0.55	0.79	-	125,125,125,125	0
56	MG	IA	105	1/1	0.91	0.17	-	80,80,80,80	0
56	MG	B	3415	1/1	0.94	0.41	-	42,42,42,42	0
56	MG	GB	2990	1/1	0.92	0.61	-	63,63,63,63	0
56	MG	B	3113	1/1	0.89	0.17	-	65,65,65,65	0
56	MG	B	3558	1/1	0.76	0.32	-	64,64,64,64	0
56	MG	FB	1677	1/1	0.76	0.43	-	67,67,67,67	0
56	MG	B	3727	1/1	0.91	0.53	-	49,49,49,49	0
56	MG	B	3378	1/1	0.97	0.25	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	SC	202	1/1	0.34	0.41	-	92,92,92,92	0
56	MG	WC	202	1/1	0.76	0.24	-	121,121,121,121	0
56	MG	FB	1782	1/1	0.90	0.21	-	91,91,91,91	0
56	MG	GB	2955	1/1	0.85	0.24	-	69,69,69,69	0
56	MG	A	1632	1/1	0.87	0.25	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.