



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2016 – 10:14 AM EST

PDB ID : 5J88  
Title : Structure of the E coli 70S ribosome with the U1060A mutation in 16S rRNA  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-07  
Resolution : 3.32 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](mailto: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.

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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-20028320  
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-20028320

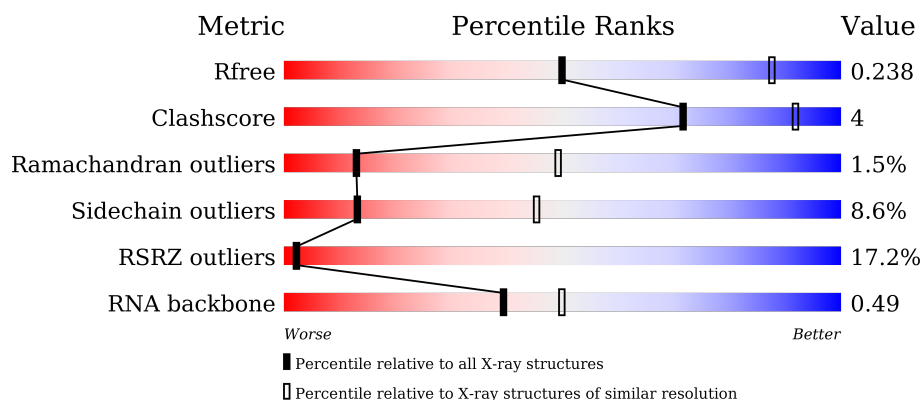
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)
RNA backbone	2183	1002 (3.84-2.80)

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  $\geq 3$ , 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	AA	1534	<div> <div>7%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	BA	1534	<div> <div>17%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
2	AB	224	<div> <div>25%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	BB	224	<div> <div>20%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	129	
11	BK	129	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	


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Mol	Chain	Length	Quality of chain
42	CO	127	
42	DO	127	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	100	
48	DU	100	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	76	
51	DX	76	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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	AA	1612	-	-	-	X
56	MG	AA	1639	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	AA	1657	-	-	-	X
56	MG	AA	1661	-	-	-	X
56	MG	BA	1624	-	-	-	X
56	MG	BA	1627	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3039	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3109	-	-	-	X
56	MG	CA	3131	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3150	-	-	-	X
56	MG	DA	3122	-	-	-	X
56	MG	DA	3126	-	-	-	X
56	MG	DA	3127	-	-	-	X
56	MG	DA	3147	-	-	-	X
56	MG	DA	3163	-	-	-	X
56	MG	DA	3177	-	-	-	X
56	MG	DA	3182	-	-	-	X
57	PG4	AA	1670	-	-	-	X
57	PG4	BA	1642	-	-	-	X
57	PG4	DA	3193	-	-	-	X
57	PG4	DA	3216	-	-	-	X
57	PG4	DS	202	-	-	-	X
58	MPD	AA	1671	-	-	-	X
58	MPD	AA	1676	-	-	-	X
58	MPD	DA	3192	-	-	-	X
58	MPD	DA	3204	-	-	-	X
58	MPD	DA	3207	-	-	-	X
58	MPD	DA	3210	-	-	-	X
58	MPD	DE	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MPD	DE	302	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	DA	3184	-	-	-	X
59	PUT	DA	3189	-	-	-	X
59	PUT	DA	3195	-	-	-	X
59	PUT	DA	3205	-	-	-	X
59	PUT	DA	3213	-	-	-	X
59	PUT	DA	3219	-	-	-	X
59	PUT	DA	3221	-	-	-	X
59	PUT	DA	3222	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3201	-	-	-	X
61	PEG	DA	3218	-	-	-	X
61	PEG	DA	3226	-	-	-	X
61	PEG	DL	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	D0	101	-	-	-	X
62	EDO	D1	101	-	-	-	X
62	EDO	DA	3197	-	-	-	X
62	EDO	DA	3198	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	D3	101	-	-	-	X
63	PGE	DA	3186	-	-	-	X
63	PGE	DA	3214	-	-	-	X
63	PGE	DA	3217	-	-	-	X
63	PGE	DA	3225	-	-	-	X
63	PGE	DD	301	-	-	-	X
63	PGE	DU	201	-	-	-	X
64	SPD	DA	3183	-	-	-	X
64	SPD	DA	3187	-	-	-	X
64	SPD	DA	3224	-	-	-	X
65	1PE	DA	3203	-	-	-	X
66	ACY	DA	3202	-	-	X	-



## 2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295119 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 a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32932	14695	6044	10659	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32910	14685	6039	10653	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1060	A	U	conflict	GB 675819282
BA	1060	A	U	conflict	GB 675819282

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
33	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
35	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
36	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
38	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
39	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
40	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
41	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
42	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O	S	0	0	0
			892	552	178	162				
43	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
44	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CR	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
45	DR	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
46	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
50	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
51	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
52	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
53	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 54 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 55 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

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

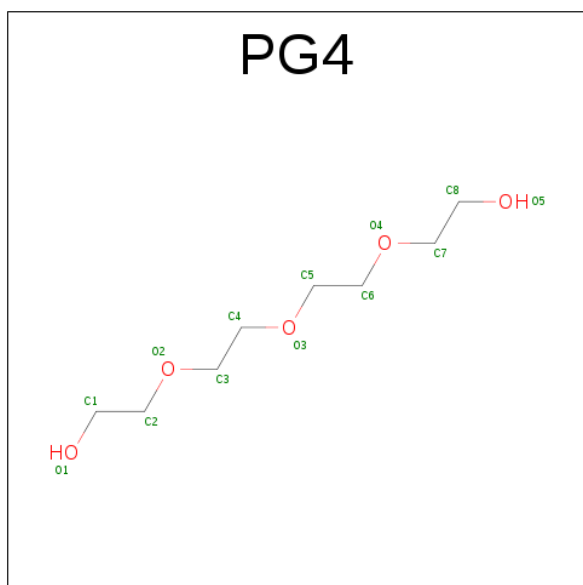
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	41	Total	Mg	0	0
			41	41		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		
56	AA	70	Total	Mg	0	0
			70	70		
56	DA	184	Total	Mg	0	0
			184	184		

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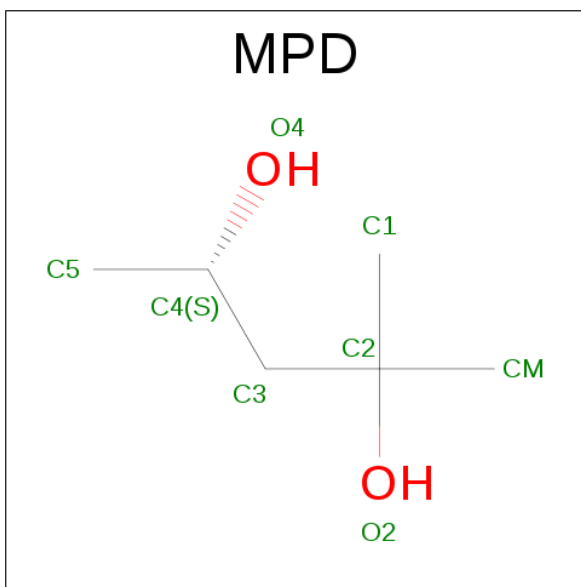
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	1	Total	Mg	0	0
			1	1		

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



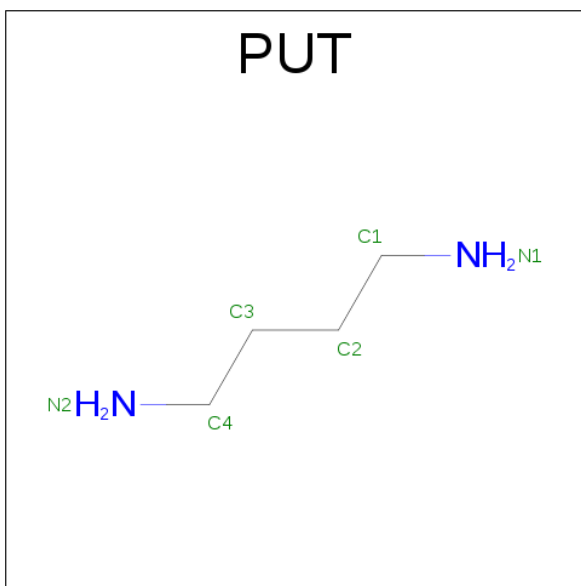
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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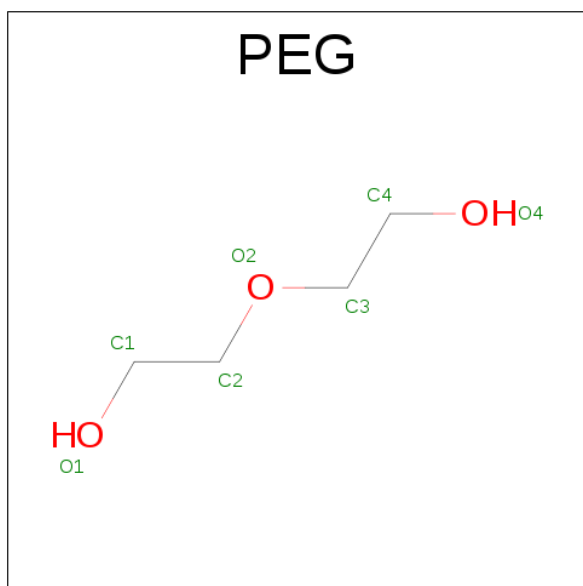
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C5	1	Total	Zn	0	0
			1	1		
60	AB	1	Total	Zn	0	0
			1	1		
60	D5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



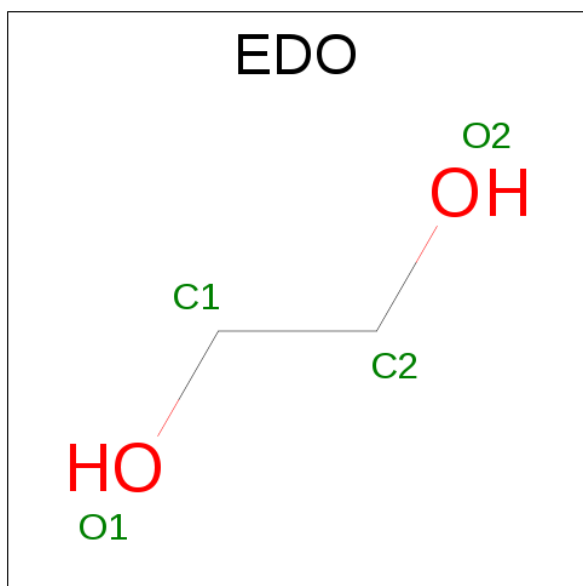
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	D0	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

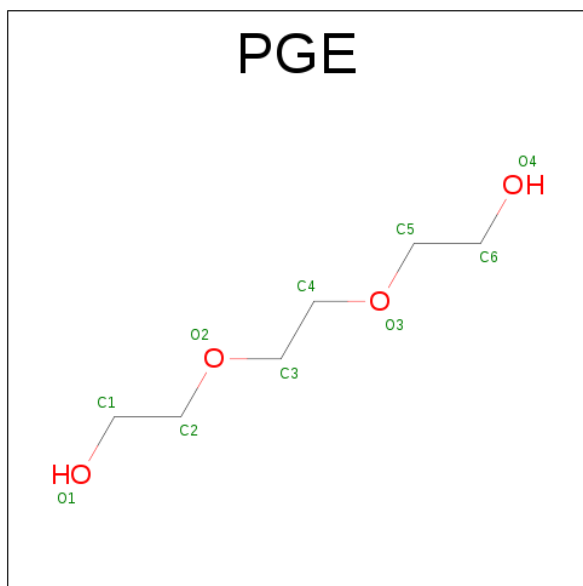
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



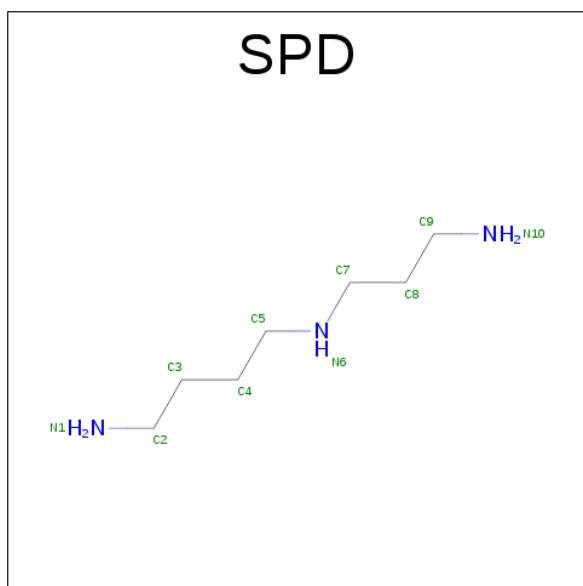
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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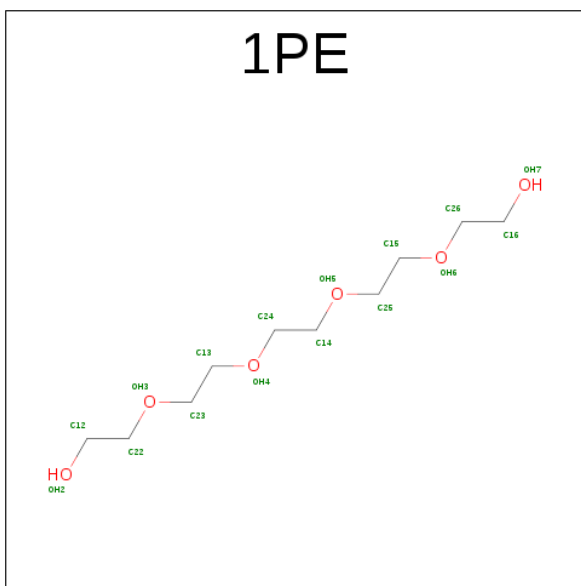
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



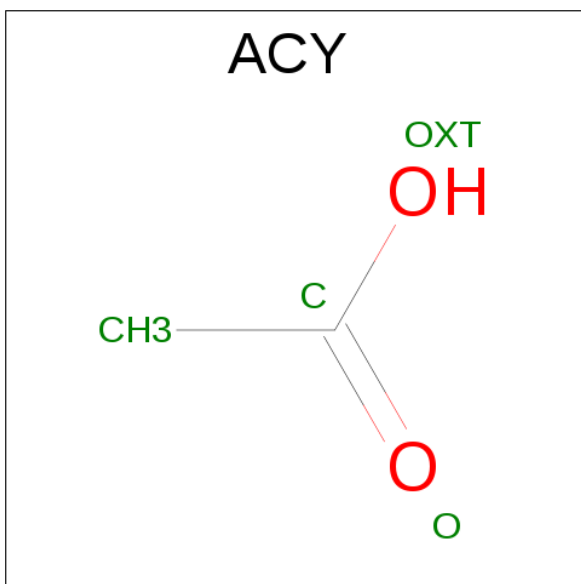
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



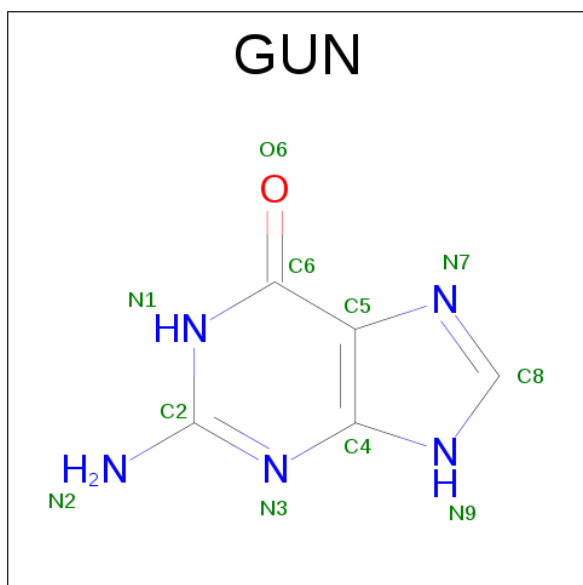
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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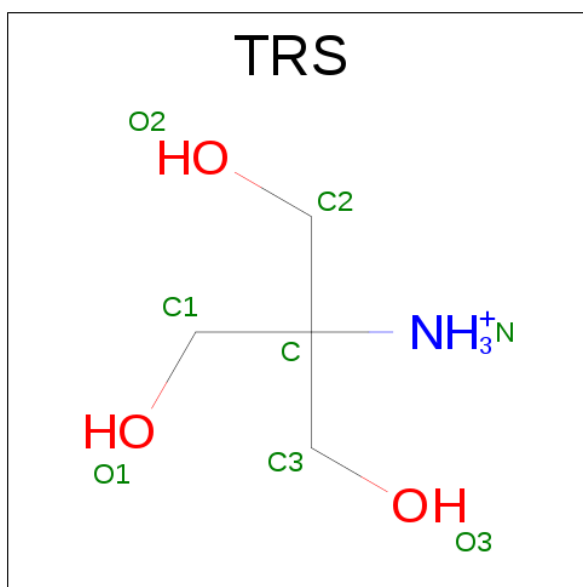
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula:  $C_5H_5N_5O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
67	DA	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	2	Total	O	0	0
			2	2		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	3	Total	O	0	0
			3	3		
69	AK	5	Total	O	0	0
			5	5		
69	AL	7	Total	O	0	0
			7	7		
69	AM	4	Total	O	0	0
			4	4		
69	AN	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	1	Total 1	O 1	0	0
69	AP	1	Total 1	O 1	0	0
69	AQ	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	4	Total 4	O 4	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	3	Total 3	O 3	0	0
69	BL	3	Total 3	O 3	0	0
69	BN	1	Total 1	O 1	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	4	Total 4	O 4	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	5	Total 5	O 5	0	0
69	D1	37	Total 37	O 37	0	0
69	D2	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	30	Total 30	O 30	0	0
69	D4	40	Total 40	O 40	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	11	Total 11	O 11	0	0
69	CD	4	Total 4	O 4	0	0
69	CA	696	Total 696	O 696	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	97	Total 97	O 97	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	54	Total 54	O 54	0	0
69	DF	13	Total 13	O 13	0	0
69	DG	9	Total 9	O 9	0	0

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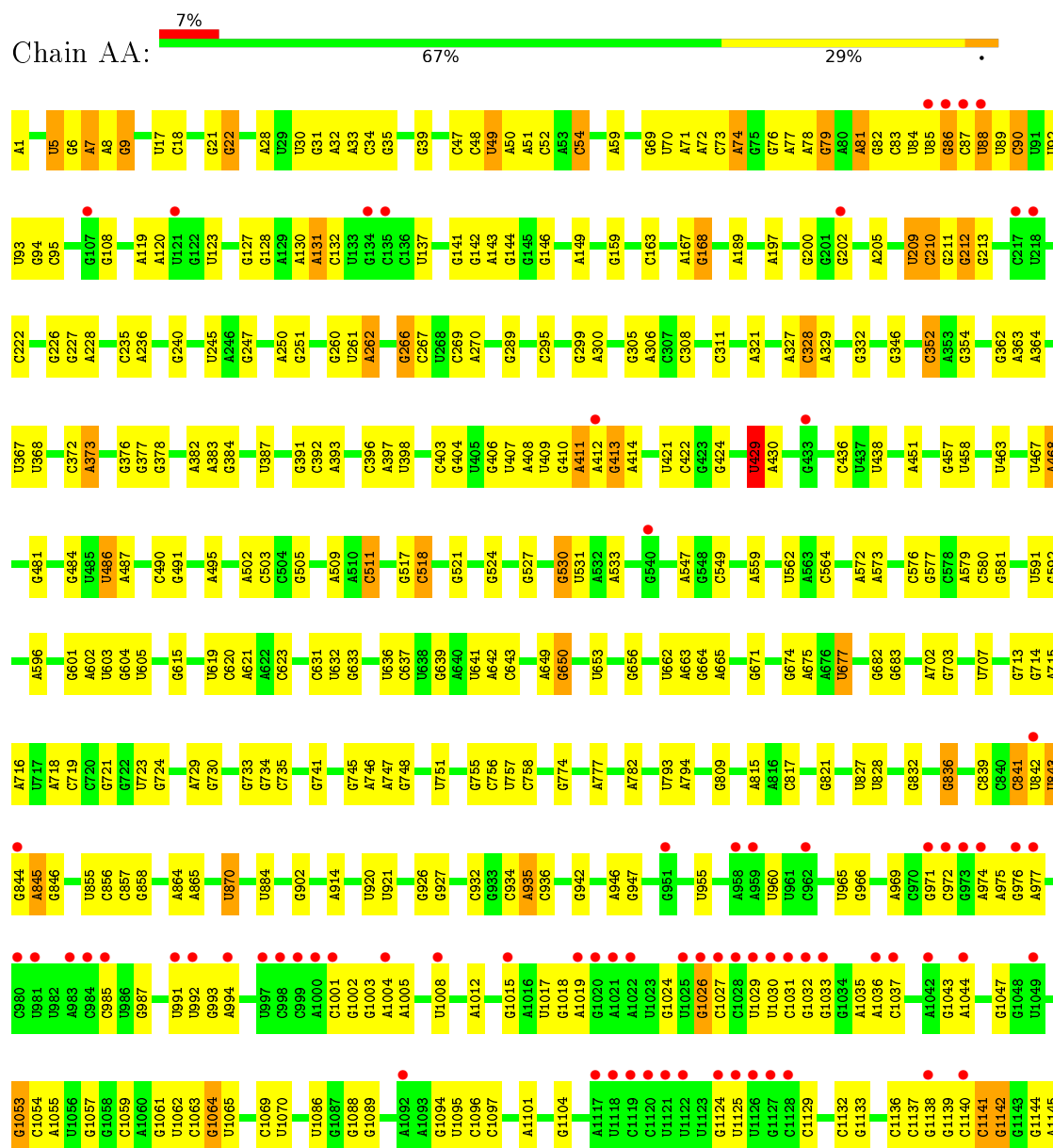
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DH	2	Total 2	O 2	0	0
69	DK	61	Total 61	O 61	0	0
69	DL	50	Total 50	O 50	0	0
69	DM	60	Total 60	O 60	0	0
69	DN	81	Total 81	O 81	0	0
69	DO	42	Total 42	O 42	0	0
69	DP	42	Total 42	O 42	0	0
69	DQ	32	Total 32	O 32	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	52	Total 52	O 52	0	0
69	DT	65	Total 65	O 65	0	0
69	DU	24	Total 24	O 24	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	33	Total 33	O 33	0	0
69	DX	33	Total 33	O 33	0	0
69	DY	11	Total 11	O 11	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	203	Total 203	O 203	0	0
69	DA	4824	Total 4824	O 4824	0	0

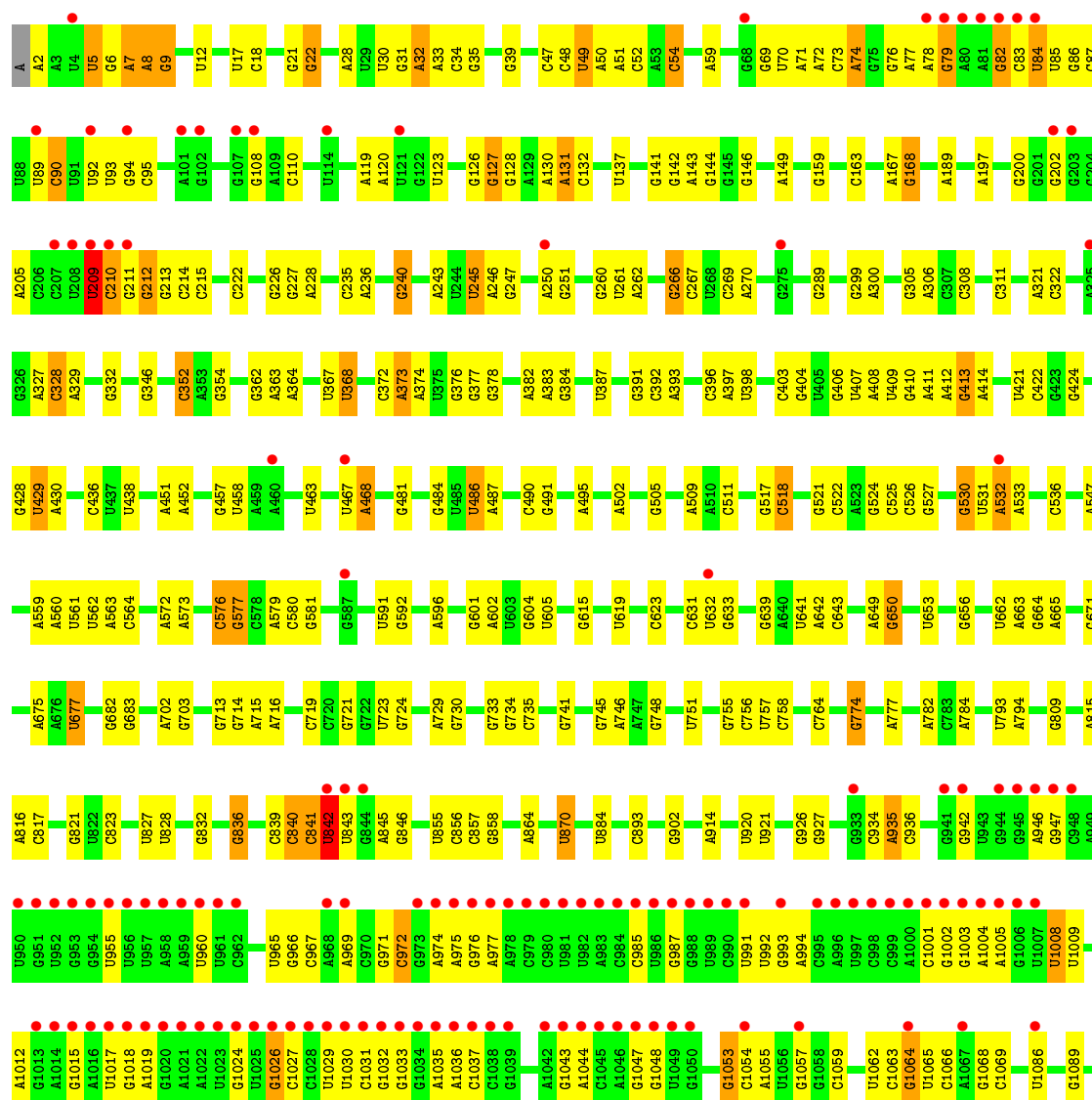


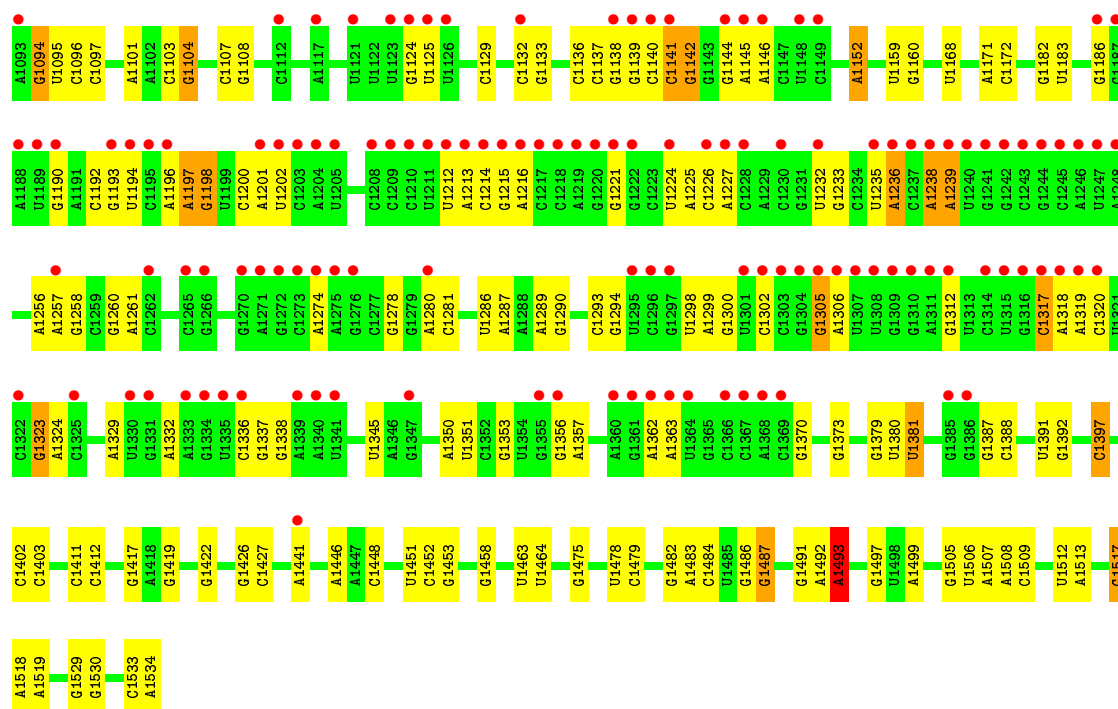
### 3 Residue-property plots

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.

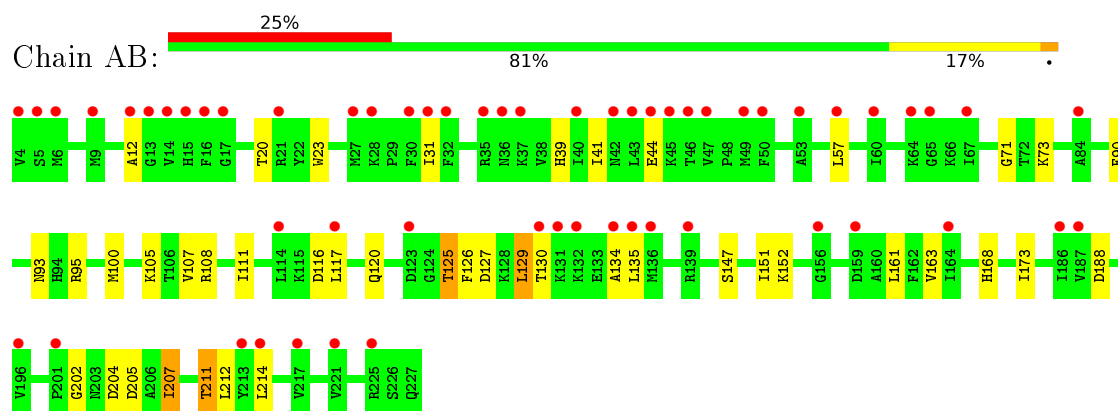
#### • Molecule 1: 16S rRNA



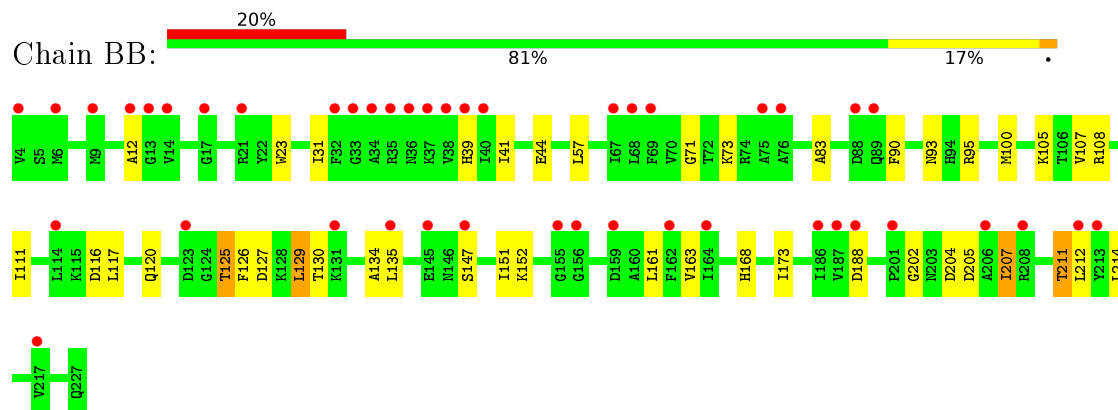




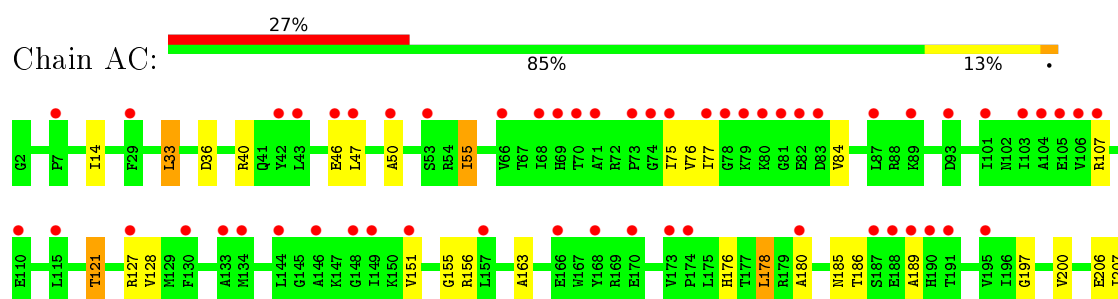
• Molecule 2: 30S ribosomal protein S2



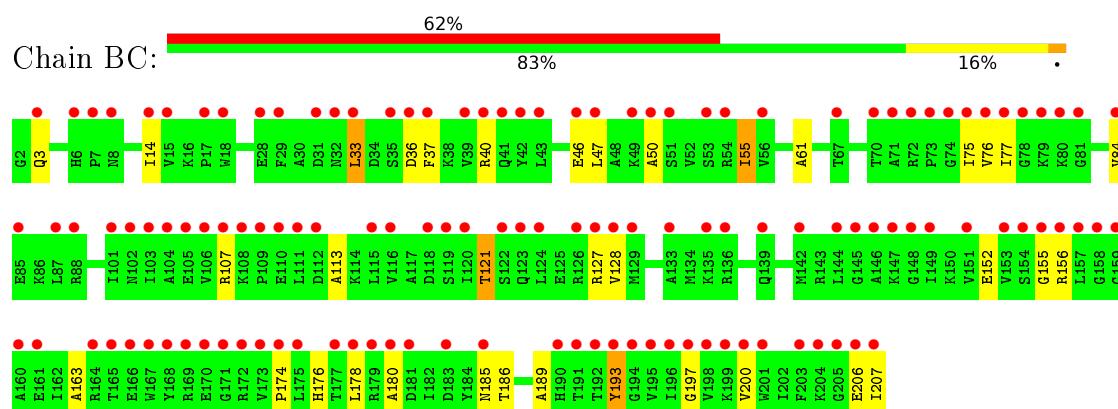
• Molecule 2: 30S ribosomal protein S2



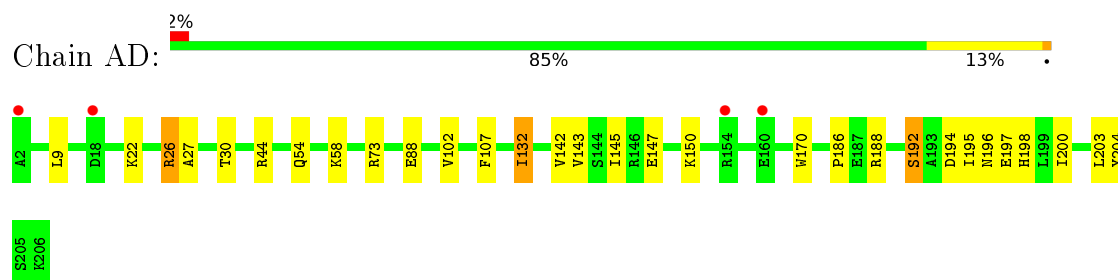
• Molecule 3: 30S ribosomal protein S3



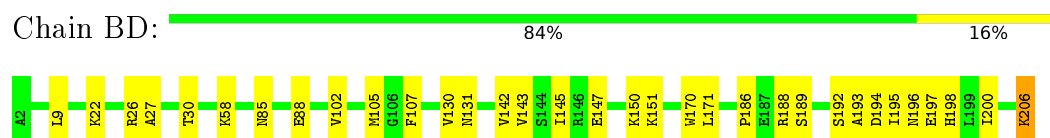
- Molecule 3: 30S ribosomal protein S3



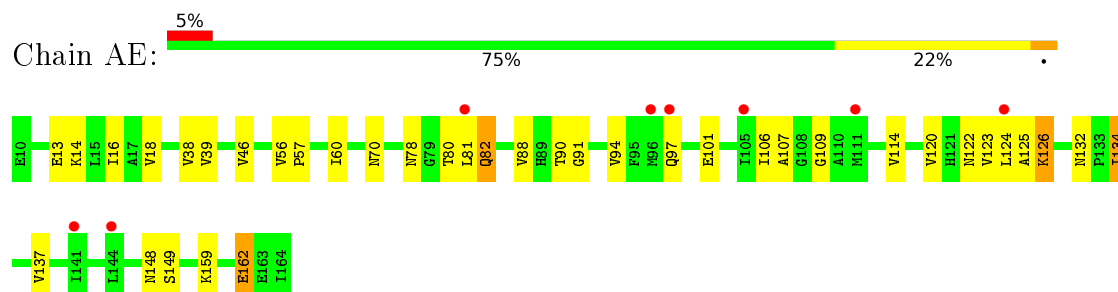
- Molecule 4: 30S ribosomal protein S4



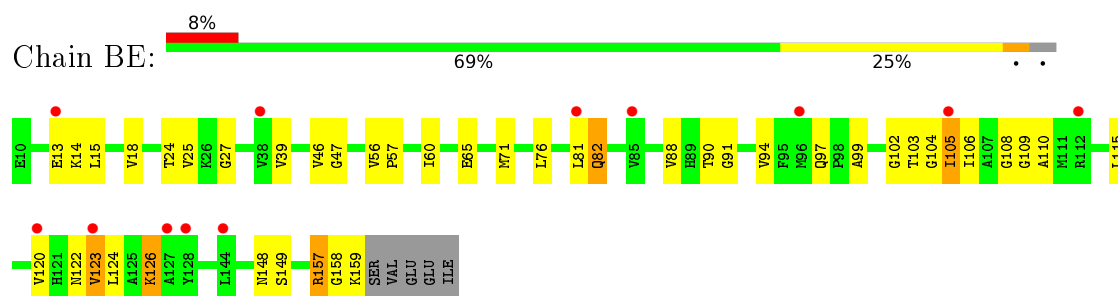
- Molecule 4: 30S ribosomal protein S4



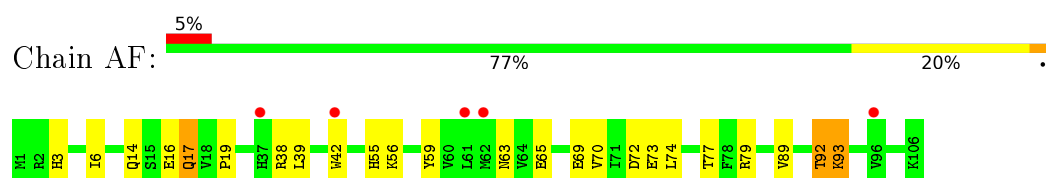
- Molecule 5: 30S ribosomal protein S5



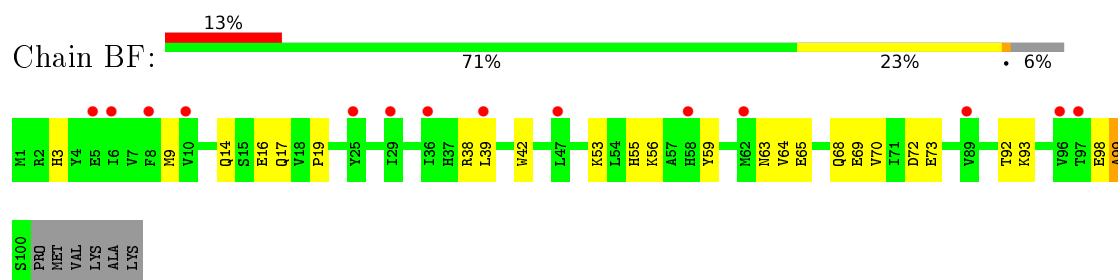
- Molecule 5: 30S ribosomal protein S5



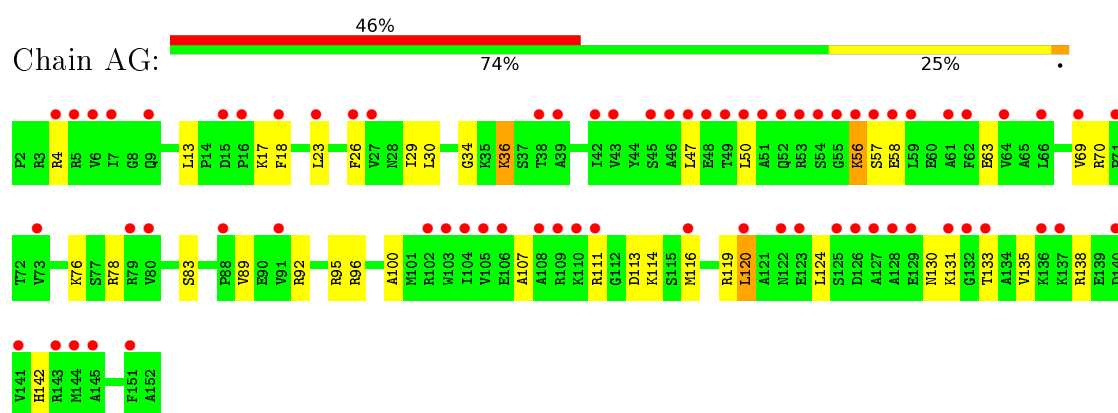
- Molecule 6: 30S ribosomal protein S6



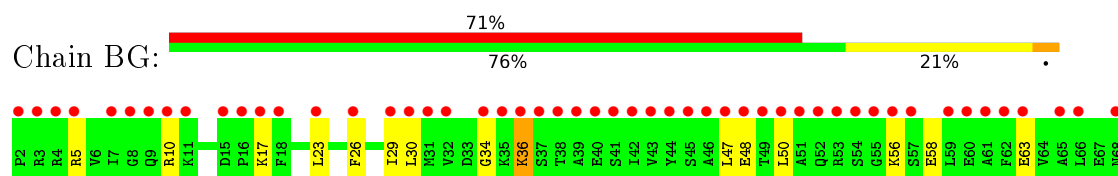
- Molecule 6: 30S ribosomal protein S6

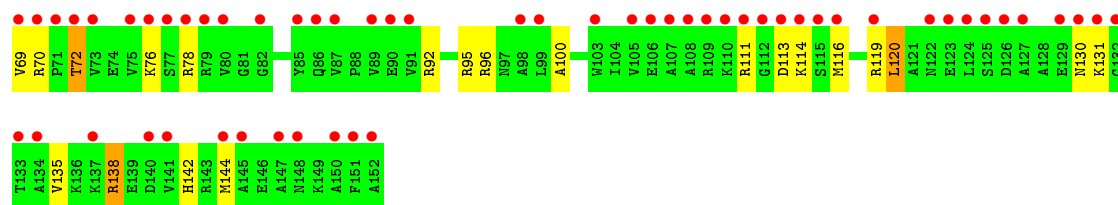


- Molecule 7: 30S ribosomal protein S7

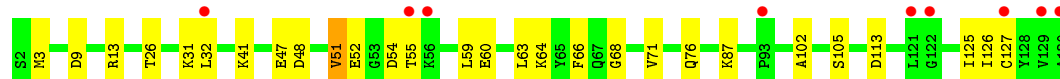
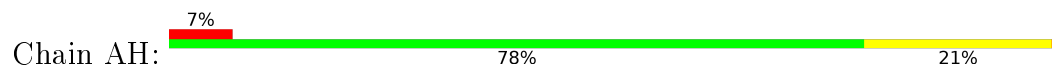


- Molecule 7: 30S ribosomal protein S7

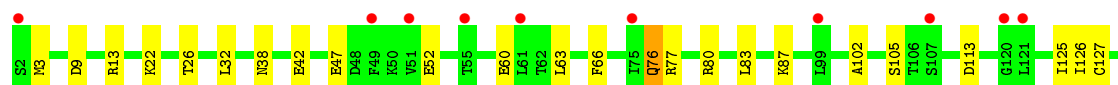
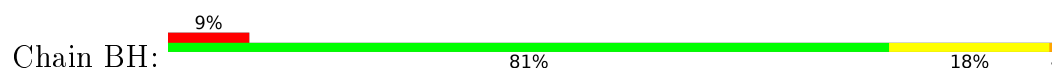




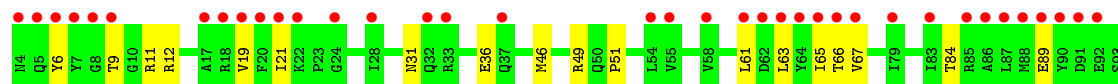
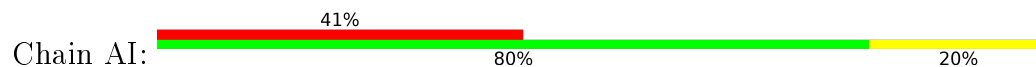
• Molecule 8: 30S ribosomal protein S8



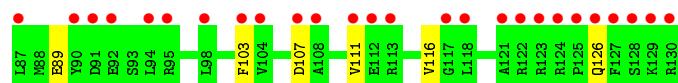
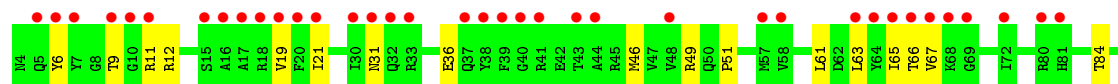
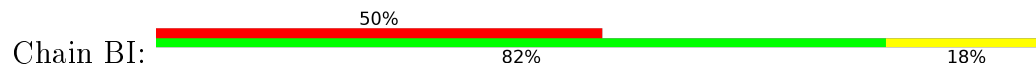
• Molecule 8: 30S ribosomal protein S8



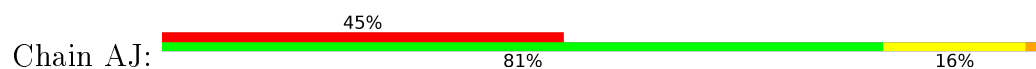
• Molecule 9: 30S ribosomal protein S9

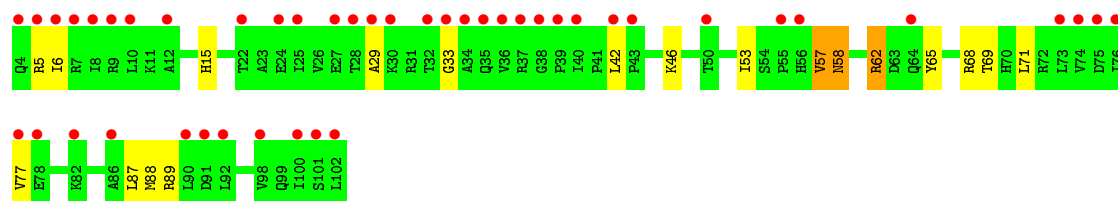


• Molecule 9: 30S ribosomal protein S9

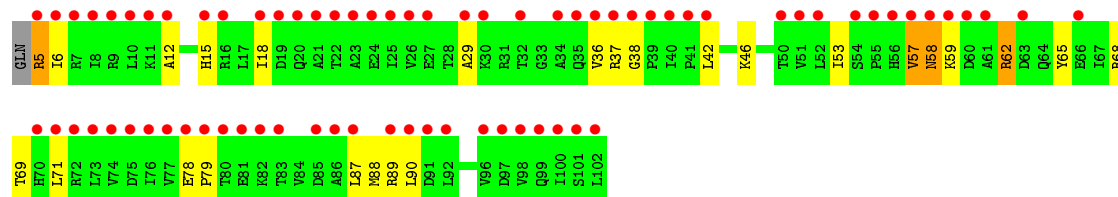
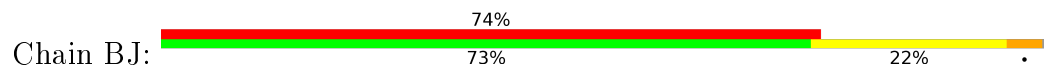


• Molecule 10: 30S ribosomal protein S10

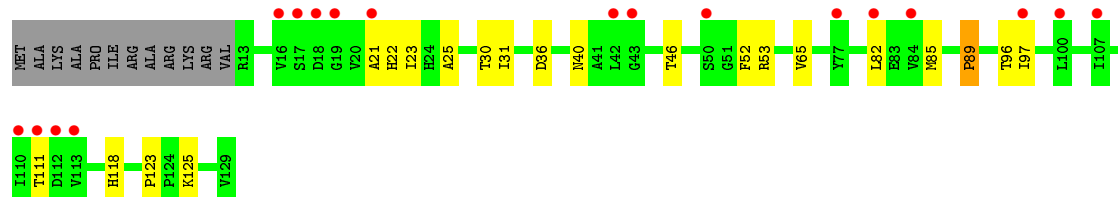
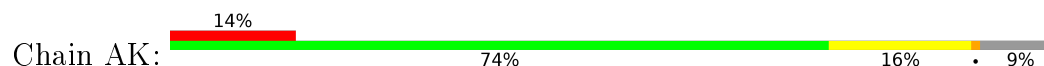




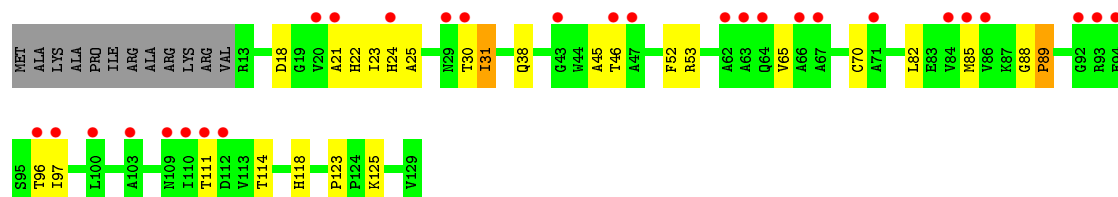
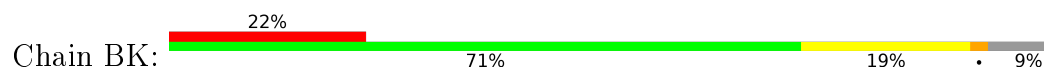
- Molecule 10: 30S ribosomal protein S10



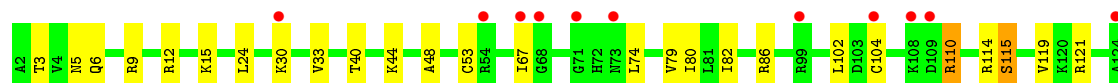
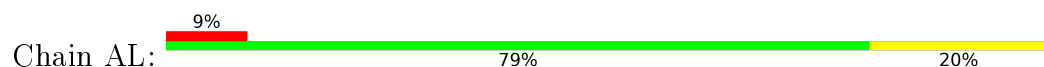
- Molecule 11: 30S ribosomal protein S11



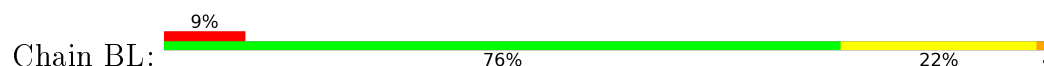
- Molecule 11: 30S ribosomal protein S11

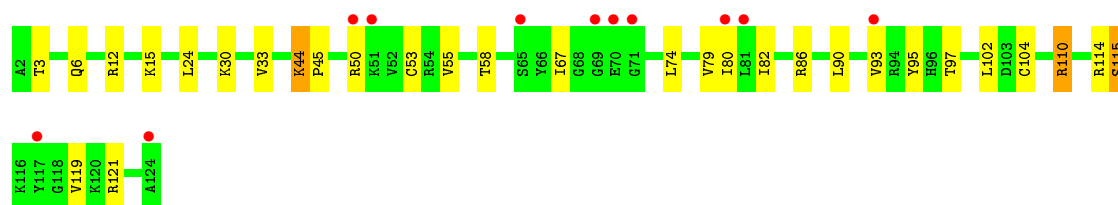


- Molecule 12: 30S ribosomal protein S12

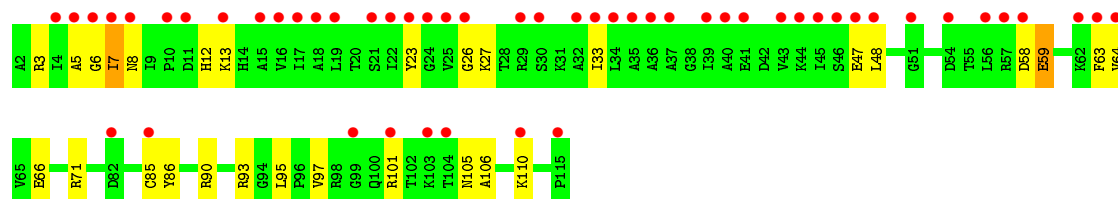
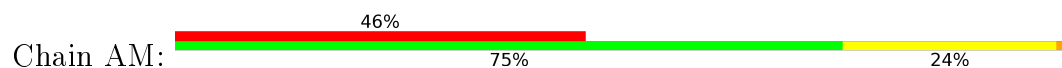


- Molecule 12: 30S ribosomal protein S12

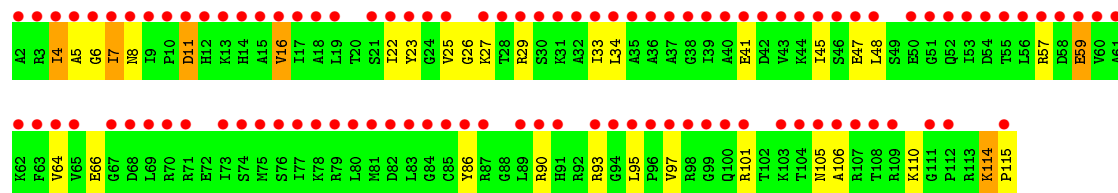
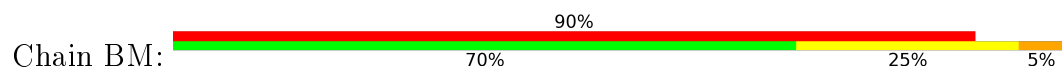




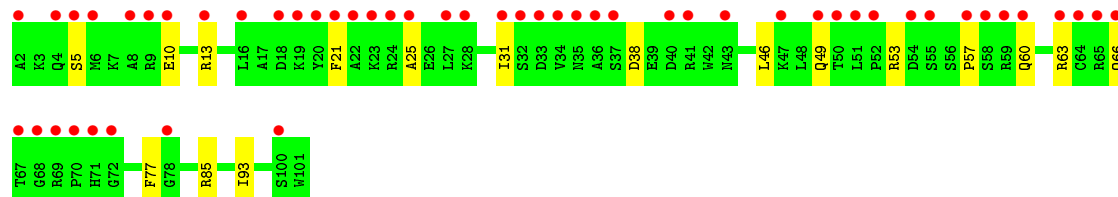
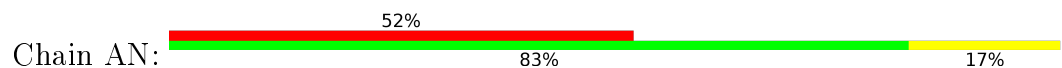
- Molecule 13: 30S ribosomal protein S13



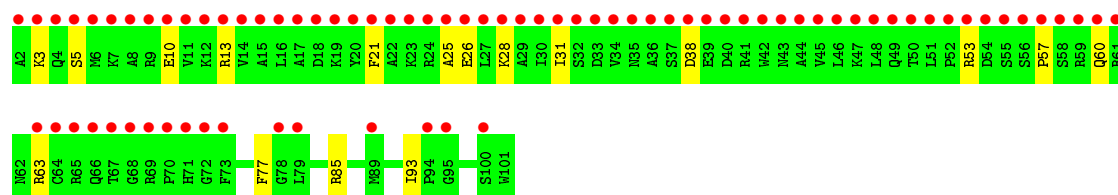
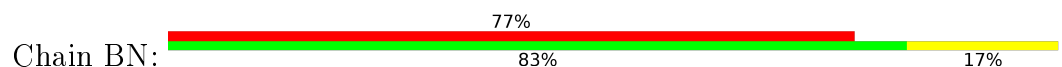
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

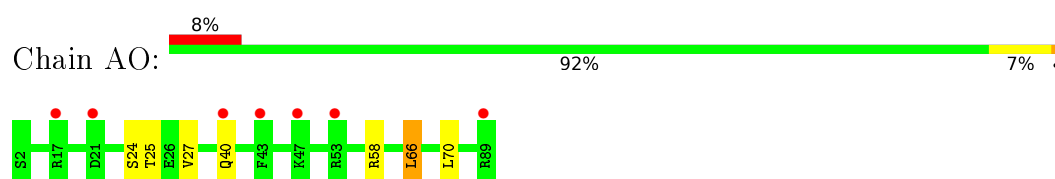


- Molecule 14: 30S ribosomal protein S14

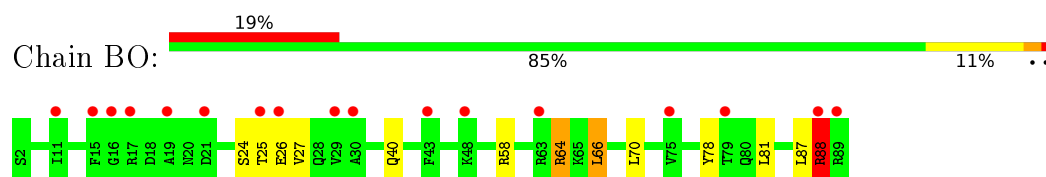


- Molecule 15: 30S ribosomal protein S15

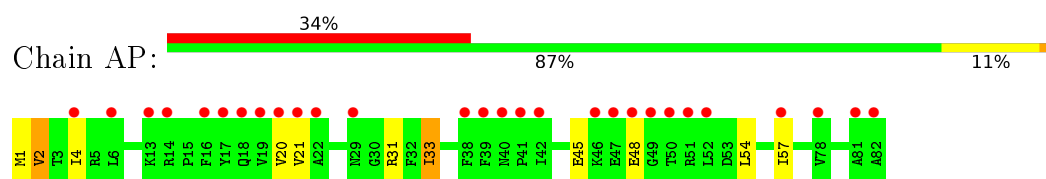




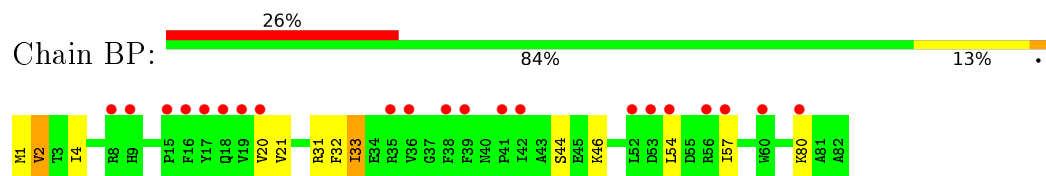
- Molecule 15: 30S ribosomal protein S15



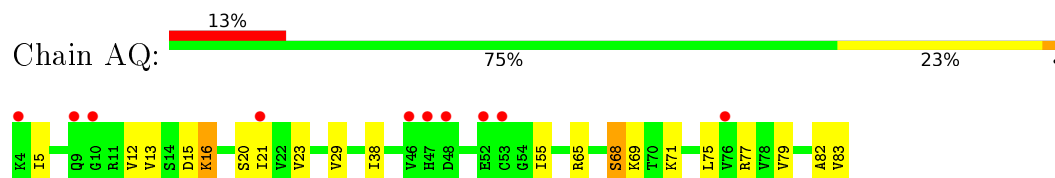
- Molecule 16: 30S ribosomal protein S16



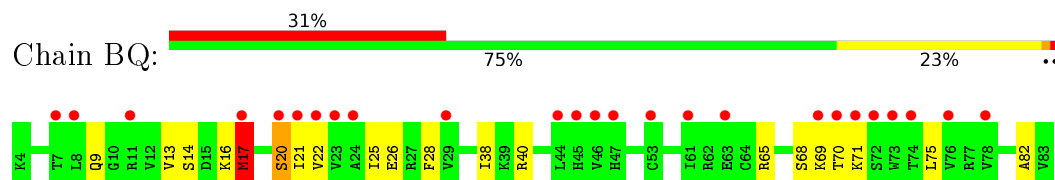
- Molecule 16: 30S ribosomal protein S16



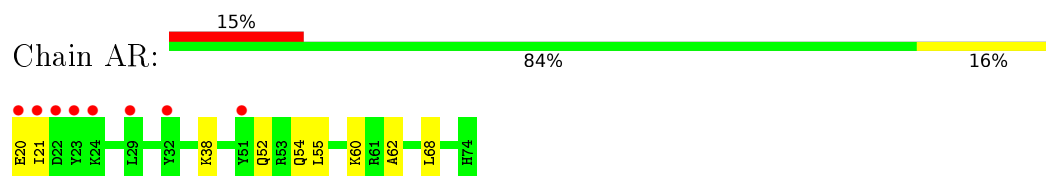
- Molecule 17: 30S ribosomal protein S17



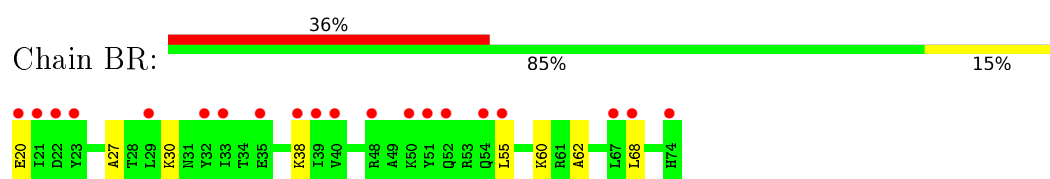
- Molecule 17: 30S ribosomal protein S17



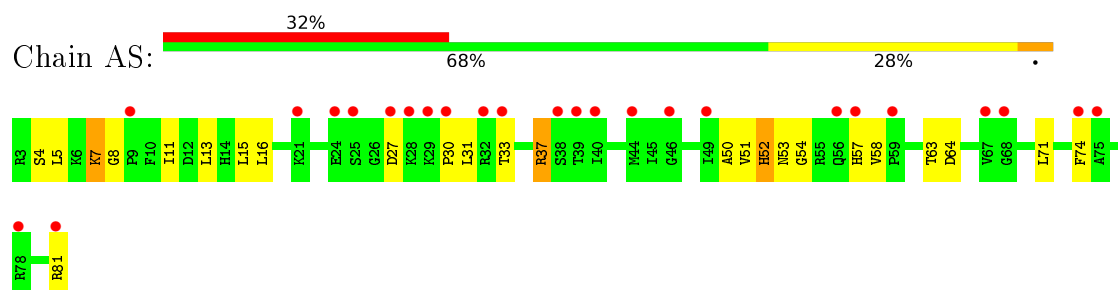
- Molecule 18: 30S ribosomal protein S18



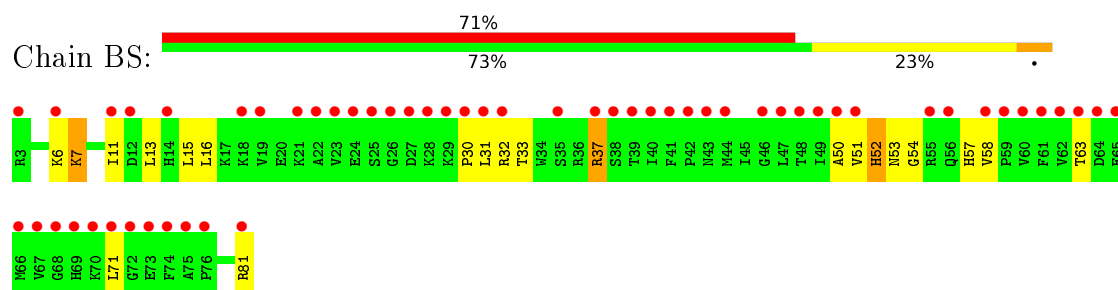
- Molecule 18: 30S ribosomal protein S18



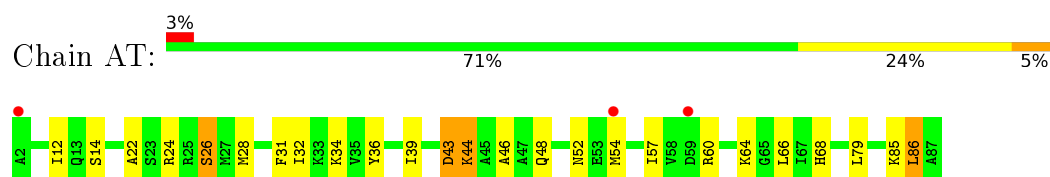
- Molecule 19: 30S ribosomal protein S19



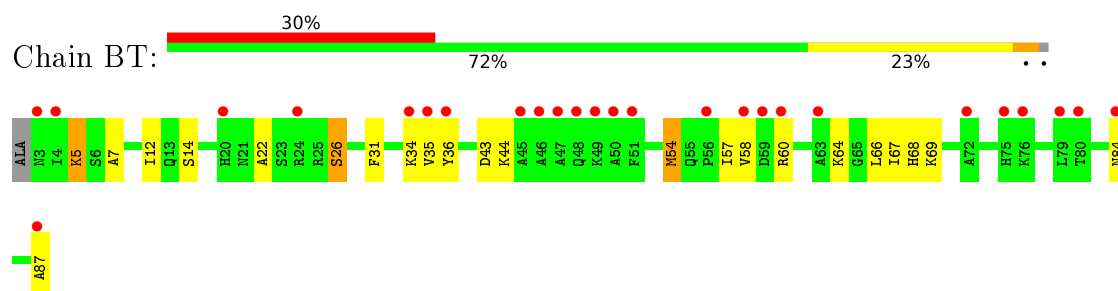
- Molecule 19: 30S ribosomal protein S19



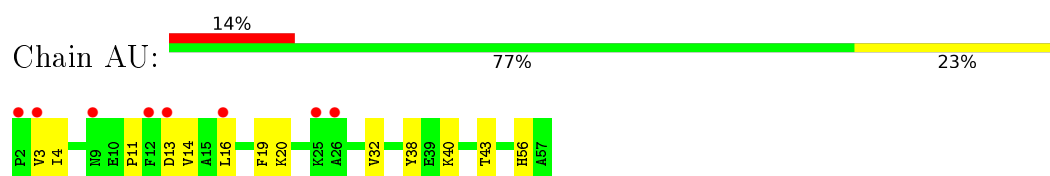
- Molecule 20: 30S ribosomal protein S20



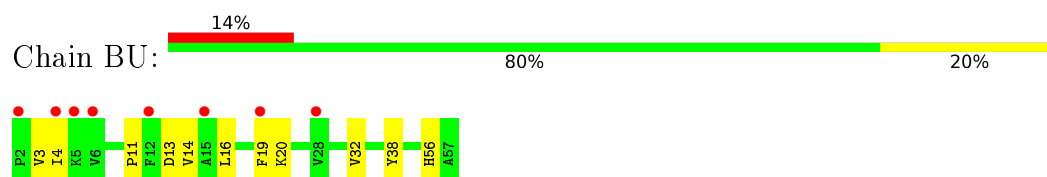
- Molecule 20: 30S ribosomal protein S20



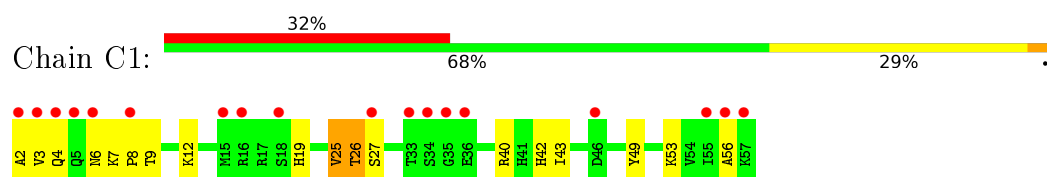
- Molecule 21: 30S ribosomal protein S21



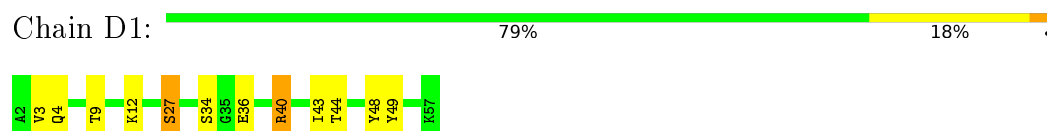
- Molecule 21: 30S ribosomal protein S21



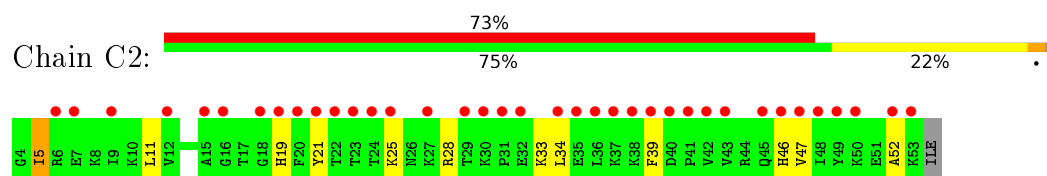
- Molecule 22: 50S ribosomal protein L32



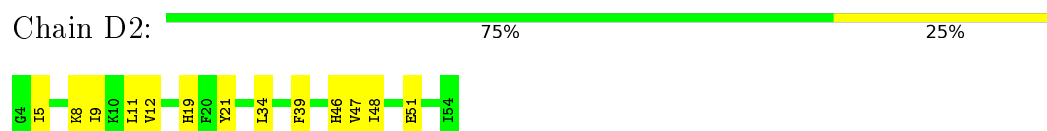
- Molecule 22: 50S ribosomal protein L32



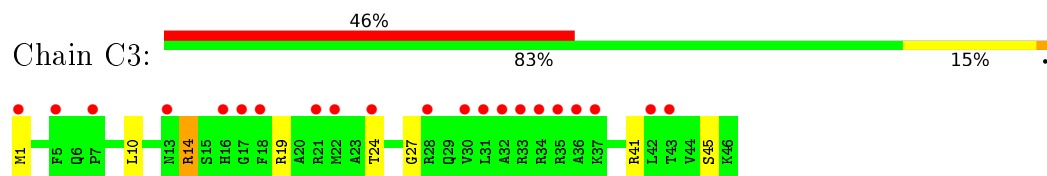
- Molecule 23: 50S ribosomal protein L33



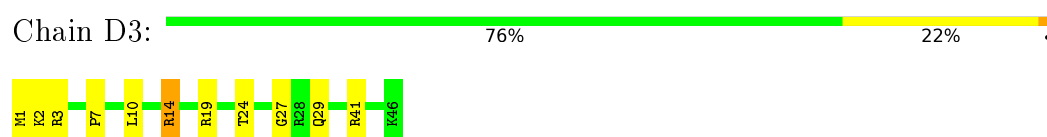
- Molecule 23: 50S ribosomal protein L33



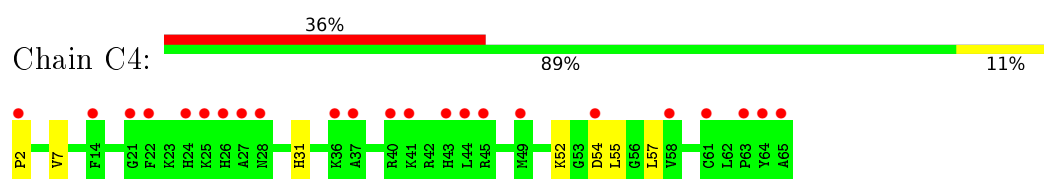
- Molecule 24: 50S ribosomal protein L34



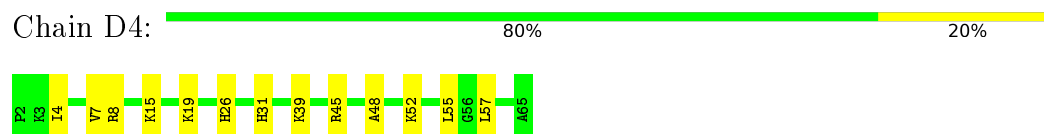
- Molecule 24: 50S ribosomal protein L34



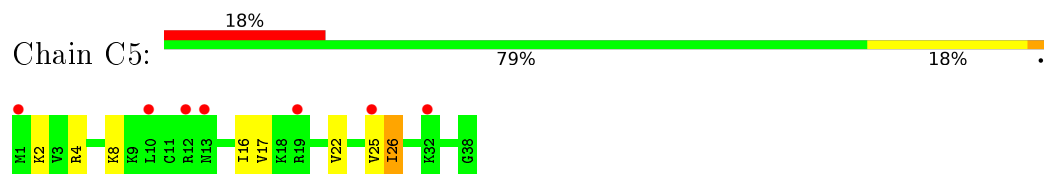
- Molecule 25: 50S ribosomal protein L35



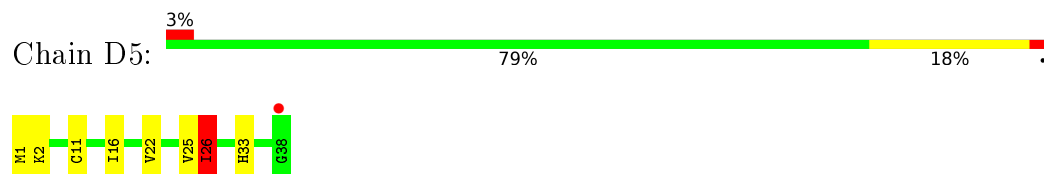
- Molecule 25: 50S ribosomal protein L35



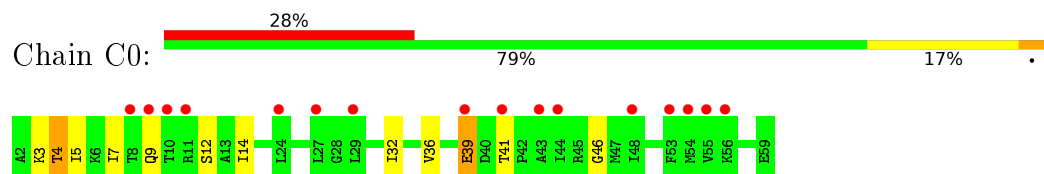
- Molecule 26: 50S ribosomal protein L36



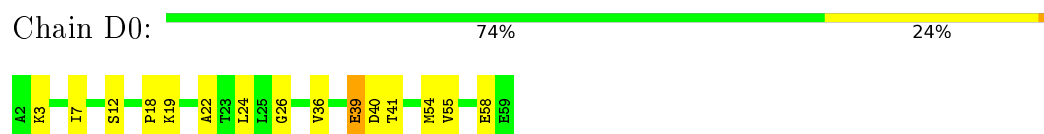
- Molecule 26: 50S ribosomal protein L36



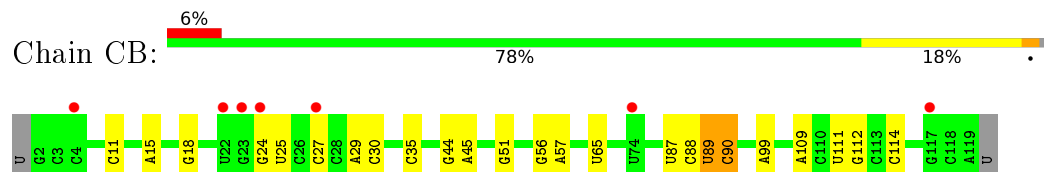
- Molecule 27: 50S ribosomal protein L30



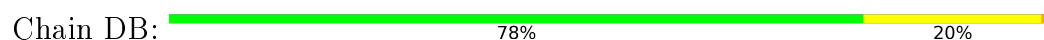
- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 5S rRNA

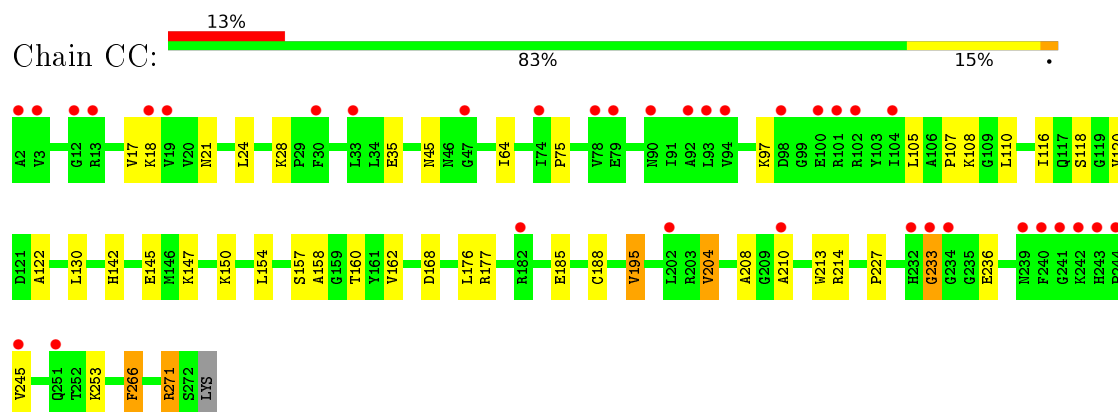


- Molecule 28: 5S rRNA

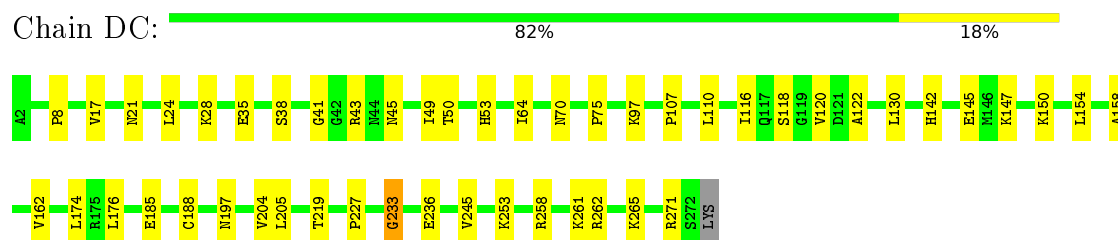




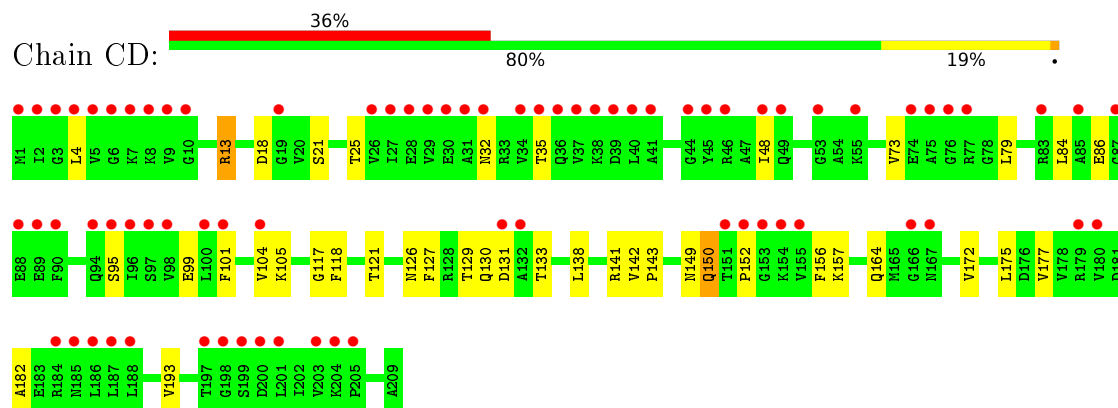
• Molecule 29: 50S ribosomal protein L2



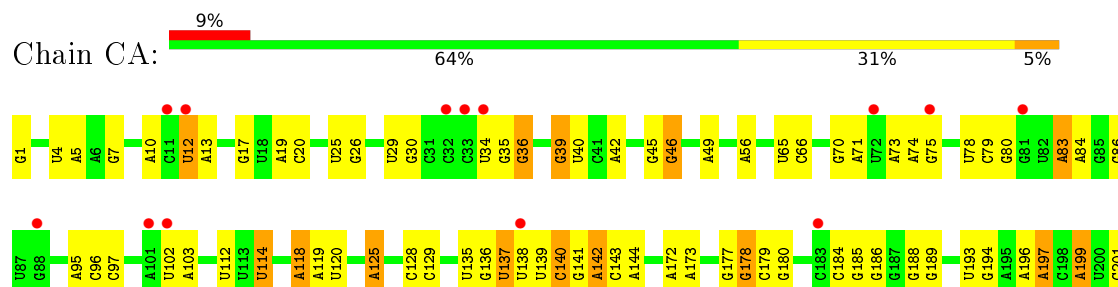
• Molecule 29: 50S ribosomal protein L2

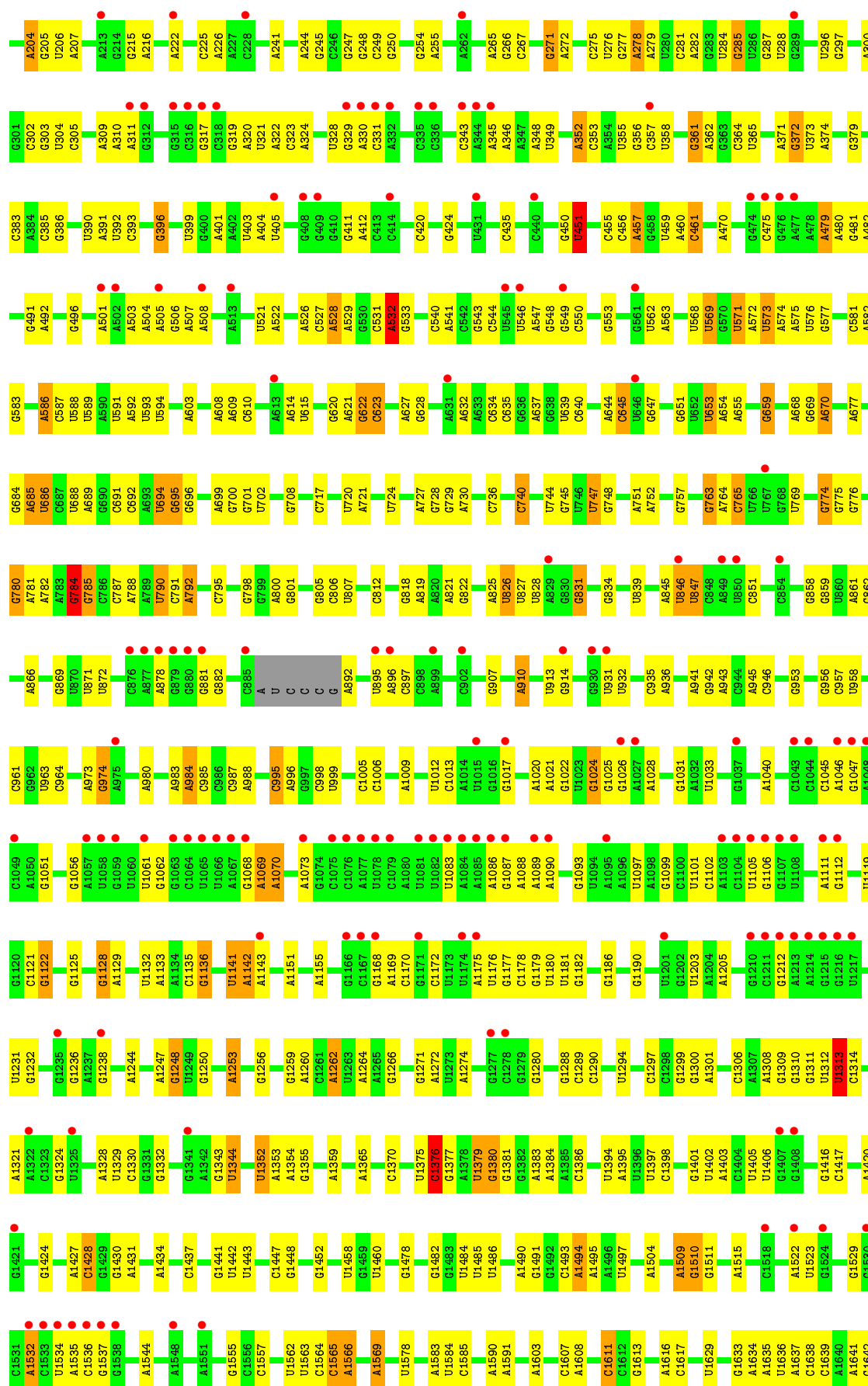


• Molecule 30: 50S ribosomal protein L3

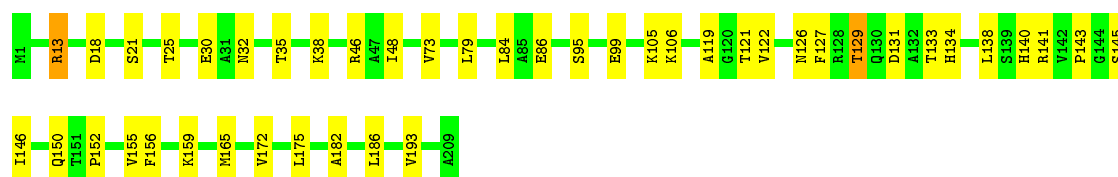


• Molecule 31: 23S rRNA

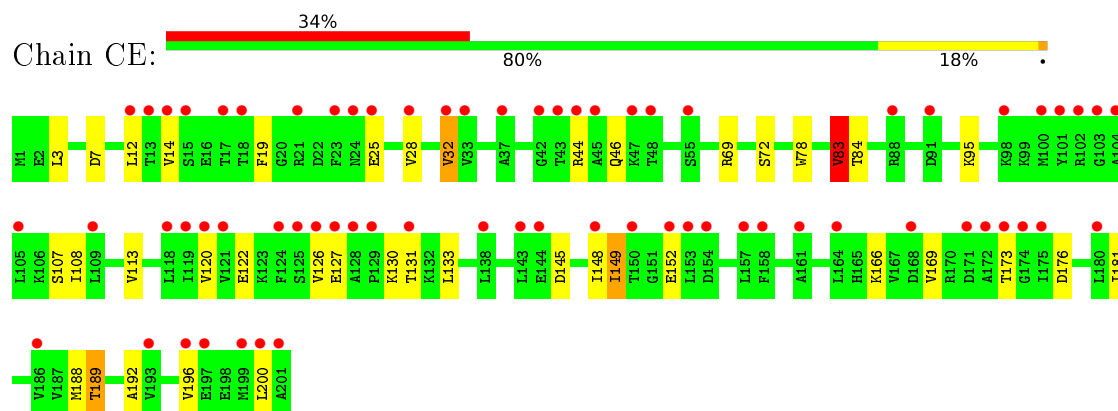




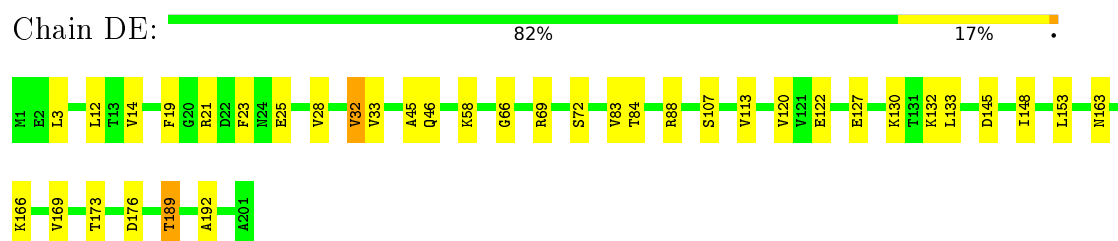




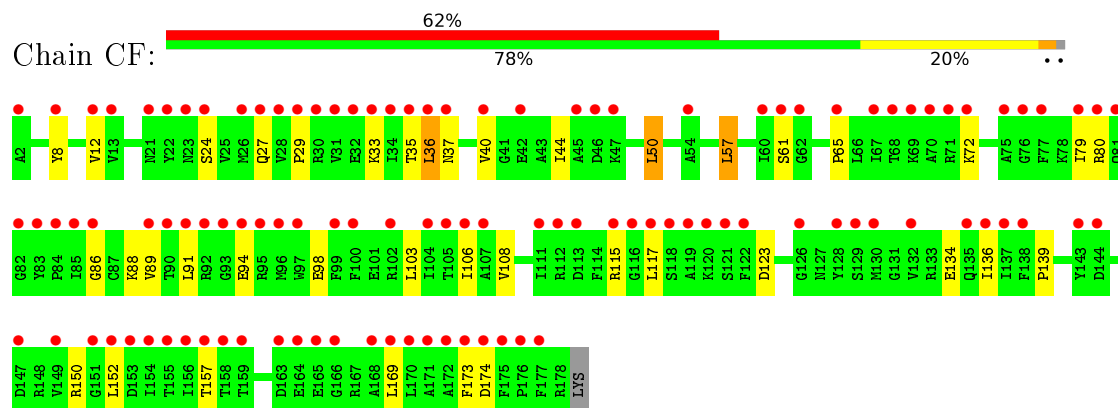
- Molecule 33: 50S ribosomal protein L4



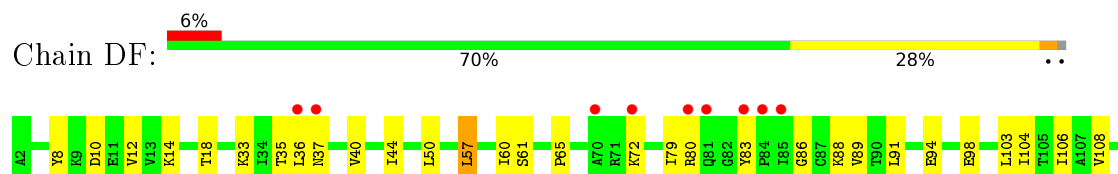
- Molecule 33: 50S ribosomal protein L4



- Molecule 34: 50S ribosomal protein L5



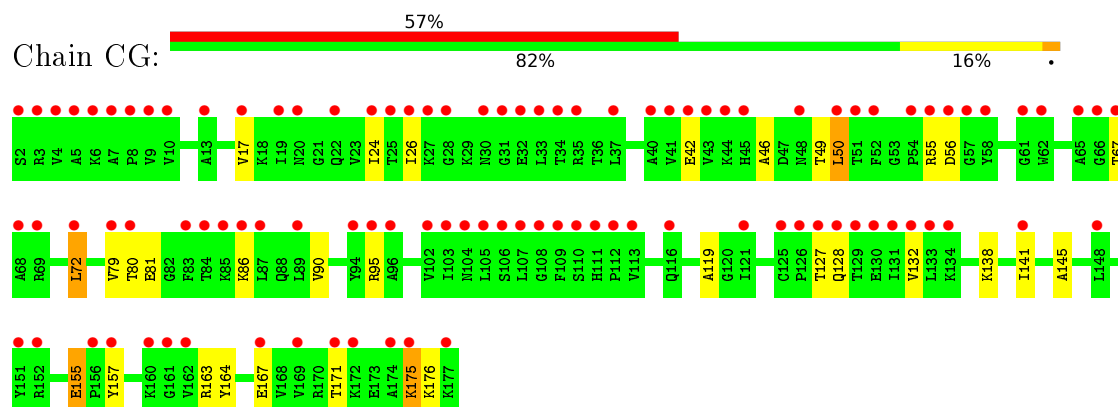
- Molecule 34: 50S ribosomal protein L5



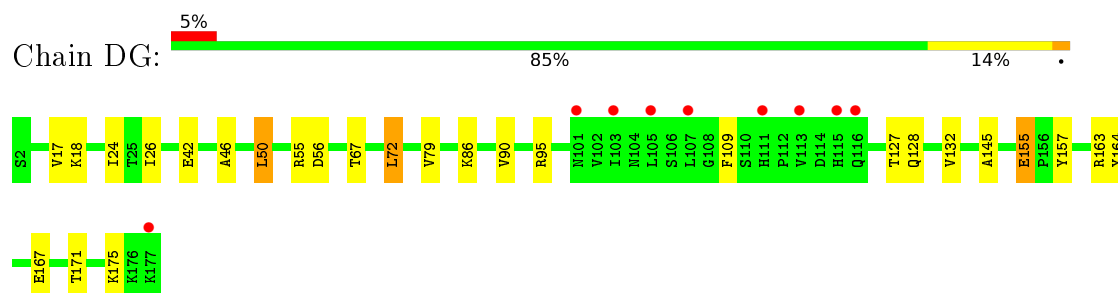




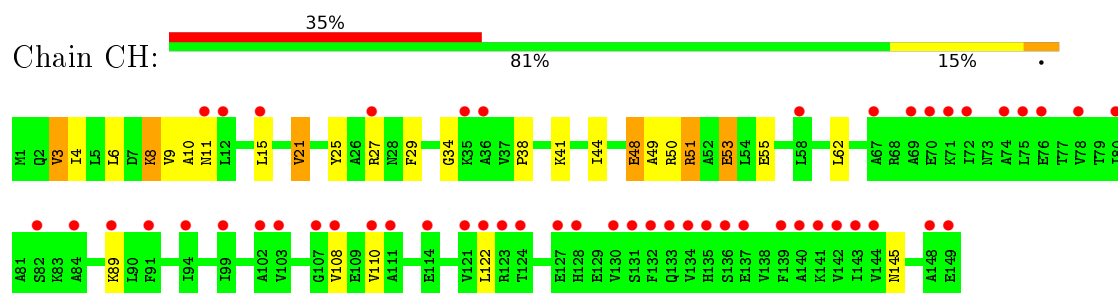
• Molecule 35: 50S ribosomal protein L6



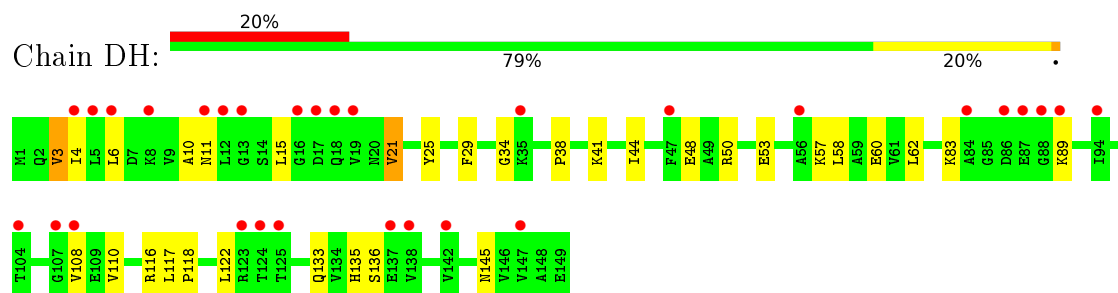
• Molecule 35: 50S ribosomal protein L6



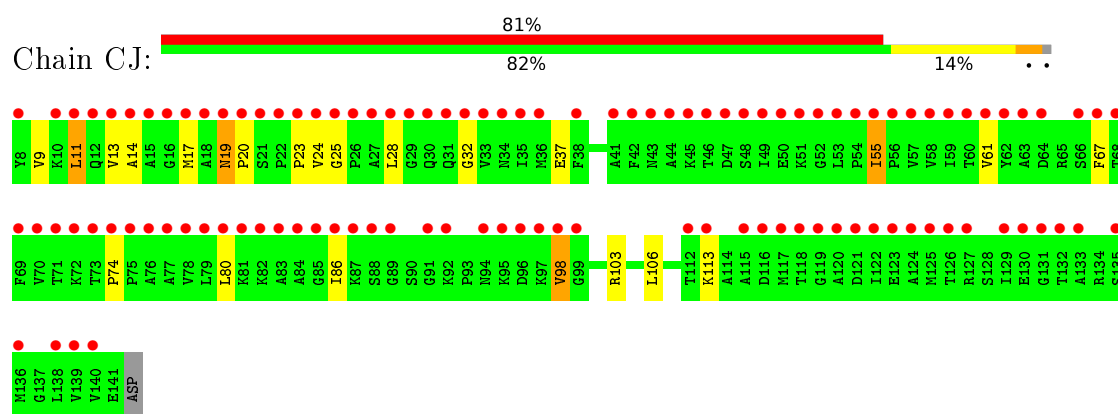
• Molecule 36: 50S ribosomal protein L9



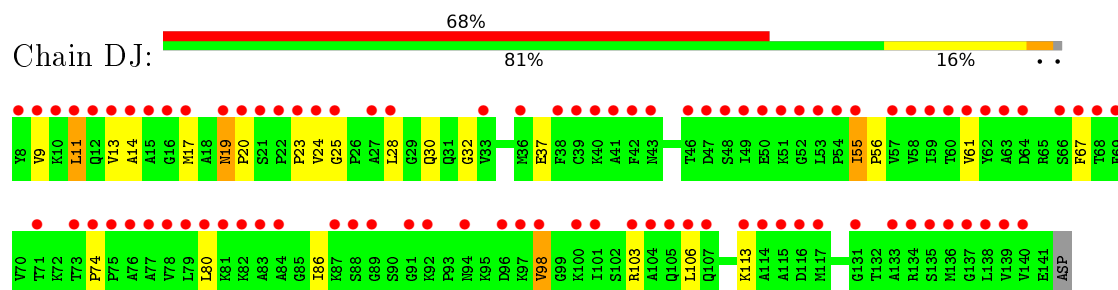
• Molecule 36: 50S ribosomal protein L9



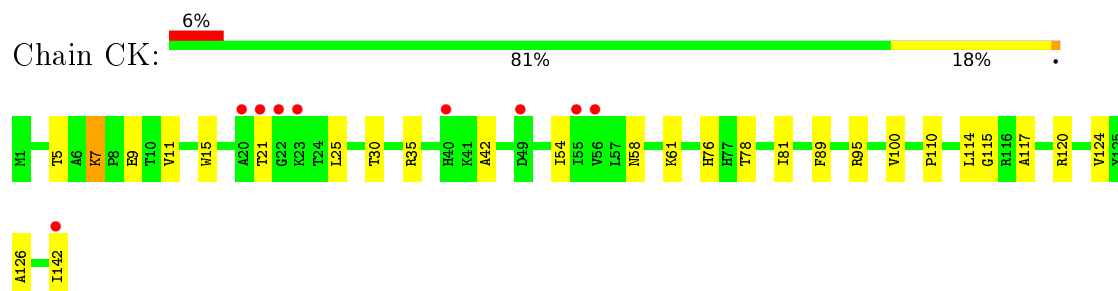
• Molecule 37: 50S ribosomal protein L11



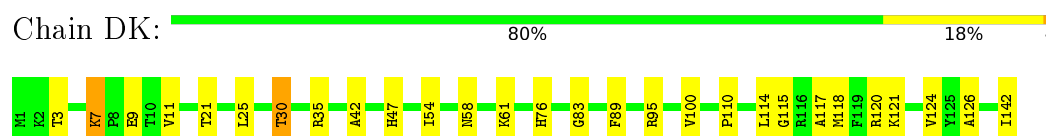
- Molecule 37: 50S ribosomal protein L11



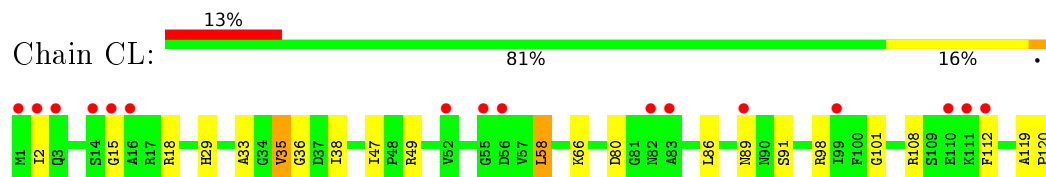
- Molecule 38: 50S ribosomal protein L13



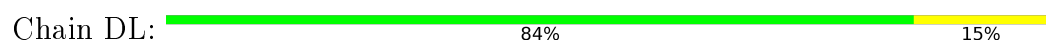
- Molecule 38: 50S ribosomal protein L13



- Molecule 39: 50S ribosomal protein L14

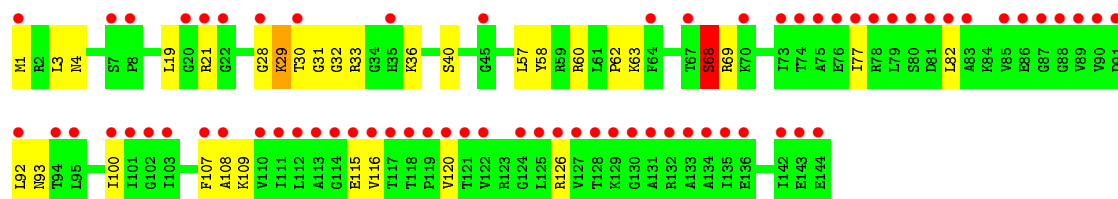
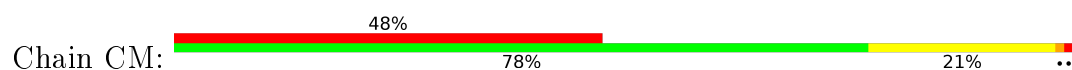


- Molecule 39: 50S ribosomal protein L14

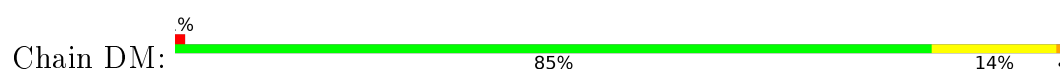




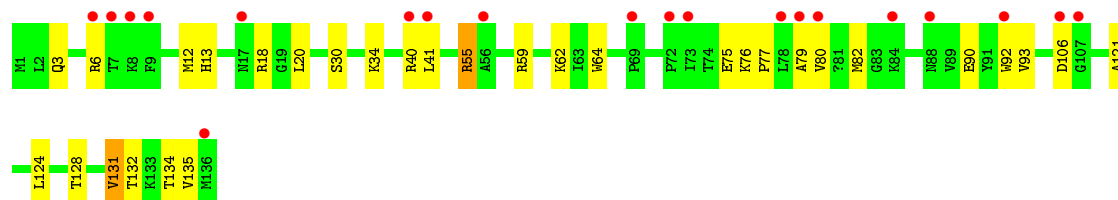
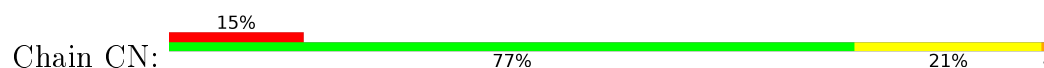
• Molecule 40: 50S ribosomal protein L15



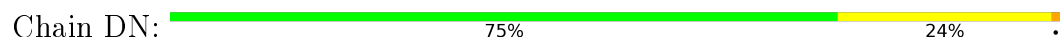
• Molecule 40: 50S ribosomal protein L15



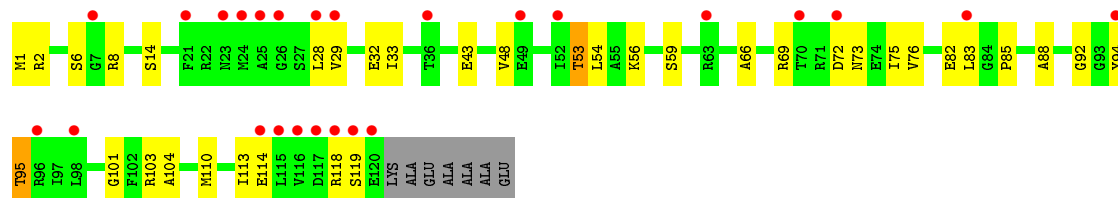
• Molecule 41: 50S ribosomal protein L16



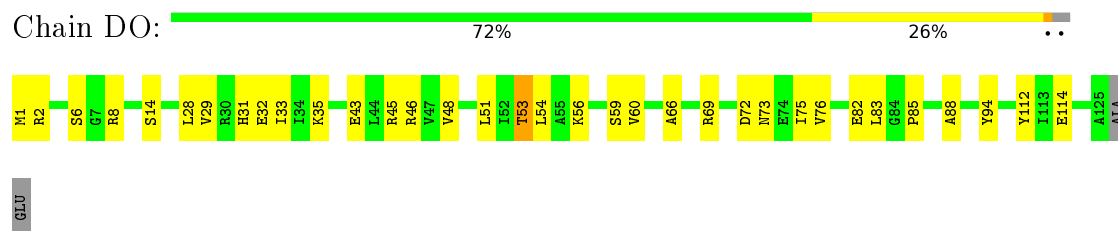
• Molecule 41: 50S ribosomal protein L16



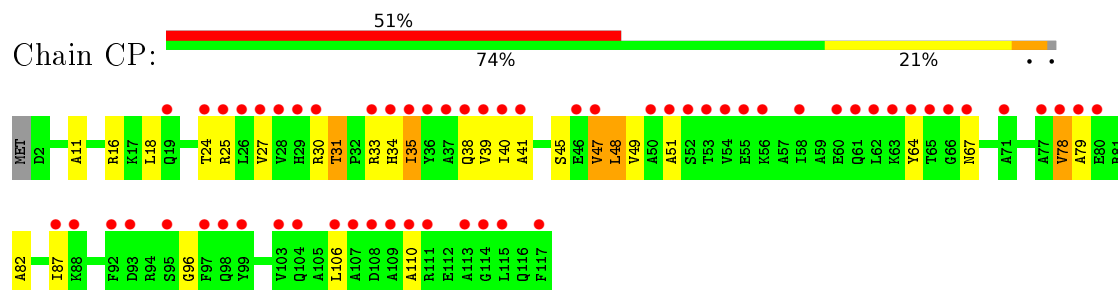
• Molecule 42: 50S ribosomal protein L17



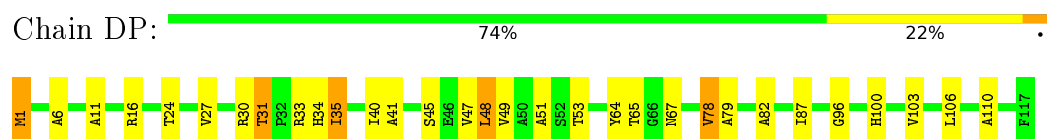
- Molecule 42: 50S ribosomal protein L17



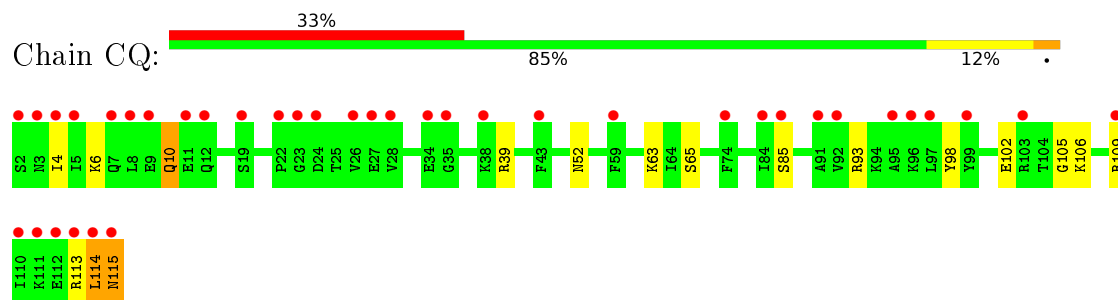
- Molecule 43: 50S ribosomal protein L18



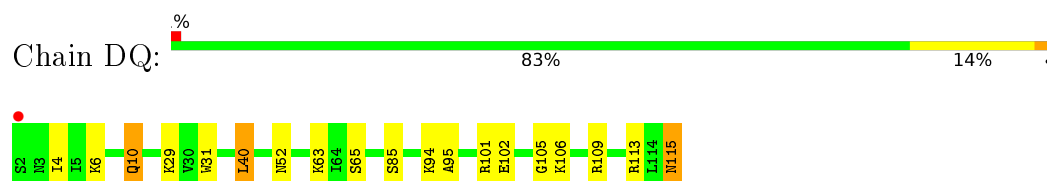
- Molecule 43: 50S ribosomal protein L18



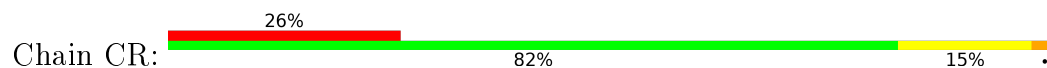
- Molecule 44: 50S ribosomal protein L19

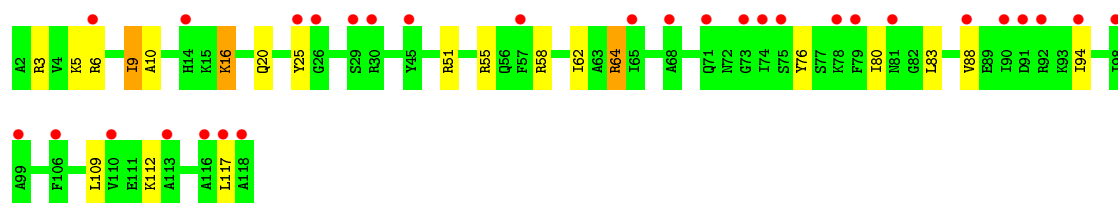


- Molecule 44: 50S ribosomal protein L19



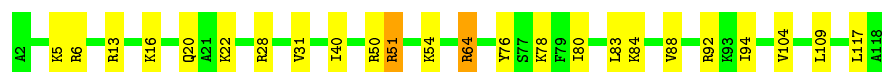
- Molecule 45: 50S ribosomal protein L20





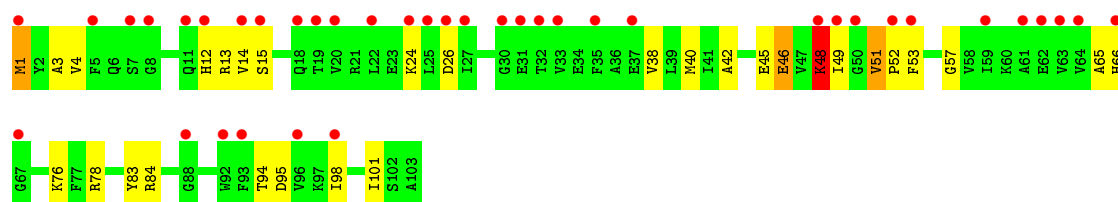
- Molecule 45: 50S ribosomal protein L20

Chain DR: 79% 19%



- Molecule 46: 50S ribosomal protein L21

Chain CS: 38% 71% 25%



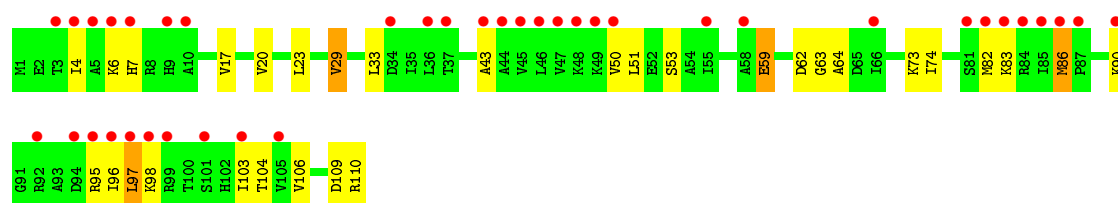
- Molecule 46: 50S ribosomal protein L21

Chain DS: 71% 26%



- Molecule 47: 50S ribosomal protein L22

Chain CT: 35% 72% 25%

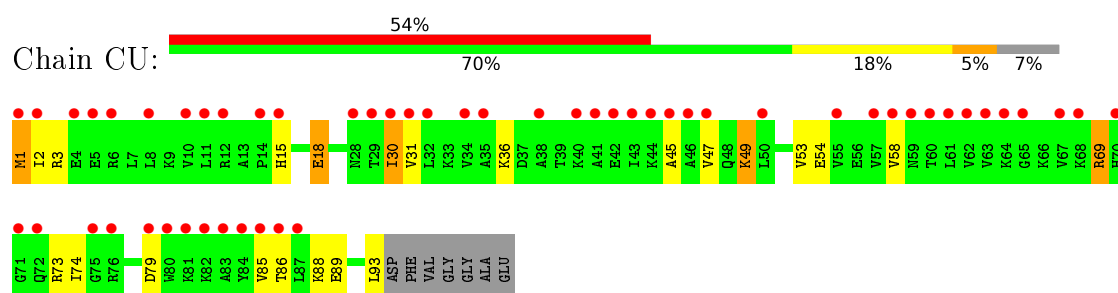


- Molecule 47: 50S ribosomal protein L22

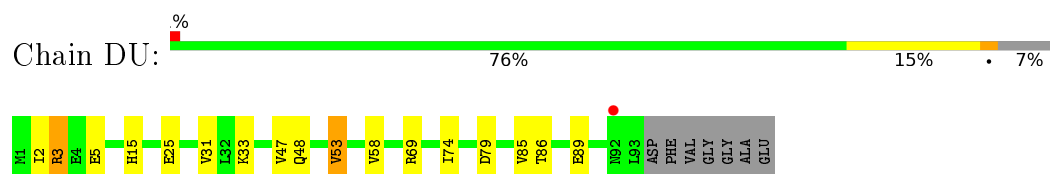
Chain DT: 78% 22%



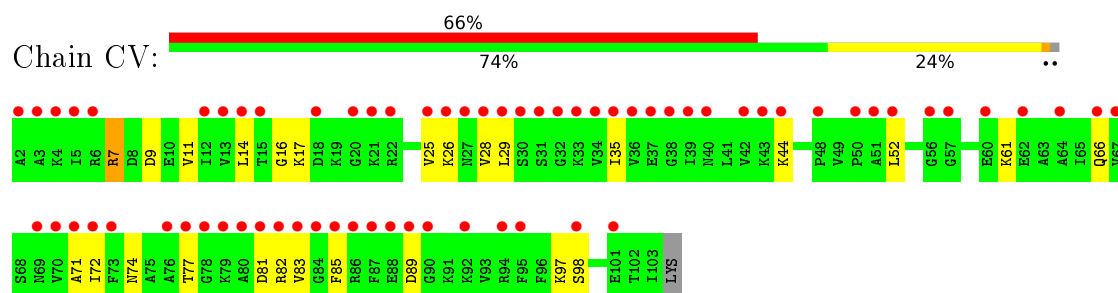
- Molecule 48: 50S ribosomal protein L23



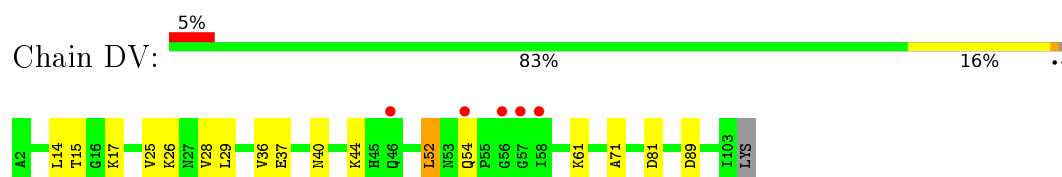
- Molecule 48: 50S ribosomal protein L23



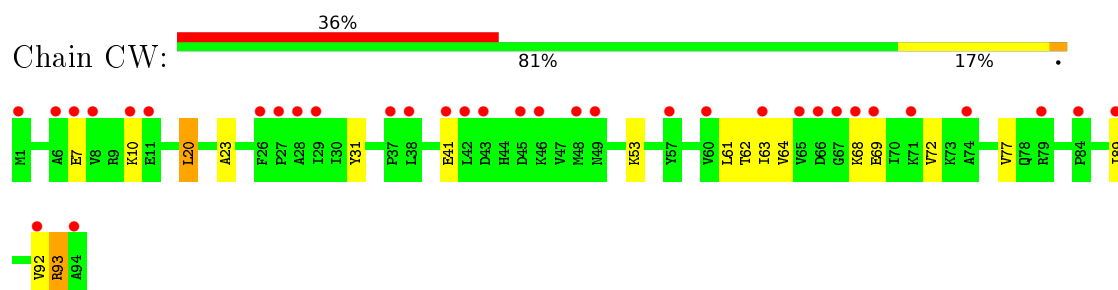
- Molecule 49: 50S ribosomal protein L24



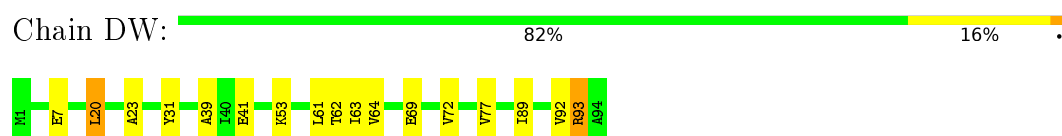
- Molecule 49: 50S ribosomal protein L24



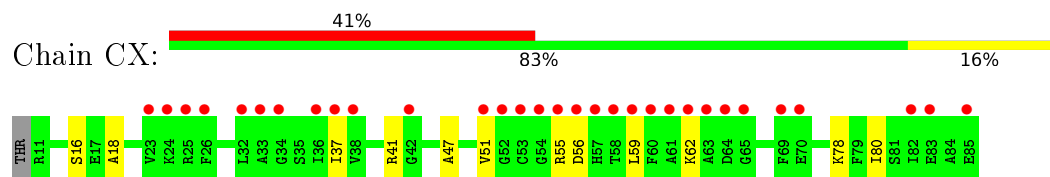
- Molecule 50: 50S ribosomal protein L25



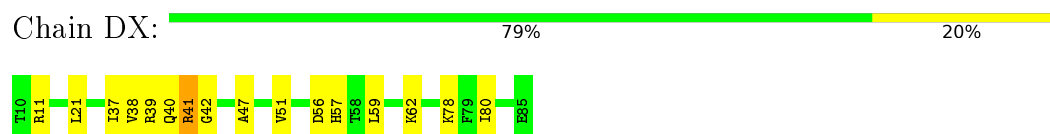
- Molecule 50: 50S ribosomal protein L25



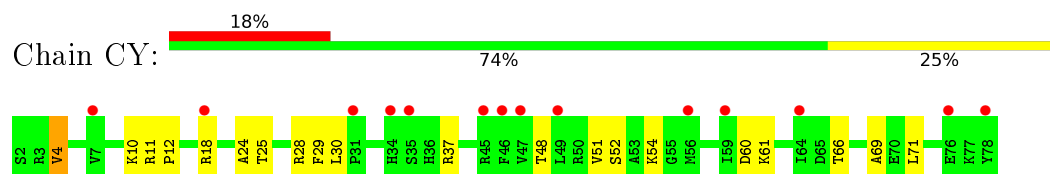
- Molecule 51: 50S ribosomal protein L27



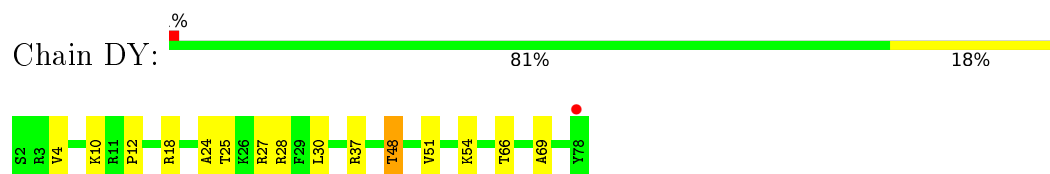
- Molecule 51: 50S ribosomal protein L27



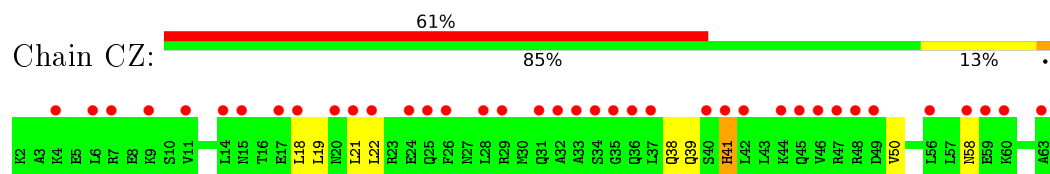
- Molecule 52: 50S ribosomal protein L28



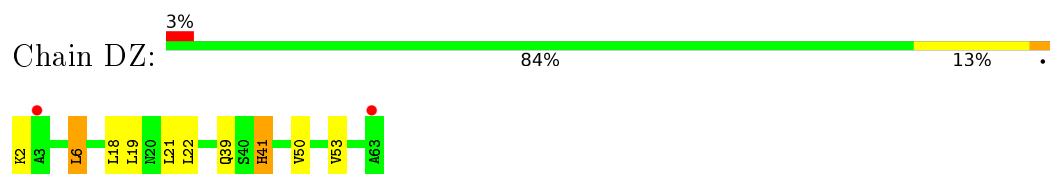
- Molecule 52: 50S ribosomal protein L28



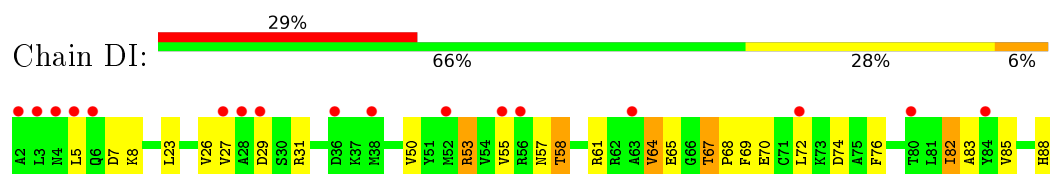
- Molecule 53: 50S ribosomal protein L29

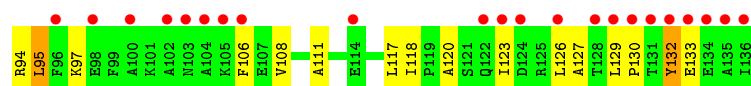


- Molecule 53: 50S ribosomal protein L29

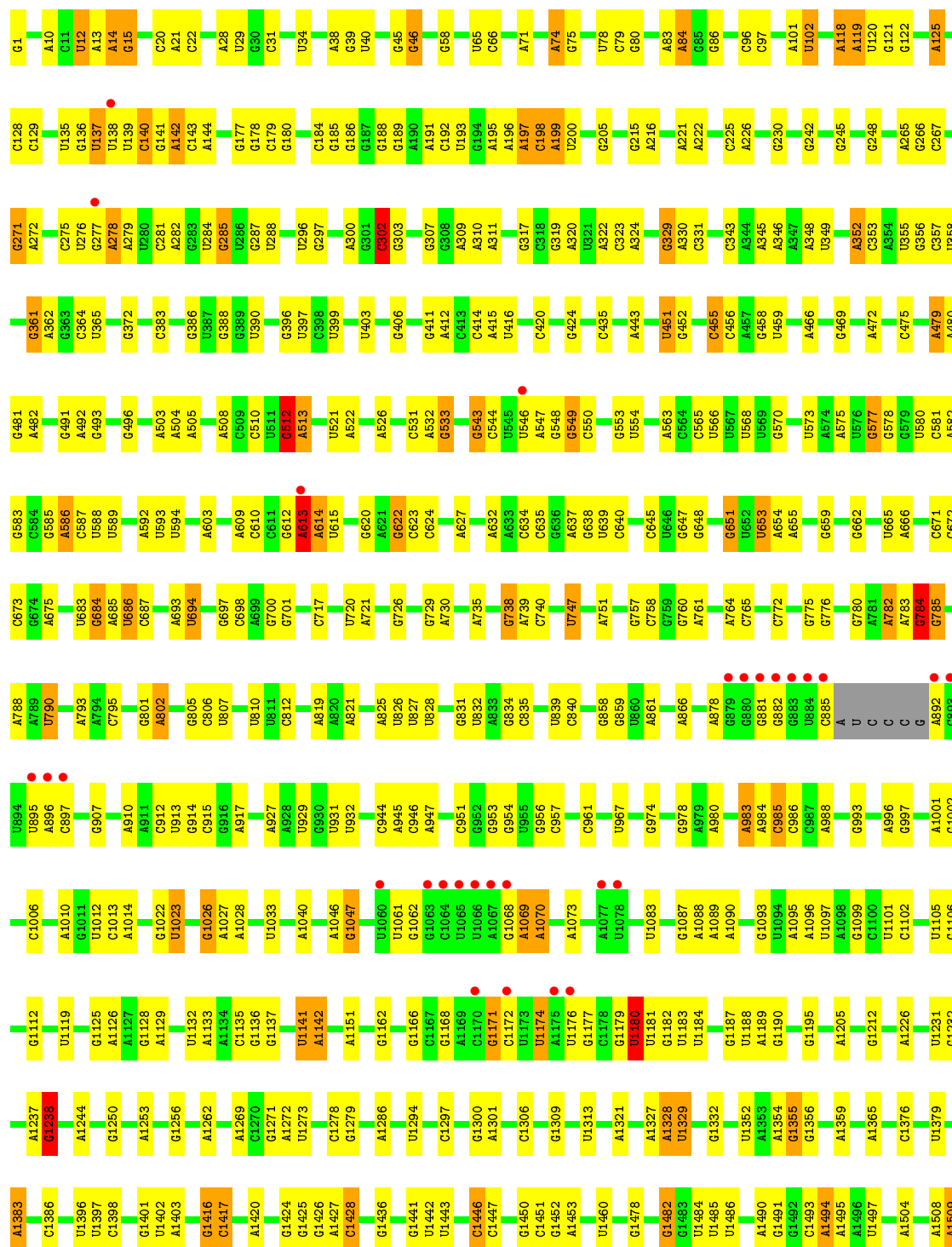


- Molecule 54: 50S ribosomal protein L10





• Molecule 55: 23S rRNA





A2887	U2783	G2673	A2547	A2439	A2340	A2225	U2131	G2050	G1961	G1649	G1510
C2888	U2784	C2681	U2548	C2440	G2341	U2233	U2132	A2051	U1796	G1659	G1511
G2895	C2768	C2689	G2557	U2441	C2342	G2234	G2133	A2052	G1797	A1515	A1515
C2901	U2789	U2689	C2558	U2344	U2343	U2344	A2134	C2055	G1798	G1663	U1523
G2902	G2791	U2690	C2559	G2447	G2345	G2346	A2135	G2056	G1799	A1664	U1523
U	U2695	U2695	U2563	U2448	C2347	G2239	G2140	G2057	A1801	A1665	G1529
U2796	U2449	A2450	A2564	U2450	C2347	U2243	G2141	A2060	A1808	G1674	G1529
C2703	A2461	A2461	A2565	A2461	C2351	G2255	A2142	G2061	U1970	G1675	A1532
U2797	G2464	G2464	A2566	G2464	C2354	C2258	C2145	G2062	U1971	A1676	C1533
A2799	C2465	C2465	G2567	C2465	C2357	U2259	A2146	C2063	G1972	G1813	U1534
A2800	A2572	A2572	A2572	A2572	G2364	C2260	A2147	C2064	G1973	G1813	A1535
G2811	C2573	C2573	A2573	A2469	G2365	G2261	U2148	C2065	G1974	C1816	C1536
G2812	A2577	A2577	G2578	G2472	G2366	U2262	U2149	G2066	U1976	G1826	G1537
A2813	G2581	G2581	G2581	U2473	A2366	U2267	U2151	U2068	G1979	G1699	A1544
C2815	G2582	G2582	G2582	U2474	A2367	A2268	G2152	G2069	A1981	G1699	A1544
U2818	U2585	U2585	U2585	U2475	A2377	A2268	G2153	A2077	C1985	U1714	C1547
G2819	U2586	U2586	U2586	U2476	A2378	A2273	A2158	A2082	U1991	G1715	U1554
A2820	U2587	U2587	U2587	U2477	A2381	A2274	G2159	G2083	G1992	U1720	C1557
A2821	U2588	U2588	U2588	U2478	G2382	A2278	C2160	G2087	U1993	G1721	C1558
G2822	U2589	U2589	U2589	U2479	G2383	G2279	C2161	G2093	C1997	A1722	U1562
A2823	U2596	U2596	U2596	G2480	C2384	G2280	A2162	A2094	G1869	U1729	U1563
G2824	G2603	G2603	G2603	U2491	C2385	A2281	A2163	A2095	C1870	G1730	U1563
C2830	U2613	U2613	U2613	U2492	A2386	G2282	C2164	C2096	A1871	G1731	A1566
A2835	U2614	U2614	U2614	U2493	U2387	G2283	C2165	A2097	A1872	G1738	A1569
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G2846	G2607	G2607	G2607	U2495	U2393	A2287	U2167	A2014	A1885	A1744	U1578
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G2848	U2609	U2609	U2609	G2502	U2402	U2292	A2170	G2018	U1747	A1746	U1584
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A2850	U2611	U2611	U2611	U2404	A2406	G2308	A2172	A2020	G1906	A1586	A1586
G2851	U2612	U2612	U2612	U2405	U2407	G2308	C2174	C2023	G1907	G1587	G1587
C2755	U2613	U2613	U2613	U2406	U2408	A2311	C2175	U2026	G1753	U1754	U1588
G2762	U2614	U2614	U2614	U2407	G2409	U2312	A2176	C1914	A1755	A1590	A1590
A2763	U2615	U2615	U2615	U2408	G2410	C2313	C2177	G2027	C1914	A1591	A1591
U2764	U2616	U2616	U2616	U2409	U2418	U2320	U2178	U2030	U1758	C1604	C1604
A2765	U2617	U2617	U2617	U2410	U2419	U2321	U2179	A1928	A1759	C1607	C1607
C2766	U2618	U2618	U2618	U2411	U2420	G2325	U2180	G1929	C1764	A1608	A1608
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C2771	U2623	U2623	U2623	U2416	A2425	U2330	U2185	G2036	U1781	A1641	A1641
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	U2633	U2633	U2633	U2426	U2440	U2340	G2218				
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	U2636	U2636	U2636	U2429	U2443	U2343	G2221				
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	U2638	U2638	U2638	U2431	U2445	U2345	G2223				
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	U2640	U2640	U2640	U2433	U2447	U2347	G2225				
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	U2691	U2691	U2691	U2484	U2498	U2398	G2276				
	U2692	U2692	U2692	U2485	U2499	U2399	G2277				
	U2693	U2693	U2693	U2486	U2500	U2400	G2278				
	U2694	U2694	U2694	U2487	U2501	U2401	G2279				
	U2695	U2695	U2695	U2488	U2502	U2402	G2280				
	U2696	U2696	U2696	U2489	U2503	U2403	G2281				
	U2697	U2697	U2697	U2490	U2504	U2404	G2282				
	U2698	U2698	U2698	U2491	U2505	U2405	G2283				
	U2699	U2699	U2699	U2492							

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.55Å 433.65Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.32 48.13 – 3.32	Depositor EDS
% Data completeness (in resolution range)	83.3 (48.13-3.32) 83.3 (48.13-3.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	40.28 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.176 , 0.219 0.191 , 0.238	Depositor DCC
$R_{free}$ test set	2784 reflections (0.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 128.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	295119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, D2T, UR3, 7MG, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, H2U, SPD, EDO, MEQ, OMU, PUT, 4OC, 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	AA	1.02	13/36596 (0.0%)	0.86	4/57086 (0.0%)
1	BA	1.01	12/36571 (0.0%)	0.86	3/57047 (0.0%)
2	AB	0.45	0/1784	0.65	0/2403
2	BB	0.43	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.66	0/2225
3	BC	0.48	0/1652	0.66	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.46	0/1665	0.69	0/2227
5	AE	0.47	0/1157	0.78	0/1557
5	BE	0.45	0/1118	0.81	0/1504
6	AF	0.44	0/881	0.71	0/1189
6	BF	0.45	0/835	0.76	0/1128
7	AG	0.49	0/1196	0.65	0/1602
7	BG	0.48	0/1196	0.64	0/1602
8	AH	0.42	0/989	0.68	0/1326
8	BH	0.41	0/989	0.67	0/1326
9	AI	0.44	0/1034	0.67	0/1375
9	BI	0.45	0/1034	0.66	0/1375
10	AJ	0.46	0/806	0.67	0/1089
10	BJ	0.52	0/797	0.71	0/1077
11	AK	0.47	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.45	0/960	0.74	0/1286
12	BL	0.43	0/960	0.72	0/1286
13	AM	0.51	0/893	0.74	1/1193 (0.1%)
13	BM	0.53	0/893	0.73	0/1193
14	AN	0.48	0/817	0.65	0/1088
14	BN	0.47	0/817	0.65	0/1088
15	AO	0.47	0/722	0.65	0/964
15	BO	0.43	0/722	0.64	0/964
16	AP	0.48	0/659	0.73	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	BP	0.47	0/659	0.75	0/884
17	AQ	0.47	0/658	0.73	0/881
17	BQ	0.47	0/658	0.75	0/881
18	AR	0.50	0/463	0.70	0/621
18	BR	0.49	0/463	0.69	0/621
19	AS	0.51	0/653	0.63	0/877
19	BS	0.51	0/653	0.64	0/877
20	AT	0.47	0/676	0.68	0/895
20	BT	0.50	0/671	0.70	0/888
21	AU	0.42	0/472	0.62	0/627
21	BU	0.40	0/472	0.63	0/627
22	C1	0.49	0/450	0.69	0/599
22	D1	0.61	0/450	0.75	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.49	0/421	0.70	0/561
24	C3	0.44	0/380	0.71	0/498
24	D3	0.54	0/380	0.74	0/498
25	C4	0.44	0/513	0.64	0/676
25	D4	0.52	0/513	0.68	0/676
26	C5	0.44	0/303	0.74	0/397
26	D5	0.60	1/303 (0.3%)	0.75	0/397
27	C0	0.53	0/453	0.75	0/605
27	D0	0.61	0/467	0.79	0/623
28	CB	1.01	1/2828 (0.0%)	0.90	1/4410 (0.0%)
28	DB	1.10	3/2872 (0.1%)	0.91	0/4478
29	CC	0.45	0/2121	0.74	0/2852
29	DC	0.49	0/2121	0.75	0/2852
30	CD	0.44	0/1586	0.68	0/2134
31	CA	1.05	65/69165 (0.1%)	0.88	16/107896 (0.0%)
32	DD	0.53	0/1576	0.70	0/2119
33	CE	0.43	0/1571	0.72	0/2113
33	DE	0.48	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.69	0/1926
34	DF	0.47	0/1434	0.73	0/1926
35	CG	0.41	0/1343	0.68	1/1816 (0.1%)
35	DG	0.45	0/1343	0.67	0/1816
36	CH	0.46	0/1121	0.72	1/1515 (0.1%)
36	DH	0.47	0/1121	0.70	0/1515
37	CJ	0.54	0/993	0.68	0/1341
37	DJ	0.54	0/993	0.68	0/1341
38	CK	0.43	0/1152	0.71	0/1551
38	DK	0.58	0/1152	0.75	0/1551
39	CL	0.47	0/947	0.75	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DL	0.53	0/955	0.77	0/1279
40	CM	0.45	0/1062	0.73	1/1413 (0.1%)
40	DM	0.51	0/1062	0.71	0/1413
41	CN	0.45	0/1081	0.72	0/1443
41	DN	0.55	0/1092	0.78	0/1457
42	CO	0.45	0/973	0.72	0/1301
42	DO	0.59	0/1006	0.78	0/1345
43	CP	0.44	0/902	0.70	0/1209
43	DP	0.51	0/910	0.70	0/1219
44	CQ	0.42	0/929	0.75	0/1242
44	DQ	0.50	0/929	0.74	0/1242
45	CR	0.47	0/960	0.70	0/1278
45	DR	0.61	0/960	0.75	0/1278
46	CS	0.45	0/829	0.77	0/1107
46	DS	0.59	0/829	0.82	0/1107
47	CT	0.42	0/864	0.78	0/1156
47	DT	0.57	0/864	0.80	0/1156
48	CU	0.46	0/744	0.72	0/994
48	DU	0.52	0/744	0.72	0/994
49	CV	0.47	0/787	0.79	0/1051
49	DV	0.49	0/787	0.82	0/1051
50	CW	0.42	0/766	0.69	0/1025
50	DW	0.52	0/766	0.71	0/1025
51	CX	0.39	0/576	0.66	0/762
51	DX	0.51	0/598	0.69	0/790
52	CY	0.40	0/635	0.70	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.44	0/502	0.69	0/667
53	DZ	0.50	0/502	0.69	0/667
54	DI	0.52	0/1037	0.78	1/1402 (0.1%)
55	DA	1.19	83/69364 (0.1%)	0.93	24/108207 (0.0%)
All	All	0.95	178/309271 (0.1%)	0.85	53/462220 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	BJ	0	1
28	DB	0	1
31	CA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DA	0	26
All	All	0	29

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-10.08	1.26	1.42
31	CA	2225	A	C3'-O3'	9.82	1.55	1.42
31	CA	1936	A	N9-C4	-9.23	1.32	1.37
55	DA	2097	A	O5'-C5'	-8.54	1.29	1.42
55	DA	2585	U	C1'-N1	8.38	1.61	1.48
1	BA	5	U	C1'-N1	7.67	1.60	1.48
55	DA	12	U	C1'-N1	7.64	1.60	1.48
31	CA	769	U	C1'-N1	7.56	1.60	1.48
31	CA	2232	C	C1'-N1	7.42	1.59	1.48
55	DA	673	C	C3'-O3'	-7.20	1.32	1.42
55	DA	790	U	C1'-N1	7.15	1.59	1.48
55	DA	2585	U	C3'-O3'	7.08	1.52	1.42
55	DA	2068	U	C3'-O3'	-7.06	1.32	1.42
1	AA	632	U	C1'-N1	6.96	1.59	1.48
55	DA	2426	A	C3'-O3'	6.89	1.51	1.42
31	CA	1657	U	C1'-N1	6.82	1.58	1.48
1	AA	1195	C	C1'-N1	6.80	1.58	1.48
55	DA	2127	G	C3'-O3'	6.79	1.51	1.42
31	CA	1825	U	C1'-N1	6.69	1.58	1.48
31	CA	1313	U	C1'-N1	6.65	1.58	1.48
31	CA	995	C	O5'-C5'	-6.62	1.32	1.42
31	CA	12	U	C1'-N1	6.57	1.58	1.48
31	CA	1938	A	N9-C4	6.54	1.41	1.37
31	CA	2465	C	C1'-N1	6.54	1.58	1.48
31	CA	790	U	C1'-N1	6.54	1.58	1.48
31	CA	2215	C	C1'-N1	6.52	1.58	1.48
31	CA	1940	U	C3'-O3'	6.50	1.51	1.42
1	BA	1397	C	N1-C2	6.45	1.46	1.40
55	DA	784	G	C3'-O3'	6.42	1.51	1.42
1	BA	632	U	C1'-N1	6.37	1.58	1.48
1	AA	5	U	C1'-N1	6.33	1.58	1.48
31	CA	2425	A	C3'-O3'	6.33	1.51	1.42
55	DA	1126	A	N9-C4	6.32	1.41	1.37
55	DA	1188	U	C2-N3	-6.30	1.33	1.37
31	CA	1670	C	C3'-O3'	6.19	1.50	1.42
55	DA	2402	U	N1-C2	6.19	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2585	U	N1-C2	6.18	1.44	1.38
1	AA	1397	C	N1-C6	6.15	1.40	1.37
31	CA	461	C	C1'-N1	6.15	1.57	1.48
55	DA	2031	A	N7-C5	-6.09	1.35	1.39
31	CA	1777	U	C1'-N1	6.08	1.57	1.48
31	CA	2263	C	C1'-N1	6.06	1.57	1.48
55	DA	793	A	N7-C5	-6.04	1.35	1.39
55	DA	1547	C	C1'-N1	6.02	1.57	1.48
55	DA	2729	G	C3'-O3'	-6.02	1.33	1.42
55	DA	1778	U	C4'-C3'	-6.01	1.46	1.53
31	CA	532	A	C3'-O3'	6.01	1.50	1.42
31	CA	1993	U	C1'-N1	6.01	1.57	1.48
1	BA	764	C	C1'-N1	5.99	1.57	1.48
31	CA	271	G	C3'-O3'	5.99	1.50	1.42
31	CA	1376	C	C1'-N1	5.94	1.57	1.48
55	DA	2502	G	O5'-C5'	-5.94	1.33	1.42
55	DA	662	G	N7-C5	-5.93	1.35	1.39
31	CA	2354	C	C1'-N1	5.91	1.57	1.48
31	CA	1584	U	C1'-N1	5.91	1.57	1.48
55	DA	12	U	P-O5'	5.89	1.65	1.59
31	CA	2443	C	C1'-N1	5.88	1.57	1.48
55	DA	1534	U	C1'-N1	5.88	1.57	1.48
55	DA	140	C	C1'-N1	5.87	1.57	1.48
31	CA	2779	U	C1'-N1	5.85	1.57	1.48
55	DA	954	G	C5-C6	5.79	1.48	1.42
55	DA	1785	A	N7-C5	-5.79	1.35	1.39
55	DA	526	A	N3-C4	5.76	1.38	1.34
55	DA	416	U	C1'-N1	5.75	1.57	1.48
31	CA	2006	C	C1'-N1	5.74	1.57	1.48
1	BA	1008	U	O5'-C5'	-5.71	1.33	1.42
1	AA	1059	C	C1'-N1	5.70	1.57	1.48
31	CA	653	U	C1'-N1	5.70	1.57	1.48
55	DA	2268	A	N7-C5	-5.68	1.35	1.39
31	CA	784	G	C3'-O3'	5.68	1.50	1.42
55	DA	102	U	N1-C2	5.67	1.43	1.38
31	CA	2680	U	C3'-O3'	5.67	1.50	1.42
31	CA	20	C	C1'-N1	5.63	1.57	1.48
1	BA	842	U	C3'-O3'	5.63	1.50	1.42
1	AA	295	C	C1'-N1	5.62	1.57	1.48
55	DA	585	G	C2-N3	5.60	1.37	1.32
31	CA	1633	G	C3'-O3'	5.59	1.50	1.42
31	CA	1656	C	C1'-N1	5.57	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2586	U	C1'-N1	5.57	1.57	1.48
55	DA	653	U	C1'-N1	5.56	1.57	1.48
55	DA	1383	A	N7-C5	-5.56	1.35	1.39
55	DA	2781	A	N7-C5	-5.56	1.35	1.39
28	DB	35	C	N1-C6	5.55	1.40	1.37
31	CA	691	C	C1'-N1	5.55	1.57	1.48
31	CA	2233	U	C1'-N1	5.55	1.57	1.48
31	CA	1352	U	C1'-N1	5.54	1.57	1.48
55	DA	978	G	C6-N1	5.51	1.43	1.39
1	AA	932	C	C1'-N1	5.51	1.57	1.48
31	CA	1314	C	C1'-N1	5.50	1.57	1.48
55	DA	1664	A	N7-C5	-5.50	1.35	1.39
55	DA	2220	U	C1'-N1	5.50	1.56	1.48
31	CA	1774	C	C1'-N1	5.49	1.56	1.48
55	DA	790	U	P-O5'	5.49	1.65	1.59
55	DA	2239	G	C3'-O3'	-5.48	1.34	1.42
1	AA	137	U	C1'-N1	5.47	1.56	1.48
1	BA	209	U	C1'-N1	5.47	1.56	1.48
55	DA	2055	C	C3'-O3'	-5.47	1.34	1.42
28	DB	11	C	C1'-N1	5.47	1.56	1.48
55	DA	1584	U	C1'-N1	5.45	1.56	1.48
55	DA	2077	A	N7-C5	-5.45	1.35	1.39
1	BA	1059	C	C1'-N1	5.44	1.56	1.48
31	CA	2104	C	C1'-N1	5.44	1.56	1.48
55	DA	2850	A	N7-C5	-5.42	1.35	1.39
1	BA	137	U	C1'-N1	5.42	1.56	1.48
55	DA	2542	A	C6-N6	-5.40	1.29	1.33
1	BA	222	C	C1'-N1	5.40	1.56	1.48
1	AA	603	U	C1'-N1	5.40	1.56	1.48
55	DA	2354	C	O5'-C5'	-5.39	1.34	1.42
55	DA	2005	A	C6-N1	5.38	1.39	1.35
31	CA	1253	A	P-O5'	5.37	1.65	1.59
55	DA	1446	C	C1'-N1	5.37	1.56	1.48
55	DA	2158	A	C3'-O3'	5.36	1.49	1.42
31	CA	1557	C	C1'-N1	5.36	1.56	1.48
31	CA	2320	U	C1'-N1	5.36	1.56	1.48
55	DA	967	U	C1'-N1	5.36	1.56	1.48
55	DA	2425	A	C3'-O3'	5.35	1.49	1.42
55	DA	2506	U	C1'-N1	5.35	1.56	1.48
55	DA	2342	C	C1'-N1	5.35	1.56	1.48
55	DA	1659	G	C3'-O3'	-5.34	1.34	1.42
31	CA	140	C	C1'-N1	5.32	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	692	C	C1'-N1	5.31	1.56	1.48
1	AA	222	C	C1'-N1	5.28	1.56	1.48
55	DA	549	G	C3'-O3'	5.27	1.49	1.42
31	CA	826	U	C1'-N1	5.26	1.56	1.48
55	DA	2901	C	C1'-N1	5.26	1.56	1.48
55	DA	275	C	C1'-N1	5.25	1.56	1.48
28	DB	91	C	C1'-N1	5.24	1.56	1.48
31	CA	623	C	C1'-N1	5.23	1.56	1.48
55	DA	2472	G	N7-C5	-5.23	1.36	1.39
31	CA	1981	A	C3'-O3'	5.21	1.49	1.42
55	DA	443	A	N7-C5	-5.21	1.36	1.39
55	DA	613	A	N9-C4	5.21	1.41	1.37
1	AA	549	C	C1'-N1	5.20	1.56	1.48
55	DA	2578	G	C5-C4	-5.19	1.34	1.38
55	DA	2402	U	C1'-N1	5.19	1.56	1.48
31	CA	1658	C	C1'-N1	5.18	1.56	1.48
31	CA	2619	C	C1'-N1	5.18	1.56	1.48
31	CA	562	U	C1'-N1	5.17	1.56	1.48
55	DA	735	A	N3-C4	5.17	1.38	1.34
55	DA	694	U	C1'-N1	5.16	1.56	1.48
55	DA	1180	U	C1'-N1	5.15	1.56	1.48
1	AA	503	C	C1'-N1	5.15	1.56	1.48
31	CA	1375	U	C1'-N1	5.14	1.56	1.48
31	CA	635	C	C1'-N1	5.13	1.56	1.48
55	DA	2406	A	P-O5'	5.12	1.64	1.59
31	CA	114	U	C1'-N1	5.12	1.56	1.48
1	BA	1493	A	C3'-O3'	5.11	1.49	1.42
31	CA	801	G	C3'-O3'	5.10	1.49	1.42
55	DA	810	U	N1-C2	5.10	1.43	1.38
55	DA	1913	A	C3'-O3'	5.10	1.49	1.42
55	DA	2491	U	C1'-N1	5.10	1.56	1.48
31	CA	275	C	C1'-N1	5.10	1.56	1.48
31	CA	2385	C	C1'-N1	5.09	1.56	1.48
55	DA	951	C	N1-C6	5.09	1.40	1.37
31	CA	2823	A	C3'-O3'	5.09	1.49	1.42
31	CA	2656	U	C1'-N1	5.08	1.56	1.48
55	DA	533	G	N7-C5	-5.08	1.36	1.39
55	DA	635	C	C1'-N1	5.08	1.56	1.48
1	BA	823	C	C1'-N1	5.08	1.56	1.48
28	CB	11	C	C1'-N1	5.08	1.56	1.48
31	CA	1994	C	C1'-N1	5.08	1.56	1.48
55	DA	1174	U	C1'-N1	5.08	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	29	U	C1'-N1	5.08	1.56	1.48
55	DA	578	G	N7-C5	-5.07	1.36	1.39
55	DA	469	G	C3'-O3'	-5.06	1.35	1.42
31	CA	2581	G	N3-C4	5.06	1.39	1.35
55	DA	1714	U	C1'-N1	5.05	1.56	1.48
55	DA	701	G	N3-C4	5.05	1.39	1.35
55	DA	1665	A	N7-C5	-5.04	1.36	1.39
31	CA	1629	U	C1'-N1	5.04	1.56	1.48
31	CA	2658	C	C1'-N1	5.04	1.56	1.48
55	DA	458	G	N3-C4	5.03	1.39	1.35
55	DA	2442	C	C3'-O3'	-5.03	1.35	1.42
1	AA	1196	A	N9-C4	5.02	1.40	1.37
55	DA	2769	U	C3'-O3'	-5.02	1.35	1.42
26	D5	26	ILE	CG1-CD1	5.01	1.85	1.50
55	DA	632	A	N7-C5	-5.01	1.36	1.39
31	CA	2342	C	C1'-N1	5.00	1.56	1.48

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	9.57	115.86	108.20
31	CA	2425	A	P-O3'-C3'	8.79	130.24	119.70
31	CA	271	G	P-O3'-C3'	7.72	128.96	119.70
1	BA	2	A	OP1-P-OP2	-7.50	108.34	119.60
1	AA	1	A	OP1-P-OP2	-7.15	108.88	119.60
55	DA	892	A	OP1-P-OP2	-7.06	109.01	119.60
54	DI	132	TYR	C-N-CA	7.02	139.24	121.70
55	DA	2585	U	P-O3'-C3'	6.93	128.01	119.70
55	DA	1	G	OP1-P-OP2	-6.92	109.23	119.60
31	CA	892	A	OP1-P-OP2	-6.85	109.32	119.60
31	CA	1786	A	C1'-O4'-C4'	-6.60	104.62	109.90
55	DA	512	G	O4'-C1'-N9	6.55	113.44	108.20
55	DA	2825	G	O4'-C1'-N9	6.38	113.31	108.20
55	DA	199	A	C1'-O4'-C4'	-6.29	104.87	109.90
1	BA	7	A	C1'-O4'-C4'	-6.22	104.93	109.90
1	BA	893	C	C3'-C2'-C1'	-6.15	96.58	101.50
55	DA	479	A	C3'-C2'-C1'	-6.12	96.60	101.50
55	DA	613	A	O4'-C1'-N9	6.05	113.04	108.20
55	DA	1023	U	C4'-C3'-C2'	-6.03	96.58	102.60
55	DA	2848	G	O4'-C1'-N9	5.97	112.98	108.20
55	DA	271	G	P-O3'-C3'	5.84	126.71	119.70
31	CA	974	G	N9-C1'-C2'	5.79	121.52	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2225	A	P-O3'-C3'	5.78	126.63	119.70
31	CA	199	A	C1'-O4'-C4'	-5.76	105.29	109.90
31	CA	784	G	P-O3'-C3'	5.75	126.61	119.70
31	CA	479	A	C3'-C2'-C1'	-5.73	96.92	101.50
1	AA	7	A	C1'-O4'-C4'	-5.68	105.35	109.90
55	DA	1648	U	O4'-C1'-N1	5.58	112.66	108.20
40	CM	68	SER	C-N-CA	5.57	135.63	121.70
55	DA	2825	G	C4'-C3'-C2'	-5.49	97.11	102.60
55	DA	242	G	C3'-C2'-C1'	-5.47	97.12	101.50
31	CA	2680	U	P-O3'-C3'	5.47	126.27	119.70
13	AM	12	HIS	C-N-CA	5.47	135.37	121.70
31	CA	1128	G	C1'-O4'-C4'	-5.46	105.53	109.90
1	AA	841	C	P-O3'-C3'	5.43	126.21	119.70
31	CA	2095	A	C5'-C4'-C3'	-5.39	107.37	116.00
55	DA	242	G	C1'-O4'-C4'	-5.37	105.60	109.90
55	DA	2436	G	C4'-C3'-C2'	-5.34	97.26	102.60
55	DA	451	U	C1'-O4'-C4'	-5.33	105.64	109.90
36	CH	8	LYS	C-N-CA	5.31	134.98	121.70
55	DA	458	G	C3'-C2'-C1'	-5.31	97.25	101.50
31	CA	2035	G	C1'-O4'-C4'	-5.28	105.67	109.90
55	DA	302	C	C5'-C4'-O4'	5.21	115.35	109.10
55	DA	2238	G	C1'-O4'-C4'	-5.18	105.76	109.90
35	CG	175	LYS	C-N-CA	5.17	134.62	121.70
31	CA	1379	U	P-O3'-C3'	5.14	125.87	119.70
55	DA	2447	G	C3'-C2'-C1'	-5.14	97.39	101.50
31	CA	451	U	C1'-O4'-C4'	-5.12	105.80	109.90
55	DA	2127	G	P-O3'-C3'	5.12	125.84	119.70
55	DA	1800	C	C1'-O4'-C4'	-5.11	105.81	109.90
1	AA	429	U	C1'-O4'-C4'	-5.10	105.82	109.90
31	CA	204	A	C3'-C2'-C1'	-5.03	97.47	101.50
55	DA	479	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	BJ	37	ARG	Mainchain
31	CA	780	G	Sidechain
55	DA	1047	G	Sidechain
55	DA	1162	G	Sidechain
55	DA	1238	G	Sidechain
55	DA	1682	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	1773	A	Sidechain
55	DA	1985	C	Sidechain
55	DA	2010	G	Sidechain
55	DA	2286	G	Sidechain
55	DA	2351	G	Sidechain
55	DA	2512	C	Sidechain
55	DA	2516	A	Sidechain
55	DA	2518	A	Sidechain
55	DA	2582	G	Sidechain
55	DA	2588	G	Sidechain
55	DA	2728	U	Sidechain
55	DA	2825	G	Sidechain
55	DA	329	G	Sidechain
55	DA	452	G	Sidechain
55	DA	512	G	Sidechain
55	DA	577	G	Sidechain
55	DA	700	G	Sidechain
55	DA	726	G	Sidechain
55	DA	953	G	Sidechain
55	DA	956	G	Sidechain
55	DA	980	A	Sidechain
55	DA	983	A	Sidechain
28	DB	13	G	Sidechain

## 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	AA	32932	0	16593	164	0
1	BA	32910	0	16582	182	0
2	AB	1753	0	1780	14	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	18	0
4	BD	1643	0	1707	19	0
5	AE	1144	0	1185	17	0
5	BE	1105	0	1148	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	862	0	864	12	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	17	0
7	BG	1182	0	1238	16	0
8	AH	979	0	1031	9	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	11	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	8	0
10	BJ	787	0	828	11	0
11	AK	877	0	887	11	0
11	BK	877	0	887	13	0
12	AL	957	0	1017	14	0
12	BL	957	0	1017	16	0
13	AM	884	0	941	11	0
13	BM	884	0	941	14	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	3	0
15	BO	714	0	734	7	0
16	AP	649	0	666	5	0
16	BP	649	0	666	8	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	5	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	11	0
20	BT	665	0	714	8	0
21	AU	465	0	491	6	0
21	BU	465	0	491	5	0
22	C1	444	0	458	17	0
22	D1	444	0	458	10	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	7	0
25	C4	504	0	572	3	0
25	D4	504	0	572	7	0
26	C5	302	0	340	5	0
26	D5	302	0	340	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C0	449	0	488	4	0
27	D0	463	0	504	7	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	10	0
29	CC	2082	0	2154	24	0
29	DC	2082	0	2154	22	0
30	CD	1565	0	1616	22	0
31	CA	62229	0	31319	399	0
32	DD	1576	0	1627	29	0
33	CE	1552	0	1619	20	0
33	DE	1552	0	1619	20	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	26	0
35	CG	1323	0	1371	16	0
35	DG	1323	0	1371	14	0
36	CH	1110	0	1148	9	0
36	DH	1110	0	1148	10	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	10	0
38	CK	1129	0	1162	13	0
38	DK	1129	0	1162	14	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	7	0
40	CM	1053	0	1129	21	0
40	DM	1053	0	1129	16	0
41	CN	1075	0	1154	15	0
41	DN	1092	0	1177	17	0
42	CO	960	0	1000	16	0
42	DO	993	0	1034	16	0
43	CP	892	0	923	14	0
43	DP	900	0	935	17	0
44	CQ	917	0	962	8	0
44	DQ	917	0	962	14	0
45	CR	947	0	1019	13	0
45	DR	947	0	1019	20	0
46	CS	816	0	839	16	0
46	DS	816	0	839	20	0
47	CT	857	0	922	16	0
47	DT	857	0	922	14	0
48	CU	738	0	807	9	0
48	DU	738	0	807	6	0
49	CV	779	0	831	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	DV	779	0	831	8	0
50	CW	753	0	780	6	0
50	DW	753	0	780	7	0
51	CX	569	0	581	8	0
51	DX	591	0	606	14	0
52	CY	625	0	652	11	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	5	0
53	DZ	501	0	531	6	0
54	DI	1023	0	1052	26	0
55	DA	62423	0	31411	382	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	0	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	1	0
57	DS	13	0	18	0	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	4	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	1	0
61	DA	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	1	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	4	0
62	DB	8	0	12	0	0
63	D1	10	0	14	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	2	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	3	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	5	0	0	0	0
69	AL	7	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	1	0
69	AO	1	0	0	0	0
69	AP	1	0	0	0	0
69	AQ	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	4	0	0	0	0
69	BA	287	0	0	2	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0
69	BL	3	0	0	0	0
69	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BO	1	0	0	0	0
69	BP	4	0	0	0	0
69	BR	1	0	0	0	0
69	BT	5	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	CA	696	0	0	3	0
69	CB	13	0	0	0	0
69	CC	11	0	0	0	0
69	CD	4	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	2	0
69	D1	37	0	0	0	0
69	D2	5	0	0	0	0
69	D3	30	0	0	0	0
69	D4	40	0	0	1	0
69	D5	13	0	0	1	0
69	DA	4824	0	0	39	0
69	DB	203	0	0	3	0
69	DC	100	0	0	1	0
69	DD	97	0	0	5	0
69	DE	54	0	0	2	0
69	DF	13	0	0	1	0
69	DG	9	0	0	0	0
69	DH	2	0	0	0	0
69	DK	61	0	0	0	0
69	DL	50	0	0	0	0
69	DM	60	0	0	0	0
69	DN	81	0	0	1	0
69	DO	42	0	0	1	0
69	DP	42	0	0	2	0
69	DQ	32	0	0	1	0
69	DR	68	0	0	3	0
69	DS	52	0	0	5	0
69	DT	65	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DU	24	0	0	0	0
69	DV	19	0	0	1	0
69	DW	33	0	0	1	0
69	DX	33	0	0	2	0
69	DY	11	0	0	1	0
69	DZ	7	0	0	0	0
All	All	295119	0	194415	2066	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 4.

All (2066) 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)
26:D5:26:ILE:CD1	26:D5:26:ILE:CG1	1.85	1.50
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.16
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.62	0.99
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.44	0.95
31:CA:1311:G:H21	31:CA:1603:A:H62	1.16	0.94
54:DI:67:THR:HG22	54:DI:68:PRO:HA	1.52	0.91
31:CA:1936:A:H2	31:CA:1943:U:H3	1.15	0.91
51:DX:41[A]:ARG:HH12	55:DA:2262:U:H5''	1.39	0.88
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.56	0.87
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.56	0.87
55:DA:1975:G:H21	63:DA:3225:PGE:H22	1.39	0.86
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.57	0.86
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.57	0.86
40:DM:60:ARG:HH21	55:DA:2428:G:N2	1.72	0.86
2:AB:31:ILE:HG21	2:AB:39:HIS:HD2	1.42	0.85
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.07	0.84
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.60	0.84
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.60	0.83
32:DD:140:HIS:HB3	69:DD:485:HOH:O	1.76	0.83
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.59	0.83
2:BB:31:ILE:HG21	2:BB:39:HIS:HD2	1.43	0.82
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.62	0.82
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.82
55:DA:1927:A:H2'	55:DA:1928:A:C8	2.15	0.82
1:AA:1063:C:H2'	1:AA:1064:G:C8	2.15	0.82
55:DA:2796:U:H3	55:DA:2799:A:H61	1.24	0.82
29:CC:17:VAL:HB	29:CC:204:VAL:CG1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.62	0.80
31:CA:694:U:OP1	31:CA:1569:A:H1'	1.83	0.79
31:CA:206:U:H2'	31:CA:207:A:H8	1.46	0.79
47:DT:90:LYS:HA	55:DA:751:A:H5'	1.62	0.79
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.09	0.78
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.63	0.78
31:CA:2428:G:N2	40:CM:60:ARG:HH21	1.79	0.78
1:AA:81:A:H61	1:AA:86:G:H1	1.29	0.78
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	1.66	0.78
31:CA:751:A:H5'	47:CT:90:LYS:HA	1.66	0.78
1:BA:841:C:H3'	1:BA:842:U:H5''	1.66	0.78
31:CA:193:U:H2'	31:CA:194:G:H8	1.49	0.77
31:CA:450:G:H2'	31:CA:451:U:H5''	1.65	0.76
34:DF:158:THR:HG23	34:DF:160:ALA:H	1.50	0.76
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.67	0.76
33:DE:21:ARG:HD2	69:DE:432:HOH:O	1.85	0.76
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.68	0.76
55:DA:758:C:O2	55:DA:1981:A:H2	1.69	0.75
29:DC:41:GLY:O	29:DC:43:ARG:HD2	1.87	0.75
40:DM:60:ARG:HH21	55:DA:2428:G:H21	1.33	0.75
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.69	0.75
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.52	0.75
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.68	0.74
33:DE:130:LYS:HB2	33:DE:133:LEU:HD12	1.69	0.74
43:DP:103:VAL:HG23	69:DP:313:HOH:O	1.87	0.74
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.68	0.74
49:DV:37:GLU:HB3	69:DV:206:HOH:O	1.88	0.74
31:CA:2641:G:H5''	38:CK:78:THR:HB	1.69	0.73
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.69	0.73
29:CC:266:PHE:CD1	29:CC:266:PHE:N	2.57	0.73
31:CA:1203:U:H5'	40:CM:3:LEU:HD12	1.70	0.73
29:CC:266:PHE:H	29:CC:266:PHE:HD1	1.33	0.73
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.70	0.72
1:BA:82:G:H1	1:BA:84:U:H5	1.37	0.72
1:BA:1107:C:OP1	3:BC:174:PRO:HB3	1.90	0.71
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.71	0.71
1:BA:518:C:H2'	1:BA:530:G:C8	2.25	0.71
45:DR:20:GLN:HG2	57:DR:201:PG4:H42	1.73	0.71
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.72	0.71
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.54	0.71
1:BA:664:G:H22	1:BA:741:G:H1	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.72	0.71
31:CA:118:A:N3	31:CA:178:G:H1'	2.06	0.71
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.57	0.70
31:CA:1936:A:N6	31:CA:1963:U:H3	1.90	0.70
1:AA:518:C:H2'	1:AA:530:G:C8	2.27	0.70
29:DC:258:ARG:HD2	55:DA:1799:G:OP1	1.92	0.70
55:DA:671:C:O2'	55:DA:672:C:H5'	1.92	0.70
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	1.74	0.70
55:DA:1137:G:H5''	59:DA:3213:PUT:H12	1.73	0.69
1:AA:202:G:HO2'	1:AA:468:A:H8	1.40	0.69
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.73	0.69
1:BA:967:5MC:HM53	1:BA:1197:A:N6	2.07	0.69
1:AA:403:C:H5'	4:AD:132:ILE:HG23	1.74	0.69
35:DG:95:ARG:HG2	35:DG:128:GLN:HB3	1.75	0.69
34:DF:80:ARG:HB3	34:DF:83:TYR:CZ	2.28	0.69
33:CE:130:LYS:HB2	33:CE:133:LEU:HD12	1.73	0.69
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.75	0.68
1:AA:664:G:H22	1:AA:741:G:H1	1.39	0.68
31:CA:784:G:H5'	31:CA:785:G:OP1	1.93	0.68
35:CG:95:ARG:HG2	35:CG:128:GLN:HB3	1.76	0.68
31:CA:532:A:N1	31:CA:2020:A:H1'	2.08	0.68
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.76	0.68
31:CA:1936:A:H2	31:CA:1943:U:N3	1.90	0.68
31:CA:2428:G:H21	40:CM:60:ARG:HH21	1.40	0.68
45:DR:28:ARG:HD3	69:DR:310:HOH:O	1.94	0.68
12:AL:114:ARG:HB3	12:AL:119:VAL:HB	1.76	0.68
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.75	0.68
55:DA:414:C:H2'	55:DA:415:A:C8	2.29	0.68
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.58	0.68
39:DL:2:ILE:HB	39:DL:33:ALA:HB3	1.76	0.67
1:BA:841:C:H3'	1:BA:842:U:C5'	2.24	0.67
33:CE:126:VAL:CG2	33:CE:133:LEU:HB3	2.24	0.67
29:DC:107:PRO:HD2	29:DC:110:LEU:HD22	1.76	0.67
54:DI:85:VAL:HG11	54:DI:91:ALA:HB3	1.75	0.67
6:AF:16:GLU:HG2	4:BD:193:ALA:HB2	1.77	0.67
41:DN:19:GLY:HA2	69:DB:338:HOH:O	1.92	0.67
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.58	0.67
42:DO:53:THR:HA	42:DO:56:LYS:HD2	1.77	0.67
1:BA:715:A:H2'	1:BA:716:A:C8	2.30	0.67
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.09	0.67
1:AA:715:A:H2'	1:AA:716:A:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.60	0.67
31:CA:910:A:H62	41:CN:12:MET:HA	1.57	0.67
49:CV:7:ARG:O	49:CV:25:VAL:HB	1.94	0.67
1:BA:1305:G:H21	1:BA:1332:A:H2	1.44	0.66
43:CP:18:LEU:HD23	43:CP:25:ARG:HD3	1.76	0.66
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.60	0.66
31:CA:2394:C:H5''	40:CM:63:LYS:HE2	1.76	0.66
31:CA:1779:U:H5	31:CA:1784:A:N7	1.93	0.66
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.31	0.66
39:CL:2:ILE:HB	39:CL:33:ALA:HB3	1.76	0.66
55:DA:2751:G:H2'	69:DA:4887:HOH:O	1.94	0.66
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.26	0.66
49:CV:82:ARG:HB2	49:CV:97:LYS:HG3	1.78	0.66
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.60	0.66
1:AA:1197:A:H3'	1:AA:1197:A:OP2	1.96	0.66
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.78	0.66
55:DA:74:A:N3	55:DA:74:A:H5''	2.11	0.66
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.77	0.66
43:DP:64:TYR:HB3	43:DP:67:ASN:HD22	1.61	0.65
43:CP:64:TYR:HB3	43:CP:67:ASN:HD22	1.62	0.65
55:DA:1002:G:H5'	61:DA:3201:PEG:H32	1.78	0.65
40:DM:63:LYS:HE2	55:DA:2394:C:H5''	1.78	0.65
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.77	0.65
45:DR:94:ILE:HG21	46:DS:4:VAL:HG11	1.79	0.65
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.77	0.65
31:CA:2326:C:O2'	31:CA:2327:A:H8	1.80	0.65
55:DA:1026:G:H2'	55:DA:1027:A:H8	1.62	0.65
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.79	0.65
31:CA:2366:A:H4'	51:CX:62:LYS:HE3	1.79	0.65
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.77	0.65
55:DA:2255:G:H21	68:DA:3220:TRS:H12	1.62	0.65
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	1.79	0.64
2:AB:31:ILE:HG21	2:AB:39:HIS:CD2	2.30	0.64
42:CO:53:THR:HA	42:CO:56:LYS:HD2	1.78	0.64
32:DD:122:VAL:HG23	69:DD:411:HOH:O	1.97	0.64
46:DS:73:LYS:HZ2	58:DS:203:MPD:H53	1.60	0.64
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.80	0.64
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.96	0.64
12:BL:114:ARG:HB3	12:BL:119:VAL:HB	1.78	0.64
55:DA:2052:A:H3'	69:DA:3584:HOH:O	1.96	0.64
45:CR:94:ILE:HG21	46:CS:4:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.79	0.64
1:AA:1144:G:H21	1:AA:1146:A:H62	1.46	0.64
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.80	0.64
33:DE:3:LEU:HD12	33:DE:14:VAL:HG11	1.80	0.63
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.79	0.63
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.81	0.63
55:DA:1778:U:H2'	55:DA:1784:A:N6	2.13	0.63
44:DQ:31:TRP:CE2	44:DQ:40:LEU:HD21	2.34	0.63
1:AA:1305:G:H21	1:AA:1332:A:H2	1.44	0.63
38:CK:117:ALA:HA	38:CK:120:ARG:HD2	1.81	0.63
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.80	0.63
1:AA:677:U:H3	1:AA:713:G:H22	1.45	0.63
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.34	0.63
40:DM:36:LYS:HE2	55:DA:807:U:OP1	1.98	0.63
1:BA:1063:C:H42	1:BA:1193:G:H1	1.47	0.63
1:BA:202:G:HO2'	1:BA:468:A:H8	1.45	0.63
1:BA:677:U:H3	1:BA:713:G:H22	1.43	0.63
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.80	0.63
55:DA:1975:G:H21	63:DA:3225:PGE:C2	2.07	0.63
29:DC:38:SER:HA	69:DA:5917:HOH:O	1.98	0.63
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.81	0.62
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.62	0.62
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.64	0.62
27:D0:39:GLU:HB2	27:D0:41:THR:HG23	1.80	0.62
55:DA:1965:C:OP1	55:DA:1966:A:H2'	1.99	0.62
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.34	0.62
27:C0:39:GLU:HB2	27:C0:41:THR:HG23	1.81	0.62
24:C3:19:ARG:HD3	31:CA:125:A:OP2	1.99	0.62
29:CC:17:VAL:HB	29:CC:204:VAL:HG12	1.78	0.62
29:CC:45:ASN:ND2	31:CA:1812:U:H1'	2.14	0.62
53:DZ:2:LYS:HB3	53:DZ:6:LEU:HD12	1.80	0.62
1:BA:1144:G:H21	1:BA:1146:A:H62	1.47	0.62
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.34	0.62
31:CA:1827:U:H2'	31:CA:1828:G:O4'	2.00	0.62
18:AR:62:ALA:HB3	18:AR:68:LEU:HD12	1.82	0.62
31:CA:528:A:H3'	31:CA:528:A:C8	2.35	0.62
33:CE:3:LEU:HD12	33:CE:14:VAL:HG11	1.82	0.62
55:DA:588:U:H2'	55:DA:589:U:C6	2.34	0.62
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.82	0.62
22:D1:34:SER:OG	22:D1:36:GLU:HB2	2.00	0.62
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:197:A:H2	31:CA:2434:A:H62	1.48	0.62
31:CA:571:U:H4'	31:CA:573:U:H5	1.64	0.62
1:BA:663:A:H5'	1:BA:836:G:OP1	1.98	0.62
55:DA:2162:G:H5''	55:DA:2171:A:H2'	1.82	0.62
1:AA:663:A:H5'	1:AA:836:G:OP1	1.99	0.61
31:CA:1707:G:H1	31:CA:1751:U:H3	1.47	0.61
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.64	0.61
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.35	0.61
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.15	0.61
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.81	0.61
18:BR:62:ALA:HB3	18:BR:68:LEU:HD12	1.82	0.61
31:CA:320:A:H4'	31:CA:322:A:N7	2.15	0.61
38:DK:117:ALA:HA	38:DK:120:ARG:HD2	1.81	0.61
41:DN:62:LYS:HD3	41:DN:64:TRP:CZ2	2.36	0.61
31:CA:1760:C:H2'	31:CA:1761:C:O4'	2.00	0.61
1:BA:1063:C:N4	1:BA:1193:G:H1	1.97	0.61
45:DR:78:LYS:HA	69:DA:6376:HOH:O	2.01	0.61
1:AA:209:U:H4'	1:AA:210:C:OP2	1.99	0.61
31:CA:806:C:H2'	31:CA:807:U:C6	2.36	0.61
14:AN:66:GLN:HB2	69:AN:202:HOH:O	2.01	0.61
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.83	0.61
38:CK:110:PRO:O	38:CK:115:GLY:HA3	2.01	0.61
55:DA:1141:U:H4'	55:DA:1142:A:O4'	2.01	0.61
1:AA:1314:C:H41	19:AS:4:SER:HA	1.66	0.60
31:CA:1155:A:H5''	45:CR:55:ARG:HD3	1.81	0.60
42:DO:60:VAL:HB	69:DO:217:HOH:O	2.00	0.60
31:CA:588:U:H2'	31:CA:589:U:C6	2.36	0.60
54:DI:5:LEU:HA	54:DI:8:LYS:HB2	1.83	0.60
50:DW:63:ILE:HD12	50:DW:72:VAL:HG21	1.83	0.60
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.84	0.60
1:AA:707:U:H5''	11:AK:22:HIS:CD2	2.37	0.60
55:DA:1913:A:H4'	55:DA:1913:A:OP1	2.01	0.60
1:AA:1421:G:H3'	69:AA:1814:HOH:O	2.02	0.60
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.82	0.60
31:CA:2443:C:H2'	31:CA:2444:G:O4'	2.01	0.60
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.67	0.60
31:CA:1006:C:O4'	38:CK:30:THR:HG23	2.01	0.60
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.03	0.60
29:DC:45:ASN:ND2	55:DA:1812:U:H1'	2.15	0.60
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.84	0.60
31:CA:1709:U:H2'	31:CA:1710:G:H8	1.66	0.60
31:CA:2326:C:O2'	31:CA:2327:A:C8	2.55	0.60
55:DA:2402:U:O2	55:DA:2402:U:H2'	2.01	0.60
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	1.83	0.60
26:D5:1:MET:HG2	69:D5:202:HOH:O	2.01	0.60
42:CO:73:ASN:HA	42:CO:76:VAL:HG22	1.84	0.60
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.32	0.60
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.83	0.60
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.84	0.59
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.84	0.59
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.66	0.59
43:CP:49:VAL:HG21	43:CP:82:ALA:HA	1.84	0.59
32:DD:150[B]:MEQ:HG3	55:DA:2032:G:N3	2.17	0.59
51:DX:56:ASP:OD1	55:DA:2364:C:H4'	2.02	0.59
31:CA:1974:C:H3'	69:CA:3320:HOH:O	2.03	0.59
45:DR:50:ARG:O	45:DR:54:LYS:HD2	2.02	0.59
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	1.84	0.59
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.83	0.59
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.84	0.59
1:BA:33:A:H2'	1:BA:34:C:C6	2.37	0.59
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.17	0.59
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.67	0.59
55:DA:1424:G:H21	63:DA:3214:PGE:H32	1.67	0.59
32:DD:30:GLU:HB3	69:DD:457:HOH:O	2.03	0.59
1:BA:967:5MC:HN42	1:BA:1197:A:H61	1.48	0.59
55:DA:2783:U:H2'	55:DA:2784:U:H6	1.67	0.59
2:BB:31:ILE:HG21	2:BB:39:HIS:CD2	2.31	0.59
31:CA:135:U:H3	31:CA:144:A:H61	1.51	0.59
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.84	0.59
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.67	0.59
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.83	0.59
50:CW:63:ILE:HD12	50:CW:72:VAL:HG21	1.85	0.59
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.03	0.59
54:DI:67:THR:CG2	54:DI:68:PRO:HA	2.29	0.59
6:AF:92:THR:HG22	6:AF:93:LYS:HE2	1.85	0.58
31:CA:320:A:H2'	33:CE:131:THR:HG21	1.83	0.58
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.67	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
55:DA:45:G:H5''	55:DA:46:G:H5'	1.85	0.58
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1770:G:H4'	31:CA:1938:A:OP1	2.03	0.58
55:DA:2771:C:H2'	55:DA:2772:C:H6	1.68	0.58
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.84	0.58
31:CA:29:U:H2'	31:CA:30:G:C8	2.37	0.58
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.85	0.58
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.19	0.58
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.49	0.58
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.85	0.58
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.68	0.58
31:CA:142:A:H1'	48:CU:1:MET:HB3	1.85	0.58
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.85	0.58
33:CE:28:VAL:O	33:CE:32:VAL:HG23	2.04	0.58
41:CN:62:LYS:HD3	41:CN:64:TRP:CZ2	2.37	0.58
53:DZ:41:HIS:CD2	55:DA:96:C:H4'	2.38	0.58
1:AA:54:C:H2'	1:AA:352:C:H41	1.69	0.58
1:AA:73:C:HO2'	1:AA:74:A:H8	1.51	0.58
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.85	0.58
1:BA:54:C:H2'	1:BA:352:C:H41	1.69	0.58
31:CA:45:G:H5''	31:CA:46:G:H5'	1.85	0.58
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.85	0.58
31:CA:2469:A:H4'	41:CN:55:ARG:HD3	1.86	0.58
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.86	0.58
40:DM:32:GLY:HA2	55:DA:1190:G:H5''	1.84	0.58
55:DA:2557:G:H2'	55:DA:2558:C:C6	2.39	0.58
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.39	0.58
42:DO:73:ASN:HA	42:DO:76:VAL:HG22	1.85	0.58
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.86	0.58
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.58
31:CA:1796:U:H2'	31:CA:1797:G:C8	2.39	0.58
31:CA:1812:U:H2'	31:CA:1813:G:C8	2.38	0.58
31:CA:1936:A:H61	31:CA:1963:U:H3	1.50	0.58
31:CA:846:U:H1'	31:CA:847:U:H5	1.68	0.58
31:CA:586:A:H5'	33:CE:84:THR:HG21	1.84	0.58
33:CE:108:ILE:HG22	40:CM:1:MET:SD	2.43	0.57
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.70	0.57
41:CN:30:SER:H	41:CN:106:ASP:HB3	1.68	0.57
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.86	0.57
47:DT:75:PHE:CZ	65:DA:3185:1PE:H142	2.39	0.57
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.03	0.57
1:BA:73:C:HO2'	1:BA:74:A:H8	1.50	0.57
31:CA:1311:G:H21	31:CA:1603:A:N6	1.95	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:582:A:H2'	31:CA:583:G:C8	2.39	0.57
55:DA:944:C:H2'	69:DA:6066:HOH:O	2.04	0.57
41:DN:30:SER:H	41:DN:106:ASP:HB3	1.69	0.57
43:DP:49:VAL:HG21	43:DP:82:ALA:HA	1.86	0.57
1:AA:79:G:H22	1:AA:90:C:H42	1.52	0.57
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	1.87	0.57
55:DA:2063:C:O2	55:DA:2450:A:N1	2.37	0.57
51:DX:40:GLN:HG3	51:DX:42:GLY:O	2.05	0.57
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.85	0.57
22:C1:7:LYS:HD2	31:CA:1262:A:C2	2.39	0.57
50:CW:20:LEU:HD21	50:CW:41:GLU:HB2	1.85	0.57
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	1.86	0.57
1:AA:1063:C:H2'	1:AA:1064:G:H8	1.64	0.57
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	1.86	0.57
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.34	0.57
50:DW:20:LEU:HD21	50:DW:41:GLU:HB2	1.85	0.57
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.86	0.57
31:CA:35:G:H2'	31:CA:36:G:O4'	2.04	0.57
31:CA:96:C:H4'	53:CZ:41:HIS:CD2	2.40	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.35	0.57
55:DA:2728:U:HO2'	55:DA:2729:G:H8	1.51	0.57
55:DA:2783:U:H2'	55:DA:2784:U:C6	2.39	0.57
38:DK:110:PRO:O	38:DK:115:GLY:HA3	2.04	0.57
43:DP:48:LEU:HD12	43:DP:87:ILE:HD11	1.87	0.57
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.87	0.57
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.86	0.57
31:CA:528:A:C2	31:CA:2043:C:H4'	2.40	0.57
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.39	0.57
31:CA:1203:U:H1'	40:CM:4:ASN:HB3	1.87	0.57
55:DA:1885:A:H2'	55:DA:1886:U:O4'	2.04	0.57
10:BJ:42:LEU:HB2	10:BJ:71:LEU:HB3	1.86	0.56
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.05	0.56
1:AA:33:A:H2'	1:AA:34:C:C6	2.39	0.56
22:D1:4:GLN:HA	55:DA:2615:U:C2	2.41	0.56
31:CA:2491:U:HO2'	31:CA:2492:U:H5	1.54	0.56
34:CF:24:SER:H	34:CF:27:GLN:NE2	2.03	0.56
29:DC:158:ALA:HB1	29:DC:197:ASN:O	2.04	0.56
45:DR:16:LYS:O	45:DR:20:GLN:HG3	2.05	0.56
14:AN:13:ARG:HB3	14:AN:60:GLN:HG2	1.87	0.56
45:DR:22:LYS:HE3	55:DA:20:C:OP1	2.06	0.56
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1327:A:H2'	55:DA:1328:A:O4'	2.06	0.56
55:DA:135:U:H3	55:DA:144:A:H61	1.51	0.56
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.86	0.56
28:CB:114:C:H1'	43:CP:47:VAL:HG11	1.86	0.56
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.56
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.86	0.56
3:BC:40:ARG:HG2	3:BC:55:ILE:HG21	1.87	0.56
31:CA:677:A:O2'	31:CA:2071:A:H5'	2.05	0.56
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.70	0.56
55:DA:320:A:H4'	55:DA:322:A:N7	2.20	0.56
1:BA:576:C:H3'	1:BA:577:G:H5''	1.86	0.56
1:BA:840:C:H2'	1:BA:841:C:O4'	2.06	0.56
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.87	0.56
43:DP:16:ARG:HD3	69:DP:310:HOH:O	2.06	0.56
5:AE:97:GLN:HE21	5:AE:124:LEU:HD13	1.71	0.56
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.41	0.56
33:CE:46:GLN:HB3	33:CE:83:VAL:HG21	1.87	0.56
35:CG:90:VAL:HG21	35:CG:163:ARG:HE	1.71	0.56
32:DD:48:ILE:HG23	32:DD:84:LEU:HD11	1.88	0.56
35:DG:90:VAL:HG21	35:DG:163:ARG:HE	1.70	0.56
1:BA:79:G:H22	1:BA:90:C:H42	1.54	0.56
14:BN:13:ARG:HB3	14:BN:60:GLN:HG2	1.88	0.56
31:CA:2114:A:N6	31:CA:2119:A:H62	2.03	0.56
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.05	0.56
31:CA:459:U:H2'	31:CA:460:A:H8	1.69	0.56
34:DF:138:PHE:HE2	34:DF:152:LEU:HD21	1.71	0.56
35:DG:26:ILE:HG22	35:DG:79:VAL:HG21	1.88	0.56
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.36	0.56
52:CY:37:ARG:HG2	52:CY:48:THR:HG22	1.87	0.56
24:D3:7:PRO:HG2	55:DA:1309:G:H4'	1.87	0.56
1:AA:1350:A:H2	7:AG:34:GLY:HA3	1.70	0.55
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.06	0.55
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.87	0.55
55:DA:683:U:H2'	55:DA:684:G:H5''	1.88	0.55
55:DA:760:G:H2'	55:DA:761:A:O4'	2.06	0.55
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.42	0.55
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.55
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.07	0.55
31:CA:744:U:H4'	31:CA:1658:C:H4'	1.88	0.55
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.89	0.55
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:27:ARG:HH12	36:CH:38:PRO:HG3	1.71	0.55
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.41	0.55
1:AA:674:G:H3'	69:AA:1714:HOH:O	2.05	0.55
31:CA:540:C:H2'	31:CA:541:A:C8	2.41	0.55
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.37	0.55
35:DG:67:THR:HG23	55:DA:2747:G:O2'	2.06	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.88	0.55
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.89	0.55
31:CA:528:A:H3'	31:CA:528:A:H8	1.71	0.55
55:DA:912:C:O2'	55:DA:913:U:H5'	2.07	0.55
29:DC:17:VAL:HB	29:DC:204:VAL:HB	1.88	0.55
50:DW:39:ALA:HB3	69:DW:105:HOH:O	2.06	0.55
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.86	0.55
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.89	0.55
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.06	0.55
55:DA:2771:C:H2'	55:DA:2772:C:C6	2.41	0.55
12:AL:3:THR:HB	12:AL:6:GLN:HB2	1.86	0.55
1:BA:1350:A:H2	7:BG:34:GLY:HA3	1.70	0.55
55:DA:1952:A:H4'	69:DA:5281:HOH:O	2.07	0.55
40:DM:60:ARG:NH2	55:DA:2428:G:N2	2.51	0.55
34:DF:60:ILE:HG12	34:DF:138:PHE:CD2	2.42	0.55
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.72	0.55
16:BP:2:VAL:CG2	16:BP:33:ILE:HD11	2.36	0.55
31:CA:321:U:H5''	33:CE:131:THR:HG23	1.89	0.55
31:CA:373:U:H2'	31:CA:374:A:H8	1.71	0.55
37:DJ:30:GLN:HE22	55:DA:1095:A:H61	1.54	0.55
55:DA:1532:A:H5''	55:DA:1532:A:H8	1.72	0.55
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.55
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	1.88	0.55
41:DN:75:GLU:HB2	41:DN:90:GLU:HG3	1.89	0.55
49:DV:52:LEU:HD13	49:DV:54:GLN:HE21	1.72	0.55
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.07	0.54
31:CA:1509:A:O2'	31:CA:1510:G:H8	1.90	0.54
31:CA:2557:G:H2'	31:CA:2558:C:C6	2.42	0.54
31:CA:373:U:H2'	31:CA:374:A:C8	2.41	0.54
1:AA:269:C:H2'	1:AA:270:A:C8	2.42	0.54
1:AA:76:G:H1	1:AA:93:U:H3	1.55	0.54
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.43	0.54
33:CE:149:ILE:HG23	33:CE:188:MET:HG2	1.90	0.54
34:CF:24:SER:H	34:CF:27:GLN:HE21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.54
55:DA:20:C:H2'	55:DA:21:A:H8	1.72	0.54
55:DA:784:G:H5'	55:DA:785:G:OP1	2.08	0.54
14:BN:21:PHE:HA	14:BN:25:ALA:HB3	1.87	0.54
1:BA:751:U:H4'	15:BO:24:SER:HA	1.89	0.54
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.07	0.54
55:DA:1509:A:O2'	55:DA:1510:G:H8	1.89	0.54
35:DG:24:ILE:HG21	35:DG:72:LEU:HD21	1.88	0.54
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.73	0.54
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.89	0.54
12:BL:79:VAL:HG12	12:BL:102:LEU:HD23	1.90	0.54
31:CA:2105:U:H2'	31:CA:2106:U:C6	2.42	0.54
31:CA:2267:A:H5''	31:CA:2268:A:H5'	1.90	0.54
52:CY:4:VAL:HG13	52:CY:11:ARG:HG3	1.89	0.54
55:DA:414:C:H2'	55:DA:415:A:H8	1.73	0.54
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.87	0.54
3:AC:121:THR:HA	3:AC:189:ALA:HB2	1.88	0.54
45:CR:16:LYS:O	45:CR:20:GLN:HG3	2.08	0.54
34:DF:65:PRO:HA	34:DF:89:VAL:HG23	1.89	0.54
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.89	0.54
55:DA:2887[B]:A:N3	55:DA:2887[B]:A:H2'	2.22	0.54
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.54
1:BA:209:U:O2	1:BA:209:U:H2'	2.08	0.54
1:BA:76:G:H1	1:BA:93:U:H3	1.54	0.54
42:CO:28:LEU:HD23	42:CO:48:VAL:HG11	1.90	0.54
34:DF:8:TYR:HB2	34:DF:173:PHE:HZ	1.73	0.54
42:DO:28:LEU:HD23	42:DO:48:VAL:HG11	1.88	0.54
1:BA:591:U:H2'	1:BA:592:G:C8	2.42	0.54
3:BC:121:THR:HA	3:BC:189:ALA:HB2	1.89	0.54
31:CA:1936:A:N6	31:CA:1963:U:N3	2.54	0.54
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.89	0.54
46:CS:49:ILE:HD12	46:CS:52:PRO:HA	1.90	0.54
6:AF:42:TRP:HB2	6:AF:59:TYR:HB2	1.90	0.54
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.89	0.54
31:CA:1738:G:HO2'	31:CA:1739:A:H8	1.55	0.54
31:CA:1796:U:H2'	31:CA:1797:G:H8	1.73	0.54
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.89	0.54
55:DA:2767:C:H2'	55:DA:2768:U:H6	1.73	0.54
46:DS:20:VAL:HG22	69:DS:339:HOH:O	2.07	0.54
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.89	0.53
13:BM:33:ILE:HG23	13:BM:59:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:241:A:N1	31:CA:255:A:H5''	2.23	0.53
27:D0:3[B]:LYS:O	27:D0:40:ASP:HB2	2.08	0.53
44:DQ:94:LYS:CE	55:DA:1754:A:C8	2.92	0.53
53:DZ:39:GLN:HB3	53:DZ:41:HIS:CE1	2.44	0.53
1:AA:1411:C:H2'	1:AA:1412:C:C6	2.44	0.53
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.08	0.53
31:CA:699:A:H2'	31:CA:700:G:O4'	2.09	0.53
31:CA:685:A:H5''	31:CA:774:G:O6	2.08	0.53
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.90	0.53
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.91	0.53
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.43	0.53
23:D2:9:ILE:HD13	23:D2:51:GLU:HG3	1.88	0.53
55:DA:1812:U:H2'	55:DA:1813:G:C8	2.44	0.53
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.43	0.53
34:CF:8:TYR:HB2	34:CF:173:PHE:HZ	1.73	0.53
44:CQ:4:ILE:H	44:CQ:4:ILE:HD12	1.73	0.53
55:DA:985:C:H2'	55:DA:986:C:H6	1.73	0.53
1:AA:260:G:H2'	1:AA:261:U:C6	2.44	0.53
1:AA:591:U:H2'	1:AA:592:G:C8	2.43	0.53
1:BA:490:C:H2'	1:BA:491:G:H8	1.74	0.53
31:CA:2598:A:H2'	31:CA:2599:G:O4'	2.09	0.53
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.91	0.53
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.44	0.53
31:CA:1532:A:H8	31:CA:1532:A:H5''	1.73	0.53
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.91	0.53
47:DT:93:ALA:HB2	55:DA:1614:A:C2	2.44	0.53
1:AA:1373:G:H5'	7:AG:36:LYS:HB2	1.91	0.53
31:CA:1564:C:H2'	31:CA:1565:C:C6	2.44	0.53
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.91	0.53
55:DA:693:A:H2'	55:DA:694:U:O4'	2.08	0.53
43:DP:79:ALA:HB2	43:DP:110:ALA:HA	1.91	0.53
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.73	0.53
1:BA:269:C:H2'	1:BA:270:A:C8	2.43	0.53
31:CA:1308:A:H2'	31:CA:1309:G:O4'	2.09	0.53
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.44	0.53
55:DA:2105:U:O4	55:DA:2184:A:H2	1.92	0.53
1:BA:260:G:H2'	1:BA:261:U:C6	2.44	0.53
31:CA:2747:G:O2'	35:CG:67:THR:HG23	2.09	0.53
22:D1:40:ARG:NH2	55:DA:2884[B]:U:H2'	2.24	0.53
22:D1:44:THR:HG23	22:D1:48:TYR:O	2.09	0.53
55:DA:2128:G:H1	55:DA:2160:C:H42	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.43	0.53
55:DA:623:C:H2'	55:DA:624:C:C6	2.44	0.53
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.91	0.53
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.91	0.53
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.90	0.53
1:AA:751:U:H4'	15:AO:24:SER:HA	1.90	0.53
31:CA:2189:U:H2'	31:CA:2190:G:C8	2.43	0.53
31:CA:2261:C:C2	31:CA:2280:G:N2	2.77	0.53
31:CA:457:A:N1	31:CA:470:A:H5''	2.24	0.53
31:CA:780:G:H8	31:CA:780:G:O5'	1.90	0.53
55:DA:1166:G:N2	55:DA:1184:U:H1'	2.24	0.53
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.74	0.52
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.92	0.52
55:DA:1722:A:N6	55:DA:1738:G:H1'	2.24	0.52
55:DA:1753:G:N2	55:DA:1755:A:H3'	2.25	0.52
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.09	0.52
35:CG:24:ILE:HG21	35:CG:72:LEU:HD21	1.90	0.52
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.90	0.52
40:DM:60:ARG:HD3	55:DA:2428:G:H21	1.74	0.52
55:DA:795:C:H1'	69:DA:4280:HOH:O	2.08	0.52
29:DC:43:ARG:HG3	29:DC:49:ILE:HA	1.91	0.52
50:DW:72:VAL:HG12	50:DW:93:ARG:HA	1.91	0.52
31:CA:2064:C:H1'	31:CA:2450:A:C6	2.45	0.52
41:CN:75:GLU:HB2	41:CN:90:GLU:HG3	1.91	0.52
55:DA:14:A:H5''	55:DA:15:G:OP2	2.09	0.52
55:DA:612:G:H4'	55:DA:613:A:C2	2.43	0.52
32:DD:134:HIS:HE1	69:DA:5373:HOH:O	1.92	0.52
44:DQ:4:ILE:H	44:DQ:4:ILE:HD12	1.74	0.52
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.44	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.45	0.52
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	1.90	0.52
1:AA:1381:U:H1'	7:AG:78:ARG:HE	1.75	0.52
6:BF:42:TRP:HB2	6:BF:59:TYR:HB2	1.92	0.52
31:CA:581:C:H2'	31:CA:582:A:C8	2.44	0.52
30:CD:129:THR:HG22	30:CD:141:ARG:HA	1.91	0.52
53:CZ:39:GLN:HB3	53:CZ:41:HIS:CE1	2.44	0.52
55:DA:2183:A:H2'	55:DA:2184:A:C8	2.44	0.52
55:DA:2408:U:H2'	55:DA:2409:G:C8	2.45	0.52
1:BA:1001:C:H2'	1:BA:1002:G:C8	2.45	0.52
19:BS:52:HIS:HD2	19:BS:54:GLY:H	1.58	0.52
31:CA:861:A:H2'	31:CA:862:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:587:C:O2'	40:CM:19:LEU:HD13	2.09	0.52
43:CP:79:ALA:HB2	43:CP:110:ALA:HA	1.90	0.52
55:DA:2037:A:H2'	55:DA:2038:G:C8	2.44	0.52
55:DA:2703:C:H2'	55:DA:2704:C:H6	1.74	0.52
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.91	0.52
31:CA:568:U:C1'	31:CA:2030:6MZ:H9C1	2.31	0.52
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	1.92	0.52
44:DQ:101:ARG:HD2	69:DQ:322:HOH:O	2.10	0.52
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.92	0.52
1:BA:1373:G:H5'	7:BG:36:LYS:HB2	1.92	0.52
31:CA:2888:C:H2'	31:CA:2889:C:C6	2.45	0.52
40:DM:57:LEU:HA	40:DM:60:ARG:HE	1.75	0.52
1:AA:718:A:C8	11:AK:118:HIS:HB3	2.45	0.52
16:AP:2:VAL:CG2	16:AP:33:ILE:HD11	2.40	0.52
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.90	0.52
31:CA:1248:G:O2'	45:CR:3:ARG:HA	2.10	0.52
31:CA:568:U:H1'	31:CA:2030:6MZ:C9	2.29	0.52
30:CD:121:THR:HG21	30:CD:143:PRO:HB3	1.92	0.52
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.45	0.52
43:DP:11:ALA:HB2	43:DP:96:GLY:N	2.25	0.52
13:AM:33:ILE:HG23	13:AM:59:GLU:HB3	1.91	0.52
55:DA:2097:A:H8	55:DA:2097:A:H5''	1.76	0.52
55:DA:2402:U:H2'	55:DA:2403:C:H5'	1.91	0.52
33:DE:46:GLN:HB3	33:DE:83:VAL:HG21	1.92	0.52
38:DK:21:THR:HG23	38:DK:61:LYS:HB3	1.92	0.52
1:BA:403:C:H2'	1:BA:404:G:O4'	2.10	0.51
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.91	0.51
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.24	0.51
31:CA:2262:U:OP2	51:CX:16:SER:HB2	2.10	0.51
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.92	0.51
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.92	0.51
1:BA:212:G:H2'	1:BA:213:G:C8	2.44	0.51
1:BA:967:5MC:N4	1:BA:1197:A:H61	2.08	0.51
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.11	0.51
40:CM:57:LEU:HA	40:CM:60:ARG:HE	1.75	0.51
42:CO:103:ARG:HD3	42:CO:110:MET:SD	2.50	0.51
55:DA:20:C:H2'	55:DA:21:A:C8	2.44	0.51
1:AA:412:A:H3'	1:AA:413:G:H5'	1.92	0.51
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	1.92	0.51
1:BA:1458:G:H5''	20:BT:26:SER:HB3	1.93	0.51
55:DA:2563:U:H1'	55:DA:2566:A:N6	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:582:A:H2'	55:DA:583:G:C8	2.46	0.51
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	1.92	0.51
42:DO:82:GLU:O	42:DO:85:PRO:HD2	2.10	0.51
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.45	0.51
1:BA:12:U:H4'	1:BA:526:C:H4'	1.93	0.51
35:CG:26:ILE:HG22	35:CG:79:VAL:HG21	1.91	0.51
38:CK:21:THR:HG23	38:CK:61:LYS:HB3	1.93	0.51
55:DA:1416:G:HO2'	55:DA:1417:C:H6	1.59	0.51
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.45	0.51
42:CO:82:GLU:O	42:CO:85:PRO:HD2	2.10	0.51
25:D4:57:LEU:HD11	55:DA:834:G:H5'	1.93	0.51
39:DL:101:GLY:O	39:DL:120:PRO:HD2	2.11	0.51
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.46	0.51
1:BA:429:U:H5''	4:BD:9:LEU:HD12	1.92	0.51
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.45	0.51
6:AF:17:GLN:HG3	4:BD:189:SER:HB2	1.92	0.51
46:DS:65:ALA:HB3	46:DS:95:ASP:HB2	1.92	0.51
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.92	0.51
8:AH:51:VAL:HG13	8:AH:59:LEU:HD12	1.93	0.51
46:CS:65:ALA:HB3	46:CS:95:ASP:HB2	1.93	0.51
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.92	0.51
38:DK:42:ALA:O	45:DR:64:ARG:HD3	2.10	0.51
40:DM:57:LEU:HB2	40:DM:60:ARG:HH11	1.75	0.51
1:AA:77:A:H2'	1:AA:78:A:C8	2.46	0.51
5:AE:82:GLN:HG2	5:AE:149:SER:HA	1.93	0.51
1:AA:1317:C:OP1	14:AN:57:PRO:HD2	2.11	0.51
16:BP:2:VAL:HG21	16:BP:33:ILE:HD11	1.93	0.51
45:CR:9:ILE:HG13	45:CR:10:ALA:N	2.26	0.51
35:DG:42:GLU:HA	35:DG:55:ARG:HH21	1.75	0.51
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.93	0.51
45:DR:64:ARG:HD2	69:DR:323:HOH:O	2.09	0.51
46:DS:24:LYS:HE3	69:DS:312:HOH:O	2.10	0.51
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	1.92	0.51
31:CA:1353:A:H2'	31:CA:1354:A:C8	2.46	0.51
31:CA:1380:G:H2'	31:CA:1381:G:H8	1.75	0.51
31:CA:2408:U:H2'	31:CA:2409:G:C8	2.46	0.51
35:CG:42:GLU:HA	35:CG:55:ARG:HH21	1.75	0.51
55:DA:1720:U:H2'	55:DA:1721:G:O4'	2.11	0.51
55:DA:296:U:H2'	55:DA:297:G:C8	2.46	0.51
36:DH:3:VAL:HG12	36:DH:38:PRO:HA	1.93	0.51
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:27:VAL:HG22	54:DI:82:ILE:HG22	1.93	0.51
11:AK:23:ILE:HG21	11:AK:96:THR:HG21	1.93	0.51
1:BA:579:A:H2'	1:BA:580:C:C6	2.46	0.51
1:BA:643:C:H5'	8:BH:32:LEU:HD13	1.93	0.51
31:CA:1991:U:H6	31:CA:1991:U:H5''	1.76	0.51
30:CD:48:ILE:HG23	30:CD:84:LEU:HD11	1.91	0.51
33:CE:148:ILE:HB	33:CE:169:VAL:HG22	1.93	0.51
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.93	0.51
23:D2:19:HIS:HE1	23:D2:21:TYR:CE1	2.29	0.51
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.46	0.51
32:DD:35:THR:HG22	32:DD:73:VAL:HG21	1.93	0.51
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	1.93	0.51
4:AD:192:SER:HB3	4:AD:195:ILE:HD12	1.93	0.50
5:AE:107:ALA:CB	5:AE:125:ALA:HB3	2.40	0.50
8:AH:102:ALA:HB3	8:AH:113:ASP:HB3	1.93	0.50
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.76	0.50
22:C1:7:LYS:HD2	31:CA:1262:A:H2	1.76	0.50
22:C1:3:VAL:HG21	31:CA:2016:U:H1'	1.93	0.50
34:CF:65:PRO:HA	34:CF:89:VAL:HG23	1.91	0.50
41:DN:3:GLN:HG3	41:DN:92:TRP:CD1	2.46	0.50
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.93	0.50
1:BA:1197:A:H3'	1:BA:1198:G:C5'	2.42	0.50
1:BA:17:U:H2'	1:BA:18:C:C6	2.47	0.50
9:BI:84:THR:HG21	9:BI:103:PHE:HB2	1.93	0.50
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.76	0.50
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.92	0.50
31:CA:1170:C:H42	31:CA:1178:C:H41	1.58	0.50
35:CG:90:VAL:HG21	35:CG:163:ARG:NE	2.27	0.50
36:CH:3:VAL:HG12	36:CH:38:PRO:HA	1.91	0.50
55:DA:118:A:N3	55:DA:178:G:H1'	2.25	0.50
55:DA:2126:A:H61	55:DA:2163:A:H5'	1.75	0.50
32:DD:121:THR:HG21	32:DD:143:PRO:HB3	1.92	0.50
35:DG:90:VAL:HG21	35:DG:163:ARG:NE	2.26	0.50
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.47	0.50
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.77	0.50
10:BJ:53:ILE:HG13	14:BN:85:ARG:HD2	1.93	0.50
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.47	0.50
22:C1:19:HIS:HE1	31:CA:2624:G:H1'	1.75	0.50
31:CA:526:A:N6	31:CA:2626:C:H4'	2.26	0.50
31:CA:296:U:H2'	31:CA:297:G:C8	2.46	0.50
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.46	0.50
55:DA:284:U:H2'	55:DA:285:G:H8	1.75	0.50
19:AS:52:HIS:HD2	19:AS:54:GLY:H	1.59	0.50
11:BK:23:ILE:HG21	11:BK:96:THR:HG21	1.94	0.50
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.60	0.50
31:CA:806:C:H2'	31:CA:807:U:H6	1.76	0.50
50:CW:64:VAL:HG22	50:CW:69:GLU:HG2	1.94	0.50
55:DA:2133:G:H2'	55:DA:2157:G:H1	1.76	0.50
55:DA:31:C:O3'	55:DA:1238:G:H5''	2.12	0.50
28:DB:111:U:H2'	28:DB:112:G:C8	2.45	0.50
28:DB:1:U:H2'	28:DB:2:G:C8	2.46	0.50
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.94	0.50
32:DD:99:GLU:CG	32:DD:182:ALA:HB2	2.41	0.50
1:AA:1061:G:H1	1:AA:1195:C:H41	1.59	0.50
1:BA:1194:U:H5'	5:BE:27:GLY:CA	2.42	0.50
1:BA:407:U:H2'	1:BA:408:A:C8	2.47	0.50
19:BS:52:HIS:CD2	19:BS:54:GLY:H	2.30	0.50
31:CA:1720:U:H2'	31:CA:1721:G:O4'	2.11	0.50
31:CA:644:A:H2'	31:CA:645:C:O4'	2.12	0.50
52:CY:12:PRO:HB3	52:CY:30:LEU:HD23	1.93	0.50
55:DA:610:C:H5'	69:DA:3623:HOH:O	2.10	0.50
34:DF:103:LEU:HG	34:DF:108:VAL:HG23	1.94	0.50
43:DP:33:ARG:HD2	69:DB:319:HOH:O	2.10	0.50
52:DY:27:ARG:HD3	69:DY:101:HOH:O	2.10	0.50
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	1.92	0.50
39:CL:101:GLY:O	39:CL:120:PRO:HD2	2.11	0.50
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.93	0.50
55:DA:581:C:H2'	55:DA:582:A:C8	2.46	0.50
55:DA:825:A:OP1	59:DA:3223:PUT:H12	2.12	0.50
41:DN:100:LYS:HD3	69:DN:320:HOH:O	2.10	0.50
1:AA:212:G:H2'	1:AA:213:G:C8	2.46	0.50
1:AA:490:C:H2'	1:AA:491:G:H8	1.75	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.94	0.50
20:AT:57:ILE:HD12	20:AT:60:ARG:HE	1.76	0.50
5:BE:82:GLN:HG2	5:BE:149:SER:HA	1.93	0.50
12:BL:30:LYS:O	12:BL:82:ILE:HG22	2.11	0.50
20:BT:57:ILE:HD12	20:BT:60:ARG:HE	1.77	0.50
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.12	0.50
53:CZ:39:GLN:HB3	53:CZ:41:HIS:HE1	1.77	0.50
55:DA:1181:U:H2'	55:DA:1182:G:C8	2.46	0.50
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1381:U:H1'	7:BG:78:ARG:HE	1.76	0.50
8:BH:102:ALA:HB3	8:BH:113:ASP:HB3	1.93	0.50
23:C2:19:HIS:HE1	23:C2:21:TYR:CE1	2.29	0.50
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.93	0.50
50:CW:72:VAL:HG12	50:CW:93:ARG:HA	1.92	0.50
55:DA:1975:G:N2	63:DA:3225:PGE:H22	2.19	0.50
40:DM:53:GLY:HA3	55:DA:826:U:O2'	2.12	0.50
53:DZ:39:GLN:HB3	53:DZ:41:HIS:HE1	1.77	0.50
1:AA:1232:U:H5''	9:AI:126:GLN:HB3	1.94	0.50
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.93	0.50
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.94	0.50
1:AA:1458:G:H5''	20:AT:26:SER:HB3	1.93	0.50
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.46	0.50
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.77	0.50
31:CA:284:U:H2'	31:CA:285:G:H8	1.77	0.50
69:D0:216:HOH:O	55:DA:927:A:H1'	2.11	0.50
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.94	0.50
54:DI:111:ALA:O	54:DI:118:ILE:HB	2.11	0.50
1:AA:429:U:H5''	4:AD:9:LEU:HD12	1.94	0.49
1:BA:1317:C:OP1	14:BN:57:PRO:HD2	2.12	0.49
26:C5:8:LYS:HE3	31:CA:1031:G:H5''	1.93	0.49
31:CA:1783:A:N1	31:CA:2587:A:H2'	2.26	0.49
29:CC:162:VAL:HG22	29:CC:176:LEU:HA	1.94	0.49
55:DA:2133:G:H21	55:DA:2158:A:N6	2.09	0.49
55:DA:881:G:H1	55:DA:895:U:H3	1.60	0.49
46:DS:73:LYS:NZ	58:DS:203:MPD:H53	2.26	0.49
1:BA:21:G:H2'	1:BA:22:G:C8	2.47	0.49
6:BF:3:HIS:HA	6:BF:65:GLU:HA	1.94	0.49
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.49
7:BG:70:ARG:HG2	7:BG:96:ARG:HG2	1.94	0.49
29:CC:160:THR:O	29:CC:195:VAL:HG13	2.12	0.49
30:CD:99:GLU:CG	30:CD:182:ALA:HB2	2.42	0.49
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.94	0.49
31:CA:396:G:H1'	52:CY:29:PHE:CD2	2.47	0.49
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.12	0.49
46:DS:58:VAL:HG12	46:DS:102:SER:HB2	1.94	0.49
1:AA:403:C:H2'	1:AA:404:G:O4'	2.12	0.49
1:BA:745:G:H2'	1:BA:746:A:C8	2.47	0.49
2:BB:100:MET:HA	2:BB:107:VAL:HG21	1.93	0.49
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.95	0.49
31:CA:281:C:H2'	31:CA:282:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:111:U:H2'	28:CB:112:G:C8	2.47	0.49
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.76	0.49
45:CR:112:LYS:HD3	46:CS:48:LYS:HE2	1.94	0.49
55:DA:1425:G:H2'	55:DA:1426:G:C8	2.47	0.49
55:DA:839:U:H2'	55:DA:840:C:C6	2.48	0.49
49:DV:17:LYS:HE3	49:DV:40:ASN:HA	1.94	0.49
2:AB:100:MET:HA	2:AB:107:VAL:HG21	1.93	0.49
3:AC:14:ILE:HG21	3:AC:178:LEU:HB3	1.93	0.49
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.46	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:NE1	2.26	0.49
55:DA:137:U:H3	55:DA:142:A:H61	1.60	0.49
55:DA:2577:A:H5''	55:DA:2578:G:H5'	1.93	0.49
55:DA:648:G:H5''	69:DA:6963:HOH:O	2.12	0.49
29:DC:162:VAL:HG22	29:DC:176:LEU:HA	1.94	0.49
33:DE:148:ILE:HB	33:DE:169:VAL:HG22	1.93	0.49
50:DW:64:VAL:HG22	50:DW:69:GLU:HG2	1.94	0.49
1:AA:745:G:H2'	1:AA:746:A:C8	2.48	0.49
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.11	0.49
31:CA:83:A:H2	31:CA:103:A:N7	2.09	0.49
31:CA:695:G:H4'	31:CA:1380:G:H5'	1.94	0.49
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.94	0.49
36:CH:49:ALA:O	36:CH:53:GLU:HB2	2.13	0.49
38:CK:42:ALA:O	45:CR:64:ARG:HD3	2.12	0.49
43:CP:11:ALA:HB2	43:CP:96:GLY:N	2.27	0.49
55:DA:1436:G:N2	55:DA:1557:C:C2	2.81	0.49
29:DC:75:PRO:HG2	29:DC:97:LYS:HD3	1.95	0.49
1:AA:86:G:H21	1:AA:87:C:H41	1.61	0.49
7:AG:70:ARG:HG2	7:AG:96:ARG:HG2	1.94	0.49
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.43	0.49
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.49
55:DA:2258:C:H4'	55:DA:2259:U:OP2	2.12	0.49
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.95	0.49
45:DR:84:LYS:HG3	62:DA:3002:EDO:H22	1.94	0.49
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.60	0.49
1:AA:643:C:H5'	8:AH:32:LEU:HD13	1.95	0.49
1:BA:1096:C:H2'	1:BA:1097:C:C6	2.48	0.49
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	1.92	0.49
9:BI:31:ASN:HD21	9:BI:67:VAL:H	1.61	0.49
40:CM:57:LEU:HB2	40:CM:60:ARG:HH11	1.77	0.49
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.49
1:AA:17:U:H2'	1:AA:18:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.13	0.49
1:BA:77:A:H2'	1:BA:78:A:C8	2.47	0.49
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	1.95	0.49
31:CA:1299:G:H2'	31:CA:1639:C:N4	2.27	0.49
31:CA:1380:G:H1'	31:CA:1569:A:N6	2.28	0.49
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.95	0.49
25:D4:8:ARG:HD2	55:DA:245:G:O6	2.13	0.49
55:DA:388:G:N7	55:DA:390:U:H2'	2.27	0.49
55:DA:821:A:H1'	69:DA:3397:HOH:O	2.13	0.49
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.94	0.49
1:AA:719:C:O2'	18:AR:38:LYS:HB3	2.13	0.49
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.42	0.49
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	1.95	0.49
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.94	0.49
5:BE:97:GLN:HE21	5:BE:124:LEU:HD13	1.76	0.49
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.42	0.49
31:CA:247:G:N7	31:CA:249:C:C2	2.81	0.49
55:DA:740:C:H5"	55:DA:1784:A:OP1	2.12	0.49
34:DF:158:THR:HG23	34:DF:160:ALA:N	2.25	0.49
46:DS:1:MET:HA	46:DS:42:ALA:O	2.13	0.49
52:DY:18:ARG:NH2	52:DY:24:ALA:HB2	2.27	0.49
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.94	0.49
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.24	0.49
41:CN:3:GLN:HG3	41:CN:92:TRP:CD1	2.47	0.49
26:D5:16:ILE:CD1	26:D5:25:VAL:HG22	2.43	0.49
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.95	0.49
38:DK:47:HIS:HE1	69:DA:4185:HOH:O	1.96	0.49
1:AA:1096:C:H2'	1:AA:1097:C:C6	2.47	0.48
1:AA:1239:A:H62	1:AA:1299:A:H62	1.61	0.48
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.28	0.48
55:DA:1014:A:H1'	69:DA:5823:HOH:O	2.12	0.48
55:DA:118:A:C8	55:DA:119:A:C8	3.01	0.48
55:DA:2343:U:H2'	55:DA:2344:U:C6	2.48	0.48
55:DA:2427:C:H5"	55:DA:2428:G:OP1	2.12	0.48
55:DA:284:U:H2'	55:DA:285:G:C8	2.48	0.48
9:AI:84:THR:HG21	9:AI:103:PHE:HB2	1.94	0.48
1:BA:1216:A:H5"	14:BN:5:SER:HB3	1.96	0.48
4:BD:147:GLU:HA	4:BD:150:LYS:HD2	1.95	0.48
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.48
31:CA:881:G:H1	31:CA:895:U:H3	1.60	0.48
34:CF:103:LEU:HG	34:CF:108:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C1:42:HIS:CD2	42:CO:101:GLY:H	2.31	0.48
55:DA:195:A:H61	55:DA:198:C:H3'	1.77	0.48
29:DC:162:VAL:CG1	29:DC:174:LEU:HD22	2.43	0.48
52:DY:12:PRO:HB3	52:DY:30:LEU:HD23	1.94	0.48
6:AF:74:LEU:O	6:AF:77:THR:HG22	2.13	0.48
16:AP:2:VAL:HG21	16:AP:33:ILE:HD11	1.95	0.48
19:AS:52:HIS:CD2	19:AS:54:GLY:H	2.31	0.48
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.48
1:BA:429:U:H1'	1:BA:430:A:H5''	1.95	0.48
1:BA:202:G:O2'	1:BA:468:A:H8	1.96	0.48
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.48	0.48
44:DQ:6:LYS:O	44:DQ:10:GLN:HG2	2.14	0.48
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.61	0.48
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	1.95	0.48
1:BA:392:C:H2'	1:BA:393:A:C8	2.49	0.48
31:CA:1056:G:H4'	31:CA:1086:A:C8	2.48	0.48
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.47	0.48
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.13	0.48
31:CA:279:A:H61	31:CA:361:G:H1'	1.79	0.48
34:CF:33:LYS:HG3	34:CF:157:THR:HB	1.95	0.48
37:CJ:86:ILE:HG21	37:CJ:98:VAL:HB	1.96	0.48
31:CA:2393:U:H5''	40:CM:62:PRO:HB3	1.95	0.48
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	1.94	0.48
28:DB:81:G:H1'	69:DB:339:HOH:O	2.13	0.48
41:DN:123:LYS:HB3	55:DA:2484:G:H1'	1.95	0.48
19:BS:32:ARG:HE	19:BS:57:HIS:CD2	2.31	0.48
26:C5:16:ILE:CD1	26:C5:25:VAL:HG22	2.43	0.48
31:CA:1093:G:H1'	31:CA:1099:G:N2	2.27	0.48
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.28	0.48
1:AA:407:U:H2'	1:AA:408:A:C8	2.49	0.48
1:AA:601:G:H2'	1:AA:602:A:C8	2.49	0.48
1:AA:1216:A:H5''	14:AN:5:SER:HB3	1.95	0.48
1:BA:719:C:O2'	18:BR:38:LYS:HB3	2.13	0.48
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.96	0.48
7:BG:72:THR:HG22	7:BG:96:ARG:HH12	1.77	0.48
31:CA:785:G:O2'	31:CA:1779:U:H5''	2.13	0.48
31:CA:818:G:H5'	31:CA:839:U:OP1	2.14	0.48
33:CE:126:VAL:HG21	33:CE:133:LEU:HB3	1.95	0.48
55:DA:1622:G:H1'	69:DA:6193:HOH:O	2.14	0.48
55:DA:1935:G:H1'	55:DA:1964:G:N2	2.28	0.48
55:DA:2018:G:H2'	55:DA:2019:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD12	1.96	0.48
1:AA:1239:A:H62	1:AA:1299:A:N6	2.12	0.48
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.79	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.49	0.48
1:AA:429:U:H1'	1:AA:430:A:H5''	1.95	0.48
4:AD:73:ARG:HG3	4:AD:204:TYR:CE1	2.48	0.48
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	1.96	0.48
1:BA:1232:U:H5''	9:BI:126:GLN:HB3	1.96	0.48
31:CA:1310:G:H1'	31:CA:1611:C:H5''	1.96	0.48
46:CS:46:GLU:CD	46:CS:46:GLU:H	2.16	0.48
31:CA:2271:G:OP1	51:CX:18:ALA:HB1	2.13	0.48
55:DA:281:C:H2'	55:DA:282:A:C8	2.48	0.48
42:DO:85:PRO:HA	42:DO:88:ALA:HB2	1.95	0.48
9:AI:31:ASN:HD21	9:AI:67:VAL:H	1.61	0.48
1:BA:601:G:H2'	1:BA:602:A:C8	2.49	0.48
5:BE:18:VAL:HG11	5:BE:56:VAL:HG13	1.96	0.48
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.48	0.48
31:CA:763:G:H2'	31:CA:765:C:OP2	2.12	0.48
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:C6	2.49	0.48
54:DI:58:THR:HB	55:DA:1046:A:H4'	1.95	0.48
38:DK:30:THR:HG22	55:DA:1006:C:O4'	2.14	0.48
43:DP:1:MET:HB3	43:DP:6:ALA:HB2	1.95	0.48
1:AA:412:A:H3'	1:AA:413:G:C5'	2.43	0.48
1:AA:662:U:H2'	1:AA:663:A:C8	2.49	0.48
12:AL:53:CYS:HB3	12:AL:67:ILE:HD11	1.96	0.48
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.14	0.48
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.48	0.48
31:CA:2849:U:H4'	31:CA:2868:A:C2	2.48	0.48
31:CA:364:C:H2'	31:CA:365:U:C6	2.48	0.48
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.95	0.48
31:CA:2364:C:H4'	51:CX:56:ASP:OD1	2.14	0.48
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.49	0.48
55:DA:296:U:H2'	55:DA:297:G:H8	1.79	0.48
1:AA:1057:G:O3'	3:AC:197:GLY:HA3	2.14	0.48
13:BM:106:ALA:HB3	13:BM:110:LYS:HE3	1.96	0.48
31:CA:137:U:H3	31:CA:142:A:H61	1.62	0.48
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.95	0.48
55:DA:1441:G:H2'	55:DA:1442:U:C6	2.49	0.48
55:DA:1428:C:C5	55:DA:1569:A:H5''	2.49	0.48
37:DJ:86:ILE:HG21	37:DJ:98:VAL:HB	1.95	0.48
31:CA:1776:G:N2	31:CA:1789:A:H1'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:831:G:O5'	31:CA:831:G:H8	1.96	0.47
35:CG:138:LYS:HA	35:CG:141:ILE:HG22	1.96	0.47
55:DA:142:A:H2'	55:DA:143:C:C6	2.49	0.47
55:DA:622:G:H5''	55:DA:622:G:H8	1.79	0.47
24:D3:2:LYS:HE2	55:DA:687:C:H5''	1.96	0.47
27:D0:12:SER:HB3	55:DA:988:A:P	2.54	0.47
38:DK:58:ASN:HA	38:DK:126:ALA:O	2.14	0.47
45:DR:104:VAL:HG11	46:DS:45:GLU:HA	1.96	0.47
1:BA:1239:A:H62	1:BA:1299:A:N6	2.13	0.47
1:BA:649:A:H2'	1:BA:650:G:O4'	2.14	0.47
1:BA:662:U:H2'	1:BA:663:A:C8	2.49	0.47
1:BA:714:G:H2'	1:BA:715:A:C8	2.49	0.47
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.49	0.47
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.49	0.47
31:CA:1999:C:H5''	31:CA:2723:C:O2'	2.15	0.47
31:CA:528:A:C8	31:CA:528:A:C3'	2.97	0.47
31:CA:942:G:H4'	31:CA:1190:G:H5'	1.96	0.47
49:CV:82:ARG:CB	49:CV:97:LYS:HG3	2.43	0.47
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.96	0.47
55:DA:21:A:H2'	55:DA:22:C:O4'	2.14	0.47
55:DA:364:C:H2'	55:DA:365:U:C6	2.49	0.47
1:AA:620:C:C2	4:AD:132:ILE:HG21	2.50	0.47
19:AS:51:VAL:HG21	19:AS:71:LEU:HB3	1.97	0.47
3:BC:14:ILE:HG21	3:BC:178:LEU:HB3	1.96	0.47
5:BE:13:GLU:HB3	5:BE:39:VAL:HG12	1.96	0.47
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.79	0.47
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.29	0.47
46:CS:78:ARG:HB2	46:CS:83:TYR:HD1	1.79	0.47
55:DA:1746:A:H2'	55:DA:1747:U:C6	2.50	0.47
55:DA:2543:G:H2'	55:DA:2544:G:C8	2.49	0.47
44:DQ:95:ALA:HB3	69:DA:4560:HOH:O	2.13	0.47
6:AF:6:ILE:HG13	6:AF:89:VAL:HG23	1.95	0.47
4:BD:192:SER:HB3	4:BD:195:ILE:HD12	1.96	0.47
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.29	0.47
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	1.97	0.47
31:CA:980:A:C4	31:CA:1136:G:O4'	2.68	0.47
38:CK:58:ASN:HA	38:CK:126:ALA:O	2.15	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.61	0.47
55:DA:1796:U:H2'	55:DA:1797:G:H8	1.78	0.47
29:DC:21:ASN:HB3	29:DC:24:LEU:HG	1.97	0.47
1:AA:714:G:H2'	1:AA:715:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.30	0.47
1:BA:1239:A:H62	1:BA:1299:A:H62	1.61	0.47
9:BI:12:ARG:HG3	9:BI:107:ASP:HB3	1.96	0.47
31:CA:1998:A:H2'	31:CA:1999:C:O4'	2.14	0.47
28:DB:18:G:H1	28:DB:65:U:H3	1.62	0.47
39:DL:113:MET:HE1	39:DL:116:ILE:HD11	1.94	0.47
48:DU:58:VAL:HG22	48:DU:85:VAL:HG22	1.96	0.47
1:AA:202:G:O2'	1:AA:468:A:H8	1.96	0.47
31:CA:1441:G:H2'	31:CA:1442:U:C6	2.50	0.47
31:CA:688:U:H2'	31:CA:689:A:H8	1.80	0.47
44:DQ:31:TRP:CD2	44:DQ:40:LEU:HD21	2.49	0.47
1:AA:392:C:H2'	1:AA:393:A:C8	2.49	0.47
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.50	0.47
1:BA:429:U:C5'	4:BD:9:LEU:HD12	2.45	0.47
31:CA:142:A:H2'	31:CA:143:C:C6	2.50	0.47
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.15	0.47
31:CA:2189:U:O2'	31:CA:2190:G:H5'	2.15	0.47
31:CA:2520:C:H2'	31:CA:2521:C:H6	1.79	0.47
31:CA:460:A:H2'	31:CA:461:C:O4'	2.15	0.47
31:CA:736:C:O5'	31:CA:736:C:H6	1.98	0.47
31:CA:787:C:H5''	31:CA:788:A:H5'	1.97	0.47
31:CA:987:C:H2'	31:CA:988:A:O4'	2.14	0.47
55:DA:1590:A:H2'	55:DA:1591:A:C8	2.50	0.47
40:DM:62:PRO:HB3	55:DA:2393:U:H5''	1.96	0.47
55:DA:2869:G:H2'	55:DA:2870:C:O4'	2.15	0.47
54:DI:93:ALA:O	54:DI:97:LYS:HG3	2.14	0.47
42:DO:56:LYS:HE3	42:DO:94:TYR:OH	2.14	0.47
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.14	0.47
31:CA:1775:U:H2'	31:CA:1776:G:O4'	2.14	0.47
30:CD:150:GLN:NE2	31:CA:2032:G:H1'	2.29	0.47
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.78	0.47
29:CC:147:LYS:HB2	29:CC:150:LYS:HD2	1.96	0.47
55:DA:1069:A:H5'	55:DA:1070:A:H8	1.80	0.47
55:DA:553:G:H2'	55:DA:554:U:O4'	2.14	0.47
38:DK:9:GLU:HG3	69:DA:5367:HOH:O	2.15	0.47
1:AA:1061:G:H1	1:AA:1195:C:N4	2.13	0.47
1:AA:649:A:H2'	1:AA:650:G:O4'	2.14	0.47
4:AD:147:GLU:HA	4:AD:150:LYS:HD2	1.96	0.47
5:AE:13:GLU:HB3	5:AE:39:VAL:HG12	1.96	0.47
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.80	0.47
1:BA:1069:C:O2'	1:BA:1192:C:H1'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.50	0.47
31:CA:1428:C:C5	31:CA:1569:A:H5''	2.49	0.47
31:CA:25:U:H2'	31:CA:26:G:O4'	2.15	0.47
31:CA:296:U:H2'	31:CA:297:G:H8	1.80	0.47
35:CG:24:ILE:HD12	35:CG:72:LEU:HD11	1.97	0.47
55:DA:2723:C:H2'	55:DA:2724:U:O4'	2.15	0.47
32:DD:150[A]:MEQ:OE1	55:DA:2032:G:H1'	2.15	0.47
44:DQ:6:LYS:HG3	61:DQ:201:PEG:H41	1.97	0.47
1:BA:1512:U:H2'	1:BA:1513:A:C8	2.50	0.47
7:BG:47:LEU:HD22	7:BG:58:GLU:HG2	1.96	0.47
31:CA:1343:G:H2'	31:CA:1344:U:C6	2.49	0.47
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.50	0.47
31:CA:279:A:N6	31:CA:361:G:H1'	2.29	0.47
55:DA:1180:U:H5''	55:DA:1180:U:H6	1.80	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
55:DA:1278:C:H2'	55:DA:1279:G:H8	1.79	0.47
55:DA:1641:A:H2'	55:DA:1642:G:O4'	2.15	0.47
43:DP:100:HIS:CD2	28:DB:48:U:H4'	2.50	0.47
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.30	0.47
1:AA:392:C:H2'	1:AA:393:A:H8	1.80	0.47
13:AM:85:CYS:HB3	19:AS:74:PHE:CE1	2.49	0.47
1:BA:784:A:H4'	31:CA:1837:C:OP1	2.14	0.47
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.50	0.47
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.97	0.47
55:DA:279:A:N6	55:DA:361:G:H1'	2.30	0.47
40:DM:81:ASP:HA	40:DM:84:LYS:HD2	1.97	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.15	0.46
5:BE:106:ILE:HG13	5:BE:123:VAL:O	2.15	0.46
31:CA:571:U:H1'	31:CA:573:U:C6	2.50	0.46
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.97	0.46
31:CA:2313:C:H5''	34:CF:88:LYS:HD3	1.98	0.46
42:CO:54:LEU:HD23	42:CO:66:ALA:HB2	1.97	0.46
42:CO:72:ASP:OD2	42:CO:75:ILE:HG12	2.15	0.46
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.78	0.46
55:DA:2026:U:H2'	55:DA:2027:G:O4'	2.15	0.46
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.96	0.46
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.62	0.46
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.97	0.46
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.97	0.46
31:CA:1641:A:H2'	31:CA:1642:G:O4'	2.16	0.46
31:CA:1813:G:H2'	31:CA:1814:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:284:U:H2'	31:CA:285:G:C8	2.50	0.46
31:CA:372:G:H5''	52:CY:61:LYS:HD3	1.97	0.46
55:DA:1682:G:H3'	69:DA:4329:HOH:O	2.15	0.46
55:DA:2377:A:H2'	55:DA:2378:A:C8	2.50	0.46
55:DA:697:G:H2'	55:DA:698:C:C6	2.50	0.46
29:DC:147:LYS:HB2	29:DC:150:LYS:HD2	1.97	0.46
42:DO:72:ASP:OD2	42:DO:75:ILE:HG12	2.15	0.46
43:DP:41:ALA:HB2	43:DP:48:LEU:HD23	1.97	0.46
49:DV:14:LEU:HD11	49:DV:71:ALA:HB2	1.97	0.46
1:BA:1057:G:O3'	3:BC:197:GLY:HA3	2.15	0.46
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.97	0.46
11:BK:111:THR:HG23	21:BU:3:VAL:HG22	1.96	0.46
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.50	0.46
31:CA:392:U:H2'	31:CA:393:C:H6	1.79	0.46
38:DK:35:ARG:HB3	38:DK:54:ILE:HD11	1.97	0.46
46:DS:37:GLU:HB3	46:DS:53:PHE:CE1	2.51	0.46
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.51	0.46
1:AA:857:C:H2'	1:AA:858:G:O4'	2.15	0.46
7:AG:47:LEU:HD22	7:AG:58:GLU:HG2	1.98	0.46
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.81	0.46
1:BA:1026:G:H1	1:BA:1035:A:H2	1.62	0.46
1:BA:59:A:H5''	1:BA:387:U:H5''	1.97	0.46
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.79	0.46
24:C3:24:THR:HG23	24:C3:27:GLY:HA3	1.97	0.46
31:CA:1754:A:H8	31:CA:1754:A:O5'	1.98	0.46
31:CA:569:U:H5''	31:CA:821:A:C2	2.50	0.46
55:DA:1424:G:H2'	55:DA:1425:G:O4'	2.15	0.46
55:DA:136:G:H1	55:DA:143:C:H42	1.62	0.46
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.16	0.46
55:DA:2402:U:C2'	55:DA:2403:C:H5'	2.45	0.46
55:DA:352:A:H8	55:DA:352:A:H5''	1.80	0.46
47:DT:17:VAL:HA	47:DT:43:ALA:HB1	1.96	0.46
1:AA:1141:C:O2'	1:AA:1142:G:H8	1.99	0.46
1:AA:34:C:H2'	1:AA:35:G:C8	2.50	0.46
16:AP:54:LEU:HA	16:AP:57:ILE:HD12	1.97	0.46
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	1.98	0.46
1:BA:1194:U:C5'	5:BE:27:GLY:HA2	2.45	0.46
6:BF:16:GLU:O	6:BF:19:PRO:HD2	2.15	0.46
16:BP:4:ILE:HD13	16:BP:57:ILE:HG23	1.97	0.46
19:BS:51:VAL:HG21	19:BS:71:LEU:HB3	1.98	0.46
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2233:U:H2'	31:CA:2234:G:C8	2.50	0.46
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.15	0.46
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.96	0.46
42:DO:35:LYS:HB2	42:DO:112:TYR:CE1	2.51	0.46
46:DS:22:LEU:HA	69:DS:311:HOH:O	2.15	0.46
6:AF:16:GLU:O	6:AF:19:PRO:HD2	2.16	0.46
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.46
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.98	0.46
20:AT:48:GLN:HE21	20:AT:52:ASN:ND2	2.13	0.46
31:CA:355:U:H2'	31:CA:356:G:C8	2.51	0.46
55:DA:570:G:H2'	55:DA:2030:6MZ:N7	2.31	0.46
41:DN:16:ARG:HB3	28:DB:90:C:OP1	2.16	0.46
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46
1:BA:490:C:H2'	1:BA:491:G:C8	2.50	0.46
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.43	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.97	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1974:C:H2'	31:CA:1975:G:H8	1.81	0.46
31:CA:2718:G:OP1	44:CQ:98:TYR:HD2	1.99	0.46
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.46
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.97	0.46
44:CQ:6:LYS:O	44:CQ:10:GLN:HG2	2.16	0.46
52:CY:18:ARG:NH2	52:CY:24:ALA:HB2	2.31	0.46
55:DA:2328:A:H2'	55:DA:2329:U:C6	2.51	0.46
55:DA:2626:C:H2'	55:DA:2627:G:O4'	2.16	0.46
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.50	0.46
55:DA:639:U:H2'	55:DA:640:C:C6	2.51	0.46
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.98	0.46
1:AA:373:A:H61	1:AA:391:G:H1'	1.81	0.46
4:AD:54:GLN:HB3	4:AD:203:LEU:HD13	1.97	0.46
13:AM:93:ARG:HH12	19:AS:81:ARG:HH21	1.63	0.46
1:BA:392:C:H2'	1:BA:393:A:H8	1.79	0.46
28:CB:18:G:H1	28:CB:65:U:H3	1.62	0.46
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.46
41:CN:34:LYS:HE3	41:CN:131:VAL:HG11	1.98	0.46
55:DA:225:C:H2'	55:DA:226:A:O4'	2.16	0.46
55:DA:2461:A:H1'	55:DA:2492:U:C2	2.51	0.46
55:DA:279:A:H61	55:DA:361:G:H1'	1.79	0.46
55:DA:2830:C:H5'	69:DA:4054:HOH:O	2.16	0.46
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.96	0.46
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:73:C:O2'	1:BA:74:A:H8	1.99	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.97	0.46
16:BP:54:LEU:HA	16:BP:57:ILE:HD12	1.98	0.46
31:CA:1783:A:C2	31:CA:2588:G:O4'	2.69	0.46
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.46
31:CA:2547:A:H2'	31:CA:2548:U:C6	2.51	0.46
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.31	0.46
42:CO:85:PRO:HA	42:CO:88:ALA:HB2	1.97	0.46
55:DA:2609:U:C5	62:DA:3194:EDO:H12	2.51	0.46
34:DF:33:LYS:HG3	34:DF:157:THR:HB	1.96	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
13:AM:106:ALA:HB3	13:AM:110:LYS:HE3	1.98	0.46
1:BA:34:C:H2'	1:BA:35:G:C8	2.51	0.46
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.98	0.46
31:CA:2544:G:H5'	31:CA:2645:G:N2	2.31	0.46
31:CA:352:A:H5"	31:CA:352:A:H8	1.81	0.46
55:DA:2065:C:H2'	55:DA:2066:C:O4'	2.16	0.46
55:DA:2097:A:C8	55:DA:2097:A:H5"	2.50	0.46
55:DA:2267:A:H5"	55:DA:2268:A:H5'	1.98	0.46
25:D4:45:ARG:HD3	55:DA:2418:A:OP1	2.16	0.46
55:DA:2558:C:H2'	55:DA:2559:C:O4'	2.16	0.46
55:DA:2643:G:H2'	55:DA:2644:G:O4'	2.16	0.46
32:DD:129:THR:HG22	32:DD:141:ARG:HA	1.98	0.46
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	1.98	0.46
1:AA:429:U:C5'	4:AD:9:LEU:HD12	2.47	0.45
1:AA:579:A:H2'	1:AA:580:C:C6	2.51	0.45
1:AA:73:C:O2'	1:AA:74:A:H8	1.98	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.96	0.45
11:AK:21:ALA:HB2	11:AK:82:LEU:HD13	1.98	0.45
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.45
1:BA:1103:C:H2'	1:BA:1104:G:O4'	2.16	0.45
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.97	0.45
31:CA:2461:A:H1'	31:CA:2492:U:C2	2.51	0.45
31:CA:2886:A:C2	31:CA:2887:A:H1'	2.51	0.45
38:CK:35:ARG:HB3	38:CK:54:ILE:HD11	1.98	0.45
55:DA:1532:A:C8	55:DA:1532:A:H5"	2.51	0.45
47:DT:93:ALA:HB2	55:DA:1614:A:N1	2.31	0.45
55:DA:2141:G:H2'	55:DA:2142:A:C8	2.52	0.45
66:DA:3202:ACY:H2	69:DA:5043:HOH:O	2.15	0.45
55:DA:355:U:H2'	55:DA:356:G:C8	2.51	0.45
55:DA:455:C:N3	55:DA:472:A:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:634:C:H6	55:DA:634:C:O5'	1.99	0.45
29:DC:8:PRO:O	55:DA:1695:G:H1'	2.16	0.45
33:DE:33:VAL:HG22	58:DA:3192:MPD:C1	2.39	0.45
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.81	0.45
69:AA:1745:HOH:O	12:AL:115:SER:HB3	2.16	0.45
16:AP:4:ILE:HD13	16:AP:57:ILE:HG23	1.98	0.45
20:AT:39:ILE:HG23	20:AT:86:LEU:HD11	1.98	0.45
1:BA:1305:G:HO2'	1:BA:1306:A:H8	1.61	0.45
1:BA:857:C:H2'	1:BA:858:G:O4'	2.16	0.45
31:CA:2377:A:H2'	31:CA:2378:A:C8	2.50	0.45
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.15	0.45
43:CP:41:ALA:HB2	43:CP:48:LEU:HD23	1.97	0.45
35:DG:24:ILE:HD12	35:DG:72:LEU:HD11	1.97	0.45
45:DR:76:TYR:CZ	45:DR:80:ILE:HG13	2.50	0.45
49:DV:52:LEU:C	49:DV:54:GLN:H	2.18	0.45
1:AA:1026:G:H1	1:AA:1035:A:H2	1.63	0.45
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.45
1:AA:623:C:H6	1:AA:623:C:O5'	2.00	0.45
6:AF:3:HIS:HA	6:AF:65:GLU:HA	1.98	0.45
1:BA:502:A:OP1	12:BL:115:SER:HB2	2.17	0.45
1:BA:920:U:H2'	1:BA:921:U:C6	2.51	0.45
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.98	0.45
46:CS:1:MET:HA	46:CS:42:ALA:O	2.16	0.45
49:CV:72:ILE:HG12	49:CV:83:VAL:HG23	1.99	0.45
55:DA:1426:G:O5'	55:DA:1426:G:H8	1.98	0.45
29:DC:50:THR:OG1	55:DA:1813:G:H1'	2.17	0.45
33:DE:58:LYS:HD2	55:DA:675:A:OP1	2.17	0.45
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.14	0.45
48:DU:33:LYS:HE2	63:DU:201:PGE:H32	1.98	0.45
1:AA:1069:C:H4'	1:AA:1192:C:O2	2.16	0.45
1:AA:920:U:H2'	1:AA:921:U:C6	2.51	0.45
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.99	0.45
1:BA:1141:C:O2'	1:BA:1142:G:H8	1.99	0.45
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.99	0.45
21:BU:11:PRO:HG2	21:BU:14:VAL:HB	1.98	0.45
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.97	0.45
31:CA:2182:U:H2'	31:CA:2183:A:C8	2.51	0.45
41:CN:40:ARG:HD3	41:CN:93:VAL:HG21	1.99	0.45
44:CQ:114:LEU:HD22	44:CQ:114:LEU:H	1.82	0.45
55:DA:1796:U:H2'	55:DA:1797:G:C8	2.52	0.45
55:DA:191:A:H2'	55:DA:192:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.98	0.45
34:DF:122:PHE:CE2	34:DF:167:ARG:HD3	2.52	0.45
34:DF:88:LYS:HD3	55:DA:2313:C:H5''	1.99	0.45
46:DS:72:VAL:HG13	69:DS:346:HOH:O	2.16	0.45
5:BE:99:ALA:HB3	5:BE:122:ASN:HB3	1.97	0.45
7:BG:26:PHE:HA	7:BG:29:ILE:HD12	1.97	0.45
41:CN:121:ALA:HA	41:CN:124:LEU:HD12	1.98	0.45
23:D2:8:LYS:HE2	55:DA:2420:C:H5''	1.97	0.45
55:DA:1237:A:H4'	55:DA:1238:G:OP1	2.16	0.45
55:DA:2557:G:H2'	55:DA:2558:C:H6	1.82	0.45
41:DN:77:PRO:HG2	41:DN:80:VAL:HG21	1.97	0.45
45:DR:78:LYS:HG2	69:DA:6376:HOH:O	2.17	0.45
1:AA:167:A:H2'	1:AA:168:G:O4'	2.17	0.45
9:AI:12:ARG:HG3	9:AI:107:ASP:HB3	1.98	0.45
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.16	0.45
1:BA:212:G:H2'	1:BA:213:G:H8	1.80	0.45
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.51	0.45
31:CA:197:A:H2	31:CA:2434:A:N6	2.14	0.45
31:CA:2101:A:H2'	31:CA:2102:G:H8	1.81	0.45
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.99	0.45
24:D3:24:THR:HG23	24:D3:27:GLY:HA3	1.98	0.45
55:DA:2014:A:H2'	55:DA:2015:A:C8	2.51	0.45
55:DA:2047:C:C5	66:DA:3202:ACY:H3	2.51	0.45
42:DO:45:ARG:HD2	69:DA:5551:HOH:O	2.16	0.45
1:AA:1190:G:H5'	3:AC:176:HIS:CE1	2.51	0.45
5:BE:105:ILE:H	5:BE:123:VAL:H	1.65	0.45
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.32	0.45
31:CA:1380:G:H1'	31:CA:1569:A:H61	1.81	0.45
31:CA:1590:A:H2'	31:CA:1591:A:C8	2.52	0.45
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.16	0.45
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.52	0.45
42:DO:54:LEU:HD23	42:DO:66:ALA:HB2	1.98	0.45
2:AB:207:ILE:HG13	2:AB:207:ILE:H	1.60	0.45
1:BA:123:U:H5''	1:BA:311:C:O2'	2.17	0.45
1:BA:729:A:H2'	1:BA:730:G:O4'	2.16	0.45
4:BD:88:GLU:HG2	4:BD:188:ARG:HD3	1.97	0.45
15:BO:64:ARG:HH12	15:BO:88:ARG:NH1	2.15	0.45
31:CA:136:G:H1	31:CA:143:C:H42	1.64	0.45
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.17	0.45
55:DA:1179:G:H2'	55:DA:1180:U:C6	2.51	0.45
55:DA:780:G:H2'	55:DA:782:A:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:825:A:H2'	55:DA:826:U:O4'	2.17	0.45
32:DD:159:LYS:HE2	69:DA:4766:HOH:O	2.16	0.45
41:DN:19:GLY:O	41:DN:97:GLN:HB3	2.17	0.45
42:DO:29:VAL:HG13	42:DO:83:LEU:HD11	1.98	0.45
51:DX:57:HIS:N	51:DX:57:HIS:CD2	2.85	0.45
1:AA:1484:C:O2'	55:DA:1961:C:H5'	2.16	0.45
1:AA:843:U:H1'	1:AA:845:A:C6	2.52	0.45
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.99	0.45
5:AE:18:VAL:HG11	5:AE:56:VAL:HG13	1.99	0.45
7:AG:26:PHE:HA	7:AG:29:ILE:HD12	1.99	0.45
1:BA:328:C:O2	1:BA:328:C:H2'	2.16	0.45
1:BA:1194:U:H5'	5:BE:27:GLY:HA2	1.97	0.45
9:BI:84:THR:HG21	9:BI:103:PHE:CB	2.47	0.45
31:CA:1069:A:H5'	31:CA:1070:A:H8	1.81	0.45
31:CA:1121:C:H2'	31:CA:1122:G:O4'	2.17	0.45
31:CA:790:U:H3	31:CA:795:C:H5'	1.82	0.45
22:D1:3:VAL:HG22	22:D1:4:GLN:H	1.81	0.45
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.51	0.45
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.99	0.45
54:DI:53:ARG:HD2	54:DI:55:VAL:HG23	1.97	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	1.98	0.45
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.81	0.45
1:BA:1197:A:H3'	1:BA:1198:G:H5''	1.99	0.45
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.82	0.45
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.45
1:BA:82:G:N1	1:BA:84:U:H5	2.10	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.98	0.45
31:CA:206:U:H2'	31:CA:207:A:C8	2.37	0.45
31:CA:2364:C:OP1	51:CX:55:ARG:HD3	2.17	0.45
55:DA:2182:U:H2'	55:DA:2183:A:C8	2.52	0.45
55:DA:2345:G:N3	55:DA:2381:A:H2'	2.32	0.45
55:DA:2903:U:H3'	69:DA:6757:HOH:O	2.17	0.45
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.52	0.44
1:AA:235:C:H2'	1:AA:236:A:C8	2.52	0.44
19:AS:53:ASN:HD22	19:AS:58:VAL:HG23	1.82	0.44
1:BA:32:A:H2'	1:BA:33:A:C8	2.52	0.44
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.44
1:BA:373:A:H61	1:BA:391:G:H1'	1.82	0.44
12:BL:53:CYS:HB3	12:BL:67:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BS:53:ASN:HD22	19:BS:58:VAL:HG23	1.81	0.44
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.52	0.44
31:CA:1532:A:C8	31:CA:1532:A:H5''	2.51	0.44
31:CA:2141:G:H2'	31:CA:2142:A:C8	2.53	0.44
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.99	0.44
22:C1:42:HIS:HD2	42:CO:101:GLY:H	1.63	0.44
27:D0:19:LYS:O	27:D0:22:ALA:HB3	2.17	0.44
55:DA:1401:G:H2'	55:DA:1402:U:C6	2.52	0.44
1:AA:1494:G:C8	55:DA:1913:A:C2	3.05	0.44
55:DA:2767:C:H2'	55:DA:2768:U:C6	2.52	0.44
55:DA:466:A:O4'	55:DA:683:U:H4'	2.16	0.44
36:DH:29:PHE:HB2	55:DA:2198:A:C2	2.52	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	1.99	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HB	1.99	0.44
1:BA:1063:C:H2'	1:BA:1064:G:C8	2.52	0.44
1:BA:591:U:H2'	1:BA:592:G:H8	1.83	0.44
2:BB:207:ILE:HG13	2:BB:207:ILE:H	1.61	0.44
5:BE:13:GLU:CB	5:BE:39:VAL:HG12	2.47	0.44
7:BG:138:ARG:HE	7:BG:138:ARG:HB3	1.62	0.44
31:CA:225:C:H2'	31:CA:226:A:O4'	2.17	0.44
31:CA:2261:C:H1'	31:CA:2388:A:N3	2.32	0.44
31:CA:593:U:H2'	31:CA:594:U:C6	2.53	0.44
31:CA:686:U:H2'	31:CA:788:A:N1	2.32	0.44
28:CB:29:A:H2'	28:CB:30:C:C6	2.53	0.44
55:DA:1171:G:H1'	55:DA:1179:G:N2	2.32	0.44
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.16	0.44
55:DA:1979:U:OP1	59:DA:3212:PUT:H32	2.17	0.44
55:DA:739:A:H2'	69:DA:7494:HOH:O	2.18	0.44
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.98	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.82	0.44
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.82	0.44
13:BM:93:ARG:HH12	19:BS:81:ARG:HH21	1.66	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.83	0.44
29:CC:271:ARG:HD3	31:CA:1819:A:H2	1.83	0.44
29:CC:107:PRO:HB3	29:CC:142:HIS:NE2	2.32	0.44
31:CA:2428:G:H21	40:CM:60:ARG:HD3	1.83	0.44
42:CO:8:ARG:HE	42:CO:43:GLU:HG2	1.83	0.44
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	2.00	0.44
25:D4:4:ILE:HD11	55:DA:592:A:N3	2.33	0.44
55:DA:2184:A:H8	55:DA:2184:A:O5'	2.01	0.44
55:DA:2578:G:OP2	55:DA:2578:G:H4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:278:A:H2'	55:DA:278:A:N3	2.33	0.44
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.99	0.44
17:AQ:77:ARG:NH2	17:AQ:79:VAL:HG22	2.33	0.44
11:AK:111:THR:HG23	21:AU:3:VAL:HG22	2.00	0.44
1:BA:623:C:H6	1:BA:623:C:O5'	2.01	0.44
11:BK:21:ALA:HB2	11:BK:82:LEU:HD13	1.99	0.44
31:CA:392:U:H2'	31:CA:393:C:C6	2.53	0.44
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.99	0.44
43:CP:16:ARG:HD2	43:CP:16:ARG:HA	1.81	0.44
55:DA:128:C:H2'	55:DA:129:C:C6	2.53	0.44
55:DA:757:G:H5''	69:DA:3996:HOH:O	2.18	0.44
55:DA:78:U:H2'	55:DA:79:C:C6	2.53	0.44
55:DA:96:C:H2'	55:DA:97:C:H6	1.83	0.44
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.99	0.44
46:DS:76:LYS:O	46:DS:84:ARG:HA	2.17	0.44
51:DX:39:ARG:HD3	69:DX:117:HOH:O	2.16	0.44
1:AA:123:U:H5''	1:AA:311:C:O2'	2.18	0.44
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.17	0.44
1:AA:212:G:H2'	1:AA:213:G:H8	1.81	0.44
1:AA:946:A:H2'	1:AA:947:G:C8	2.53	0.44
18:AR:52:GLN:HA	18:AR:55:LEU:HD12	1.98	0.44
1:BA:243:A:C2	1:BA:245:U:C2	3.05	0.44
31:CA:128:C:H2'	31:CA:129:C:C6	2.52	0.44
31:CA:1344:U:O2'	31:CA:1384:A:H2'	2.17	0.44
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.52	0.44
31:CA:2014:A:H2'	31:CA:2015:A:C8	2.52	0.44
37:CJ:55:ILE:HD12	37:CJ:74:PRO:HD3	1.99	0.44
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.99	0.44
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	2.00	0.44
45:DR:40:ILE:HG12	58:DS:203:MPD:H31	2.00	0.44
49:DV:25:VAL:HA	49:DV:36:VAL:HG22	1.98	0.44
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.33	0.44
31:CA:2641:G:H2'	31:CA:2642:G:H8	1.83	0.44
31:CA:96:C:H2'	31:CA:97:C:H6	1.82	0.44
29:CC:145:GLU:HB2	29:CC:188:CYS:HB3	1.99	0.44
50:CW:77:VAL:HG23	50:CW:89:ILE:HG12	2.00	0.44
55:DA:1278:C:H2'	55:DA:1279:G:C8	2.53	0.44
25:D4:19:LYS:HB2	55:DA:651:G:OP1	2.18	0.44
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.44
40:DM:19:LEU:HD12	55:DA:587:C:O2'	2.18	0.44
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.99	0.44
1:BA:522:C:H41	12:BL:50:ARG:NH2	2.15	0.44
1:BA:935:A:H2'	1:BA:936:C:C6	2.53	0.44
1:BA:532:A:N1	3:BC:193:TYR:HB3	2.33	0.44
31:CA:278:A:N3	31:CA:278:A:H2'	2.33	0.44
31:CA:576:U:H2'	31:CA:577:G:C8	2.52	0.44
31:CA:78:U:H2'	31:CA:79:C:C6	2.53	0.44
30:CD:104:VAL:HG23	30:CD:177:VAL:HG21	2.00	0.44
55:DA:1442:U:H2'	55:DA:1443:U:C6	2.52	0.44
55:DA:1965:C:OP1	55:DA:1966:A:C2'	2.66	0.44
55:DA:2607:G:H2'	55:DA:2608:G:O4'	2.17	0.44
55:DA:2681:C:C2	55:DA:2724:U:O4	2.71	0.44
47:DT:6:LYS:HA	47:DT:103:ILE:O	2.18	0.44
48:DU:15:HIS:HB3	48:DU:31:VAL:HG12	2.00	0.44
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.83	0.44
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.81	0.44
1:BA:407:U:H2'	1:BA:408:A:H8	1.83	0.44
18:BR:20:GLU:HA	18:BR:55:LEU:HD23	2.00	0.44
22:C1:2:ALA:N	31:CA:2577:A:H2	2.16	0.44
31:CA:1401:G:H2'	31:CA:1402:U:C6	2.53	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.53	0.44
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.83	0.44
48:CU:15:HIS:HB3	48:CU:31:VAL:HG12	1.99	0.44
48:CU:58:VAL:HG22	48:CU:85:VAL:HG22	1.98	0.44
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.82	0.44
54:DI:50:VAL:CG1	54:DI:92:ALA:HB2	2.48	0.44
41:DN:34:LYS:HE3	41:DN:131:VAL:HG11	1.98	0.44
51:DX:47:ALA:HB1	51:DX:51:VAL:O	2.17	0.44
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.99	0.44
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.18	0.44
6:AF:93:LYS:HE2	6:AF:93:LYS:H	1.82	0.44
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.99	0.44
12:AL:5:ASN:O	12:AL:9:ARG:HD2	2.18	0.44
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	2.00	0.44
17:BQ:9:GLN:O	17:BQ:25:ILE:HG23	2.18	0.44
23:C2:39:PHE:HB2	23:C2:46:HIS:CE1	2.53	0.44
1:BA:1517:G:H1'	31:CA:1919:A:O3'	2.17	0.44
31:CA:571:U:H1'	31:CA:573:U:H6	1.82	0.44
36:CH:21:VAL:HG21	36:CH:25:TYR:HD2	1.82	0.44
55:DA:2849:U:N3	55:DA:2867:G:O4'	2.50	0.44
55:DA:577:G:H1'	69:DA:3571:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.00	0.44
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.33	0.44
37:DJ:55:ILE:HD12	37:DJ:74:PRO:HD3	1.99	0.44
42:DO:8:ARG:HE	42:DO:43:GLU:HG2	1.83	0.44
1:BA:235:C:H2'	1:BA:236:A:C8	2.53	0.43
1:BA:946:A:H2'	1:BA:947:G:C8	2.53	0.43
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.82	0.43
7:BG:116:MET:HA	7:BG:119:ARG:HB2	2.00	0.43
10:BJ:46:LYS:HG2	10:BJ:68:ARG:HG2	1.99	0.43
31:CA:1024:G:H3'	31:CA:1025:G:H2'	1.99	0.43
31:CA:12:U:O2	31:CA:12:U:H2'	2.17	0.43
31:CA:1791:A:N6	31:CA:1828:G:O2'	2.51	0.43
30:CD:118:PHE:HZ	31:CA:2048:G:H21	1.66	0.43
47:CT:6:LYS:HG2	47:CT:104:THR:HG23	2.00	0.43
55:DA:320:A:H4'	55:DA:322:A:C8	2.53	0.43
55:DA:492:A:H2'	55:DA:493:G:O4'	2.18	0.43
55:DA:729:G:H2'	55:DA:1775:U:H1'	2.00	0.43
55:DA:739:A:H1'	55:DA:740:C:H5	1.83	0.43
34:DF:14:LYS:O	34:DF:18:THR:HG22	2.18	0.43
44:DQ:113:ARG:HG2	44:DQ:115:ASN:HD21	1.83	0.43
1:AA:490:C:H2'	1:AA:491:G:C8	2.52	0.43
5:AE:13:GLU:CB	5:AE:39:VAL:HG12	2.47	0.43
21:AU:11:PRO:HG2	21:AU:14:VAL:HB	1.99	0.43
1:BA:363:A:H2'	1:BA:364:A:O4'	2.18	0.43
1:BA:604:G:H2'	1:BA:605:U:O4'	2.18	0.43
12:BL:90:LEU:HD23	12:BL:93:VAL:HG21	2.00	0.43
31:CA:2006:C:H2'	31:CA:2007:U:C6	2.53	0.43
31:CA:2582:G:C2	31:CA:2583:G:C8	3.06	0.43
31:CA:727:A:H2'	31:CA:728:G:C8	2.53	0.43
27:C0:46:GLY:HA3	31:CA:851:C:O2'	2.19	0.43
55:DA:521:U:H2'	55:DA:522:A:C8	2.53	0.43
33:DE:145:ASP:HA	33:DE:166:LYS:HB3	2.01	0.43
50:DW:77:VAL:HG23	50:DW:89:ILE:HG12	2.01	0.43
1:AA:756:C:H2'	1:AA:757:U:O4'	2.19	0.43
9:AI:84:THR:HG21	9:AI:103:PHE:CB	2.47	0.43
1:BA:994:A:N1	1:BA:1047:G:H4'	2.33	0.43
20:BT:22:ALA:O	20:BT:26:SER:HB2	2.18	0.43
31:CA:1280:G:H1	31:CA:1290:C:H42	1.67	0.43
31:CA:197:A:C2	31:CA:2434:A:N6	2.84	0.43
31:CA:2771:C:H2'	31:CA:2772:C:H6	1.83	0.43
33:CE:108:ILE:HG21	33:CE:181:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:CO:29:VAL:HG13	42:CO:83:LEU:HD11	2.00	0.43
44:CQ:113:ARG:HG2	44:CQ:115:ASN:HD21	1.82	0.43
49:CV:72:ILE:H	49:CV:72:ILE:HG13	1.64	0.43
27:D0:24:LEU:HD11	27:D0:54:MET:CE	2.48	0.43
55:DA:1354:A:H2'	55:DA:1355:G:O4'	2.18	0.43
55:DA:1485:U:H2'	55:DA:1486:U:C6	2.53	0.43
55:DA:2123:G:H2'	55:DA:2124:G:H8	1.82	0.43
32:DD:119:ALA:HB3	32:DD:165:MET:HB2	1.99	0.43
36:DH:116:ARG:HH21	36:DH:133:GLN:HB2	1.83	0.43
1:AA:729:A:H2'	1:AA:730:G:O4'	2.17	0.43
1:AA:855:U:H2'	1:AA:856:C:C6	2.53	0.43
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	2.00	0.43
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.54	0.43
1:BA:167:A:H2'	1:BA:168:G:O4'	2.18	0.43
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.82	0.43
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.53	0.43
31:CA:1826:G:C6	31:CA:1827:U:C4	3.06	0.43
31:CA:2840:C:H5''	42:CO:53:THR:HG21	1.99	0.43
31:CA:609:A:H2'	31:CA:610:C:O4'	2.19	0.43
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.19	0.43
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	2.00	0.43
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	2.00	0.43
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.19	0.43
31:CA:492:A:H2	47:CT:7:HIS:NE2	2.16	0.43
55:DA:2101:A:H2'	55:DA:2102:G:H8	1.83	0.43
35:DG:155:GLU:HG2	35:DG:157:TYR:H	1.84	0.43
43:DP:30:ARG:HG3	43:DP:35:ILE:HD12	2.00	0.43
47:DT:6:LYS:HG2	47:DT:104:THR:HG23	2.00	0.43
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.53	0.43
1:AA:682:G:H2'	1:AA:683:G:H8	1.83	0.43
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.43
3:AC:180:ALA:HA	3:AC:206:GLU:HA	2.01	0.43
8:AH:64:LYS:HB3	8:AH:71:VAL:HG21	2.01	0.43
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	2.00	0.43
1:BA:1417:G:C6	1:BA:1482:G:C6	3.07	0.43
13:BM:23:TYR:HB3	13:BM:66:GLU:HA	2.00	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1447:C:H2'	31:CA:1448:G:H8	1.84	0.43
31:CA:521:U:H2'	31:CA:522:A:C8	2.53	0.43
31:CA:56:A:H61	31:CA:114:U:H3	1.66	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.01	0.43
47:CT:17:VAL:HA	47:CT:43:ALA:HB1	2.00	0.43
47:CT:62:ASP:HB3	47:CT:63:GLY:H	1.73	0.43
47:CT:95:ARG:CZ	47:CT:97:LEU:HD21	2.49	0.43
55:DA:861:A:C2	55:DA:917:A:C4	3.06	0.43
34:DF:40:VAL:HG23	34:DF:86:GLY:HA2	2.00	0.43
1:AA:1500:A:H5''	1:AA:1508:A:H5''	2.01	0.43
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	2.00	0.43
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	2.01	0.43
8:AH:76:GLN:O	8:AH:127:CYS:HB2	2.19	0.43
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.99	0.43
12:AL:80:ILE:HG22	12:AL:104:CYS:HB2	2.00	0.43
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.19	0.43
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.99	0.43
6:BF:3:HIS:CD2	6:BF:92:THR:HG23	2.53	0.43
24:C3:10:LEU:O	24:C3:14:ARG:HB2	2.18	0.43
31:CA:2027:G:C6	31:CA:2028:U:C4	3.07	0.43
31:CA:2781:A:H5''	31:CA:2782:G:H5'	2.01	0.43
31:CA:685:A:H1'	31:CA:688:U:O4	2.18	0.43
30:CD:172:VAL:HG12	30:CD:175:LEU:HD21	2.01	0.43
47:CT:6:LYS:HA	47:CT:103:ILE:O	2.18	0.43
22:D1:40:ARG:HH22	55:DA:2884[B]:U:H2'	1.84	0.43
52:DY:10:LYS:HD3	55:DA:397:U:OP2	2.19	0.43
55:DA:738:G:C6	55:DA:739:A:C6	3.07	0.43
32:DD:105:LYS:HD3	32:DD:106:LYS:HG3	1.99	0.43
1:AA:1373:G:C5'	7:AG:36:LYS:HB2	2.48	0.43
1:AA:994:A:N1	1:AA:1047:G:H4'	2.34	0.43
20:AT:31:PHE:HA	20:AT:34:LYS:HD2	2.00	0.43
1:BA:1486:G:H2'	1:BA:1487:G:O4'	2.17	0.43
1:BA:601:G:H2'	1:BA:602:A:H8	1.84	0.43
4:BD:105:MET:HE2	4:BD:171:LEU:HD22	2.01	0.43
9:BI:6:TYR:HB2	9:BI:21:ILE:HB	1.99	0.43
15:BO:64:ARG:HH22	15:BO:88:ARG:NH2	2.17	0.43
25:C4:2:PRO:N	31:CA:591:U:H1'	2.34	0.43
31:CA:1484:U:H2'	31:CA:1485:U:C6	2.54	0.43
31:CA:1485:U:H2'	31:CA:1486:U:C6	2.53	0.43
31:CA:184:C:H2'	31:CA:185:G:C8	2.54	0.43
31:CA:2179:C:H2'	31:CA:2180:U:C6	2.53	0.43
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.18	0.43
31:CA:2636:C:H2'	31:CA:2637:U:H6	1.82	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:21:ASN:HB3	29:CC:24:LEU:HG	2.00	0.43
55:DA:1759:A:H4'	55:DA:2715:C:O4'	2.18	0.43
55:DA:307:G:N2	55:DA:309:A:H3'	2.33	0.43
55:DA:831:G:C6	55:DA:832:U:C4	3.07	0.43
46:DS:53:PHE:HB3	69:DS:301:HOH:O	2.18	0.43
1:AA:1387:G:H2'	1:AA:1388:C:C6	2.53	0.43
1:AA:363:A:H2'	1:AA:364:A:O4'	2.18	0.43
1:AA:409:U:H2'	1:AA:410:G:O4'	2.19	0.43
1:AA:502:A:OP1	12:AL:115:SER:HB2	2.19	0.43
1:AA:601:G:H2'	1:AA:602:A:H8	1.84	0.43
1:AA:865:A:H8	1:AA:865:A:O5'	2.02	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.43
1:BA:855:U:H2'	1:BA:856:C:C6	2.54	0.43
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.00	0.43
31:CA:1170:C:H42	31:CA:1178:C:N4	2.16	0.43
31:CA:1231:U:H2'	31:CA:1232:G:H8	1.83	0.43
31:CA:1442:U:H2'	31:CA:1443:U:C6	2.53	0.43
31:CA:1939:5MU:H3'	69:CA:3666:HOH:O	2.17	0.43
31:CA:2024:G:C4	31:CA:2040:G:N2	2.87	0.43
38:CK:89:PHE:CE2	38:CK:100:VAL:HG11	2.54	0.43
43:CP:30:ARG:HG3	43:CP:35:ILE:HD12	2.00	0.43
55:DA:357:C:H2'	55:DA:358:U:C6	2.54	0.43
33:DE:72:SER:HB2	69:DE:449:HOH:O	2.19	0.43
36:DH:57:LYS:HA	36:DH:60:GLU:HG2	2.00	0.43
40:DM:109:LYS:HA	40:DM:126:ARG:O	2.18	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.42	0.43
46:DS:45:GLU:HG3	46:DS:46:GLU:OE2	2.18	0.43
1:AA:59:A:H5''	1:AA:387:U:H5''	2.00	0.43
1:AA:591:U:H2'	1:AA:592:G:H8	1.84	0.43
1:AA:81:A:H2	1:AA:88:U:H3	1.66	0.43
1:BA:409:U:H2'	1:BA:410:G:O4'	2.19	0.43
9:BI:51:PRO:HB3	9:BI:84:THR:HG23	2.00	0.43
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.53	0.43
30:CD:157:LYS:CG	31:CA:2619:C:H5''	2.48	0.43
31:CA:825:A:H2'	31:CA:826:U:O4'	2.19	0.43
33:CE:145:ASP:HA	33:CE:166:LYS:HB3	2.01	0.43
40:CM:21:ARG:HA	40:CM:21:ARG:HD3	1.77	0.43
53:CZ:21:LEU:HB3	53:CZ:50:VAL:HG22	2.01	0.43
55:DA:1484:U:H2'	55:DA:1485:U:C6	2.54	0.43
55:DA:2243:U:O2	55:DA:2434:A:C2	2.72	0.43
55:DA:834:G:H2'	55:DA:835:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:233:GLY:HA3	69:DC:347:HOH:O	2.19	0.43
1:AA:49:U:O2	1:AA:362:G:H1'	2.19	0.43
1:AA:935:A:H2'	1:AA:936:C:C6	2.54	0.43
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.54	0.43
1:BA:214:C:H2'	1:BA:215:C:H6	1.83	0.43
1:BA:299:G:H2'	1:BA:300:A:C8	2.54	0.43
8:BH:22:LYS:O	8:BH:63:LEU:HD12	2.19	0.43
15:BO:26:GLU:HG3	15:BO:81:LEU:HD22	2.01	0.43
15:BO:78:TYR:HE1	15:BO:88:ARG:HH21	1.67	0.43
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.19	0.43
29:CC:18:LYS:HE3	31:CA:1565:C:H5'	2.01	0.43
31:CA:2123:G:O5'	31:CA:2123:G:H8	2.02	0.43
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.18	0.43
34:CF:40:VAL:HG23	34:CF:86:GLY:HA2	1.99	0.43
55:DA:1001:A:O5'	55:DA:1001:A:H8	2.01	0.43
55:DA:1093:G:H1'	55:DA:1099:G:N2	2.34	0.43
55:DA:1494:A:H2'	55:DA:1495:A:C8	2.53	0.43
41:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.49	0.43
53:DZ:18:LEU:HB2	53:DZ:53:VAL:HG11	2.01	0.43
13:AM:23:TYR:HB3	13:AM:66:GLU:HA	2.00	0.42
4:BD:102:VAL:HG13	4:BD:107:PHE:HB2	2.00	0.42
30:CD:104:VAL:CG2	30:CD:177:VAL:HG21	2.48	0.42
36:CH:48:GLU:HA	36:CH:51:ARG:HB3	2.00	0.42
55:DA:184:C:H2'	55:DA:185:G:C8	2.54	0.42
29:DC:145:GLU:HB2	29:DC:188:CYS:HB3	2.00	0.42
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	2.00	0.42
33:DE:28:VAL:O	33:DE:32:VAL:HG23	2.19	0.42
41:DN:121:ALA:HA	41:DN:124:LEU:HD12	2.01	0.42
1:AA:604:G:H2'	1:AA:605:U:O4'	2.18	0.42
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.54	0.42
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	2.01	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.01	0.42
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	2.00	0.42
27:C0:12:SER:HB3	31:CA:988:A:P	2.59	0.42
31:CA:935:C:H2'	31:CA:936:A:C8	2.54	0.42
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.19	0.42
24:D3:10:LEU:O	24:D3:14:ARG:HB2	2.19	0.42
25:D4:39:LYS:HB3	69:D4:133:HOH:O	2.18	0.42
55:DA:1183:U:H2'	55:DA:1184:U:C6	2.54	0.42
55:DA:1847:A:O5'	55:DA:1847:A:H8	2.01	0.42
55:DA:2747:G:O6	55:DA:2755:C:H5''	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2848:G:H1'	55:DA:2867:G:N2	2.33	0.42
55:DA:2609:U:H5	62:DA:3194:EDO:H12	1.84	0.42
55:DA:720:U:H2'	55:DA:721:A:C8	2.55	0.42
34:DF:118:SER:OG	34:DF:120:LYS:HG3	2.19	0.42
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	2.01	0.42
1:AA:1293:C:H2'	1:AA:1294:G:C8	2.54	0.42
19:AS:64:ASP:HB3	34:DF:115:ARG:HH21	1.83	0.42
1:BA:1387:G:H2'	1:BA:1388:C:C6	2.54	0.42
26:C5:17:VAL:HG11	26:C5:26:ILE:HD12	2.01	0.42
31:CA:1562:U:H2'	31:CA:1563:U:O4'	2.19	0.42
31:CA:1825:U:H6	31:CA:1825:U:O5'	2.02	0.42
31:CA:459:U:H2'	31:CA:460:A:C8	2.50	0.42
31:CA:540:C:H2'	31:CA:541:A:H8	1.84	0.42
31:CA:622:G:H2'	31:CA:623:C:C6	2.54	0.42
31:CA:720:U:H2'	31:CA:721:A:C8	2.54	0.42
30:CD:101:PHE:HA	30:CD:104:VAL:HG13	2.01	0.42
55:DA:2105:U:O4	55:DA:2184:A:C2	2.71	0.42
55:DA:2133:G:H2'	55:DA:2157:G:H22	1.83	0.42
55:DA:2621:G:H5''	69:DA:4246:HOH:O	2.19	0.42
55:DA:2721:A:H2'	55:DA:2722:G:O4'	2.18	0.42
55:DA:2852:G:H4'	69:DA:5849:HOH:O	2.19	0.42
52:DY:66:THR:O	52:DY:69:ALA:HB3	2.19	0.42
7:AG:56:LYS:HB3	7:AG:57:SER:H	1.63	0.42
1:BA:1293:C:H2'	1:BA:1294:G:C8	2.55	0.42
1:BA:631:C:H6	1:BA:631:C:O5'	2.02	0.42
1:BA:756:C:H2'	1:BA:757:U:O4'	2.19	0.42
1:BA:1373:G:C5'	7:BG:36:LYS:HB2	2.49	0.42
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	2.01	0.42
31:CA:2282:G:OP1	31:CA:2283:C:H1'	2.19	0.42
31:CA:2341:G:H2'	31:CA:2342:C:O4'	2.19	0.42
31:CA:39:G:H2'	31:CA:40:U:C6	2.54	0.42
31:CA:70:G:H5''	31:CA:112:U:O2	2.19	0.42
28:CB:90:C:H5'	41:CN:18:ARG:HA	2.02	0.42
46:CS:24:LYS:HA	46:CS:94:THR:OG1	2.20	0.42
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.18	0.42
52:CY:51:VAL:HG22	52:CY:52:SER:O	2.18	0.42
55:DA:1231:U:H2'	55:DA:1232:G:H8	1.84	0.42
55:DA:1976:U:H1'	63:DA:3225:PGE:H2	2.01	0.42
55:DA:2741:A:H2'	55:DA:2742:G:O4'	2.19	0.42
55:DA:2845:U:H2'	55:DA:2846:G:O4'	2.20	0.42
35:DG:145:ALA:HB1	35:DG:164:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.00	0.42
38:DK:3:THR:HA	69:DR:307:HOH:O	2.19	0.42
46:DS:73:LYS:HZ2	58:DS:203:MPD:C5	2.28	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.54	0.42
1:BA:1491:G:H2'	1:BA:1492:A:C8	2.55	0.42
10:BJ:29:ALA:HB2	10:BJ:87:LEU:HD11	2.02	0.42
31:CA:1677:A:C8	31:CA:1677:A:H5''	2.55	0.42
31:CA:2494:G:O3'	41:CN:79:ALA:HA	2.18	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.54	0.42
31:CA:740:C:H5'	31:CA:1784:A:H3'	2.02	0.42
55:DA:1446:C:H2'	55:DA:1447:C:C6	2.54	0.42
55:DA:2064:C:H2'	55:DA:2065:C:C6	2.55	0.42
55:DA:2341:G:H2'	55:DA:2342:C:O4'	2.20	0.42
55:DA:2636:C:H2'	55:DA:2637:U:H6	1.82	0.42
55:DA:609:A:H2'	55:DA:610:C:O4'	2.20	0.42
32:DD:143:PRO:HA	69:DD:410:HOH:O	2.20	0.42
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	2.01	0.42
1:BA:682:G:H2'	1:BA:683:G:H8	1.84	0.42
5:BE:47:GLY:HA3	5:BE:71:MET:HG2	2.01	0.42
31:CA:2520:C:H2'	31:CA:2521:C:C6	2.55	0.42
31:CA:2569:G:H5''	31:CA:2569:G:C8	2.55	0.42
31:CA:2641:G:H2'	31:CA:2642:G:C8	2.55	0.42
31:CA:374:A:C2	31:CA:401:A:C4	3.08	0.42
31:CA:396:G:H1'	52:CY:29:PHE:HD2	1.83	0.42
31:CA:740:C:H42	31:CA:757:G:H1	1.66	0.42
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.52	0.42
33:CE:126:VAL:HG23	33:CE:133:LEU:HB3	1.98	0.42
37:CJ:37:GLU:HB3	37:CJ:67:PHE:HZ	1.84	0.42
50:CW:31:TYR:O	50:CW:92:VAL:HA	2.20	0.42
51:CX:47:ALA:HB1	51:CX:51:VAL:O	2.19	0.42
55:DA:1028:A:H61	55:DA:1125:G:H2'	1.81	0.42
55:DA:1604:C:H5'	69:DA:3982:HOH:O	2.18	0.42
55:DA:348:A:H2'	55:DA:349:U:O4'	2.20	0.42
40:DM:36:LYS:HB3	69:DA:4844:HOH:O	2.20	0.42
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	2.02	0.42
53:DZ:21:LEU:HB3	53:DZ:50:VAL:HG22	2.01	0.42
1:AA:486:U:H2'	1:AA:487:A:H8	1.85	0.42
7:AG:116:MET:HA	7:AG:119:ARG:HB2	2.00	0.42
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	2.01	0.42
1:BA:1508:A:H2'	1:BA:1509:C:O4'	2.19	0.42
1:BA:322:C:H41	1:BA:328:C:H6	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:211:THR:HA	2:BB:214:LEU:HB2	2.01	0.42
3:BC:180:ALA:HA	3:BC:206:GLU:HA	2.01	0.42
11:BK:31:ILE:HA	11:BK:46:THR:HG22	2.02	0.42
31:CA:1093:G:H1'	31:CA:1099:G:H22	1.84	0.42
31:CA:1635:A:H2'	31:CA:1636:U:O4'	2.19	0.42
35:CG:145:ALA:HB1	35:CG:164:TYR:HE1	1.85	0.42
49:CV:14:LEU:HD11	49:CV:71:ALA:HB2	2.01	0.42
55:DA:2824:C:C4	55:DA:2825:G:C5	3.07	0.42
55:DA:28:A:H1'	55:DA:513:A:C2	2.55	0.42
32:DD:145:SER:O	55:DA:2512:C:H1'	2.19	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.01	0.42
19:AS:11:ILE:HG12	19:AS:16:LEU:HD13	2.02	0.42
11:BK:123:PRO:HD2	21:BU:38:TYR:HB2	2.01	0.42
20:BT:35:VAL:HG21	20:BT:54:MET:HG2	2.01	0.42
31:CA:2207:C:H2'	31:CA:2208:C:C6	2.55	0.42
31:CA:300:A:H1'	31:CA:319:G:H1'	2.02	0.42
31:CA:19:A:O2'	31:CA:553:G:H4'	2.19	0.42
31:CA:668:A:H2'	31:CA:670:A:H62	1.85	0.42
34:CF:29:PRO:HB2	34:CF:169:LEU:HD22	2.02	0.42
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.19	0.42
55:DA:1313:U:O2	55:DA:1313:U:H2'	2.19	0.42
55:DA:1446:C:O5'	55:DA:1446:C:H6	2.02	0.42
28:DB:29:A:H2'	28:DB:30:C:C6	2.54	0.42
32:DD:146:ILE:HD12	32:DD:155:VAL:CG2	2.50	0.42
1:AA:299:G:H2'	1:AA:300:A:C8	2.54	0.42
10:AJ:29:ALA:HB2	10:AJ:87:LEU:HD11	2.02	0.42
20:AT:28:MET:HG2	20:AT:32:ILE:HD11	2.02	0.42
1:BA:1426:G:H2'	1:BA:1427:C:O4'	2.20	0.42
1:BA:413:G:H1'	1:BA:428:G:H21	1.84	0.42
1:BA:580:C:H2'	1:BA:581:G:O4'	2.19	0.42
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	2.02	0.42
31:CA:1376:C:H2'	31:CA:1377:G:O4'	2.20	0.42
31:CA:573:U:N3	31:CA:2030:6MZ:H3'	2.34	0.42
31:CA:956:G:H5''	41:CN:76:LYS:HG3	2.02	0.42
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	2.02	0.42
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:H6	1.85	0.42
55:DA:2813:A:H2	55:DA:2887[A]:A:N1	2.18	0.42
55:DA:593:U:H2'	55:DA:594:U:C6	2.55	0.42
55:DA:686:U:H2'	55:DA:788:A:N1	2.34	0.42
29:DC:107:PRO:HB3	29:DC:142:HIS:NE2	2.34	0.42
32:DD:133:THR:HG21	55:DA:1676:A:H1'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DH:21:VAL:HG21	36:DH:25:TYR:HD2	1.85	0.42
38:DK:114:LEU:O	38:DK:117:ALA:HB3	2.19	0.42
41:DN:5:LYS:HE2	69:DA:6106:HOH:O	2.20	0.42
46:DS:3:ALA:HB3	46:DS:101:ILE:HD12	2.02	0.42
46:DS:24:LYS:HA	46:DS:94:THR:OG1	2.19	0.42
48:DU:3:ARG:HD3	48:DU:5:GLU:H	1.85	0.42
50:DW:31:TYR:O	50:DW:92:VAL:HA	2.20	0.42
1:AA:227:G:H2'	1:AA:228:A:O4'	2.20	0.42
9:AI:51:PRO:HB3	9:AI:84:THR:HG23	2.00	0.42
1:BA:131:A:H2'	1:BA:132:C:C6	2.54	0.42
1:BA:382:A:H2'	1:BA:383:A:C8	2.54	0.42
20:BT:31:PHE:HA	20:BT:34:LYS:HD2	2.01	0.42
22:C1:2:ALA:N	31:CA:2577:A:C2	2.88	0.42
22:C1:6:ASN:ND2	31:CA:2020:A:H62	2.18	0.42
31:CA:1847:A:H8	31:CA:1847:A:O5'	2.03	0.42
31:CA:745:1MG:O2'	31:CA:748:G:H1'	2.19	0.42
38:CK:114:LEU:O	38:CK:117:ALA:HB3	2.20	0.42
45:CR:83:LEU:HB3	45:CR:88:VAL:HB	2.01	0.42
55:DA:121:G:H2'	55:DA:122:G:H8	1.85	0.42
55:DA:2706:A:O5'	55:DA:2706:A:H8	2.03	0.42
45:DR:92:ARG:HB2	55:DA:997:G:OP1	2.20	0.42
32:DD:172:VAL:HG12	32:DD:175:LEU:HD21	2.01	0.42
41:DN:57:VAL:HA	41:DN:112:LEU:HD21	2.02	0.42
20:AT:22:ALA:O	20:AT:26:SER:HB2	2.20	0.41
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	2.01	0.41
1:BA:374:A:OP1	1:BA:452:A:N1	2.53	0.41
1:BA:517:G:O2'	1:BA:530:G:H4'	2.20	0.41
1:BA:827:U:H2'	1:BA:870:U:O4	2.19	0.41
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.35	0.41
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.02	0.41
25:C4:57:LEU:HD11	31:CA:834:G:H5'	2.02	0.41
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	2.02	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5"	2.02	0.41
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.02	0.41
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.72	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.55	0.41
55:DA:2243:U:O2	55:DA:2434:A:H2	2.02	0.41
55:DA:39:G:H2'	55:DA:40:U:C6	2.55	0.41
55:DA:543:G:H5"	55:DA:543:G:H8	1.85	0.41
37:DJ:37:GLU:HB3	37:DJ:67:PHE:HZ	1.84	0.41
45:DR:13:ARG:HD2	69:DA:3914:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:116:MET:O	7:AG:120:LEU:HB2	2.19	0.41
2:BB:90:PHE:HB3	2:BB:151:ILE:HG22	2.02	0.41
5:BE:15:LEU:HD11	5:BE:18:VAL:HG23	2.02	0.41
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	2.02	0.41
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.55	0.41
31:CA:787:C:H3'	31:CA:791:C:H41	1.85	0.41
40:CM:109:LYS:HA	40:CM:126:ARG:O	2.20	0.41
55:DA:2740:A:C6	55:DA:2764:A:C8	3.08	0.41
55:DA:612:G:H2'	55:DA:614:A:C8	2.55	0.41
33:DE:66:GLY:HA2	55:DA:2060:A:OP2	2.20	0.41
38:DK:118:MET:HA	38:DK:121:LYS:NZ	2.35	0.41
1:AA:1426:G:H2'	1:AA:1427:C:O4'	2.20	0.41
1:AA:1533:C:H5'	1:AA:1534:A:OP1	2.20	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	2.02	0.41
9:BI:46:MET:HA	9:BI:49:ARG:HD2	2.02	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
31:CA:1259:G:H2'	31:CA:1260:A:C8	2.55	0.41
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.39	0.41
31:CA:2198:A:C2	36:CH:29:PHE:HB2	2.55	0.41
31:CA:2428:G:N2	40:CM:60:ARG:NH2	2.58	0.41
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.19	0.41
31:CA:1190:G:H5''	40:CM:32:GLY:HA2	2.02	0.41
52:CY:66:THR:O	52:CY:69:ALA:HB3	2.20	0.41
22:D1:27:SER:HA	69:DA:4108:HOH:O	2.20	0.41
55:DA:1450:G:C6	55:DA:1451:C:N4	2.88	0.41
55:DA:1562:U:H2'	55:DA:1563:U:O4'	2.20	0.41
55:DA:179:C:H2'	55:DA:180:G:O4'	2.21	0.41
55:DA:2005:A:H5''	69:DA:4377:HOH:O	2.20	0.41
55:DA:565:C:H2'	55:DA:566:U:O4'	2.20	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.00	0.41
1:AA:636:U:H2'	1:AA:637:C:C6	2.55	0.41
8:AH:41:LYS:HD2	8:AH:48:ASP:HA	2.02	0.41
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.55	0.41
1:BA:1190:G:H5'	3:BC:176:HIS:CE1	2.55	0.41
35:CG:155:GLU:HG2	35:CG:157:TYR:H	1.85	0.41
31:CA:2849:U:P	44:CQ:93:ARG:HH21	2.43	0.41
49:CV:11:VAL:HG12	49:CV:72:ILE:HA	2.01	0.41
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.85	0.41
55:DA:1554:U:H1'	59:DA:3219:PUT:H32	2.03	0.41
55:DA:198:C:O5'	55:DA:198:C:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DX:62:LYS:HE3	55:DA:2366:A:H4'	2.01	0.41
55:DA:2822:G:H2'	55:DA:2823:A:H5''	2.03	0.41
55:DA:300:A:H1'	55:DA:319:G:H1'	2.02	0.41
32:DD:38:LYS:O	32:DD:46:ARG:HA	2.20	0.41
54:DI:91:ALA:O	54:DI:95:LEU:HB2	2.20	0.41
45:DR:83:LEU:HB3	45:DR:88:VAL:HB	2.01	0.41
51:DX:39:ARG:HA	69:DX:110:HOH:O	2.19	0.41
1:AA:1017:U:H2'	1:AA:1018:G:H8	1.86	0.41
1:AA:1417:G:C6	1:AA:1482:G:C6	3.08	0.41
1:AA:262:A:H5'	20:AT:68:HIS:HB3	2.03	0.41
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.41
8:BH:38:ASN:O	8:BH:42:GLU:HG3	2.21	0.41
31:CA:1:G:H1	31:CA:2902:C:H42	1.68	0.41
31:CA:708:G:N2	31:CA:724:U:H1'	2.36	0.41
31:CA:984:A:H2'	31:CA:984:A:N3	2.35	0.41
46:CS:38:VAL:CG2	46:CS:57:GLY:HA3	2.50	0.41
24:D3:19:ARG:HD3	55:DA:125:A:OP2	2.21	0.41
55:DA:1093:G:H1'	55:DA:1099:G:H22	1.85	0.41
55:DA:1195:G:N3	55:DA:1226:A:H2	2.19	0.41
55:DA:1286:A:C6	55:DA:1329:U:C2	3.08	0.41
55:DA:1664:A:O5'	55:DA:1664:A:C8	2.73	0.41
55:DA:189:G:H2'	55:DA:205:G:N2	2.36	0.41
55:DA:2714:G:O2'	55:DA:2715:C:H5'	2.20	0.41
55:DA:622:G:C8	55:DA:622:G:H5''	2.55	0.41
28:DB:1:U:H2'	28:DB:2:G:H8	1.83	0.41
54:DI:132:TYR:HD2	54:DI:133:GLU:HG2	1.84	0.41
38:DK:89:PHE:CE2	38:DK:100:VAL:HG11	2.55	0.41
42:DO:31:HIS:C	42:DO:33:ILE:H	2.24	0.41
52:DY:18:ARG:HH21	52:DY:24:ALA:HB2	1.85	0.41
1:AA:827:U:H2'	1:AA:870:U:O4	2.20	0.41
15:AO:66:LEU:H	15:AO:66:LEU:HG	1.71	0.41
1:BA:562:U:H5	12:BL:15:LYS:HE2	1.85	0.41
31:CA:323:C:H6	31:CA:1205:A:N1	2.18	0.41
31:CA:5:A:C2	31:CA:2899:A:C2	3.09	0.41
31:CA:871:U:H2'	31:CA:872:U:C6	2.55	0.41
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	2.01	0.41
26:D5:11:CYS:HB3	26:D5:33:HIS:HE1	1.85	0.41
55:DA:1189:A:H2'	55:DA:1190:G:O4'	2.21	0.41
55:DA:2057:G:H5'	69:DA:5229:HOH:O	2.20	0.41
62:DA:3194:EDO:H22	69:DA:7234:HOH:O	2.19	0.41
34:DF:104:ILE:HD11	34:DF:175:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DO:51:LEU:HA	42:DO:51:LEU:HD23	1.87	0.41
1:AA:517:G:O2'	1:AA:530:G:H4'	2.21	0.41
2:BB:117:LEU:HA	2:BB:120:GLN:HG2	2.01	0.41
6:BF:64:VAL:HG12	6:BF:65:GLU:N	2.36	0.41
12:BL:80:ILE:HG22	12:BL:104:CYS:HB2	2.01	0.41
12:BL:3:THR:HB	12:BL:6:GLN:HB2	2.03	0.41
16:BP:20:VAL:HG11	16:BP:32:PHE:HB2	2.02	0.41
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.21	0.41
31:CA:348:A:H2'	31:CA:349:U:O4'	2.20	0.41
30:CD:130:GLN:NE2	30:CD:142:VAL:HG23	2.35	0.41
40:CM:28:GLY:O	40:CM:29:LYS:C	2.58	0.41
31:CA:2250:G:N7	41:CN:82:MET:HB2	2.34	0.41
46:CS:3:ALA:HA	46:CS:40:MET:O	2.21	0.41
47:CT:20:VAL:O	47:CT:23:LEU:HB2	2.21	0.41
48:CU:47:VAL:HG11	48:CU:85:VAL:HG11	2.02	0.41
55:DA:819:A:C4	55:DA:1189:A:C2	3.09	0.41
55:DA:1832:C:N4	55:DA:1833:C:C4	2.89	0.41
55:DA:2438:U:O2'	55:DA:2439:A:H5''	2.21	0.41
55:DA:2695:U:H3'	69:DA:4531:HOH:O	2.21	0.41
55:DA:323:C:H6	55:DA:1205:A:N1	2.19	0.41
55:DA:83:A:H2'	55:DA:84:A:C8	2.56	0.41
33:DE:163:ASN:HB2	55:DA:322:A:OP2	2.20	0.41
34:DF:162:SER:HB2	69:DF:207:HOH:O	2.20	0.41
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	2.03	0.41
47:DT:20:VAL:O	47:DT:23:LEU:HB2	2.20	0.41
48:DU:47:VAL:HG11	48:DU:85:VAL:HG11	2.02	0.41
48:DU:48:GLN:HG2	48:DU:53:VAL:O	2.20	0.41
51:DX:41[A]:ARG:HG3	55:DA:2386:A:C2	2.55	0.41
52:DY:37:ARG:HG3	52:DY:48:THR:HG23	2.03	0.41
1:AA:631:C:O5'	1:AA:631:C:H6	2.04	0.41
1:AA:746:A:H2'	1:AA:747:A:C8	2.55	0.41
2:AB:90:PHE:HB3	2:AB:151:ILE:HG22	2.02	0.41
7:AG:107:ALA:HB1	7:AG:133:THR:HB	2.03	0.41
11:AK:36:ASP:OD2	11:AK:40:ASN:HB2	2.21	0.41
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	2.03	0.41
1:BA:1017:U:H2'	1:BA:1018:G:H8	1.85	0.41
1:BA:126:G:H2'	1:BA:127:G:O4'	2.21	0.41
1:BA:202:G:H1	1:BA:215:C:H42	1.69	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.01	0.41
31:CA:2660:A:H2'	31:CA:2661:G:C8	2.56	0.41
31:CA:287:G:H2'	31:CA:288:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:214:ARG:NH1	31:CA:1566:A:H5'	2.36	0.41
33:CE:19:PHE:HB3	33:CE:113:VAL:HG21	2.03	0.41
55:DA:1585:C:H2'	55:DA:1586:A:O4'	2.21	0.41
55:DA:2019:A:H2	55:DA:2035:G:H22	1.69	0.41
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.41
55:DA:2519:U:C6	55:DA:2542:A:N6	2.89	0.41
35:DG:109:PHE:CD1	55:DA:2667:C:H1'	2.55	0.41
55:DA:302:C:H2'	55:DA:303:G:H8	1.86	0.41
45:DR:92:ARG:NH1	55:DA:997:G:H5''	2.36	0.41
34:DF:40:VAL:HG21	34:DF:50:LEU:HD12	2.03	0.41
36:DH:135:HIS:CG	36:DH:136:SER:H	2.39	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.55	0.41
2:AB:12:ALA:HB2	2:AB:212:LEU:HD13	2.02	0.41
9:AI:46:MET:HA	9:AI:49:ARG:HD2	2.02	0.41
1:BA:240:G:H5''	1:BA:240:G:C8	2.56	0.41
1:BA:486:U:H2'	1:BA:487:A:H8	1.85	0.41
15:BO:24:SER:HB3	15:BO:27:VAL:HG23	2.03	0.41
31:CA:1676:A:H2'	31:CA:1677:A:O4'	2.20	0.41
31:CA:2146:C:H4'	31:CA:2147:A:O5'	2.21	0.41
30:CD:117:GLY:HA2	30:CD:164:GLN:HE22	1.85	0.41
39:CL:119:ALA:HA	39:CL:120:PRO:HD3	1.91	0.41
27:D0:18:PRO:HD2	69:D0:206:HOH:O	2.21	0.41
55:DA:1356:G:C2	55:DA:1376:C:O2	2.74	0.41
55:DA:1782:U:H2'	55:DA:1783:A:H5'	2.03	0.41
55:DA:2082:A:H2'	55:DA:2083:G:O4'	2.20	0.41
55:DA:2660:A:H2'	55:DA:2661:G:C8	2.56	0.41
33:DE:45:ALA:HB3	55:DA:38:A:H5'	2.02	0.41
1:AA:382:A:H2'	1:AA:383:A:C8	2.56	0.41
1:AA:580:C:H2'	1:AA:581:G:O4'	2.21	0.41
1:AA:845:A:O4'	1:AA:845:A:P	2.79	0.41
2:AB:211:THR:HA	2:AB:214:LEU:HB2	2.01	0.41
11:AK:31:ILE:HA	11:AK:46:THR:HG22	2.02	0.41
1:BA:536:C:OP1	69:BA:1701:HOH:O	2.22	0.41
7:BG:116:MET:O	7:BG:120:LEU:HB2	2.20	0.41
15:BO:66:LEU:H	15:BO:66:LEU:HG	1.71	0.41
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	2.02	0.41
55:DA:287:G:H2'	55:DA:288:U:C6	2.56	0.41
37:DJ:55:ILE:HA	37:DJ:56:PRO:HD3	2.00	0.41
47:DT:100:THR:HG21	69:DT:346:HOH:O	2.21	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.02	0.41
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1088:G:H21	1:AA:1167:A:H62	1.69	0.41
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.21	0.41
1:AA:845:A:H2'	1:AA:846:G:O4'	2.21	0.41
17:AQ:12:VAL:HG12	17:AQ:55:ILE:HA	2.03	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.03	0.41
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.55	0.41
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.41
1:BA:368:U:O4	36:DH:83:LYS:HB2	2.21	0.41
1:BA:577:G:C1'	1:BA:816:A:H2'	2.51	0.41
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	2.02	0.41
5:BE:57:PRO:HA	5:BE:60:ILE:HG13	2.02	0.41
12:BL:82:ILE:HD11	12:BL:95:TYR:HB2	2.03	0.41
19:BS:11:ILE:HG12	19:BS:16:LEU:HD13	2.02	0.41
31:CA:172:A:H2'	31:CA:173:A:C8	2.56	0.41
31:CA:379:G:O4'	31:CA:2232:C:H5''	2.21	0.41
31:CA:297:G:H5''	49:CV:85:PHE:HB2	2.02	0.41
46:CS:76:LYS:O	46:CS:84:ARG:HA	2.21	0.41
55:DA:1782:U:H3'	69:DA:4190:HOH:O	2.21	0.41
55:DA:665:U:H2'	55:DA:666:A:H8	1.85	0.41
46:DS:3:ALA:HA	46:DS:40:MET:O	2.21	0.41
47:DT:20:VAL:HA	47:DT:23:LEU:HD12	2.03	0.41
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.21	0.40
11:AK:52:PHE:CE2	11:AK:65:VAL:HG21	2.56	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.40
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.36	0.40
1:BA:377:G:H2'	1:BA:378:G:H8	1.86	0.40
22:C1:12:LYS:HA	22:C1:12:LYS:HD2	1.70	0.40
31:CA:528:A:N1	31:CA:2042:A:H2'	2.36	0.40
31:CA:2598:A:C8	31:CA:2599:G:H1'	2.56	0.40
31:CA:65:U:H2'	31:CA:66:C:C6	2.56	0.40
28:CB:24:G:H1'	28:CB:27:C:N4	2.36	0.40
42:CO:92:GLY:HA2	42:CO:94:TYR:CZ	2.56	0.40
43:CP:39:VAL:HG11	43:CP:87:ILE:HG21	2.03	0.40
27:D0:26:GLY:O	55:DA:929:U:H1'	2.21	0.40
55:DA:2261:C:H1'	55:DA:2388:A:N3	2.35	0.40
49:DV:15:THR:HG23	55:DA:310:A:H5''	2.03	0.40
55:DA:65:U:H2'	55:DA:66:C:C6	2.56	0.40
54:DI:64:VAL:CG2	54:DI:69:PHE:HB2	2.50	0.40
11:AK:123:PRO:HD2	21:AU:38:TYR:HB2	2.03	0.40
20:AT:44:LYS:HG3	20:AT:44:LYS:H	1.48	0.40
21:AU:40:LYS:HB2	21:AU:43:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:562:U:H4'	1:BA:563:A:O5'	2.21	0.40
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.86	0.40
31:CA:189:G:H2'	31:CA:205:G:N2	2.37	0.40
31:CA:1940:U:H5''	31:CA:1965:C:C5	2.55	0.40
31:CA:2538:C:H2'	31:CA:2539:C:C6	2.56	0.40
31:CA:244:A:H62	31:CA:254:G:H21	1.70	0.40
31:CA:304:U:H2'	31:CA:305:C:C6	2.56	0.40
33:CE:196:VAL:HG13	33:CE:200:LEU:HD13	2.03	0.40
39:CL:35:VAL:HB	39:CL:36:GLY:H	1.66	0.40
55:DA:2042:A:H2	69:DA:7342:HOH:O	2.04	0.40
36:DH:117:LEU:HA	36:DH:118:PRO:HD3	2.00	0.40
5:AE:80:THR:HB	5:AE:122:ASN:HB2	2.03	0.40
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.02	0.40
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	2.02	0.40
2:BB:83:ALA:HB3	2:BB:214:LEU:HD22	2.02	0.40
8:BH:76:GLN:O	8:BH:127:CYS:HB2	2.21	0.40
31:CA:2328:A:H8	31:CA:2328:A:O5'	2.04	0.40
31:CA:2464:G:C2	31:CA:2465:C:H1'	2.57	0.40
31:CA:2693:G:H2'	31:CA:2694:G:H8	1.85	0.40
31:CA:302:C:H2'	31:CA:303:G:H8	1.85	0.40
34:CF:40:VAL:HG21	34:CF:50:LEU:HD12	2.04	0.40
34:CF:8:TYR:HB2	34:CF:173:PHE:CZ	2.55	0.40
39:CL:15:GLY:HA2	39:CL:47:ILE:HG12	2.03	0.40
25:D4:26:HIS:NE2	25:D4:48:ALA:HB2	2.36	0.40
44:DQ:94:LYS:HE2	55:DA:1754:A:C8	2.56	0.40
55:DA:638:G:H2'	55:DA:639:U:C6	2.57	0.40
29:DC:53:HIS:NE2	29:DC:219:THR:HG23	2.37	0.40
32:DD:175:LEU:HA	69:DD:435:HOH:O	2.22	0.40
1:AA:1235:U:H2'	1:AA:1236:A:O4'	2.22	0.40
1:AA:377:G:H2'	1:AA:378:G:H8	1.87	0.40
2:AB:117:LEU:HA	2:AB:120:GLN:HG2	2.03	0.40
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.56	0.40
1:AA:511:C:H5'	4:AD:44:ARG:CZ	2.52	0.40
15:AO:24:SER:HB3	15:AO:27:VAL:HG23	2.04	0.40
1:BA:1235:U:H2'	1:BA:1236:A:O4'	2.22	0.40
10:BJ:59:LYS:H	10:BJ:59:LYS:HG3	1.66	0.40
11:BK:52:PHE:CE2	11:BK:65:VAL:HG21	2.56	0.40
13:BM:4:ILE:HA	13:BM:57:ARG:HG2	2.04	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.40
31:CA:1313:U:H5'	69:CA:3366:HOH:O	2.21	0.40
31:CA:179:C:H2'	31:CA:180:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:7:G:H4'	38:CK:15:TRP:CZ2	2.56	0.40
31:CA:2547:A:H4'	39:CL:29:HIS:NE2	2.36	0.40
47:CT:29:VAL:O	47:CT:33:LEU:HD12	2.21	0.40
55:DA:2498:OMC:HM23	55:DA:2498:OMC:H1'	1.95	0.40
55:DA:2538:C:H2'	55:DA:2539:C:C6	2.57	0.40
34:DF:138:PHE:HA	34:DF:139:PRO:HD3	1.93	0.40
34:DF:175:PHE:HA	34:DF:176:PRO:HD3	1.95	0.40
43:DP:53:THR:HB	43:DP:65:THR:HG22	2.04	0.40
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.57	0.40
1:AA:407:U:H2'	1:AA:408:A:H8	1.86	0.40
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.50	0.40
1:AA:562:U:H5	12:AL:15:LYS:HE2	1.86	0.40
1:BA:110:C:H1'	69:BA:1786:HOH:O	2.21	0.40
1:BA:227:G:H2'	1:BA:228:A:O4'	2.20	0.40
1:BA:240:G:OP1	1:BA:240:G:H4'	2.22	0.40
10:BJ:12:ALA:HB3	10:BJ:18:ILE:HB	2.03	0.40
12:BL:44:LYS:HB2	12:BL:45:PRO:HD3	2.03	0.40
31:CA:2066:C:O2'	31:CA:2067:G:H5'	2.22	0.40
31:CA:4:U:H2'	31:CA:5:A:C8	2.57	0.40
31:CA:963:U:H2'	31:CA:964:C:C6	2.56	0.40
48:CU:30:ILE:HG22	48:CU:85:VAL:HB	2.02	0.40
49:CV:26:LYS:HB2	49:CV:35:ILE:HG22	2.04	0.40
24:D3:3:ARG:HB2	55:DA:1612:C:O2'	2.21	0.40
55:DA:192:C:O2'	55:DA:802:A:H1'	2.21	0.40
55:DA:2521:C:H2'	55:DA:2522:U:C6	2.57	0.40
55:DA:2844:G:H2'	55:DA:2845:U:O4'	2.22	0.40
33:DE:132:LYS:HD2	55:DA:320:A:OP2	2.21	0.40
33:DE:19:PHE:HB3	33:DE:113:VAL:HG21	2.03	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	
2	AB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	8	40
2	BB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	8	40
3	AC	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	19	59
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	13	49
4	AD	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	15	53
5	BE	148/155 (96%)	126 (85%)	17 (12%)	5 (3%)	5	30
6	AF	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	19	59
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	5	33
7	AG	149/151 (99%)	137 (92%)	10 (7%)	2 (1%)	15	53
7	BG	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	15	53
8	AH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	12	48
8	BH	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	24	63
9	AI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
9	BI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
10	AJ	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	5	33
10	BJ	96/99 (97%)	78 (81%)	14 (15%)	4 (4%)	3	25
11	AK	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	21	61
11	BK	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	21	61
12	AL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	11	47
12	BL	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	11	47
13	AM	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	4	29
13	BM	112/114 (98%)	96 (86%)	10 (9%)	6 (5%)	2	18
14	AN	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	19	59
14	BN	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	19	59
15	AO	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	BO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	16	54
16	AP	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7	38
16	BP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	4	27
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	4	27
17	BQ	78/80 (98%)	69 (88%)	5 (6%)	4 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	6 (8%)	3 (4%)	4	26
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	7	37
20	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	BT	83/86 (96%)	78 (94%)	4 (5%)	1 (1%)	16	54
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	45 (83%)	6 (11%)	3 (6%)	2	17
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	4 (8%)	1 (2%)	9	42
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	40
24	D3	44/46 (96%)	44 (100%)	0	0	100	100
25	C4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12	48
25	D4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12	48
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	4	29
27	D0	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
29	CC	269/272 (99%)	243 (90%)	21 (8%)	5 (2%)	10	45
29	DC	269/272 (99%)	245 (91%)	19 (7%)	5 (2%)	10	45
30	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	14	50
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
33	CE	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	34	72
33	DE	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
34	CF	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
34	DF	175/178 (98%)	163 (93%)	12 (7%)	0	100	100
35	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	8	40
35	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	30	69
36	CH	147/149 (99%)	129 (88%)	12 (8%)	6 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DH	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	6	36
37	CJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	5	34
37	DJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	5	34
38	CK	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	9	42
38	DK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	42
39	CL	120/123 (98%)	111 (92%)	7 (6%)	2 (2%)	11	47
39	DL	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	24	63
40	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	3	25
40	DM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	9	42
41	CN	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	DN	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	CO	118/127 (93%)	98 (83%)	16 (14%)	4 (3%)	5	30
42	DO	123/127 (97%)	106 (86%)	16 (13%)	1 (1%)	24	63
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	CQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	21	61
44	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	21	61
45	CR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
45	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
46	CS	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	9	43
46	DS	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	19	59
47	CT	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
47	DT	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	21	61
48	CU	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	17	57
48	DU	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	17	57
49	CV	100/103 (97%)	85 (85%)	12 (12%)	3 (3%)	5	34
49	DV	100/103 (97%)	87 (87%)	11 (11%)	2 (2%)	9	43
50	CW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	17	57
50	DW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	17	57
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	CY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
52	DY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
53	CZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	11	47
53	DZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	11	47
54	DI	133/135 (98%)	112 (84%)	17 (13%)	4 (3%)	5	34
All	All	11407/11679 (98%)	10425 (91%)	815 (7%)	167 (2%)	13	49

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	ARG
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA
22	C1	25	VAL
22	C1	27	SER
23	C2	5	ILE
27	C0	4	THR
2	BB	95	ARG
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
13	BM	7	ILE
17	BQ	82	ALA
20	BT	5	LYS
29	CC	108	LYS
29	CC	158	ALA
33	CE	83	VAL
35	CG	46	ALA
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
40	CM	29	LYS
48	CU	89	GLU
35	DG	46	ALA
36	DH	11	ASN

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Mol	Chain	Res	Type
37	DJ	19	ASN
49	DV	52	LEU
54	DI	91	ALA
3	AC	127	ARG
5	AE	162	GLU
8	AH	66	PHE
10	AJ	33	GLY
10	AJ	57	VAL
11	AK	89	PRO
14	AN	38	ASP
16	AP	31	ARG
19	AS	31	LEU
3	BC	61	ALA
3	BC	127	ARG
5	BE	110	ALA
6	BF	99	ALA
8	BH	66	PHE
10	BJ	38	GLY
10	BJ	57	VAL
11	BK	89	PRO
13	BM	5	ALA
14	BN	38	ASP
15	BO	88	ARG
16	BP	31	ARG
17	BQ	16	LYS
17	BQ	70	THR
29	CC	122	ALA
29	DC	122	ALA
29	DC	261	LYS
36	CH	11	ASN
38	CK	95	ARG
39	CL	35	VAL
40	CM	30	THR
40	CM	36	LYS
40	CM	69	ARG
44	CQ	105	GLY
49	CV	89	ASP
38	DK	95	ARG
40	DM	29	LYS
40	DM	36	LYS
44	DQ	105	GLY
46	DS	44	GLY

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Mol	Chain	Res	Type
48	DU	89	GLU
49	DV	89	ASP
54	DI	130	PRO
2	AB	127	ASP
7	AG	56	LYS
10	AJ	58	ASN
12	AL	48	ALA
12	AL	74	LEU
19	AS	8	GLY
22	C1	26	THR
2	BB	127	ASP
5	BE	103	THR
5	BE	109	GLY
7	BG	56	LYS
10	BJ	36	VAL
10	BJ	58	ASN
13	BM	114	LYS
19	BS	7	LYS
19	BS	31	LEU
29	CC	233	GLY
29	CC	253	LYS
30	CD	105	LYS
29	DC	233	GLY
36	CH	9	VAL
36	CH	122	LEU
37	CJ	23	PRO
37	CJ	32	GLY
39	CL	108	ARG
42	CO	119	SER
49	CV	7	ARG
49	CV	17	LYS
36	DH	122	LEU
37	DJ	23	PRO
37	DJ	32	GLY
39	DL	108	ARG
5	AE	109	GLY
6	AF	56	LYS
13	AM	7	ILE
17	AQ	16	LYS
17	AQ	68	SER
24	C3	45	SER
6	BF	56	LYS

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Mol	Chain	Res	Type
12	BL	74	LEU
13	BM	47	GLU
16	BP	44	SER
16	BP	80	LYS
30	CD	86	GLU
37	CJ	25	GLY
53	CZ	41	HIS
37	DJ	25	GLY
50	DW	23	ALA
53	DZ	41	HIS
54	DI	88	HIS
2	AB	125	THR
7	AG	17	LYS
13	AM	47	GLU
13	AM	105	ASN
16	AP	45	GLU
19	AS	7	LYS
2	BB	125	THR
5	BE	24	THR
7	BG	17	LYS
12	BL	44	LYS
13	BM	4	ILE
13	BM	105	ASN
17	BQ	17	MET
30	CD	149	ASN
29	DC	253	LYS
29	DC	262	ARG
36	CH	8	LYS
36	CH	34	GLY
40	CM	58	TYR
42	CO	32	GLU
42	CO	104	ALA
42	CO	118	ARG
46	CS	53	PHE
50	CW	23	ALA
38	DK	25	LEU
40	DM	58	TYR
42	DO	32	GLU
54	DI	108	VAL
8	AH	68	GLY
38	CK	25	LEU
40	CM	68	SER

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Mol	Chain	Res	Type
46	CS	48	LYS
36	DH	10	ALA
36	DH	34	GLY
47	DT	66	ILE
2	AB	71	GLY
2	BB	71	GLY
25	D4	7	VAL
27	C0	14	ILE
25	C4	7	VAL
5	BE	25	VAL
38	DK	83	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	
2	AB	186/186 (100%)	168 (90%)	18 (10%)	10	37
2	BB	186/186 (100%)	168 (90%)	18 (10%)	10	37
3	AC	170/170 (100%)	158 (93%)	12 (7%)	18	55
3	BC	170/170 (100%)	155 (91%)	15 (9%)	12	43
4	AD	172/172 (100%)	163 (95%)	9 (5%)	29	67
4	BD	172/172 (100%)	162 (94%)	10 (6%)	25	63
5	AE	118/118 (100%)	102 (86%)	16 (14%)	5	21
5	BE	113/118 (96%)	97 (86%)	16 (14%)	4	19
6	AF	92/92 (100%)	83 (90%)	9 (10%)	10	37
6	BF	87/92 (95%)	77 (88%)	10 (12%)	7	29
7	AG	124/124 (100%)	108 (87%)	16 (13%)	5	23
7	BG	124/124 (100%)	107 (86%)	17 (14%)	4	20
8	AH	104/104 (100%)	92 (88%)	12 (12%)	7	29
8	BH	104/104 (100%)	93 (89%)	11 (11%)	8	32
9	AI	105/105 (100%)	97 (92%)	8 (8%)	16	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BI	105/105 (100%)	97 (92%)	8 (8%)	16	51
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	19	57
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	8	33
11	AK	90/99 (91%)	86 (96%)	4 (4%)	35	72
11	BK	90/99 (91%)	81 (90%)	9 (10%)	9	35
12	AL	102/102 (100%)	96 (94%)	6 (6%)	24	63
12	BL	102/102 (100%)	95 (93%)	7 (7%)	19	57
13	AM	92/92 (100%)	81 (88%)	11 (12%)	6	27
13	BM	92/92 (100%)	81 (88%)	11 (12%)	6	27
14	AN	83/83 (100%)	81 (98%)	2 (2%)	57	83
14	BN	83/83 (100%)	81 (98%)	2 (2%)	57	83
15	AO	76/76 (100%)	71 (93%)	5 (7%)	21	58
15	BO	76/76 (100%)	68 (90%)	8 (10%)	8	33
16	AP	65/65 (100%)	60 (92%)	5 (8%)	16	51
16	BP	65/65 (100%)	61 (94%)	4 (6%)	23	60
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	6	26
17	BQ	74/74 (100%)	64 (86%)	10 (14%)	5	21
18	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	63 (90%)	7 (10%)	9	35
19	BS	70/70 (100%)	64 (91%)	6 (9%)	13	45
20	AT	65/65 (100%)	54 (83%)	11 (17%)	2	12
20	BT	65/65 (100%)	54 (83%)	11 (17%)	2	12
21	AU	48/48 (100%)	44 (92%)	4 (8%)	14	47
21	BU	48/48 (100%)	44 (92%)	4 (8%)	14	47
22	C1	47/47 (100%)	46 (98%)	1 (2%)	61	84
22	D1	47/47 (100%)	45 (96%)	2 (4%)	35	72
23	C2	45/46 (98%)	42 (93%)	3 (7%)	20	58
23	D2	45/46 (98%)	41 (91%)	4 (9%)	12	43
24	C3	38/38 (100%)	35 (92%)	3 (8%)	15	49
24	D3	38/38 (100%)	35 (92%)	3 (8%)	15	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	C4	51/51 (100%)	48 (94%)	3 (6%)	24	63
25	D4	51/51 (100%)	47 (92%)	4 (8%)	16	50
26	C5	34/34 (100%)	31 (91%)	3 (9%)	12	43
26	D5	34/34 (100%)	31 (91%)	3 (9%)	12	43
27	C0	48/48 (100%)	42 (88%)	6 (12%)	6	24
27	D0	49/48 (102%)	44 (90%)	5 (10%)	9	35
29	CC	216/217 (100%)	202 (94%)	14 (6%)	21	59
29	DC	216/217 (100%)	204 (94%)	12 (6%)	26	65
30	CD	164/164 (100%)	154 (94%)	10 (6%)	23	61
32	DD	163/163 (100%)	153 (94%)	10 (6%)	23	61
33	CE	165/165 (100%)	147 (89%)	18 (11%)	8	31
33	DE	165/165 (100%)	153 (93%)	12 (7%)	17	53
34	CF	148/149 (99%)	131 (88%)	17 (12%)	7	29
34	DF	148/149 (99%)	132 (89%)	16 (11%)	8	32
35	CG	137/137 (100%)	129 (94%)	8 (6%)	25	63
35	DG	137/137 (100%)	129 (94%)	8 (6%)	25	63
36	CH	114/114 (100%)	100 (88%)	14 (12%)	6	25
36	DH	114/114 (100%)	101 (89%)	13 (11%)	7	29
37	CJ	104/105 (99%)	95 (91%)	9 (9%)	13	44
37	DJ	104/105 (99%)	95 (91%)	9 (9%)	13	44
38	CK	116/116 (100%)	110 (95%)	6 (5%)	29	67
38	DK	116/116 (100%)	111 (96%)	5 (4%)	35	72
39	CL	103/104 (99%)	95 (92%)	8 (8%)	16	50
39	DL	104/104 (100%)	93 (89%)	11 (11%)	8	32
40	CM	103/103 (100%)	94 (91%)	9 (9%)	13	44
40	DM	103/103 (100%)	97 (94%)	6 (6%)	25	63
41	CN	108/108 (100%)	98 (91%)	10 (9%)	11	39
41	DN	109/108 (101%)	98 (90%)	11 (10%)	9	35
42	CO	100/103 (97%)	92 (92%)	8 (8%)	15	49
42	DO	102/103 (99%)	94 (92%)	8 (8%)	16	50
43	CP	86/87 (99%)	77 (90%)	9 (10%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DP	87/87 (100%)	78 (90%)	9 (10%)	9	34
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	15	48
44	DQ	99/99 (100%)	92 (93%)	7 (7%)	18	55
45	CR	89/89 (100%)	81 (91%)	8 (9%)	12	42
45	DR	89/89 (100%)	83 (93%)	6 (7%)	20	58
46	CS	84/84 (100%)	74 (88%)	10 (12%)	6	27
46	DS	84/84 (100%)	75 (89%)	9 (11%)	8	32
47	CT	93/93 (100%)	83 (89%)	10 (11%)	8	32
47	DT	93/93 (100%)	85 (91%)	8 (9%)	13	45
48	CU	80/84 (95%)	67 (84%)	13 (16%)	3	13
48	DU	80/84 (95%)	72 (90%)	8 (10%)	9	35
49	CV	83/84 (99%)	75 (90%)	8 (10%)	10	38
49	DV	83/84 (99%)	77 (93%)	6 (7%)	18	54
50	CW	78/78 (100%)	70 (90%)	8 (10%)	9	34
50	DW	78/78 (100%)	72 (92%)	6 (8%)	16	51
51	CX	56/58 (97%)	54 (96%)	2 (4%)	42	76
51	DX	58/58 (100%)	54 (93%)	4 (7%)	19	57
52	CY	67/67 (100%)	63 (94%)	4 (6%)	24	62
52	DY	67/67 (100%)	62 (92%)	5 (8%)	17	52
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	17	52
53	DZ	54/54 (100%)	51 (94%)	3 (6%)	26	65
54	DI	103/103 (100%)	91 (88%)	12 (12%)	7	28
All	All	9461/9514 (99%)	8645 (91%)	816 (9%)	13	45

All (816) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	57	LEU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	AB	116	ASP
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	147	SER
2	AB	161	LEU
2	AB	168	HIS
2	AB	205	ASP
2	AB	207	ILE
2	AB	211	THR
3	AC	33	LEU
3	AC	36	ASP
3	AC	46	GLU
3	AC	55	ILE
3	AC	75	ILE
3	AC	107	ARG
3	AC	121	THR
3	AC	128	VAL
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
3	AC	207	ILE
4	AD	22	LYS
4	AD	26	ARG
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	192	SER
4	AD	194	ASP
4	AD	196	ASN
4	AD	198	HIS
5	AE	14	LYS
5	AE	46	VAL
5	AE	70	ASN
5	AE	78	ASN
5	AE	81	LEU
5	AE	82	GLN
5	AE	88	VAL
5	AE	94	VAL
5	AE	101	GLU
5	AE	120	VAL

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Mol	Chain	Res	Type
5	AE	123	VAL
5	AE	126	LYS
5	AE	134	ILE
5	AE	148	ASN
5	AE	159	LYS
5	AE	162	GLU
6	AF	14	GLN
6	AF	17	GLN
6	AF	39	LEU
6	AF	55	HIS
6	AF	69	GLU
6	AF	72	ASP
6	AF	79	ARG
6	AF	92	THR
6	AF	93	LYS
7	AG	4	ARG
7	AG	13	LEU
7	AG	18	PHE
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	63	GLU
7	AG	76	LYS
7	AG	83	SER
7	AG	89	VAL
7	AG	92	ARG
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	138	ARG
7	AG	142	HIS
8	AH	3	MET
8	AH	9	ASP
8	AH	13	ARG
8	AH	26	THR
8	AH	31	LYS
8	AH	47	GLU
8	AH	51	VAL
8	AH	52	GLU
8	AH	54	ASP
8	AH	55	THR
8	AH	60	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	AH	63	LEU
9	AI	9	THR
9	AI	11	ARG
9	AI	36	GLU
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	89	GLU
9	AI	111	VAL
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	65	TYR
10	AJ	69	THR
10	AJ	88	MET
10	AJ	89	ARG
11	AK	53	ARG
11	AK	85	MET
11	AK	97	ILE
11	AK	125	LYS
12	AL	24	LEU
12	AL	40	THR
12	AL	86	ARG
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	3	ARG
13	AM	7	ILE
13	AM	8	ASN
13	AM	13	LYS
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	59	GLU
13	AM	64	VAL
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
14	AN	77	PHE
15	AO	25	THR
15	AO	40	GLN
15	AO	58	ARG
15	AO	66	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	AO	70	LEU
16	AP	1	MET
16	AP	2	VAL
16	AP	20	VAL
16	AP	33	ILE
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	13	VAL
17	AQ	16	LYS
17	AQ	20	SER
17	AQ	29	VAL
17	AQ	38	ILE
17	AQ	65	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	20	GLU
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	37	ARG
19	AS	52	HIS
19	AS	63	THR
20	AT	12	ILE
20	AT	14	SER
20	AT	24	ARG
20	AT	26	SER
20	AT	43	ASP
20	AT	44	LYS
20	AT	54	MET
20	AT	64	LYS
20	AT	66	LEU
20	AT	85	LYS
20	AT	86	LEU
21	AU	13	ASP
21	AU	16	LEU
21	AU	20	LYS
21	AU	56	HIS
22	C1	40	ARG
23	C2	5	ILE
23	C2	28	ARG
23	C2	47	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	C3	1	MET
24	C3	14	ARG
24	C3	41	ARG
25	C4	31	HIS
25	C4	52	LYS
25	C4	55	LEU
26	C5	2	LYS
26	C5	22	VAL
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	7	ILE
27	C0	36	VAL
27	C0	39	GLU
2	BB	23	TRP
2	BB	44	GLU
2	BB	57	LEU
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	116	ASP
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	147	SER
2	BB	161	LEU
2	BB	168	HIS
2	BB	205	ASP
2	BB	207	ILE
2	BB	211	THR
3	BC	3	GLN
3	BC	33	LEU
3	BC	36	ASP
3	BC	37	PHE
3	BC	46	GLU
3	BC	55	ILE
3	BC	75	ILE
3	BC	107	ARG
3	BC	121	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	BC	128	VAL
3	BC	152	GLU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
3	BC	207	ILE
4	BD	22	LYS
4	BD	26	ARG
4	BD	130	VAL
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	194	ASP
4	BD	196	ASN
4	BD	198	HIS
4	BD	206	LYS
5	BE	14	LYS
5	BE	46	VAL
5	BE	65	GLU
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	105	ILE
5	BE	115	LEU
5	BE	120	VAL
5	BE	123	VAL
5	BE	126	LYS
5	BE	148	ASN
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	17	GLN
6	BF	39	LEU
6	BF	53	LYS
6	BF	55	HIS
6	BF	68	GLN
6	BF	69	GLU
6	BF	72	ASP
6	BF	93	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	BG	5	ARG
7	BG	10	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	76	LYS
7	BG	92	ARG
7	BG	95	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	138	ARG
7	BG	142	HIS
7	BG	144	MET
8	BH	3	MET
8	BH	9	ASP
8	BH	13	ARG
8	BH	26	THR
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
9	BI	9	THR
9	BI	11	ARG
9	BI	36	GLU
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	89	GLU
9	BI	111	VAL
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	65	TYR
10	BJ	69	THR
10	BJ	78	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	53	ARG
11	BK	85	MET
11	BK	97	ILE
11	BK	118	HIS
11	BK	125	LYS
12	BL	24	LEU
12	BL	55	VAL
12	BL	58	THR
12	BL	86	ARG
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	7	ILE
13	BM	8	ASN
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	29	ARG
13	BM	41	GLU
13	BM	48	LEU
13	BM	59	GLU
13	BM	64	VAL
13	BM	101	ARG
14	BN	26	GLU
14	BN	77	PHE
15	BO	25	THR
15	BO	40	GLN
15	BO	58	ARG
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	87	LEU
15	BO	88	ARG
16	BP	1	MET
16	BP	2	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	BP	33	ILE
16	BP	46	LYS
17	BQ	13	VAL
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	28	PHE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	65	ARG
17	BQ	75	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	37	ARG
19	BS	52	HIS
19	BS	63	THR
20	BT	12	ILE
20	BT	14	SER
20	BT	26	SER
20	BT	36	TYR
20	BT	43	ASP
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	20	LYS
21	BU	56	HIS
22	D1	27	SER
22	D1	40	ARG
23	D2	5	ILE
23	D2	12	VAL
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
24	D3	14	ARG
24	D3	41	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	D4	15	LYS
25	D4	31	HIS
25	D4	52	LYS
25	D4	55	LEU
26	D5	2	LYS
26	D5	22	VAL
26	D5	26	ILE
27	D0	7	ILE
27	D0	36	VAL
27	D0	39	GLU
27	D0	55	VAL
27	D0	58	GLU
29	CC	28	LYS
29	CC	116	ILE
29	CC	118	SER
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	185	GLU
29	CC	195	VAL
29	CC	204	VAL
29	CC	236	GLU
29	CC	245	VAL
29	CC	266	PHE
29	CC	271	ARG
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	32	ASN
30	CD	79	LEU
30	CD	95	SER
30	CD	126	ASN
30	CD	131	ASP
30	CD	138	LEU
30	CD	150	GLN
29	DC	28	LYS
29	DC	70	ASN
29	DC	116	ILE
29	DC	118	SER
29	DC	120	VAL
29	DC	130	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	DC	185	GLU
29	DC	205	LEU
29	DC	236	GLU
29	DC	245	VAL
29	DC	265	LYS
29	DC	271	ARG
32	DD	13	ARG
32	DD	18	ASP
32	DD	32	ASN
32	DD	79	LEU
32	DD	86	GLU
32	DD	95	SER
32	DD	126	ASN
32	DD	129	THR
32	DD	131	ASP
32	DD	138	LEU
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	32	VAL
33	CE	44	ARG
33	CE	69	ARG
33	CE	72	SER
33	CE	78	TRP
33	CE	83	VAL
33	CE	107	SER
33	CE	120	VAL
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	173	THR
33	CE	176	ASP
33	CE	189	THR
34	CF	35	THR
34	CF	36	LEU
34	CF	37	ASN
34	CF	50	LEU
34	CF	57	LEU
34	CF	72	LYS
34	CF	80	ARG
34	CF	94	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	CF	98	GLU
34	CF	115	ARG
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	136	ILE
34	CF	150	ARG
34	CF	152	LEU
34	CF	174	ASP
35	CG	49	THR
35	CG	50	LEU
35	CG	56	ASP
35	CG	72	LEU
35	CG	127	THR
35	CG	155	GLU
35	CG	167	GLU
35	CG	171	THR
36	CH	3	VAL
36	CH	6	LEU
36	CH	15	LEU
36	CH	21	VAL
36	CH	48	GLU
36	CH	50	ARG
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	62	LEU
36	CH	89	LYS
36	CH	108	VAL
36	CH	110	VAL
36	CH	145	ASN
37	CJ	9	VAL
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	55	ILE
37	CJ	61	VAL
37	CJ	80	LEU
37	CJ	98	VAL
37	CJ	113	LYS
38	CK	5	THR
38	CK	7	LYS

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Mol	Chain	Res	Type
38	CK	9	GLU
38	CK	76	HIS
38	CK	124	VAL
38	CK	142	ILE
39	CL	18	ARG
39	CL	49	ARG
39	CL	58	LEU
39	CL	66	LYS
39	CL	80	ASP
39	CL	89	ASN
39	CL	91	SER
39	CL	98	ARG
40	CM	33	ARG
40	CM	40	SER
40	CM	68	SER
40	CM	92	LEU
40	CM	93	ASN
40	CM	100	ILE
40	CM	107	PHE
40	CM	115	GLU
40	CM	120	VAL
41	CN	6	ARG
41	CN	13	HIS
41	CN	20	LEU
41	CN	55	ARG
41	CN	59	ARG
41	CN	128	THR
41	CN	131	VAL
41	CN	132	THR
41	CN	134	THR
41	CN	135	VAL
42	CO	1	MET
42	CO	2	ARG
42	CO	6	SER
42	CO	14	SER
42	CO	53	THR
42	CO	59	SER
42	CO	69	ARG
42	CO	95	THR
43	CP	24	THR
43	CP	31	THR
43	CP	35	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	CP	38	GLN
43	CP	45	SER
43	CP	47	VAL
43	CP	48	LEU
43	CP	78	VAL
43	CP	106	LEU
44	CQ	10	GLN
44	CQ	39	ARG
44	CQ	63	LYS
44	CQ	65	SER
44	CQ	85	SER
44	CQ	102	GLU
44	CQ	114	LEU
44	CQ	115	ASN
45	CR	5	LYS
45	CR	6	ARG
45	CR	9	ILE
45	CR	16	LYS
45	CR	51	ARG
45	CR	64	ARG
45	CR	109	LEU
45	CR	117	LEU
46	CS	1	MET
46	CS	12	HIS
46	CS	13	ARG
46	CS	15	SER
46	CS	26	ASP
46	CS	45	GLU
46	CS	46	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	66	HIS
47	CT	29	VAL
47	CT	50	VAL
47	CT	53	SER
47	CT	59	GLU
47	CT	74	ILE
47	CT	83	LYS
47	CT	86	MET
47	CT	97	LEU
47	CT	109	ASP
47	CT	110	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG
48	CU	18	GLU
48	CU	30	ILE
48	CU	36	LYS
48	CU	49	LYS
48	CU	53	VAL
48	CU	69	ARG
48	CU	73	ARG
48	CU	79	ASP
48	CU	86	THR
48	CU	93	LEU
49	CV	9	ASP
49	CV	28	VAL
49	CV	29	LEU
49	CV	44	LYS
49	CV	52	LEU
49	CV	61	LYS
49	CV	81	ASP
49	CV	98	SER
50	CW	7	GLU
50	CW	10	LYS
50	CW	20	LEU
50	CW	53	LYS
50	CW	61	LEU
50	CW	62	THR
50	CW	68	LYS
50	CW	93	ARG
51	CX	41	ARG
51	CX	78	LYS
52	CY	4	VAL
52	CY	25	THR
52	CY	28	ARG
52	CY	71	LEU
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	22	LEU
53	CZ	58	ASN
33	DE	12	LEU
33	DE	32	VAL
33	DE	69	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	DE	88	ARG
33	DE	107	SER
33	DE	120	VAL
33	DE	122	GLU
33	DE	127	GLU
33	DE	153	LEU
33	DE	173	THR
33	DE	176	ASP
33	DE	189	THR
34	DF	10	ASP
34	DF	35	THR
34	DF	37	ASN
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	98	GLU
34	DF	117	LEU
34	DF	134	GLU
34	DF	136	ILE
34	DF	148	ARG
34	DF	150	ARG
34	DF	152	LEU
34	DF	158	THR
34	DF	174	ASP
34	DF	178	ARG
35	DG	18	LYS
35	DG	50	LEU
35	DG	56	ASP
35	DG	72	LEU
35	DG	127	THR
35	DG	155	GLU
35	DG	167	GLU
35	DG	171	THR
36	DH	3	VAL
36	DH	6	LEU
36	DH	15	LEU
36	DH	21	VAL
36	DH	48	GLU
36	DH	50	ARG
36	DH	53	GLU
36	DH	58	LEU
36	DH	62	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	DH	89	LYS
36	DH	108	VAL
36	DH	110	VAL
36	DH	145	ASN
37	DJ	9	VAL
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	55	ILE
37	DJ	61	VAL
37	DJ	80	LEU
37	DJ	98	VAL
37	DJ	113	LYS
38	DK	7	LYS
38	DK	30	THR
38	DK	76	HIS
38	DK	124	VAL
38	DK	142	ILE
39	DL	18	ARG
39	DL	49	ARG
39	DL	58	LEU
39	DL	66	LYS
39	DL	75	SER
39	DL	80	ASP
39	DL	89	ASN
39	DL	91	SER
39	DL	109	SER
39	DL	110	GLU
39	DL	113	MET
40	DM	40	SER
40	DM	86	GLU
40	DM	92	LEU
40	DM	107	PHE
40	DM	115	GLU
40	DM	120	VAL
41	DN	6	ARG
41	DN	10	ARG
41	DN	55	ARG
41	DN	58	LYS
41	DN	100	LYS
41	DN	126	ILE
41	DN	128	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	DN	131	VAL
41	DN	132	THR
41	DN	134	THR
41	DN	135	VAL
42	DO	1	MET
42	DO	2	ARG
42	DO	6	SER
42	DO	14	SER
42	DO	46	ARG
42	DO	53	THR
42	DO	59	SER
42	DO	69	ARG
43	DP	1	MET
43	DP	24	THR
43	DP	31	THR
43	DP	35	ILE
43	DP	45	SER
43	DP	47	VAL
43	DP	48	LEU
43	DP	78	VAL
43	DP	106	LEU
44	DQ	10	GLN
44	DQ	40	LEU
44	DQ	63	LYS
44	DQ	65	SER
44	DQ	85	SER
44	DQ	102	GLU
44	DQ	115	ASN
45	DR	5	LYS
45	DR	6	ARG
45	DR	51	ARG
45	DR	64	ARG
45	DR	109	LEU
45	DR	117	LEU
46	DS	1	MET
46	DS	7	SER
46	DS	13	ARG
46	DS	15	SER
46	DS	20	VAL
46	DS	26	ASP
46	DS	38	VAL
46	DS	58	VAL

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Mol	Chain	Res	Type
46	DS	66	HIS
47	DT	29	VAL
47	DT	50	VAL
47	DT	53	SER
47	DT	59	GLU
47	DT	74	ILE
47	DT	86	MET
47	DT	109	ASP
47	DT	110	ARG
48	DU	2	ILE
48	DU	3	ARG
48	DU	25	GLU
48	DU	53	VAL
48	DU	69	ARG
48	DU	74	ILE
48	DU	79	ASP
48	DU	86	THR
49	DV	26	LYS
49	DV	28	VAL
49	DV	29	LEU
49	DV	44	LYS
49	DV	61	LYS
49	DV	81	ASP
50	DW	7	GLU
50	DW	20	LEU
50	DW	53	LYS
50	DW	61	LEU
50	DW	62	THR
50	DW	93	ARG
51	DX	11	ARG
51	DX	41[A]	ARG
51	DX	41[B]	ARG
51	DX	78	LYS
52	DY	4	VAL
52	DY	25	THR
52	DY	28	ARG
52	DY	48	THR
52	DY	51	VAL
53	DZ	6	LEU
53	DZ	19	LEU
53	DZ	22	LEU
54	DI	7	ASP

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Mol	Chain	Res	Type
54	DI	23	LEU
54	DI	31	ARG
54	DI	53	ARG
54	DI	58	THR
54	DI	61	ARG
54	DI	64	VAL
54	DI	67	THR
54	DI	74	ASP
54	DI	82	ILE
54	DI	95	LEU
54	DI	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	93	ASN
2	AB	120	GLN
2	AB	177	ASN
3	AC	139	GLN
4	AD	136	GLN
4	AD	196	ASN
5	AE	82	GLN
5	AE	89	HIS
5	AE	97	GLN
6	AF	14	GLN
6	AF	63	ASN
7	AG	97	ASN
9	AI	31	ASN
10	AJ	58	ASN
11	AK	24	HIS
11	AK	101	ASN
16	AP	63	GLN
19	AS	52	HIS
19	AS	53	ASN
19	AS	56	GLN
19	AS	57	HIS
20	AT	48	GLN
22	C1	6	ASN
22	C1	42	HIS
2	BB	39	HIS
2	BB	93	ASN

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Mol	Chain	Res	Type
2	BB	120	GLN
2	BB	177	ASN
3	BC	139	GLN
5	BE	82	GLN
5	BE	89	HIS
5	BE	97	GLN
6	BF	14	GLN
7	BG	97	ASN
7	BG	142	HIS
9	BI	31	ASN
11	BK	101	ASN
16	BP	63	GLN
19	BS	53	ASN
19	BS	57	HIS
20	BT	13	GLN
20	BT	20	HIS
29	CC	45	ASN
29	CC	70	ASN
30	CD	130	GLN
30	CD	150	GLN
30	CD	164	GLN
29	DC	45	ASN
29	DC	70	ASN
34	CF	27	GLN
35	CG	38	ASN
37	CJ	43	ASN
38	CK	47	HIS
40	CM	38	GLN
43	CP	100	HIS
49	CV	74	ASN
52	CY	16	ASN
35	DG	22	GLN
37	DJ	30	GLN
37	DJ	43	ASN
38	DK	47	HIS
41	DN	60	GLN
42	DO	13	ASN
43	DP	38	GLN
44	DQ	115	ASN
45	DR	56	GLN
49	DV	54	GLN
50	DW	24	ASN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	296 (19%)	48 (3%)
1	BA	1529/1534 (99%)	300 (19%)	52 (3%)
28	CB	117/120 (97%)	13 (11%)	2 (1%)
28	DB	119/120 (99%)	13 (10%)	1 (0%)
31	CA	2892/2904 (99%)	572 (19%)	110 (3%)
55	DA	2880/2904 (99%)	490 (17%)	73 (2%)
All	All	9067/9116 (99%)	1684 (18%)	286 (3%)

All (1684) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	49	U
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	79	G
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U

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Mol	Chain	Res	Type
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	119	A
1	AA	120	A
1	AA	127	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	146	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	189	A
1	AA	197	A
1	AA	200	G
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	306	A
1	AA	308	C
1	AA	321	A
1	AA	328	C
1	AA	329	A

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Mol	Chain	Res	Type
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	368	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	396	C
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	467	U
1	AA	468	A
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	505	G
1	AA	509	A
1	AA	511	C
1	AA	521	G
1	AA	524	G
1	AA	527	7MG
1	AA	530	G
1	AA	531	U
1	AA	533	A
1	AA	547	A

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Mol	Chain	Res	Type
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	615	G
1	AA	633	G
1	AA	639	G
1	AA	642	A
1	AA	650	G
1	AA	653	U
1	AA	656	G
1	AA	665	A
1	AA	671	G
1	AA	675	A
1	AA	677	U
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	758	C
1	AA	774	G
1	AA	777	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	809	G
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U

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Mol	Chain	Res	Type
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	884	U
1	AA	902	G
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	955	U
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	985	C
1	AA	987	G
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1053	G
1	AA	1054	C

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Mol	Chain	Res	Type
1	AA	1055	A
1	AA	1064	G
1	AA	1065	U
1	AA	1070	U
1	AA	1086	U
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1145	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1182	G
1	AA	1183	U
1	AA	1184	G
1	AA	1186	G
1	AA	1196	A
1	AA	1197	A
1	AA	1198	G
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1221	G
1	AA	1224	U
1	AA	1225	A

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Mol	Chain	Res	Type
1	AA	1226	C
1	AA	1227	A
1	AA	1233	G
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1258	G
1	AA	1260	G
1	AA	1274	A
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1323	G
1	AA	1338	G
1	AA	1351	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1422	G
1	AA	1441	A
1	AA	1446	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1483	A

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Mol	Chain	Res	Type
1	AA	1484	C
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	5	U
1	BA	6	G
1	BA	7	A
1	BA	8	A
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	31	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	49	U
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	54	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	79	G
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G

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Mol	Chain	Res	Type
1	BA	87	C
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	119	A
1	BA	120	A
1	BA	127	G
1	BA	128	G
1	BA	130	A
1	BA	131	A
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	146	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	189	A
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	306	A
1	BA	308	C
1	BA	321	A
1	BA	328	C

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Mol	Chain	Res	Type
1	BA	329	A
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	368	U
1	BA	372	C
1	BA	373	A
1	BA	376	G
1	BA	384	G
1	BA	396	C
1	BA	397	A
1	BA	398	U
1	BA	406	G
1	BA	411	A
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	436	C
1	BA	451	A
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	505	G
1	BA	509	A
1	BA	511	C
1	BA	521	G
1	BA	524	G
1	BA	525	C
1	BA	527	7MG
1	BA	530	G

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Mol	Chain	Res	Type
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	564	C
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	596	A
1	BA	615	G
1	BA	633	G
1	BA	639	G
1	BA	642	A
1	BA	650	G
1	BA	653	U
1	BA	656	G
1	BA	665	A
1	BA	671	G
1	BA	675	A
1	BA	677	U
1	BA	702	A
1	BA	703	G
1	BA	721	G
1	BA	723	U
1	BA	724	G
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	758	C
1	BA	774	G
1	BA	777	A
1	BA	782	A
1	BA	793	U
1	BA	794	A
1	BA	809	G
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U

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Mol	Chain	Res	Type
1	BA	832	G
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	845	A
1	BA	846	G
1	BA	902	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	942	G
1	BA	955	U
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	972	C
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	985	C
1	BA	987	G
1	BA	992	U
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G

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Mol	Chain	Res	Type
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1044	A
1	BA	1053	G
1	BA	1054	C
1	BA	1055	A
1	BA	1064	G
1	BA	1065	U
1	BA	1066	C
1	BA	1086	U
1	BA	1089	G
1	BA	1094	G
1	BA	1095	U
1	BA	1101	A
1	BA	1104	G
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1182	G
1	BA	1183	U
1	BA	1186	G
1	BA	1196	A
1	BA	1197	A
1	BA	1198	G
1	BA	1201	A
1	BA	1202	U
1	BA	1212	U
1	BA	1213	A

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Mol	Chain	Res	Type
1	BA	1214	C
1	BA	1215	G
1	BA	1221	G
1	BA	1224	U
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1233	G
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1258	G
1	BA	1260	G
1	BA	1261	A
1	BA	1274	A
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1318	A
1	BA	1319	A
1	BA	1320	C
1	BA	1323	G
1	BA	1337	G
1	BA	1338	G
1	BA	1351	U
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1419	G
1	BA	1422	G
1	BA	1441	A

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Mol	Chain	Res	Type
1	BA	1446	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1483	A
1	BA	1484	C
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1505	G
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	51	G
28	CB	56	G
28	CB	57	A
28	CB	87	U
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	13	A
31	CA	34	U
31	CA	36	G
31	CA	39	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	71	A

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Mol	Chain	Res	Type
31	CA	73	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	86	G
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	177	G
31	CA	178	G
31	CA	186	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	201	C
31	CA	204	A
31	CA	215	G
31	CA	216	A
31	CA	222	A
31	CA	245	G
31	CA	248	G
31	CA	250	G
31	CA	265	A
31	CA	266	G
31	CA	267	C
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	285	G
31	CA	310	A
31	CA	311	A

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Mol	Chain	Res	Type
31	CA	317	G
31	CA	324	A
31	CA	329	G
31	CA	330	A
31	CA	331	C
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	361	G
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	383	C
31	CA	385	C
31	CA	386	G
31	CA	391	A
31	CA	396	G
31	CA	399	U
31	CA	403	U
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	435	C
31	CA	451	U
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	475	C
31	CA	479	A
31	CA	480	A
31	CA	481	G
31	CA	482	A
31	CA	491	G
31	CA	496	G
31	CA	501	A
31	CA	504	A
31	CA	505	A
31	CA	507	A
31	CA	508	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	CA	527	C
31	CA	528	A
31	CA	529	A
31	CA	531	C
31	CA	532	A
31	CA	533	G
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	548	G
31	CA	549	G
31	CA	550	C
31	CA	563	A
31	CA	569	U
31	CA	572	A
31	CA	573	U
31	CA	574	A
31	CA	575	A
31	CA	586	A
31	CA	592	A
31	CA	603	A
31	CA	614	A
31	CA	615	U
31	CA	620	G
31	CA	621	A
31	CA	622	G
31	CA	627	A
31	CA	628	G
31	CA	632	A
31	CA	634	C
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	651	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	659	G
31	CA	669	G
31	CA	670	A
31	CA	684	G

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Mol	Chain	Res	Type
31	CA	685	A
31	CA	686	U
31	CA	694	U
31	CA	695	G
31	CA	696	G
31	CA	701	G
31	CA	702	U
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	763	G
31	CA	764	A
31	CA	765	C
31	CA	774	G
31	CA	775	G
31	CA	776	G
31	CA	781	A
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	800	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	831	G
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	866	A
31	CA	869	G
31	CA	878	A
31	CA	882	G
31	CA	896	A
31	CA	897	C
31	CA	907	G

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Mol	Chain	Res	Type
31	CA	910	A
31	CA	914	G
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	957	C
31	CA	961	C
31	CA	973	A
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	999	U
31	CA	1009	A
31	CA	1012	U
31	CA	1013	C
31	CA	1017	G
31	CA	1020	A
31	CA	1021	A
31	CA	1022	G
31	CA	1024	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1051	G
31	CA	1061	U
31	CA	1062	G
31	CA	1068	G
31	CA	1069	A
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1090	A
31	CA	1097	U

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Mol	Chain	Res	Type
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1141	U
31	CA	1142	A
31	CA	1143	A
31	CA	1151	A
31	CA	1168	G
31	CA	1169	A
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1244	A
31	CA	1247	A
31	CA	1248	G
31	CA	1250	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1288	G
31	CA	1289	C
31	CA	1294	U
31	CA	1300	G
31	CA	1301	A
31	CA	1306	C

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Mol	Chain	Res	Type
31	CA	1312	U
31	CA	1313	U
31	CA	1321	A
31	CA	1328	A
31	CA	1329	U
31	CA	1330	C
31	CA	1332	G
31	CA	1344	U
31	CA	1352	U
31	CA	1355	G
31	CA	1359	A
31	CA	1365	A
31	CA	1370	C
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1386	C
31	CA	1395	A
31	CA	1398	C
31	CA	1403	A
31	CA	1416	G
31	CA	1417	C
31	CA	1420	A
31	CA	1424	G
31	CA	1427	A
31	CA	1428	C
31	CA	1434	A
31	CA	1437	C
31	CA	1452	G
31	CA	1458	U
31	CA	1460	U
31	CA	1478	G
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1504	A
31	CA	1509	A
31	CA	1510	G

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Mol	Chain	Res	Type
31	CA	1515	A
31	CA	1522	A
31	CA	1523	U
31	CA	1529	G
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1544	A
31	CA	1555	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1611	C
31	CA	1613	G
31	CA	1617	C
31	CA	1634	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1663	G
31	CA	1664	A
31	CA	1674	G
31	CA	1677	A
31	CA	1694	C
31	CA	1697	G
31	CA	1698	A
31	CA	1699	G
31	CA	1703	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1754	A

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Mol	Chain	Res	Type
31	CA	1758	U
31	CA	1764	C
31	CA	1773	A
31	CA	1781	U
31	CA	1782	U
31	CA	1784	A
31	CA	1786	A
31	CA	1787	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U
31	CA	1815	A
31	CA	1816	C
31	CA	1821	A
31	CA	1822	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1833	C
31	CA	1834	U
31	CA	1839	G
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1902	C
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1928	A
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1934	C
31	CA	1938	A
31	CA	1940	U
31	CA	1955	U

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Mol	Chain	Res	Type
31	CA	1965	C
31	CA	1966	A
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1992	G
31	CA	1993	U
31	CA	1997	C
31	CA	2020	A
31	CA	2022	U
31	CA	2023	C
31	CA	2027	G
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2046	G
31	CA	2049	G
31	CA	2051	A
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	7MG
31	CA	2072	C
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2101	A
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A

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Mol	Chain	Res	Type
31	CA	2120	G
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2145	C
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2161	C
31	CA	2162	G
31	CA	2163	A
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2243	U
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2282	G
31	CA	2283	C
31	CA	2287	A

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Mol	Chain	Res	Type
31	CA	2288	A
31	CA	2305	U
31	CA	2311	A
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2357	G
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2436	G
31	CA	2441	U
31	CA	2446	G
31	CA	2448	A
31	CA	2449	U
31	CA	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2491	U
31	CA	2498	OMC
31	CA	2502	G
31	CA	2505	G
31	CA	2512	C
31	CA	2513	A
31	CA	2518	A

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Mol	Chain	Res	Type
31	CA	2520	C
31	CA	2529	G
31	CA	2535	G
31	CA	2543	G
31	CA	2544	G
31	CA	2547	A
31	CA	2554	U
31	CA	2564	A
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2582	G
31	CA	2585	U
31	CA	2600	A
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2673	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2733	A
31	CA	2744	G
31	CA	2748	A
31	CA	2762	C
31	CA	2765	A
31	CA	2776	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2791	G
31	CA	2794	C
31	CA	2798	U

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Mol	Chain	Res	Type
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2867	G
31	CA	2870	C
31	CA	2872	A
31	CA	2879	A
31	CA	2883	A
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G
28	DB	25	U
28	DB	35	C
28	DB	37	C
28	DB	44	G
28	DB	45	A
28	DB	51	G
28	DB	56	G
28	DB	57	A
28	DB	87	U
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	13	A
55	DA	14	A
55	DA	15	G
55	DA	34	U
55	DA	46	G
55	DA	58	G
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G

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Mol	Chain	Res	Type
55	DA	84	A
55	DA	86	G
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	125	A
55	DA	137	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	186	G
55	DA	188	G
55	DA	193	U
55	DA	196	A
55	DA	197	A
55	DA	198	C
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	230	G
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	267	C
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	285	G
55	DA	302	C
55	DA	311	A
55	DA	317	G
55	DA	324	A
55	DA	329	G
55	DA	330	A

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Mol	Chain	Res	Type
55	DA	331	C
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	361	G
55	DA	362	A
55	DA	372	G
55	DA	383	C
55	DA	386	G
55	DA	396	G
55	DA	399	U
55	DA	403	U
55	DA	406	G
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	435	C
55	DA	451	U
55	DA	455	C
55	DA	456	C
55	DA	459	U
55	DA	475	C
55	DA	479	A
55	DA	480	A
55	DA	481	G
55	DA	482	A
55	DA	491	G
55	DA	496	G
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	510	C
55	DA	513	A
55	DA	531	C
55	DA	532	A
55	DA	533	G
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A

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Mol	Chain	Res	Type
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	620	G
55	DA	622	G
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	651	G
55	DA	653	U
55	DA	654	A
55	DA	655	A
55	DA	659	G
55	DA	684	G
55	DA	685	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	738	G
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	772	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	783	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	801	G
55	DA	802	A
55	DA	805	G

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Mol	Chain	Res	Type
55	DA	806	C
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	866	A
55	DA	878	A
55	DA	882	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	907	G
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	947	A
55	DA	957	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	984	A
55	DA	985	C
55	DA	996	A
55	DA	1010	A
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1023	U
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1061	U
55	DA	1062	G
55	DA	1068	G
55	DA	1069	A
55	DA	1070	A
55	DA	1073	A

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Mol	Chain	Res	Type
55	DA	1083	U
55	DA	1088	A
55	DA	1090	A
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1119	U
55	DA	1128	G
55	DA	1129	A
55	DA	1132	U
55	DA	1133	A
55	DA	1135	C
55	DA	1136	G
55	DA	1141	U
55	DA	1142	A
55	DA	1151	A
55	DA	1168	G
55	DA	1172	C
55	DA	1174	U
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1212	G
55	DA	1238	G
55	DA	1244	A
55	DA	1250	G
55	DA	1253	A
55	DA	1256	G
55	DA	1262	A
55	DA	1269	A
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1294	U
55	DA	1297	C
55	DA	1300	G
55	DA	1301	A
55	DA	1306	C
55	DA	1321	A
55	DA	1328	A
55	DA	1332	G
55	DA	1352	U

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Mol	Chain	Res	Type
55	DA	1355	G
55	DA	1359	A
55	DA	1365	A
55	DA	1379	U
55	DA	1383	A
55	DA	1386	C
55	DA	1398	C
55	DA	1403	A
55	DA	1416	G
55	DA	1417	C
55	DA	1420	A
55	DA	1427	A
55	DA	1428	C
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1478	G
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1504	A
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1529	G
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1537	G
55	DA	1544	A
55	DA	1554	U
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C

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Mol	Chain	Res	Type
55	DA	1608	A
55	DA	1613	G
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1663	G
55	DA	1674	G
55	DA	1694	C
55	DA	1699	G
55	DA	1715	G
55	DA	1729	U
55	DA	1730	C
55	DA	1738	G
55	DA	1744	A
55	DA	1750	G
55	DA	1758	U
55	DA	1764	C
55	DA	1773	A
55	DA	1781	U
55	DA	1782	U
55	DA	1786	A
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1812	U
55	DA	1816	C
55	DA	1826	G
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1900	A
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1927	A
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U

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Mol	Chain	Res	Type
55	DA	1932	A
55	DA	1938	A
55	DA	1941	C
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1974	C
55	DA	1991	U
55	DA	1992	G
55	DA	1993	U
55	DA	1997	C
55	DA	2020	A
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2049	G
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	7MG
55	DA	2093	G
55	DA	2095	A
55	DA	2097	A
55	DA	2100	G
55	DA	2101	A
55	DA	2105	U
55	DA	2108	A
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2121	G
55	DA	2123	G

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Mol	Chain	Res	Type
55	DA	2125	G
55	DA	2126	A
55	DA	2127	G
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2147	A
55	DA	2148	G
55	DA	2157	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2185	U
55	DA	2186	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2278	A

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Mol	Chain	Res	Type
55	DA	2280	G
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2288	A
55	DA	2292	U
55	DA	2305	U
55	DA	2308	G
55	DA	2311	A
55	DA	2312	U
55	DA	2320	U
55	DA	2325	G
55	DA	2327	A
55	DA	2328	A
55	DA	2331	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2350	C
55	DA	2357	G
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2410	G
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2426	A
55	DA	2427	C
55	DA	2434	A
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2464	G
55	DA	2465	C
55	DA	2469	A
55	DA	2474	U
55	DA	2476	A
55	DA	2478	A
55	DA	2480	C

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Mol	Chain	Res	Type
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G
55	DA	2518	A
55	DA	2520	C
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2564	A
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2578	G
55	DA	2582	G
55	DA	2585	U
55	DA	2586	U
55	DA	2596	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2621	G
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2673	G
55	DA	2689	U
55	DA	2690	U
55	DA	2706	A
55	DA	2714	G
55	DA	2719	G
55	DA	2720	U
55	DA	2721	A
55	DA	2726	A
55	DA	2729	G
55	DA	2733	A
55	DA	2744	G
55	DA	2748	A
55	DA	2762	C
55	DA	2765	A
55	DA	2769	U
55	DA	2778	A

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Mol	Chain	Res	Type
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2811	G
55	DA	2815	C
55	DA	2818	U
55	DA	2820	A
55	DA	2821	A
55	DA	2825	G
55	DA	2835	A
55	DA	2836	U
55	DA	2861	U
55	DA	2867	G
55	DA	2872	A
55	DA	2879	A
55	DA	2883	A

All (286) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	30	U
1	AA	49	U
1	AA	70	U
1	AA	89	U
1	AA	142	G
1	AA	209	U
1	AA	250	A
1	AA	305	G
1	AA	327	A
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	438	U
1	AA	518	C
1	AA	559	A
1	AA	576	C
1	AA	641	U
1	AA	702	A
1	AA	733	G
1	AA	793	U

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Mol	Chain	Res	Type
1	AA	841	C
1	AA	870	U
1	AA	884	U
1	AA	965	U
1	AA	971	G
1	AA	974	A
1	AA	991	U
1	AA	992	U
1	AA	1053	G
1	AA	1129	C
1	AA	1136	C
1	AA	1137	C
1	AA	1140	C
1	AA	1141	C
1	AA	1195	C
1	AA	1197	A
1	AA	1224	U
1	AA	1225	A
1	AA	1278	G
1	AA	1281	C
1	AA	1319	A
1	AA	1345	U
1	AA	1380	U
1	AA	1397	C
1	AA	1432	G
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	30	U
1	BA	49	U
1	BA	70	U
1	BA	83	C
1	BA	86	G
1	BA	89	U
1	BA	142	G
1	BA	209	U
1	BA	246	A
1	BA	250	A
1	BA	305	G
1	BA	327	A
1	BA	367	U
1	BA	422	C

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Mol	Chain	Res	Type
1	BA	438	U
1	BA	518	C
1	BA	559	A
1	BA	561	U
1	BA	576	C
1	BA	641	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	870	U
1	BA	884	U
1	BA	965	U
1	BA	971	G
1	BA	974	A
1	BA	991	U
1	BA	992	U
1	BA	1008	U
1	BA	1053	G
1	BA	1129	C
1	BA	1136	C
1	BA	1137	C
1	BA	1140	C
1	BA	1141	C
1	BA	1196	A
1	BA	1224	U
1	BA	1225	A
1	BA	1278	G
1	BA	1281	C
1	BA	1319	A
1	BA	1345	U
1	BA	1362	A
1	BA	1363	A
1	BA	1380	U
1	BA	1397	C
1	BA	1452	C
28	CB	51	G
28	CB	89	U
31	CA	83	A
31	CA	137	U
31	CA	138	U
31	CA	139	U

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Mol	Chain	Res	Type
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	215	G
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	361	G
31	CA	386	G
31	CA	390	U
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	531	C
31	CA	571	U
31	CA	572	A
31	CA	573	U
31	CA	603	A
31	CA	620	G
31	CA	637	A
31	CA	669	G
31	CA	684	G
31	CA	685	A
31	CA	752	A
31	CA	764	A
31	CA	774	G
31	CA	781	A
31	CA	784	G
31	CA	827	U
31	CA	846	U
31	CA	913	U
31	CA	945	A
31	CA	957	C
31	CA	973	A
31	CA	984	A
31	CA	1021	A

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Mol	Chain	Res	Type
31	CA	1045	C
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1087	G
31	CA	1089	A
31	CA	1128	G
31	CA	1133	A
31	CA	1141	U
31	CA	1212	G
31	CA	1247	A
31	CA	1288	G
31	CA	1300	G
31	CA	1329	U
31	CA	1379	U
31	CA	1397	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1776	G
31	CA	1786	A
31	CA	1800	C
31	CA	1818	U
31	CA	1838	C
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1937	A
31	CA	1970	A
31	CA	2035	G
31	CA	2043	C
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2145	C
31	CA	2146	C
31	CA	2157	G

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Mol	Chain	Res	Type
31	CA	2164	C
31	CA	2225	A
31	CA	2238	G
31	CA	2282	G
31	CA	2286	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2426	A
31	CA	2448	A
31	CA	2468	A
31	CA	2542	A
31	CA	2572	A
31	CA	2645	G
31	CA	2680	U
31	CA	2776	A
31	CA	2778	A
31	CA	2779	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
28	DB	51	G
55	DA	119	A
55	DA	125	A
55	DA	137	U
55	DA	138	U
55	DA	141	G
55	DA	177	G
55	DA	196	A
55	DA	199	A
55	DA	215	G
55	DA	271	G
55	DA	278	A
55	DA	345	A
55	DA	361	G
55	DA	403	U
55	DA	411	G
55	DA	455	C
55	DA	503	A
55	DA	512	G
55	DA	603	A

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Mol	Chain	Res	Type
55	DA	614	A
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	858	G
55	DA	945	A
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1089	A
55	DA	1128	G
55	DA	1133	A
55	DA	1171	G
55	DA	1300	G
55	DA	1329	U
55	DA	1396	U
55	DA	1397	U
55	DA	1420	A
55	DA	1427	A
55	DA	1490	A
55	DA	1509	A
55	DA	1535	A
55	DA	1558	C
55	DA	1607	C
55	DA	1647	U
55	DA	1786	A
55	DA	1800	C
55	DA	1870	C
55	DA	1871	A
55	DA	1900	A
55	DA	1939	5MU
55	DA	2035	G
55	DA	2051	A
55	DA	2097	A
55	DA	2119	A
55	DA	2126	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A

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Mol	Chain	Res	Type
55	DA	2164	C
55	DA	2238	G
55	DA	2282	G
55	DA	2286	G
55	DA	2311	A
55	DA	2406	A
55	DA	2423	U
55	DA	2572	A
55	DA	2581	G
55	DA	2585	U
55	DA	2866	U
55	DA	2873	A

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

75 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	AA	1207	1	18,26,27	1.12	2 (11%)	21,38,41	2.57	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.79	0	21,32,35	1.28	3 (14%)
1	5MC	AA	1407	1	14,22,23	0.83	1 (7%)	17,32,35	0.74	1 (5%)
1	UR3	AA	1498	1	13,22,23	0.99	1 (7%)	18,32,35	0.76	1 (5%)
1	2MG	AA	1516	1	18,26,27	1.08	2 (11%)	21,38,41	2.55	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.62	0	15,38,41	0.56	0
1	MA6	AA	1519	1	18,26,27	0.78	0	15,38,41	0.64	0
1	PSU	AA	516	1,56	15,21,22	1.36	3 (20%)	16,30,33	3.50	2 (12%)
1	7MG	AA	527	1	20,26,27	2.27	4 (20%)	23,39,42	3.10	5 (21%)
1	2MG	AA	966	1	18,26,27	1.30	2 (11%)	21,38,41	2.50	4 (19%)
1	5MC	AA	967	1	14,22,23	0.89	1 (7%)	17,32,35	0.69	1 (5%)
12	D2T	AL	89	12	4,9,10	0.54	0	4,11,13	1.46	1 (25%)
1	2MG	BA	1207	1	18,26,27	1.16	2 (11%)	21,38,41	2.56	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	BA	1402	1	15,23,24	0.80	0	21,32,35	1.25	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.93	1 (7%)	17,32,35	0.69	1 (5%)
1	UR3	BA	1498	1	13,22,23	0.99	1 (7%)	18,32,35	0.76	0
1	2MG	BA	1516	1	18,26,27	1.14	2 (11%)	21,38,41	2.60	4 (19%)
1	MA6	BA	1518	1	18,26,27	0.62	0	15,38,41	0.54	0
1	MA6	BA	1519	1	18,26,27	0.73	0	15,38,41	0.65	0
1	PSU	BA	516	1	15,21,22	1.34	3 (20%)	16,30,33	3.48	2 (12%)
1	7MG	BA	527	1	20,26,27	2.30	4 (20%)	23,39,42	2.83	5 (21%)
1	2MG	BA	966	1	18,26,27	1.24	2 (11%)	21,38,41	2.57	4 (19%)
1	5MC	BA	967	1	14,22,23	0.90	0	17,32,35	0.68	1 (5%)
12	D2T	BL	89	12	4,9,10	0.61	0	4,11,13	1.49	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.71	0	15,36,39	0.69	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.10	1 (5%)	21,38,41	2.56	4 (19%)
31	PSU	CA	1911	31	15,21,22	1.20	2 (13%)	16,30,33	3.48	2 (12%)
31	3TD	CA	1915	31	15,22,23	1.11	3 (20%)	17,32,35	1.11	2 (11%)
31	PSU	CA	1917	31	15,21,22	1.23	2 (13%)	16,30,33	3.48	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.06	1 (7%)	16,32,35	4.74	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.77	1 (7%)	17,32,35	0.70	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.65	0	15,36,39	0.82	1 (6%)
31	7MG	CA	2069	31	20,26,27	2.26	5 (25%)	23,39,42	2.79	4 (17%)
31	OMG	CA	2251	31	18,26,27	1.14	2 (11%)	21,38,41	2.74	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.10	1 (5%)	21,38,41	2.48	3 (14%)
31	PSU	CA	2457	31	15,21,22	1.43	3 (20%)	16,30,33	3.48	1 (6%)
31	OMC	CA	2498	31,56	15,22,23	0.88	1 (6%)	20,31,34	0.49	0
31	2MA	CA	2503	31	17,25,26	0.96	0	18,37,40	1.24	4 (22%)
31	PSU	CA	2504	31	15,21,22	1.13	2 (13%)	16,30,33	3.47	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.21	2 (14%)	19,31,34	2.94	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.28	2 (13%)	16,30,33	3.59	3 (18%)
31	PSU	CA	2605	31	15,21,22	1.15	2 (13%)	16,30,33	3.51	1 (6%)
31	1MG	CA	745	31	17,26,27	1.14	2 (11%)	19,39,42	1.16	2 (10%)
31	PSU	CA	746	31,56	15,21,22	1.31	2 (13%)	16,30,33	3.50	1 (6%)
31	5MU	CA	747	31	13,22,23	1.07	1 (7%)	16,32,35	4.78	3 (18%)
31	PSU	CA	955	31	15,21,22	1.11	2 (13%)	16,30,33	3.47	2 (12%)
41	4D4	CN	81	41	7,11,12	0.63	0	5,13,15	1.06	0
55	6MZ	DA	1618	55	17,25,26	1.04	0	15,36,39	0.72	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	2MG	DA	1835	55	18,26,27	1.18	2 (11%)	21,38,41	2.60	4 (19%)
55	PSU	DA	1911	55	15,21,22	1.23	2 (13%)	16,30,33	3.44	2 (12%)
55	3TD	DA	1915	55	15,22,23	1.03	1 (6%)	17,32,35	1.13	2 (11%)
55	PSU	DA	1917	55	15,21,22	1.35	3 (20%)	16,30,33	3.45	1 (6%)
55	5MU	DA	1939	55	13,22,23	1.51	2 (15%)	16,32,35	4.79	3 (18%)
55	5MC	DA	1962	55	14,22,23	0.97	1 (7%)	17,32,35	0.72	1 (5%)
55	6MZ	DA	2030	55	17,25,26	0.71	0	15,36,39	0.67	0
55	7MG	DA	2069	55	20,26,27	2.34	4 (20%)	23,39,42	2.98	3 (13%)
55	OMG	DA	2251	55	18,26,27	0.92	1 (5%)	21,38,41	2.72	4 (19%)
55	2MG	DA	2445	55	18,26,27	1.02	1 (5%)	21,38,41	2.57	4 (19%)
55	H2U	DA	2449	55	17,21,22	0.59	0	23,30,33	0.52	0
55	PSU	DA	2457	55	15,21,22	1.36	3 (20%)	16,30,33	3.47	1 (6%)
55	OMC	DA	2498	55,56	15,22,23	0.98	1 (6%)	20,31,34	0.55	0
55	2MA	DA	2503	55,56	17,25,26	0.86	0	18,37,40	1.13	2 (11%)
55	PSU	DA	2504	55	15,21,22	1.15	2 (13%)	16,30,33	3.47	1 (6%)
55	OMU	DA	2552	55	14,22,23	1.15	2 (14%)	19,31,34	2.94	2 (10%)
55	PSU	DA	2580	55	15,21,22	1.25	2 (13%)	16,30,33	3.59	2 (12%)
55	PSU	DA	2604	55	15,21,22	1.49	4 (26%)	16,30,33	3.53	1 (6%)
55	PSU	DA	2605	55	15,21,22	1.21	2 (13%)	16,30,33	3.44	1 (6%)
55	1MG	DA	745	55	17,26,27	1.11	1 (5%)	19,39,42	1.05	2 (10%)
55	PSU	DA	746	55,56	15,21,22	1.78	3 (20%)	16,30,33	3.53	2 (12%)
55	5MU	DA	747	55	13,22,23	1.20	2 (15%)	16,32,35	4.80	3 (18%)
55	PSU	DA	955	55	15,21,22	1.41	3 (20%)	16,30,33	3.52	3 (18%)
32	MEQ	DD	150[A]	32	7,9,10	0.34	0	8,10,12	1.89	1 (12%)
32	MEQ	DD	150[B]	32	7,9,10	1.69	1 (14%)	8,10,12	1.89	2 (25%)
41	4D4	DN	81[A]	-	7,11,12	0.96	1 (14%)	5,13,15	1.12	1 (20%)
41	4D4	DN	81[B]	-	7,11,12	1.13	1 (14%)	5,13,15	0.91	0

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	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	AL	89	12	-	0/2/12/14	0/0/0/0
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	BA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	BA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	7MG	BA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	7MG	CA	2069	31	-	0/7/37/38	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/5/27/28	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/5/27/28	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	31,56	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
41	4D4	CN	81	41	-	0/8/12/14	0/0/0/0
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	2MG	DA	1835	55	-	0/5/27/28	0/3/3/3
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/3/25/26	0/2/2/2
55	5MC	DA	1962	55	-	0/3/25/26	0/2/2/2
55	6MZ	DA	2030	55	-	0/5/27/28	0/3/3/3
55	7MG	DA	2069	55	-	0/7/37/38	0/3/3/3
55	OMG	DA	2251	55	-	0/5/27/28	0/3/3/3
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/5/27/28	0/2/2/2
55	2MA	DA	2503	55,56	-	0/3/25/26	0/3/3/3
55	PSU	DA	2504	55	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/5/27/28	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
55	PSU	DA	746	55,56	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/3/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	0/7/9/11	0/0/0/0
32	MEQ	DD	150[B]	32	-	0/7/9/11	0/0/0/0
41	4D4	DN	81[A]	-	-	0/8/12/14	0/0/0/0
41	4D4	DN	81[B]	-	-	0/8/12/14	0/0/0/0

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2069	7MG	C8-N9	-8.61	1.33	1.45
1	BA	527	7MG	C8-N9	-8.55	1.33	1.45
31	CA	2069	7MG	C8-N9	-8.30	1.33	1.45
1	AA	527	7MG	C8-N9	-8.28	1.33	1.45
55	DA	746	PSU	O4'-C1'	-3.85	1.38	1.44
55	DA	746	PSU	C2'-C1'	-3.47	1.50	1.53
55	DA	1939	5MU	C2'-C1'	-3.16	1.48	1.53
55	DA	2604	PSU	C5-C1'	-2.77	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	516	PSU	C5-C1'	-2.50	1.50	1.52
55	DA	1917	PSU	C5-C1'	-2.48	1.50	1.52
31	CA	2069	7MG	C8-N7	-2.46	1.32	1.43
31	CA	746	PSU	O4'-C1'	-2.40	1.40	1.44
1	AA	527	7MG	C8-N7	-2.40	1.32	1.43
55	DA	2604	PSU	O3'-C3'	-2.38	1.37	1.43
55	DA	2604	PSU	C6-C5	-2.31	1.35	1.38
55	DA	955	PSU	C6-C5	-2.31	1.35	1.38
55	DA	955	PSU	C2'-C1'	-2.30	1.51	1.53
55	DA	2457	PSU	C5-C1'	-2.22	1.50	1.52
31	CA	1915	3TD	C6-C5	-2.21	1.35	1.38
55	DA	747	5MU	C6-C5	-2.20	1.34	1.40
55	DA	1911	PSU	C6-C5	-2.20	1.35	1.38
55	DA	2457	PSU	C6-C5	-2.19	1.35	1.38
1	BA	527	7MG	C8-N7	-2.19	1.33	1.43
55	DA	1915	3TD	C6-C5	-2.19	1.35	1.38
1	BA	516	PSU	C5-C1'	-2.18	1.50	1.52
1	BA	516	PSU	C6-C5	-2.18	1.35	1.38
55	DA	2069	7MG	C8-N7	-2.17	1.33	1.43
31	CA	1917	PSU	C6-C5	-2.15	1.35	1.38
31	CA	1911	PSU	C6-C5	-2.15	1.35	1.38
1	AA	516	PSU	C6-C5	-2.12	1.35	1.38
31	CA	2069	7MG	C1'-N9	-2.11	1.40	1.44
55	DA	1962	5MC	C6-C5	-2.11	1.34	1.40
55	DA	2504	PSU	C6-C5	-2.10	1.35	1.38
31	CA	2457	PSU	C6-C5	-2.09	1.35	1.38
55	DA	1917	PSU	C6-C5	-2.09	1.35	1.38
55	DA	2605	PSU	C6-C5	-2.08	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.08	1.35	1.38
1	AA	1407	5MC	C6-C5	-2.07	1.34	1.40
31	CA	1962	5MC	C6-C5	-2.05	1.34	1.40
31	CA	2457	PSU	C5-C1'	-2.05	1.50	1.52
31	CA	2504	PSU	C6-C5	-2.04	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.04	1.34	1.40
31	CA	2580	PSU	O4'-C1'	-2.04	1.41	1.44
31	CA	955	PSU	C6-C5	-2.03	1.35	1.38
31	CA	1915	3TD	C5-C1'	-2.02	1.50	1.52
55	DA	2580	PSU	C6-C5	-2.01	1.35	1.38
1	AA	967	5MC	C6-C5	-2.00	1.34	1.40
55	DA	2498	OMC	C6-N1	2.06	1.38	1.35
31	CA	745	1MG	C6-N1	2.06	1.41	1.38
31	CA	2251	OMG	C6-C5	2.08	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2069	7MG	C6-C5	2.15	1.44	1.41
31	CA	2498	OMC	C6-N1	2.15	1.38	1.35
55	DA	745	1MG	C6-C5	2.17	1.45	1.40
41	DN	81[A]	4D4	CB-CA	2.23	1.58	1.54
31	CA	1915	3TD	C4-N3	2.27	1.41	1.38
1	AA	1207	2MG	C6-C5	2.27	1.45	1.41
1	BA	1516	2MG	C6-C5	2.29	1.45	1.41
1	AA	1516	2MG	C6-C5	2.31	1.46	1.41
31	CA	2552	OMU	C6-N1	2.33	1.38	1.35
1	BA	1498	UR3	C6-N1	2.43	1.38	1.35
1	BA	1207	2MG	C6-C5	2.44	1.46	1.41
55	DA	2552	OMU	C6-N1	2.45	1.38	1.35
1	AA	527	7MG	C6-C5	2.58	1.45	1.41
55	DA	1835	2MG	C6-C5	2.63	1.46	1.41
1	BA	966	2MG	C6-C5	2.69	1.46	1.41
55	DA	2604	PSU	C4-N3	2.69	1.37	1.33
55	DA	2445	2MG	C6-N1	2.70	1.37	1.33
41	DN	81[B]	4D4	CB-CA	2.74	1.59	1.54
55	DA	1835	2MG	C6-N1	2.77	1.38	1.33
55	DA	2552	OMU	C4-N3	2.78	1.38	1.33
1	AA	1498	UR3	C6-N1	2.81	1.39	1.35
55	DA	747	5MU	C4-N3	2.91	1.38	1.33
1	BA	527	7MG	C6-N1	2.99	1.38	1.33
31	CA	1939	5MU	C4-N3	3.00	1.38	1.33
55	DA	955	PSU	C4-N3	3.01	1.38	1.33
55	DA	2580	PSU	C4-N3	3.02	1.38	1.33
55	DA	2069	7MG	C6-N1	3.05	1.38	1.33
55	DA	2457	PSU	C4-N3	3.06	1.38	1.33
31	CA	745	1MG	C6-C5	3.08	1.46	1.40
55	DA	2251	OMG	C6-N1	3.13	1.38	1.33
31	CA	747	5MU	C4-N3	3.13	1.38	1.33
31	CA	2251	OMG	C6-N1	3.13	1.38	1.33
1	AA	966	2MG	C6-C5	3.15	1.47	1.41
31	CA	1835	2MG	C6-N1	3.18	1.38	1.33
1	BA	527	7MG	C6-C5	3.18	1.45	1.41
31	CA	1917	PSU	C4-N3	3.21	1.38	1.33
31	CA	2445	2MG	C6-N1	3.21	1.38	1.33
55	DA	746	PSU	C4-N3	3.21	1.38	1.33
31	CA	2605	PSU	C4-N3	3.22	1.38	1.33
1	AA	1516	2MG	C6-N1	3.22	1.38	1.33
31	CA	2457	PSU	C4-N3	3.26	1.38	1.33
55	DA	1939	5MU	C4-N3	3.26	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2069	7MG	C6-N1	3.26	1.38	1.33
31	CA	955	PSU	C4-N3	3.28	1.38	1.33
31	CA	1911	PSU	C4-N3	3.29	1.39	1.33
55	DA	1911	PSU	C4-N3	3.31	1.39	1.33
1	AA	1207	2MG	C6-N1	3.32	1.39	1.33
1	BA	516	PSU	C4-N3	3.34	1.39	1.33
55	DA	1917	PSU	C4-N3	3.36	1.39	1.33
1	AA	516	PSU	C4-N3	3.36	1.39	1.33
31	CA	2552	OMU	C4-N3	3.36	1.39	1.33
55	DA	2504	PSU	C4-N3	3.38	1.39	1.33
1	BA	1207	2MG	C6-N1	3.38	1.39	1.33
55	DA	2605	PSU	C4-N3	3.38	1.39	1.33
31	CA	2580	PSU	C4-N3	3.39	1.39	1.33
31	CA	2504	PSU	C4-N3	3.43	1.39	1.33
55	DA	2069	7MG	C6-C5	3.43	1.46	1.41
31	CA	746	PSU	C4-N3	3.46	1.39	1.33
1	BA	1516	2MG	C6-N1	3.47	1.39	1.33
1	BA	966	2MG	C6-N1	3.48	1.39	1.33
1	AA	527	7MG	C6-N1	3.53	1.39	1.33
1	AA	966	2MG	C6-N1	3.56	1.39	1.33
32	DD	150[B]	MEQ	CB-CA	4.27	1.59	1.53

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	747	5MU	C5-C4-N3	-12.15	115.15	125.35
31	CA	747	5MU	C5-C4-N3	-12.12	115.17	125.35
55	DA	1939	5MU	C5-C4-N3	-12.07	115.22	125.35
31	CA	1939	5MU	C5-C4-N3	-12.02	115.26	125.35
55	DA	1835	2MG	C5-C6-N1	-9.00	111.75	123.52
31	CA	2069	7MG	C5-C6-N1	-8.75	110.36	123.39
31	CA	1835	2MG	C5-C6-N1	-8.72	112.12	123.52
1	AA	1207	2MG	C5-C6-N1	-8.63	112.24	123.52
31	CA	2445	2MG	C5-C6-N1	-8.59	112.30	123.52
31	CA	2251	OMG	C5-C6-N1	-8.58	112.31	123.52
1	BA	1516	2MG	C5-C6-N1	-8.57	112.32	123.52
1	AA	527	7MG	C5-C6-N1	-8.55	110.67	123.39
1	BA	966	2MG	C5-C6-N1	-8.54	112.36	123.52
55	DA	2069	7MG	C5-C4-N3	-8.47	118.11	126.74
1	AA	527	7MG	C5-C4-N3	-8.46	118.12	126.74
1	BA	1207	2MG	C5-C6-N1	-8.42	112.51	123.52
55	DA	2445	2MG	C5-C6-N1	-8.40	112.54	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	2251	OMG	C5-C6-N1	-8.40	112.54	123.52
1	AA	1516	2MG	C5-C6-N1	-8.37	112.58	123.52
1	AA	966	2MG	C5-C6-N1	-8.36	112.60	123.52
55	DA	2069	7MG	C5-C6-N1	-8.35	110.95	123.39
1	BA	527	7MG	C5-C6-N1	-8.29	111.05	123.39
1	BA	527	7MG	C5-C4-N3	-7.01	119.60	126.74
31	CA	2069	7MG	C5-C4-N3	-6.17	120.45	126.74
32	DD	150[A]	MEQ	CG-CB-CA	-4.78	103.16	114.03
31	CA	745	1MG	C6-C5-C4	-3.78	117.23	119.93
31	CA	2552	OMU	C5-C4-N3	-3.53	114.62	123.28
55	DA	2552	OMU	C5-C4-N3	-3.42	114.88	123.28
55	DA	2251	OMG	N3-C2-N1	-3.31	123.05	127.56
55	DA	746	PSU	C4-C5-C1'	-3.10	116.00	121.22
1	AA	966	2MG	C6-C5-C4	-3.09	117.33	120.86
31	CA	2251	OMG	N3-C2-N1	-3.07	123.38	127.56
31	CA	1915	3TD	C5-C4-N3	-3.06	116.16	118.65
55	DA	1915	3TD	C5-C4-N3	-3.02	116.19	118.65
1	AA	1516	2MG	C6-C5-C4	-3.00	117.43	120.86
1	BA	966	2MG	C6-C5-C4	-2.89	117.55	120.86
1	BA	1516	2MG	C6-C5-C4	-2.89	117.55	120.86
1	BA	1207	2MG	C6-C5-C4	-2.89	117.56	120.86
55	DA	2445	2MG	C6-C5-C4	-2.82	117.63	120.86
55	DA	745	1MG	C5-C6-N1	-2.75	114.75	118.35
1	AA	1207	2MG	C6-C5-C4	-2.65	117.83	120.86
55	DA	955	PSU	C4-C5-C1'	-2.64	116.77	121.22
31	CA	2445	2MG	C6-C5-C4	-2.55	117.95	120.86
31	CA	2503	2MA	C6-C5-C4	-2.53	115.12	119.67
31	CA	2251	OMG	C6-C5-C4	-2.49	118.01	120.86
55	DA	1835	2MG	C6-C5-C4	-2.48	118.02	120.86
31	CA	1835	2MG	C6-C5-C4	-2.48	118.02	120.86
55	DA	2503	2MA	C6-C5-C4	-2.36	115.44	119.67
31	CA	745	1MG	C5-C6-N1	-2.35	115.27	118.35
41	DN	81[A]	4D4	O-C-CA	-2.20	119.68	125.69
1	AA	1402	4OC	C6-C5-C4	-2.19	116.56	117.42
55	DA	2580	PSU	C4-C5-C1'	-2.14	117.62	121.22
1	BA	527	7MG	N1-C2-N3	-2.12	122.05	125.51
55	DA	2251	OMG	C6-C5-C4	-2.11	118.45	120.86
55	DA	745	1MG	C6-C5-C4	-2.10	118.43	119.93
1	AA	527	7MG	N1-C2-N3	-2.09	122.09	125.51
31	CA	2503	2MA	N3-C2-N1	-2.02	121.64	125.60
31	CA	955	PSU	C3'-C2'-C1'	-2.02	99.32	101.71
31	CA	1939	5MU	C5M-C5-C6	2.02	122.72	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	CM2-C2-N3	2.03	120.68	117.22
31	CA	2580	PSU	C3'-C2'-C1'	2.04	104.14	101.71
1	AA	966	2MG	CM2-N2-C2	2.05	125.34	123.03
1	AA	1498	UR3	C6-C5-C4	2.06	121.11	117.30
55	DA	747	5MU	C5M-C5-C6	2.07	122.83	118.63
1	AA	527	7MG	C8-N9-C1'	2.08	128.67	122.43
1	BA	527	7MG	C8-N9-C1'	2.08	128.68	122.43
31	CA	1618	6MZ	C2-N1-C6	2.08	117.97	116.47
31	CA	2069	7MG	C8-N9-C1'	2.12	128.78	122.43
31	CA	747	5MU	C5M-C5-C6	2.13	122.95	118.63
1	BA	1407	5MC	CM5-C5-C6	2.14	122.96	118.63
55	DA	1835	2MG	N2-C2-N3	2.15	119.43	116.94
31	CA	1911	PSU	O4'-C1'-C2'	2.15	107.02	104.69
12	AL	89	D2T	C-CA-N	2.16	114.71	109.95
31	CA	1835	2MG	N2-C2-N3	2.18	119.47	116.94
1	BA	1516	2MG	N2-C2-N3	2.20	119.49	116.94
1	BA	967	5MC	CM5-C5-C6	2.23	123.16	118.63
1	AA	967	5MC	CM5-C5-C6	2.24	123.17	118.63
55	DA	1939	5MU	C5M-C5-C6	2.24	123.18	118.63
55	DA	2445	2MG	N2-C2-N3	2.25	119.55	116.94
55	DA	1962	5MC	CM5-C5-C6	2.26	123.22	118.63
55	DA	2503	2MA	C2-N3-C4	2.27	116.38	115.29
1	AA	1516	2MG	N2-C2-N3	2.28	119.59	116.94
12	BL	89	D2T	C-CA-N	2.28	114.99	109.95
1	BA	516	PSU	O4'-C1'-C2'	2.29	107.17	104.69
1	AA	1207	2MG	N2-C2-N3	2.30	119.61	116.94
1	AA	1407	5MC	CM5-C5-C6	2.32	123.33	118.63
31	CA	1962	5MC	CM5-C5-C6	2.33	123.35	118.63
55	DA	1618	6MZ	C2-N1-C6	2.37	118.17	116.47
55	DA	1911	PSU	O4'-C1'-C2'	2.37	107.25	104.69
1	AA	516	PSU	O4'-C1'-C2'	2.43	107.32	104.69
1	BA	966	2MG	N2-C2-N3	2.43	119.77	116.94
31	CA	1915	3TD	O4'-C1'-C2'	2.47	107.36	104.69
55	DA	955	PSU	O4'-C1'-C2'	2.48	107.37	104.69
1	BA	1207	2MG	N2-C2-N3	2.54	119.89	116.94
31	CA	2030	6MZ	C2-N1-C6	2.59	118.34	116.47
55	DA	1915	3TD	O4'-C1'-C2'	2.62	107.52	104.69
1	AA	1402	4OC	CM4-N4-C4	3.06	125.45	122.87
32	DD	150[B]	MEQ	CB-CG-CD	3.07	120.29	113.26
31	CA	2503	2MA	C2-N3-C4	3.11	116.79	115.29
31	CA	2580	PSU	O4'-C1'-C2'	3.14	108.09	104.69
1	BA	1402	4OC	CM4-N4-C4	3.18	125.55	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	DD	150[B]	MEQ	CB-CA-N	3.54	120.51	110.54
1	BA	1402	4OC	C2-N3-C4	4.11	120.66	115.43
1	AA	1402	4OC	C2-N3-C4	4.16	120.72	115.43
31	CA	2445	2MG	C6-N1-C2	6.31	124.28	115.24
1	AA	966	2MG	C6-N1-C2	6.32	124.29	115.24
1	AA	1516	2MG	C6-N1-C2	6.59	124.68	115.24
1	BA	966	2MG	C6-N1-C2	6.64	124.74	115.24
31	CA	1835	2MG	C6-N1-C2	6.64	124.75	115.24
1	BA	1207	2MG	C6-N1-C2	6.65	124.76	115.24
1	BA	1516	2MG	C6-N1-C2	6.65	124.76	115.24
1	AA	1207	2MG	C6-N1-C2	6.65	124.77	115.24
55	DA	1835	2MG	C6-N1-C2	6.67	124.80	115.24
55	DA	2445	2MG	C6-N1-C2	6.69	124.81	115.24
31	CA	2069	7MG	C6-N1-C2	6.98	124.06	115.88
55	DA	2069	7MG	C6-N1-C2	7.02	124.10	115.88
1	BA	527	7MG	C6-N1-C2	7.05	124.14	115.88
1	AA	527	7MG	C6-N1-C2	7.45	124.61	115.88
31	CA	2251	OMG	C6-N1-C2	7.91	125.15	115.88
55	DA	2251	OMG	C6-N1-C2	7.96	125.20	115.88
31	CA	2552	OMU	C4-N3-C2	12.14	127.00	114.21
55	DA	2552	OMU	C4-N3-C2	12.21	127.07	114.21
55	DA	2605	PSU	C4-N3-C2	13.30	126.25	115.16
55	DA	955	PSU	C4-N3-C2	13.37	126.31	115.16
55	DA	1911	PSU	C4-N3-C2	13.41	126.35	115.16
55	DA	2457	PSU	C4-N3-C2	13.43	126.36	115.16
1	BA	516	PSU	C4-N3-C2	13.49	126.41	115.16
31	CA	955	PSU	C4-N3-C2	13.51	126.43	115.16
55	DA	1917	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	1911	PSU	C4-N3-C2	13.55	126.47	115.16
55	DA	2604	PSU	C4-N3-C2	13.56	126.47	115.16
31	CA	746	PSU	C4-N3-C2	13.57	126.48	115.16
1	AA	516	PSU	C4-N3-C2	13.57	126.48	115.16
31	CA	2580	PSU	C4-N3-C2	13.57	126.48	115.16
55	DA	746	PSU	C4-N3-C2	13.57	126.48	115.16
31	CA	2457	PSU	C4-N3-C2	13.59	126.50	115.16
31	CA	2605	PSU	C4-N3-C2	13.62	126.52	115.16
31	CA	2504	PSU	C4-N3-C2	13.62	126.53	115.16
55	DA	2504	PSU	C4-N3-C2	13.63	126.53	115.16
31	CA	1917	PSU	C4-N3-C2	13.68	126.57	115.16
55	DA	2580	PSU	C4-N3-C2	13.73	126.61	115.16
31	CA	1939	5MU	C4-N3-C2	14.39	127.17	115.16
55	DA	1939	5MU	C4-N3-C2	14.43	127.20	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	747	5MU	C4-N3-C2	14.52	127.27	115.16
55	DA	747	5MU	C4-N3-C2	14.60	127.34	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1402	4OC	1	0
1	AA	1518	MA6	1	0
1	AA	1519	MA6	1	0
1	BA	1402	4OC	1	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
1	BA	967	5MC	3	0
31	CA	1939	5MU	1	0
31	CA	2030	6MZ	5	0
31	CA	745	1MG	1	0
31	CA	747	5MU	1	0
55	DA	2030	6MZ	2	0
55	DA	2498	OMC	1	0
55	DA	747	5MU	1	0
32	DD	150[A]	MEQ	2	0
32	DD	150[B]	MEQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 for Mogul analysis.

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	$\# Z  > 2$
57	PG4	AA	1670	-	12,12,12	0.19	0	11,11,11	0.21	0
58	MPD	AA	1671	-	6,7,7	0.24	0	6,10,10	0.44	0
59	PUT	AA	1672	-	5,5,5	0.13	0	4,4,4	0.21	0
59	PUT	AA	1673	-	5,5,5	0.18	0	4,4,4	0.14	0
59	PUT	AA	1674	-	5,5,5	0.19	0	4,4,4	0.18	0
59	PUT	AA	1675	-	5,5,5	0.23	0	4,4,4	0.09	0
58	MPD	AA	1676	-	6,7,7	0.43	0	6,10,10	0.35	0
61	PEG	AL	201	-	6,6,6	0.21	0	5,5,5	0.15	0
57	PG4	BA	1642	-	12,12,12	0.24	0	11,11,11	0.19	0
62	EDO	D0	101	-	3,3,3	0.60	0	2,2,2	0.62	0
62	EDO	D1	101	-	3,3,3	0.65	0	2,2,2	0.27	0
63	PGE	D1	102	-	9,9,9	0.12	0	8,8,8	0.14	0
63	PGE	D3	101	-	9,9,9	0.24	0	8,8,8	0.09	0
61	PEG	D3	102	-	6,6,6	0.23	0	5,5,5	0.18	0
62	EDO	DA	3002	-	3,3,3	0.60	0	2,2,2	0.21	0
62	EDO	DA	3003	-	3,3,3	0.64	0	2,2,2	0.38	0
64	SPD	DA	3183	-	9,9,9	0.24	0	8,8,8	0.32	0
59	PUT	DA	3184	-	5,5,5	0.20	0	4,4,4	0.22	0
65	1PE	DA	3185	-	15,15,15	0.21	0	14,14,14	0.15	0
63	PGE	DA	3186	-	9,9,9	0.34	0	8,8,8	0.35	0
64	SPD	DA	3187	-	9,9,9	0.14	0	8,8,8	0.24	0
59	PUT	DA	3188	-	5,5,5	0.16	0	4,4,4	0.21	0
59	PUT	DA	3189	-	5,5,5	0.11	0	4,4,4	0.28	0
58	MPD	DA	3190	-	6,7,7	0.37	0	6,10,10	0.46	0
66	ACY	DA	3191	-	0,3,3	0.00	-	0,3,3	0.00	-
58	MPD	DA	3192	-	6,7,7	0.47	0	6,10,10	0.52	0
57	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.25	0
62	EDO	DA	3194	-	3,3,3	0.71	0	2,2,2	0.09	0
59	PUT	DA	3195	-	5,5,5	0.32	0	4,4,4	0.24	0
66	ACY	DA	3196	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3197	-	3,3,3	0.64	0	2,2,2	0.20	0
62	EDO	DA	3198	-	3,3,3	0.72	0	2,2,2	0.27	0
61	PEG	DA	3199	-	6,6,6	0.20	0	5,5,5	0.12	0
61	PEG	DA	3200	-	6,6,6	0.25	0	5,5,5	0.07	0
61	PEG	DA	3201	-	6,6,6	0.16	0	5,5,5	0.14	0
66	ACY	DA	3202	-	0,3,3	0.00	-	0,3,3	0.00	-
65	1PE	DA	3203	-	15,15,15	0.23	0	14,14,14	0.25	0
58	MPD	DA	3204	-	6,7,7	0.46	0	6,10,10	0.43	0
59	PUT	DA	3205	-	5,5,5	0.22	0	4,4,4	0.21	0
64	SPD	DA	3206	-	9,9,9	0.25	0	8,8,8	0.22	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	MPD	DA	3207	-	6,7,7	0.31	0	6,10,10	0.45	0
62	EDO	DA	3208	-	3,3,3	0.57	0	2,2,2	0.37	0
62	EDO	DA	3209	-	3,3,3	0.51	0	2,2,2	0.39	0
58	MPD	DA	3210	-	6,7,7	0.38	0	6,10,10	0.21	0
67	GUN	DA	3211	-	9,12,12	1.47	1 (11%)	7,17,17	4.92	5 (71%)
59	PUT	DA	3212	-	5,5,5	0.29	0	4,4,4	0.13	0
59	PUT	DA	3213	-	5,5,5	0.28	0	4,4,4	0.20	0
63	PGE	DA	3214	-	9,9,9	0.26	0	8,8,8	0.34	0
62	EDO	DA	3215	-	3,3,3	0.69	0	2,2,2	0.28	0
57	PG4	DA	3216	-	12,12,12	0.16	0	11,11,11	0.15	0
63	PGE	DA	3217	-	9,9,9	0.24	0	8,8,8	0.18	0
61	PEG	DA	3218	-	6,6,6	0.17	0	5,5,5	0.08	0
59	PUT	DA	3219	-	5,5,5	0.24	0	4,4,4	0.18	0
68	TRS	DA	3220	-	7,7,7	0.39	0	9,9,9	0.32	0
59	PUT	DA	3221	-	5,5,5	0.29	0	4,4,4	0.12	0
59	PUT	DA	3222	-	5,5,5	0.31	0	4,4,4	0.47	0
59	PUT	DA	3223	-	5,5,5	0.25	0	4,4,4	0.19	0
64	SPD	DA	3224	-	9,9,9	0.15	0	8,8,8	0.25	0
63	PGE	DA	3225	-	9,9,9	0.28	0	8,8,8	0.31	0
61	PEG	DA	3226	-	6,6,6	0.22	0	5,5,5	0.05	0
61	PEG	DA	3227	-	6,6,6	0.27	0	5,5,5	0.14	0
62	EDO	DB	210	-	3,3,3	0.66	0	2,2,2	0.20	0
62	EDO	DB	211	-	3,3,3	0.56	0	2,2,2	0.37	0
63	PGE	DD	301	-	9,9,9	0.23	0	8,8,8	0.15	0
58	MPD	DE	301	-	6,7,7	0.42	0	6,10,10	0.40	0
58	MPD	DE	302	-	6,7,7	0.53	0	6,10,10	0.70	0
58	MPD	DK	201	-	6,7,7	0.56	0	6,10,10	0.37	0
61	PEG	DL	201	-	6,6,6	0.12	0	5,5,5	0.11	0
59	PUT	DM	201	-	5,5,5	0.25	0	4,4,4	0.28	0
58	MPD	DN	201	-	6,7,7	0.66	0	6,10,10	0.44	0
61	PEG	DP	201	-	6,6,6	0.18	0	5,5,5	0.11	0
61	PEG	DQ	201	-	6,6,6	0.24	0	5,5,5	0.09	0
57	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
57	PG4	DR	201	-	12,12,12	0.23	0	11,11,11	0.25	0
63	PGE	DS	201	-	9,9,9	0.24	0	8,8,8	0.18	0
57	PG4	DS	202	-	12,12,12	0.20	0	11,11,11	0.23	0
58	MPD	DS	203	-	6,7,7	0.37	0	6,10,10	0.30	0
58	MPD	DT	201	-	6,7,7	0.51	0	6,10,10	0.13	0
58	MPD	DT	202	-	6,7,7	0.46	0	6,10,10	0.50	0
63	PGE	DU	201	-	9,9,9	0.34	0	8,8,8	0.28	0

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
57	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
58	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
59	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
58	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
57	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
62	EDO	D0	101	-	-	0/1/1/1	0/0/0/0
62	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
63	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
63	PGE	D3	101	-	-	0/7/7/7	0/0/0/0
61	PEG	D3	102	-	-	0/4/4/4	0/0/0/0
62	EDO	DA	3002	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
64	SPD	DA	3183	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3184	-	-	0/3/3/3	0/0/0/0
65	1PE	DA	3185	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3186	-	-	0/7/7/7	0/0/0/0
64	SPD	DA	3187	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3188	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3189	-	-	0/3/3/3	0/0/0/0
58	MPD	DA	3190	-	-	0/5/5/5	0/0/0/0
66	ACY	DA	3191	-	-	0/0/0/0	0/0/0/0
58	MPD	DA	3192	-	-	0/5/5/5	0/0/0/0
57	PG4	DA	3193	-	-	0/10/10/10	0/0/0/0
62	EDO	DA	3194	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3195	-	-	0/3/3/3	0/0/0/0
66	ACY	DA	3196	-	-	0/0/0/0	0/0/0/0
62	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3198	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3200	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3201	-	-	0/4/4/4	0/0/0/0
66	ACY	DA	3202	-	-	0/0/0/0	0/0/0/0
65	1PE	DA	3203	-	-	0/13/13/13	0/0/0/0
58	MPD	DA	3204	-	-	0/5/5/5	0/0/0/0
59	PUT	DA	3205	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3206	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3207	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	EDO	DA	3208	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3209	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3210	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3211	-	-	0/0/0/0	0/2/2/2
59	PUT	DA	3212	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3213	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3214	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3215	-	-	0/1/1/1	0/0/0/0
57	PG4	DA	3216	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3217	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3218	-	-	0/4/4/4	0/0/0/0
59	PUT	DA	3219	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3220	-	-	0/9/9/9	0/0/0/0
59	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3222	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3223	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3224	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3225	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3226	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3227	-	-	0/4/4/4	0/0/0/0
62	EDO	DB	210	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
63	PGE	DD	301	-	-	0/7/7/7	0/0/0/0
58	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
58	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
58	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
59	PUT	DM	201	-	-	0/3/3/3	0/0/0/0
58	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
57	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
57	PG4	DR	201	-	-	0/10/10/10	0/0/0/0
63	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
57	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
58	MPD	DS	203	-	-	0/5/5/5	0/0/0/0
58	MPD	DT	201	-	-	0/5/5/5	0/0/0/0
58	MPD	DT	202	-	-	0/5/5/5	0/0/0/0
63	PGE	DU	201	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3211	GUN	C6-N1	3.57	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3211	GUN	C5-C6-N1	-8.45	112.48	123.52
67	DA	3211	GUN	C5-C4-N9	-3.62	104.70	111.12
67	DA	3211	GUN	N3-C2-N1	-3.48	122.82	127.56
67	DA	3211	GUN	C6-C5-C4	-2.53	117.96	120.86
67	DA	3211	GUN	C6-N1-C2	8.06	125.32	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	1642	PG4	1	0
61	D3	102	PEG	1	0
62	DA	3002	EDO	1	0
65	DA	3185	1PE	1	0
58	DA	3192	MPD	2	0
62	DA	3194	EDO	3	0
61	DA	3201	PEG	1	0
66	DA	3202	ACY	2	0
59	DA	3212	PUT	1	0
59	DA	3213	PUT	1	0
63	DA	3214	PGE	1	0
59	DA	3219	PUT	1	0
68	DA	3220	TRS	1	0
59	DA	3223	PUT	1	0
63	DA	3225	PGE	4	0
61	DQ	201	PEG	1	0
57	DR	201	PG4	1	0
58	DS	203	MPD	4	0
63	DU	201	PGE	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	0.31	110 (7%) 18 18	65, 138, 270, 291	0
1	BA	1522/1534 (99%)	0.84	260 (17%) 2 2	86, 162, 293, 294	0
2	AB	224/224 (100%)	1.18	57 (25%) 1 1	108, 156, 231, 272	0
2	BB	224/224 (100%)	1.03	44 (19%) 1 2	138, 181, 229, 262	0
3	AC	206/206 (100%)	1.31	56 (27%) 1 1	138, 174, 208, 228	0
3	BC	206/206 (100%)	3.38	127 (61%) 0 0	223, 253, 269, 279	0
4	AD	205/205 (100%)	0.24	4 (1%) 68 67	100, 145, 174, 190	0
4	BD	205/205 (100%)	-0.20	0 100 100	71, 100, 137, 174	0
5	AE	155/155 (100%)	0.39	8 (5%) 31 29	83, 119, 150, 176	0
5	BE	150/155 (96%)	0.43	12 (8%) 15 14	92, 125, 168, 236	0
6	AF	106/106 (100%)	0.01	5 (4%) 35 34	89, 126, 149, 187	0
6	BF	100/106 (94%)	0.73	14 (14%) 4 4	135, 162, 188, 196	0
7	AG	151/151 (100%)	1.99	70 (46%) 0 0	159, 186, 216, 229	0
7	BG	151/151 (100%)	4.00	107 (70%) 0 0	198, 247, 263, 268	0
8	AH	129/129 (100%)	0.47	9 (6%) 19 19	89, 122, 148, 158	0
8	BH	129/129 (100%)	0.33	11 (8%) 13 13	119, 151, 179, 192	0
9	AI	127/127 (100%)	2.23	52 (40%) 0 1	168, 196, 251, 270	0
9	BI	127/127 (100%)	2.81	63 (49%) 0 0	198, 234, 277, 283	0
10	AJ	99/99 (100%)	2.37	45 (45%) 0 0	169, 190, 228, 238	0
10	BJ	98/99 (98%)	4.87	73 (74%) 0 0	209, 248, 280, 287	0
11	AK	117/129 (90%)	0.76	18 (15%) 3 3	77, 139, 174, 190	0
11	BK	117/129 (90%)	1.21	28 (23%) 1 1	111, 166, 186, 202	0
12	AL	122/123 (99%)	0.47	11 (9%) 12 11	78, 112, 137, 178	0
12	BL	122/123 (99%)	0.63	11 (9%) 12 11	96, 121, 148, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	2.14	52 (45%) 0 0	167, 198, 220, 233	0
13	BM	114/114 (100%)	4.72	103 (90%) 0 0	254, 271, 288, 292	0
14	AN	100/100 (100%)	2.50	52 (52%) 0 0	166, 188, 252, 260	0
14	BN	100/100 (100%)	4.57	77 (77%) 0 0	226, 252, 282, 288	0
15	AO	88/88 (100%)	0.30	7 (7%) 15 14	75, 109, 142, 169	0
15	BO	88/88 (100%)	0.94	17 (19%) 2 2	127, 160, 180, 197	0
16	AP	82/82 (100%)	1.41	28 (34%) 0 1	88, 128, 168, 195	0
16	BP	82/82 (100%)	1.13	21 (25%) 1 1	106, 136, 168, 184	0
17	AQ	80/80 (100%)	0.58	10 (12%) 5 5	86, 115, 149, 157	0
17	BQ	80/80 (100%)	1.41	25 (31%) 1 1	120, 159, 182, 197	0
18	AR	55/55 (100%)	0.71	8 (14%) 3 3	86, 116, 172, 194	0
18	BR	55/55 (100%)	1.76	20 (36%) 0 1	126, 143, 173, 216	0
19	AS	79/79 (100%)	1.36	25 (31%) 1 1	180, 201, 215, 222	0
19	BS	79/79 (100%)	4.58	56 (70%) 0 0	229, 265, 274, 278	0
20	AT	86/86 (100%)	0.24	3 (3%) 48 46	91, 122, 151, 161	0
20	BT	85/86 (98%)	1.68	26 (30%) 1 1	136, 157, 183, 193	0
21	AU	56/56 (100%)	1.16	8 (14%) 4 3	114, 146, 208, 223	0
21	BU	56/56 (100%)	0.65	8 (14%) 4 3	112, 151, 191, 204	0
22	C1	56/56 (100%)	1.67	18 (32%) 1 1	131, 187, 206, 219	0
22	D1	56/56 (100%)	-0.35	0 100 100	31, 57, 81, 120	0
23	C2	50/51 (98%)	3.50	37 (74%) 0 0	179, 197, 215, 237	0
23	D2	51/51 (100%)	0.18	0 100 100	81, 98, 130, 145	0
24	C3	46/46 (100%)	1.91	21 (45%) 0 0	129, 153, 170, 177	0
24	D3	46/46 (100%)	-0.11	0 100 100	42, 51, 71, 143	0
25	C4	64/64 (100%)	1.44	23 (35%) 0 1	145, 165, 182, 187	0
25	D4	64/64 (100%)	-0.18	0 100 100	51, 64, 78, 105	0
26	C5	38/38 (100%)	1.27	7 (18%) 2 2	126, 153, 166, 174	0
26	D5	38/38 (100%)	0.07	1 (2%) 59 58	52, 68, 95, 120	0
27	C0	58/58 (100%)	1.24	16 (27%) 1 1	123, 142, 171, 180	0
27	D0	58/58 (100%)	-0.34	0 100 100	36, 49, 85, 112	0
28	CB	118/120 (98%)	0.57	7 (5%) 26 24	134, 208, 253, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	-0.18	0 <span>100</span> <span>100</span>	45, 87, 138, 167	0
29	CC	271/272 (99%)	0.71	35 (12%) <span>5</span> <span>4</span>	102, 130, 160, 176	0
29	DC	271/272 (99%)	-0.19	0 <span>100</span> <span>100</span>	42, 75, 106, 142	0
30	CD	209/209 (100%)	1.64	75 (35%) <span>0</span> <span>1</span>	100, 154, 179, 193	0
31	CA	2876/2904 (99%)	0.63	269 (9%) <span>11</span> <span>11</span>	92, 184, 267, 286	0
32	DD	208/209 (99%)	-0.24	0 <span>100</span> <span>100</span>	27, 55, 93, 121	0
33	CE	201/201 (100%)	1.60	68 (33%) <span>0</span> <span>1</span>	133, 193, 233, 243	0
33	DE	201/201 (100%)	-0.05	0 <span>100</span> <span>100</span>	30, 82, 132, 150	0
34	CF	177/178 (99%)	2.61	110 (62%) <span>0</span> <span>0</span>	212, 233, 249, 254	0
34	DF	177/178 (99%)	0.33	10 (5%) <span>28</span> <span>27</span>	79, 120, 170, 188	0
35	CG	176/176 (100%)	2.56	100 (56%) <span>0</span> <span>0</span>	168, 196, 232, 244	0
35	DG	176/176 (100%)	0.08	9 (5%) <span>32</span> <span>30</span>	57, 93, 122, 156	0
36	CH	149/149 (100%)	1.58	52 (34%) <span>0</span> <span>1</span>	131, 172, 197, 208	0
36	DH	149/149 (100%)	1.18	30 (20%) <span>1</span> <span>1</span>	83, 173, 211, 231	0
37	CJ	134/135 (99%)	5.46	110 (82%) <span>0</span> <span>0</span>	259, 279, 289, 291	0
37	DJ	134/135 (99%)	3.81	92 (68%) <span>0</span> <span>0</span>	228, 249, 266, 272	0
38	CK	142/142 (100%)	0.65	9 (6%) <span>23</span> <span>23</span>	115, 144, 168, 182	0
38	DK	142/142 (100%)	-0.32	0 <span>100</span> <span>100</span>	28, 49, 82, 106	0
39	CL	122/123 (99%)	0.68	16 (13%) <span>5</span> <span>4</span>	105, 133, 168, 181	0
39	DL	123/123 (100%)	-0.23	0 <span>100</span> <span>100</span>	43, 62, 95, 135	0
40	CM	144/144 (100%)	2.54	69 (47%) <span>0</span> <span>0</span>	131, 195, 243, 260	0
40	DM	144/144 (100%)	-0.18	1 (0%) <span>89</span> <span>88</span>	26, 78, 114, 152	0
41	CN	135/136 (99%)	0.88	20 (14%) <span>3</span> <span>3</span>	107, 145, 176, 205	0
41	DN	135/136 (99%)	-0.38	0 <span>100</span> <span>100</span>	36, 59, 90, 112	0
42	CO	120/127 (94%)	1.25	25 (20%) <span>1</span> <span>1</span>	127, 158, 186, 233	0
42	DO	125/127 (98%)	-0.26	0 <span>100</span> <span>100</span>	33, 52, 96, 155	0
43	CP	116/117 (99%)	2.36	60 (51%) <span>0</span> <span>0</span>	165, 195, 217, 223	0
43	DP	117/117 (100%)	-0.08	0 <span>100</span> <span>100</span>	56, 84, 121, 136	0
44	CQ	114/114 (100%)	1.49	38 (33%) <span>0</span> <span>1</span>	124, 150, 174, 186	0
44	DQ	114/114 (100%)	-0.22	1 (0%) <span>85</span> <span>86</span>	47, 72, 105, 135	0
45	CR	117/117 (100%)	1.35	30 (25%) <span>1</span> <span>1</span>	117, 144, 166, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	DR	117/117 (100%)	-0.17	0 100 100	24, 41, 63, 114	0
46	CS	103/103 (100%)	1.94	39 (37%) 0 1	117, 159, 195, 202	0
46	DS	103/103 (100%)	-0.25	0 100 100	30, 55, 92, 126	0
47	CT	110/110 (100%)	1.58	39 (35%) 0 1	140, 171, 196, 207	0
47	DT	110/110 (100%)	-0.28	0 100 100	26, 45, 79, 128	0
48	CU	93/100 (93%)	2.62	54 (58%) 0 0	159, 194, 219, 229	0
48	DU	93/100 (93%)	0.26	1 (1%) 82 82	51, 73, 136, 154	0
49	CV	102/103 (99%)	3.13	68 (66%) 0 0	157, 198, 231, 242	0
49	DV	102/103 (99%)	0.08	5 (4%) 33 31	57, 82, 126, 156	0
50	CW	94/94 (100%)	1.56	34 (36%) 0 1	133, 172, 186, 192	0
50	DW	94/94 (100%)	-0.30	0 100 100	43, 73, 110, 119	0
51	CX	75/76 (98%)	1.95	31 (41%) 0 1	129, 161, 175, 206	0
51	DX	76/76 (100%)	-0.35	0 100 100	36, 62, 92, 157	0
52	CY	77/77 (100%)	0.86	14 (18%) 2 2	120, 145, 173, 185	0
52	DY	77/77 (100%)	-0.10	1 (1%) 79 79	56, 76, 111, 130	0
53	CZ	62/62 (100%)	2.62	38 (61%) 0 0	177, 199, 210, 217	0
53	DZ	62/62 (100%)	0.32	2 (3%) 51 50	65, 97, 136, 174	0
54	DI	135/135 (100%)	1.30	39 (28%) 1 1	104, 179, 244, 266	1 (0%)
55	DA	2873/2904 (98%)	0.06	78 (2%) 58 57	29, 65, 231, 294	0
All	All	20634/20795 (99%)	0.86	3543 (17%) 2 2	24, 144, 266, 294	1 (0%)

All (3543) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	CJ	13	VAL	34.4
9	BI	126	GLN	26.7
9	BI	128	SER	23.2
37	DJ	54	PRO	20.5
1	BA	1302	C	20.3
10	BJ	41	PRO	19.5
3	BC	197	GLY	19.0
10	BJ	74	VAL	18.5
10	BJ	75	ASP	18.2
3	BC	196	ILE	17.9
37	CJ	14	ALA	17.3

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Mol	Chain	Res	Type	RSRZ
3	BC	198	VAL	17.2
37	DJ	53	LEU	16.8
3	BC	195	VAL	16.7
1	BA	985	C	16.6
37	CJ	12	GLN	16.3
9	BI	127	PHE	16.2
1	BA	1242	G	16.1
19	BS	29	LYS	15.8
10	BJ	77	VAL	15.7
7	BG	42	ILE	15.5
10	BJ	8	ILE	15.5
7	BG	39	ALA	15.5
1	BA	1241	G	15.5
37	CJ	23	PRO	15.2
10	BJ	73	LEU	15.1
55	DA	2120	G	15.0
37	CJ	69	PHE	15.0
3	BC	159	GLY	14.5
7	BG	38	THR	14.5
9	AI	127	PHE	14.3
14	BN	37	SER	14.1
1	BA	1305	G	14.0
19	BS	66	MET	13.8
14	BN	36	ALA	13.7
19	BS	30	PRO	13.5
14	AN	21	PHE	13.5
13	BM	95	LEU	13.5
3	BC	193	TYR	13.4
35	CG	32	GLU	13.4
37	DJ	13	VAL	13.2
31	CA	1068	G	13.1
37	CJ	57	VAL	13.1
31	CA	1067	A	12.9
9	AI	130	ARG	12.6
14	BN	55	SER	12.6
13	BM	45	ILE	12.6
18	BR	20	GLU	12.4
37	CJ	87	LYS	12.3
7	BG	45	SER	12.2
37	CJ	54	PRO	12.2
7	BG	112	GLY	12.2
40	CM	81	ASP	12.1

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Mol	Chain	Res	Type	RSRZ
10	BJ	9	ARG	12.1
30	CD	6	GLY	12.1
7	BG	43	VAL	12.0
9	BI	31	ASN	12.0
19	BS	60	VAL	11.9
37	DJ	79	LEU	11.8
37	CJ	88	SER	11.7
13	BM	104	THR	11.5
1	BA	1016	A	11.5
37	CJ	20	PRO	11.4
1	BA	983	A	11.4
10	BJ	72	ARG	11.3
37	CJ	51	LYS	11.3
37	CJ	11	LEU	11.2
37	DJ	76	ALA	11.2
37	CJ	55	ILE	11.1
13	BM	83	LEU	11.0
37	CJ	42	PHE	11.0
13	BM	108	THR	10.9
13	BM	40	ALA	10.9
37	CJ	53	LEU	10.9
46	CS	50	GLY	10.8
1	BA	1201	A	10.8
55	DA	2116	G	10.8
1	BA	1274	A	10.7
1	BA	1243	C	10.7
19	BS	61	PHE	10.6
9	AI	128	SER	10.6
37	CJ	71	THR	10.5
1	BA	1049	U	10.5
37	CJ	24	VAL	10.5
3	BC	181	ASP	10.4
13	BM	33	ILE	10.4
43	CP	64	TYR	10.4
34	CF	153	ASP	10.4
1	BA	986	U	10.3
10	BJ	26	VAL	10.3
31	CA	2126	A	10.3
14	BN	72	GLY	10.3
7	BG	65	ALA	10.2
37	DJ	59	ILE	10.2
31	CA	331	C	10.2

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Mol	Chain	Res	Type	RSRZ
3	BC	128	VAL	10.1
13	BM	39	ILE	10.1
1	BA	987	G	10.1
7	BG	62	PHE	10.0
19	BS	48	THR	10.0
31	CA	2172	U	10.0
10	BJ	22	THR	10.0
37	DJ	12	GLN	10.0
37	DJ	23	PRO	9.9
13	BM	84	GLY	9.9
10	BJ	40	ILE	9.9
35	CG	2	SER	9.9
7	BG	49	THR	9.9
14	BN	67	THR	9.9
14	BN	54	ASP	9.8
37	CJ	21	SER	9.8
1	BA	954	G	9.8
9	AI	126	GLN	9.8
9	BI	17	ALA	9.8
51	CX	54	GLY	9.8
13	BM	10	PRO	9.7
1	BA	984	C	9.7
10	BJ	7	ARG	9.7
23	C2	52	ALA	9.7
37	DJ	21	SER	9.7
3	BC	192	THR	9.7
31	CA	1087	G	9.6
14	AN	24	ARG	9.6
37	DJ	67	PHE	9.5
14	BN	4	GLN	9.5
49	CV	89	ASP	9.5
10	BJ	10	LEU	9.4
19	BS	49	ILE	9.4
10	BJ	76	ILE	9.4
37	DJ	80	LEU	9.4
14	BN	60	GLN	9.2
7	BG	41	SER	9.2
40	CM	120	VAL	9.2
1	BA	1196	A	9.2
1	BA	1024	G	9.1
31	CA	1537	G	9.1
3	BC	156	ARG	9.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	CJ	22	PRO	9.1
7	BG	69	VAL	9.1
37	DJ	20	PRO	9.0
7	BG	116	MET	9.0
48	CU	15	HIS	9.0
1	BA	1307	U	9.0
48	CU	83	ALA	9.0
1	BA	1022	A	8.9
37	CJ	116	ASP	8.9
55	DA	2110	G	8.9
54	DI	131	THR	8.9
23	C2	21	TYR	8.9
37	CJ	83	ALA	8.9
37	DJ	55	ILE	8.9
10	BJ	35	GLN	8.9
1	BA	955	U	8.8
1	BA	1331	G	8.8
14	AN	55	SER	8.8
7	BG	66	LEU	8.8
14	BN	13	ARG	8.7
37	CJ	126	THR	8.7
3	BC	157	LEU	8.7
10	BJ	42	LEU	8.7
31	CA	2402	U	8.7
7	BG	73	VAL	8.7
10	BJ	6	ILE	8.6
37	CJ	86	ILE	8.6
1	BA	962	C	8.6
37	CJ	77	ALA	8.6
34	CF	128	TYR	8.6
37	CJ	60	THR	8.6
3	BC	71	ALA	8.6
14	BN	15	ALA	8.6
13	BM	24	GLY	8.5
9	AI	90	TYR	8.5
1	BA	1020	G	8.5
14	BN	6	MET	8.5
14	BN	35	ASN	8.4
21	AU	2	PRO	8.4
1	BA	1025	U	8.4
13	BM	64	VAL	8.4
55	DA	2111	U	8.4

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Mol	Chain	Res	Type	RSRZ
1	BA	1244	G	8.3
37	CJ	80	LEU	8.3
43	CP	66	GLY	8.3
3	BC	164	ARG	8.3
14	BN	2	ALA	8.3
7	BG	148	ASN	8.3
1	BA	1306	A	8.3
19	BS	24	GLU	8.3
13	BM	105	ASN	8.3
10	BJ	23	ALA	8.2
37	DJ	88	SER	8.2
43	CP	65	THR	8.2
1	AA	1030	U	8.2
14	BN	5	SER	8.2
37	CJ	82	LYS	8.2
10	AJ	75	ASP	8.2
37	CJ	52	GLY	8.2
1	BA	958	A	8.2
7	BG	18	PHE	8.2
14	AN	25	ALA	8.2
14	BN	44	ALA	8.2
13	BM	29	ARG	8.2
19	BS	63	THR	8.2
19	BS	75	ALA	8.2
3	BC	172	ARG	8.2
31	CA	2174	C	8.2
43	CP	63	LYS	8.1
37	CJ	73	THR	8.1
19	BS	41	PHE	8.1
9	AI	89	GLU	8.1
14	BN	22	ALA	8.1
40	CM	80	SER	8.1
1	BA	1219	A	8.1
37	DJ	135	SER	8.0
13	BM	32	ALA	8.0
43	CP	52	SER	8.0
31	CA	2123	G	8.0
40	CM	78	ARG	8.0
31	CA	1066	U	8.0
13	BM	96	PRO	8.0
37	DJ	24	VAL	8.0
37	DJ	14	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1217	C	7.9
1	BA	1240	U	7.9
31	CA	931	U	7.9
9	BI	16	ALA	7.9
7	BG	111	ARG	7.9
35	CG	111	HIS	7.9
7	AG	50	LEU	7.9
14	BN	68	GLY	7.9
51	CX	56	ASP	7.9
7	BG	91	VAL	7.9
1	BA	953	G	7.8
10	BJ	37	ARG	7.8
10	AJ	8	ILE	7.7
37	DJ	77	ALA	7.7
1	BA	1204	A	7.7
7	BG	54	SER	7.7
40	CM	77	ILE	7.7
40	CM	113	ALA	7.7
23	C2	36	LEU	7.7
49	CV	36	VAL	7.7
3	BC	174	PRO	7.7
44	CQ	110	ILE	7.7
19	BS	76	PRO	7.7
14	BN	58	SER	7.6
54	DI	130	PRO	7.6
31	CA	1084	A	7.6
7	BG	72	THR	7.6
1	BA	981	U	7.6
9	BI	130	ARG	7.6
49	CV	18	ASP	7.6
1	BA	1296	C	7.6
10	BJ	71	LEU	7.5
46	CS	20	VAL	7.5
36	DH	87	GLU	7.5
49	CV	69	ASN	7.5
7	BG	107	ALA	7.5
3	BC	155	GLY	7.5
37	DJ	22	PRO	7.5
10	BJ	39	PRO	7.5
10	AJ	36	VAL	7.5
46	CS	96	VAL	7.5
19	BS	65	GLU	7.5

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Mol	Chain	Res	Type	RSRZ
49	CV	35	ILE	7.5
37	CJ	45	LYS	7.4
14	BN	28	LYS	7.4
19	BS	59	PRO	7.4
9	AI	125	PRO	7.4
1	AA	1032	G	7.4
14	AN	23	LYS	7.4
31	CA	2125	G	7.4
7	BG	15	ASP	7.3
55	DA	2121	G	7.3
3	BC	158	GLY	7.3
3	BC	78	GLY	7.3
7	AG	54	SER	7.3
34	CF	85	ILE	7.3
49	CV	3	ALA	7.2
7	BG	52	GLN	7.2
9	BI	125	PRO	7.2
14	BN	8	ALA	7.2
1	AA	1031	C	7.2
1	BA	1028	C	7.2
19	BS	37	ARG	7.2
10	AJ	91	ASP	7.2
37	CJ	33	VAL	7.1
13	BM	63	PHE	7.1
14	BN	20	TYR	7.1
54	DI	2	ALA	7.1
1	BA	1031	C	7.1
13	AM	30	SER	7.1
3	BC	206	GLU	7.1
40	CM	115	GLU	7.1
9	AI	18	ARG	7.1
13	BM	23	TYR	7.1
37	CJ	46	THR	7.1
48	CU	60	THR	7.1
14	BN	32	SER	7.0
37	CJ	59	ILE	7.0
13	BM	94	GLY	7.0
14	BN	52	PRO	7.0
13	BM	58	ASP	7.0
9	AI	20	PHE	7.0
55	DA	2172	U	7.0
13	AM	64	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
37	CJ	50	GLU	7.0
19	BS	43	ASN	6.9
7	BG	2	PRO	6.9
49	CV	29	LEU	6.9
31	CA	1175	A	6.9
13	BM	11	ASP	6.9
19	BS	67	VAL	6.9
1	BA	1032	G	6.9
14	BN	51	LEU	6.9
1	BA	1218	C	6.8
7	BG	8	GLY	6.8
7	BG	71	PRO	6.8
55	DA	2127	G	6.8
23	C2	42	VAL	6.8
43	CP	40	ILE	6.8
10	AJ	43	PRO	6.8
10	BJ	25	ILE	6.8
35	CG	107	LEU	6.8
10	AJ	74	VAL	6.7
19	BS	62	VAL	6.7
37	CJ	56	PRO	6.7
1	BA	209	U	6.7
1	BA	988	G	6.7
13	BM	48	LEU	6.7
46	CS	27	ILE	6.7
19	BS	71	LEU	6.7
7	AG	49	THR	6.7
19	BS	39	THR	6.7
42	CO	118	ARG	6.7
55	DA	896	A	6.7
7	BG	103	TRP	6.7
9	AI	104	VAL	6.7
40	CM	82	LEU	6.7
1	BA	1030	U	6.7
7	BG	105	VAL	6.6
31	CA	2110	G	6.6
23	C2	24	THR	6.6
10	BJ	70	HIS	6.6
37	CJ	68	THR	6.6
14	AN	32	SER	6.6
10	AJ	76	ILE	6.6
14	BN	3	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	BA	1033	G	6.6
33	CE	143	LEU	6.6
53	CZ	29	ARG	6.6
49	CV	31	SER	6.6
37	CJ	63	ALA	6.5
10	AJ	35	GLN	6.5
9	BI	66	THR	6.5
9	AI	17	ALA	6.5
37	CJ	61	VAL	6.5
3	BC	127	ARG	6.5
48	CU	55	VAL	6.5
30	CD	200	ASP	6.5
43	CP	51	ALA	6.5
43	CP	53	THR	6.5
1	BA	982	U	6.5
40	CM	79	LEU	6.5
3	BC	79	LYS	6.5
30	CD	26	VAL	6.5
9	BI	20	PHE	6.5
55	DA	884	U	6.5
35	CG	103	ILE	6.4
10	BJ	12	ALA	6.4
48	CU	43	ILE	6.4
7	BG	82	GLY	6.4
40	CM	114	GLY	6.4
34	CF	27	GLN	6.4
3	BC	53	SER	6.4
49	CV	33	LYS	6.4
19	BS	12	ASP	6.4
23	C2	37	LYS	6.4
14	AN	67	THR	6.4
55	DA	2125	G	6.4
1	BA	1019	A	6.4
1	BA	1304	G	6.4
31	CA	1104	C	6.4
49	CV	13	VAL	6.4
37	CJ	47	ASP	6.4
1	AA	984	C	6.4
49	CV	80	ALA	6.4
14	BN	59	ARG	6.4
31	CA	2127	G	6.4
48	CU	61	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
54	DI	136	ILE	6.3
22	C1	57	LYS	6.3
10	AJ	73	LEU	6.3
37	DJ	42	PHE	6.3
48	CU	59	ASN	6.3
37	CJ	28	LEU	6.3
1	BA	959	A	6.3
1	BA	1048	G	6.3
13	BM	17	ILE	6.3
19	BS	23	VAL	6.3
49	CV	83	VAL	6.3
19	BS	40	ILE	6.3
1	AA	1125	U	6.3
7	BG	131	LYS	6.3
7	AG	58	GLU	6.3
49	CV	32	GLY	6.3
37	CJ	81	LYS	6.3
9	AI	21	ILE	6.3
1	BA	1023	U	6.3
10	AJ	6	ILE	6.3
9	AI	6	TYR	6.2
14	BN	78	GLY	6.2
19	BS	50	ALA	6.2
1	BA	1021	A	6.2
13	AM	24	GLY	6.2
7	BG	16	PRO	6.2
49	CV	40	ASN	6.2
55	DA	2175	C	6.2
13	BM	46	SER	6.2
37	CJ	67	PHE	6.2
55	DA	2124	G	6.2
37	CJ	75	PRO	6.2
13	BM	41	GLU	6.2
7	BG	30	LEU	6.2
14	BN	30	ILE	6.2
10	BJ	38	GLY	6.2
40	CM	101	ILE	6.2
13	AM	40	ALA	6.2
1	AA	1286	U	6.1
7	AG	62	PHE	6.1
2	BB	213	TYR	6.1
3	BC	168	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
55	DA	2174	C	6.1
31	CA	2124	G	6.1
19	BS	28	LYS	6.1
1	BA	1026	G	6.1
31	CA	2797	U	6.1
35	CG	52	PHE	6.1
54	DI	134	GLU	6.1
13	BM	36	ALA	6.1
19	BS	32	ARG	6.1
3	BC	170	GLU	6.1
20	BT	4	ILE	6.1
10	AJ	56	HIS	6.1
35	CG	151	TYR	6.1
49	CV	87	PHE	6.1
3	BC	160	ALA	6.1
37	DJ	52	GLY	6.1
37	CJ	76	ALA	6.0
37	CJ	138	LEU	6.0
35	CG	105	LEU	6.0
14	BN	16	LEU	6.0
1	AA	87	C	6.0
7	BG	133	THR	6.0
43	CP	50	ALA	6.0
14	BN	48	LEU	6.0
23	C2	47	VAL	6.0
9	BI	9	THR	6.0
55	DA	2118	U	6.0
37	CJ	25	GLY	6.0
34	CF	84	PRO	6.0
31	CA	1103	A	6.0
14	BN	61	ARG	6.0
37	DJ	68	THR	6.0
15	BO	17	ARG	6.0
3	BC	73	PRO	6.0
30	CD	199	SER	6.0
10	AJ	101	SER	5.9
33	CE	200	LEU	5.9
40	CM	92	LEU	5.9
13	BM	54	ASP	5.9
35	CG	33	LEU	5.9
49	CV	70	VAL	5.9
34	CF	152	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
14	AN	50	THR	5.9
34	CF	91	LEU	5.9
43	CP	29	HIS	5.9
19	BS	31	LEU	5.9
37	CJ	121	ASP	5.9
2	BB	67	ILE	5.9
40	CM	132	ARG	5.9
1	BA	1210	C	5.9
13	BM	34	LEU	5.9
10	BJ	97	ASP	5.9
7	AG	7	ILE	5.9
10	BJ	19	ASP	5.9
49	CV	88	GLU	5.9
3	BC	43	LEU	5.9
3	BC	194	GLY	5.8
10	AJ	5	ARG	5.8
30	CD	4	LEU	5.8
3	AC	68	ILE	5.8
7	BG	132	GLY	5.8
40	CM	102	GLY	5.8
1	AA	1025	U	5.8
19	BS	72	GLY	5.8
13	AM	33	ILE	5.8
7	BG	150	ALA	5.8
1	BA	1015	G	5.8
1	BA	1029	U	5.8
14	AN	20	TYR	5.8
9	BI	67	VAL	5.8
13	AM	15	ALA	5.8
7	BG	53	ARG	5.8
7	AG	61	ALA	5.8
18	BR	51	TYR	5.8
13	BM	109	ARG	5.8
30	CD	9	VAL	5.8
10	AJ	34	ALA	5.8
3	BC	171	GLY	5.8
1	BA	980	C	5.8
13	BM	13	LYS	5.8
10	BJ	102	LEU	5.8
37	CJ	129	ILE	5.7
1	BA	1126	U	5.7
14	BN	43	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
37	CJ	10	LYS	5.7
31	CA	2667	C	5.7
13	AM	41	GLU	5.7
33	CE	172	ALA	5.7
37	DJ	11	LEU	5.7
3	BC	179	ARG	5.7
31	CA	2168	G	5.7
51	CX	55	ARG	5.7
3	BC	116	VAL	5.7
35	CG	131	ILE	5.7
46	CS	88	GLY	5.7
3	BC	36	ASP	5.7
35	CG	40	ALA	5.7
40	CM	130	GLY	5.7
1	BA	1208	C	5.7
3	BC	120	ILE	5.7
10	BJ	11	LYS	5.7
37	CJ	58	VAL	5.7
1	BA	1237	C	5.7
37	CJ	62	TYR	5.7
23	C2	46	HIS	5.7
34	CF	23	ASN	5.7
13	BM	35	ALA	5.7
31	CA	1057	A	5.7
10	BJ	21	ALA	5.6
13	AM	32	ALA	5.6
44	CQ	91	ALA	5.6
33	CE	14	VAL	5.6
1	BA	1018	G	5.6
1	BA	1221	G	5.6
37	CJ	38	PHE	5.6
10	BJ	50	THR	5.6
7	BG	106	GLU	5.6
23	C2	43	VAL	5.6
3	BC	80	LYS	5.6
47	CT	97	LEU	5.6
35	CG	9	VAL	5.6
48	CU	8	LEU	5.6
10	AJ	29	ALA	5.6
13	BM	97	VAL	5.6
23	C2	40	ASP	5.6
19	BS	38	SER	5.6

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Mol	Chain	Res	Type	RSRZ
13	BM	6	GLY	5.6
13	BM	18	ALA	5.6
19	BS	74	PHE	5.6
1	BA	1038	C	5.6
37	CJ	41	ALA	5.6
40	CM	131	ALA	5.6
37	CJ	17	MET	5.6
53	CZ	56	LEU	5.6
31	CA	2173	A	5.6
49	CV	12	ILE	5.6
2	AB	36	ASN	5.6
14	BN	18	ASP	5.5
20	BT	3	ASN	5.5
48	CU	47	VAL	5.5
2	AB	123	ASP	5.5
50	CW	43	ASP	5.5
33	CE	128	ALA	5.5
38	CK	142	ILE	5.5
14	AN	31	ILE	5.5
3	AC	77	ILE	5.5
30	CD	186	LEU	5.5
34	CF	144	ASP	5.5
7	BG	4	ARG	5.5
11	AK	19	GLY	5.5
37	CJ	74	PRO	5.5
31	CA	1083	U	5.5
9	BI	117	GLY	5.5
37	DJ	73	THR	5.5
40	CM	121	THR	5.5
19	BS	26	GLY	5.5
37	DJ	38	PHE	5.5
30	CD	8	LYS	5.5
14	AN	54	ASP	5.5
3	AC	103	ILE	5.5
11	BK	110	ILE	5.5
40	CM	117	THR	5.4
10	BJ	91	ASP	5.4
37	CJ	19	ASN	5.4
37	CJ	31	GLN	5.4
9	AI	129	LYS	5.4
19	BS	22	ALA	5.4
51	CX	53	CYS	5.4

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Mol	Chain	Res	Type	RSRZ
3	AC	82	GLU	5.4
30	CD	10	GLY	5.4
35	CG	104	ASN	5.4
53	CZ	45	GLN	5.4
34	CF	173	PHE	5.4
31	CA	345	A	5.4
37	DJ	78	VAL	5.4
13	BM	56	LEU	5.4
7	BG	152	ALA	5.4
33	CE	144	GLU	5.4
55	DA	879	G	5.4
48	CU	75	GLY	5.4
3	BC	109	PRO	5.4
54	DI	128	THR	5.4
17	AQ	53	CYS	5.4
37	CJ	18	ALA	5.4
1	AA	86	G	5.4
34	CF	34	ILE	5.4
13	BM	16	VAL	5.4
31	CA	2666	C	5.4
13	AM	29	ARG	5.4
49	CV	72	ILE	5.4
41	CN	136	MET	5.4
3	BC	119	SER	5.4
45	CR	29	SER	5.4
31	CA	2120	G	5.4
25	C4	61	CYS	5.4
51	CX	26	PHE	5.4
37	CJ	78	VAL	5.3
48	CU	2	ILE	5.3
31	CA	1085	A	5.3
14	BN	66	GLN	5.3
50	CW	28	ALA	5.3
33	CE	126	VAL	5.3
34	CF	105	THR	5.3
23	C2	39	PHE	5.3
1	BA	976	G	5.3
1	BA	1276	G	5.3
10	AJ	25	ILE	5.3
9	BI	38	TYR	5.3
3	BC	39	VAL	5.3
27	C0	10	THR	5.3

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Mol	Chain	Res	Type	RSRZ
34	CF	155	THR	5.3
1	BA	1148	U	5.3
1	BA	1125	U	5.3
1	BA	1273	C	5.3
13	BM	30	SER	5.3
14	AN	37	SER	5.3
13	AM	19	LEU	5.3
10	BJ	15	HIS	5.3
42	CO	25	ALA	5.3
37	CJ	96	ASP	5.3
13	BM	103	LYS	5.3
23	C2	41	PRO	5.3
34	CF	95	ARG	5.3
3	AC	105	GLU	5.3
50	CW	45	ASP	5.3
53	CZ	15	ASN	5.3
31	CA	75	G	5.3
33	CE	103	GLY	5.3
9	AI	123	ARG	5.3
20	BT	76	LYS	5.3
34	CF	130	MET	5.3
40	CM	100	ILE	5.3
10	BJ	87	LEU	5.3
42	CO	26	GLY	5.2
3	BC	84	VAL	5.2
37	DJ	28	LEU	5.2
7	BG	17	LYS	5.2
9	AI	95	ARG	5.2
34	CF	67	ILE	5.2
43	CP	38	GLN	5.2
48	CU	10	VAL	5.2
1	BA	1017	U	5.2
9	AI	19	VAL	5.2
3	AC	81	GLY	5.2
40	CM	142	ILE	5.2
31	CA	1105	U	5.2
3	BC	8	ASN	5.2
7	BG	37	SER	5.2
48	CU	58	VAL	5.2
31	CA	1065	U	5.2
14	AN	9	ARG	5.2
14	AN	28	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
22	C1	36	GLU	5.2
24	C3	17	GLY	5.2
37	DJ	71	THR	5.2
14	BN	27	LEU	5.2
9	BI	103	PHE	5.2
43	CP	117	PHE	5.2
55	DA	883	G	5.2
35	CG	57	GLY	5.2
43	CP	46	GLU	5.2
13	BM	2	ALA	5.2
30	CD	198	GLY	5.2
1	BA	973	G	5.2
7	AG	53	ARG	5.2
13	AM	25	VAL	5.2
37	DJ	19	ASN	5.1
51	CX	59	LEU	5.1
3	BC	35	SER	5.1
13	BM	21	SER	5.1
14	BN	31	ILE	5.1
40	CM	126	ARG	5.1
49	CV	28	VAL	5.1
55	DA	2109	U	5.1
37	DJ	87	LYS	5.1
37	DJ	137	GLY	5.1
19	BS	25	SER	5.1
25	C4	36	LYS	5.1
29	CC	18	LYS	5.1
19	BS	27	ASP	5.1
1	BA	1003	G	5.1
17	BQ	70	THR	5.1
1	BA	1275	A	5.1
34	CF	24	SER	5.1
13	BM	22	ILE	5.1
47	CT	94	ASP	5.1
37	DJ	40	LYS	5.1
33	CE	157	LEU	5.1
35	CG	110	SER	5.1
49	CV	39	ILE	5.1
35	CG	94	TYR	5.1
35	CG	108	GLY	5.1
20	BT	35	VAL	5.1
33	CE	127	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
7	BG	109	ARG	5.0
1	BA	211	G	5.0
37	DJ	96	ASP	5.0
10	BJ	56	HIS	5.0
55	DA	885	C	5.0
19	AS	33	THR	5.0
1	BA	1270	G	5.0
1	BA	1297	G	5.0
37	DJ	116	ASP	5.0
37	CJ	89	GLY	5.0
2	BB	14	VAL	5.0
31	CA	2162	G	5.0
2	AB	30	PHE	5.0
47	CT	5	ALA	5.0
14	BN	56	SER	5.0
36	CH	142	VAL	5.0
3	AC	168	TYR	5.0
9	BI	32	GLN	5.0
33	CE	153	LEU	5.0
23	C2	29	THR	5.0
7	BG	151	PHE	5.0
7	AG	6	VAL	5.0
35	CG	58	TYR	5.0
13	AM	11	ASP	5.0
22	C1	55	ILE	5.0
37	CJ	43	ASN	5.0
34	CF	92	ARG	5.0
42	CO	120	GLU	5.0
11	BK	112	ASP	5.0
14	BN	71	HIS	5.0
9	BI	90	TYR	5.0
9	BI	39	PHE	5.0
7	BG	48	GLU	5.0
30	CD	75	ALA	5.0
40	CM	75	ALA	5.0
3	BC	165	THR	5.0
19	BS	47	LEU	5.0
13	AM	63	PHE	5.0
23	C2	53	LYS	5.0
47	CT	103	ILE	5.0
13	AM	115	PRO	5.0
37	CJ	72	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
3	BC	180	ALA	4.9
7	AG	4	ARG	4.9
12	AL	124	ALA	4.9
13	BM	37	ALA	4.9
48	CU	35	ALA	4.9
16	BP	52	LEU	4.9
2	AB	46	THR	4.9
20	BT	59	ASP	4.9
1	BA	1205	U	4.9
3	BC	177	THR	4.9
35	CG	109	PHE	4.9
1	AA	1126	U	4.9
1	AA	1127	G	4.9
37	DJ	138	LEU	4.9
7	BG	55	GLY	4.9
49	CV	78	GLY	4.9
29	CC	232	HIS	4.9
49	CV	77	THR	4.9
7	BG	51	ALA	4.9
31	CA	2111	U	4.9
30	CD	31	ALA	4.9
11	BK	109	ASN	4.9
13	BM	38	GLY	4.9
14	BN	9	ARG	4.9
14	BN	53	ARG	4.9
53	CZ	36	GLN	4.9
10	AJ	24	GLU	4.9
30	CD	96	ILE	4.9
55	DA	2163	A	4.9
3	AC	79	LYS	4.9
30	CD	180	VAL	4.9
26	C5	1	MET	4.9
36	CH	132	PHE	4.9
46	CS	32	THR	4.9
37	CJ	130	GLU	4.9
40	CM	89	VAL	4.9
34	CF	119	ALA	4.9
43	CP	36	TYR	4.9
1	BA	956	U	4.9
31	CA	2128	G	4.9
13	AM	99	GLY	4.9
2	AB	131	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	BA	1245	C	4.9
7	AG	52	GLN	4.9
37	CJ	8	TYR	4.9
46	CS	52	PRO	4.9
13	AM	34	LEU	4.8
1	BA	1309	G	4.8
49	CV	5	ILE	4.8
14	BN	17	ALA	4.8
7	BG	34	GLY	4.8
11	AK	111	THR	4.8
34	CF	106	ILE	4.8
35	CG	84	THR	4.8
10	BJ	101	SER	4.8
7	BG	113	ASP	4.8
11	BK	96	THR	4.8
29	CC	241	GLY	4.8
14	BN	49	GLN	4.8
1	BA	1220	G	4.8
31	CA	2171	A	4.8
33	CE	119	ILE	4.8
44	CQ	43	PHE	4.8
1	BA	1004	A	4.8
14	BN	21	PHE	4.8
44	CQ	9	GLU	4.8
33	CE	173	THR	4.8
3	BC	207	ILE	4.8
3	AC	78	GLY	4.8
9	BI	40	GLY	4.8
46	CS	24	LYS	4.8
7	AG	123	GLU	4.8
31	CA	846	U	4.8
36	DH	137	GLU	4.8
48	CU	40	LYS	4.8
35	CG	56	ASP	4.8
10	AJ	7	ARG	4.8
53	CZ	22	LEU	4.8
37	DJ	82	LYS	4.8
1	BA	82	G	4.8
42	CO	29	VAL	4.8
25	C4	64	TYR	4.7
29	CC	242	LYS	4.7
35	CG	106	SER	4.7

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Mol	Chain	Res	Type	RSRZ
39	CL	110	GLU	4.7
40	CM	144	GLU	4.7
43	CP	27	VAL	4.7
1	BA	1027	C	4.7
37	DJ	25	GLY	4.7
11	BK	64	GLN	4.7
13	BM	31	LYS	4.7
14	BN	50	THR	4.7
41	CN	80	VAL	4.7
13	BM	77	ILE	4.7
35	CG	26	ILE	4.7
54	DI	132	TYR	4.7
19	BS	35	SER	4.7
14	AN	8	ALA	4.7
3	AC	166	GLU	4.7
9	BI	123	ARG	4.7
48	CU	71	GLY	4.7
24	C3	42	LEU	4.7
3	BC	205	GLY	4.7
37	DJ	36	MET	4.7
1	BA	1271	A	4.7
19	BS	14	HIS	4.7
7	AG	110	LYS	4.7
10	BJ	80	THR	4.7
39	CL	83	ALA	4.7
43	CP	37	ALA	4.7
51	CX	63	ALA	4.7
7	BG	35	LYS	4.7
14	BN	24	ARG	4.7
50	CW	7	GLU	4.7
35	CG	152	ARG	4.7
44	CQ	111	LYS	4.7
49	CV	81	ASP	4.7
3	BC	85	GLU	4.7
3	BC	154	SER	4.7
7	AG	122	ASN	4.7
42	CO	28	LEU	4.7
35	CG	126	PRO	4.7
27	C0	8	THR	4.7
9	BI	65	ILE	4.7
34	CF	35	THR	4.7
14	BN	79	LEU	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	BM	101	ARG	4.6
30	CD	77	ARG	4.6
37	DJ	8	TYR	4.6
13	BM	12	HIS	4.6
9	BI	44	ALA	4.6
2	AB	37	LYS	4.6
19	BS	81	ARG	4.6
53	CZ	18	LEU	4.6
1	AA	1281	C	4.6
1	BA	79	G	4.6
1	BA	948	C	4.6
43	CP	92	PHE	4.6
7	AG	48	GLU	4.6
14	AN	22	ALA	4.6
52	CY	78	TYR	4.6
31	CA	1536	C	4.6
3	AC	47	LEU	4.6
9	BI	41	ARG	4.6
3	AC	110	GLU	4.6
9	BI	21	ILE	4.6
31	CA	2150	C	4.6
23	C2	20	PHE	4.6
54	DI	3	LEU	4.6
34	CF	86	GLY	4.6
37	CJ	26	PRO	4.6
43	CP	39	VAL	4.6
55	DA	2132	U	4.6
13	BM	111	GLY	4.6
37	DJ	89	GLY	4.6
37	DJ	133	ALA	4.6
37	CJ	91	GLY	4.6
43	CP	103	VAL	4.6
33	CE	47	LYS	4.6
34	CF	69	LYS	4.6
7	BG	126	ASP	4.6
53	CZ	49	ASP	4.6
55	DA	2123	G	4.6
13	BM	67	GLY	4.5
2	BB	37	LYS	4.5
9	BI	11	ARG	4.5
10	BJ	20	GLN	4.5
22	C1	34	SER	4.5

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Mol	Chain	Res	Type	RSRZ
31	CA	329	G	4.5
35	CG	43	VAL	4.5
13	BM	51	GLY	4.5
43	CP	93	ASP	4.5
7	BG	79	ARG	4.5
17	BQ	46	VAL	4.5
40	CM	116	VAL	4.5
7	AG	46	ALA	4.5
7	BG	78	ARG	4.5
7	BG	31	MET	4.5
34	CF	31	VAL	4.5
7	BG	77	SER	4.5
27	C0	56	LYS	4.5
31	CA	1213	A	4.5
37	CJ	44	ALA	4.5
31	CA	1064	C	4.5
37	CJ	79	LEU	4.5
48	CU	84	TYR	4.5
23	C2	25	LYS	4.5
2	BB	201	PRO	4.5
55	DA	2115	G	4.5
1	BA	1303	C	4.5
10	BJ	58	ASN	4.5
13	AM	16	VAL	4.5
24	C3	35	ARG	4.5
13	BM	89	LEU	4.5
1	AA	1285	A	4.5
1	BA	996	A	4.5
13	AM	48	LEU	4.5
44	CQ	3	ASN	4.5
34	CF	76	GLY	4.5
40	CM	28	GLY	4.5
37	DJ	9	VAL	4.5
51	CX	23	VAL	4.5
7	BG	134	ALA	4.5
17	BQ	24	ALA	4.5
55	DA	2167	U	4.4
37	DJ	83	ALA	4.4
43	CP	107	ALA	4.4
1	BA	1039	G	4.4
1	BA	1050	G	4.4
3	BC	77	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
48	CU	42	GLU	4.4
3	AC	83	ASP	4.4
20	BT	49	LYS	4.4
47	CT	44	ALA	4.4
6	BF	8	PHE	4.4
19	AS	68	GLY	4.4
37	DJ	131	GLY	4.4
45	CR	74	ILE	4.4
11	BK	111	THR	4.4
7	BG	115	SER	4.4
10	BJ	36	VAL	4.4
36	CH	11	ASN	4.4
2	AB	32	PHE	4.4
31	CA	2122	U	4.4
1	BA	1001	C	4.4
34	CF	104	ILE	4.4
10	BJ	90	LEU	4.4
3	BC	129	MET	4.4
1	BA	1341	U	4.4
3	BC	46	GLU	4.4
3	BC	191	THR	4.4
55	DA	2106	U	4.4
17	BQ	21	ILE	4.4
44	CQ	97	LEU	4.4
47	CT	82	MET	4.4
10	BJ	81	GLU	4.4
13	BM	19	LEU	4.4
19	BS	42	PRO	4.4
29	CC	244	PRO	4.4
3	BC	51	SER	4.4
11	BK	67	ALA	4.4
34	CF	177	PHE	4.4
48	CU	46	ALA	4.4
10	BJ	100	ILE	4.4
41	CN	72	PRO	4.4
19	BS	44	MET	4.4
14	BN	10	GLU	4.4
17	BQ	47	HIS	4.4
31	CA	1082	U	4.4
49	CV	86	ARG	4.4
53	CZ	59	GLU	4.4
34	CF	175	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
3	BC	122	SER	4.4
11	AK	110	ILE	4.4
22	C1	27	SER	4.4
29	CC	233	GLY	4.4
21	AU	16	LEU	4.4
21	BU	12	PHE	4.4
31	CA	2175	C	4.4
16	AP	47	GLU	4.4
3	BC	15	VAL	4.3
55	DA	880	G	4.3
31	CA	2665	A	4.3
55	DA	2108	A	4.3
37	CJ	64	ASP	4.3
23	C2	19	HIS	4.3
55	DA	1729	U	4.3
47	CT	43	ALA	4.3
35	CG	24	ILE	4.3
7	AG	57	SER	4.3
1	BA	1280	A	4.3
13	AM	7	ILE	4.3
37	CJ	131	GLY	4.3
31	CA	2383	G	4.3
47	CT	47	VAL	4.3
35	CG	112	PRO	4.3
49	CV	90	GLY	4.3
54	DI	129	LEU	4.3
10	BJ	27	GLU	4.3
2	AB	139	ARG	4.3
3	BC	173	VAL	4.3
9	AI	63	LEU	4.3
7	BG	26	PHE	4.3
37	CJ	117	MET	4.3
37	CJ	136	MET	4.3
31	CA	12	U	4.3
2	AB	35	ARG	4.3
37	CJ	32	GLY	4.3
3	AC	43	LEU	4.3
13	BM	5	ALA	4.3
37	DJ	16	GLY	4.3
53	CZ	11	VAL	4.3
31	CA	1086	A	4.3
37	CJ	34	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
47	CT	48	LYS	4.3
11	BK	85	MET	4.3
1	BA	1047	G	4.3
13	BM	74	SER	4.3
14	AN	66	GLN	4.3
13	BM	14	HIS	4.3
1	BA	977	A	4.3
13	AM	18	ALA	4.3
34	CF	97	TRP	4.3
45	CR	71	GLN	4.3
7	BG	46	ALA	4.3
41	CN	84	LYS	4.2
31	CA	1870	C	4.2
10	AJ	39	PRO	4.2
49	CV	52	LEU	4.2
13	BM	8	ASN	4.2
13	BM	9	ILE	4.2
14	AN	78	GLY	4.2
55	DA	882	G	4.2
1	BA	1212	U	4.2
31	CA	1078	U	4.2
14	BN	69	ARG	4.2
33	CE	131	THR	4.2
3	BC	14	ILE	4.2
13	BM	68	ASP	4.2
22	C1	46	ASP	4.2
35	CG	4	VAL	4.2
33	CE	201	ALA	4.2
37	CJ	27	ALA	4.2
9	BI	64	TYR	4.2
37	DJ	58	VAL	4.2
49	CV	42	VAL	4.2
7	BG	147	ALA	4.2
11	BK	63	ALA	4.2
24	C3	32	ALA	4.2
39	CL	14	SER	4.2
1	BA	1035	A	4.2
1	BA	1317	C	4.2
2	BB	89	GLN	4.2
37	DJ	49	ILE	4.2
42	CO	24	MET	4.2
10	BJ	63	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
31	CA	2627	G	4.2
34	CF	36	LEU	4.2
36	CH	12	LEU	4.2
14	BN	14	VAL	4.2
37	CJ	85	GLY	4.2
45	CR	79	PHE	4.2
2	AB	135	LEU	4.2
36	CH	122	LEU	4.2
23	C2	18	GLY	4.2
43	CP	87	ILE	4.2
55	DA	881	G	4.2
1	BA	998	C	4.2
37	CJ	120	ALA	4.2
51	CX	25	ARG	4.2
49	CV	51	ALA	4.2
1	BA	1209	C	4.2
31	CA	1106	G	4.2
7	AG	137	LYS	4.2
30	CD	55	LYS	4.2
31	CA	2181	U	4.2
40	CM	90	VAL	4.2
24	C3	33	ARG	4.2
50	CW	42	LEU	4.2
31	CA	879	G	4.2
35	CG	25	THR	4.2
40	CM	127	VAL	4.2
10	AJ	40	ILE	4.2
1	BA	1037	C	4.1
24	C3	28	ARG	4.1
20	BT	47	ALA	4.1
19	BS	58	VAL	4.1
34	CF	151	GLY	4.1
13	AM	45	ILE	4.1
51	CX	58	THR	4.1
37	DJ	94	ASN	4.1
30	CD	44	GLY	4.1
36	CH	130	VAL	4.1
34	CF	96	MET	4.1
55	DA	2122	U	4.1
1	BA	968	A	4.1
14	BN	47	LYS	4.1
30	CD	151	THR	4.1

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Mol	Chain	Res	Type	RSRZ
3	BC	153	VAL	4.1
13	BM	65	VAL	4.1
19	BS	51	VAL	4.1
49	CV	6	ARG	4.1
30	CD	27	ILE	4.1
35	CG	148	LEU	4.1
55	DA	2169	A	4.1
7	AG	45	SER	4.1
37	CJ	48	SER	4.1
9	BI	30	ILE	4.1
37	CJ	115	ALA	4.1
1	AA	1000	A	4.1
31	CA	878	A	4.1
53	CZ	6	LEU	4.1
3	BC	204	LYS	4.1
16	AP	38	PHE	4.1
18	BR	74	HIS	4.1
1	BA	946	A	4.1
23	C2	38	LYS	4.1
7	BG	127	ALA	4.1
20	BT	87	ALA	4.1
24	C3	18	PHE	4.1
29	CC	2	ALA	4.1
1	BA	1034	G	4.1
16	AP	17	TYR	4.1
22	C1	33	THR	4.1
10	BJ	60	ASP	4.1
33	CE	23	PHE	4.1
1	AA	1196	A	4.1
42	CO	116	VAL	4.1
34	CF	37	ASN	4.1
51	CX	52	GLY	4.1
10	AJ	42	LEU	4.1
35	CG	7	ALA	4.1
36	CH	148	ALA	4.1
7	BG	36	LYS	4.1
49	CV	37	GLU	4.1
34	CF	136	ILE	4.1
34	CF	154	ILE	4.1
37	DJ	69	PHE	4.0
3	BC	126	ARG	4.0
9	AI	91	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
9	BI	121	ALA	4.0
14	BN	38	ASP	4.0
34	CF	40	VAL	4.0
37	DJ	104	ALA	4.0
36	CH	72	ILE	4.0
1	BA	1044	A	4.0
3	AC	80	LYS	4.0
31	CA	1524	G	4.0
14	BN	57	PRO	4.0
34	CF	29	PRO	4.0
47	CT	7	HIS	4.0
7	AG	111	ARG	4.0
29	CC	3	VAL	4.0
35	CG	65	ALA	4.0
36	CH	84	ALA	4.0
46	CS	63	VAL	4.0
7	AG	38	THR	4.0
35	CG	89	LEU	4.0
2	AB	9	MET	4.0
7	AG	106	GLU	4.0
31	CA	1167	C	4.0
1	AA	1148	U	4.0
3	BC	103	ILE	4.0
40	CM	70	LYS	4.0
31	CA	2800	A	4.0
2	AB	12	ALA	4.0
37	CJ	99	GLY	4.0
40	CM	108	ALA	4.0
37	DJ	134	ARG	4.0
9	AI	5	GLN	4.0
16	AP	39	PHE	4.0
2	BB	187	VAL	4.0
31	CA	877	A	4.0
12	BL	124	ALA	4.0
30	CD	154	LYS	4.0
1	BA	1330	U	4.0
46	CS	31	GLU	4.0
17	BQ	23	VAL	4.0
30	CD	76	GLY	4.0
47	CT	98	LYS	4.0
1	BA	1236	A	4.0
25	C4	37	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
53	CZ	42	LEU	4.0
35	CG	83	PHE	4.0
30	CD	38	LYS	4.0
14	AN	68	GLY	4.0
14	BN	100	SER	4.0
31	CA	546	U	4.0
44	CQ	85	SER	4.0
48	CU	63	VAL	4.0
34	CF	26	MET	4.0
1	BA	979	C	4.0
1	BA	1322	C	4.0
18	AR	23	TYR	4.0
13	BM	52	GLN	4.0
17	BQ	73	TRP	4.0
50	CW	69	GLU	4.0
7	AG	140	ASP	4.0
13	BM	99	GLY	4.0
7	BG	144	MET	4.0
53	CZ	28	LEU	4.0
34	CF	71	ARG	4.0
22	C1	4	GLN	4.0
3	BC	185	ASN	4.0
53	CZ	58	ASN	4.0
16	BP	54	LEU	4.0
33	CE	199	MET	4.0
1	BA	1295	U	3.9
40	CM	76	GLU	3.9
7	BG	87	VAL	3.9
9	BI	104	VAL	3.9
49	CV	71	ALA	3.9
31	CA	2149	U	3.9
3	BC	102	ASN	3.9
48	CU	14	PRO	3.9
33	CE	104	ALA	3.9
34	CF	83	TYR	3.9
40	CM	118	THR	3.9
37	CJ	66	SER	3.9
2	AB	43	LEU	3.9
37	DJ	81	LYS	3.9
53	CZ	17	GLU	3.9
53	CZ	24	GLU	3.9
1	AA	1320	C	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1203	C	3.9
16	BP	57	ILE	3.9
9	BI	7	TYR	3.9
24	C3	30	VAL	3.9
30	CD	203	VAL	3.9
37	DJ	57	VAL	3.9
46	CS	19	THR	3.9
49	CV	84	GLY	3.9
13	AM	17	ILE	3.9
14	AN	57	PRO	3.9
1	AA	1033	G	3.9
9	BI	37	GLN	3.9
34	CF	100	PHE	3.9
7	BG	29	ILE	3.9
10	AJ	100	ILE	3.9
3	BC	112	ASP	3.9
1	BA	1239	A	3.9
18	BR	48	ARG	3.9
40	CM	8	PRO	3.9
37	DJ	63	ALA	3.9
35	CG	62	TRP	3.9
11	BK	94	GLU	3.9
43	CP	110	ALA	3.9
3	AC	157	LEU	3.9
22	C1	3	VAL	3.9
35	CG	44	LYS	3.9
37	CJ	113	LYS	3.9
2	BB	21	ARG	3.9
1	BA	842	U	3.9
16	AP	20	VAL	3.9
2	BB	208	ARG	3.9
3	AC	74	GLY	3.9
19	BS	73	GLU	3.9
36	CH	94	ILE	3.9
48	CU	72	GLN	3.9
30	CD	185	ASN	3.9
35	CG	27	LYS	3.9
49	CV	26	LYS	3.9
51	CX	51	VAL	3.8
53	CZ	37	LEU	3.8
49	CV	15	THR	3.8
3	AC	134	MET	3.8

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Mol	Chain	Res	Type	RSRZ
24	C3	22	MET	3.8
9	BI	108	ALA	3.8
34	CF	107	ALA	3.8
48	CU	87	LEU	3.8
31	CA	1538	G	3.8
14	BN	23	LYS	3.8
31	CA	2118	U	3.8
1	BA	999	C	3.8
55	DA	1064	C	3.8
3	BC	133	ALA	3.8
13	AM	54	ASP	3.8
39	CL	111	LYS	3.8
2	AB	44	GLU	3.8
1	BA	989	U	3.8
1	BA	1211	U	3.8
2	AB	47	VAL	3.8
13	BM	43	VAL	3.8
7	BG	137	LYS	3.8
31	CA	33	C	3.8
1	AA	1260	G	3.8
2	BB	159	ASP	3.8
55	DA	2162	G	3.8
10	BJ	24	GLU	3.8
14	BN	11	VAL	3.8
18	AR	24	LYS	3.8
31	CA	613	A	3.8
35	CG	10	VAL	3.8
42	CO	52	ILE	3.8
7	BG	99	LEU	3.8
31	CA	289	G	3.8
35	CG	132	VAL	3.8
7	AG	133	THR	3.8
43	CP	30	ARG	3.8
31	CA	2154	A	3.8
7	AG	59	LEU	3.8
52	CY	49	LEU	3.8
13	BM	71	ARG	3.8
1	AA	1020	G	3.8
1	AA	1138	G	3.8
34	CF	158	THR	3.8
1	BA	997	U	3.8
17	BQ	61	ILE	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	AB	6	MET	3.8
7	BG	141	VAL	3.8
14	AN	6	MET	3.8
48	CU	67	VAL	3.8
30	CD	166	GLY	3.8
31	CA	1075	C	3.8
45	CR	99	ALA	3.8
14	BN	19	LYS	3.8
7	BG	50	LEU	3.8
45	CR	117	LEU	3.8
49	CV	95	PHE	3.8
21	AU	26	ALA	3.8
35	CG	5	ALA	3.8
37	CJ	15	ALA	3.8
3	AC	53	SER	3.8
43	CP	26	LEU	3.8
2	BB	123	ASP	3.8
18	AR	20	GLU	3.8
31	CA	1048	A	3.8
16	BP	42	ILE	3.8
20	BT	80	THR	3.8
37	DJ	113	LYS	3.7
1	AA	1008	U	3.7
14	BN	65	ARG	3.7
50	CW	27	PRO	3.7
3	BC	101	ILE	3.7
9	BI	43	THR	3.7
35	CG	102	VAL	3.7
16	AP	41	PRO	3.7
21	BU	2	PRO	3.7
35	CG	133	LEU	3.7
36	CH	108	VAL	3.7
13	BM	57	ARG	3.7
39	CL	15	GLY	3.7
31	CA	2803	G	3.7
42	CO	119	SER	3.7
55	DA	2117	A	3.7
14	AN	40	ASP	3.7
24	C3	13	ASN	3.7
36	DH	142	VAL	3.7
13	BM	90	ARG	3.7
13	BM	93	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
14	AN	5	SER	3.7
47	CT	3	THR	3.7
14	AN	33	ASP	3.7
30	CD	45	TYR	3.7
40	CM	91	ASP	3.7
3	BC	200	VAL	3.7
31	CA	1731	G	3.7
34	CF	132	VAL	3.7
35	CG	162	VAL	3.7
37	DJ	61	VAL	3.7
3	BC	161	GLU	3.7
33	CE	152	GLU	3.7
9	AI	66	THR	3.7
9	AI	62	ASP	3.7
47	CT	84	ARG	3.7
1	BA	1308	U	3.7
7	AG	144	MET	3.7
10	BJ	78	GLU	3.7
3	BC	104	ALA	3.7
40	CM	133	ALA	3.7
34	CF	117	LEU	3.7
19	AS	25	SER	3.7
3	BC	201	TRP	3.7
44	CQ	24	ASP	3.7
26	C5	32	LYS	3.7
43	CP	88	LYS	3.7
1	AA	1049	U	3.7
30	CD	184	ARG	3.7
31	CA	1168	G	3.7
11	BK	29	ASN	3.7
10	BJ	16	ARG	3.7
2	AB	186	ILE	3.7
37	CJ	35	ILE	3.7
43	CP	99	TYR	3.7
30	CD	49	GLN	3.7
8	BH	55	THR	3.7
30	CD	28	GLU	3.7
34	CF	164	GLU	3.7
29	CC	102	ARG	3.7
31	CA	1535	A	3.7
37	CJ	132	THR	3.7
31	CA	32	C	3.7

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Mol	Chain	Res	Type	RSRZ
41	CN	6	ARG	3.7
10	BJ	98	VAL	3.7
31	CA	2801	G	3.7
29	CC	100	GLU	3.7
35	CG	22	GLN	3.7
7	BG	119	ARG	3.7
18	BR	67	LEU	3.7
29	CC	33	LEU	3.7
31	CA	101	A	3.7
31	CA	2119	A	3.7
34	DF	83	TYR	3.7
37	CJ	98	VAL	3.7
17	AQ	9	GLN	3.7
1	BA	1006	G	3.6
31	CA	2819	G	3.6
13	AM	46	SER	3.6
14	BN	25	ALA	3.6
37	DJ	114	ALA	3.6
7	AG	69	VAL	3.6
35	CG	130	GLU	3.6
1	BA	1121	U	3.6
9	AI	9	THR	3.6
35	CG	54	PRO	3.6
33	CE	175	ILE	3.6
48	CU	76	ARG	3.6
54	DI	104	ALA	3.6
48	CU	82	LYS	3.6
53	CZ	31	GLN	3.6
55	DA	1067	A	3.6
55	DA	2126	A	3.6
55	DA	2164	C	3.6
7	BG	63	GLU	3.6
15	BO	15	PHE	3.6
14	BN	29	ALA	3.6
36	CH	137	GLU	3.6
37	CJ	139	VAL	3.6
47	CT	105	VAL	3.6
1	BA	1235	U	3.6
9	AI	7	TYR	3.6
2	AB	65	GLY	3.6
46	CS	30	GLY	3.6
14	BN	64	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
34	CF	156	ILE	3.6
36	CH	143	ILE	3.6
54	DI	6	GLN	3.6
20	BT	51	PHE	3.6
1	AA	844	G	3.6
1	BA	1002	G	3.6
8	BH	2	SER	3.6
30	CD	95	SER	3.6
37	DJ	46	THR	3.6
13	BM	59	GLU	3.6
44	CQ	8	LEU	3.6
53	CZ	26	PHE	3.6
1	BA	1222	G	3.6
30	CD	2	ILE	3.6
33	CE	186	VAL	3.6
53	CZ	47	ARG	3.6
54	DI	55	VAL	3.6
3	BC	70	THR	3.6
13	BM	85	CYS	3.6
10	AJ	37	ARG	3.6
3	BC	178	LEU	3.6
9	BI	6	TYR	3.6
2	AB	201	PRO	3.6
25	C4	2	PRO	3.6
7	BG	123	GLU	3.6
3	BC	147	LYS	3.6
14	BN	45	VAL	3.6
33	CE	148	ILE	3.6
40	CM	136	GLU	3.6
37	DJ	51	LYS	3.6
40	CM	94	THR	3.6
9	BI	81	HIS	3.6
14	AN	51	LEU	3.6
17	BQ	8	LEU	3.6
1	BA	1124	G	3.6
29	CC	47	GLY	3.6
34	CF	170	LEU	3.6
1	AA	1243	C	3.5
9	BI	68	LYS	3.5
14	AN	52	PRO	3.5
13	AM	39	ILE	3.5
24	C3	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
34	CF	32	GLU	3.5
39	CL	2	ILE	3.5
44	CQ	84	ILE	3.5
53	CZ	20	ASN	3.5
34	CF	22	TYR	3.5
37	DJ	66	SER	3.5
1	BA	1007	U	3.5
13	BM	7	ILE	3.5
19	AS	67	VAL	3.5
31	CA	2245	U	3.5
35	CG	41	VAL	3.5
2	AB	225	ARG	3.5
7	AG	39	ALA	3.5
55	DA	1175	A	3.5
21	AU	12	PHE	3.5
34	CF	28	VAL	3.5
36	CH	110	VAL	3.5
37	CJ	49	ILE	3.5
47	CT	66	ILE	3.5
2	BB	206	ALA	3.5
11	BK	93	ARG	3.5
31	CA	1534	U	3.5
7	AG	56	LYS	3.5
8	AH	122	GLY	3.5
1	AA	1128	C	3.5
19	AS	74	PHE	3.5
30	CD	29	VAL	3.5
22	C1	5	GLN	3.5
10	BJ	30	LYS	3.5
13	AM	5	ALA	3.5
37	CJ	119	GLY	3.5
40	CM	125	LEU	3.5
53	CZ	33	ALA	3.5
9	AI	92	GLU	3.5
3	AC	66	VAL	3.5
19	BS	19	VAL	3.5
36	CH	144	VAL	3.5
50	CW	89	ILE	3.5
1	AA	959	A	3.5
1	BA	1238	A	3.5
2	BB	34	ALA	3.5
16	AP	22	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
34	CF	126	GLY	3.5
3	AC	101	ILE	3.5
5	BE	120	VAL	3.5
40	CM	110	VAL	3.5
53	CZ	14	LEU	3.5
3	BC	7	PRO	3.5
7	BG	86	GLN	3.5
1	AA	977	A	3.5
1	BA	975	A	3.5
1	BA	1046	A	3.5
1	AA	1029	U	3.5
3	BC	106	VAL	3.5
6	BF	10	VAL	3.5
13	BM	4	ILE	3.5
25	C4	24	HIS	3.5
30	CD	152	PRO	3.5
47	CT	87	PRO	3.5
1	BA	1367	C	3.5
37	DJ	33	VAL	3.5
55	DA	2170	A	3.5
40	CM	135	ILE	3.5
7	BG	140	ASP	3.5
2	BB	156	GLY	3.5
16	AP	81	ALA	3.5
23	C2	23	THR	3.5
37	CJ	97	LYS	3.5
6	BF	39	LEU	3.5
14	AN	71	HIS	3.5
17	AQ	47	HIS	3.5
19	BS	69	HIS	3.5
1	BA	952	U	3.5
1	BA	957	U	3.5
13	BM	98	ARG	3.5
14	BN	73	PHE	3.5
34	CF	112	ARG	3.5
33	CE	33	VAL	3.5
9	BI	98	LEU	3.5
2	BB	33	GLY	3.5
37	DJ	17	MET	3.5
13	AM	8	ASN	3.5
27	C0	9	GLN	3.5
40	CM	134	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
10	BJ	55	PRO	3.5
13	BM	70	ARG	3.5
22	C1	15	MET	3.5
46	CS	35	PHE	3.5
10	BJ	34	ALA	3.5
27	C0	55	VAL	3.4
31	CA	2156	G	3.4
41	CN	69	PRO	3.4
3	AC	170	GLU	3.4
3	BC	190	HIS	3.4
12	BL	70	GLU	3.4
10	AJ	90	LEU	3.4
27	C0	48	ILE	3.4
35	CG	6	LYS	3.4
44	CQ	4	ILE	3.4
1	AA	1022	A	3.4
37	DJ	39	CYS	3.4
41	CN	79	ALA	3.4
13	BM	62	LYS	3.4
30	CD	5	VAL	3.4
49	CV	79	LYS	3.4
48	DU	92	ASN	3.4
9	BI	129	LYS	3.4
20	BT	60	ARG	3.4
3	BC	144	LEU	3.4
1	BA	1314	C	3.4
3	BC	40	ARG	3.4
34	CF	129	SER	3.4
24	C3	31	LEU	3.4
29	CC	245	VAL	3.4
19	AS	49	ILE	3.4
31	CA	896	A	3.4
44	CQ	115	ASN	3.4
52	CY	46	PHE	3.4
1	BA	1364	U	3.4
3	BC	50	ALA	3.4
11	BK	84	VAL	3.4
55	DA	2165	C	3.4
45	CR	26	GLY	3.4
1	BA	1014	A	3.4
7	BG	90	GLU	3.4
21	AU	9	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
39	CL	89	ASN	3.4
3	BC	111	LEU	3.4
55	DA	2152	G	3.4
14	BN	95	GLY	3.4
37	CJ	125	MET	3.4
49	CV	27	ASN	3.4
1	AA	1280	A	3.4
7	BG	108	ALA	3.4
44	CQ	28	VAL	3.4
46	CS	61	ALA	3.4
13	BM	55	THR	3.4
33	CE	17	THR	3.4
7	AG	26	PHE	3.4
13	BM	100	GLN	3.4
31	CA	2109	U	3.4
31	CA	476	G	3.4
3	BC	124	LEU	3.4
19	AS	32	ARG	3.4
45	CR	116	ALA	3.4
23	C2	49	TYR	3.4
1	BA	1036	A	3.4
10	AJ	28	THR	3.4
31	CA	344	A	3.4
31	CA	501	A	3.4
36	DH	47	PHE	3.4
13	BM	47	GLU	3.4
30	CD	30	GLU	3.4
13	BM	81	MET	3.4
9	BI	18	ARG	3.4
1	BA	1013	G	3.4
3	BC	105	GLU	3.4
15	BO	25	THR	3.4
1	AA	1332	A	3.4
49	CV	22	ARG	3.4
35	CG	169	VAL	3.4
40	CM	83	ALA	3.4
43	CP	58	ILE	3.4
1	BA	1356	G	3.4
31	CA	2802	G	3.4
4	AD	154	ARG	3.4
35	CG	86	LYS	3.4
7	AG	43	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
44	CQ	92	VAL	3.3
54	DI	5	LEU	3.3
30	CD	90	PHE	3.3
55	DA	892	A	3.3
3	BC	74	GLY	3.3
29	CC	251	GLN	3.3
34	CF	42	GLU	3.3
37	CJ	95	LYS	3.3
37	DJ	50	GLU	3.3
12	AL	67	ILE	3.3
31	CA	2449	U	3.3
54	DI	84	TYR	3.3
1	BA	1216	A	3.3
2	BB	145	GLU	3.3
14	BN	39	GLU	3.3
16	BP	60	TRP	3.3
43	CP	35	ILE	3.3
52	CY	45	ARG	3.3
55	DA	1065	U	3.3
1	BA	1246	A	3.3
7	BG	23	LEU	3.3
7	BG	32	VAL	3.3
7	BG	75	VAL	3.3
9	AI	67	VAL	3.3
33	CE	193	VAL	3.3
47	CT	86	MET	3.3
7	BG	145	ALA	3.3
9	BI	122	ARG	3.3
10	BJ	89	ARG	3.3
30	CD	101	PHE	3.3
7	AG	55	GLY	3.3
31	CA	2628	C	3.3
42	CO	96	ARG	3.3
49	CV	85	PHE	3.3
1	AA	1042	A	3.3
3	AC	104	ALA	3.3
44	CQ	2	SER	3.3
10	BJ	79	PRO	3.3
7	AG	136	LYS	3.3
13	BM	44	LYS	3.3
33	CE	154	ASP	3.3
53	CZ	60	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
29	CC	30	PHE	3.3
7	BG	60	GLU	3.3
13	AM	35	ALA	3.3
37	CJ	16	GLY	3.3
7	BG	80	VAL	3.3
14	AN	41	ARG	3.3
46	CS	25	LEU	3.3
31	CA	2151	U	3.3
41	CN	73	ILE	3.3
49	DV	56	GLY	3.3
55	DA	2149	U	3.3
29	CC	93	LEU	3.3
1	BA	1316	G	3.3
31	CA	1862	G	3.3
40	CM	22	GLY	3.3
31	CA	1058	U	3.3
31	CA	2796	U	3.3
40	DM	104	GLN	3.3
1	AA	1044	A	3.3
6	BF	5	GLU	3.3
16	BP	53	ASP	3.3
36	DH	86	ASP	3.3
7	BG	5	ARG	3.3
20	AT	2	ALA	3.3
48	CU	44	LYS	3.3
7	BG	68	ASN	3.3
20	BT	75	HIS	3.3
31	CA	880	G	3.3
48	CU	32	LEU	3.3
49	CV	50	PRO	3.3
3	BC	166	GLU	3.3
7	BG	76	LYS	3.3
16	AP	46	LYS	3.3
7	AG	109	ARG	3.3
23	C2	6	ARG	3.3
51	CX	85	GLU	3.3
53	CZ	32	ALA	3.3
7	BG	44	TYR	3.3
1	BA	1363	A	3.3
33	CE	24	ASN	3.3
43	CP	54	VAL	3.3
31	CA	138	U	3.3

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Mol	Chain	Res	Type	RSRZ
55	DA	2133	G	3.3
2	BB	9	MET	3.3
31	CA	2177	C	3.3
7	AG	127	ALA	3.3
7	BG	7	ILE	3.3
20	BT	72	ALA	3.3
35	CG	141	ILE	3.3
25	C4	25	LYS	3.3
29	CC	94	VAL	3.3
43	CP	34	HIS	3.3
51	CX	69	PHE	3.3
19	AS	24	GLU	3.2
35	CG	35	ARG	3.2
3	BC	148	GLY	3.2
13	AM	4	ILE	3.2
14	BN	33	ASP	3.2
37	DJ	47	ASP	3.2
3	BC	72	ARG	3.2
31	CA	431	U	3.2
49	CV	76	ALA	3.2
1	AA	1001	C	3.2
16	AP	78	VAL	3.2
17	BQ	53	CYS	3.2
48	CU	5	GLU	3.2
3	BC	81	GLY	3.2
18	BR	39	ILE	3.2
3	BC	42	TYR	3.2
18	BR	23	TYR	3.2
31	CA	646	U	3.2
35	CG	127	THR	3.2
7	AG	66	LEU	3.2
16	AP	6	LEU	3.2
30	CD	201	LEU	3.2
50	CW	46	LYS	3.2
31	CA	930	G	3.2
39	CL	16	ALA	3.2
54	DI	135	ALA	3.2
2	AB	16	PHE	3.2
35	CG	157	TYR	3.2
21	AU	3	VAL	3.2
43	CP	28	VAL	3.2
45	CR	75	SER	3.2

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Mol	Chain	Res	Type	RSRZ
13	BM	53	ILE	3.2
1	BA	995	C	3.2
14	BN	42	TRP	3.2
36	CH	67	ALA	3.2
1	AA	973	G	3.2
31	CA	81	G	3.2
49	CV	21	LYS	3.2
55	DA	1731	G	3.2
1	AA	997	U	3.2
15	BO	21	ASP	3.2
2	AB	15	HIS	3.2
3	AC	144	LEU	3.2
9	AI	37	GLN	3.2
11	BK	66	ALA	3.2
54	DI	106	PHE	3.2
1	AA	962	C	3.2
9	AI	94	LEU	3.2
40	CM	112	LEU	3.2
51	CX	37	ILE	3.2
17	BQ	45	HIS	3.2
7	AG	51	ALA	3.2
11	BK	86	VAL	3.2
16	AP	16	PHE	3.2
1	BA	1146	A	3.2
19	AS	21	LYS	3.2
19	BS	21	LYS	3.2
7	BG	129	GLU	3.2
13	BM	3	ARG	3.2
9	BI	94	LEU	3.2
44	CQ	95	ALA	3.2
36	CH	103	VAL	3.2
40	CM	119	PRO	3.2
30	CD	89	GLU	3.2
51	CX	70	GLU	3.2
55	DA	1068	G	3.2
40	CM	88	GLY	3.2
42	CO	83	LEU	3.2
45	CR	98	ILE	3.2
31	CA	885	C	3.2
34	CF	159	THR	3.2
43	CP	61	GLN	3.2
55	DA	893	C	3.2

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Mol	Chain	Res	Type	RSRZ
11	BK	24	HIS	3.2
7	AG	71	PRO	3.2
3	BC	33	LEU	3.2
36	DH	12	LEU	3.2
21	BU	5	LYS	3.2
40	CM	73	ILE	3.2
36	CH	91	PHE	3.2
9	BI	58	VAL	3.2
12	BL	50	ARG	3.2
13	BM	61	ALA	3.2
18	BR	35	GLU	3.2
31	CA	1076	C	3.2
35	CG	121	ILE	3.2
35	DG	103	ILE	3.2
47	CT	36	LEU	3.2
37	CJ	94	ASN	3.2
1	BA	1257	A	3.2
1	BA	1312	G	3.2
2	AB	130	THR	3.2
11	AK	21	ALA	3.2
16	BP	9	HIS	3.2
25	C4	43	HIS	3.2
31	CA	2799	A	3.2
3	BC	47	LEU	3.1
39	CL	99	ILE	3.1
3	BC	107	ARG	3.1
33	CE	100	MET	3.1
50	CW	26	PHE	3.1
43	CP	113	ALA	3.1
34	CF	68	THR	3.1
1	AA	971	G	3.1
36	DH	88	GLY	3.1
1	BA	1366	C	3.1
25	C4	49	MET	3.1
31	CA	336	C	3.1
31	CA	1044	C	3.1
52	CY	47	VAL	3.1
2	AB	64	LYS	3.1
36	CH	133	GLN	3.1
53	DZ	3	ALA	3.1
33	CE	15	SER	3.1
36	CH	82	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	AC	70	THR	3.1
10	BJ	52	LEU	3.1
37	DJ	106	LEU	3.1
10	BJ	18	ILE	3.1
45	CR	65	ILE	3.1
1	BA	1086	U	3.1
14	BN	12	LYS	3.1
31	CA	102	U	3.1
31	CA	850	U	3.1
50	CW	94	ALA	3.1
3	BC	87	LEU	3.1
7	BG	70	ARG	3.1
48	CU	12	ARG	3.1
11	BK	30	THR	3.1
19	BS	11	ILE	3.1
34	CF	147	ASP	3.1
39	CL	56	ASP	3.1
10	BJ	57	VAL	3.1
7	AG	5	ARG	3.1
37	CJ	124	ALA	3.1
46	CS	1	MET	3.1
1	AA	991	U	3.1
10	AJ	30	LYS	3.1
14	AN	19	LYS	3.1
1	AA	974	A	3.1
51	CX	57	HIS	3.1
34	CF	176	PRO	3.1
55	DA	897	C	3.1
55	DA	2153	C	3.1
2	AB	217	VAL	3.1
1	BA	844	G	3.1
29	CC	92	ALA	3.1
35	CG	96	ALA	3.1
54	DI	28	ALA	3.1
14	BN	7	LYS	3.1
29	CC	240	PHE	3.1
3	AC	151	VAL	3.1
34	CF	46	ASP	3.1
34	CF	89	VAL	3.1
35	CG	113	VAL	3.1
13	AM	104	THR	3.1
43	CP	62	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	CF	82	GLY	3.1
30	CD	46	ARG	3.1
45	CR	30	ARG	3.1
2	BB	36	ASN	3.1
9	AI	88	MET	3.1
40	CM	122	VAL	3.1
13	AM	23	TYR	3.1
31	CA	2170	A	3.1
2	BB	40	ILE	3.1
13	BM	25	VAL	3.1
30	CD	88	GLU	3.1
35	DG	105	LEU	3.1
16	AP	57	ILE	3.1
38	CK	55	ILE	3.1
11	BK	62	ALA	3.1
18	AR	29	LEU	3.1
14	AN	13	ARG	3.1
33	CE	161	ALA	3.1
1	BA	1315	U	3.1
47	CT	101	SER	3.1
53	CZ	40	SER	3.1
12	BL	93	VAL	3.1
21	BU	28	VAL	3.1
34	CF	165	GLU	3.1
1	BA	1362	A	3.1
9	BI	124	ARG	3.1
10	AJ	102	LEU	3.1
31	CA	316	C	3.1
33	CE	43	THR	3.0
1	BA	1347	G	3.0
31	CA	1210	G	3.0
7	AG	108	ALA	3.0
11	BK	21	ALA	3.0
35	CG	61	GLY	3.0
35	CG	66	GLY	3.0
55	DA	2119	A	3.0
3	BC	118	ASP	3.0
19	BS	56	GLN	3.0
36	CH	149	GLU	3.0
51	CX	64	ASP	3.0
48	CU	31	VAL	3.0
14	AN	16	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
23	C2	34	LEU	3.0
33	CE	12	LEU	3.0
2	AB	213	TYR	3.0
44	CQ	23	GLY	3.0
1	BA	1145	A	3.0
14	AN	34	VAL	3.0
30	CD	155	VAL	3.0
33	CE	32	VAL	3.0
31	CA	1174	U	3.0
36	DH	5	LEU	3.0
2	BB	35	ARG	3.0
23	C2	32	GLU	3.0
47	CT	96	ILE	3.0
36	DH	123	ARG	3.0
3	BC	123	GLN	3.0
1	BA	1000	A	3.0
1	BA	1230	C	3.0
28	CB	23	G	3.0
31	CA	312	G	3.0
6	BF	96	VAL	3.0
6	AF	42	TRP	3.0
29	CC	202	LEU	3.0
1	AA	1028	C	3.0
13	BM	107	ARG	3.0
31	CA	1732	C	3.0
34	CF	54	ALA	3.0
40	CM	21	ARG	3.0
50	CW	6	ALA	3.0
1	BA	1310	G	3.0
2	AB	31	ILE	3.0
31	CA	2891	U	3.0
55	DA	1063	G	3.0
13	BM	60	VAL	3.0
14	AN	47	LYS	3.0
14	BN	70	PRO	3.0
16	AP	21	VAL	3.0
37	DJ	92	LYS	3.0
35	CG	50	LEU	3.0
20	BT	84	ASN	3.0
3	BC	28	GLU	3.0
9	AI	8	GLY	3.0
14	AN	72	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	CE	45	ALA	3.0
36	CH	74	ALA	3.0
1	AA	1322	C	3.0
2	BB	4	VAL	3.0
3	BC	76	VAL	3.0
18	BR	55	LEU	3.0
1	BA	1186	G	3.0
31	CA	513	A	3.0
31	CA	2152	G	3.0
31	CA	2169	A	3.0
14	BN	63	ARG	3.0
34	CF	122	PHE	3.0
18	BR	33	ILE	3.0
25	C4	28	ASN	3.0
37	CJ	70	VAL	3.0
14	BN	41	ARG	3.0
49	CV	94	ARG	3.0
31	CA	502	A	3.0
55	DA	2171	A	3.0
1	BA	1272	G	3.0
13	BM	50	GLU	3.0
21	BU	15	ALA	3.0
44	CQ	27	GLU	3.0
7	BG	89	VAL	3.0
45	CR	81	ASN	3.0
11	BK	46	THR	3.0
45	CR	106	PHE	3.0
48	CU	68	LYS	3.0
55	DA	2131	U	3.0
27	C0	39	GLU	3.0
36	CH	107	GLY	3.0
37	CJ	123	GLU	3.0
3	BC	75	ILE	3.0
7	AG	79	ARG	3.0
17	AQ	4	LYS	3.0
35	CG	172	LYS	3.0
55	DA	2166	U	3.0
3	BC	151	VAL	3.0
55	DA	1170	C	3.0
1	AA	1220	G	2.9
1	AA	1244	G	2.9
7	AG	132	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
23	C2	31	PRO	3.0
31	CA	1407	G	2.9
46	CS	67	GLY	2.9
3	AC	107	ARG	2.9
3	AC	130	PHE	2.9
31	CA	1278	C	2.9
54	DI	103	ASN	2.9
31	CA	2346	A	2.9
51	CX	34	GLY	2.9
11	AK	84	VAL	2.9
13	BM	80	LEU	2.9
13	BM	86	TYR	2.9
16	BP	17	TYR	2.9
20	BT	50	ALA	2.9
30	CD	7	LYS	2.9
1	BA	1187	G	2.9
48	CU	79	ASP	2.9
54	DI	96	PHE	2.9
23	C2	48	ILE	2.9
40	CM	103	ILE	2.9
47	CT	6	LYS	2.9
31	CA	508	A	2.9
33	CE	101	TYR	2.9
47	CT	45	VAL	2.9
3	BC	203	PHE	2.9
40	CM	107	PHE	2.9
8	AH	56	LYS	2.9
14	BN	26	GLU	2.9
55	DA	546	U	2.9
14	AN	60	GLN	2.9
29	CC	234	GLY	2.9
31	CA	2136	G	2.9
49	CV	20	GLY	2.9
53	CZ	9	LYS	2.9
9	BI	118	LEU	2.9
14	AN	27	LEU	2.9
17	BQ	76	VAL	2.9
20	BT	79	LEU	2.9
29	CC	19	VAL	2.9
35	CG	37	LEU	2.9
1	BA	1112	C	2.9
31	CA	228	C	2.9

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Mol	Chain	Res	Type	RSRZ
37	DJ	60	THR	2.9
31	CA	1551	A	2.9
35	CG	125	CYS	2.9
13	AM	44	LYS	2.9
13	BM	75	MET	2.9
14	AN	18	ASP	2.9
23	C2	7	GLU	2.9
24	C3	37	LYS	2.9
17	BQ	17	MET	2.9
39	CL	1	MET	2.9
3	AC	149	ILE	2.9
14	BN	34	VAL	2.9
43	CP	41	ALA	2.9
45	CR	118	ALA	2.9
1	BA	1139	G	2.9
34	DF	72	LYS	2.9
3	BC	145	GLY	2.9
2	AB	14	VAL	2.9
3	BC	41	GLN	2.9
7	AG	91	VAL	2.9
11	AK	113	VAL	2.9
37	CJ	30	GLN	2.9
3	BC	32	ASN	2.9
24	C3	7	PRO	2.9
35	CG	68	ALA	2.9
23	C2	22	THR	2.9
1	BA	1265	C	2.9
8	BH	120	GLY	2.9
23	C2	16	GLY	2.9
31	CA	1026	G	2.9
31	CA	2161	C	2.9
37	CJ	29	GLY	2.9
48	CU	1	MET	2.9
23	C2	45	GLN	2.9
35	CG	79	VAL	2.9
36	CH	75	LEU	2.9
36	DH	18	GLN	2.9
49	CV	34	VAL	2.9
1	BA	991	U	2.9
1	BA	1005	A	2.9
14	AN	2	ALA	2.9
31	CA	505	A	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	975	A	2.9
34	CF	172	ALA	2.9
42	CO	23	ASN	2.9
36	DH	16	GLY	2.9
2	BB	38	VAL	2.9
9	BI	113	ARG	2.9
34	CF	30	ARG	2.9
18	BR	50	LYS	2.9
20	BT	34	LYS	2.9
44	CQ	7	GLN	2.9
30	CD	132	ALA	2.9
36	CH	140	ALA	2.9
1	BA	102	G	2.9
1	BA	275	G	2.9
1	BA	1334	G	2.9
30	CD	97	SER	2.9
31	CA	2155	U	2.9
36	CH	136	SER	2.9
37	DJ	48	SER	2.9
1	AA	994	A	2.9
48	CU	80	TRP	2.9
43	CP	106	LEU	2.9
53	DZ	63	ALA	2.9
3	AC	188	GLU	2.9
6	BF	58	HIS	2.9
9	BI	15	SER	2.9
31	CA	72	U	2.9
31	CA	2107	G	2.9
51	CX	42	GLY	2.9
3	AC	191	THR	2.9
13	BM	73	ILE	2.9
31	CA	1095	A	2.9
7	BG	98	ALA	2.9
8	AH	130	ALA	2.9
13	BM	42	ASP	2.9
30	CD	39	ASP	2.9
2	AB	17	GLY	2.9
19	AS	59	PRO	2.9
46	CS	12	HIS	2.9
50	CW	37	PRO	2.9
2	BB	212	LEU	2.9
31	CA	876	C	2.9

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Mol	Chain	Res	Type	RSRZ
40	CM	1	MET	2.9
43	CP	67	ASN	2.9
1	BA	1339	A	2.9
10	BJ	86	ALA	2.9
31	CA	1047	G	2.9
31	CA	1107	G	2.9
36	CH	127	GLU	2.9
18	BR	38	LYS	2.9
30	CD	3	GLY	2.9
30	CD	40	LEU	2.9
48	CU	30	ILE	2.8
10	BJ	5	ARG	2.8
16	BP	35	ARG	2.8
44	CQ	99	TYR	2.8
2	AB	21	ARG	2.8
37	DJ	103	ARG	2.8
9	AI	64	TYR	2.8
23	C2	35	GLU	2.8
1	BA	1045	C	2.8
31	CA	405	U	2.8
31	CA	2165	C	2.8
13	AM	22	ILE	2.8
17	AQ	46	VAL	2.8
1	AA	412	A	2.8
6	BF	62	MET	2.8
26	C5	19	ARG	2.8
36	DH	4	ILE	2.8
31	CA	1214	A	2.8
45	CR	92	ARG	2.8
7	BG	110	LYS	2.8
9	BI	112	GLU	2.8
20	BT	36	TYR	2.8
43	CP	55	GLU	2.8
46	CS	62	GLU	2.8
1	BA	84	U	2.8
1	BA	208	U	2.8
10	AJ	92	LEU	2.8
31	CA	2180	U	2.8
31	CA	2300	C	2.8
31	CA	2313	C	2.8
34	CF	137	ILE	2.8
34	DF	80	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
41	CN	8	LYS	2.8
50	CW	8	VAL	2.8
7	AG	151	PHE	2.8
8	BH	107	SER	2.8
31	CA	409	G	2.8
31	CA	1166	G	2.8
31	CA	2148	G	2.8
31	CA	2286	G	2.8
35	CG	31	GLY	2.8
31	CA	1533	C	2.8
3	AC	187	SER	2.8
9	BI	5	GLN	2.8
13	AM	56	LEU	2.8
16	AP	51	ARG	2.8
35	CG	95	ARG	2.8
37	DJ	105	GLN	2.8
37	DJ	97	LYS	2.8
49	CV	38	GLY	2.8
53	CZ	21	LEU	2.8
1	BA	1360	A	2.8
31	CA	1532	A	2.8
49	CV	67	VAL	2.8
1	AA	1321	U	2.8
9	BI	91	ASP	2.8
37	DJ	136	MET	2.8
31	CA	549	G	2.8
31	CA	2892	G	2.8
42	CO	117	ASP	2.8
44	CQ	22	PRO	2.8
13	AM	36	ALA	2.8
31	CA	1049	C	2.8
9	BI	10	GLY	2.8
49	DV	46	GLN	2.8
50	CW	10	LYS	2.8
13	AM	43	VAL	2.8
37	CJ	140	VAL	2.8
51	CX	36	ILE	2.8
17	BQ	7	THR	2.8
7	AG	126	ASP	2.8
33	CE	91	ASP	2.8
9	AI	24	GLY	2.8
1	BA	990	C	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	2153	C	2.8
31	CA	2877	G	2.8
35	CG	17	VAL	2.8
1	AA	1188	A	2.8
9	AI	107	ASP	2.8
18	AR	22	ASP	2.8
55	DA	2114	A	2.8
1	BA	1224	U	2.8
9	AI	32	GLN	2.8
15	BO	16	GLY	2.8
9	BI	111	VAL	2.8
40	CM	111	ILE	2.8
2	AB	5	SER	2.8
1	AA	951	G	2.8
1	BA	1190	G	2.8
7	AG	143	ARG	2.8
34	CF	80	ARG	2.8
40	CM	129	LYS	2.8
8	BH	130	ALA	2.8
34	CF	62	GLY	2.8
34	CF	113	ASP	2.8
45	CR	91	ASP	2.8
49	CV	48	PRO	2.8
1	AA	121	U	2.8
20	BT	48	GLN	2.8
37	DJ	140	VAL	2.8
2	AB	40	ILE	2.8
36	DH	94	ILE	2.8
13	AM	85	CYS	2.8
1	AA	972	C	2.8
1	BA	202	G	2.8
18	BR	32	TYR	2.8
31	CA	1211	C	2.8
34	CF	157	THR	2.8
42	CO	94	TYR	2.8
17	BQ	78	VAL	2.8
11	AK	97	ILE	2.8
5	AE	96	MET	2.8
11	BK	100	LEU	2.8
2	BB	17	GLY	2.8
1	AA	1140	C	2.8
1	BA	1320	C	2.8

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Mol	Chain	Res	Type	RSRZ
9	AI	119	ARG	2.8
4	AD	18	ASP	2.8
10	AJ	98	VAL	2.8
25	C4	26	HIS	2.8
33	CE	18	THR	2.8
34	CF	33	LYS	2.8
29	CC	98	ASP	2.8
35	DG	115	HIS	2.8
10	AJ	78	GLU	2.7
1	AA	433	G	2.7
1	AA	1319	A	2.7
1	BA	1318	A	2.7
16	BP	8	ARG	2.7
34	CF	47	LYS	2.7
42	CO	63	ARG	2.7
49	CV	56	GLY	2.7
34	CF	65	PRO	2.7
43	CP	78	VAL	2.7
46	CS	14	VAL	2.7
36	CH	70	GLU	2.7
1	AA	999	C	2.7
3	AC	89	LYS	2.7
48	CU	11	LEU	2.7
1	AA	134	G	2.7
3	BC	146	ALA	2.7
31	CA	881	G	2.7
40	CM	7	SER	2.7
11	BK	97	ILE	2.7
31	CA	2860	A	2.7
54	DI	124	ASP	2.7
3	BC	108	LYS	2.7
29	CC	101	ARG	2.7
49	CV	82	ARG	2.7
1	BA	1054	C	2.7
30	CD	19	GLY	2.7
55	DA	2161	C	2.7
16	BP	39	PHE	2.7
31	CA	2904	U	2.7
55	DA	1066	U	2.7
14	AN	70	PRO	2.7
10	AJ	22	THR	2.7
14	BN	40	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
17	BQ	44	LEU	2.7
19	AS	27	ASP	2.7
28	CB	24	G	2.7
37	DJ	10	LYS	2.7
48	CU	81	LYS	2.7
31	CA	1548	A	2.7
9	AI	103	PHE	2.7
46	CS	5	PHE	2.7
50	CW	65	VAL	2.7
1	BA	1335	U	2.7
43	CP	56	LYS	2.7
7	BG	47	LEU	2.7
7	BG	122	ASN	2.7
26	C5	10	LEU	2.7
47	CT	37	THR	2.7
51	CX	32	LEU	2.7
1	AA	1272	G	2.7
2	BB	69	PHE	2.7
31	CA	1212	G	2.7
8	AH	127	CYS	2.7
9	AI	22	LYS	2.7
30	CD	48	ILE	2.7
1	AA	88	U	2.7
1	BA	1149	C	2.7
1	BA	1336	C	2.7
10	BJ	54	SER	2.7
2	AB	42	ASN	2.7
31	CA	1046	A	2.7
31	CA	1090	A	2.7
9	BI	87	LEU	2.7
14	AN	49	GLN	2.7
31	CA	1112	G	2.7
17	BQ	72	SER	2.7
1	BA	961	U	2.7
19	AS	44	MET	2.7
2	AB	159	ASP	2.7
2	BB	131	LYS	2.7
12	AL	68	GLY	2.7
3	AC	127	ARG	2.7
11	AK	18	ASP	2.7
49	CV	25	VAL	2.7
9	AI	83	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
18	AR	32	TYR	2.7
1	BA	325	A	2.7
35	DG	177	LYS	2.7
38	CK	40	HIS	2.7
53	CZ	4	LYS	2.7
54	DI	38	MET	2.7
1	BA	107	G	2.7
2	BB	13	GLY	2.7
36	DH	13	GLY	2.7
29	CC	210	ALA	2.7
55	DA	1172	C	2.7
18	BR	29	LEU	2.7
43	CP	115	LEU	2.7
46	CS	22	LEU	2.7
27	C0	54	MET	2.7
1	BA	974	A	2.7
5	BE	38	VAL	2.7
33	CE	174	GLY	2.7
35	CG	28	GLY	2.7
29	CC	90	ASN	2.7
1	AA	1323	G	2.7
1	BA	945	G	2.7
9	AI	98	LEU	2.7
19	BS	18	LYS	2.7
31	CA	1238	G	2.7
35	DG	107	LEU	2.7
9	AI	124	ARG	2.7
15	BO	88	ARG	2.7
44	CQ	12	GLN	2.7
44	CQ	59	PHE	2.7
51	CX	38	VAL	2.7
2	BB	164	ILE	2.7
3	AC	180	ALA	2.7
7	BG	61	ALA	2.7
46	CS	49	ILE	2.7
1	BA	1248	A	2.7
9	BI	107	ASP	2.7
34	DF	81	GLN	2.7
55	DA	2178	C	2.7
21	BU	4	ILE	2.7
44	DQ	2	SER	2.6
15	BO	89	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
42	CO	36	THR	2.6
1	BA	1319	A	2.6
46	CS	18	GLN	2.6
1	BA	1132	C	2.6
31	CA	2143	C	2.6
10	AJ	10	LEU	2.6
31	CA	474	G	2.6
34	CF	169	LEU	2.6
55	DA	2140	G	2.6
16	AP	40	ASN	2.6
7	AG	105	VAL	2.6
11	BK	20	VAL	2.6
54	DI	98	GLU	2.6
1	AA	1201	A	2.6
3	BC	54	ARG	2.6
13	AM	57	ARG	2.6
31	CA	330	A	2.6
31	CA	1077	A	2.6
43	CP	111	ARG	2.6
9	BI	63	LEU	2.6
27	C0	24	LEU	2.6
46	CS	7	SER	2.6
12	BL	71	GLY	2.6
30	CD	153	GLY	2.6
31	CA	1863	G	2.6
31	CA	2121	G	2.6
34	CF	93	GLY	2.6
36	CH	134	VAL	2.6
37	CJ	92	LYS	2.6
16	AP	50	THR	2.6
2	BB	76	ALA	2.6
35	CG	72	LEU	2.6
37	CJ	122	ILE	2.6
37	DJ	115	ALA	2.6
1	BA	1340	A	2.6
19	AS	57	HIS	2.6
31	CA	1089	A	2.6
7	AG	103	TRP	2.6
16	AP	49	GLY	2.6
47	CT	49	LYS	2.6
2	AB	136	MET	2.6
36	DH	19	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
34	DF	37	ASN	2.6
2	BB	135	LEU	2.6
27	C0	43	ALA	2.6
33	CE	105	LEU	2.6
34	CF	75	ALA	2.6
19	BS	55	ARG	2.6
33	CE	25	GLU	2.6
47	CT	50	VAL	2.6
52	CY	56	MET	2.6
55	DA	2176	A	2.6
1	AA	1147	C	2.6
1	BA	83	C	2.6
1	BA	1141	C	2.6
31	CA	183	C	2.6
31	CA	2078	C	2.6
54	DI	36	ASP	2.6
8	AH	121	LEU	2.6
11	AK	82	LEU	2.6
10	AJ	86	ALA	2.6
37	DJ	41	ALA	2.6
43	CP	109	ALA	2.6
1	AA	1026	G	2.6
1	BA	108	G	2.6
26	D5	38	GLY	2.6
31	CA	1216	G	2.6
33	CE	28	VAL	2.6
13	BM	76	SER	2.6
19	BS	6	LYS	2.6
1	AA	1119	C	2.6
22	C1	56	ALA	2.6
36	CH	141	LYS	2.6
41	CN	17	ASN	2.6
10	BJ	83	THR	2.6
37	CJ	118	THR	2.6
48	CU	85	VAL	2.6
3	AC	87	LEU	2.6
14	AN	64	CYS	2.6
22	C1	18	SER	2.6
49	CV	4	LYS	2.6
1	BA	944	G	2.6
2	BB	188	ASP	2.6
31	CA	2895	G	2.6

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Mol	Chain	Res	Type	RSRZ
1	AA	1216	A	2.6
31	CA	1073	A	2.6
1	AA	1027	C	2.6
2	AB	156	GLY	2.6
11	BK	92	GLY	2.6
1	AA	1121	U	2.6
1	BA	92	U	2.6
13	BM	27	LYS	2.6
25	C4	41	LYS	2.6
36	CH	15	LEU	2.6
34	CF	135	GLN	2.6
46	CS	93	PHE	2.6
51	CX	60	PHE	2.6
51	CX	61	ALA	2.6
7	BG	40	GLU	2.6
19	AS	46	GLY	2.6
25	C4	58	VAL	2.6
54	DI	114	GLU	2.6
50	CW	84	PRO	2.6
1	AA	958	A	2.6
31	CA	2287	A	2.6
16	AP	52	LEU	2.6
29	CC	182	ARG	2.6
34	CF	60	ILE	2.6
36	CH	123	ARG	2.6
42	CO	98	LEU	2.6
1	BA	950	U	2.6
43	CP	97	PHE	2.6
7	BG	125	SER	2.6
5	BE	123	VAL	2.6
9	AI	58	VAL	2.6
16	AP	19	VAL	2.6
17	AQ	10	GLY	2.6
34	CF	94	GLU	2.6
35	CG	85	LYS	2.6
35	DG	113	VAL	2.6
2	AB	27	MET	2.6
40	CM	74	THR	2.6
52	CY	34	HIS	2.6
1	BA	942	G	2.6
1	BA	1188	A	2.6
15	BO	43	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
7	BG	85	TYR	2.6
31	CA	2129	C	2.6
9	BI	92	GLU	2.6
13	AM	110	LYS	2.6
16	BP	36	VAL	2.6
5	AE	124	LEU	2.6
20	BT	56	PRO	2.6
22	C1	8	PRO	2.6
54	DI	126	LEU	2.6
2	BB	39	HIS	2.6
6	BF	36	ILE	2.6
48	CU	70	HIS	2.6
53	CZ	41	HIS	2.6
44	CQ	74	PHE	2.5
24	C3	36	ALA	2.5
42	CO	49	GLU	2.5
2	AB	4	VAL	2.5
12	BL	65	SER	2.5
31	CA	1530	G	2.5
43	CP	47	VAL	2.5
33	CE	171	ASP	2.5
10	AJ	55	PRO	2.5
26	C5	13	ASN	2.5
7	AG	131	LYS	2.5
2	AB	134	ALA	2.5
10	BJ	29	ALA	2.5
14	AN	63	ARG	2.5
36	CH	27	ARG	2.5
43	CP	71	ALA	2.5
47	CT	95	ARG	2.5
1	AA	1019	A	2.5
1	BA	81	A	2.5
34	CF	121	SER	2.5
35	CG	87	LEU	2.5
5	BE	96	MET	2.5
1	BA	993	G	2.5
1	BA	1144	G	2.5
36	CH	99	ILE	2.5
54	DI	4	ASN	2.5
10	AJ	27	GLU	2.5
13	BM	87	ARG	2.5
34	CF	143	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
37	DJ	107	GLN	2.5
3	AC	148	GLY	2.5
53	CZ	35	GLY	2.5
7	BG	56	LYS	2.5
1	BA	1247	U	2.5
18	AR	21	ILE	2.5
34	CF	99	PHE	2.5
50	CW	29	ILE	2.5
1	BA	78	A	2.5
13	AM	101	ARG	2.5
43	CP	25	ARG	2.5
30	CD	32	ASN	2.5
55	DA	1847	A	2.5
10	BJ	99	GLN	2.5
13	BM	28	THR	2.5
33	CE	120	VAL	2.5
33	CE	121	VAL	2.5
35	CG	51	THR	2.5
44	CQ	26	VAL	2.5
49	CV	66	GLN	2.5
50	CW	67	GLY	2.5
5	AE	81	LEU	2.5
51	CX	24	LYS	2.5
30	CD	179	ARG	2.5
14	AN	100	SER	2.5
2	AB	84	ALA	2.5
5	BE	127	ALA	2.5
1	BA	1325	C	2.5
18	BR	40	VAL	2.5
52	DY	78	TYR	2.5
53	CZ	25	GLN	2.5
33	CE	118	LEU	2.5
1	BA	1266	G	2.5
7	BG	57	SER	2.5
43	CP	108	ASP	2.5
44	CQ	19	SER	2.5
50	CW	41	GLU	2.5
33	CE	37	ALA	2.5
30	CD	188	LEU	2.5
35	CG	128	GLN	2.5
48	CU	41	ALA	2.5
55	DA	1060	U	2.5

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Mol	Chain	Res	Type	RSRZ
9	AI	4	ASN	2.5
9	AI	33	ARG	2.5
35	CG	3	ARG	2.5
1	BA	1140	C	2.5
31	CA	357	C	2.5
3	AC	73	PRO	2.5
1	BA	947	G	2.5
2	AB	13	GLY	2.5
40	CM	20	GLY	2.5
40	CM	85	VAL	2.5
41	CN	106	ASP	2.5
43	CP	95	SER	2.5
53	CZ	63	ALA	2.5
6	BF	47	LEU	2.5
8	BH	121	LEU	2.5
34	CF	81	GLN	2.5
35	CG	116	GLN	2.5
7	AG	104	ILE	2.5
23	C2	9	ILE	2.5
45	CR	90	ILE	2.5
31	CA	262	A	2.5
31	CA	1143	A	2.5
49	CV	62	GLU	2.5
2	AB	221	VAL	2.5
35	CG	69	ARG	2.5
48	CU	50	LEU	2.5
10	BJ	82	LYS	2.5
31	CA	767	U	2.5
35	CG	19	ILE	2.5
36	CH	114	GLU	2.5
50	CW	1	MET	2.5
9	BI	33	ARG	2.5
16	AP	82	ALA	2.5
20	BT	45	ALA	2.5
30	CD	37	VAL	2.5
30	CD	53	GLY	2.5
31	CA	1043	C	2.5
41	CN	78	LEU	2.5
2	AB	132	LYS	2.5
37	DJ	100	LYS	2.5
16	AP	42	ILE	2.5
1	BA	1202	U	2.5

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Mol	Chain	Res	Type	RSRZ
36	CH	76	GLU	2.5
44	CQ	34	GLU	2.5
33	CE	150	THR	2.5
48	CU	86	THR	2.5
1	BA	933	G	2.5
2	AB	57	LEU	2.5
4	AD	2	ALA	2.5
30	CD	104	VAL	2.5
31	CA	561	G	2.5
37	DJ	27	ALA	2.5
3	BC	183	ASP	2.5
46	CS	26	ASP	2.5
53	CZ	44	LYS	2.5
1	BA	250	A	2.5
49	CV	30	SER	2.5
52	CY	18	ARG	2.5
2	BB	155	GLY	2.5
9	AI	54	LEU	2.5
29	CC	78	VAL	2.5
35	CG	67	THR	2.5
35	CG	129	THR	2.5
50	CW	60	VAL	2.5
13	BM	106	ALA	2.5
35	CG	134	LYS	2.5
13	BM	115	PRO	2.5
1	BA	1057	G	2.5
7	AG	15	ASP	2.5
54	DI	122	GLN	2.5
17	BQ	63	GLU	2.5
31	CA	315	G	2.5
31	CA	317	G	2.5
31	CA	2668	G	2.5
43	CP	60	GLU	2.5
31	CA	2045	C	2.4
1	AA	1021	A	2.4
19	BS	46	GLY	2.4
25	C4	44	LEU	2.4
31	CA	311	A	2.4
36	DH	35	LYS	2.4
43	CP	114	GLY	2.4
1	AA	981	U	2.4
2	AB	164	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
47	CT	99	ARG	2.4
35	CG	42	GLU	2.4
24	C3	16	HIS	2.4
2	AB	45	LYS	2.4
3	BC	199	LYS	2.4
1	BA	1043	G	2.4
2	AB	214	LEU	2.4
8	BH	99	LEU	2.4
31	CA	1171	G	2.4
31	CA	1215	G	2.4
31	CA	1874	C	2.4
31	CA	1984	G	2.4
2	BB	75	ALA	2.4
23	C2	15	ALA	2.4
31	CA	2163	A	2.4
31	CA	2176	A	2.4
43	CP	33	ARG	2.4
11	AK	107	ILE	2.4
17	BQ	22	VAL	2.4
42	CO	115	LEU	2.4
48	CU	62	VAL	2.4
49	CV	57	GLY	2.4
3	AC	50	ALA	2.4
7	AG	128	ALA	2.4
14	AN	36	ALA	2.4
25	C4	14	PHE	2.4
1	AA	135	C	2.4
1	AA	980	C	2.4
1	AA	985	C	2.4
14	AN	10	GLU	2.4
46	CS	11	GLN	2.4
54	DI	133	GLU	2.4
1	BA	1189	U	2.4
31	CA	1880	U	2.4
3	BC	6	HIS	2.4
7	AG	64	VAL	2.4
48	CU	65	GLY	2.4
35	CG	174	ALA	2.4
45	CR	68	ALA	2.4
43	CP	80	GLU	2.4
6	AF	61	LEU	2.4
1	BA	68	G	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	969	A	2.4
3	AC	93	ASP	2.4
36	CH	36	ALA	2.4
36	CH	102	ALA	2.4
48	CU	45	ALA	2.4
13	BM	112	PRO	2.4
19	AS	30	PRO	2.4
33	CE	88	ARG	2.4
29	CC	12	GLY	2.4
37	DJ	91	GLY	2.4
27	C0	53	PHE	2.4
41	CN	9	PHE	2.4
6	BF	25	TYR	2.4
5	BE	13	GLU	2.4
9	AI	65	ILE	2.4
31	CA	2138	G	2.4
34	CF	118	SER	2.4
34	DF	85	ILE	2.4
40	CM	86	GLU	2.4
3	BC	88	ARG	2.4
7	BG	59	LEU	2.4
9	BI	48	VAL	2.4
25	C4	63	PRO	2.4
34	CF	149	VAL	2.4
54	DI	72	LEU	2.4
13	AM	10	PRO	2.4
35	CG	8	PRO	2.4
35	CG	171	THR	2.4
25	C4	22	PHE	2.4
54	DI	105	LYS	2.4
3	AC	133	ALA	2.4
3	BC	31	ASP	2.4
47	CT	85	ILE	2.4
1	AA	983	A	2.4
1	AA	1036	A	2.4
1	BA	978	A	2.4
31	CA	332	A	2.4
36	DH	108	VAL	2.4
1	BA	94	G	2.4
1	BA	203	G	2.4
40	CM	87	GLY	2.4
49	CV	44	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
24	C3	43	THR	2.4
33	CE	129	PRO	2.4
35	CG	80	THR	2.4
3	AC	146	ALA	2.4
20	BT	46	ALA	2.4
30	CD	41	ALA	2.4
37	DJ	15	ALA	2.4
31	CA	545	U	2.4
52	CY	64	ILE	2.4
1	AA	998	C	2.4
10	AJ	38	GLY	2.4
10	AJ	77	VAL	2.4
23	C2	12	VAL	2.4
37	CJ	135	SER	2.4
38	CK	22	GLY	2.4
51	CX	65	GLY	2.4
1	BA	101	A	2.4
10	AJ	9	ARG	2.4
15	BO	19	ALA	2.4
19	AS	75	ALA	2.4
42	CO	114	GLU	2.4
48	CU	29	THR	2.4
52	CY	76	GLU	2.4
1	BA	1386	G	2.4
34	CF	120	LYS	2.4
35	CG	177	LYS	2.4
46	CS	92	TRP	2.4
50	CW	63	ILE	2.4
9	AI	87	LEU	2.4
31	CA	1217	U	2.4
21	BU	19	PHE	2.4
34	CF	77	PHE	2.4
50	CW	11	GLU	2.4
1	BA	1311	A	2.4
10	AJ	50	THR	2.4
37	DJ	101	ILE	2.4
2	BB	68	LEU	2.4
3	AC	195	VAL	2.4
15	BO	29	VAL	2.4
34	CF	12	VAL	2.4
1	AA	1124	G	2.4
1	BA	843	U	2.4

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Mol	Chain	Res	Type	RSRZ
34	CF	166	GLY	2.4
13	AM	21	SER	2.4
14	AN	69	ARG	2.4
24	C3	34	ARG	2.4
53	CZ	34	SER	2.4
54	DI	52	MET	2.4
55	DA	2151	U	2.4
7	BG	130	ASN	2.4
35	CG	34	THR	2.4
36	CH	80	ILE	2.4
35	CG	45	HIS	2.4
41	CN	41	LEU	2.4
31	CA	2783	U	2.3
1	BA	1361	G	2.3
3	AC	7	PRO	2.3
30	CD	187	LEU	2.3
25	C4	40	ARG	2.3
30	CD	197	THR	2.3
47	CT	9	HIS	2.3
36	CH	139	PHE	2.3
45	CR	57	PHE	2.3
54	DI	29	ASP	2.3
18	BR	21	ILE	2.3
37	DJ	84	ALA	2.3
48	CU	38	ALA	2.3
34	CF	102	ARG	2.3
53	CZ	48	ARG	2.3
7	AG	141	VAL	2.3
10	BJ	96	VAL	2.3
3	BC	67	THR	2.3
3	BC	135	LYS	2.3
6	BF	97	THR	2.3
10	AJ	32	THR	2.3
31	CA	408	G	2.3
38	CK	23	LYS	2.3
51	CX	62	LYS	2.3
3	BC	3	GLN	2.3
18	BR	22	ASP	2.3
49	DV	54	GLN	2.3
5	AE	144	LEU	2.3
17	BQ	20	SER	2.3
35	CG	13	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
46	CS	59	ILE	2.3
7	AG	18	PHE	2.3
17	BQ	71	LYS	2.3
38	CK	56	VAL	2.3
2	AB	49	MET	2.3
48	CU	4	GLU	2.3
33	CE	168	ASP	2.3
34	CF	163	ASP	2.3
13	BM	79	ARG	2.3
50	CW	79	ARG	2.3
2	BB	12	ALA	2.3
2	BB	186	ILE	2.3
8	BH	75	ILE	2.3
52	CY	59	ILE	2.3
15	AO	43	PHE	2.3
16	BP	20	VAL	2.3
33	CE	196	VAL	2.3
1	BA	121	U	2.3
1	BA	467	U	2.3
55	DA	613	A	2.3
13	AM	47	GLU	2.3
36	DH	11	ASN	2.3
39	CL	3	GLN	2.3
39	CL	82	ASN	2.3
41	CN	92	TRP	2.3
51	CX	83	GLU	2.3
2	AB	28	LYS	2.3
10	AJ	12	ALA	2.3
23	C2	50	LYS	2.3
27	C0	29	LEU	2.3
30	CD	100	LEU	2.3
36	CH	111	ALA	2.3
2	BB	217	VAL	2.3
1	BA	1138	G	2.3
16	BP	41	PRO	2.3
28	CB	27	C	2.3
31	CA	318	C	2.3
36	DH	147	VAL	2.3
50	CW	92	VAL	2.3
31	CA	1063	G	2.3
31	CA	2116	G	2.3
33	CE	55	SER	2.3

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Mol	Chain	Res	Type	RSRZ
36	DH	107	GLY	2.3
1	AA	842	U	2.3
1	AA	1212	U	2.3
7	BG	10	ARG	2.3
9	BI	57	MET	2.3
15	AO	17	ARG	2.3
17	AQ	52	GLU	2.3
29	CC	79	GLU	2.3
44	CQ	109	ARG	2.3
1	AA	1197	A	2.3
1	BA	1333	A	2.3
31	CA	829	A	2.3
31	CA	1847	A	2.3
31	CA	2147	A	2.3
7	AG	23	LEU	2.3
33	CE	180	LEU	2.3
36	DH	8	LYS	2.3
19	AS	40	ILE	2.3
5	BE	85	VAL	2.3
36	CH	121	VAL	2.3
45	CR	73	GLY	2.3
10	BJ	66	GLU	2.3
19	AS	29	LYS	2.3
31	CA	343	C	2.3
37	CJ	36	MET	2.3
44	CQ	38	LYS	2.3
28	CB	117	G	2.3
31	CA	1017	G	2.3
31	CA	1277	G	2.3
1	AA	1117	A	2.3
11	BK	71	ALA	2.3
25	C4	65	ALA	2.3
30	CD	35	THR	2.3
30	CD	34	VAL	2.3
31	CA	1111	A	2.3
31	CA	1322	A	2.3
45	CR	25	TYR	2.3
44	CQ	112	GLU	2.3
1	BA	210	C	2.3
10	AJ	64	GLN	2.3
51	CX	82	ILE	2.3
3	AC	29	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	51	VAL	2.3
30	CD	131	ASP	2.3
36	DH	138	VAL	2.3
37	CJ	133	ALA	2.3
37	DJ	43	ASN	2.3
40	CM	64	PHE	2.3
50	CW	49	ASN	2.3
55	DA	1078	U	2.3
12	AL	54	ARG	2.3
1	AA	1347	G	2.3
31	CA	477	A	2.3
31	CA	1734	G	2.3
31	CA	2159	G	2.3
44	CQ	11	GLU	2.3
16	BP	18	GLN	2.3
9	BI	95	ARG	2.3
54	DI	63	ALA	2.3
1	BA	960	U	2.3
22	C1	6	ASN	2.3
35	CG	48	ASN	2.3
38	CK	21	THR	2.3
48	CU	64	LYS	2.3
1	BA	1213	A	2.3
1	BA	1355	G	2.3
5	BE	81	LEU	2.3
11	AK	42	LEU	2.3
55	DA	2128	G	2.3
12	BL	80	ILE	2.3
8	BH	49	PHE	2.3
33	CE	125	SER	2.3
46	CS	15	SER	2.3
26	C5	25	VAL	2.3
46	CS	53	PHE	2.3
53	CZ	46	VAL	2.3
1	BA	1214	C	2.3
10	BJ	85	ASP	2.3
19	AS	39	THR	2.3
27	C0	41	THR	2.3
31	CA	335	C	2.3
36	DH	124	THR	2.3
7	AG	116	MET	2.3
7	BG	3	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
30	CD	205	PRO	2.3
47	CT	92	ARG	2.3
15	AO	47	LYS	2.3
47	CT	55	ILE	2.3
1	AA	1346	A	2.3
1	BA	80	A	2.3
7	AG	80	VAL	2.3
8	BH	51	VAL	2.3
31	CA	2435	A	2.3
40	CM	35	HIS	2.3
54	DI	27	VAL	2.3
30	CD	74	GLU	2.2
31	CA	914	G	2.2
31	CA	2112	G	2.2
34	CF	116	GLY	2.2
16	AP	14	ARG	2.2
19	AS	78	ARG	2.2
22	C1	16	ARG	2.2
28	CB	22	U	2.2
31	CA	1742	U	2.2
37	DJ	74	PRO	2.2
44	CQ	96	LYS	2.2
50	CW	68	LYS	2.2
2	BB	32	PHE	2.2
20	BT	58	VAL	2.2
47	CT	10	ALA	2.2
49	CV	98	SER	2.2
1	BA	1067	A	2.2
15	AO	53	ARG	2.2
37	CJ	127	ARG	2.2
2	AB	114	LEU	2.2
8	AH	32	LEU	2.2
12	AL	109	ASP	2.2
14	AN	43	ASN	2.2
23	C2	27	LYS	2.2
31	CA	1341	G	2.2
47	CT	90	LYS	2.2
1	AA	1364	U	2.2
5	AE	141	ILE	2.2
9	BI	72	ILE	2.2
43	CP	24	THR	2.2
7	AG	73	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
45	CR	88	VAL	2.2
55	DA	138	U	2.2
7	AG	129	GLU	2.2
34	CF	171	ALA	2.2
54	DI	56	ARG	2.2
7	AG	120	LEU	2.2
7	BG	124	LEU	2.2
15	BO	48	LYS	2.2
17	BQ	69	LYS	2.2
33	CE	138	LEU	2.2
1	AA	1092	A	2.2
2	BB	88	ASP	2.2
16	BP	16	PHE	2.2
36	CH	124	THR	2.2
2	AB	53	ALA	2.2
13	AM	37	ALA	2.2
25	C4	27	ALA	2.2
31	CA	1873	G	2.2
1	AA	1149	C	2.2
45	CR	14	HIS	2.2
46	CS	66	HIS	2.2
13	BM	69	LEU	2.2
2	AB	50	PHE	2.2
3	AC	106	VAL	2.2
5	AE	105	ILE	2.2
16	BP	38	PHE	2.2
33	CE	124	PHE	2.2
13	BM	82	ASP	2.2
3	BC	17	PRO	2.2
9	AI	86	ALA	2.2
11	AK	43	GLY	2.2
17	BQ	74	THR	2.2
7	BG	9	GLN	2.2
15	AO	40	GLN	2.2
36	CH	35	LYS	2.2
1	BA	1232	U	2.2
31	CA	34	U	2.2
31	CA	895	U	2.2
31	CA	1061	U	2.2
31	CA	2344	U	2.2
33	CE	164	LEU	2.2
36	CH	58	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	88	G	2.2
31	CA	1421	G	2.2
1	BA	1195	C	2.2
6	BF	6	ILE	2.2
9	BI	19	VAL	2.2
17	AQ	21	ILE	2.2
31	CA	2651	C	2.2
48	CU	57	VAL	2.2
3	BC	110	GLU	2.2
12	AL	30	LYS	2.2
15	BO	26	GLU	2.2
7	AG	145	ALA	2.2
19	BS	68	GLY	2.2
37	DJ	64	ASP	2.2
50	CW	71	LYS	2.2
37	CJ	84	ALA	2.2
40	CM	30	THR	2.2
1	BA	114	U	2.2
3	AC	69	HIS	2.2
29	CC	243	HIS	2.2
31	CA	2650	U	2.2
55	DA	1077	A	2.2
3	BC	142	MET	2.2
34	CF	138	PHE	2.2
49	CV	73	PHE	2.2
2	AB	187	VAL	2.2
3	AC	173	VAL	2.2
37	DJ	139	VAL	2.2
1	AA	976	G	2.2
1	AA	1302	C	2.2
31	CA	854	C	2.2
31	CA	2527	C	2.2
46	CS	8	GLY	2.2
3	AC	71	ALA	2.2
3	AC	115	LEU	2.2
3	BC	139	GLN	2.2
19	BS	64	ASP	2.2
36	DH	17	ASP	2.2
54	DI	102	ALA	2.2
33	CE	13	THR	2.2
36	DH	125	THR	2.2
13	AM	103	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
30	CD	98	VAL	2.2
31	CA	1325	U	2.2
36	CH	78	VAL	2.2
13	AM	51	GLY	2.2
1	AA	217	C	2.2
8	BH	61	LEU	2.2
10	BJ	92	LEU	2.2
11	AK	112	ASP	2.2
14	BN	46	LEU	2.2
21	AU	13	ASP	2.2
36	DH	6	LEU	2.2
43	CP	104	GLN	2.2
1	BA	1064	G	2.2
3	BC	169	ARG	2.2
9	AI	85	ARG	2.2
10	BJ	32	THR	2.2
12	BL	51	LYS	2.2
29	CC	239	ASN	2.2
31	CA	1037	G	2.2
31	CA	2144	G	2.2
33	CE	48	THR	2.2
40	CM	128	THR	2.2
48	CU	6	ARG	2.2
33	CE	158	PHE	2.2
34	DF	175	PHE	2.2
55	DA	2107	G	2.2
6	AF	62	MET	2.2
29	CC	74	ILE	2.2
49	DV	58	ILE	2.2
31	CA	1015	U	2.2
1	BA	1117	A	2.2
5	BE	128	TYR	2.2
5	BE	144	LEU	2.2
11	BK	47	ALA	2.2
54	DI	100	ALA	2.2
7	BG	114	LYS	2.2
13	AM	62	LYS	2.2
15	AO	21	ASP	2.2
15	AO	89	ARG	2.2
20	AT	59	ASP	2.2
25	C4	45	ARG	2.2
41	CN	40	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
52	CY	31	PRO	2.2
1	BA	1369	C	2.2
24	C3	24	THR	2.2
31	CA	11	C	2.2
34	CF	21	ASN	2.2
9	AI	55	VAL	2.2
20	BT	20	HIS	2.2
34	CF	79	ILE	2.2
31	CA	1807	G	2.2
55	DA	277	G	2.2
1	AA	1122	U	2.2
1	BA	89	U	2.2
7	AG	125	SER	2.2
29	CC	13	ARG	2.2
30	CD	85	ALA	2.2
31	CA	1081	U	2.2
34	CF	70	ALA	2.2
36	CH	131	SER	2.2
47	CT	46	LEU	2.2
6	BF	29	ILE	2.2
34	CF	90	THR	2.2
37	CJ	112	THR	2.2
44	CQ	5	ILE	2.2
1	BA	207	C	2.2
11	BK	43	GLY	2.2
31	CA	1079	C	2.2
42	CO	7	GLY	2.2
3	AC	42	TYR	2.2
12	AL	108	LYS	2.2
20	BT	24	ARG	2.2
44	CQ	113	ARG	2.2
3	AC	189	ALA	2.2
3	BC	115	LEU	2.2
7	AG	47	LEU	2.2
11	BK	103	ALA	2.2
19	AS	38	SER	2.2
20	BT	63	ALA	2.2
1	BA	1301	U	2.2
1	AA	1215	G	2.2
31	CA	1059	G	2.2
29	CC	104	ILE	2.2
34	CF	174	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1441	A	2.2
14	BN	89	MET	2.2
46	CS	98	ILE	2.2
16	BP	80	LYS	2.2
17	BQ	11	ARG	2.2
31	CA	899	A	2.2
40	CM	124	GLY	2.2
44	CQ	35	GLY	2.2
2	BB	114	LEU	2.1
44	CQ	114	LEU	2.1
31	CA	1518	C	2.1
34	CF	45	ALA	2.1
36	CH	69	ALA	2.1
50	CW	57	TYR	2.1
1	AA	1120	C	2.1
1	BA	1228	C	2.1
51	CX	33	ALA	2.1
1	AA	992	U	2.1
16	AP	18	GLN	2.1
31	CA	1201	U	2.1
3	AC	75	ILE	2.1
13	AM	58	ASP	2.1
30	CD	1	MET	2.1
35	CG	167	GLU	2.1
38	CK	49	ASP	2.1
48	CU	34	VAL	2.1
36	CH	89	LYS	2.1
49	CV	101	GLU	2.1
50	CW	66	ASP	2.1
6	AF	37	HIS	2.1
14	AN	35	ASN	2.1
35	DG	111	HIS	2.1
34	CF	2	ALA	2.1
50	CW	74	ALA	2.1
35	DG	116	GLN	2.1
33	CE	102	ARG	2.1
34	CF	61	SER	2.1
1	BA	1123	U	2.1
19	AS	9	PRO	2.1
45	CR	78	LYS	2.1
46	CS	64	VAL	2.1
55	DA	2150	C	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	2743	U	2.1
49	DV	57	GLY	2.1
8	AH	55	THR	2.1
15	BO	30	ALA	2.1
41	CN	56	ALA	2.1
1	AA	1373	G	2.1
9	BI	80	ARG	2.1
35	CG	175	LYS	2.1
15	BO	11	ILE	2.1
54	DI	123	ILE	2.1
1	AA	1118	U	2.1
28	CB	74	U	2.1
31	CA	414	C	2.1
34	DF	36	LEU	2.1
47	CT	34	ASP	2.1
3	BC	37	PHE	2.1
13	BM	15	ALA	2.1
34	CF	8	TYR	2.1
49	CV	43	LYS	2.1
54	DI	80	THR	2.1
3	AC	46	GLU	2.1
1	BA	1193	G	2.1
25	C4	21	GLY	2.1
31	CA	2782	G	2.1
1	BA	1262	C	2.1
2	BB	162	PHE	2.1
7	BG	11	LYS	2.1
12	AL	99	ARG	2.1
12	BL	117	TYR	2.1
13	AM	13	LYS	2.1
19	AS	56	GLN	2.1
43	CP	19	GLN	2.1
12	BL	81	LEU	2.1
13	AM	26	GLY	2.1
35	CG	161	GLY	2.1
7	AG	102	ARG	2.1
11	AK	50	SER	2.1
35	CG	156	PRO	2.1
14	AN	65	ARG	2.1
19	AS	81	ARG	2.1
45	CR	6	ARG	2.1
47	CT	81	SER	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AA	1150	A	2.1
17	AQ	48	ASP	2.1
31	CA	1522	A	2.1
31	CA	1235	G	2.1
43	CP	79	ALA	2.1
55	DA	895	U	2.1
55	DA	1176	U	2.1
7	AG	27	VAL	2.1
7	AG	9	GLN	2.1
9	BI	69	GLY	2.1
39	CL	55	GLY	2.1
13	BM	78	LYS	2.1
23	C2	30	LYS	2.1
30	CD	83	ARG	2.1
34	CF	115	ARG	2.1
53	CZ	7	ARG	2.1
3	BC	29	PHE	2.1
7	AG	16	PRO	2.1
14	BN	94	PRO	2.1
16	BP	15	PRO	2.1
11	AK	17	SER	2.1
10	BJ	61	ALA	2.1
25	C4	54	ASP	2.1
27	C0	44	ILE	2.1
52	CY	7	VAL	2.1
1	BA	4	U	2.1
31	CA	440	C	2.1
33	CE	21	ARG	2.1
35	CG	20	ASN	2.1
35	CG	30	ASN	2.1
41	CN	88	ASN	2.1
42	CO	70	THR	2.1
50	CW	38	LEU	2.1
55	DA	2168	G	2.1
22	C1	2	ALA	2.1
8	AH	129	VAL	2.1
3	BC	167	TRP	2.1
9	AI	28	ILE	2.1
34	CF	13	VAL	2.1
35	CG	160	LYS	2.1
36	CH	135	HIS	2.1
1	AA	85	U	2.1

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Mol	Chain	Res	Type	RSRZ
10	AJ	4	GLN	2.1
11	AK	100	LEU	2.1
30	CD	94	GLN	2.1
33	CE	109	LEU	2.1
1	BA	1093	A	2.1
24	C3	5	PHE	2.1
35	DG	101	ASN	2.1
48	CU	28	ASN	2.1
11	AK	77	TYR	2.1
18	AR	51	TYR	2.1
31	CA	902	C	2.1
31	CA	2000	C	2.1
31	CA	2178	C	2.1
35	CG	55	ARG	2.1
36	DH	89	LYS	2.1
43	CP	77	ALA	2.1
47	CT	58	ALA	2.1
49	CV	64	ALA	2.1
3	BC	149	ILE	2.1
6	AF	96	VAL	2.1
12	AL	104	CYS	2.1
21	BU	6	VAL	2.1
45	CR	110	VAL	2.1
52	CY	35	SER	2.1
2	AB	117	LEU	2.1
13	BM	91	HIS	2.1
42	CO	72	ASP	2.1
5	AE	111	MET	2.1
14	AN	4	GLN	2.1
1	AA	218	U	2.1
15	BO	79	THR	2.1
40	CM	67	THR	2.1
1	AA	1004	A	2.1
1	AA	1170	A	2.1
31	CA	849	A	2.1
5	BE	112	ARG	2.1
16	BP	56	ARG	2.1
49	CV	92	LYS	2.1
1	AA	1245	C	2.1
1	AA	1273	C	2.1
12	BL	69	GLY	2.1
14	AN	58	SER	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	475	C	2.1
31	CA	2793	C	2.1
1	AA	540	G	2.1
20	AT	54	MET	2.1
4	AD	160	GLU	2.1
12	AL	73	ASN	2.1
33	CE	197	GLU	2.1
34	DF	84	PRO	2.1
36	DH	84	ALA	2.1
36	DH	104	THR	2.1
37	DJ	62	TYR	2.1
40	CM	143	GLU	2.1
17	AQ	76	VAL	2.1
38	CK	20	ALA	2.1
7	AG	42	ILE	2.1
18	BR	68	LEU	2.1
30	CD	87	GLY	2.1
31	CA	631	A	2.1
45	CR	94	ILE	2.1
33	CE	42	GLY	2.1
41	CN	107	GLY	2.1
1	AA	1037	C	2.1
3	BC	18	TRP	2.0
18	BR	54	GLN	2.0
28	CB	4	C	2.1
19	BS	3	ARG	2.0
19	BS	70	LYS	2.0
37	DJ	117	MET	2.1
44	CQ	103	ARG	2.0
1	AA	202	G	2.0
8	AH	93	PRO	2.0
11	AK	16	VAL	2.0
15	BO	75	VAL	2.0
49	CV	2	ALA	2.0
34	CF	111	ILE	2.0
47	CT	4	ILE	2.0
12	AL	71	GLY	2.0
40	CM	45	GLY	2.0
49	CV	14	LEU	2.0
1	BA	1227	A	2.0
2	BB	147	SER	2.0
34	CF	72	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1226	C	2.0
16	AP	48	GLU	2.0
34	DF	70	ALA	2.0
36	DH	56	ALA	2.0
37	DJ	98	VAL	2.0
46	CS	33	VAL	2.0
1	BA	1194	U	2.0
10	AJ	33	GLY	2.0
13	AM	6	GLY	2.0
41	CN	7	THR	2.0
31	CA	1108	U	2.0
36	CH	71	LYS	2.0
46	CS	48	LYS	2.0
3	BC	136	ARG	2.0
42	CO	21	PHE	2.0
3	AC	190	HIS	2.0
1	BA	1042	A	2.0
31	CA	213	A	2.0
27	C0	27	LEU	2.0
34	CF	168	ALA	2.0
39	CL	52	VAL	2.0
2	AB	67	ILE	2.0
5	BE	105	ILE	2.0
3	AC	174	PRO	2.0
7	AG	88	PRO	2.0
19	AS	28	LYS	2.0
16	AP	29	ASN	2.0
30	CD	167	ASN	2.0
1	BA	632	U	2.0
2	BB	6	MET	2.0
50	CW	48	MET	2.0
1	AA	107	G	2.0
1	AA	1015	G	2.0
1	BA	941	G	2.0
1	BA	951	G	2.0
1	BA	1215	G	2.0
1	BA	1385	G	2.0
31	CA	1408	G	2.0
43	CP	98	GLN	2.0
3	BC	49	LYS	2.0
6	BF	89	VAL	2.0
13	AM	82	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
36	CH	128	HIS	2.0
10	BJ	59	LYS	2.0
15	BO	63	ARG	2.0
16	AP	4	ILE	2.0
16	AP	13	LYS	2.0
1	BA	460	A	2.0
1	BA	1368	A	2.0
22	C1	35	GLY	2.0
24	C3	21	ARG	2.0
1	AA	1224	U	2.0
5	AE	97	GLN	2.0
30	CD	36	GLN	2.0
49	CV	60	GLU	2.0
2	AB	196	VAL	2.0
10	AJ	82	LYS	2.0
31	CA	1729	U	2.0
16	BP	19	VAL	2.0
2	AB	60	ILE	2.0
3	BC	175	LEU	2.0
9	AI	79	ILE	2.0
33	CE	44	ARG	2.0
45	CR	113	ALA	2.0
1	BA	587	G	2.0
31	CA	2526	G	2.0
39	CL	112	PHE	2.0
37	DJ	75	PRO	2.0
1	AA	1225	A	2.0
1	BA	532	A	2.0
31	CA	222	A	2.0
31	CA	1027	A	2.0
46	CS	37	GLU	2.0
18	BR	52	GLN	2.0
21	AU	25	LYS	2.0
30	CD	204	LYS	2.0
31	CA	1868	C	2.0
31	CA	1958	C	2.0
33	CE	98	LYS	2.0
47	CT	83	LYS	2.0
3	BC	56	VAL	2.0
9	AI	61	LEU	2.0
14	AN	59	ARG	2.0
17	BQ	29	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
26	C5	12	ARG	2.0
27	C0	11	ARG	2.0
40	CM	95	LEU	2.0
45	CR	45	TYR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	2MA	DA	2503	23/24	0.99	0.21	-	44,51,58,62	0
31	OMC	CA	2498	21/22	0.92	0.29	-	116,124,130,132	0
31	3TD	CA	1915	21/22	0.87	0.19	-	162,165,170,171	0
1	2MG	BA	966	24/25	0.43	0.57	-	258,264,268,268	0
55	OMU	DA	2552	21/22	0.99	0.21	-	45,48,52,57	0
55	PSU	DA	2504	20/21	0.98	0.19	-	50,51,54,56	0
55	7MG	DA	2069	24/25	0.99	0.18	-	41,48,53,53	0
1	2MG	BA	1207	24/25	0.70	0.39	-	256,257,258,259	0
31	PSU	CA	955	20/21	0.91	0.17	-	126,130,135,136	0
31	OMG	CA	2251	24/25	0.92	0.26	-	111,114,115,116	0
31	PSU	CA	2504	20/21	0.93	0.21	-	106,114,117,120	0
41	4D4	DN	81[B]	12/13	0.98	0.23	-	37,45,50,50	9
41	4D4	DN	81[A]	12/13	0.98	0.23	-	49,59,65,66	9
31	2MG	CA	1835	24/25	0.94	0.21	-	100,103,106,110	0
1	4OC	BA	1402	22/23	0.94	0.19	-	111,116,127,128	0
55	6MZ	DA	2030	23/24	0.99	0.20	-	27,33,38,40	0
1	UR3	BA	1498	21/22	0.95	0.15	-	118,122,126,127	0
31	2MA	CA	2503	23/24	0.94	0.23	-	117,126,137,138	0
1	MA6	BA	1519	24/25	0.94	0.24	-	100,102,107,110	0
1	2MG	AA	966	24/25	0.78	0.24	-	211,213,215,216	0
55	PSU	DA	2604	20/21	0.99	0.17	-	58,63,70,72	0
55	PSU	DA	2580	20/21	0.99	0.20	-	30,35,41,43	0
1	2MG	AA	1516	24/25	0.96	0.17	-	74,82,84,86	0
1	MA6	AA	1518	24/25	0.97	0.16	-	67,77,81,85	0
1	PSU	BA	516	20/21	0.90	0.14	-	111,121,128,129	0
32	MEQ	DD	150[B]	10/11	0.98	0.28	-	35,38,44,45	10
55	PSU	DA	1911	20/21	0.95	0.14	-	107,118,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	D2T	BL	89	10/11	0.94	0.39	-	106,110,113,114	0
1	2MG	BA	1516	24/25	0.93	0.19	-	105,110,116,117	0
1	5MC	AA	1407	21/22	0.96	0.16	-	80,88,90,91	0
31	PSU	CA	1911	20/21	0.92	0.14	-	152,158,159,161	0
32	MEQ	DD	150[A]	10/11	0.98	0.28	-	31,32,37,37	10
55	OMG	DA	2251	24/25	0.99	0.18	-	29,48,54,62	0
31	PSU	CA	2457	20/21	0.96	0.19	-	118,122,126,127	0
55	PSU	DA	2605	20/21	0.98	0.17	-	51,59,64,65	0
55	5MU	DA	747	21/22	0.99	0.19	-	41,43,52,58	0
1	5MC	AA	967	21/22	0.75	0.28	-	214,216,219,220	0
1	7MG	BA	527	24/25	0.95	0.18	-	100,108,118,120	0
55	2MG	DA	1835	24/25	0.96	0.21	-	59,65,71,72	0
1	7MG	AA	527	24/25	0.96	0.16	-	102,109,115,118	0
31	PSU	CA	746	20/21	0.90	0.20	-	135,137,142,142	0
41	4D4	CN	81	12/13	0.92	0.42	-	118,121,132,133	0
55	5MC	DA	1962	21/22	0.98	0.19	-	46,61,65,66	0
55	PSU	DA	955	20/21	0.99	0.19	-	32,35,39,41	0
31	1MG	CA	745	24/25	0.94	0.17	-	123,126,132,134	0
31	5MU	CA	1939	21/22	0.95	0.17	-	95,99,105,107	0
31	PSU	CA	1917	20/21	0.91	0.17	-	132,140,149,149	0
31	5MC	CA	1962	21/22	0.96	0.20	-	103,106,110,112	0
1	5MC	BA	1407	21/22	0.95	0.14	-	111,121,124,125	0
55	PSU	DA	746	20/21	1.00	0.18	-	38,44,46,47	0
12	D2T	AL	89	10/11	0.95	0.29	-	109,114,125,128	0
55	PSU	DA	1917	20/21	0.97	0.13	-	109,113,119,119	0
31	PSU	CA	2605	20/21	0.96	0.17	-	97,101,106,106	0
31	6MZ	CA	1618	23/24	0.94	0.29	-	160,164,168,172	0
1	MA6	BA	1518	24/25	0.93	0.24	-	91,97,102,103	0
31	PSU	CA	2580	20/21	0.95	0.18	-	118,125,130,131	0
31	6MZ	CA	2030	23/24	0.94	0.19	-	117,125,134,134	0
55	2MG	DA	2445	24/25	0.99	0.20	-	39,45,50,62	0
55	OMC	DA	2498	21/22	0.99	0.21	-	37,39,46,47	0
55	6MZ	DA	1618	23/24	0.99	0.20	-	34,42,47,49	0
55	1MG	DA	745	24/25	0.99	0.19	-	31,37,42,44	0
1	MA6	AA	1519	24/25	0.97	0.20	-	72,76,80,81	0
31	7MG	CA	2069	24/25	0.94	0.19	-	104,111,124,124	0
55	PSU	DA	2457	20/21	0.99	0.18	-	44,46,52,53	0
1	UR3	AA	1498	21/22	0.97	0.18	-	86,92,97,100	0
55	5MU	DA	1939	21/22	0.99	0.20	-	53,58,65,69	0
1	4OC	AA	1402	22/23	0.96	0.17	-	94,99,103,104	0
55	3TD	DA	1915	21/22	0.96	0.12	-	133,140,146,147	0
31	OMU	CA	2552	21/22	0.87	0.44	-	106,111,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	5MU	CA	747	21/22	0.92	0.17	-	131,134,136,137	0
1	2MG	AA	1207	24/25	0.80	0.19	-	234,239,241,243	0
1	PSU	AA	516	20/21	0.94	0.15	-	135,138,139,141	0
1	5MC	BA	967	21/22	0.55	0.62	-	258,263,266,266	0
31	2MG	CA	2445	24/25	0.94	0.28	-	103,109,112,114	0
55	H2U	DA	2449	20/21	0.99	0.23	-	33,39,46,46	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
59	PUT	AA	1674	6/6	0.79	0.76	49.74	109,113,116,117	0
59	PUT	DA	3184	6/6	0.92	0.43	40.68	65,70,74,74	0
63	PGE	DA	3214	10/10	0.86	0.60	35.42	67,87,91,92	0
58	MPD	DA	3204	8/8	0.85	0.61	26.85	116,119,125,127	0
59	PUT	DA	3195	6/6	0.69	0.45	24.30	100,104,108,108	0
56	MG	CA	3003	1/1	0.94	1.78	24.19	272,272,272,272	0
56	MG	CA	3150	1/1	0.96	0.77	23.58	79,79,79,79	0
56	MG	BA	1627	1/1	0.93	0.67	20.55	203,203,203,203	0
61	PEG	D3	102	7/7	0.66	1.32	19.37	136,138,140,140	0
56	MG	DA	3163	1/1	0.60	0.52	19.12	87,87,87,87	0
61	PEG	DA	3201	7/7	0.81	0.47	18.71	146,150,151,152	0
57	PG4	DA	3193	13/13	0.88	0.96	18.04	109,113,119,120	0
63	PGE	DA	3217	10/10	0.90	0.34	15.13	87,89,93,94	0
58	MPD	AA	1676	8/8	0.86	0.63	14.70	145,146,148,148	0
64	SPD	DA	3183	10/10	0.93	0.45	14.31	80,95,97,98	0
56	MG	DA	3147	1/1	0.70	0.29	14.04	108,108,108,108	0
59	PUT	DA	3222	6/6	0.92	0.31	13.95	77,81,83,83	0
61	PEG	DA	3226	7/7	0.87	0.32	12.65	125,126,131,131	0
56	MG	CA	3022	1/1	0.78	0.72	12.38	259,259,259,259	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	PUT	AA	1673	6/6	0.77	0.67	12.25	142,145,148,150	0
64	SPD	DA	3224	10/10	0.91	0.30	11.90	58,71,88,88	0
56	MG	DA	3177	1/1	0.96	0.37	11.79	52,52,52,52	0
56	MG	DA	3182	1/1	0.71	0.43	11.65	55,55,55,55	0
62	EDO	DA	3198	4/4	0.72	0.43	11.23	109,110,112,112	0
57	PG4	BA	1642	13/13	0.89	0.46	10.99	113,117,132,132	0
56	MG	AA	1642	1/1	0.84	0.78	10.34	275,275,275,275	0
59	PUT	DA	3221	6/6	0.82	0.45	9.87	112,120,122,122	0
56	MG	AA	1661	1/1	0.89	0.67	9.75	223,223,223,223	0
59	PUT	DA	3219	6/6	0.86	0.29	9.73	100,102,103,103	0
63	PGE	DA	3225	10/10	0.81	0.39	9.55	100,120,131,131	0
58	MPD	DA	3207	8/8	0.89	0.44	9.19	121,125,128,129	0
56	MG	CA	3026	1/1	0.73	1.03	8.82	245,245,245,245	0
58	MPD	DA	3192	8/8	0.95	0.57	8.19	84,90,92,94	0
63	PGE	DD	301	10/10	0.89	0.31	8.11	120,122,129,130	0
58	MPD	DE	301	8/8	0.69	1.05	8.05	172,174,179,179	0
62	EDO	DA	3197	4/4	0.93	0.29	7.14	75,76,77,77	0
61	PEG	DA	3200	7/7	0.72	0.35	6.96	124,124,125,125	0
62	EDO	D0	101	4/4	0.92	0.26	6.90	79,80,85,89	0
63	PGE	D1	102	10/10	0.83	0.36	6.87	142,145,152,153	0
56	MG	DA	3126	1/1	0.93	0.31	6.70	77,77,77,77	0
63	PGE	D3	101	10/10	0.81	0.54	6.70	121,123,125,126	0
57	PG4	DA	3216	13/13	0.89	0.28	6.45	111,122,132,134	0
61	PEG	DA	3218	7/7	0.77	0.29	6.24	179,180,181,181	0
56	MG	CA	3056	1/1	0.70	0.48	5.92	77,77,77,77	0
56	MG	DA	3122	1/1	0.97	0.28	5.88	48,48,48,48	0
61	PEG	DQ	201	7/7	0.51	0.82	5.84	162,166,170,170	0
56	MG	BA	1624	1/1	0.18	2.21	5.79	293,293,293,293	0
65	1PE	DA	3203	16/16	0.92	0.30	5.53	98,105,109,109	0
56	MG	AA	1639	1/1	0.98	0.49	5.47	225,225,225,225	0
58	MPD	AA	1671	8/8	0.91	0.69	5.25	143,144,147,148	0
56	MG	CA	3039	1/1	0.92	0.58	5.22	190,190,190,190	0
56	MG	CA	3133	1/1	0.87	0.32	5.05	110,110,110,110	0
59	PUT	DA	3213	6/6	0.82	0.27	5.01	156,156,157,157	0
58	MPD	DA	3210	8/8	0.92	0.30	4.89	110,118,123,125	0
57	PG4	AA	1670	13/13	0.82	0.26	4.72	111,116,118,119	0
64	SPD	DA	3187	10/10	0.94	0.26	4.69	78,82,85,85	0
58	MPD	DE	302	8/8	0.93	0.41	4.42	101,102,103,104	0
56	MG	DA	3127	1/1	0.98	0.45	4.32	69,69,69,69	0
62	EDO	D1	101	4/4	0.91	0.23	4.28	70,71,73,75	0
59	PUT	DA	3189	6/6	0.95	0.25	4.02	49,55,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3109	1/1	0.93	0.34	3.60	67,67,67,67	0
61	PEG	DL	201	7/7	0.88	0.31	3.33	102,103,109,110	0
59	PUT	DA	3205	6/6	0.92	0.30	3.28	106,108,108,109	0
56	MG	AA	1612	1/1	0.92	0.36	3.14	77,77,77,77	0
63	PGE	DU	201	10/10	0.86	0.45	2.77	135,141,147,147	0
56	MG	CA	3131	1/1	0.87	0.34	2.58	123,123,123,123	0
63	PGE	DA	3186	10/10	0.95	0.21	2.32	58,65,71,71	0
57	PG4	DS	202	13/13	0.90	0.31	2.25	72,73,85,86	0
67	GUN	DA	3211	11/11	0.91	0.26	1.85	116,122,123,124	0
56	MG	BA	1613	1/1	0.99	0.26	1.80	149,149,149,149	0
56	MG	BA	1612	1/1	0.89	0.23	1.76	262,262,262,262	0
56	MG	CA	3037	1/1	0.98	0.27	1.53	234,234,234,234	0
56	MG	BA	1618	1/1	0.97	0.22	1.29	172,172,172,172	0
56	MG	BA	1601	1/1	0.97	0.22	1.26	135,135,135,135	0
64	SPD	DA	3206	10/10	0.71	0.23	1.25	142,143,144,144	0
63	PGE	DS	201	10/10	0.87	0.34	1.21	96,99,101,101	0
56	MG	DA	3084	1/1	1.00	0.18	1.19	55,55,55,55	0
56	MG	CA	3100	1/1	0.98	0.25	1.19	243,243,243,243	0
61	PEG	AL	201	7/7	0.64	0.30	1.18	132,133,135,136	0
57	PG4	DQ	202	13/13	0.84	0.26	1.13	84,89,100,101	0
65	1PE	DA	3185	16/16	0.94	0.21	0.91	74,89,123,123	0
59	PUT	AA	1672	6/6	0.52	0.30	0.70	149,150,150,150	0
56	MG	DA	3023	1/1	0.99	0.22	0.49	57,57,57,57	0
56	MG	AA	1657	1/1	0.95	0.46	0.43	134,134,134,134	0
56	MG	DD	302	1/1	0.97	0.22	0.24	62,62,62,62	0
56	MG	CA	3032	1/1	0.92	0.35	0.20	197,197,197,197	0
56	MG	CA	3027	1/1	0.96	0.21	-0.13	88,88,88,88	0
56	MG	CA	3153	1/1	0.96	0.20	-0.13	77,77,77,77	0
56	MG	CA	3086	1/1	0.98	0.21	-0.19	106,106,106,106	0
59	PUT	DM	201	6/6	0.95	0.21	-0.20	63,66,74,75	0
58	MPD	DS	203	8/8	0.98	0.22	-0.30	62,64,65,67	0
59	PUT	DA	3188	6/6	0.93	0.20	-0.37	89,93,93,94	0
56	MG	DA	3135	1/1	0.97	0.16	-0.47	146,146,146,146	0
56	MG	DA	3094	1/1	0.98	0.19	-0.78	29,29,29,29	0
56	MG	DA	3029	1/1	0.99	0.21	-0.82	44,44,44,44	0
56	MG	AA	1662	1/1	0.94	0.20	-0.83	164,164,164,164	0
56	MG	CA	3031	1/1	0.94	0.19	-0.84	128,128,128,128	0
56	MG	CA	3019	1/1	0.86	0.21	-0.92	87,87,87,87	0
56	MG	DA	3099	1/1	0.97	0.19	-1.05	45,45,45,45	0
56	MG	CA	3102	1/1	0.99	0.11	-1.11	99,99,99,99	0
56	MG	CA	3009	1/1	0.80	0.15	-1.17	259,259,259,259	0
56	MG	CA	3089	1/1	0.99	0.21	-1.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1663	1/1	0.82	0.24	-1.37	230,230,230,230	0
56	MG	DA	3037	1/1	1.00	0.16	-1.41	13,13,13,13	0
56	MG	CB	202	1/1	0.99	0.09	-1.47	116,116,116,116	0
56	MG	CA	3105	1/1	0.62	0.18	-1.54	252,252,252,252	0
56	MG	AA	1668	1/1	0.96	0.13	-1.64	110,110,110,110	0
56	MG	CA	3011	1/1	0.98	0.17	-1.66	95,95,95,95	0
56	MG	CA	3103	1/1	0.96	0.15	-1.68	176,176,176,176	0
56	MG	BA	1632	1/1	0.99	0.12	-1.69	74,74,74,74	0
56	MG	BA	1608	1/1	0.98	0.19	-1.69	144,144,144,144	0
60	ZN	C5	101	1/1	0.93	0.07	-1.71	175,175,175,175	0
56	MG	DA	3013	1/1	0.99	0.20	-1.71	13,13,13,13	0
56	MG	AA	1677	1/1	0.87	0.08	-1.73	101,101,101,101	0
56	MG	DB	204	1/1	0.94	0.16	-1.74	85,85,85,85	0
56	MG	CA	3101	1/1	0.95	0.12	-1.75	239,239,239,239	0
60	ZN	D5	101	1/1	1.00	0.10	-1.77	84,84,84,84	0
56	MG	BA	1615	1/1	0.98	0.16	-1.79	103,103,103,103	0
56	MG	BA	1620	1/1	0.94	0.12	-1.82	172,172,172,172	0
56	MG	DA	3112	1/1	0.99	0.18	-1.85	46,46,46,46	0
56	MG	DA	3093	1/1	0.99	0.17	-1.91	23,23,23,23	0
56	MG	AA	1656	1/1	0.89	0.11	-1.93	274,274,274,274	0
56	MG	BA	1602	1/1	0.97	0.11	-1.97	102,102,102,102	0
56	MG	DA	3004	1/1	0.98	0.14	-2.00	149,149,149,149	0
56	MG	CA	3080	1/1	0.82	0.11	-2.00	108,108,108,108	0
56	MG	DA	3026	1/1	0.99	0.18	-2.01	228,228,228,228	0
56	MG	CA	3094	1/1	0.86	0.11	-2.23	132,132,132,132	0
56	MG	CA	3044	1/1	0.98	0.17	-2.24	113,113,113,113	0
56	MG	BA	1614	1/1	0.98	0.14	-2.32	217,217,217,217	0
56	MG	CB	201	1/1	0.87	0.06	-2.41	235,235,235,235	0
56	MG	DA	3140	1/1	0.99	0.18	-2.43	51,51,51,51	0
56	MG	DA	3097	1/1	0.97	0.11	-2.48	75,75,75,75	0
56	MG	CA	3054	1/1	0.89	0.12	-2.49	122,122,122,122	0
56	MG	CA	3040	1/1	0.94	0.13	-2.54	122,122,122,122	0
56	MG	CA	3099	1/1	0.93	0.12	-2.61	174,174,174,174	0
56	MG	AA	1651	1/1	0.99	0.13	-2.70	75,75,75,75	0
56	MG	CA	3018	1/1	0.93	0.10	-2.78	147,147,147,147	0
60	ZN	AB	301	1/1	0.95	0.04	-2.80	165,165,165,165	0
56	MG	BA	1617	1/1	0.96	0.12	-2.80	165,165,165,165	0
56	MG	CA	3006	1/1	0.81	0.10	-2.85	221,221,221,221	0
56	MG	AA	1644	1/1	0.99	0.14	-2.86	180,180,180,180	0
56	MG	CA	3063	1/1	0.97	0.13	-2.89	155,155,155,155	0
56	MG	BA	1610	1/1	0.94	0.07	-2.90	107,107,107,107	0
56	MG	AA	1637	1/1	0.95	0.15	-2.94	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	202	1/1	0.99	0.10	-3.03	56,56,56,56	0
56	MG	CA	3024	1/1	0.98	0.06	-3.05	85,85,85,85	0
56	MG	DA	3095	1/1	0.96	0.14	-3.08	65,65,65,65	0
56	MG	DA	3054	1/1	0.98	0.17	-3.14	167,167,167,167	0
56	MG	AA	1629	1/1	0.99	0.10	-3.22	110,110,110,110	0
56	MG	DA	3009	1/1	0.99	0.12	-3.44	39,39,39,39	0
56	MG	AA	1643	1/1	0.98	0.14	-3.52	70,70,70,70	0
56	MG	CA	3033	1/1	0.97	0.09	-3.56	150,150,150,150	0
56	MG	DA	3027	1/1	0.99	0.20	-3.57	49,49,49,49	0
56	MG	DA	3047	1/1	0.99	0.13	-3.65	42,42,42,42	0
56	MG	AA	1631	1/1	0.98	0.09	-3.74	75,75,75,75	0
56	MG	BA	1622	1/1	0.96	0.10	-3.81	240,240,240,240	0
56	MG	DA	3090	1/1	0.99	0.17	-3.83	26,26,26,26	0
56	MG	CA	3030	1/1	0.89	0.09	-3.84	82,82,82,82	0
56	MG	DA	3050	1/1	0.99	0.13	-4.08	41,41,41,41	0
56	MG	CA	3020	1/1	0.96	0.15	-4.09	116,116,116,116	0
56	MG	CA	3008	1/1	0.90	0.09	-4.12	202,202,202,202	0
56	MG	DA	3043	1/1	0.98	0.14	-4.18	40,40,40,40	0
56	MG	AA	1653	1/1	0.95	0.06	-4.38	108,108,108,108	0
56	MG	DA	3024	1/1	1.00	0.17	-4.45	44,44,44,44	0
56	MG	DA	3022	1/1	0.99	0.13	-4.49	40,40,40,40	0
56	MG	DA	3014	1/1	0.99	0.17	-4.56	31,31,31,31	0
56	MG	AA	1648	1/1	0.96	0.05	-4.58	84,84,84,84	0
56	MG	DA	3007	1/1	0.96	0.09	-4.59	127,127,127,127	0
56	MG	AA	1646	1/1	0.99	0.11	-4.71	80,80,80,80	0
56	MG	CA	3144	1/1	0.98	0.06	-4.76	66,66,66,66	0
56	MG	BA	1605	1/1	0.98	0.08	-4.81	136,136,136,136	0
56	MG	DA	3092	1/1	0.99	0.12	-4.84	50,50,50,50	0
56	MG	DA	3046	1/1	1.00	0.18	-4.89	27,27,27,27	0
56	MG	DA	3102	1/1	0.99	0.13	-5.00	32,32,32,32	0
56	MG	DA	3061	1/1	0.99	0.14	-5.10	44,44,44,44	0
56	MG	DB	201	1/1	0.96	0.11	-5.20	121,121,121,121	0
56	MG	DA	3228	1/1	0.99	0.14	-5.28	18,18,18,18	0
56	MG	CA	3049	1/1	0.99	0.12	-5.29	53,53,53,53	0
56	MG	DA	3063	1/1	0.99	0.15	-5.30	111,111,111,111	0
56	MG	DA	3031	1/1	0.98	0.16	-5.54	51,51,51,51	0
56	MG	DA	3033	1/1	0.95	0.13	-5.60	46,46,46,46	0
56	MG	DA	3058	1/1	1.00	0.09	-5.73	66,66,66,66	0
56	MG	DA	3035	1/1	0.99	0.14	-5.90	24,24,24,24	0
56	MG	DA	3110	1/1	1.00	0.16	-5.94	31,31,31,31	0
56	MG	DA	3071	1/1	0.98	0.08	-6.00	56,56,56,56	0
56	MG	CA	3041	1/1	0.99	0.08	-6.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3017	1/1	0.99	0.12	-6.34	34,34,34,34	0
56	MG	DA	3109	1/1	0.99	0.16	-6.48	38,38,38,38	0
56	MG	DA	3064	1/1	1.00	0.14	-6.75	75,75,75,75	0
56	MG	DA	3081	1/1	0.99	0.07	-6.85	46,46,46,46	0
56	MG	AA	1649	1/1	0.97	0.06	-8.01	111,111,111,111	0
56	MG	DA	3150	1/1	0.98	0.08	-8.50	72,72,72,72	0
56	MG	CA	3013	1/1	0.99	0.11	-8.81	71,71,71,71	0
56	MG	DA	3066	1/1	0.99	0.12	-12.32	43,43,43,43	0
56	MG	CA	3124	1/1	0.39	0.28	-	159,159,159,159	0
56	MG	CA	3143	1/1	0.95	0.14	-	72,72,72,72	0
56	MG	CA	3078	1/1	0.98	0.29	-	198,198,198,198	0
59	PUT	DA	3212	6/6	0.85	0.22	-	114,115,117,117	0
56	MG	DA	3128	1/1	0.88	1.11	-	57,57,57,57	0
56	MG	DA	3018	1/1	0.99	0.10	-	95,95,95,95	0
56	MG	AA	1628	1/1	0.23	0.26	-	137,137,137,137	0
56	MG	BA	1619	1/1	0.89	0.47	-	228,228,228,228	0
56	MG	AA	1604	1/1	0.77	0.66	-	79,79,79,79	0
56	MG	DA	3059	1/1	0.99	0.07	-	25,25,25,25	0
56	MG	DA	3015	1/1	0.99	0.16	-	78,78,78,78	0
58	MPD	DT	202	8/8	0.75	0.37	-	138,139,144,145	0
56	MG	DA	3137	1/1	0.59	0.34	-	61,61,61,61	0
56	MG	AA	1665	1/1	0.76	0.71	-	274,274,274,274	0
56	MG	CA	3154	1/1	0.38	0.71	-	110,110,110,110	0
56	MG	DA	3088	1/1	0.98	0.09	-	75,75,75,75	0
56	MG	DA	3057	1/1	1.00	0.14	-	28,28,28,28	0
56	MG	BA	1625	1/1	0.77	0.76	-	288,288,288,288	0
56	MG	DA	3083	1/1	0.99	0.07	-	57,57,57,57	0
56	MG	DA	3152	1/1	0.57	0.27	-	115,115,115,115	0
56	MG	CA	3045	1/1	0.98	0.07	-	167,167,167,167	0
56	MG	DA	3117	1/1	0.97	0.12	-	70,70,70,70	0
56	MG	DA	3041	1/1	1.00	0.23	-	22,22,22,22	0
56	MG	CA	3051	1/1	0.96	0.39	-	248,248,248,248	0
56	MG	AA	1640	1/1	0.96	0.11	-	131,131,131,131	0
56	MG	AA	1619	1/1	0.95	0.54	-	122,122,122,122	0
56	MG	BA	1641	1/1	0.86	0.37	-	140,140,140,140	0
56	MG	DA	3052	1/1	0.99	0.29	-	251,251,251,251	0
56	MG	DA	3107	1/1	0.99	0.15	-	50,50,50,50	0
56	MG	DA	3166	1/1	0.97	0.35	-	74,74,74,74	0
56	MG	CA	3012	1/1	0.97	0.14	-	115,115,115,115	0
56	MG	DA	3144	1/1	0.93	0.62	-	79,79,79,79	0
56	MG	BA	1634	1/1	0.86	0.10	-	216,216,216,216	0
56	MG	AA	1632	1/1	0.97	0.10	-	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3108	1/1	0.98	0.08	-	36,36,36,36	0
56	MG	CA	3060	1/1	0.87	0.42	-	238,238,238,238	0
56	MG	DA	3180	1/1	0.89	0.81	-	77,77,77,77	0
56	MG	DA	3167	1/1	0.97	0.43	-	97,97,97,97	0
56	MG	DA	3179	1/1	0.94	1.13	-	85,85,85,85	0
56	MG	CA	3067	1/1	0.86	0.21	-	274,274,274,274	0
56	MG	DA	3173	1/1	0.97	0.87	-	100,100,100,100	0
58	MPD	DA	3190	8/8	0.89	0.31	-	100,102,103,106	0
62	EDO	DA	3194	4/4	0.83	0.31	-	89,90,90,90	0
56	MG	CA	3016	1/1	0.97	0.91	-	218,218,218,218	0
56	MG	DA	3181	1/1	0.97	0.29	-	66,66,66,66	0
56	MG	CA	3141	1/1	0.89	0.22	-	78,78,78,78	0
56	MG	CA	3138	1/1	0.91	0.12	-	98,98,98,98	0
56	MG	DB	207	1/1	0.94	0.77	-	92,92,92,92	0
56	MG	AA	1601	1/1	0.84	0.76	-	62,62,62,62	0
56	MG	CA	3076	1/1	0.99	0.31	-	218,218,218,218	0
56	MG	CA	3135	1/1	0.61	0.48	-	78,78,78,78	0
56	MG	CA	3010	1/1	0.93	0.10	-	259,259,259,259	0
56	MG	DA	3060	1/1	0.99	0.14	-	23,23,23,23	0
56	MG	DA	3039	1/1	1.00	0.12	-	34,34,34,34	0
56	MG	CA	3132	1/1	0.18	0.61	-	157,157,157,157	0
56	MG	CA	3023	1/1	0.95	0.39	-	255,255,255,255	0
56	MG	CA	3106	1/1	0.94	0.13	-	74,74,74,74	0
56	MG	CA	3097	1/1	0.96	0.14	-	112,112,112,112	0
56	MG	BA	1638	1/1	0.81	0.44	-	65,65,65,65	0
56	MG	CA	3065	1/1	0.96	0.15	-	115,115,115,115	0
56	MG	AA	1615	1/1	0.68	0.68	-	129,129,129,129	0
56	MG	AA	1634	1/1	0.95	0.32	-	179,179,179,179	0
56	MG	AA	1659	1/1	0.78	0.33	-	273,273,273,273	0
56	MG	AA	1641	1/1	0.94	0.06	-	122,122,122,122	0
56	MG	DA	3072	1/1	0.99	0.20	-	86,86,86,86	0
56	MG	CA	3127	1/1	0.97	0.14	-	73,73,73,73	0
56	MG	AA	1618	1/1	0.54	0.11	-	172,172,172,172	0
56	MG	AA	1621	1/1	0.64	0.51	-	97,97,97,97	0
56	MG	DA	3034	1/1	1.00	0.16	-	44,44,44,44	0
56	MG	BA	1623	1/1	0.62	0.87	-	277,277,277,277	0
56	MG	AA	1622	1/1	0.24	0.84	-	106,106,106,106	0
56	MG	DA	3118	1/1	0.95	0.10	-	31,31,31,31	0
61	PEG	DP	201	7/7	0.69	0.68	-	149,153,164,165	0
56	MG	CA	3046	1/1	0.95	0.13	-	99,99,99,99	0
56	MG	DA	3019	1/1	1.00	0.27	-	16,16,16,16	0
56	MG	AA	1635	1/1	0.96	0.14	-	220,220,220,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3062	1/1	0.93	0.27	-	269,269,269,269	0
58	MPD	DN	201	8/8	0.91	0.35	-	109,117,119,121	0
56	MG	CA	3122	1/1	0.80	0.52	-	89,89,89,89	0
56	MG	DA	3123	1/1	0.80	0.36	-	84,84,84,84	0
56	MG	CA	3048	1/1	0.89	0.16	-	147,147,147,147	0
56	MG	DA	3133	1/1	0.89	0.26	-	52,52,52,52	0
56	MG	CA	3053	1/1	0.92	0.11	-	86,86,86,86	0
56	MG	DA	3101	1/1	0.99	0.15	-	90,90,90,90	0
56	MG	DA	3051	1/1	0.99	0.13	-	37,37,37,37	0
56	MG	AA	1611	1/1	0.94	0.15	-	133,133,133,133	0
56	MG	CA	3155	1/1	0.93	0.26	-	181,181,181,181	0
56	MG	CA	3130	1/1	0.80	0.13	-	84,84,84,84	0
56	MG	DA	3085	1/1	0.98	0.13	-	100,100,100,100	0
56	MG	DA	3134	1/1	0.81	0.60	-	98,98,98,98	0
56	MG	BA	1626	1/1	0.72	0.91	-	255,255,255,255	0
56	MG	DA	3154	1/1	0.84	0.35	-	60,60,60,60	0
56	MG	CA	3149	1/1	0.92	0.44	-	76,76,76,76	0
56	MG	CA	3042	1/1	0.98	0.06	-	96,96,96,96	0
56	MG	CA	3083	1/1	0.91	0.34	-	254,254,254,254	0
68	TRS	DA	3220	8/8	0.69	0.79	-	184,187,190,191	0
56	MG	BA	1640	1/1	0.99	0.08	-	103,103,103,103	0
56	MG	DA	3086	1/1	0.99	0.09	-	82,82,82,82	0
56	MG	DA	3091	1/1	1.00	0.13	-	29,29,29,29	0
56	MG	CA	3110	1/1	0.86	0.35	-	129,129,129,129	0
56	MG	AA	1636	1/1	0.98	0.39	-	209,209,209,209	0
56	MG	CA	3001	1/1	0.87	0.29	-	291,291,291,291	0
56	MG	AA	1647	1/1	0.91	0.30	-	145,145,145,145	0
56	MG	AA	1660	1/1	0.62	0.53	-	283,283,283,283	0
56	MG	DA	3159	1/1	0.98	0.15	-	131,131,131,131	0
56	MG	DA	3169	1/1	0.98	0.11	-	41,41,41,41	0
56	MG	DA	3171	1/1	0.86	0.81	-	111,111,111,111	0
56	MG	CA	3140	1/1	0.69	0.53	-	108,108,108,108	0
56	MG	CA	3021	1/1	0.88	1.32	-	253,253,253,253	0
56	MG	AA	1602	1/1	0.80	0.44	-	78,78,78,78	0
56	MG	CA	3113	1/1	0.76	0.44	-	76,76,76,76	0
56	MG	CA	3081	1/1	0.97	0.16	-	254,254,254,254	0
56	MG	DA	3174	1/1	0.96	0.23	-	87,87,87,87	0
56	MG	CA	3038	1/1	0.92	0.17	-	252,252,252,252	0
61	PEG	DA	3227	7/7	0.84	0.34	-	109,114,120,120	0
56	MG	DA	3087	1/1	1.00	0.19	-	32,32,32,32	0
56	MG	AA	1664	1/1	0.96	0.71	-	265,265,265,265	0
56	MG	CA	3028	1/1	0.92	0.80	-	284,284,284,284	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	1628	1/1	0.97	0.15	-	120,120,120,120	0
56	MG	CA	3128	1/1	0.86	0.35	-	116,116,116,116	0
56	MG	DA	3172	1/1	0.90	0.39	-	85,85,85,85	0
56	MG	DB	203	1/1	0.99	0.10	-	88,88,88,88	0
56	MG	DA	3143	1/1	0.93	0.31	-	63,63,63,63	0
56	MG	AA	1620	1/1	0.82	0.81	-	116,116,116,116	0
56	MG	DA	3230	1/1	1.00	0.13	-	76,76,76,76	0
56	MG	CA	3068	1/1	0.93	0.26	-	174,174,174,174	0
66	ACY	DA	3202	4/4	0.97	0.19	-	93,96,96,97	0
56	MG	BA	1631	1/1	0.96	0.11	-	132,132,132,132	0
56	MG	CA	3071	1/1	0.84	0.34	-	228,228,228,228	0
56	MG	CA	3092	1/1	0.76	0.08	-	163,163,163,163	0
56	MG	CA	3085	1/1	0.94	0.08	-	116,116,116,116	0
56	MG	DA	3151	1/1	0.98	0.25	-	48,48,48,48	0
56	MG	CA	3017	1/1	0.97	0.12	-	192,192,192,192	0
56	MG	DA	3080	1/1	0.95	0.10	-	195,195,195,195	0
56	MG	DA	3005	1/1	0.99	0.13	-	67,67,67,67	0
56	MG	CA	3139	1/1	0.17	0.83	-	140,140,140,140	0
56	MG	DA	3076	1/1	0.99	0.19	-	46,46,46,46	0
56	MG	DA	3012	1/1	0.97	0.14	-	141,141,141,141	0
56	MG	DA	3138	1/1	0.92	0.34	-	29,29,29,29	1
56	MG	DA	3089	1/1	0.99	0.15	-	24,24,24,24	0
56	MG	BA	1606	1/1	0.83	0.17	-	270,270,270,270	0
56	MG	BA	1604	1/1	0.85	0.48	-	257,257,257,257	0
56	MG	DA	3038	1/1	0.99	0.11	-	35,35,35,35	0
56	MG	CA	3120	1/1	0.92	0.14	-	130,130,130,130	0
56	MG	DB	208	1/1	0.99	0.17	-	57,57,57,57	0
56	MG	CA	3058	1/1	0.95	0.14	-	124,124,124,124	0
56	MG	DA	3175	1/1	0.96	0.60	-	115,115,115,115	0
56	MG	DA	3075	1/1	1.00	0.18	-	25,25,25,25	0
56	MG	CB	203	1/1	0.92	0.15	-	237,237,237,237	0
56	MG	CA	3070	1/1	0.91	0.31	-	234,234,234,234	0
56	MG	BA	1609	1/1	0.96	0.13	-	156,156,156,156	0
56	MG	DA	3006	1/1	0.99	0.11	-	266,266,266,266	0
56	MG	DA	3104	1/1	1.00	0.22	-	43,43,43,43	0
56	MG	CA	3096	1/1	0.92	0.08	-	89,89,89,89	0
56	MG	AA	1650	1/1	0.97	0.13	-	115,115,115,115	0
56	MG	BA	1639	1/1	0.92	0.27	-	117,117,117,117	0
56	MG	CA	3152	1/1	0.91	0.16	-	160,160,160,160	0
56	MG	AA	1616	1/1	0.52	0.69	-	105,105,105,105	0
56	MG	CA	3147	1/1	0.91	0.25	-	36,36,36,36	1
62	EDO	DA	3215	4/4	0.88	0.32	-	64,67,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1627	1/1	0.27	1.20	-	115,115,115,115	0
56	MG	DA	3178	1/1	0.82	0.34	-	93,93,93,93	0
59	PUT	DA	3223	6/6	0.97	0.19	-	75,81,84,84	0
56	MG	DA	3114	1/1	0.99	0.08	-	52,52,52,52	0
56	MG	DA	3020	1/1	0.99	0.06	-	69,69,69,69	0
56	MG	CA	3118	1/1	0.87	0.51	-	87,87,87,87	0
56	MG	AA	1667	1/1	0.98	0.14	-	76,76,76,76	0
56	MG	DA	3231	1/1	0.98	0.26	-	70,70,70,70	0
56	MG	DA	3068	1/1	0.99	0.20	-	43,43,43,43	0
56	MG	AA	1608	1/1	0.94	0.36	-	128,128,128,128	0
56	MG	CA	3126	1/1	0.56	0.36	-	115,115,115,115	0
56	MG	DA	3065	1/1	1.00	0.13	-	41,41,41,41	0
56	MG	DB	209	1/1	0.96	0.15	-	83,83,83,83	0
56	MG	DA	3067	1/1	0.98	0.11	-	75,75,75,75	0
56	MG	DA	3111	1/1	0.98	0.46	-	283,283,283,283	0
62	EDO	DA	3002	4/4	0.72	0.61	-	176,176,176,177	0
56	MG	CA	3117	1/1	0.91	0.13	-	59,59,59,59	0
56	MG	DA	3036	1/1	1.00	0.18	-	32,32,32,32	0
56	MG	CA	3108	1/1	0.96	0.23	-	89,89,89,89	0
56	MG	CA	3156	1/1	0.87	0.16	-	263,263,263,263	0
56	MG	DA	3158	1/1	0.86	0.49	-	107,107,107,107	0
56	MG	DA	3113	1/1	0.99	0.16	-	113,113,113,113	0
56	MG	BA	1616	1/1	0.95	0.12	-	151,151,151,151	0
56	MG	DA	3148	1/1	0.82	0.22	-	67,67,67,67	0
56	MG	AA	1630	1/1	0.96	0.20	-	205,205,205,205	0
56	MG	DA	3156	1/1	0.55	0.68	-	83,83,83,83	0
56	MG	BA	1633	1/1	0.94	0.55	-	237,237,237,237	0
56	MG	CA	3091	1/1	0.97	0.09	-	81,81,81,81	0
56	MG	CA	3034	1/1	0.82	0.14	-	228,228,228,228	0
56	MG	DA	3100	1/1	1.00	0.20	-	34,34,34,34	0
56	MG	AA	1638	1/1	0.93	0.14	-	142,142,142,142	0
62	EDO	DA	3209	4/4	0.91	0.62	-	94,96,98,99	0
56	MG	CA	3036	1/1	0.93	0.15	-	227,227,227,227	0
56	MG	DA	3045	1/1	0.99	0.10	-	73,73,73,73	0
56	MG	AA	1606	1/1	0.89	0.14	-	124,124,124,124	0
56	MG	CA	3151	1/1	0.81	0.55	-	102,102,102,102	0
56	MG	DA	3103	1/1	0.99	0.15	-	59,59,59,59	0
56	MG	CA	3087	1/1	0.92	0.17	-	232,232,232,232	0
66	ACY	DA	3196	4/4	0.96	0.24	-	61,69,69,72	0
56	MG	CA	3115	1/1	0.97	0.30	-	111,111,111,111	0
56	MG	DA	3073	1/1	1.00	0.16	-	40,40,40,40	0
56	MG	DA	3074	1/1	0.99	0.12	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	PUT	AA	1675	6/6	0.37	0.60	-	172,174,174,175	0
56	MG	AA	1626	1/1	0.71	0.95	-	120,120,120,120	0
58	MPD	DK	201	8/8	0.83	0.27	-	125,126,127,127	0
56	MG	DA	3165	1/1	0.90	0.27	-	63,63,63,63	0
56	MG	AA	1666	1/1	0.99	0.07	-	100,100,100,100	0
56	MG	CA	3107	1/1	0.90	0.34	-	81,81,81,81	0
56	MG	DR	202	1/1	0.97	0.30	-	269,269,269,269	0
56	MG	DA	3164	1/1	0.95	0.26	-	78,78,78,78	0
56	MG	BA	1629	1/1	0.91	1.34	-	217,217,217,217	0
56	MG	DA	3139	1/1	0.97	0.13	-	42,42,42,42	0
56	MG	DA	3136	1/1	0.99	0.19	-	72,72,72,72	0
56	MG	DA	3070	1/1	0.99	0.12	-	151,151,151,151	0
56	MG	CA	3029	1/1	0.95	0.17	-	143,143,143,143	0
56	MG	CA	3137	1/1	0.91	0.31	-	164,164,164,164	0
56	MG	AA	1669	1/1	0.99	0.25	-	239,239,239,239	0
56	MG	CA	3136	1/1	0.94	0.24	-	107,107,107,107	0
58	MPD	DT	201	8/8	0.87	0.31	-	110,115,125,126	0
56	MG	DA	3142	1/1	0.96	0.26	-	80,80,80,80	0
56	MG	CA	3121	1/1	0.92	0.23	-	83,83,83,83	0
57	PG4	DR	201	13/13	0.61	0.34	-	156,168,173,173	0
56	MG	AA	1607	1/1	0.95	0.48	-	90,90,90,90	0
56	MG	CA	3064	1/1	0.92	0.30	-	271,271,271,271	0
56	MG	CA	3079	1/1	0.97	0.28	-	131,131,131,131	0
56	MG	DA	3040	1/1	0.99	0.09	-	55,55,55,55	0
56	MG	CA	3146	1/1	0.87	0.10	-	174,174,174,174	0
56	MG	AA	1624	1/1	0.83	0.30	-	82,82,82,82	0
56	MG	DM	202	1/1	0.99	0.04	-	90,90,90,90	0
56	MG	CA	3061	1/1	0.43	0.19	-	270,270,270,270	0
56	MG	DA	3168	1/1	0.51	0.54	-	119,119,119,119	0
56	MG	DA	3001	1/1	0.91	0.45	-	47,47,47,47	0
56	MG	DA	3141	1/1	0.95	0.41	-	80,80,80,80	0
56	MG	AA	1658	1/1	0.91	0.34	-	212,212,212,212	0
56	MG	CA	3055	1/1	0.79	0.10	-	193,193,193,193	0
56	MG	DA	3044	1/1	0.97	0.08	-	124,124,124,124	0
56	MG	DA	3098	1/1	0.90	0.21	-	246,246,246,246	0
56	MG	DA	3130	1/1	0.27	0.89	-	109,109,109,109	0
56	MG	CA	3088	1/1	0.99	0.13	-	86,86,86,86	0
56	MG	CA	3074	1/1	0.98	0.10	-	145,145,145,145	0
56	MG	DA	3028	1/1	0.99	0.10	-	116,116,116,116	0
56	MG	CA	3077	1/1	0.78	0.43	-	244,244,244,244	0
56	MG	DA	3229	1/1	0.99	0.08	-	107,107,107,107	0
56	MG	CA	3125	1/1	0.84	0.28	-	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3079	1/1	0.95	0.31	-	179,179,179,179	0
56	MG	BA	1603	1/1	0.91	0.21	-	278,278,278,278	0
56	MG	AA	1625	1/1	0.77	0.57	-	83,83,83,83	0
56	MG	AA	1655	1/1	0.97	0.08	-	152,152,152,152	0
56	MG	DB	206	1/1	0.92	0.31	-	73,73,73,73	0
56	MG	DA	3055	1/1	0.99	0.25	-	52,52,52,52	0
56	MG	CA	3142	1/1	0.86	0.17	-	102,102,102,102	0
56	MG	CA	3095	1/1	0.97	0.12	-	174,174,174,174	0
56	MG	DA	3119	1/1	1.00	0.30	-	41,41,41,41	0
56	MG	DA	3121	1/1	0.94	0.52	-	111,111,111,111	0
56	MG	AA	1613	1/1	0.91	0.62	-	80,80,80,80	0
56	MG	BA	1621	1/1	0.99	0.17	-	45,45,45,45	0
56	MG	BA	1611	1/1	0.98	0.13	-	84,84,84,84	0
56	MG	CA	3015	1/1	0.98	0.22	-	84,84,84,84	0
56	MG	DA	3116	1/1	0.99	0.10	-	72,72,72,72	0
56	MG	CA	3114	1/1	0.95	0.31	-	67,67,67,67	0
56	MG	CA	3002	1/1	0.92	0.15	-	224,224,224,224	0
56	MG	AA	1645	1/1	0.97	0.13	-	70,70,70,70	0
56	MG	CA	3014	1/1	0.89	0.19	-	273,273,273,273	0
56	MG	CA	3112	1/1	0.96	0.37	-	103,103,103,103	0
56	MG	CA	3025	1/1	0.98	0.12	-	133,133,133,133	0
56	MG	DA	3125	1/1	0.91	0.22	-	51,51,51,51	0
56	MG	DA	3069	1/1	1.00	0.10	-	64,64,64,64	0
56	MG	CA	3123	1/1	0.80	0.69	-	142,142,142,142	0
56	MG	CA	3116	1/1	0.76	0.41	-	92,92,92,92	0
56	MG	DA	3155	1/1	0.81	0.40	-	86,86,86,86	0
56	MG	DA	3157	1/1	0.84	0.26	-	74,74,74,74	0
56	MG	CA	3047	1/1	0.91	0.26	-	100,100,100,100	0
56	MG	DA	3129	1/1	0.89	0.22	-	51,51,51,51	0
56	MG	BA	1637	1/1	0.28	0.54	-	121,121,121,121	0
56	MG	DA	3048	1/1	0.98	0.12	-	59,59,59,59	0
62	EDO	DB	211	4/4	0.96	0.22	-	131,131,132,133	0
62	EDO	DA	3208	4/4	0.97	0.21	-	111,113,113,113	0
56	MG	DA	3025	1/1	0.99	0.11	-	57,57,57,57	0
56	MG	DA	3016	1/1	0.99	0.17	-	74,74,74,74	0
56	MG	CA	3066	1/1	0.94	0.11	-	91,91,91,91	0
56	MG	CA	3075	1/1	0.54	1.11	-	231,231,231,231	0
56	MG	CA	3082	1/1	0.96	0.26	-	168,168,168,168	0
56	MG	AA	1603	1/1	0.52	0.67	-	111,111,111,111	0
56	MG	DA	3124	1/1	0.90	0.52	-	90,90,90,90	0
56	MG	CA	3098	1/1	0.99	0.08	-	98,98,98,98	0
56	MG	CA	3119	1/1	0.84	0.38	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3148	1/1	0.90	0.41	-	43,43,43,43	1
56	MG	DA	3176	1/1	0.84	0.31	-	81,81,81,81	0
56	MG	DA	3160	1/1	0.86	0.37	-	64,64,64,64	0
56	MG	DA	3077	1/1	0.99	0.12	-	71,71,71,71	0
56	MG	CA	3073	1/1	0.97	0.23	-	139,139,139,139	0
56	MG	CA	3005	1/1	0.97	0.37	-	233,233,233,233	0
56	MG	DA	3170	1/1	0.80	0.18	-	59,59,59,59	0
56	MG	CA	3129	1/1	0.93	0.13	-	135,135,135,135	0
56	MG	CA	3104	1/1	0.47	0.46	-	249,249,249,249	0
56	MG	CA	3069	1/1	0.98	0.14	-	107,107,107,107	0
56	MG	DA	3146	1/1	0.93	0.28	-	76,76,76,76	0
56	MG	DA	3162	1/1	0.76	0.30	-	79,79,79,79	0
56	MG	DA	3082	1/1	0.99	0.11	-	109,109,109,109	0
56	MG	DA	3145	1/1	0.95	0.19	-	45,45,45,45	0
56	MG	CA	3043	1/1	0.99	0.06	-	90,90,90,90	0
56	MG	DA	3153	1/1	0.91	0.29	-	102,102,102,102	0
56	MG	CA	3004	1/1	0.95	0.11	-	192,192,192,192	0
56	MG	BA	1630	1/1	0.85	0.07	-	197,197,197,197	0
56	MG	DA	3131	1/1	0.92	0.24	-	83,83,83,83	0
56	MG	AA	1617	1/1	0.94	0.21	-	88,88,88,88	0
61	PEG	DA	3199	7/7	0.84	0.46	-	99,106,112,113	0
56	MG	DA	3011	1/1	1.00	0.10	-	23,23,23,23	0
56	MG	CA	3052	1/1	0.91	0.07	-	124,124,124,124	0
56	MG	DA	3021	1/1	1.00	0.14	-	31,31,31,31	0
56	MG	DA	3078	1/1	0.99	0.06	-	47,47,47,47	0
56	MG	AA	1609	1/1	0.86	0.56	-	107,107,107,107	0
56	MG	DA	3008	1/1	0.96	0.12	-	280,280,280,280	0
66	ACY	DA	3191	4/4	0.95	0.26	-	79,80,81,81	0
56	MG	CA	3090	1/1	0.92	0.16	-	187,187,187,187	0
56	MG	AA	1633	1/1	0.99	0.12	-	116,116,116,116	0
56	MG	DA	3010	1/1	0.99	0.11	-	48,48,48,48	0
56	MG	CA	3111	1/1	0.88	0.29	-	103,103,103,103	0
56	MG	DA	3105	1/1	0.99	0.17	-	33,33,33,33	0
56	MG	CA	3062	1/1	0.94	0.11	-	168,168,168,168	0
56	MG	DA	3106	1/1	0.99	0.15	-	45,45,45,45	0
56	MG	DA	3132	1/1	0.94	0.21	-	56,56,56,56	0
62	EDO	DA	3003	4/4	0.80	0.28	-	135,137,140,141	0
56	MG	CA	3007	1/1	0.47	0.67	-	257,257,257,257	0
56	MG	CA	3035	1/1	0.99	0.20	-	100,100,100,100	0
56	MG	DA	3149	1/1	0.97	0.24	-	96,96,96,96	0
56	MG	BA	1636	1/1	0.88	0.47	-	77,77,77,77	0
56	MG	CA	3084	1/1	0.94	0.21	-	172,172,172,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3096	1/1	0.99	0.14	-	28,28,28,28	0
56	MG	CA	3134	1/1	0.93	0.12	-	167,167,167,167	0
56	MG	AA	1614	1/1	0.92	0.13	-	83,83,83,83	0
56	MG	DA	3115	1/1	0.98	0.20	-	52,52,52,52	0
56	MG	CA	3057	1/1	0.91	0.14	-	111,111,111,111	0
56	MG	AA	1652	1/1	0.98	0.26	-	42,42,42,42	0
56	MG	DA	3049	1/1	1.00	0.14	-	52,52,52,52	0
56	MG	CA	3072	1/1	0.88	1.06	-	258,258,258,258	0
56	MG	BA	1607	1/1	0.96	0.24	-	280,280,280,280	0
56	MG	CA	3050	1/1	0.96	0.18	-	166,166,166,166	0
56	MG	DA	3030	1/1	0.98	0.20	-	88,88,88,88	0
56	MG	AA	1610	1/1	0.82	0.28	-	99,99,99,99	0
56	MG	CA	3145	1/1	0.60	0.98	-	78,78,78,78	0
56	MG	CA	3093	1/1	0.82	0.16	-	143,143,143,143	0
56	MG	DA	3042	1/1	0.99	0.11	-	87,87,87,87	0
56	MG	BA	1635	1/1	0.80	0.16	-	209,209,209,209	0
56	MG	DA	3053	1/1	0.98	0.10	-	54,54,54,54	0
56	MG	DA	3032	1/1	0.99	0.19	-	33,33,33,33	0
56	MG	DB	205	1/1	0.95	0.66	-	148,148,148,148	0
56	MG	DA	3056	1/1	0.99	0.22	-	55,55,55,55	0
56	MG	AA	1623	1/1	0.63	0.76	-	87,87,87,87	0
62	EDO	DB	210	4/4	0.76	0.39	-	125,126,126,127	0
56	MG	DA	3161	1/1	0.90	0.22	-	73,73,73,73	0
56	MG	DA	3120	1/1	0.96	0.55	-	66,66,66,66	0
56	MG	AA	1654	1/1	0.89	0.14	-	178,178,178,178	0
56	MG	AA	1605	1/1	0.79	0.52	-	87,87,87,87	0
56	MG	CA	3059	1/1	0.92	0.10	-	118,118,118,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.