



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:08 PM GMT

PDB ID : 4V8H
Title : Crystal structure of HPF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.10 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

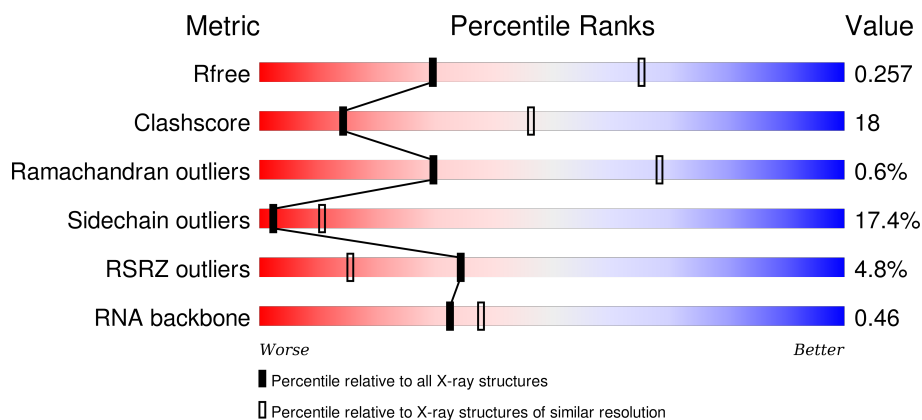
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>4%</div> <div>23% 45% 24% 7%</div> </div>
1	CA	1522	<div> <div>4%</div> <div>23% 45% 23% 7%</div> </div>
2	AB	256	<div> <div>4%</div> <div>37% 40% 13% 10%</div> </div>
2	CB	256	<div> <div>5%</div> <div>35% 41% 13% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AX	101	
22	CX	101	
23	BA	2913	
23	DA	2913	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	


























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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	



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Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	

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
54	MG	AA	1610	-	-	-	X
54	MG	AA	1612	-	-	-	X
54	MG	AA	1618	-	-	-	X
54	MG	AA	1619	-	-	-	X
54	MG	AA	1624	-	-	-	X
54	MG	AA	1629	-	-	-	X
54	MG	AA	1633	-	-	-	X
54	MG	AA	1639	-	-	-	X
54	MG	AA	1650	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1660	-	-	-	X
54	MG	AA	1668	-	-	-	X
54	MG	AA	1671	-	-	-	X
54	MG	AA	1672	-	-	-	X
54	MG	AA	1680	-	-	-	X
54	MG	AA	1684	-	-	-	X
54	MG	AA	1711	-	-	-	X
54	MG	AA	1712	-	-	-	X
54	MG	AD	302	-	-	-	X
54	MG	B3	101	-	-	-	X
54	MG	BA	3006	-	-	-	X
54	MG	BA	3011	-	-	-	X
54	MG	BA	3015	-	-	-	X
54	MG	BA	3019	-	-	-	X
54	MG	BA	3026	-	-	-	X
54	MG	BA	3031	-	-	-	X
54	MG	BA	3037	-	-	-	X
54	MG	BA	3040	-	-	-	X
54	MG	BA	3042	-	-	-	X
54	MG	BA	3046	-	-	-	X
54	MG	BA	3050	-	-	-	X
54	MG	BA	3061	-	-	-	X
54	MG	BA	3064	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3065	-	-	-	X
54	MG	BA	3069	-	-	-	X
54	MG	BA	3089	-	-	-	X
54	MG	BA	3102	-	-	-	X
54	MG	BA	3103	-	-	-	X
54	MG	BA	3105	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3127	-	-	-	X
54	MG	BA	3129	-	-	-	X
54	MG	BA	3130	-	-	-	X
54	MG	BA	3145	-	-	-	X
54	MG	BA	3154	-	-	-	X
54	MG	BA	3157	-	-	-	X
54	MG	BA	3159	-	-	-	X
54	MG	BA	3167	-	-	-	X
54	MG	BA	3170	-	-	-	X
54	MG	BA	3172	-	-	-	X
54	MG	BA	3188	-	-	-	X
54	MG	BA	3189	-	-	-	X
54	MG	BA	3194	-	-	-	X
54	MG	BA	3212	-	-	-	X
54	MG	BA	3226	-	-	-	X
54	MG	BA	3245	-	-	-	X
54	MG	BA	3246	-	-	-	X
54	MG	BA	3247	-	-	-	X
54	MG	BA	3248	-	-	-	X
54	MG	BA	3249	-	-	-	X
54	MG	BA	3250	-	-	-	X
54	MG	BA	3251	-	-	-	X
54	MG	BA	3252	-	-	-	X
54	MG	BA	3253	-	-	-	X
54	MG	BA	3255	-	-	-	X
54	MG	BA	3256	-	-	-	X
54	MG	BA	3257	-	-	-	X
54	MG	BA	3259	-	-	-	X
54	MG	BA	3262	-	-	-	X
54	MG	BA	3264	-	-	-	X
54	MG	BA	3265	-	-	-	X
54	MG	BA	3270	-	-	-	X
54	MG	BA	3273	-	-	-	X
54	MG	BA	3278	-	-	-	X
54	MG	BA	3279	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3282	-	-	-	X
54	MG	BA	3284	-	-	-	X
54	MG	BA	3333	-	-	-	X
54	MG	BA	3337	-	-	-	X
54	MG	BA	3368	-	-	-	X
54	MG	BA	3397	-	-	-	X
54	MG	BA	3419	-	-	-	X
54	MG	BA	3424	-	-	-	X
54	MG	BA	3451	-	-	-	X
54	MG	BA	3455	-	-	-	X
54	MG	BA	3456	-	-	-	X
54	MG	BA	3467	-	-	-	X
54	MG	BA	3473	-	-	-	X
54	MG	BA	3484	-	-	-	X
54	MG	BA	3492	-	-	-	X
54	MG	BA	3502	-	-	-	X
54	MG	BA	3574	-	-	-	X
54	MG	BA	3590	-	-	-	X
54	MG	BA	3595	-	-	-	X
54	MG	BB	206	-	-	-	X
54	MG	BB	212	-	-	-	X
54	MG	BB	220	-	-	-	X
54	MG	BD	301	-	-	-	X
54	MG	BE	301	-	-	-	X
54	MG	CA	1607	-	-	-	X
54	MG	CA	1611	-	-	-	X
54	MG	CA	1613	-	-	-	X
54	MG	CA	1619	-	-	-	X
54	MG	CA	1645	-	-	-	X
54	MG	CA	1685	-	-	-	X
54	MG	CA	1689	-	-	-	X
54	MG	CA	1690	-	-	-	X
54	MG	CA	1741	-	-	-	X
54	MG	CA	1749	-	-	-	X
54	MG	CA	1751	-	-	-	X
54	MG	CQ	201	-	-	-	X
54	MG	DA	3006	-	-	-	X
54	MG	DA	3008	-	-	-	X
54	MG	DA	3010	-	-	-	X
54	MG	DA	3011	-	-	-	X
54	MG	DA	3014	-	-	-	X
54	MG	DA	3017	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3029	-	-	-	X
54	MG	DA	3039	-	-	-	X
54	MG	DA	3040	-	-	-	X
54	MG	DA	3041	-	-	-	X
54	MG	DA	3042	-	-	-	X
54	MG	DA	3044	-	-	-	X
54	MG	DA	3052	-	-	-	X
54	MG	DA	3063	-	-	-	X
54	MG	DA	3069	-	-	-	X
54	MG	DA	3083	-	-	-	X
54	MG	DA	3091	-	-	-	X
54	MG	DA	3092	-	-	-	X
54	MG	DA	3096	-	-	-	X
54	MG	DA	3100	-	-	-	X
54	MG	DA	3123	-	-	-	X
54	MG	DA	3125	-	-	-	X
54	MG	DA	3128	-	-	-	X
54	MG	DA	3130	-	-	-	X
54	MG	DA	3131	-	-	-	X
54	MG	DA	3133	-	-	-	X
54	MG	DA	3146	-	-	-	X
54	MG	DA	3150	-	-	-	X
54	MG	DA	3156	-	-	-	X
54	MG	DA	3157	-	-	-	X
54	MG	DA	3162	-	-	-	X
54	MG	DA	3163	-	-	-	X
54	MG	DA	3164	-	-	-	X
54	MG	DA	3167	-	-	-	X
54	MG	DA	3178	-	-	-	X
54	MG	DA	3182	-	-	-	X
54	MG	DA	3183	-	-	-	X
54	MG	DA	3196	-	-	-	X
54	MG	DA	3197	-	-	-	X
54	MG	DA	3203	-	-	-	X
54	MG	DA	3205	-	-	-	X
54	MG	DA	3209	-	-	-	X
54	MG	DA	3219	-	-	-	X
54	MG	DA	3221	-	-	-	X
54	MG	DA	3224	-	-	-	X
54	MG	DA	3229	-	-	-	X
54	MG	DA	3230	-	-	-	X
54	MG	DA	3231	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3232	-	-	-	X
54	MG	DA	3241	-	-	-	X
54	MG	DA	3242	-	-	-	X
54	MG	DA	3244	-	-	-	X
54	MG	DA	3247	-	-	-	X
54	MG	DA	3257	-	-	-	X
54	MG	DA	3266	-	-	-	X
54	MG	DA	3269	-	-	-	X
54	MG	DA	3272	-	-	-	X
54	MG	DA	3276	-	-	-	X
54	MG	DA	3284	-	-	-	X
54	MG	DA	3293	-	-	-	X
54	MG	DA	3302	-	-	-	X
54	MG	DA	3303	-	-	-	X
54	MG	DA	3304	-	-	-	X
54	MG	DA	3305	-	-	-	X
54	MG	DA	3307	-	-	-	X
54	MG	DA	3308	-	-	-	X
54	MG	DA	3309	-	-	-	X
54	MG	DA	3311	-	-	-	X
54	MG	DA	3321	-	-	-	X
54	MG	DA	3337	-	-	-	X
54	MG	DA	3338	-	-	-	X
54	MG	DA	3345	-	-	-	X
54	MG	DA	3353	-	-	-	X
54	MG	DA	3366	-	-	-	X
54	MG	DA	3373	-	-	-	X
54	MG	DA	3374	-	-	-	X
54	MG	DA	3382	-	-	-	X
54	MG	DA	3414	-	-	-	X
54	MG	DA	3420	-	-	-	X
54	MG	DA	3441	-	-	-	X
54	MG	DA	3449	-	-	-	X
54	MG	DA	3473	-	-	-	X
54	MG	DA	3491	-	-	-	X
54	MG	DA	3514	-	-	-	X
54	MG	DA	3549	-	-	-	X
54	MG	DA	3570	-	-	-	X
54	MG	DA	3573	-	-	-	X
54	MG	DA	3578	-	-	-	X
54	MG	DB	201	-	-	-	X
54	MG	DD	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DF	301	-	-	-	X
54	MG	DR	202	-	-	-	X
54	MG	DR	203	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286308 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			
1	CA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	230	Total	C	N	O	S	0	0	0
			1787	1141	319	322	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

- 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
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			663	410	132	121	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			828	516	155	154	3	0	0
11	CK	114	Total	C	N	O	S		
			828	516	155	154	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			905	567	178	159	1	0	0
12	CL	122	Total	C	N	O	S		
			905	567	178	159	1	0	0

- 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		
			804	497	164	142	1	0	0
13	CM	114	Total	C	N	O	S		
			804	497	164	142	1	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			478	303	99	72	4	0	0
14	CN	60	Total	C	N	O	S		
			478	303	99	72	4	0	0

- 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		
			724	453	143	126	2	0	0
15	CO	88	Total	C	N	O	S		
			724	453	143	126	2	0	0

- 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
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	87	Total	C	N	O	S	0	0	0
			665	410	142	111	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a protein called Probable sigma(54) modulation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AX	95	Total	C	N	O	S	0	0	0
			631	396	116	118	1			
22	CX	95	Total	C	N	O	S	0	0	0
			601	378	108	114	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	96	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	97	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	98	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	99	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	100	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	101	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	96	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	97	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	98	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	99	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	100	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	101	HIS	-	EXPRESSION TAG	UNP P0AFX0

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2837	Total	C	N	O	P	0	0	0
			61112	27197	11440	19639	2836			
23	DA	2814	Total	C	N	O	P	0	0	0
			60621	26978	11351	19479	2813			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	?	-	U	DELETION	GB AP008226.1
BA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
24	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	275	Total	C	N	O	S	0	0	0
			2135	1349	422	361	3			
25	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
26	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
28	DG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
29	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1037	666	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			953	608	168	176	1			

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
31	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
32	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
33	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
34	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			
36	DS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
38	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
40	DW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	201	Total	C	N	O	S	0	0	0
			1536	980	272	282	2			
43	DZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
45	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
46	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 50 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
51	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	660	Total	Mg	0	0
			660	660		
54	CA	162	Total	Mg	0	0
			162	162		
54	DQ	2	Total	Mg	0	0
			2	2		
54	DF	1	Total	Mg	0	0
			1	1		
54	B8	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BE	5	Total 5	Mg 5	0	0
54	B1	1	Total 1	Mg 1	0	0
54	BP	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	23	Total 23	Mg 23	0	0
54	BT	2	Total 2	Mg 2	0	0
54	D8	2	Total 2	Mg 2	0	0
54	B9	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	3	Total 3	Mg 3	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	135	Total 135	Mg 135	0	0
54	BQ	4	Total 4	Mg 4	0	0
54	CQ	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DD	2	Total 2	Mg 2	0	0
54	D0	2	Total 2	Mg 2	0	0
54	BG	1	Total 1	Mg 1	0	0
54	B3	1	Total 1	Mg 1	0	0
54	BR	1	Total 1	Mg 1	0	0
54	DA	598	Total 598	Mg 598	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DP	1	Total 1	Mg 1	0	0
54	BV	1	Total 1	Mg 1	0	0
54	DO	2	Total 2	Mg 2	0	0
54	DE	4	Total 4	Mg 4	0	0
54	AQ	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	1	Total 1	Mg 1	0	0
54	BS	1	Total 1	Mg 1	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	3	Total 3	Mg 3	0	0
54	B0	3	Total 3	Mg 3	0	0
54	CE	1	Total 1	Mg 1	0	0
54	BW	2	Total 2	Mg 2	0	0
54	AF	1	Total 1	Mg 1	0	0
54	DB	8	Total 8	Mg 8	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B5	1	Total 1	Zn 1	0	0
55	B4	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CD	1	Total 1	Zn 1	0	0
55	B9	1	Total 1	Zn 1	0	0
55	BY	1	Total 1	Zn 1	0	0
55	DY	1	Total 1	Zn 1	0	0
55	D5	1	Total 1	Zn 1	0	0
55	D4	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0
55	CN	1	Total 1	Zn 1	0	0
55	D6	1	Total 1	Zn 1	0	0
55	D9	1	Total 1	Zn 1	0	0
55	B6	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	268	Total 268	O 268	0	0
56	AE	1	Total 1	O 1	0	0
56	AL	1	Total 1	O 1	0	0
56	AO	1	Total 1	O 1	0	0
56	AP	1	Total 1	O 1	0	0
56	AT	1	Total 1	O 1	0	0
56	AX	1	Total 1	O 1	0	0
56	BA	1694	Total 1694	O 1694	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	57	Total 57	O 57	0	0
56	BD	20	Total 20	O 20	0	0
56	BE	11	Total 11	O 11	0	0
56	BF	6	Total 6	O 6	0	0
56	BH	1	Total 1	O 1	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	2	Total 2	O 2	0	0
56	BP	11	Total 11	O 11	0	0
56	BQ	5	Total 5	O 5	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	3	Total 3	O 3	0	0
56	BV	3	Total 3	O 3	0	0
56	BW	3	Total 3	O 3	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	4	Total 4	O 4	0	0
56	B0	8	Total 8	O 8	0	0
56	B1	2	Total 2	O 2	0	0
56	B3	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B6	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B7	5	Total 5	O 5	0	0
56	B8	10	Total 10	O 10	0	0
56	B9	1	Total 1	O 1	0	0
56	CA	265	Total 265	O 265	0	0
56	CC	1	Total 1	O 1	0	0
56	CD	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	1	Total 1	O 1	0	0
56	CP	1	Total 1	O 1	0	0
56	CQ	1	Total 1	O 1	0	0
56	CT	1	Total 1	O 1	0	0
56	CX	1	Total 1	O 1	0	0
56	DA	1174	Total 1174	O 1174	0	0
56	DB	17	Total 17	O 17	0	0
56	DD	8	Total 8	O 8	0	0
56	DE	11	Total 11	O 11	0	0
56	DF	7	Total 7	O 7	0	0
56	DN	1	Total 1	O 1	0	0
56	DO	5	Total 5	O 5	0	0

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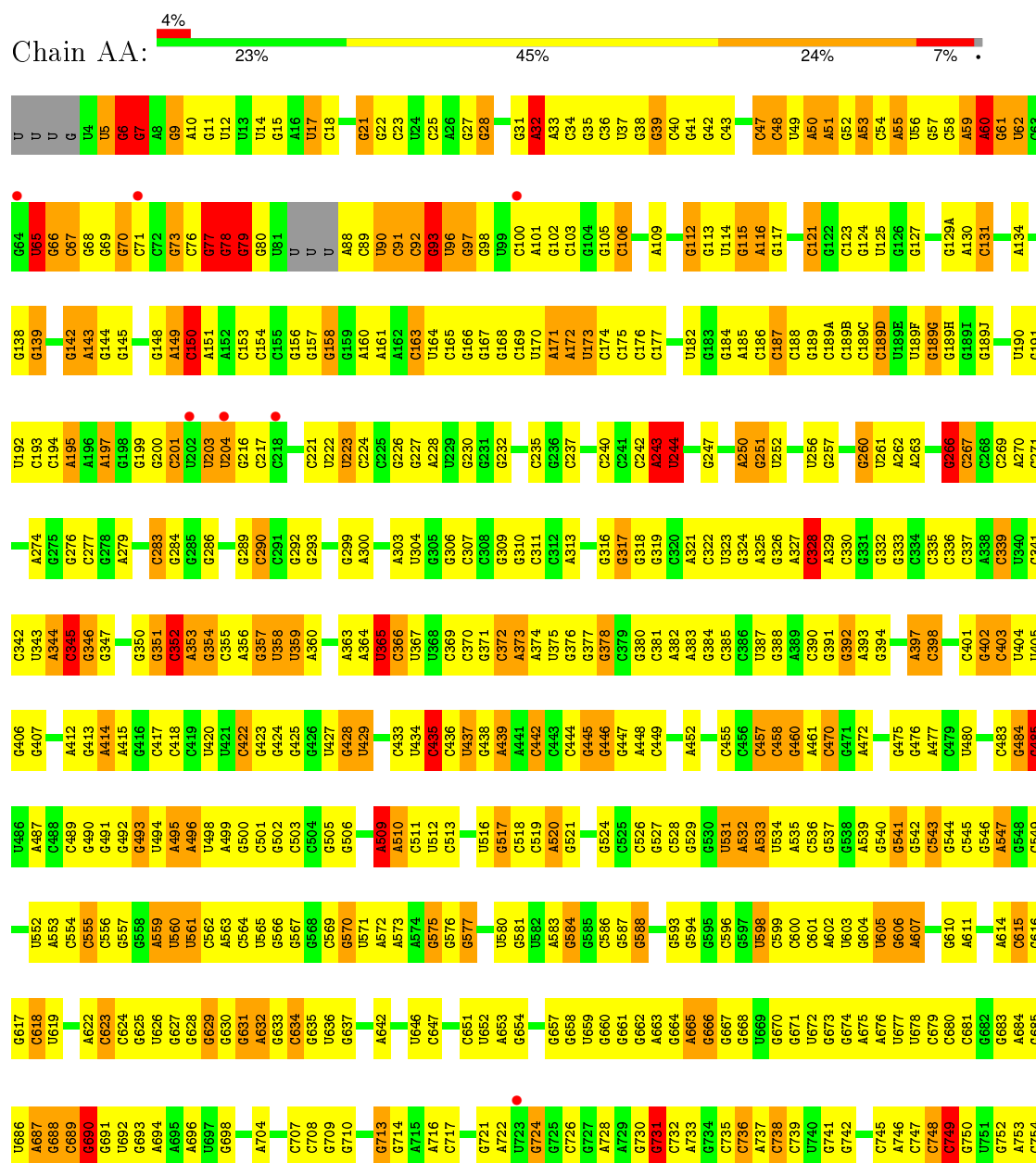
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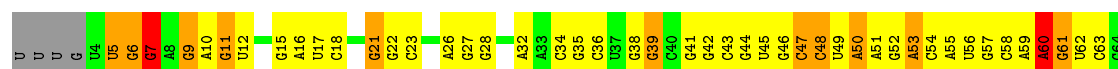
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			10	10		
56	DQ	3	Total	O	0	0
			3	3		
56	DR	2	Total	O	0	0
			2	2		
56	DT	2	Total	O	0	0
			2	2		
56	DU	5	Total	O	0	0
			5	5		
56	DV	2	Total	O	0	0
			2	2		
56	DW	2	Total	O	0	0
			2	2		
56	DX	1	Total	O	0	0
			1	1		
56	DY	2	Total	O	0	0
			2	2		
56	D0	1	Total	O	0	0
			1	1		
56	D1	5	Total	O	0	0
			5	5		
56	D3	1	Total	O	0	0
			1	1		
56	D4	1	Total	O	0	0
			1	1		
56	D7	3	Total	O	0	0
			3	3		
56	D8	1	Total	O	0	0
			1	1		

3 Residue-property plots

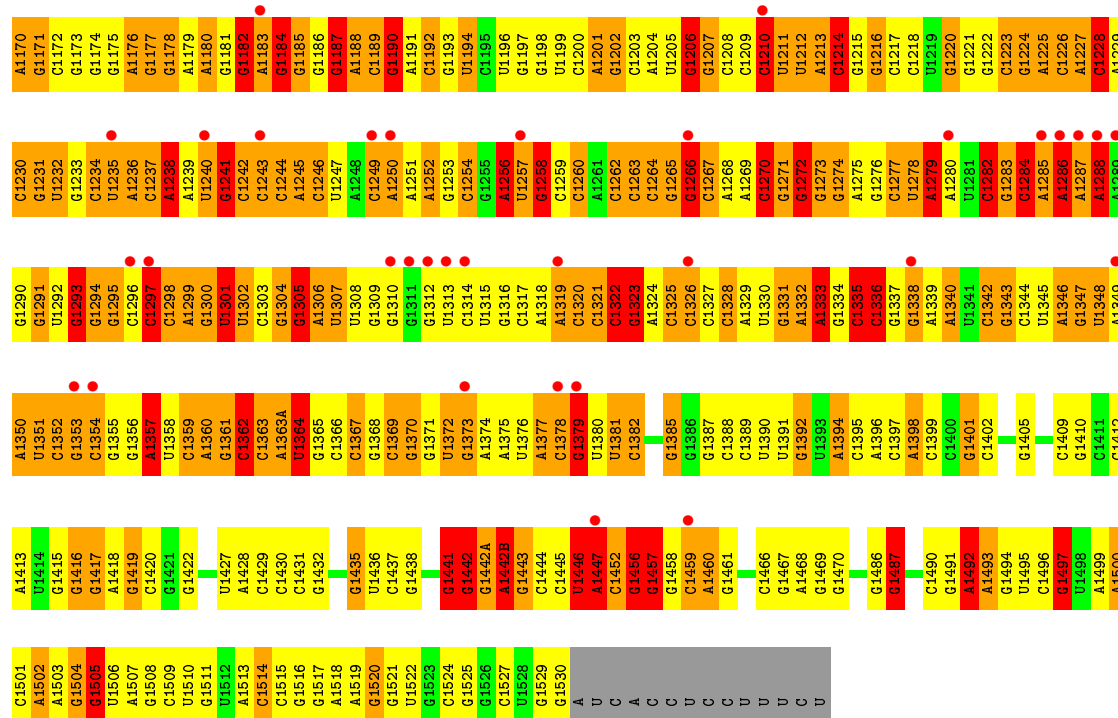
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S Ribosomal RNA

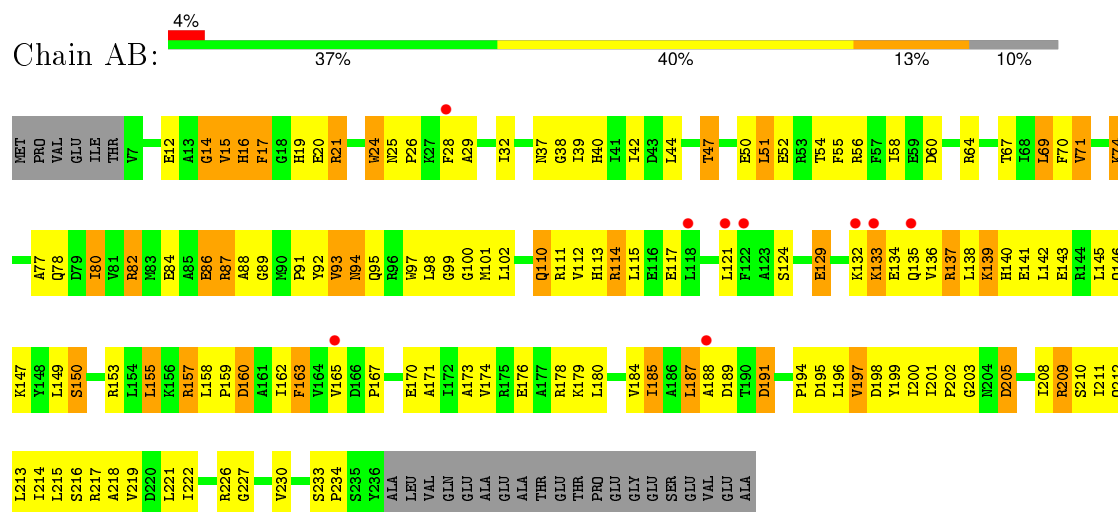




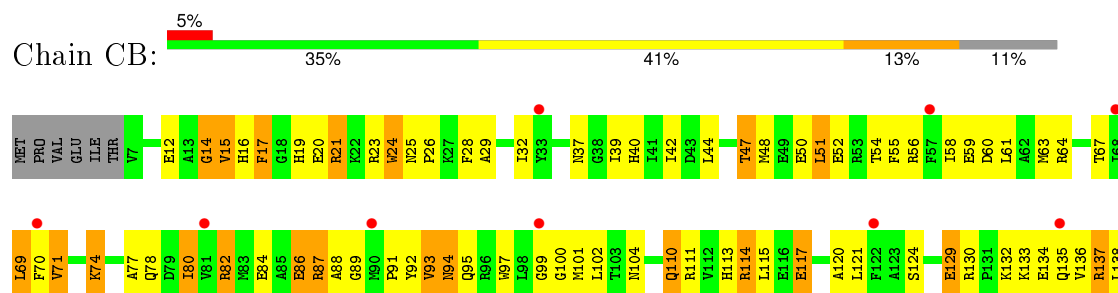
C1109	U1049	A994	C934	C856	A782	G710	U636	C569	G504	G425	A360	C290	A197	A143	U85
A1110	G1050	C995	A935	C857	C783	G713	G637	C569	G505	G426	A361	C291	A197	G144	G66
A1111	C1051	A996	C936	G858	C784	G714	G638	U571	A509	G427	U365	C292	C201	G145	C67
C1112	U1052	A997	G785	A859	G785	G714	U638	G570	A510	G428	C366	G293	U202	G146	G68
C1113	G1053	A998	A937	A860	A786	G715	A642	A572	C511	A429	U367	U294	U203	G147	G69
C1114	C1054	C999	G939	A861	A787	C717	U646	A573	C512	A430	U368	U295	U204	G148	G70
C1115	A1055	U1000	C840	U871	G791	C717	U647	A574	C513	A431	U369	U296	G216	A149	C71
C1116	U1056	A1001	G941	A865	G792	G721	C647	G575	C514	C433	C370	A297	C221	C150	C72
G1117	G1057	G1001A	G942	C866	A792	A722	U650	G577	C515	A434	C371	A298	U222	A151	G73
C1118	G1058	G1002	U943	C867	U793	U723	G650	G577	G516	C435	C372	A300	U223	C76	C77
C1119	G1059	G1003	G944	C868	A794	G724	U652	U580	C517	A436	C373	A301	U224	G77	G78
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G1121	G1061	A1005	A946	U870	C796	C726	A653	U582	C519	U438	U375	U804	G226	G	
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G1124	G1064	C1008	A873	A873	G803	G730	G658	G584	C522	C442	G378	C309	G233	U	
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C1161	A1101	A1041	A986	G925	U841	C770	U697	G628	C559	A495			G270		
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C1163	G1103	C1043	G988	G927	C849	G772	U705	G630	C561	U497			G272		
G1164	G1104	A1044	C989	G928	U850	G773	A706	G631	C562	A498			G273		
C1165	A1105	C1045	C990	G929	G851	G774	A707	A632	C563	G500			G274		
G1166	C1106	A1046	U991	C931	G852	G775	C707	G633	C564	G501			G275		
A1167	C1107	U992	C932	C932	G854	A777	C708	G634	C565	G502			G276		
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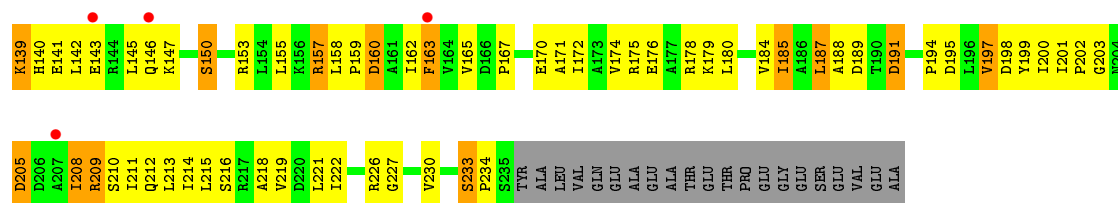


• Molecule 2: 30S Ribosomal Protein S2

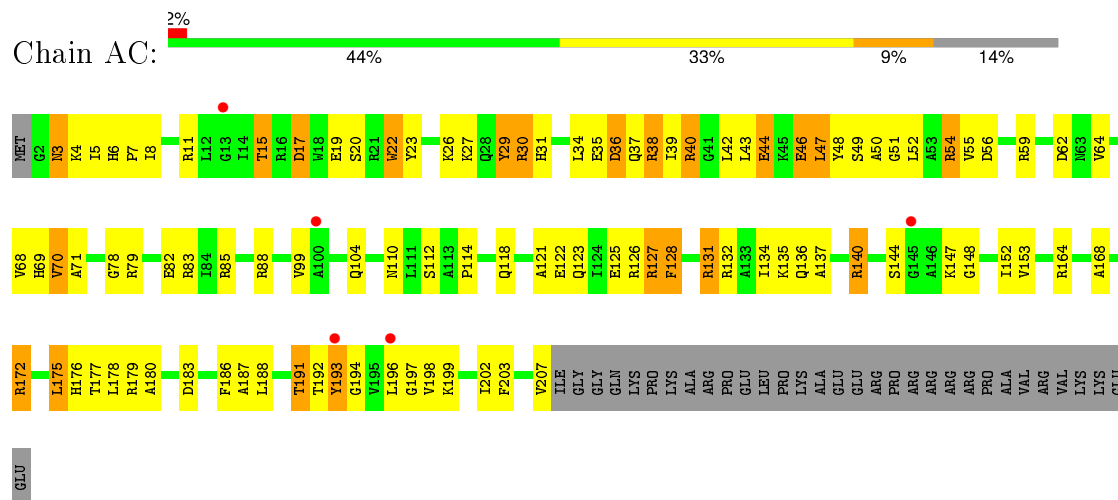


• Molecule 2: 30S Ribosomal Protein S2

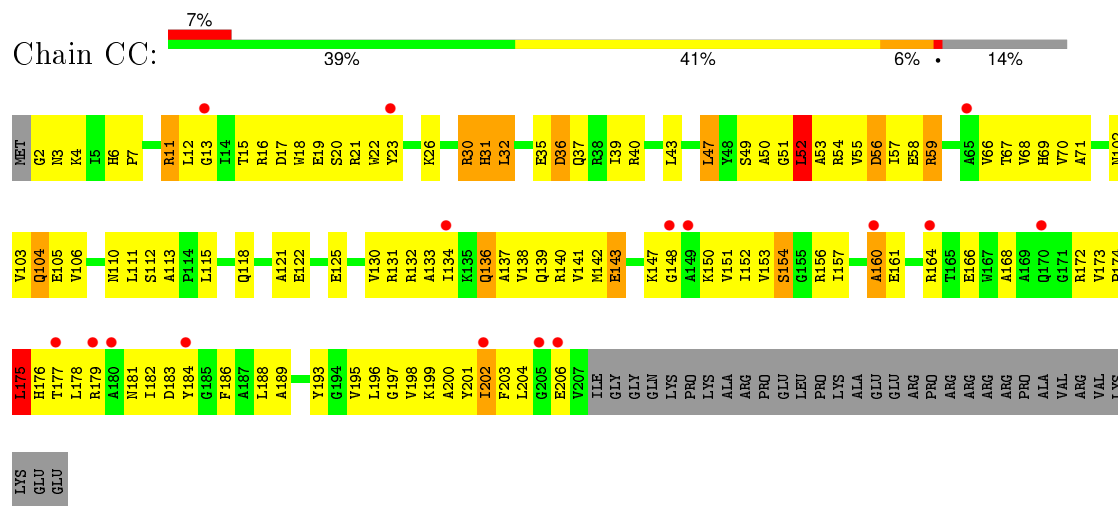




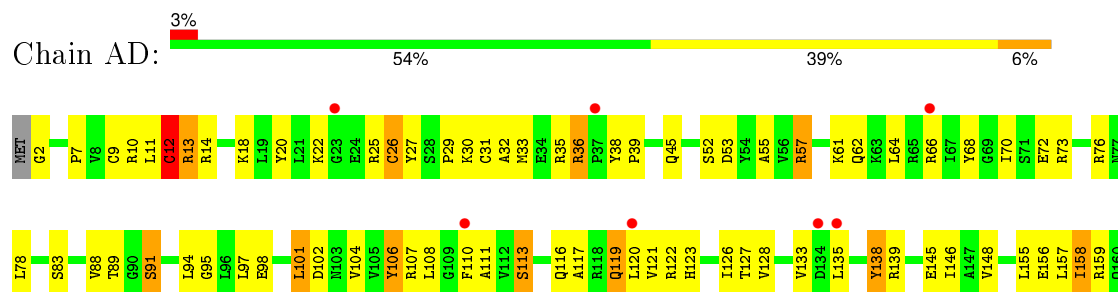
• Molecule 3: 30S Ribosomal Protein S3



• Molecule 3: 30S Ribosomal Protein S3

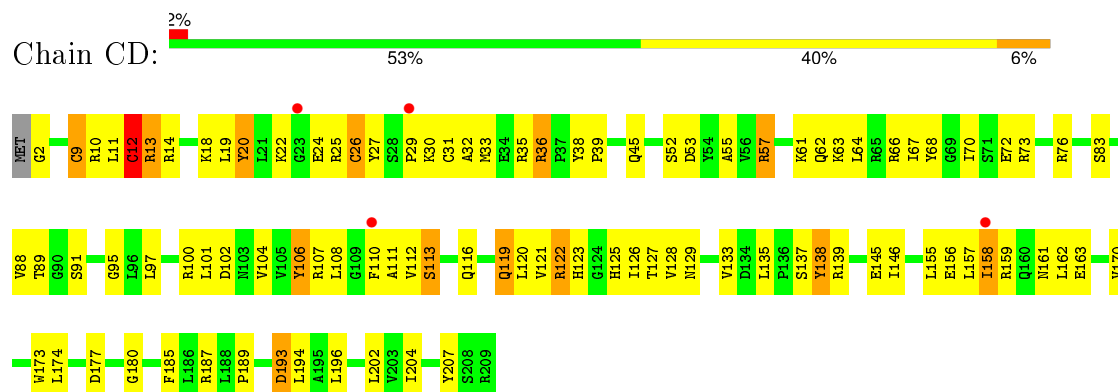


• Molecule 4: 30S Ribosomal Protein S4

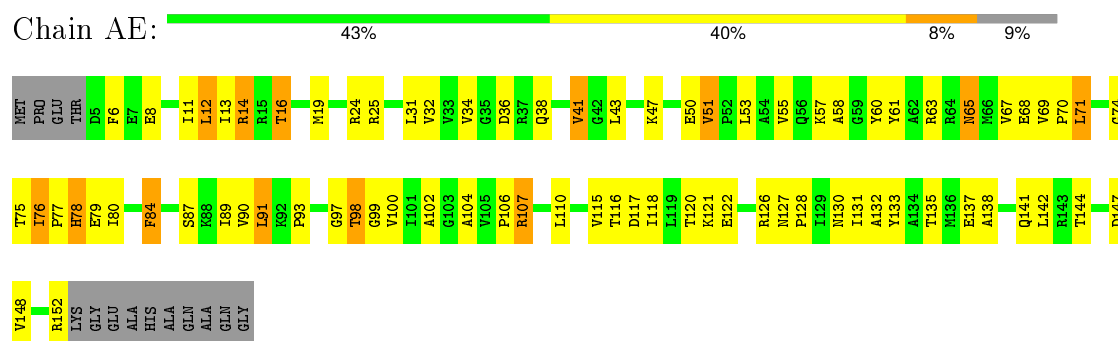




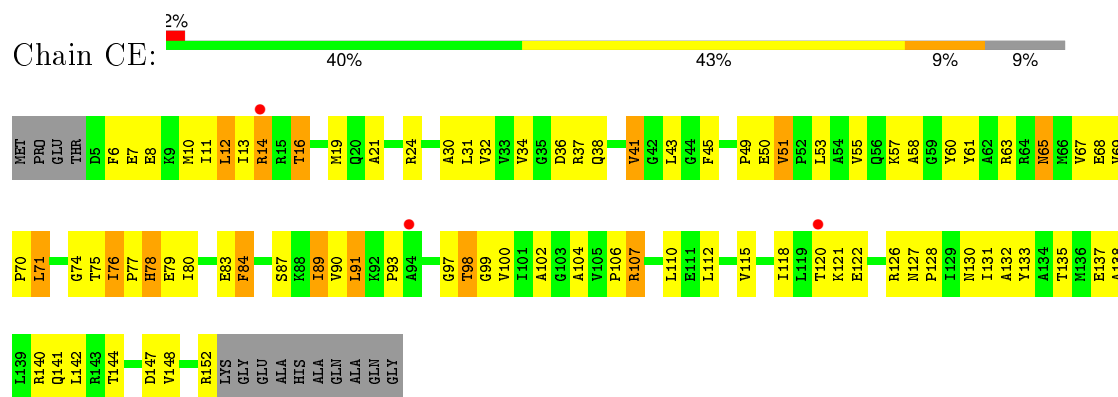
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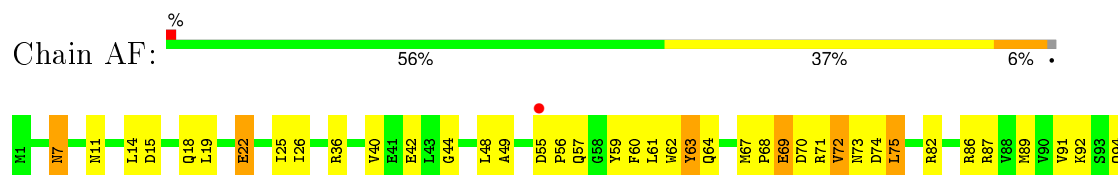
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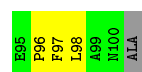


• Molecule 5: 30S Ribosomal Protein S5

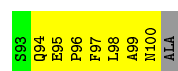
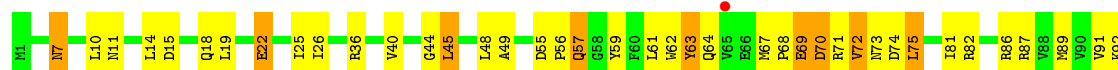


• Molecule 6: 30S Ribosomal Protein S6

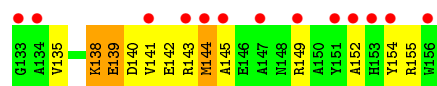
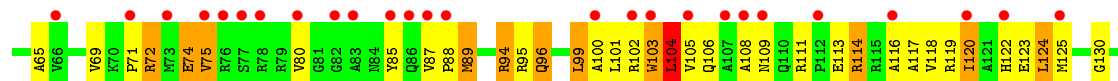
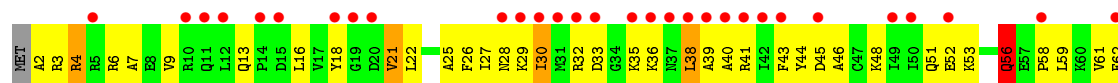
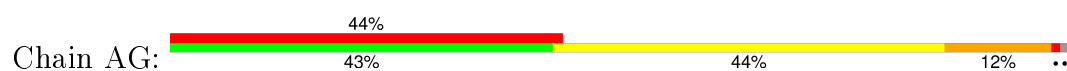




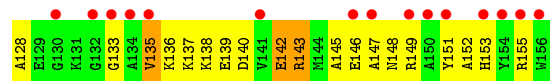
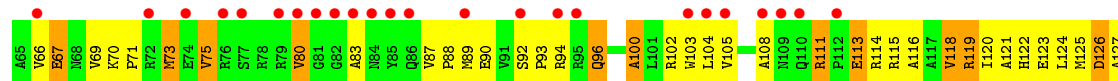
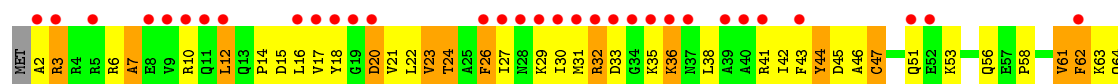
• Molecule 6: 30S Ribosomal Protein S6



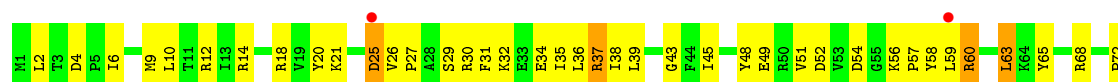
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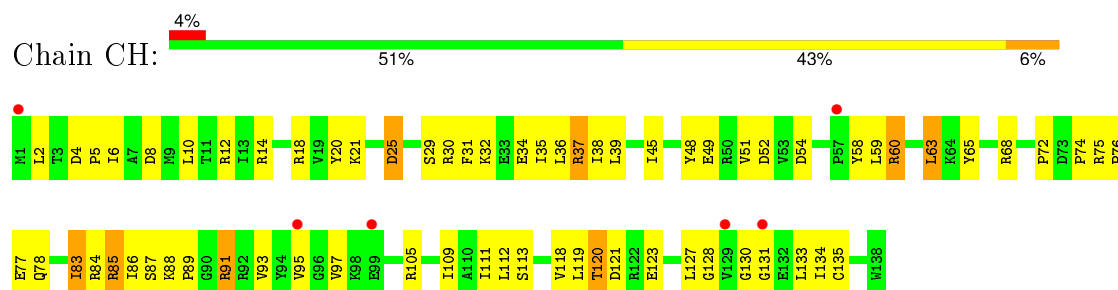
• Molecule 7: 30S Ribosomal Protein S7



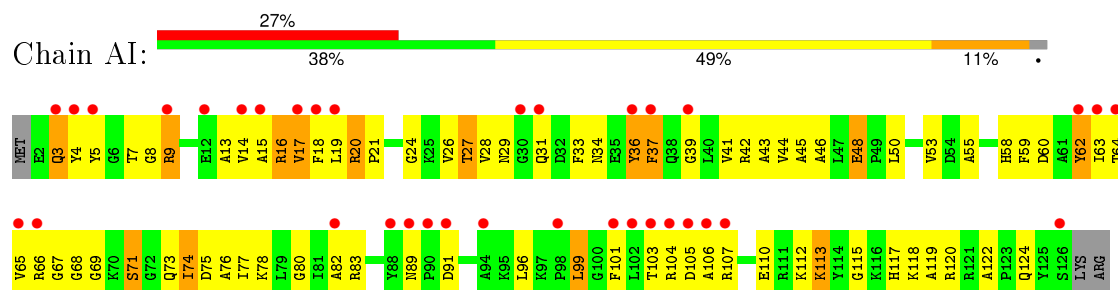
• Molecule 8: 30S Ribosomal Protein S8



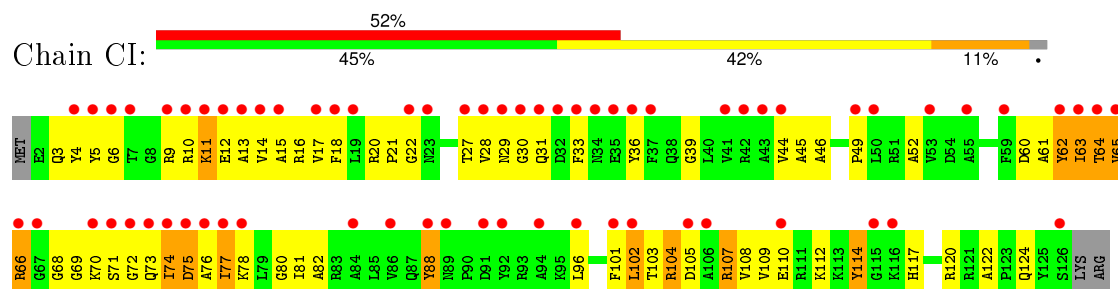
- Molecule 8: 30S Ribosomal Protein S8



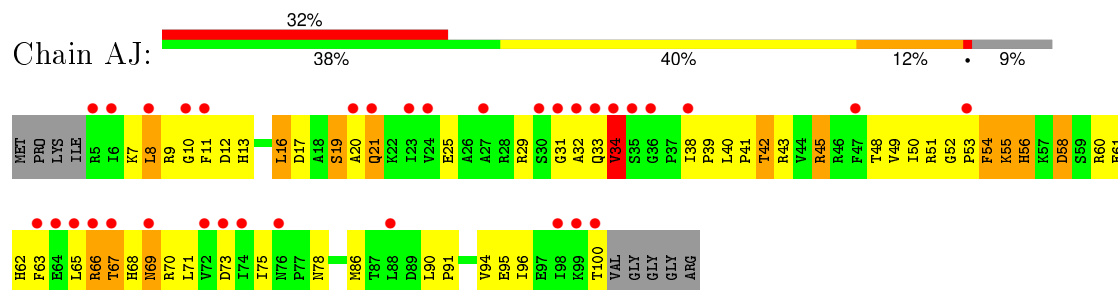
- Molecule 9: 30S Ribosomal Protein S9



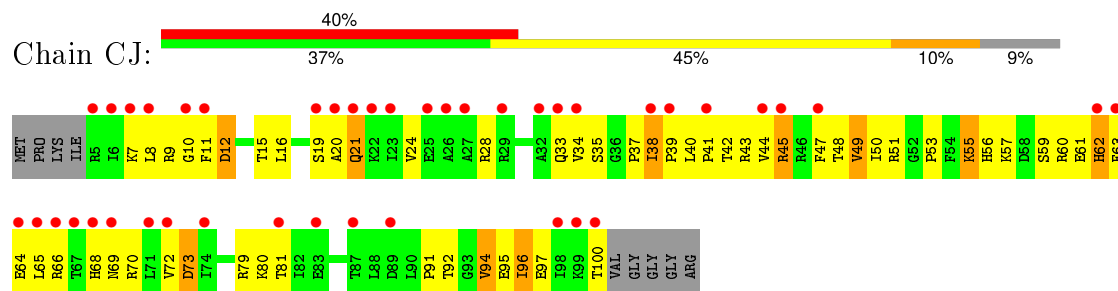
- Molecule 9: 30S Ribosomal Protein S9



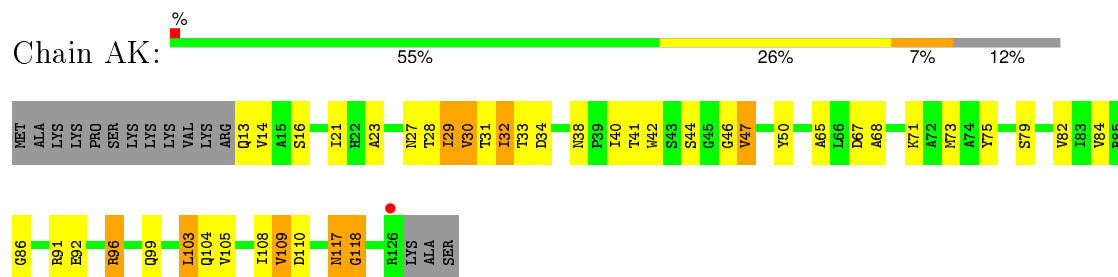
- Molecule 10: 30S Ribosomal Protein S10



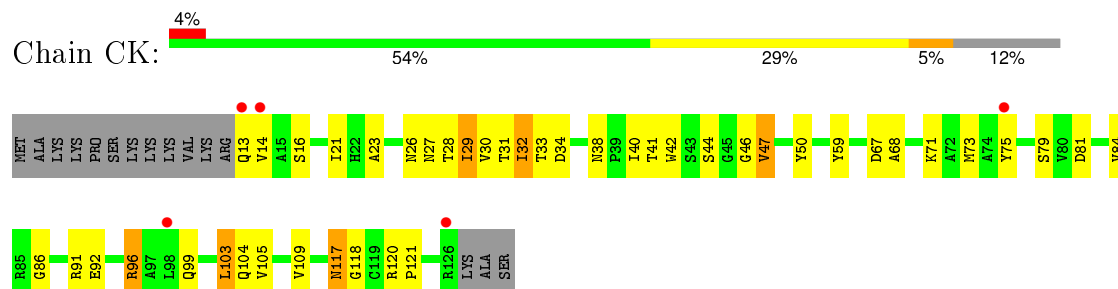
- Molecule 10: 30S Ribosomal Protein S10



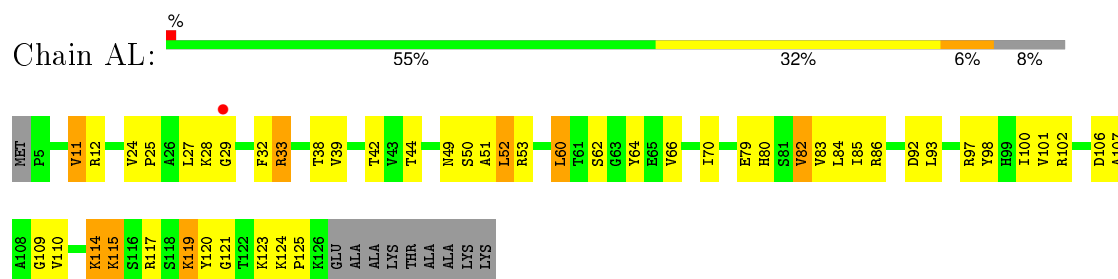
- Molecule 11: 30S Ribosomal Protein S11



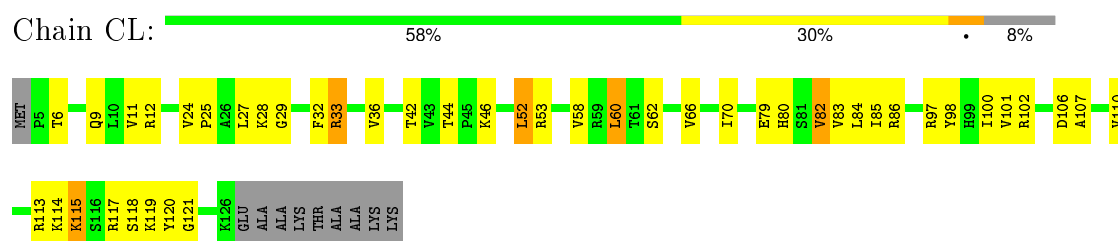
- Molecule 11: 30S Ribosomal Protein S11



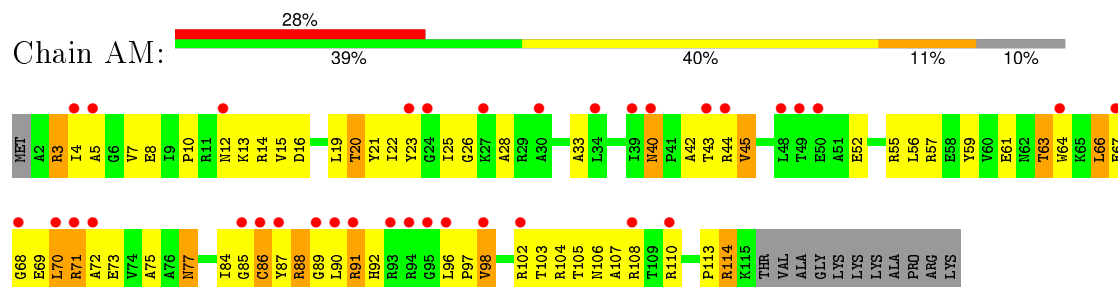
- Molecule 12: 30S Ribosomal Protein S12



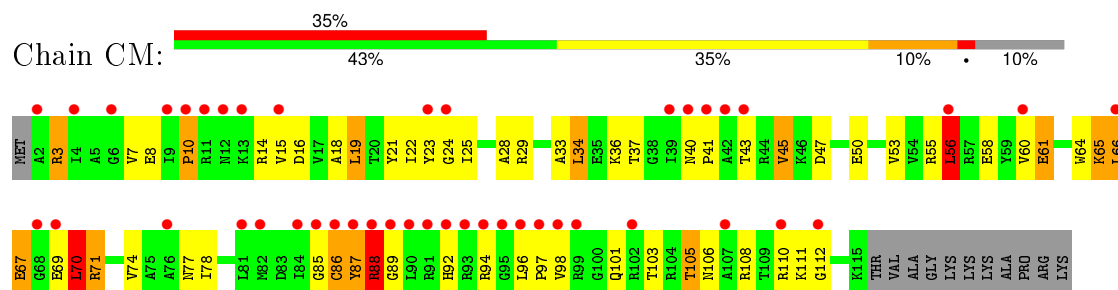
- Molecule 12: 30S Ribosomal Protein S12



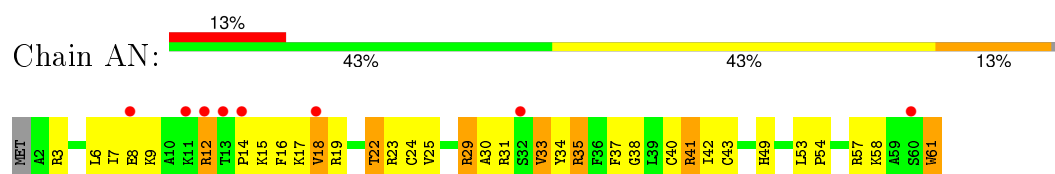
- Molecule 13: 30S Ribosomal Protein S13



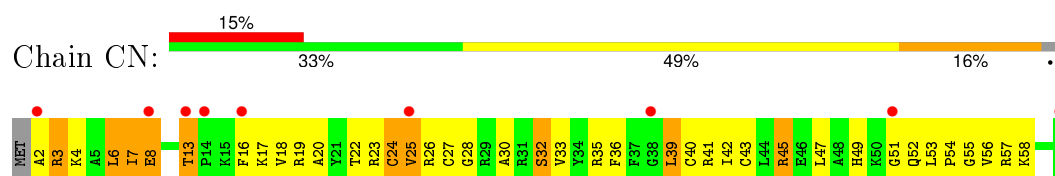
- Molecule 13: 30S Ribosomal Protein S13



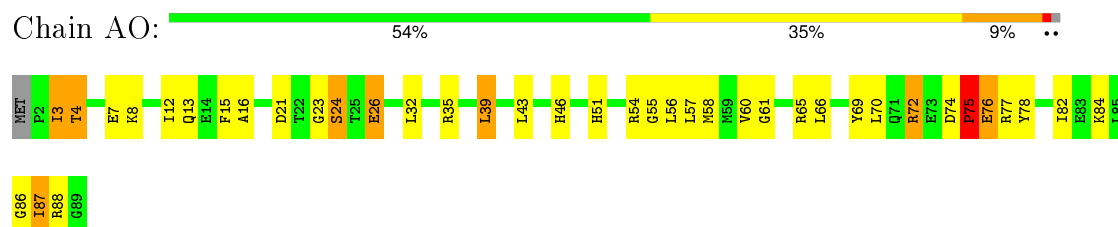
- Molecule 14: 30S Ribosomal Protein S14



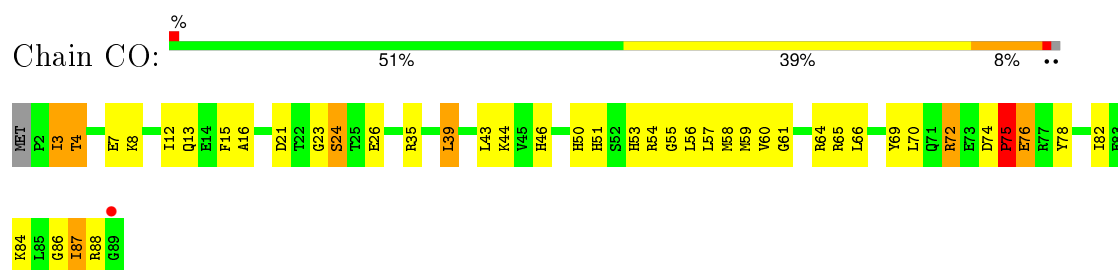
- Molecule 14: 30S Ribosomal Protein S14



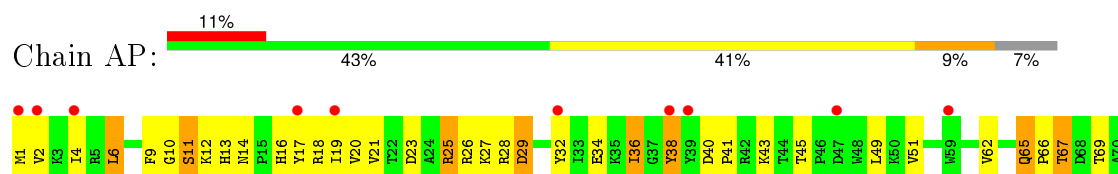
- Molecule 15: 30S Ribosomal Protein S15

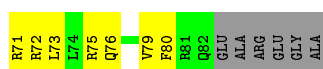


- Molecule 15: 30S Ribosomal Protein S15

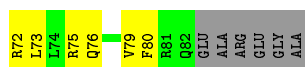
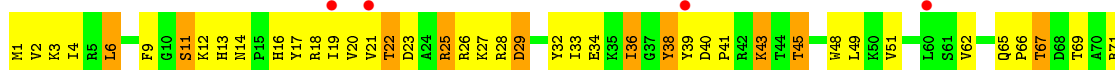
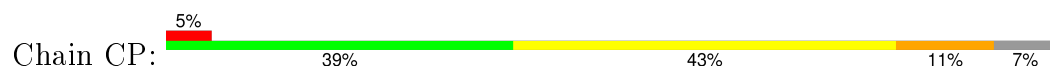


- Molecule 16: 30S Ribosomal Protein S16





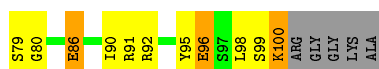
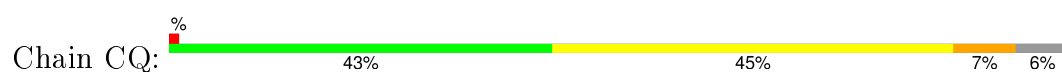
• Molecule 16: 30S Ribosomal Protein S16



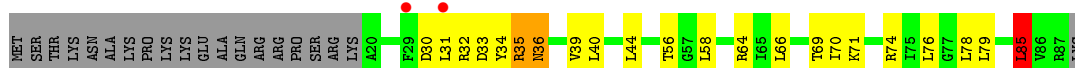
• Molecule 17: 30S Ribosomal Protein S17



• Molecule 17: 30S Ribosomal Protein S17



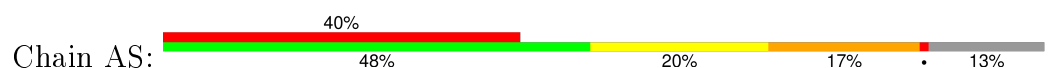
• Molecule 18: 30S Ribosomal Protein S18

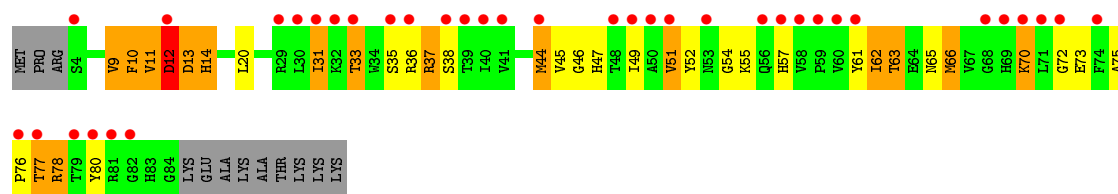


• Molecule 18: 30S Ribosomal Protein S18

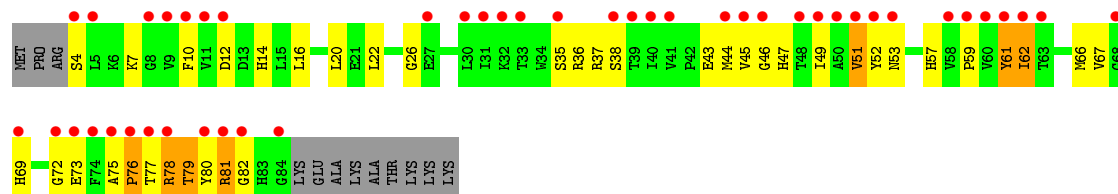


• Molecule 19: 30S Ribosomal Protein S19

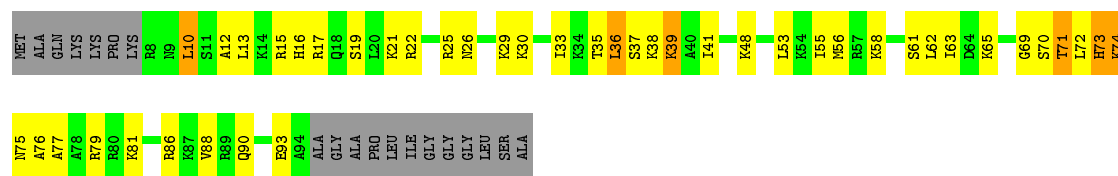




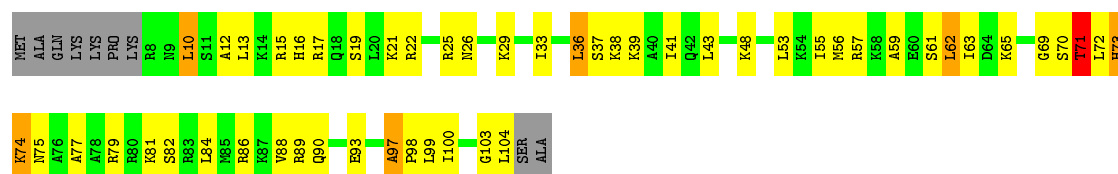
• Molecule 19: 30S Ribosomal Protein S19



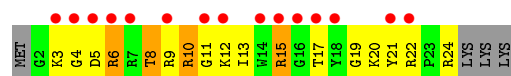
• Molecule 20: 30S Ribosomal Protein S20



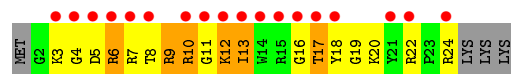
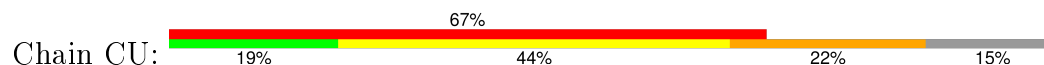
• Molecule 20: 30S Ribosomal Protein S20



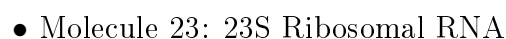
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



• Molecule 22: Probable sigma(54) modulation protein



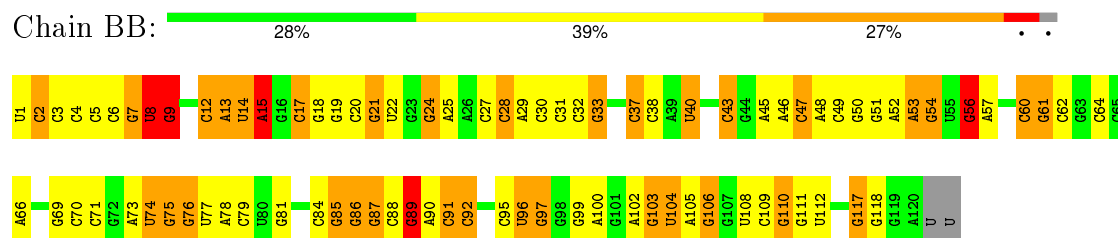
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G1606	A1335	G1393	C1327	G1262	U1198	U1129	G	G938	G938	G864	A800	G739	G674
C1607	G1336	U1394	G1328	G1200	U1199	U1130	G	G939	G939	G801	G801	A675	A675
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G1609	U1338		C1330	U1267	C1202	U1132	A	C1006	A941	G869	U803	G743	A677
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C1615	C1407		G1337	A1272	C1207	G1139	C	U1014	G947	G809	G809	C749	G683
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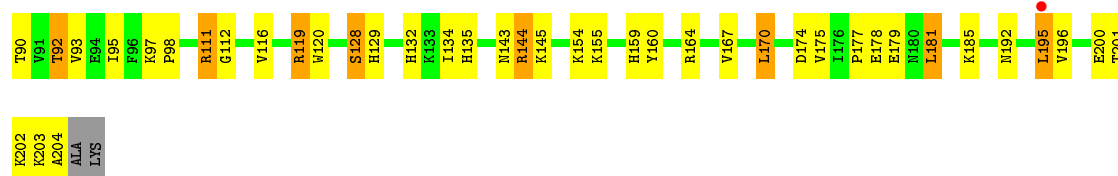
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G1812	G1744	G1649	U1578	C1505	G1425	C1351	G1283	G1212	U1136	G948	C	C1014	C815	C749
G1813	G1746	G1650	A1579	C1506	A1427	U1352	A1284	A1213	G1137		C	G1015	C816	A750
A1814	G1750	G1651	A1580	A1507	G1428	G1355	A1287	G1216	G1138	C951	C	G1016	C817	A751
A1815	C1751	A1652	A1581	A1508	G1429	G1356	C1288	G1219	G1139	G952	A	G1017	G818	A752
G1816	G1752	G1653	C1582	C1509	U1430	U1357	G1289	G1219	C1140	A953	C	C1018	A819	C753
U1817	G1753	G1654	A1583	A1509A	U1431	U1358	C1290	A1220	U1141	C955	C	U1019	A820	C754
A1818	G1755	A1655	C1584	A1509B	G1432	G1358	U1291	U1142	U1142	C956	C	A1020	A821	C755
A1819	G1756	C1656	A1586	G1510	U1433	A1359	U1292	C1222	A1142A	A957	G	U1021	U822	C756
U1820	U1757	C1657	A1587	C1511	A1434	A1360	C1293	G1223		C893	U	G1022	G823	U757
A1821	G1758	G1658	A1588	U1512	G1435	G1361	G1296	G1223	C1153	U958	U	U1023	A824	C758
G1822	A1759	G1659	G1593	C1513	G1436	A1365	C1297	G1225	C1154	U959	U	G1024	C825	G759
G1823	G1760	U1659	G1594	U1514	U1437	A1366	C1298	G1226	A1155	A960	A	G1025	U826	G760
G1826	A1762	C1663	G1595	U1518	G1438	A1367	C1299	C1230	A1156	C965	G	A1027	U828	U762
C1827	G1763	G1668	A1596	G1519	G1439	G1368	G1299	G1231	U1159		A	A1028	A829	G763
A1828	G1764	A1669	A1597	G1520	G1440	G1369	A1301	G1236	G1160	G968	G	A1029	G830	A764
A1829	C1765	C1670	C1598	G1521	G1441	C1370	A1302	G1237	C1161	U969	U	G1030	G831	G765
C1830	C1767	U1671	G1601	G1525	G1442	G1371	G1303	A1237	G1162	C970	C	G1031	U833	U767
U1833	G1772	G1674	U1602	G1526	A1445	U1372	C1304	G1238	G1163	C971	C	A1032	G	G768
U1834	A1773	C1675	A1603	U1529	G1448	A1373	C1305	G1239	G1164	G972	G	U1033	U839	G769
G1835	G1774	C1676	C1604	C1530	A1449	C1375	A1308	U1240	U1165	A973	U	G1034	C840	G770
C1836	U1775	A1677	G1605	C1531	G1450	G1376	G1309	A1241	G1166	G974	A	U1035	A841	G771
C1837	G1776	C1685	G1606	C1532	G1451	G1377	G1310	A1242	U1167	C975	A	G1036	G842	C772
G1838	U1777	U1685	C1607	G	A1452	A1378	G1311	G1243	G1169	G976	U	G1037	G843	U773
G1839	U1778	U1686	A1608	U	U1453	A1379	G1312	G1244	G1170	C977	A	C1038	C844	A774
G1840	U1779	U1688	A1609	A	G1455	A1380	U1313	A1247	G1171	G978	C	G1039	C845	G776
C1843	A1780	A1689	C1610	C	G1456	G1381	C1314	G1248	G	G979	C	C1040	C846	G776
G1844	C1781	U1692	C1611	G1537	G1459	G1382	C1315	U1249	A	U981	U	C1041	U847	A777
G1845	G1782	U1693	G1612	G1538	G1460	C1383	U1316	G1250	U982	A81	C	C1043	G848	
G1846	A1783	C1694	A1613	G1539	C1464	A1384	A1317	G1251	A	C982	C	A1045	A849	A781
A1847	U1784	U1540	A1614	U1540	G1465	G1385	C1318	G1252	G1178	C983	U	G1046	C850	A783
A1848	A1785	G1695	C1615	G1541	G1466	C1386	G1319	A1253	C1179	A984	G	A1047	G853	A784
G1849	G1786	G1696	A1616	A1542	C1467	C1387	C1320	U1254	C1180	C985	G	G1047	C	A785
G1850	A1787	C1697	C1617	C1543	G1467	G1388	A1321	U1255	C1181	C986	C	A1048	C856	C786
G1851	C1788	A1698	A1618	A1544	G1470	G1388	A1322	G1256	C1185	C987	C	C1049	C857	U787
G1852	A1789	G1699	A1619	A1545	A1471	U1391	A1325	G1257	G1186	A988	C	A1050	U858	A788
G1790	A1700	C1546	C1546	C1546	A1472		G1325	C1258	G1187	C989	C	G1051	C859	A789
A1791	A1701	C1547	C1548	C1548	A1477	U1394	U1326	C1261	C1188	A990	C	C1052	U860	C790
G1792	G1702	G1553	A1553	A1553	G1478	U1395	C1327	U1261	A1189	C991	A	C	A861	C791
G1793	G1703	G1554	A1554	A1554	U1481	U1396	G1328	G1264	G1190	C992	G	A	G862	G792
G1794	G1704	G1627	G1628	G1628	U1482	C1403	U1329	A1265	G1191	C993	G	G	A863	A793
U1796	U1709	U1629	U1629	U1629	G1482	U1404	C1330	G1266	G1192	C994	G	A	G864	G794
C1797	C1710	C1557	C1557	C1557	G1484	U1405	G1332	U1267	G1193	C995	A	G	C865	C795
U1798	C1711	A1558	A1558	A1558	G1485	U1406	C1333	A1268		A996	G	G	A866	C796
G1799	C1712	G1559	G1559	G1559	G1486	U1407	C1333	G1268	G1120	C997	G	G	C867	C797
A1799	G1712	G1560	G1560	G1560	U1488	C1408	A1336	A1269	C1121	C998	U	U	U868	A802
G1800	U1713	G1635	G1635	G1635	G1489	C1408	G1337	C1270	G1122	C935	U	U	G869	U803
G1801	G1714	A1636	A1636	A1636	U1490	U1415	G1338	G1271	C1201	A1001	C	G	A870	A804
A1802	G1717	C1564	C1564	C1564	A1490	G1416	G1339	A1272	C1202	G1002	C	G	G873	G805
A1803	G1718	C1565	C1565	C1565	C1493	G1417	G1339	U1273	G1203	G1003	C	C	G874	C806
U1804	C1804	A1567	A1567	A1567	U1494	G1418	U1340	A1276	A1204	C1005	U	U	U807	
A1805	G1721	A1567	A1567	A1567	A1494	A1418	U1341	G1277	A1127	C1006	A	A	A878	A808
G1806	A1722	A1568	A1568	A1568	A1495	A1419	A1342		G1206					

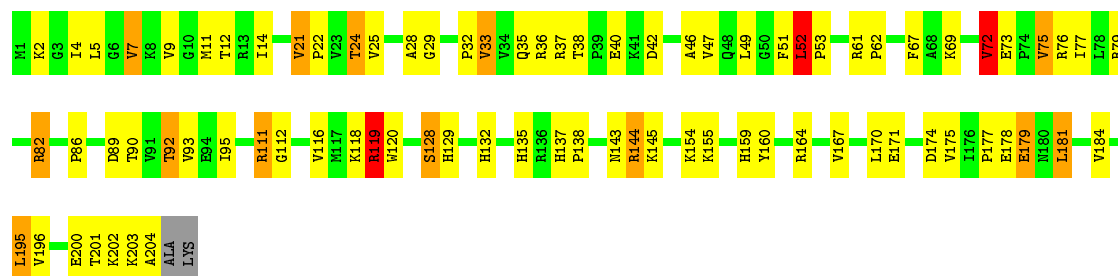
- Molecule 24: 5S Ribosomal RNA





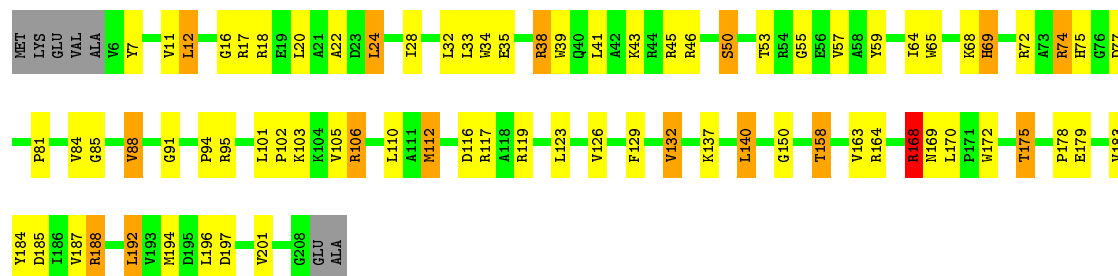
• Molecule 26: 50S Ribosomal Protein L3

Chain DE: 59% 32% 6% ..



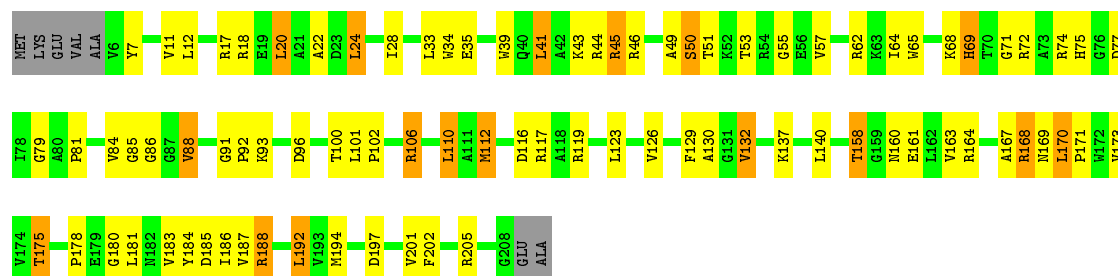
• Molecule 27: 50S Ribosomal Protein L4

Chain BF: 60% 29% 7% .



• Molecule 27: 50S Ribosomal Protein L4

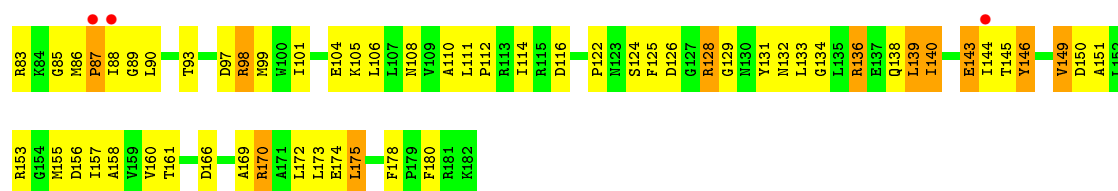
Chain DF: 55% 33% 8% .



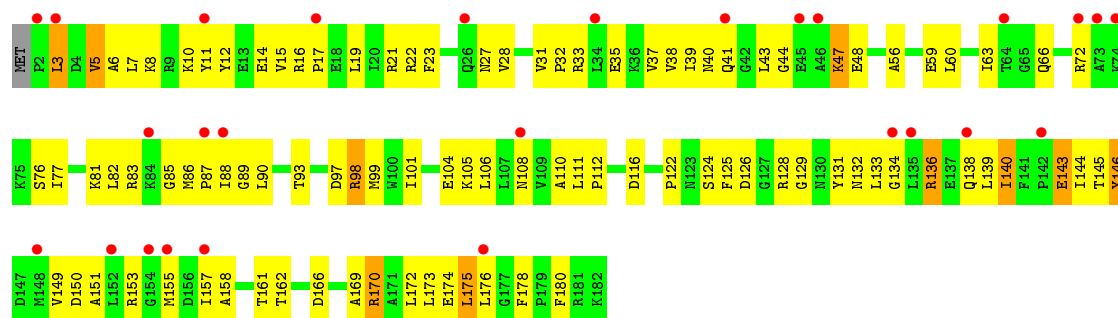
• Molecule 28: 50S Ribosomal Protein L5

Chain BG: 4% 46% 46% 8% .

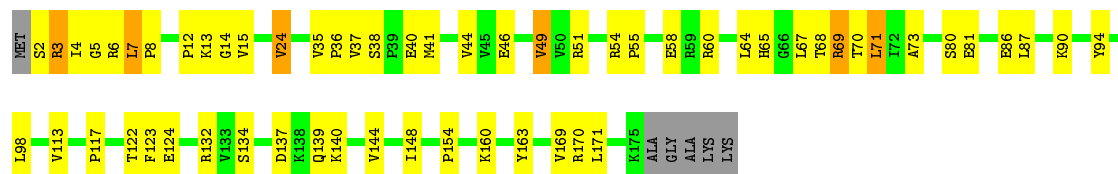




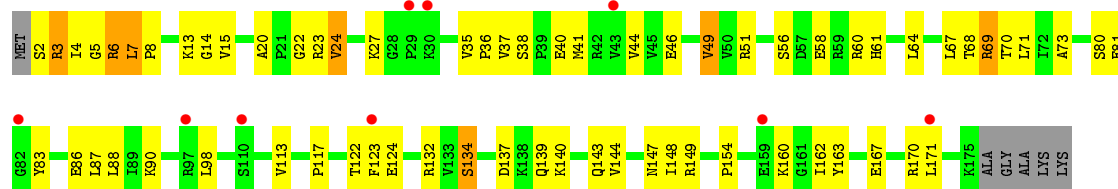
• Molecule 28: 50S Ribosomal Protein L5



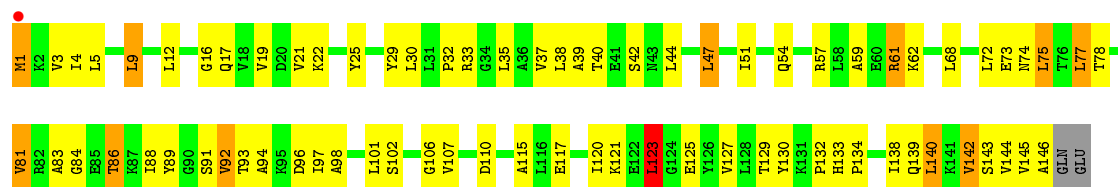
• Molecule 29: 50S Ribosomal Protein L6



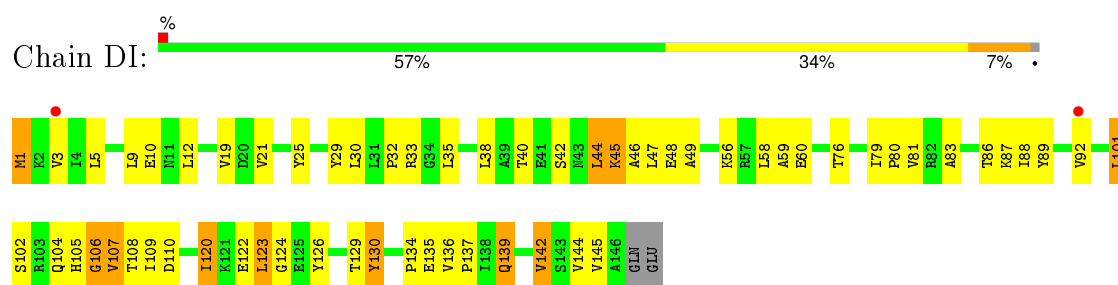
• Molecule 29: 50S Ribosomal Protein L6



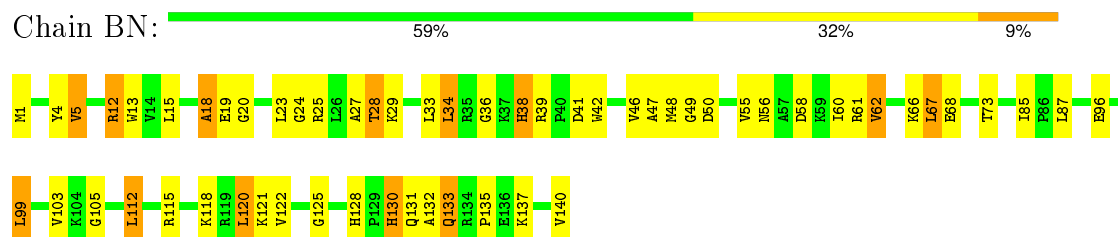
• Molecule 30: 50S Ribosomal Protein L9



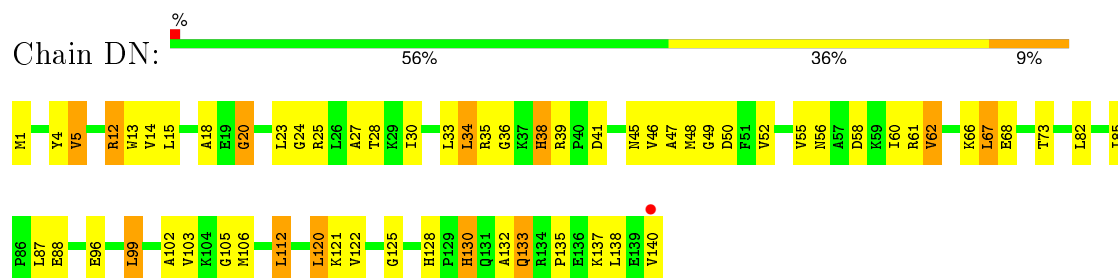
• Molecule 30: 50S Ribosomal Protein L9



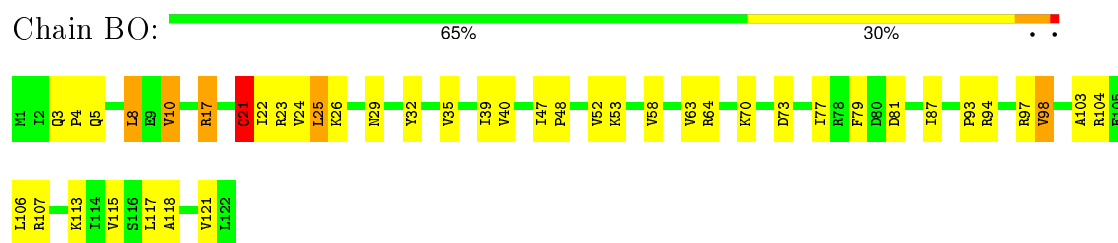
• Molecule 31: 50S Ribosomal Protein L13



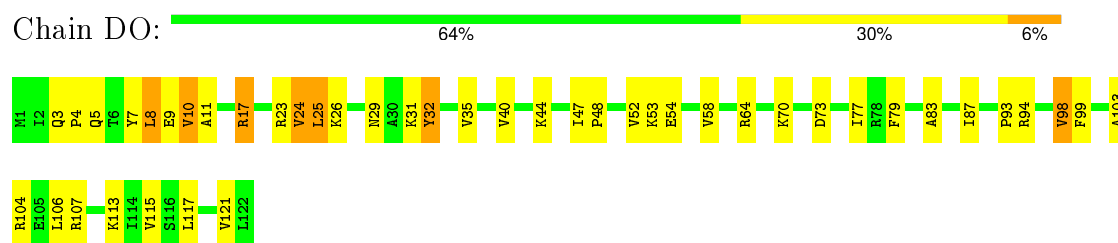
• Molecule 31: 50S Ribosomal Protein L13



• Molecule 32: 50S Ribosomal Protein L14

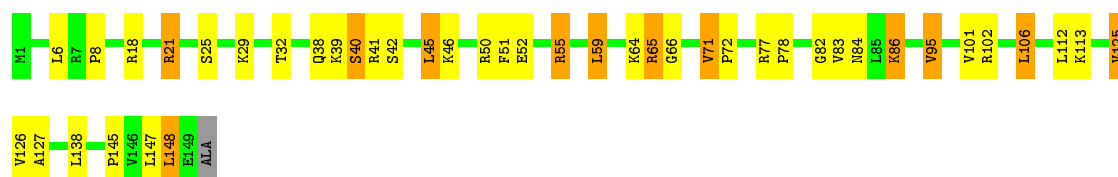


• Molecule 32: 50S Ribosomal Protein L14

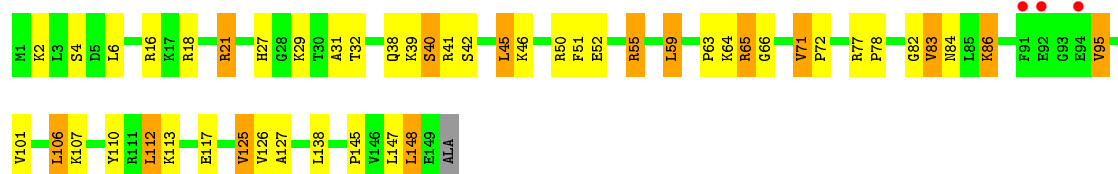


• Molecule 33: 50S Ribosomal Protein L15

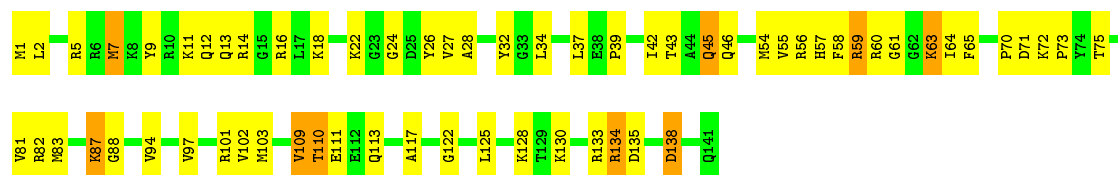




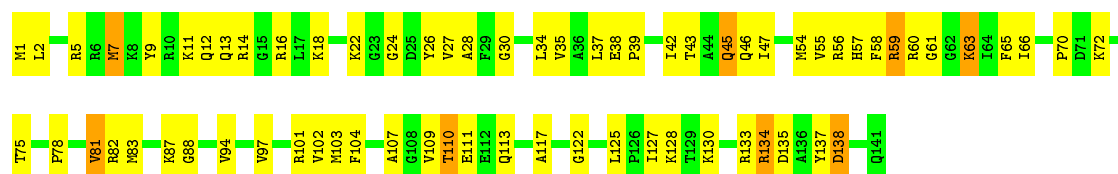
• Molecule 33: 50S Ribosomal Protein L15



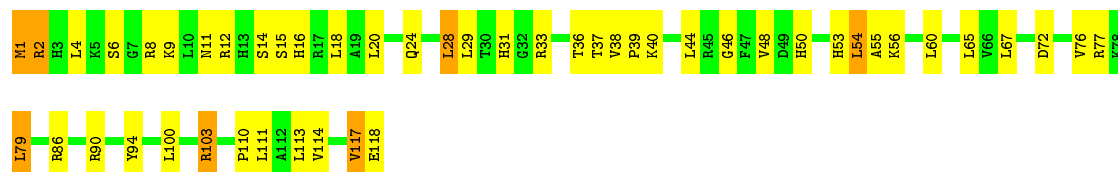
• Molecule 34: 50S Ribosomal Protein L16



• Molecule 34: 50S Ribosomal Protein L16



• Molecule 35: 50S Ribosomal Protein L17



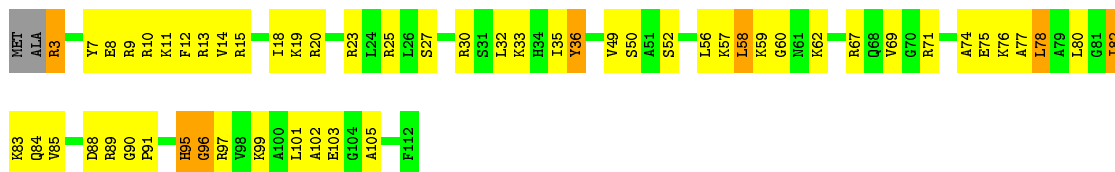
• Molecule 35: 50S Ribosomal Protein L17





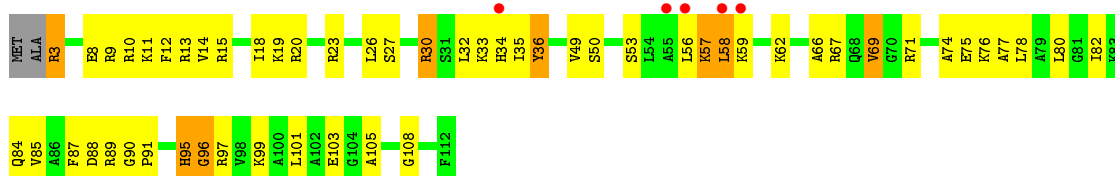
• Molecule 36: 50S Ribosomal Protein L18

Chain BS: 49% 43% 6%



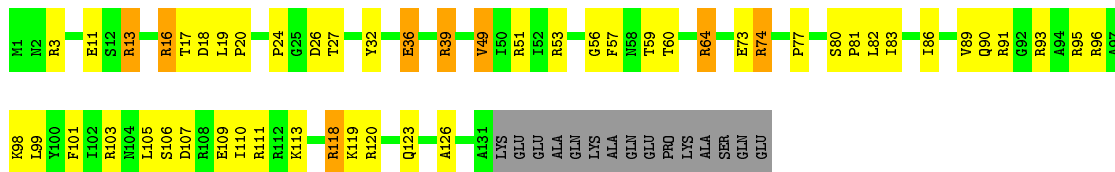
• Molecule 36: 50S Ribosomal Protein L18

Chain DS: 49% 42% 7%



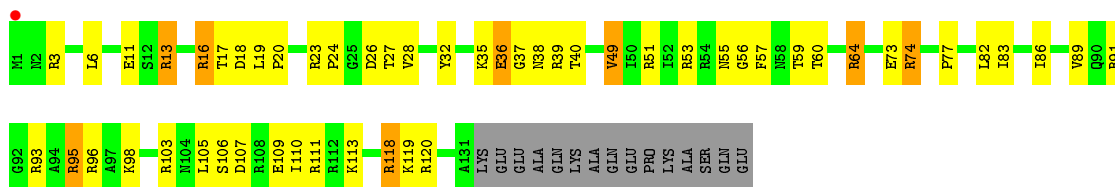
• Molecule 37: 50S Ribosomal Protein L19

Chain BT: 54% 30% 5% 10%



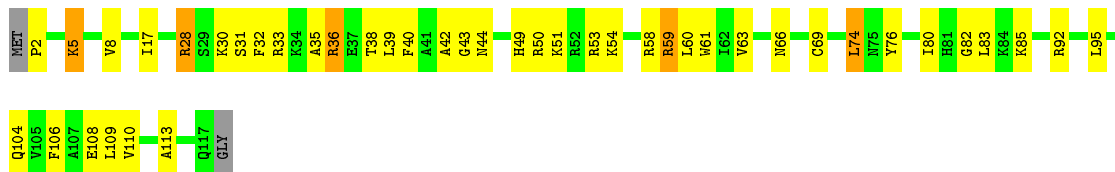
• Molecule 37: 50S Ribosomal Protein L19

Chain DT: 53% 31% 5% 10%

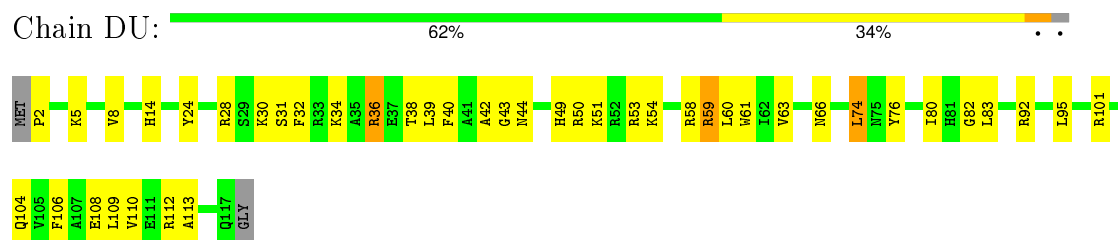


• Molecule 38: 50S Ribosomal Protein L20

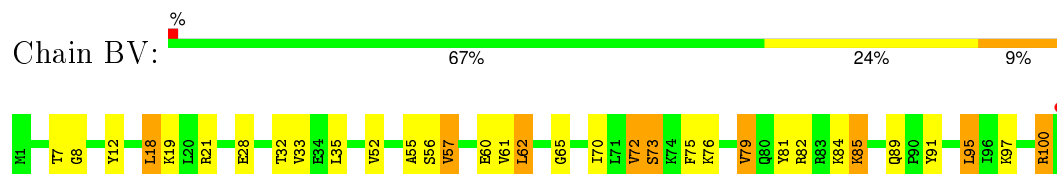
Chain BU: 62% 32%



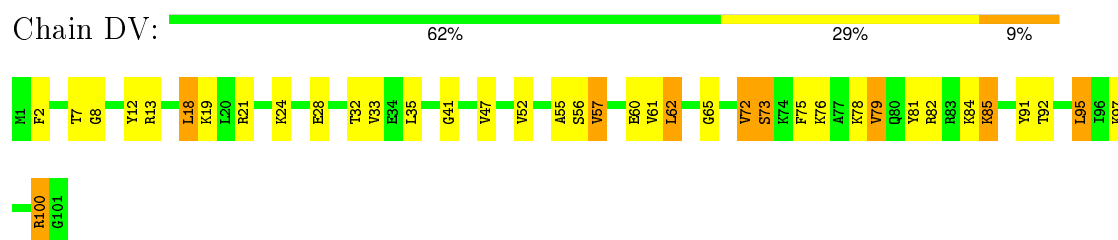
- Molecule 38: 50S Ribosomal Protein L20



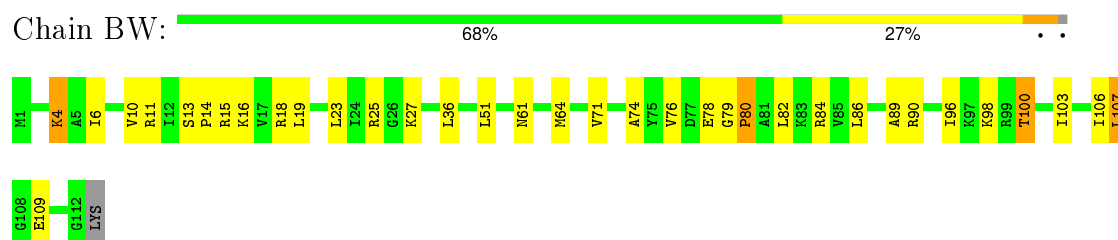
- Molecule 39: 50S Ribosomal Protein L21



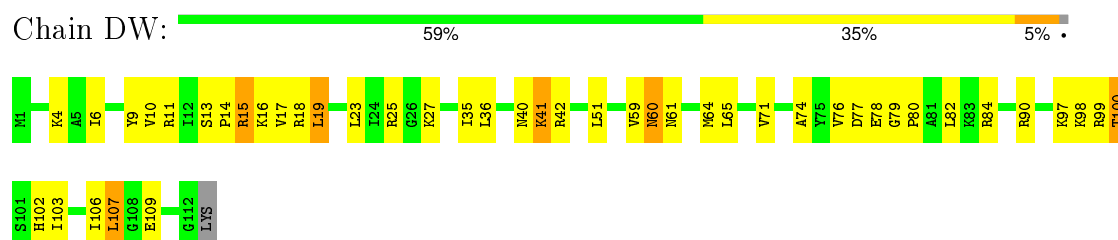
- Molecule 39: 50S Ribosomal Protein L21



- Molecule 40: 50S Ribosomal Protein L22

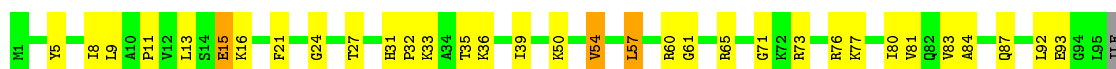


- Molecule 40: 50S Ribosomal Protein L22



- Molecule 41: 50S Ribosomal Protein L23





- Molecule 41: 50S Ribosomal Protein L23

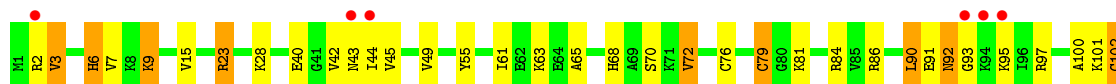


- Molecule 42: 50S Ribosomal Protein L24



THR
GLU
GLU

- Molecule 42: 50S Ribosomal Protein L24



G103
G104
D107
THR
GLU
GLU

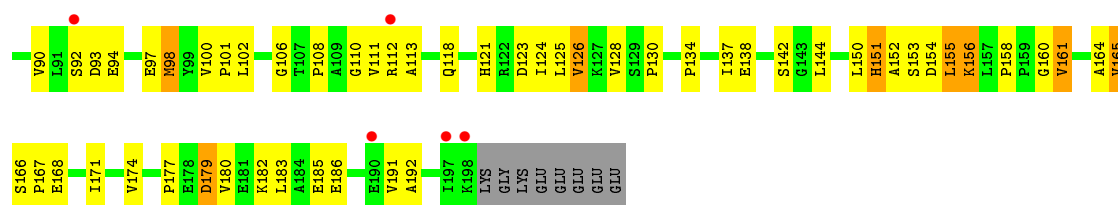
- Molecule 43: 50S Ribosomal Protein L25



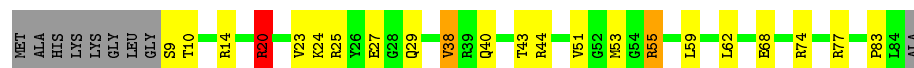
E185
E186
V191
A192
K199
G200
K201
GLU
GLU
GLU
GLU

- Molecule 43: 50S Ribosomal Protein L25





• Molecule 44: 50S Ribosomal Protein L27



• Molecule 44: 50S Ribosomal Protein L27



• Molecule 45: 50S Ribosomal Protein L28



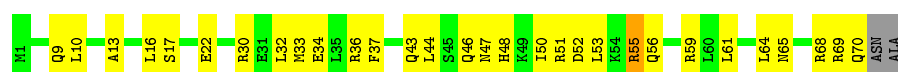
• Molecule 45: 50S Ribosomal Protein L28



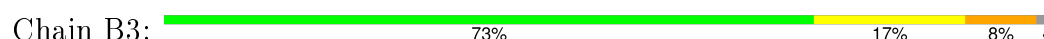
• Molecule 46: 50S Ribosomal Protein L29



• Molecule 46: 50S Ribosomal Protein L29



• Molecule 47: 50S Ribosomal Protein L30

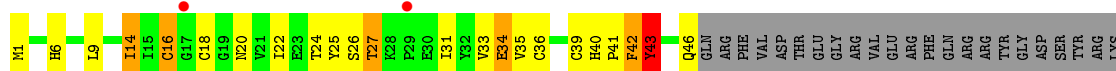




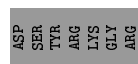
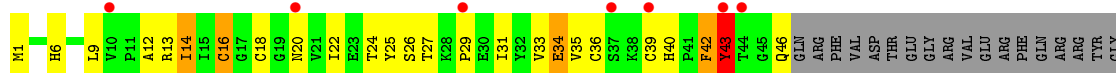
- Molecule 47: 50S Ribosomal Protein L30



- Molecule 48: 50S Ribosomal Protein L31



- Molecule 48: 50S Ribosomal Protein L31



- Molecule 49: 50S Ribosomal Protein L32



- Molecule 49: 50S Ribosomal Protein L32



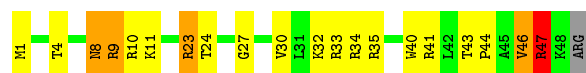
- Molecule 50: 50S Ribosomal Protein L33



- Molecule 50: 50S Ribosomal Protein L33



- Molecule 51: 50S Ribosomal Protein L34



- Molecule 51: 50S Ribosomal Protein L34



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 53: 50S Ribosomal Protein L36



- Molecule 53: 50S Ribosomal Protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.216 , 0.258 0.214 , 0.257	Depositor DCC
R_{free} test set	49855 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	286308	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	1.14	57/36123 (0.2%)	1.54	760/56379 (1.3%)
1	CA	1.11	53/36028 (0.1%)	1.55	750/56231 (1.3%)
2	AB	0.69	0/1822	0.79	1/2468 (0.0%)
2	CB	0.75	0/1809	0.79	1/2450 (0.0%)
3	AC	0.80	0/1474	0.88	0/2003
3	CC	0.78	0/1474	0.86	2/2003 (0.1%)
4	AD	0.68	2/1556 (0.1%)	0.87	3/2113 (0.1%)
4	CD	0.72	2/1556 (0.1%)	0.87	3/2113 (0.1%)
5	AE	0.61	0/1121	0.80	1/1517 (0.1%)
5	CE	0.63	0/1121	0.82	1/1517 (0.1%)
6	AF	0.59	0/790	0.73	0/1077
6	CF	0.62	0/790	0.73	0/1077
7	AG	1.04	0/1183	0.98	2/1599 (0.1%)
7	CG	0.96	0/1183	0.90	0/1599
8	AH	0.57	0/1065	0.73	0/1445
8	CH	0.58	0/1065	0.75	0/1445
9	AI	0.92	0/867	0.92	0/1180
9	CI	1.00	0/867	0.91	1/1180 (0.1%)
10	AJ	0.83	0/676	0.91	1/924 (0.1%)
10	CJ	0.90	0/676	0.97	0/924
11	AK	0.62	0/843	0.75	1/1144 (0.1%)
11	CK	0.61	0/843	0.75	1/1144 (0.1%)
12	AL	0.63	0/921	0.78	0/1247
12	CL	0.64	0/921	0.80	0/1247
13	AM	1.02	0/814	1.00	0/1107
13	CM	1.03	0/814	1.03	2/1107 (0.2%)
14	AN	0.76	0/487	0.90	0/649
14	CN	0.77	1/487 (0.2%)	0.87	1/649 (0.2%)
15	AO	0.62	0/735	0.84	0/981
15	CO	0.66	0/735	0.85	0/981
16	AP	0.63	0/667	0.82	0/905
16	CP	0.56	0/667	0.82	0/905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.66	0/836	0.84	0/1117
17	CQ	0.69	1/836 (0.1%)	0.85	0/1117
18	AR	0.59	0/519	0.76	1/699 (0.1%)
18	CR	0.63	0/519	0.76	1/699 (0.1%)
19	AS	0.96	0/574	0.87	0/781
19	CS	0.98	0/574	0.93	0/781
20	AT	0.63	0/666	0.79	0/880
20	CT	0.62	0/715	0.84	1/947 (0.1%)
21	AU	0.82	0/203	0.92	0/266
21	CU	0.91	0/203	0.97	0/266
22	AX	0.69	0/637	0.84	1/864 (0.1%)
22	CX	0.77	0/606	0.82	0/828
23	BA	1.58	572/68445 (0.8%)	1.72	2187/106848 (2.0%)
23	DA	1.21	155/67893 (0.2%)	1.65	1848/105980 (1.7%)
24	BB	1.13	6/2878 (0.2%)	1.53	60/4490 (1.3%)
24	DB	1.13	2/2878 (0.1%)	1.52	49/4490 (1.1%)
25	BD	0.90	1/2185 (0.0%)	0.91	4/2942 (0.1%)
25	DD	0.82	0/2186	0.91	2/2944 (0.1%)
26	BE	0.90	0/1588	0.92	0/2145
26	DE	0.78	0/1588	0.92	3/2145 (0.1%)
27	BF	0.91	0/1615	0.95	3/2188 (0.1%)
27	DF	0.74	0/1615	0.92	2/2188 (0.1%)
28	BG	0.61	0/1393	0.79	0/1892
28	DG	0.72	0/1393	0.81	0/1892
29	BH	0.72	0/1343	0.82	1/1820 (0.1%)
29	DH	0.66	0/1343	0.81	0/1820
30	BI	0.64	0/1052	0.87	1/1441 (0.1%)
30	DI	0.63	0/967	0.84	1/1334 (0.1%)
31	BN	0.87	0/1139	0.87	0/1538
31	DN	0.71	0/1139	0.89	1/1538 (0.1%)
32	BO	0.87	1/933 (0.1%)	0.88	1/1257 (0.1%)
32	DO	0.73	0/933	0.83	1/1257 (0.1%)
33	BP	0.84	0/1148	0.91	1/1529 (0.1%)
33	DP	0.73	0/1148	0.89	1/1529 (0.1%)
34	BQ	0.84	0/1143	0.87	1/1527 (0.1%)
34	DQ	0.74	0/1143	0.86	0/1527
35	BR	0.80	0/982	0.92	0/1312
35	DR	0.75	0/982	0.92	1/1312 (0.1%)
36	BS	0.67	0/875	0.88	1/1168 (0.1%)
36	DS	0.69	0/875	0.87	1/1168 (0.1%)
37	BT	0.83	0/1077	0.92	0/1444
37	DT	0.73	0/1077	0.90	0/1444
38	BU	1.00	1/977 (0.1%)	0.87	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	0.79	0/977	0.86	0/1301
39	BV	0.85	0/782	0.92	0/1049
39	DV	0.77	0/782	0.85	0/1049
40	BW	1.02	0/891	0.91	0/1197
40	DW	0.87	0/891	0.91	1/1197 (0.1%)
41	BX	0.91	0/756	0.88	2/1016 (0.2%)
41	DX	0.78	0/756	0.86	1/1016 (0.1%)
42	BY	0.80	1/798 (0.1%)	0.88	0/1073
42	DY	0.73	1/798 (0.1%)	0.89	0/1073
43	BZ	0.70	0/1569	0.82	1/2137 (0.0%)
43	DZ	0.72	0/1555	0.81	1/2118 (0.0%)
44	B0	0.85	0/602	0.92	1/804 (0.1%)
44	D0	0.78	0/602	0.92	0/804
45	B1	0.85	0/752	0.90	2/1003 (0.2%)
45	D1	0.80	0/752	0.89	1/1003 (0.1%)
46	B2	0.82	0/590	0.86	0/781
46	D2	0.79	0/590	0.86	0/781
47	B3	0.76	0/463	0.84	1/623 (0.2%)
47	D3	0.69	0/463	0.81	0/623
48	B4	0.68	0/358	0.84	1/487 (0.2%)
48	D4	0.85	0/358	0.83	1/487 (0.2%)
49	B5	0.93	1/469 (0.2%)	1.00	0/634
49	D5	0.86	1/469 (0.2%)	0.96	0/634
50	B6	0.93	2/456 (0.4%)	0.84	0/609
50	D6	0.75	0/456	0.87	2/609 (0.3%)
51	B7	1.03	1/426 (0.2%)	1.12	1/561 (0.2%)
51	D7	0.88	0/426	1.01	1/561 (0.2%)
52	B8	0.96	0/516	0.94	1/679 (0.1%)
52	D8	0.76	0/516	0.90	0/679
53	B9	0.79	0/300	0.95	0/395
53	D9	0.71	0/300	0.90	0/395
All	All	1.18	861/305420 (0.3%)	1.47	5724/457343 (1.3%)

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
2	AB	0	3
2	CB	0	4
3	AC	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	1
4	AD	0	1
4	CD	0	1
7	CG	0	2
9	AI	0	1
9	CI	0	1
10	AJ	0	2
10	CJ	0	2
13	AM	0	4
13	CM	0	2
14	AN	0	1
15	AO	0	1
15	CO	0	1
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
19	CS	0	1
20	AT	0	1
20	CT	0	1
23	BA	0	1
23	DA	0	1
26	BE	0	1
26	DE	0	1
27	DF	0	1
30	DI	0	1
34	BQ	0	1
34	DQ	0	1
36	BS	0	1
36	DS	0	1
41	BX	0	1
41	DX	0	1
43	BZ	0	3
43	DZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	1
48	D4	0	1
All	All	0	56

The worst 5 of 861 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1442(A)	G	N9-C4	17.19	1.51	1.38
1	AA	1442(A)	G	N9-C4	15.23	1.50	1.38
1	AA	1442(A)	G	C2-N3	15.04	1.44	1.32
1	CA	1442(A)	G	C2-N3	14.30	1.44	1.32
1	AA	1442(A)	G	N3-C4	13.24	1.44	1.35

The worst 5 of 5724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-26.14	115.53	128.60
23	DA	2296	U	N3-C4-O4	-25.95	101.23	119.40
1	AA	1442(A)	G	N3-C4-C5	-25.64	115.78	128.60
1	CA	1442(A)	G	N3-C4-N9	25.18	141.10	126.00
1	AA	1442(A)	G	N3-C4-N9	25.11	141.07	126.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	129	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	19	GLU	Peptide
3	AC	51	GLY	Peptide

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	32270	0	16286	1214	0
1	CA	32185	0	16244	1267	1
2	AB	1787	0	1752	122	0
2	CB	1775	0	1743	121	0
3	AC	1450	0	1314	92	0
3	CC	1450	0	1314	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1526	0	1415	71	0
4	CD	1526	0	1415	85	0
5	AE	1105	0	1130	56	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	31	0
6	CF	777	0	737	35	0
7	AG	1164	0	1106	87	0
7	CG	1164	0	1106	99	0
8	AH	1045	0	1033	48	0
8	CH	1045	0	1033	51	0
9	AI	852	0	742	83	0
9	CI	852	0	742	79	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	70	0
11	AK	828	0	822	29	0
11	CK	828	0	822	28	0
12	AL	905	0	916	41	0
12	CL	905	0	916	32	0
13	AM	804	0	752	58	0
13	CM	804	0	752	60	0
14	AN	478	0	497	33	0
14	CN	478	0	496	58	0
15	AO	724	0	749	34	0
15	CO	724	0	749	31	0
16	AP	651	0	638	31	0
16	CP	651	0	638	36	0
17	AQ	823	0	891	43	0
17	CQ	823	0	891	47	0
18	AR	514	0	530	25	0
18	CR	514	0	530	21	0
19	AS	560	0	466	46	0
19	CS	560	0	466	40	0
20	AT	665	0	731	34	0
20	CT	713	0	766	39	0
21	AU	199	0	208	31	0
21	CU	199	0	208	23	0
22	AX	631	0	540	20	0
22	CX	601	0	485	16	0
23	BA	61112	0	30809	1210	1
23	DA	60621	0	30566	1219	0
24	BB	2573	0	1306	56	0
24	DB	2573	0	1306	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BD	2135	0	2214	73	0
25	DD	2136	0	2218	79	0
26	BE	1555	0	1607	52	0
26	DE	1555	0	1607	56	0
27	BF	1580	0	1621	63	0
27	DF	1580	0	1621	63	0
28	BG	1368	0	1324	74	0
28	DG	1368	0	1324	86	0
29	BH	1317	0	1376	35	0
29	DH	1317	0	1376	36	0
30	BI	1037	0	1036	54	1
30	DI	953	0	858	38	0
31	BN	1112	0	1180	33	0
31	DN	1112	0	1180	44	0
32	BO	923	0	981	26	0
32	DO	923	0	981	28	0
33	BP	1131	0	1201	45	0
33	DP	1131	0	1201	55	0
34	BQ	1122	0	1179	46	0
34	DQ	1122	0	1179	49	0
35	BR	968	0	1033	32	0
35	DR	968	0	1033	36	0
36	BS	865	0	905	50	0
36	DS	865	0	905	50	0
37	BT	1063	0	1103	42	0
37	DT	1063	0	1103	43	0
38	BU	959	0	1019	34	0
38	DU	959	0	1019	35	0
39	BV	771	0	830	23	0
39	DV	771	0	830	25	0
40	BW	881	0	935	21	0
40	DW	881	0	935	31	0
41	BX	742	0	799	23	0
41	DX	742	0	799	26	0
42	BY	785	0	828	23	0
42	DY	785	0	828	23	0
43	BZ	1536	0	1518	52	0
43	DZ	1522	0	1511	65	0
44	B0	594	0	604	16	0
44	D0	594	0	604	17	0
45	B1	745	0	804	21	0
45	D1	745	0	804	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B2	588	0	643	16	0
46	D2	588	0	643	19	0
47	B3	458	0	503	8	0
47	D3	458	0	503	13	0
48	B4	349	0	336	23	0
48	D4	349	0	336	28	0
49	B5	455	0	472	13	0
49	D5	455	0	472	14	0
50	B6	449	0	462	18	0
50	D6	449	0	462	15	0
51	B7	418	0	467	14	0
51	D7	418	0	467	18	0
52	B8	509	0	565	18	0
52	D8	509	0	565	22	0
53	B9	297	0	316	9	0
53	D9	297	0	316	9	0
54	AA	135	0	0	0	0
54	AC	1	0	0	0	0
54	AD	1	0	0	0	0
54	AF	1	0	0	0	0
54	AQ	1	0	0	0	0
54	B0	3	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	1	0	0	0	0
54	B5	2	0	0	0	0
54	B8	2	0	0	0	0
54	B9	1	0	0	0	0
54	BA	660	0	0	0	0
54	BB	23	0	0	0	0
54	BD	3	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BG	1	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	4	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	2	0	0	0	0
54	BZ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	162	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	2	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	2	0	0	0	0
54	DA	598	0	0	0	0
54	DB	8	0	0	0	0
54	DD	2	0	0	0	0
54	DE	4	0	0	0	0
54	DF	1	0	0	0	0
54	DO	2	0	0	0	0
54	DP	1	0	0	0	0
54	DQ	2	0	0	0	0
54	DR	3	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	268	0	0	32	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	AX	1	0	0	0	0
56	B0	8	0	0	0	0
56	B1	2	0	0	0	0
56	B3	1	0	0	0	0
56	B5	3	0	0	0	0
56	B6	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B7	5	0	0	0	0
56	B8	10	0	0	0	0
56	B9	1	0	0	1	0
56	BA	1694	0	0	169	0
56	BB	57	0	0	3	1
56	BD	20	0	0	3	0
56	BE	11	0	0	0	0
56	BF	6	0	0	1	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	2	0	0	0	0
56	BP	11	0	0	2	0
56	BQ	5	0	0	0	0
56	BR	6	0	0	1	0
56	BT	1	0	0	0	0
56	BU	3	0	0	0	0
56	BV	3	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	4	0	0	0	0
56	CA	265	0	0	25	0
56	CC	1	0	0	2	0
56	CD	1	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	1	0
56	CL	2	0	0	1	0
56	CN	1	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D1	5	0	0	0	0
56	D3	1	0	0	0	0
56	D4	1	0	0	0	0
56	D7	3	0	0	0	0
56	D8	1	0	0	0	0
56	DA	1174	0	0	171	0
56	DB	17	0	0	0	0
56	DD	8	0	0	2	0
56	DE	11	0	0	2	0
56	DF	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DN	1	0	0	0	0
56	DO	5	0	0	1	0
56	DP	10	0	0	1	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	1	0
56	DT	2	0	0	0	0
56	DU	5	0	0	0	0
56	DV	2	0	0	1	0
56	DW	2	0	0	0	0
56	DX	1	0	0	1	0
56	DY	2	0	0	0	0
All	All	286308	0	187082	8298	2

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 18.

The worst 5 of 8298 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)
1:AA:1441:G:H2'	1:AA:1459:C:N4	1.20	1.46
1:AA:1459:C:C5	1:AA:1460:A:N6	1.79	1.44
1:AA:1441:G:C2'	1:AA:1459:C:N4	1.88	1.36
1:AA:1441:G:C2'	1:AA:1459:C:H41	1.44	1.29
1:CA:1441:G:H2'	1:CA:1459:C:N4	1.50	1.25

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BA:1594:G:OP1	56:BB:323:HOH:O[1_455]	2.18	0.02
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

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	228/256 (89%)	199 (87%)	28 (12%)	1 (0%)	39	75
2	CB	227/256 (89%)	197 (87%)	29 (13%)	1 (0%)	39	75
3	AC	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	34	72
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	CD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	AE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	65
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	15	50
7	CG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	26	65
8	AH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
8	CH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	AI	123/128 (96%)	112 (91%)	10 (8%)	1 (1%)	24	63
9	CI	123/128 (96%)	111 (90%)	11 (9%)	1 (1%)	24	63
10	AJ	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	5	26
10	CJ	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	9	37
11	AK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
11	CK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
12	AL	120/132 (91%)	110 (92%)	9 (8%)	1 (1%)	24	63
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	24	63
13	AM	112/126 (89%)	89 (80%)	21 (19%)	2 (2%)	11	42
13	CM	112/126 (89%)	87 (78%)	21 (19%)	4 (4%)	4	24
14	AN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	5	25
14	CN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	35
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	35
16	AP	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	15	50
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	15	50
19	CS	79/93 (85%)	65 (82%)	13 (16%)	1 (1%)	15	50
20	AT	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
20	CT	95/106 (90%)	84 (88%)	8 (8%)	3 (3%)	5	26
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	AX	93/101 (92%)	79 (85%)	13 (14%)	1 (1%)	17	55
22	CX	93/101 (92%)	84 (90%)	9 (10%)	0	100	100
25	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	39	75
25	DD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	39	75
26	BE	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	19	58
26	DE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	19	58
27	BF	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
27	DF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	34	72
28	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	30	68
28	DG	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
29	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	30	68
29	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	30	68
30	BI	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	14	48
30	DI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	14	48
31	BN	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	8	36
31	DN	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	8	36
32	BO	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	BP	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
33	DP	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
34	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	65
35	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
35	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
36	BS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
36	DS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
37	BT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	114 (100%)	0	0	100	100
38	DU	114/118 (97%)	114 (100%)	0	0	100	100
39	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	21	61
40	DW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	19	58
42	DY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	19	58
43	BZ	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	19	58
43	DZ	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	19	58
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
44	D0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	55
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	55
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
46	D2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
47	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	B4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
48	D4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
50	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
51	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	8	36
51	D7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	8	36
52	B8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
52	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11552/12330 (94%)	10628 (92%)	855 (7%)	69 (1%)	30	68

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	CT	100	ILE
12	AL	28	LYS
14	AN	15	LYS
16	AP	79	VAL
12	CL	28	LYS

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	178/220 (81%)	133 (75%)	45 (25%)	1	2
2	CB	177/220 (80%)	133 (75%)	44 (25%)	1	3
3	AC	114/188 (61%)	79 (69%)	35 (31%)	0	1
3	CC	114/188 (61%)	92 (81%)	22 (19%)	2	8
4	AD	141/181 (78%)	118 (84%)	23 (16%)	3	12
4	CD	141/181 (78%)	119 (84%)	22 (16%)	3	14
5	AE	108/123 (88%)	87 (81%)	21 (19%)	2	7
5	CE	108/123 (88%)	87 (81%)	21 (19%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	76/90 (84%)	61 (80%)	15 (20%)	1	7
6	CF	76/90 (84%)	58 (76%)	18 (24%)	1	3
7	AG	103/127 (81%)	73 (71%)	30 (29%)	0	1
7	CG	103/127 (81%)	68 (66%)	35 (34%)	0	0
8	AH	103/119 (87%)	82 (80%)	21 (20%)	1	6
8	CH	103/119 (87%)	83 (81%)	20 (19%)	2	7
9	AI	62/99 (63%)	47 (76%)	15 (24%)	1	3
9	CI	62/99 (63%)	47 (76%)	15 (24%)	1	3
10	AJ	53/92 (58%)	38 (72%)	15 (28%)	0	1
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0	2
11	AK	81/99 (82%)	71 (88%)	10 (12%)	6	23
11	CK	81/99 (82%)	70 (86%)	11 (14%)	5	19
12	AL	91/109 (84%)	80 (88%)	11 (12%)	6	24
12	CL	91/109 (84%)	81 (89%)	10 (11%)	8	30
13	AM	64/101 (63%)	48 (75%)	16 (25%)	1	2
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	4
14	AN	46/50 (92%)	36 (78%)	10 (22%)	1	5
14	CN	46/50 (92%)	32 (70%)	14 (30%)	0	1
15	AO	77/80 (96%)	68 (88%)	9 (12%)	7	26
15	CO	77/80 (96%)	68 (88%)	9 (12%)	7	26
16	AP	63/74 (85%)	46 (73%)	17 (27%)	0	1
16	CP	63/74 (85%)	44 (70%)	19 (30%)	0	1
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	4	15
17	CQ	94/97 (97%)	81 (86%)	13 (14%)	4	19
18	AR	49/77 (64%)	44 (90%)	5 (10%)	9	33
18	CR	49/77 (64%)	44 (90%)	5 (10%)	9	33
19	AS	43/80 (54%)	26 (60%)	17 (40%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0	2
20	AT	64/82 (78%)	55 (86%)	9 (14%)	4	18
20	CT	65/82 (79%)	55 (85%)	10 (15%)	3	14
21	AU	18/22 (82%)	13 (72%)	5 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	18/22 (82%)	11 (61%)	7 (39%)	0	0
22	AX	45/87 (52%)	34 (76%)	11 (24%)	1	3
22	CX	38/87 (44%)	29 (76%)	9 (24%)	1	3
25	BD	215/218 (99%)	182 (85%)	33 (15%)	3	14
25	DD	215/218 (99%)	183 (85%)	32 (15%)	4	15
26	BE	163/166 (98%)	135 (83%)	28 (17%)	2	11
26	DE	163/166 (98%)	137 (84%)	26 (16%)	3	13
27	BF	159/166 (96%)	135 (85%)	24 (15%)	3	15
27	DF	159/166 (96%)	134 (84%)	25 (16%)	3	13
28	BG	128/156 (82%)	109 (85%)	19 (15%)	4	16
28	DG	128/156 (82%)	109 (85%)	19 (15%)	4	16
29	BH	141/148 (95%)	123 (87%)	18 (13%)	5	21
29	DH	141/148 (95%)	123 (87%)	18 (13%)	5	21
30	BI	98/124 (79%)	81 (83%)	17 (17%)	2	11
30	DI	74/124 (60%)	60 (81%)	14 (19%)	2	8
31	BN	117/119 (98%)	98 (84%)	19 (16%)	3	12
31	DN	117/119 (98%)	98 (84%)	19 (16%)	3	12
32	BO	98/100 (98%)	82 (84%)	16 (16%)	3	12
32	DO	98/100 (98%)	83 (85%)	15 (15%)	3	14
33	BP	114/116 (98%)	99 (87%)	15 (13%)	5	20
33	DP	114/116 (98%)	99 (87%)	15 (13%)	5	20
34	BQ	111/111 (100%)	96 (86%)	15 (14%)	5	20
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	5	20
35	BR	101/101 (100%)	79 (78%)	22 (22%)	1	5
35	DR	101/101 (100%)	77 (76%)	24 (24%)	1	3
36	BS	84/88 (96%)	67 (80%)	17 (20%)	1	7
36	DS	84/88 (96%)	68 (81%)	16 (19%)	2	8
37	BT	110/127 (87%)	98 (89%)	12 (11%)	8	30
37	DT	110/127 (87%)	95 (86%)	15 (14%)	5	19
38	BU	93/94 (99%)	82 (88%)	11 (12%)	6	25
38	DU	93/94 (99%)	83 (89%)	10 (11%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BV	80/82 (98%)	63 (79%)	17 (21%)	1	6
39	DV	80/82 (98%)	63 (79%)	17 (21%)	1	6
40	BW	89/92 (97%)	81 (91%)	8 (9%)	12	41
40	DW	89/92 (97%)	78 (88%)	11 (12%)	6	23
41	BX	75/78 (96%)	71 (95%)	4 (5%)	28	64
41	DX	75/78 (96%)	70 (93%)	5 (7%)	20	56
42	BY	80/91 (88%)	64 (80%)	16 (20%)	1	7
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	6
43	BZ	159/179 (89%)	137 (86%)	22 (14%)	4	19
43	DZ	159/179 (89%)	139 (87%)	20 (13%)	5	22
44	B0	59/67 (88%)	51 (86%)	8 (14%)	5	19
44	D0	59/67 (88%)	50 (85%)	9 (15%)	3	14
45	B1	78/83 (94%)	63 (81%)	15 (19%)	2	8
45	D1	78/83 (94%)	66 (85%)	12 (15%)	3	14
46	B2	65/67 (97%)	54 (83%)	11 (17%)	2	11
46	D2	65/67 (97%)	55 (85%)	10 (15%)	3	14
47	B3	49/52 (94%)	44 (90%)	5 (10%)	9	33
47	D3	49/52 (94%)	44 (90%)	5 (10%)	9	33
48	B4	39/63 (62%)	33 (85%)	6 (15%)	3	14
48	D4	39/63 (62%)	33 (85%)	6 (15%)	3	14
49	B5	50/52 (96%)	42 (84%)	8 (16%)	3	13
49	D5	50/52 (96%)	41 (82%)	9 (18%)	2	10
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	5
50	D6	50/52 (96%)	40 (80%)	10 (20%)	1	7
51	B7	41/42 (98%)	34 (83%)	7 (17%)	2	11
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2	11
52	B8	52/55 (94%)	42 (81%)	10 (19%)	2	8
52	D8	52/55 (94%)	42 (81%)	10 (19%)	2	8
53	B9	32/34 (94%)	28 (88%)	4 (12%)	6	22
53	D9	32/34 (94%)	28 (88%)	4 (12%)	6	22
All	All	8775/10240 (86%)	7244 (83%)	1531 (17%)	2	11

5 of 1531 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	74	ARG
4	CD	158	ILE
42	DY	6	HIS
46	B2	32	LEU
2	CB	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
38	BU	49	HIS
2	CB	140	HIS
33	DP	84	ASN
39	BV	80	GLN
46	B2	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1499/1522 (98%)	385 (25%)	33 (2%)
1	CA	1495/1522 (98%)	396 (26%)	34 (2%)
23	BA	2833/2913 (97%)	609 (21%)	60 (2%)
23	DA	2807/2913 (96%)	600 (21%)	56 (1%)
24	BB	119/122 (97%)	25 (21%)	0
24	DB	119/122 (97%)	26 (21%)	0
All	All	8872/9114 (97%)	2041 (23%)	183 (2%)

5 of 2041 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	32	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2126	A

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Mol	Chain	Res	Type
1	CA	495	A
23	DA	1819	A
23	BA	2318	G
23	BA	2802	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1662 ligands modelled in this entry, 1662 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1501/1522 (98%)	0.04	61 (4%) 41 19	47, 95, 155, 169	0
1	CA	1497/1522 (98%)	0.02	68 (4%) 37 17	50, 96, 158, 171	0
2	AB	230/256 (89%)	-0.06	9 (3%) 43 21	87, 114, 134, 148	0
2	CB	229/256 (89%)	0.34	13 (5%) 27 11	92, 116, 136, 149	0
3	AC	206/239 (86%)	0.09	5 (2%) 62 39	85, 109, 127, 136	0
3	CC	206/239 (86%)	0.37	16 (7%) 16 5	94, 120, 143, 158	0
4	AD	208/209 (99%)	-0.02	7 (3%) 49 24	75, 94, 114, 125	0
4	CD	208/209 (99%)	0.06	4 (1%) 70 48	76, 93, 114, 124	0
5	AE	148/162 (91%)	-0.19	0 100 100	66, 86, 103, 125	0
5	CE	148/162 (91%)	-0.04	3 (2%) 68 46	69, 88, 104, 127	0
6	AF	100/101 (99%)	-0.29	1 (1%) 84 69	67, 82, 100, 116	0
6	CF	100/101 (99%)	-0.29	1 (1%) 84 69	70, 86, 103, 117	0
7	AG	155/156 (99%)	2.02	69 (44%) 0 0	113, 139, 153, 159	0
7	CG	155/156 (99%)	2.00	71 (45%) 0 0	122, 137, 149, 159	0
8	AH	138/138 (100%)	0.12	2 (1%) 78 60	71, 90, 100, 110	0
8	CH	138/138 (100%)	-0.02	6 (4%) 39 18	71, 92, 103, 113	0
9	AI	125/128 (97%)	1.22	35 (28%) 1 0	110, 137, 149, 154	0
9	CI	125/128 (97%)	2.67	67 (53%) 0 0	115, 139, 152, 163	0
10	AJ	96/105 (91%)	1.61	34 (35%) 0 0	92, 126, 141, 147	0
10	CJ	96/105 (91%)	2.00	42 (43%) 0 0	108, 134, 150, 160	0
11	AK	114/129 (88%)	-0.03	1 (0%) 85 72	60, 86, 108, 120	0
11	CK	114/129 (88%)	0.10	5 (4%) 38 17	63, 89, 107, 126	0
12	AL	122/132 (92%)	-0.10	1 (0%) 87 75	62, 77, 95, 112	0
12	CL	122/132 (92%)	-0.01	0 100 100	63, 77, 96, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	1.53	35 (30%) 1 0	112, 139, 150, 153	0
13	CM	114/126 (90%)	1.93	44 (38%) 0 0	116, 140, 151, 160	0
14	AN	60/61 (98%)	0.75	8 (13%) 4 2	93, 118, 131, 144	0
14	CN	60/61 (98%)	0.85	9 (15%) 3 1	103, 122, 134, 139	0
15	AO	88/89 (98%)	-0.09	0 100 100	63, 85, 103, 113	0
15	CO	88/89 (98%)	0.04	1 (1%) 82 66	63, 85, 105, 111	0
16	AP	82/88 (93%)	0.60	10 (12%) 5 2	76, 88, 110, 120	0
16	CP	82/88 (93%)	0.37	4 (4%) 33 14	73, 85, 105, 117	0
17	AQ	99/105 (94%)	0.01	1 (1%) 84 69	68, 82, 102, 106	0
17	CQ	99/105 (94%)	0.11	1 (1%) 84 69	69, 83, 101, 108	0
18	AR	68/88 (77%)	-0.08	2 (2%) 55 31	71, 82, 105, 112	0
18	CR	68/88 (77%)	0.20	1 (1%) 76 58	75, 85, 105, 117	0
19	AS	81/93 (87%)	2.43	37 (45%) 0 0	113, 138, 147, 152	0
19	CS	81/93 (87%)	2.91	45 (55%) 0 0	114, 140, 150, 153	0
20	AT	87/106 (82%)	0.34	0 100 100	75, 88, 103, 111	0
20	CT	97/106 (91%)	0.09	0 100 100	72, 86, 105, 115	0
21	AU	23/27 (85%)	3.40	15 (65%) 0 0	128, 136, 145, 154	0
21	CU	23/27 (85%)	4.34	18 (78%) 0 0	129, 137, 148, 150	0
22	AX	95/101 (94%)	0.22	5 (5%) 30 13	69, 94, 115, 123	0
22	CX	95/101 (94%)	1.14	19 (20%) 1 0	88, 106, 129, 145	0
23	BA	2837/2913 (97%)	-0.24	51 (1%) 71 50	26, 47, 132, 176	0
23	DA	2814/2913 (96%)	-0.40	81 (2%) 55 31	28, 50, 133, 176	0
24	BB	120/122 (98%)	-0.36	0 100 100	43, 72, 93, 110	0
24	DB	120/122 (98%)	-0.12	1 (0%) 87 75	48, 81, 106, 117	0
25	BD	275/276 (99%)	-0.43	0 100 100	29, 45, 63, 113	0
25	DD	275/276 (99%)	-0.43	1 (0%) 93 85	30, 47, 66, 116	0
26	BE	204/206 (99%)	-0.38	1 (0%) 91 83	28, 49, 72, 95	0
26	DE	204/206 (99%)	-0.41	0 100 100	29, 50, 76, 95	0
27	BF	203/210 (96%)	-0.39	0 100 100	29, 54, 88, 111	0
27	DF	203/210 (96%)	-0.34	0 100 100	31, 59, 90, 112	0
28	BG	181/182 (99%)	-0.00	8 (4%) 38 17	76, 110, 133, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	0.86	27 (14%) 3 1	86, 117, 138, 148	0
29	BH	174/180 (96%)	-0.28	0 100 100	54, 73, 94, 110	0
29	DH	174/180 (96%)	0.35	9 (5%) 31 13	65, 82, 101, 119	0
30	BI	146/148 (98%)	-0.37	1 (0%) 89 78	54, 81, 99, 115	0
30	DI	146/148 (98%)	-0.02	2 (1%) 78 60	56, 89, 108, 120	0
31	BN	140/140 (100%)	-0.36	0 100 100	38, 49, 78, 92	0
31	DN	140/140 (100%)	-0.26	1 (0%) 89 78	40, 54, 82, 96	0
32	BO	122/122 (100%)	-0.40	0 100 100	35, 50, 69, 77	0
32	DO	122/122 (100%)	-0.56	0 100 100	36, 52, 69, 77	0
33	BP	149/150 (99%)	-0.29	0 100 100	30, 58, 89, 105	0
33	DP	149/150 (99%)	-0.16	3 (2%) 68 46	31, 62, 92, 112	0
34	BQ	141/141 (100%)	-0.31	0 100 100	39, 54, 71, 83	0
34	DQ	141/141 (100%)	-0.34	0 100 100	41, 58, 77, 88	0
35	BR	118/118 (100%)	-0.30	0 100 100	34, 44, 58, 77	0
35	DR	118/118 (100%)	-0.31	0 100 100	36, 47, 62, 78	0
36	BS	110/112 (98%)	-0.08	0 100 100	50, 69, 89, 96	0
36	DS	110/112 (98%)	0.34	5 (4%) 37 17	55, 74, 94, 102	0
37	BT	131/146 (89%)	-0.43	0 100 100	43, 55, 92, 119	0
37	DT	131/146 (89%)	-0.35	1 (0%) 87 75	46, 57, 93, 128	0
38	BU	116/118 (98%)	-0.41	0 100 100	32, 44, 62, 71	0
38	DU	116/118 (98%)	-0.49	0 100 100	34, 48, 66, 73	0
39	BV	101/101 (100%)	-0.33	1 (0%) 84 69	29, 56, 79, 103	0
39	DV	101/101 (100%)	-0.21	0 100 100	32, 62, 85, 103	0
40	BW	112/113 (99%)	-0.41	0 100 100	33, 40, 62, 103	0
40	DW	112/113 (99%)	-0.48	0 100 100	35, 42, 67, 105	0
41	BX	95/96 (98%)	-0.26	0 100 100	38, 49, 72, 88	0
41	DX	95/96 (98%)	-0.29	1 (1%) 82 66	41, 52, 77, 90	0
42	BY	107/110 (97%)	-0.27	0 100 100	47, 61, 85, 108	0
42	DY	107/110 (97%)	0.20	6 (5%) 28 11	52, 65, 89, 113	0
43	BZ	201/206 (97%)	-0.41	0 100 100	53, 76, 99, 122	0
43	DZ	198/206 (96%)	0.05	5 (2%) 61 37	62, 81, 102, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	-0.28	0 100 100	39, 48, 64, 91	0
44	D0	76/85 (89%)	0.07	2 (2%) 59 35	43, 52, 66, 92	0
45	B1	97/98 (98%)	-0.21	0 100 100	36, 48, 82, 97	0
45	D1	97/98 (98%)	-0.16	2 (2%) 67 44	36, 51, 83, 98	0
46	B2	70/72 (97%)	-0.24	0 100 100	46, 60, 76, 107	0
46	D2	70/72 (97%)	-0.20	0 100 100	50, 64, 81, 103	0
47	B3	59/60 (98%)	-0.22	0 100 100	38, 49, 86, 97	0
47	D3	59/60 (98%)	0.17	1 (1%) 73 52	41, 53, 93, 102	0
48	B4	46/71 (64%)	-0.29	2 (4%) 39 18	101, 129, 144, 148	0
48	D4	46/71 (64%)	0.49	7 (15%) 3 1	113, 133, 144, 152	0
49	B5	59/60 (98%)	-0.53	0 100 100	30, 45, 66, 80	0
49	D5	59/60 (98%)	-0.53	0 100 100	32, 47, 68, 81	0
50	B6	53/54 (98%)	-0.54	0 100 100	42, 51, 70, 79	0
50	D6	53/54 (98%)	-0.25	2 (3%) 44 21	43, 54, 72, 82	0
51	B7	48/49 (97%)	-0.29	0 100 100	30, 34, 55, 80	0
51	D7	48/49 (97%)	-0.19	0 100 100	32, 35, 58, 84	0
52	B8	64/65 (98%)	-0.25	0 100 100	38, 43, 52, 70	0
52	D8	64/65 (98%)	-0.19	0 100 100	40, 45, 55, 70	0
53	B9	36/37 (97%)	0.28	0 100 100	44, 55, 62, 73	0
53	D9	36/37 (97%)	0.45	2 (5%) 28 11	47, 59, 68, 75	0
All	All	20641/21444 (96%)	-0.02	999 (4%) 34 15	26, 71, 144, 176	0

The worst 5 of 999 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	CU	11	GLY	12.2
19	CS	69	HIS	11.1
21	CU	12	LYS	10.6
19	CS	4	SER	10.1
19	AS	33	THR	9.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3276	1/1	0.86	0.86	73.60	60,60,60,60	0
54	MG	DA	3231	1/1	0.89	0.29	42.16	36,36,36,36	0
54	MG	CA	1645	1/1	0.85	0.93	38.10	60,60,60,60	0
54	MG	BA	3419	1/1	0.98	0.40	36.54	21,21,21,21	0
54	MG	AA	1659	1/1	0.73	0.86	34.62	70,70,70,70	0
54	MG	BA	3248	1/1	0.97	0.41	33.56	27,27,27,27	0
54	MG	DA	3162	1/1	0.92	0.36	32.54	35,35,35,35	0
54	MG	BE	301	1/1	0.91	0.43	32.35	34,34,34,34	0
54	MG	BA	3061	1/1	0.83	0.47	29.24	54,54,54,54	0
54	MG	DA	3224	1/1	0.94	0.37	25.92	32,32,32,32	0
54	MG	BA	3257	1/1	0.93	0.41	24.73	23,23,23,23	0
54	MG	DA	3302	1/1	0.96	0.51	24.51	21,21,21,21	0
54	MG	DA	3242	1/1	0.98	0.56	24.45	34,34,34,34	0
54	MG	AA	1639	1/1	0.95	0.45	23.79	67,67,67,67	0
54	MG	BA	3105	1/1	0.93	0.36	23.11	28,28,28,28	0
54	MG	DA	3244	1/1	0.92	0.52	22.96	33,33,33,33	0
54	MG	BA	3270	1/1	0.99	0.45	22.93	25,25,25,25	0
54	MG	BA	3172	1/1	0.94	0.38	22.88	47,47,47,47	0
54	MG	DA	3164	1/1	0.66	0.39	22.48	56,56,56,56	0
54	MG	AA	1668	1/1	0.94	0.57	22.20	62,62,62,62	0
54	MG	DA	3196	1/1	0.79	0.39	22.19	58,58,58,58	0
54	MG	DA	3125	1/1	0.89	0.30	22.07	50,50,50,50	0
54	MG	BA	3129	1/1	0.94	0.37	21.26	37,37,37,37	0
54	MG	DA	3157	1/1	0.96	0.35	20.74	44,44,44,44	0
54	MG	BA	3253	1/1	0.95	0.44	20.69	19,19,19,19	0
54	MG	DA	3096	1/1	0.78	0.53	20.46	59,59,59,59	0
54	MG	DA	3266	1/1	0.92	0.32	20.04	47,47,47,47	0
54	MG	BA	3167	1/1	0.96	0.45	18.93	31,31,31,31	0
54	MG	DA	3008	1/1	0.91	0.45	18.67	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3303	1/1	0.96	0.48	18.49	34,34,34,34	0
54	MG	BA	3246	1/1	0.95	0.47	18.15	20,20,20,20	0
54	MG	BA	3109	1/1	0.79	0.41	18.00	62,62,62,62	0
54	MG	DA	3272	1/1	0.93	0.38	17.80	30,30,30,30	0
54	MG	DA	3183	1/1	0.96	0.46	17.16	26,26,26,26	0
54	MG	DA	3069	1/1	0.94	0.39	15.99	42,42,42,42	0
54	MG	BA	3279	1/1	0.86	0.49	15.69	27,27,27,27	0
54	MG	DA	3373	1/1	0.97	0.27	15.67	32,32,32,32	0
54	MG	DA	3133	1/1	0.93	0.38	15.60	36,36,36,36	0
54	MG	BA	3284	1/1	0.97	0.37	15.52	24,24,24,24	0
54	MG	DA	3221	1/1	0.87	0.47	15.47	51,51,51,51	0
54	MG	CA	1689	1/1	0.96	0.38	15.32	61,61,61,61	0
54	MG	AA	1660	1/1	0.92	0.52	14.78	80,80,80,80	0
54	MG	BA	3590	1/1	0.90	0.31	14.58	31,31,31,31	0
54	MG	AA	1650	1/1	0.98	0.55	14.34	53,53,53,53	0
54	MG	DA	3041	1/1	0.96	0.51	14.14	36,36,36,36	0
54	MG	AA	1671	1/1	0.81	0.35	14.07	67,67,67,67	0
54	MG	BA	3069	1/1	0.96	0.36	13.83	42,42,42,42	0
54	MG	DA	3205	1/1	0.96	0.28	13.48	47,47,47,47	0
54	MG	BA	3247	1/1	0.96	0.47	12.80	26,26,26,26	0
54	MG	BA	3250	1/1	0.93	0.40	12.73	26,26,26,26	0
54	MG	AA	1672	1/1	0.96	0.42	12.71	46,46,46,46	0
54	MG	DA	3092	1/1	0.89	0.32	12.47	41,41,41,41	0
54	MG	DA	3311	1/1	0.95	0.36	12.29	26,26,26,26	0
54	MG	DA	3345	1/1	0.98	0.31	12.19	54,54,54,54	0
54	MG	BA	3127	1/1	0.96	0.28	12.17	38,38,38,38	0
54	MG	BA	3157	1/1	0.95	0.30	12.13	48,48,48,48	0
54	MG	DA	3131	1/1	0.95	0.32	11.92	56,56,56,56	0
54	MG	BA	3262	1/1	0.91	0.37	11.86	27,27,27,27	0
54	MG	DA	3309	1/1	0.84	0.40	11.84	28,28,28,28	0
54	MG	DA	3130	1/1	0.85	0.33	11.84	47,47,47,47	0
54	MG	BA	3282	1/1	0.97	0.34	11.64	27,27,27,27	0
54	MG	DA	3150	1/1	0.96	0.33	11.48	42,42,42,42	0
54	MG	DA	3197	1/1	0.84	0.34	11.37	49,49,49,49	0
54	MG	DA	3304	1/1	0.94	0.42	11.29	29,29,29,29	0
54	MG	AA	1610	1/1	0.96	0.41	11.17	56,56,56,56	0
54	MG	DA	3029	1/1	0.88	0.31	11.16	40,40,40,40	0
54	MG	DA	3178	1/1	0.95	0.33	10.96	32,32,32,32	0
54	MG	BA	3249	1/1	0.94	0.35	10.93	25,25,25,25	0
54	MG	BA	3256	1/1	0.93	0.34	10.91	23,23,23,23	0
54	MG	DA	3163	1/1	0.89	0.39	10.83	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DR	202	1/1	0.92	0.37	10.78	34,34,34,34	0
54	MG	BD	301	1/1	0.93	0.45	10.75	49,49,49,49	0
54	MG	DA	3321	1/1	0.90	0.42	10.70	51,51,51,51	0
54	MG	DA	3232	1/1	0.96	0.32	10.52	57,57,57,57	0
54	MG	BA	3102	1/1	0.80	0.34	10.40	44,44,44,44	0
54	MG	DA	3305	1/1	0.92	0.23	10.25	35,35,35,35	0
54	MG	BA	3255	1/1	0.95	0.31	10.16	25,25,25,25	0
54	MG	DA	3337	1/1	0.97	0.29	10.00	30,30,30,30	0
54	MG	DA	3257	1/1	0.84	0.32	9.76	56,56,56,56	0
54	MG	BA	3011	1/1	0.91	0.29	9.69	26,26,26,26	0
54	MG	BA	3278	1/1	0.96	0.38	9.69	30,30,30,30	0
54	MG	BA	3188	1/1	0.99	0.27	9.66	39,39,39,39	0
54	MG	AA	1684	1/1	0.87	0.83	9.61	60,60,60,60	0
54	MG	BB	212	1/1	0.91	0.27	9.60	60,60,60,60	0
54	MG	BA	3259	1/1	0.97	0.34	9.42	27,27,27,27	0
54	MG	BA	3064	1/1	0.97	0.24	9.32	34,34,34,34	0
54	MG	CA	1685	1/1	0.94	0.34	9.29	71,71,71,71	0
54	MG	DA	3293	1/1	0.94	0.25	9.22	33,33,33,33	0
54	MG	AA	1618	1/1	0.74	1.13	9.18	94,94,94,94	0
54	MG	BA	3473	1/1	0.94	0.23	9.07	30,30,30,30	0
54	MG	DA	3006	1/1	0.96	0.29	8.83	38,38,38,38	0
54	MG	BA	3574	1/1	0.93	0.31	8.67	33,33,33,33	0
54	MG	DA	3042	1/1	0.93	0.23	8.35	33,33,33,33	0
54	MG	CA	1749	1/1	0.97	0.23	8.32	61,61,61,61	0
54	MG	AA	1712	1/1	0.85	0.34	8.30	86,86,86,86	0
54	MG	CA	1611	1/1	0.93	0.22	8.25	43,43,43,43	0
54	MG	AA	1711	1/1	0.96	0.24	8.06	46,46,46,46	0
54	MG	DA	3308	1/1	0.86	0.31	7.93	33,33,33,33	0
54	MG	AA	1633	1/1	0.92	0.28	7.93	62,62,62,62	0
54	MG	BA	3189	1/1	0.94	0.32	7.92	41,41,41,41	0
54	MG	BA	3264	1/1	0.77	0.38	7.91	41,41,41,41	0
54	MG	CA	1741	1/1	0.97	0.32	7.80	79,79,79,79	0
54	MG	DA	3307	1/1	0.96	0.22	7.64	35,35,35,35	0
54	MG	DR	203	1/1	0.86	0.51	7.57	51,51,51,51	0
54	MG	BA	3273	1/1	0.94	0.40	7.37	37,37,37,37	0
54	MG	DA	3229	1/1	0.90	0.30	7.16	44,44,44,44	0
54	MG	BA	3245	1/1	0.95	0.34	7.08	23,23,23,23	0
54	MG	DA	3269	1/1	0.95	0.29	7.03	47,47,47,47	0
54	MG	DA	3374	1/1	0.98	0.21	7.00	37,37,37,37	0
54	MG	BA	3042	1/1	0.96	0.28	6.81	40,40,40,40	0
54	MG	AA	1624	1/1	0.90	0.37	6.72	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3284	1/1	0.79	0.22	6.69	55,55,55,55	0
54	MG	DA	3203	1/1	0.98	0.41	6.52	33,33,33,33	0
54	MG	BA	3467	1/1	0.97	0.24	6.52	30,30,30,30	0
54	MG	DA	3382	1/1	0.92	0.23	6.46	53,53,53,53	0
54	MG	AA	1612	1/1	0.88	0.31	6.44	86,86,86,86	0
54	MG	DD	302	1/1	0.96	0.41	6.40	38,38,38,38	0
54	MG	BA	3265	1/1	0.95	0.39	6.39	29,29,29,29	0
54	MG	DA	3209	1/1	0.85	0.26	6.37	51,51,51,51	0
54	MG	DA	3011	1/1	0.94	0.27	5.95	42,42,42,42	0
54	MG	DA	3182	1/1	0.94	0.31	5.82	46,46,46,46	0
54	MG	BA	3050	1/1	0.93	0.23	5.76	35,35,35,35	0
54	MG	BA	3154	1/1	0.91	0.38	5.71	50,50,50,50	0
54	MG	DA	3063	1/1	0.83	0.32	5.71	60,60,60,60	0
54	MG	BA	3089	1/1	0.97	0.33	5.68	41,41,41,41	0
54	MG	DA	3338	1/1	0.97	0.22	5.65	42,42,42,42	0
54	MG	DA	3230	1/1	0.90	0.21	5.62	45,45,45,45	0
54	MG	BA	3040	1/1	0.92	0.34	5.59	30,30,30,30	0
54	MG	DA	3420	1/1	0.97	0.22	5.55	37,37,37,37	0
54	MG	DA	3044	1/1	0.94	0.19	5.50	46,46,46,46	0
54	MG	BA	3065	1/1	0.88	0.24	5.41	41,41,41,41	0
54	MG	BA	3194	1/1	0.87	0.20	5.38	63,63,63,63	0
54	MG	DA	3146	1/1	0.89	0.18	5.29	44,44,44,44	0
54	MG	DA	3039	1/1	0.96	0.20	5.14	28,28,28,28	0
54	MG	CQ	201	1/1	0.91	0.35	5.13	62,62,62,62	0
54	MG	AA	1680	1/1	0.98	0.25	5.08	72,72,72,72	0
54	MG	BA	3424	1/1	0.85	0.21	5.06	72,72,72,72	0
54	MG	DA	3128	1/1	0.90	0.24	5.06	45,45,45,45	0
54	MG	BA	3455	1/1	0.85	0.23	5.01	22,22,22,22	0
54	MG	DA	3040	1/1	0.93	0.26	4.96	48,48,48,48	0
54	MG	BA	3397	1/1	0.88	0.17	4.92	86,86,86,86	0
54	MG	DA	3578	1/1	0.97	0.22	4.86	29,29,29,29	0
54	MG	DA	3441	1/1	0.95	0.26	4.84	48,48,48,48	0
54	MG	DA	3573	1/1	0.97	0.24	4.84	31,31,31,31	0
54	MG	B3	101	1/1	0.94	0.35	4.80	51,51,51,51	0
54	MG	DA	3353	1/1	0.85	0.21	4.65	61,61,61,61	0
54	MG	BA	3252	1/1	0.93	0.33	4.64	36,36,36,36	0
54	MG	AA	1629	1/1	0.81	0.29	4.54	44,44,44,44	0
54	MG	AD	302	1/1	0.84	0.29	4.53	77,77,77,77	0
54	MG	DA	3017	1/1	0.89	0.20	4.46	50,50,50,50	0
54	MG	BA	3103	1/1	0.92	0.20	4.45	29,29,29,29	0
54	MG	DA	3091	1/1	0.93	0.18	4.41	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3366	1/1	0.91	0.20	4.41	31,31,31,31	0
54	MG	BA	3026	1/1	0.89	0.19	4.38	52,52,52,52	0
54	MG	BA	3159	1/1	0.88	0.23	4.36	46,46,46,46	0
54	MG	DA	3156	1/1	0.95	0.20	4.32	35,35,35,35	0
54	MG	BA	3484	1/1	0.97	0.18	4.29	27,27,27,27	0
54	MG	AA	1619	1/1	0.74	0.27	4.18	86,86,86,86	0
54	MG	CA	1607	1/1	0.89	0.21	4.17	50,50,50,50	0
54	MG	CA	1751	1/1	0.88	0.26	4.04	61,61,61,61	0
54	MG	BA	3451	1/1	0.97	0.21	4.03	28,28,28,28	0
54	MG	BB	206	1/1	0.83	0.20	4.00	57,57,57,57	0
54	MG	DA	3247	1/1	0.83	0.33	3.95	67,67,67,67	0
54	MG	BA	3492	1/1	0.93	0.21	3.89	27,27,27,27	0
54	MG	BA	3502	1/1	0.98	0.24	3.86	34,34,34,34	0
54	MG	DA	3449	1/1	0.98	0.21	3.82	42,42,42,42	0
54	MG	BA	3337	1/1	0.60	0.21	3.76	49,49,49,49	0
54	MG	BA	3145	1/1	0.96	0.20	3.72	44,44,44,44	0
54	MG	DA	3167	1/1	0.83	0.21	3.45	51,51,51,51	0
54	MG	DA	3549	1/1	0.98	0.20	3.41	45,45,45,45	0
54	MG	BA	3456	1/1	0.90	0.22	3.40	32,32,32,32	0
54	MG	BA	3170	1/1	0.93	0.22	3.33	29,29,29,29	0
54	MG	DA	3514	1/1	0.94	0.19	3.33	42,42,42,42	0
54	MG	DA	3100	1/1	0.92	0.22	3.27	38,38,38,38	0
54	MG	DA	3010	1/1	0.95	0.18	3.10	42,42,42,42	0
54	MG	BA	3031	1/1	0.94	0.17	3.10	44,44,44,44	0
54	MG	BA	3333	1/1	0.87	0.19	3.01	40,40,40,40	0
54	MG	DA	3083	1/1	0.97	0.23	2.98	37,37,37,37	0
54	MG	BA	3037	1/1	0.86	0.20	2.97	75,75,75,75	0
54	MG	DA	3052	1/1	0.97	0.37	2.95	52,52,52,52	0
54	MG	BA	3226	1/1	0.96	0.22	2.77	50,50,50,50	0
54	MG	BB	220	1/1	0.97	0.18	2.75	60,60,60,60	0
54	MG	DA	3570	1/1	0.98	0.18	2.71	28,28,28,28	0
54	MG	CA	1613	1/1	0.90	0.34	2.63	66,66,66,66	0
54	MG	CA	1619	1/1	0.96	0.16	2.59	50,50,50,50	0
54	MG	BA	3006	1/1	0.97	0.19	2.57	25,25,25,25	0
54	MG	BA	3212	1/1	0.90	0.21	2.55	68,68,68,68	0
54	MG	DA	3123	1/1	0.91	0.23	2.55	53,53,53,53	0
54	MG	BA	3595	1/1	0.97	0.29	2.52	27,27,27,27	0
54	MG	DA	3241	1/1	0.95	0.27	2.49	35,35,35,35	0
54	MG	BA	3019	1/1	0.92	0.18	2.47	34,34,34,34	0
54	MG	CA	1690	1/1	0.96	0.25	2.46	64,64,64,64	0
54	MG	DB	201	1/1	0.98	0.14	2.41	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3130	1/1	0.96	0.23	2.40	43,43,43,43	0
54	MG	BA	3251	1/1	0.95	0.25	2.35	27,27,27,27	0
54	MG	DA	3014	1/1	0.97	0.19	2.33	31,31,31,31	0
54	MG	DA	3491	1/1	0.94	0.19	2.31	44,44,44,44	0
54	MG	DF	301	1/1	0.90	0.30	2.26	50,50,50,50	0
54	MG	BA	3046	1/1	0.90	0.18	2.25	36,36,36,36	0
54	MG	DA	3219	1/1	0.95	0.16	2.14	38,38,38,38	0
54	MG	DA	3473	1/1	0.94	0.21	2.12	38,38,38,38	0
54	MG	BA	3368	1/1	0.78	0.21	2.09	53,53,53,53	0
54	MG	DA	3414	1/1	0.94	0.17	2.08	51,51,51,51	0
54	MG	BA	3015	1/1	0.89	0.18	2.04	48,48,48,48	0
54	MG	DA	3397	1/1	0.85	0.19	1.98	34,34,34,34	0
54	MG	DA	3243	1/1	0.97	0.22	1.98	28,28,28,28	0
54	MG	BA	3389	1/1	0.95	0.18	1.93	46,46,46,46	0
54	MG	DA	3396	1/1	0.96	0.17	1.93	52,52,52,52	0
54	MG	DA	3496	1/1	0.97	0.20	1.90	66,66,66,66	0
54	MG	CA	1665	1/1	0.88	0.22	1.87	84,84,84,84	0
54	MG	BA	3328	1/1	0.98	0.20	1.87	30,30,30,30	0
54	MG	BA	3482	1/1	0.90	0.19	1.85	27,27,27,27	0
54	MG	BA	3500	1/1	0.98	0.17	1.84	44,44,44,44	0
54	MG	DA	3022	1/1	0.92	0.16	1.81	34,34,34,34	0
54	MG	BA	3001	1/1	0.91	0.21	1.79	43,43,43,43	0
54	MG	BA	3083	1/1	0.92	0.18	1.77	43,43,43,43	0
54	MG	DA	3248	1/1	0.90	0.18	1.75	42,42,42,42	0
54	MG	CA	1680	1/1	0.90	0.23	1.74	78,78,78,78	0
54	MG	BA	3010	1/1	0.90	0.22	1.62	39,39,39,39	0
54	MG	BA	3558	1/1	0.98	0.19	1.58	28,28,28,28	0
54	MG	CA	1729	1/1	0.90	0.17	1.56	81,81,81,81	0
54	MG	DA	3471	1/1	0.97	0.19	1.54	31,31,31,31	0
54	MG	BA	3225	1/1	0.84	0.18	1.50	44,44,44,44	0
54	MG	BA	3161	1/1	0.93	0.18	1.50	40,40,40,40	0
54	MG	BA	3360	1/1	0.97	0.23	1.46	35,35,35,35	0
54	MG	DA	3007	1/1	0.95	0.14	1.43	48,48,48,48	0
54	MG	DA	3223	1/1	0.86	0.18	1.37	54,54,54,54	0
54	MG	BA	3155	1/1	0.94	0.19	1.34	41,41,41,41	0
54	MG	DA	3216	1/1	0.94	0.15	1.32	51,51,51,51	0
54	MG	BA	3384	1/1	0.95	0.14	1.32	88,88,88,88	0
54	MG	D1	101	1/1	0.98	0.22	1.24	38,38,38,38	0
54	MG	DE	301	1/1	0.88	0.22	1.21	41,41,41,41	0
54	MG	CA	1726	1/1	0.97	0.18	1.15	52,52,52,52	0
54	MG	AA	1607	1/1	0.76	0.18	1.14	78,78,78,78	0
54	MG	BA	3030	1/1	0.89	0.20	1.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3052	1/1	0.95	0.17	1.07	52,52,52,52	0
54	MG	BA	3039	1/1	0.91	0.20	0.97	32,32,32,32	0
54	MG	BA	3471	1/1	0.89	0.18	0.94	27,27,27,27	0
54	MG	AA	1725	1/1	0.95	0.20	0.85	56,56,56,56	0
54	MG	BA	3200	1/1	0.98	0.18	0.80	31,31,31,31	0
54	MG	BA	3378	1/1	0.95	0.16	0.74	25,25,25,25	0
54	MG	DA	3417	1/1	0.87	0.16	0.69	31,31,31,31	0
54	MG	BA	3583	1/1	0.93	0.15	0.58	34,34,34,34	0
54	MG	DA	3363	1/1	0.98	0.18	0.52	26,26,26,26	0
54	MG	BA	3067	1/1	0.92	0.18	0.51	43,43,43,43	0
54	MG	CA	1703	1/1	0.94	0.18	0.50	56,56,56,56	0
54	MG	D8	102	1/1	0.85	0.28	0.49	45,45,45,45	0
54	MG	BA	3338	1/1	0.77	0.15	0.40	62,62,62,62	0
54	MG	DA	3169	1/1	0.91	0.16	0.32	45,45,45,45	0
54	MG	DA	3487	1/1	0.89	0.17	0.31	48,48,48,48	0
54	MG	BA	3468	1/1	0.91	0.18	0.31	24,24,24,24	0
54	MG	CA	1728	1/1	0.97	0.16	0.15	60,60,60,60	0
54	MG	BA	3314	1/1	0.95	0.17	0.14	37,37,37,37	0
54	MG	BG	201	1/1	0.85	0.21	0.07	60,60,60,60	0
54	MG	CA	1612	1/1	0.88	0.14	0.05	65,65,65,65	0
54	MG	BA	3385	1/1	0.85	0.15	0.03	63,63,63,63	0
54	MG	B8	101	1/1	0.99	0.21	0.02	51,51,51,51	0
54	MG	BA	3190	1/1	0.99	0.17	-0.02	27,27,27,27	0
54	MG	DA	3555	1/1	0.93	0.14	-0.03	56,56,56,56	0
54	MG	DA	3563	1/1	0.87	0.15	-0.03	70,70,70,70	0
54	MG	BB	202	1/1	0.92	0.12	-0.04	43,43,43,43	0
54	MG	DA	3477	1/1	0.94	0.15	-0.06	53,53,53,53	0
54	MG	BA	3457	1/1	0.95	0.19	-0.06	27,27,27,27	0
55	ZN	AD	301	1/1	0.96	0.28	-0.06	74,74,74,74	0
54	MG	BA	3323	1/1	0.90	0.17	-0.07	23,23,23,23	0
54	MG	BA	3027	1/1	0.93	0.15	-0.08	38,38,38,38	0
54	MG	BA	3205	1/1	0.89	0.12	-0.09	54,54,54,54	0
54	MG	DA	3404	1/1	0.98	0.14	-0.09	36,36,36,36	0
54	MG	DA	3562	1/1	0.97	0.14	-0.12	58,58,58,58	0
54	MG	CA	1737	1/1	0.93	0.13	-0.15	89,89,89,89	0
54	MG	DA	3333	1/1	0.93	0.15	-0.17	37,37,37,37	0
54	MG	DA	3568	1/1	0.94	0.11	-0.18	78,78,78,78	0
54	MG	BA	3369	1/1	0.71	0.13	-0.22	52,52,52,52	0
54	MG	DA	3418	1/1	0.98	0.15	-0.25	31,31,31,31	0
55	ZN	CD	301	1/1	0.93	0.26	-0.29	71,71,71,71	0
54	MG	DA	3375	1/1	0.93	0.14	-0.29	31,31,31,31	0
54	MG	BD	303	1/1	0.96	0.18	-0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3090	1/1	0.89	0.11	-0.34	53,53,53,53	0
54	MG	D8	101	1/1	0.94	0.15	-0.35	48,48,48,48	0
54	MG	BA	3327	1/1	0.99	0.18	-0.35	23,23,23,23	0
54	MG	BA	3458	1/1	0.92	0.17	-0.37	35,35,35,35	0
54	MG	DA	3434	1/1	0.85	0.14	-0.39	60,60,60,60	0
54	MG	DA	3047	1/1	0.94	0.15	-0.40	38,38,38,38	0
54	MG	CA	1655	1/1	0.93	0.22	-0.45	98,98,98,98	0
54	MG	DA	3015	1/1	0.93	0.13	-0.47	38,38,38,38	0
55	ZN	BY	201	1/1	0.92	0.11	-0.52	69,69,69,69	0
54	MG	DA	3558	1/1	0.93	0.15	-0.55	36,36,36,36	0
54	MG	BA	3599	1/1	0.97	0.17	-0.55	30,30,30,30	0
54	MG	CA	1709	1/1	0.96	0.13	-0.56	63,63,63,63	0
54	MG	BA	3425	1/1	0.91	0.15	-0.56	53,53,53,53	0
54	MG	DA	3051	1/1	0.95	0.14	-0.57	38,38,38,38	0
54	MG	BA	3445	1/1	0.96	0.17	-0.59	31,31,31,31	0
54	MG	BB	215	1/1	0.90	0.17	-0.62	65,65,65,65	0
54	MG	BA	3028	1/1	0.95	0.15	-0.62	22,22,22,22	0
54	MG	BA	3227	1/1	0.97	0.14	-0.62	32,32,32,32	0
54	MG	DA	3550	1/1	0.93	0.13	-0.67	58,58,58,58	0
54	MG	BA	3481	1/1	0.94	0.16	-0.67	25,25,25,25	0
54	MG	DA	3452	1/1	0.87	0.10	-0.68	90,90,90,90	0
54	MG	DA	3393	1/1	0.95	0.14	-0.77	41,41,41,41	0
55	ZN	B6	101	1/1	0.99	0.11	-0.80	48,48,48,48	0
54	MG	CA	1718	1/1	0.91	0.15	-0.84	83,83,83,83	0
54	MG	BA	3487	1/1	0.96	0.15	-0.85	20,20,20,20	0
54	MG	BA	3466	1/1	0.98	0.16	-0.85	39,39,39,39	0
54	MG	DA	3450	1/1	0.93	0.10	-0.95	67,67,67,67	0
54	MG	DA	3364	1/1	0.87	0.13	-0.98	32,32,32,32	0
54	MG	AA	1702	1/1	0.76	0.16	-0.98	68,68,68,68	0
54	MG	BA	3358	1/1	0.81	0.12	-1.00	55,55,55,55	0
54	MG	BA	3511	1/1	0.97	0.15	-1.03	32,32,32,32	0
54	MG	DA	3045	1/1	0.95	0.12	-1.04	38,38,38,38	0
54	MG	DA	3444	1/1	0.92	0.14	-1.07	41,41,41,41	0
54	MG	BA	3435	1/1	0.94	0.15	-1.07	48,48,48,48	0
54	MG	AA	1631	1/1	0.95	0.16	-1.08	41,41,41,41	0
54	MG	BA	3366	1/1	0.84	0.15	-1.12	83,83,83,83	0
55	ZN	B4	101	1/1	0.87	0.07	-1.13	199,199,199,199	0
55	ZN	AN	101	1/1	0.85	0.12	-1.13	117,117,117,117	0
55	ZN	D5	102	1/1	0.98	0.08	-1.15	69,69,69,69	0
54	MG	CA	1750	1/1	0.91	0.11	-1.15	78,78,78,78	0
54	MG	DA	3513	1/1	0.92	0.14	-1.16	34,34,34,34	0
55	ZN	D6	101	1/1	0.98	0.07	-1.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3376	1/1	0.97	0.14	-1.20	30,30,30,30	0
54	MG	DA	3476	1/1	0.82	0.13	-1.22	66,66,66,66	0
54	MG	DA	3043	1/1	0.96	0.10	-1.23	54,54,54,54	0
54	MG	DA	3564	1/1	0.95	0.10	-1.24	61,61,61,61	0
54	MG	BA	3271	1/1	0.97	0.14	-1.26	30,30,30,30	0
54	MG	BA	3218	1/1	0.90	0.15	-1.29	55,55,55,55	0
55	ZN	B5	101	1/1	0.99	0.09	-1.34	45,45,45,45	0
54	MG	BA	3475	1/1	0.98	0.14	-1.34	39,39,39,39	0
54	MG	BA	3585	1/1	0.91	0.10	-1.37	52,52,52,52	0
54	MG	BE	303	1/1	0.97	0.13	-1.38	26,26,26,26	0
54	MG	BA	3331	1/1	0.92	0.15	-1.39	48,48,48,48	0
54	MG	DA	3053	1/1	0.95	0.14	-1.45	40,40,40,40	0
54	MG	DA	3511	1/1	0.95	0.09	-1.46	49,49,49,49	0
55	ZN	D4	101	1/1	0.58	0.08	-1.48	214,214,214,214	0
54	MG	DA	3352	1/1	0.92	0.11	-1.48	33,33,33,33	0
54	MG	AA	1728	1/1	0.96	0.12	-1.49	53,53,53,53	0
54	MG	BA	3036	1/1	0.94	0.13	-1.50	36,36,36,36	0
54	MG	BA	3631	1/1	0.99	0.16	-1.50	26,26,26,26	0
54	MG	BA	3462	1/1	0.84	0.09	-1.50	43,43,43,43	0
55	ZN	B9	101	1/1	0.99	0.08	-1.53	50,50,50,50	0
54	MG	DA	3540	1/1	0.95	0.10	-1.54	53,53,53,53	0
54	MG	DA	3378	1/1	0.92	0.15	-1.59	33,33,33,33	0
54	MG	BA	3380	1/1	0.98	0.14	-1.61	26,26,26,26	0
54	MG	BA	3414	1/1	0.86	0.12	-1.61	29,29,29,29	0
54	MG	DA	3160	1/1	0.96	0.09	-1.61	42,42,42,42	0
54	MG	BA	3514	1/1	0.87	0.12	-1.62	61,61,61,61	0
54	MG	BB	201	1/1	0.95	0.12	-1.63	57,57,57,57	0
54	MG	BA	3433	1/1	0.93	0.09	-1.70	55,55,55,55	0
54	MG	DA	3370	1/1	0.88	0.10	-1.70	32,32,32,32	0
54	MG	BA	3231	1/1	0.90	0.11	-1.75	47,47,47,47	0
54	MG	BA	3446	1/1	0.94	0.15	-1.78	30,30,30,30	0
54	MG	BA	3401	1/1	0.93	0.14	-1.80	58,58,58,58	0
54	MG	BA	3332	1/1	0.90	0.09	-1.88	50,50,50,50	0
54	MG	DA	3137	1/1	0.93	0.11	-1.89	38,38,38,38	0
54	MG	BA	3033	1/1	0.95	0.10	-1.89	36,36,36,36	0
54	MG	BA	3132	1/1	0.92	0.12	-1.92	33,33,33,33	0
55	ZN	D9	101	1/1	0.95	0.06	-1.97	65,65,65,65	0
55	ZN	CN	101	1/1	0.97	0.08	-2.00	107,107,107,107	0
54	MG	BA	3495	1/1	0.94	0.13	-2.05	35,35,35,35	0
54	MG	BA	3480	1/1	0.97	0.13	-2.14	31,31,31,31	0
54	MG	BA	3444	1/1	0.93	0.11	-2.20	53,53,53,53	0
54	MG	BA	3158	1/1	0.98	0.09	-2.20	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3448	1/1	0.87	0.15	-2.20	38,38,38,38	0
54	MG	AA	1709	1/1	0.72	0.15	-2.23	101,101,101,101	0
54	MG	BA	3538	1/1	0.93	0.10	-2.33	66,66,66,66	0
54	MG	B8	102	1/1	0.94	0.10	-2.35	61,61,61,61	0
54	MG	DA	3358	1/1	0.84	0.12	-2.37	39,39,39,39	0
54	MG	DA	3502	1/1	0.98	0.11	-2.37	37,37,37,37	0
54	MG	CA	1722	1/1	0.98	0.08	-2.39	71,71,71,71	0
54	MG	BA	3508	1/1	0.96	0.14	-2.39	29,29,29,29	0
54	MG	DA	3419	1/1	0.91	0.11	-2.40	44,44,44,44	0
54	MG	AA	1634	1/1	0.91	0.10	-2.48	56,56,56,56	0
54	MG	AA	1691	1/1	0.96	0.12	-2.48	43,43,43,43	0
54	MG	DA	3403	1/1	0.99	0.07	-2.51	34,34,34,34	0
54	MG	B9	102	1/1	0.96	0.12	-2.56	28,28,28,28	0
54	MG	AA	1662	1/1	0.94	0.12	-2.58	58,58,58,58	0
54	MG	DA	3362	1/1	0.96	0.10	-2.62	26,26,26,26	0
54	MG	DA	3068	1/1	0.98	0.12	-2.63	33,33,33,33	0
54	MG	DA	3469	1/1	0.93	0.07	-2.63	56,56,56,56	0
54	MG	DA	3421	1/1	0.90	0.10	-2.64	93,93,93,93	0
54	MG	AA	1701	1/1	0.96	0.12	-2.72	48,48,48,48	0
54	MG	AA	1694	1/1	0.94	0.08	-2.73	80,80,80,80	0
54	MG	CA	1700	1/1	0.91	0.09	-2.77	70,70,70,70	0
54	MG	BA	3464	1/1	0.97	0.11	-2.81	39,39,39,39	0
54	MG	DA	3474	1/1	0.97	0.10	-2.83	30,30,30,30	0
54	MG	BA	3606	1/1	0.97	0.10	-2.84	34,34,34,34	0
54	MG	BA	3447	1/1	0.98	0.14	-2.93	29,29,29,29	0
54	MG	DA	3350	1/1	0.97	0.11	-2.99	47,47,47,47	0
54	MG	DA	3361	1/1	0.81	0.10	-3.08	30,30,30,30	0
54	MG	DA	3456	1/1	0.90	0.08	-3.08	42,42,42,42	0
54	MG	DA	3105	1/1	0.98	0.09	-3.13	46,46,46,46	0
55	ZN	DY	201	1/1	0.96	0.05	-3.13	94,94,94,94	0
54	MG	DA	3151	1/1	0.91	0.11	-3.22	43,43,43,43	0
54	MG	BA	3469	1/1	0.91	0.15	-3.28	40,40,40,40	0
54	MG	BQ	204	1/1	0.85	0.10	-3.30	43,43,43,43	0
54	MG	DA	3412	1/1	0.89	0.09	-3.33	58,58,58,58	0
54	MG	BA	3490	1/1	0.94	0.10	-3.39	28,28,28,28	0
54	MG	BA	3309	1/1	0.98	0.10	-3.40	31,31,31,31	0
54	MG	CA	1724	1/1	0.97	0.11	-3.40	49,49,49,49	0
54	MG	BA	3483	1/1	0.98	0.13	-3.42	28,28,28,28	0
54	MG	BA	3498	1/1	0.98	0.08	-3.50	32,32,32,32	0
54	MG	BA	3566	1/1	0.91	0.14	-3.50	44,44,44,44	0
54	MG	DA	3454	1/1	0.85	0.08	-3.54	64,64,64,64	0
54	MG	DA	3431	1/1	0.91	0.10	-3.55	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3601	1/1	0.91	0.14	-3.59	76,76,76,76	0
54	MG	CA	1732	1/1	0.87	0.12	-3.61	110,110,110,110	0
54	MG	BA	3578	1/1	0.91	0.10	-3.69	44,44,44,44	0
54	MG	DA	3023	1/1	0.96	0.06	-3.73	43,43,43,43	0
54	MG	BA	3355	1/1	0.93	0.14	-3.74	29,29,29,29	0
54	MG	BA	3485	1/1	0.97	0.10	-3.76	32,32,32,32	0
54	MG	BA	3560	1/1	0.95	0.08	-3.77	74,74,74,74	0
54	MG	CA	1754	1/1	0.91	0.05	-3.83	74,74,74,74	0
54	MG	CA	1628	1/1	0.93	0.09	-3.88	75,75,75,75	0
54	MG	BA	3619	1/1	0.96	0.13	-3.92	64,64,64,64	0
54	MG	DA	3377	1/1	0.99	0.07	-3.95	33,33,33,33	0
54	MG	BA	3453	1/1	0.95	0.08	-3.95	46,46,46,46	0
54	MG	DA	3038	1/1	0.99	0.08	-4.01	37,37,37,37	0
54	MG	BA	3541	1/1	0.96	0.09	-4.20	42,42,42,42	0
54	MG	BA	3517	1/1	0.95	0.11	-4.21	26,26,26,26	0
54	MG	BA	3525	1/1	0.90	0.14	-4.25	35,35,35,35	0
54	MG	BA	3411	1/1	0.87	0.08	-4.26	63,63,63,63	0
54	MG	BA	3603	1/1	0.98	0.08	-4.48	40,40,40,40	0
54	MG	BA	3416	1/1	0.99	0.08	-4.54	25,25,25,25	0
54	MG	AA	1685	1/1	0.96	0.10	-4.57	71,71,71,71	0
54	MG	DA	3579	1/1	0.94	0.08	-4.64	57,57,57,57	0
54	MG	BA	3548	1/1	0.93	0.13	-4.65	29,29,29,29	0
54	MG	DA	3574	1/1	0.95	0.07	-4.70	41,41,41,41	0
54	MG	DA	3359	1/1	0.95	0.10	-4.72	33,33,33,33	0
54	MG	DA	3406	1/1	0.95	0.07	-4.75	58,58,58,58	0
54	MG	BA	3312	1/1	0.98	0.10	-4.78	51,51,51,51	0
54	MG	DA	3501	1/1	0.96	0.08	-4.81	58,58,58,58	0
54	MG	BA	3441	1/1	0.95	0.09	-4.99	56,56,56,56	0
54	MG	BA	3629	1/1	0.96	0.09	-5.05	24,24,24,24	0
54	MG	DA	3389	1/1	0.96	0.07	-5.08	51,51,51,51	0
54	MG	DA	3411	1/1	0.92	0.11	-5.15	49,49,49,49	0
54	MG	BA	3350	1/1	0.99	0.09	-5.27	40,40,40,40	0
54	MG	DA	3539	1/1	0.94	0.09	-5.39	67,67,67,67	0
54	MG	BA	3415	1/1	0.96	0.08	-5.46	33,33,33,33	0
54	MG	DA	3369	1/1	0.96	0.07	-5.55	50,50,50,50	0
54	MG	DA	3519	1/1	0.98	0.07	-5.68	52,52,52,52	0
54	MG	BA	3555	1/1	0.94	0.12	-6.01	47,47,47,47	0
54	MG	DA	3429	1/1	0.95	0.07	-6.08	56,56,56,56	0
54	MG	BA	3463	1/1	0.99	0.09	-6.12	28,28,28,28	0
54	MG	CA	1747	1/1	0.73	0.11	-6.23	95,95,95,95	0
54	MG	BA	3336	1/1	0.94	0.11	-6.35	45,45,45,45	0
54	MG	BA	3635	1/1	0.98	0.08	-6.89	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1715	1/1	0.97	0.10	-7.07	61,61,61,61	0
54	MG	BA	3591	1/1	0.99	0.10	-8.74	34,34,34,34	0
54	MG	BA	3348	1/1	0.93	0.08	-8.76	59,59,59,59	0
54	MG	BA	3430	1/1	0.98	0.06	-12.41	49,49,49,49	0
54	MG	CA	1614	1/1	0.94	0.44	-	85,85,85,85	0
54	MG	BA	3617	1/1	0.95	0.07	-	94,94,94,94	0
54	MG	DA	3298	1/1	0.79	0.26	-	49,49,49,49	0
54	MG	DA	3356	1/1	0.94	0.16	-	60,60,60,60	0
54	MG	DP	201	1/1	0.91	0.18	-	54,54,54,54	0
54	MG	BA	3244	1/1	0.95	0.14	-	30,30,30,30	0
54	MG	CA	1684	1/1	0.73	0.33	-	91,91,91,91	0
54	MG	BA	3477	1/1	0.80	0.11	-	53,53,53,53	0
54	MG	DA	3234	1/1	0.97	0.18	-	41,41,41,41	0
54	MG	AA	1641	1/1	0.98	0.17	-	42,42,42,42	0
54	MG	DA	3466	1/1	0.80	0.15	-	68,68,68,68	0
54	MG	BA	3319	1/1	0.99	0.12	-	54,54,54,54	0
54	MG	BA	3016	1/1	0.82	0.22	-	47,47,47,47	0
54	MG	CA	1735	1/1	0.94	0.28	-	69,69,69,69	0
54	MG	DA	3301	1/1	0.95	0.46	-	50,50,50,50	0
54	MG	CA	1760	1/1	0.97	0.09	-	87,87,87,87	0
54	MG	CA	1698	1/1	0.88	0.10	-	47,47,47,47	0
54	MG	DA	3024	1/1	0.85	0.35	-	47,47,47,47	0
54	MG	DA	3387	1/1	0.89	0.11	-	60,60,60,60	0
54	MG	DA	3510	1/1	0.94	0.10	-	74,74,74,74	0
54	MG	DA	3290	1/1	0.75	0.48	-	58,58,58,58	0
54	MG	CA	1707	1/1	0.80	0.19	-	94,94,94,94	0
54	MG	BA	3035	1/1	0.88	0.19	-	45,45,45,45	0
54	MG	BA	3516	1/1	0.92	0.25	-	63,63,63,63	0
54	MG	DA	3516	1/1	0.98	0.20	-	32,32,32,32	0
54	MG	DA	3526	1/1	0.85	0.12	-	98,98,98,98	0
54	MG	DA	3260	1/1	0.89	0.20	-	41,41,41,41	0
54	MG	BA	3339	1/1	0.85	0.11	-	70,70,70,70	0
54	MG	BA	3527	1/1	0.98	0.18	-	29,29,29,29	0
54	MG	DA	3073	1/1	0.89	0.52	-	68,68,68,68	0
54	MG	DA	3055	1/1	0.80	0.32	-	56,56,56,56	0
54	MG	B0	101	1/1	0.89	0.18	-	39,39,39,39	0
54	MG	BA	3160	1/1	0.96	0.36	-	39,39,39,39	0
54	MG	AA	1615	1/1	0.94	0.36	-	54,54,54,54	0
54	MG	BA	3115	1/1	0.93	0.12	-	45,45,45,45	0
54	MG	BA	3210	1/1	0.90	0.20	-	40,40,40,40	0
54	MG	BA	3377	1/1	0.91	0.22	-	32,32,32,32	0
54	MG	DA	3453	1/1	0.96	0.07	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3609	1/1	0.86	0.10	-	75,75,75,75	0
54	MG	BA	3288	1/1	0.85	0.21	-	66,66,66,66	0
54	MG	BA	3224	1/1	0.94	0.28	-	50,50,50,50	0
54	MG	DA	3278	1/1	0.67	0.07	-	83,83,83,83	0
54	MG	BA	3275	1/1	0.95	0.29	-	26,26,26,26	0
54	MG	CA	1695	1/1	0.90	0.35	-	50,50,50,50	0
54	MG	BA	3025	1/1	0.91	0.22	-	48,48,48,48	0
54	MG	AA	1724	1/1	0.97	0.28	-	74,74,74,74	0
54	MG	BA	3580	1/1	0.87	0.15	-	49,49,49,49	0
54	MG	BA	3274	1/1	0.97	0.29	-	26,26,26,26	0
54	MG	BA	3513	1/1	0.95	0.09	-	86,86,86,86	0
54	MG	BA	3565	1/1	0.93	0.07	-	68,68,68,68	0
54	MG	BA	3174	1/1	0.95	0.18	-	32,32,32,32	0
54	MG	CA	1649	1/1	0.86	0.41	-	66,66,66,66	0
54	MG	BA	3197	1/1	0.92	0.35	-	41,41,41,41	0
54	MG	DA	3423	1/1	0.98	0.16	-	32,32,32,32	0
54	MG	BB	218	1/1	0.91	0.09	-	45,45,45,45	0
54	MG	BA	3573	1/1	0.97	0.21	-	23,23,23,23	0
54	MG	BA	3640	1/1	0.96	0.14	-	116,116,116,116	0
54	MG	BA	3607	1/1	0.94	0.17	-	99,99,99,99	0
54	MG	CA	1639	1/1	0.89	0.26	-	76,76,76,76	0
54	MG	BA	3632	1/1	0.95	0.05	-	54,54,54,54	0
54	MG	AA	1661	1/1	0.82	0.26	-	55,55,55,55	0
54	MG	CA	1716	1/1	0.90	0.15	-	102,102,102,102	0
54	MG	DA	3383	1/1	0.88	0.10	-	54,54,54,54	0
54	MG	AA	1729	1/1	0.77	0.08	-	80,80,80,80	0
54	MG	BA	3150	1/1	0.92	0.12	-	42,42,42,42	0
54	MG	DA	3238	1/1	0.90	0.45	-	56,56,56,56	0
54	MG	DA	3489	1/1	0.92	0.14	-	79,79,79,79	0
54	MG	DA	3495	1/1	0.90	0.06	-	83,83,83,83	0
54	MG	DA	3200	1/1	0.92	0.25	-	34,34,34,34	0
54	MG	BB	211	1/1	0.90	0.21	-	47,47,47,47	0
54	MG	DA	3027	1/1	0.91	0.35	-	56,56,56,56	0
54	MG	DA	3108	1/1	0.95	0.11	-	42,42,42,42	0
54	MG	BA	3056	1/1	0.89	0.16	-	57,57,57,57	0
54	MG	BA	3657	1/1	0.95	0.46	-	65,65,65,65	0
54	MG	BB	207	1/1	0.86	0.20	-	52,52,52,52	0
54	MG	BA	3594	1/1	0.90	0.05	-	86,86,86,86	0
54	MG	BA	3276	1/1	0.96	0.24	-	23,23,23,23	0
54	MG	BA	3413	1/1	0.94	0.12	-	57,57,57,57	0
54	MG	BA	3295	1/1	0.93	0.59	-	54,54,54,54	0
54	MG	DA	3289	1/1	0.85	0.58	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3596	1/1	0.98	0.07	-	48,48,48,48	0
54	MG	BA	3304	1/1	0.83	0.35	-	54,54,54,54	0
54	MG	DA	3336	1/1	0.99	0.17	-	41,41,41,41	0
54	MG	BA	3003	1/1	0.91	0.30	-	74,74,74,74	0
54	MG	CA	1602	1/1	0.91	0.40	-	62,62,62,62	0
54	MG	B5	103	1/1	0.92	0.08	-	57,57,57,57	0
54	MG	BA	3023	1/1	0.97	0.14	-	52,52,52,52	0
54	MG	BA	3341	1/1	0.94	0.05	-	44,44,44,44	0
54	MG	DA	3445	1/1	0.92	0.17	-	42,42,42,42	0
54	MG	DA	3438	1/1	0.82	0.17	-	90,90,90,90	0
54	MG	AA	1682	1/1	0.90	0.13	-	76,76,76,76	0
54	MG	CA	1635	1/1	0.86	0.10	-	60,60,60,60	0
54	MG	BA	3365	1/1	0.97	0.07	-	69,69,69,69	0
54	MG	AA	1718	1/1	0.86	0.05	-	96,96,96,96	0
54	MG	CE	201	1/1	0.69	0.57	-	77,77,77,77	0
54	MG	DA	3572	1/1	0.98	0.10	-	71,71,71,71	0
54	MG	DA	3392	1/1	0.96	0.14	-	35,35,35,35	0
54	MG	BA	3179	1/1	0.89	0.27	-	37,37,37,37	0
54	MG	BA	3310	1/1	0.97	0.35	-	23,23,23,23	0
54	MG	CA	1623	1/1	0.97	0.39	-	43,43,43,43	0
54	MG	DA	3159	1/1	0.94	0.20	-	45,45,45,45	0
54	MG	BA	3387	1/1	0.94	0.06	-	63,63,63,63	0
54	MG	AA	1681	1/1	0.87	0.24	-	50,50,50,50	0
54	MG	DA	3458	1/1	0.89	0.05	-	62,62,62,62	0
54	MG	BA	3144	1/1	0.90	0.25	-	46,46,46,46	0
54	MG	BA	3334	1/1	0.97	0.10	-	51,51,51,51	0
54	MG	DA	3239	1/1	0.79	0.55	-	58,58,58,58	0
54	MG	CA	1632	1/1	0.85	0.27	-	69,69,69,69	0
54	MG	BA	3392	1/1	0.95	0.13	-	110,110,110,110	0
54	MG	DA	3101	1/1	0.98	0.19	-	39,39,39,39	0
54	MG	BA	3047	1/1	0.97	0.31	-	35,35,35,35	0
54	MG	BA	3546	1/1	0.91	0.18	-	73,73,73,73	0
54	MG	CA	1659	1/1	0.97	0.20	-	48,48,48,48	0
54	MG	BA	3234	1/1	0.81	0.15	-	69,69,69,69	0
54	MG	AA	1727	1/1	0.91	0.09	-	61,61,61,61	0
54	MG	CA	1673	1/1	0.91	0.60	-	57,57,57,57	0
54	MG	CA	1605	1/1	0.92	0.34	-	67,67,67,67	0
54	MG	CA	1638	1/1	0.89	0.26	-	52,52,52,52	0
54	MG	BA	3412	1/1	0.96	0.17	-	78,78,78,78	0
54	MG	DA	3254	1/1	0.88	0.19	-	64,64,64,64	0
54	MG	DA	3170	1/1	0.83	0.13	-	56,56,56,56	0
54	MG	BA	3436	1/1	0.93	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BV	201	1/1	0.79	0.22	-	67,67,67,67	0
54	MG	DA	3005	1/1	0.97	0.23	-	77,77,77,77	0
54	MG	DA	3372	1/1	0.90	0.15	-	41,41,41,41	0
54	MG	BA	3075	1/1	0.85	0.19	-	46,46,46,46	0
54	MG	DA	3330	1/1	0.98	0.12	-	37,37,37,37	0
54	MG	DA	3503	1/1	0.93	0.24	-	34,34,34,34	0
54	MG	BA	3630	1/1	0.98	0.08	-	34,34,34,34	0
54	MG	BA	3423	1/1	0.99	0.17	-	33,33,33,33	0
54	MG	BA	3277	1/1	0.98	0.37	-	22,22,22,22	0
54	MG	AA	1620	1/1	0.87	0.17	-	65,65,65,65	0
54	MG	AA	1704	1/1	0.79	0.16	-	86,86,86,86	0
54	MG	BA	3302	1/1	0.97	0.14	-	47,47,47,47	0
54	MG	DR	201	1/1	0.94	0.31	-	40,40,40,40	0
54	MG	AA	1698	1/1	0.98	0.15	-	69,69,69,69	0
54	MG	DA	3566	1/1	0.98	0.13	-	54,54,54,54	0
54	MG	AA	1655	1/1	0.90	0.47	-	43,43,43,43	0
54	MG	BA	3454	1/1	0.98	0.12	-	25,25,25,25	0
54	MG	DA	3322	1/1	0.90	0.39	-	49,49,49,49	0
54	MG	DA	3075	1/1	0.71	0.26	-	58,58,58,58	0
54	MG	BA	3410	1/1	0.91	0.09	-	77,77,77,77	0
54	MG	DA	3571	1/1	0.93	0.14	-	55,55,55,55	0
54	MG	DA	3285	1/1	0.97	0.04	-	64,64,64,64	0
54	MG	DB	203	1/1	0.95	0.40	-	58,58,58,58	0
54	MG	BA	3175	1/1	0.90	0.14	-	43,43,43,43	0
54	MG	BA	3581	1/1	0.79	0.11	-	86,86,86,86	0
54	MG	BA	3216	1/1	0.79	0.30	-	43,43,43,43	0
54	MG	DA	3457	1/1	0.88	0.08	-	64,64,64,64	0
54	MG	BA	3073	1/1	0.90	0.42	-	52,52,52,52	0
54	MG	BA	3086	1/1	0.90	0.95	-	57,57,57,57	0
54	MG	BA	3593	1/1	0.70	0.21	-	84,84,84,84	0
54	MG	DA	3424	1/1	0.80	0.10	-	52,52,52,52	0
54	MG	BA	3353	1/1	0.89	0.20	-	91,91,91,91	0
54	MG	DA	3118	1/1	0.94	0.24	-	43,43,43,43	0
54	MG	BA	3296	1/1	0.96	0.22	-	43,43,43,43	0
54	MG	AA	1665	1/1	0.96	0.10	-	51,51,51,51	0
54	MG	CA	1675	1/1	0.94	0.59	-	61,61,61,61	0
54	MG	AA	1687	1/1	0.95	0.18	-	62,62,62,62	0
54	MG	BA	3202	1/1	0.95	0.16	-	48,48,48,48	0
54	MG	BA	3647	1/1	0.96	0.15	-	70,70,70,70	0
54	MG	AA	1689	1/1	0.90	0.06	-	99,99,99,99	0
54	MG	DA	3598	1/1	0.95	0.11	-	76,76,76,76	0
54	MG	BB	214	1/1	0.97	0.12	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1634	1/1	0.92	0.18	-	64,64,64,64	0
54	MG	BA	3005	1/1	0.93	0.28	-	60,60,60,60	0
54	MG	BA	3018	1/1	0.85	0.60	-	40,40,40,40	0
54	MG	DA	3533	1/1	0.97	0.10	-	89,89,89,89	0
54	MG	DA	3058	1/1	0.74	0.43	-	58,58,58,58	0
54	MG	DA	3152	1/1	0.89	0.44	-	61,61,61,61	0
54	MG	BA	3559	1/1	0.93	0.07	-	71,71,71,71	0
54	MG	CA	1723	1/1	0.96	0.13	-	55,55,55,55	0
54	MG	AA	1609	1/1	0.87	0.27	-	51,51,51,51	0
54	MG	BA	3381	1/1	0.96	0.06	-	66,66,66,66	0
54	MG	CA	1686	1/1	0.81	0.21	-	61,61,61,61	0
54	MG	CA	1748	1/1	0.97	0.06	-	58,58,58,58	0
54	MG	BA	3002	1/1	0.89	0.34	-	51,51,51,51	0
54	MG	DA	3032	1/1	0.98	0.21	-	49,49,49,49	0
54	MG	DA	3472	1/1	0.95	0.33	-	50,50,50,50	0
54	MG	BA	3382	1/1	0.94	0.19	-	100,100,100,100	0
54	MG	CA	1739	1/1	0.89	0.12	-	87,87,87,87	0
54	MG	AA	1703	1/1	0.98	0.05	-	66,66,66,66	0
54	MG	BA	3222	1/1	0.89	0.49	-	60,60,60,60	0
54	MG	BA	3351	1/1	0.95	0.08	-	60,60,60,60	0
54	MG	AA	1720	1/1	0.97	0.07	-	68,68,68,68	0
54	MG	BA	3611	1/1	0.97	0.07	-	44,44,44,44	0
54	MG	AA	1604	1/1	0.88	0.15	-	73,73,73,73	0
54	MG	DA	3082	1/1	0.96	0.42	-	36,36,36,36	0
54	MG	BA	3486	1/1	0.85	0.17	-	75,75,75,75	0
54	MG	BA	3143	1/1	0.87	0.21	-	30,30,30,30	0
54	MG	BA	3442	1/1	0.70	0.16	-	76,76,76,76	0
54	MG	BA	3322	1/1	0.97	0.08	-	37,37,37,37	0
54	MG	CA	1744	1/1	0.97	0.06	-	83,83,83,83	0
54	MG	DA	3116	1/1	0.92	0.20	-	43,43,43,43	0
54	MG	B0	103	1/1	0.94	0.12	-	89,89,89,89	0
54	MG	BA	3345	1/1	0.98	0.10	-	71,71,71,71	0
54	MG	BP	201	1/1	0.84	0.13	-	45,45,45,45	0
54	MG	BA	3068	1/1	0.84	0.40	-	50,50,50,50	0
54	MG	BA	3124	1/1	0.92	0.19	-	33,33,33,33	0
54	MG	BA	3022	1/1	0.92	0.26	-	46,46,46,46	0
54	MG	DA	3287	1/1	0.89	0.27	-	57,57,57,57	0
54	MG	BA	3217	1/1	0.89	0.23	-	41,41,41,41	0
54	MG	BA	3044	1/1	0.99	0.08	-	33,33,33,33	0
54	MG	DA	3326	1/1	0.90	0.21	-	46,46,46,46	0
54	MG	D5	101	1/1	0.85	0.35	-	52,52,52,52	0
54	MG	BA	3263	1/1	0.96	0.38	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1646	1/1	0.82	0.22	-	59,59,59,59	0
54	MG	CA	1727	1/1	0.97	0.17	-	46,46,46,46	0
54	MG	DE	302	1/1	0.94	0.35	-	21,21,21,21	0
54	MG	BA	3652	1/1	0.96	0.06	-	97,97,97,97	0
54	MG	DA	3355	1/1	0.99	0.13	-	49,49,49,49	0
54	MG	DA	3388	1/1	0.97	0.14	-	43,43,43,43	0
54	MG	AA	1605	1/1	0.93	0.17	-	66,66,66,66	0
54	MG	BA	3106	1/1	0.96	0.22	-	52,52,52,52	0
54	MG	CA	1641	1/1	0.96	0.09	-	52,52,52,52	0
54	MG	BA	3128	1/1	0.86	0.18	-	49,49,49,49	0
54	MG	CA	1647	1/1	0.97	0.15	-	86,86,86,86	0
54	MG	DA	3384	1/1	0.89	0.08	-	45,45,45,45	0
54	MG	DA	3281	1/1	0.88	0.20	-	42,42,42,42	0
54	MG	BA	3646	1/1	0.76	0.18	-	142,142,142,142	0
54	MG	DA	3470	1/1	0.90	0.10	-	47,47,47,47	0
54	MG	DA	3025	1/1	0.85	0.27	-	49,49,49,49	0
54	MG	DA	3050	1/1	0.98	0.27	-	34,34,34,34	0
54	MG	BA	3119	1/1	0.88	0.34	-	42,42,42,42	0
54	MG	BA	3504	1/1	0.82	0.14	-	65,65,65,65	0
54	MG	BA	3024	1/1	0.90	0.39	-	41,41,41,41	0
54	MG	AA	1644	1/1	0.90	0.33	-	39,39,39,39	0
54	MG	DA	3295	1/1	0.90	0.25	-	59,59,59,59	0
54	MG	BA	3269	1/1	0.82	0.48	-	35,35,35,35	0
54	MG	BA	3562	1/1	0.82	0.13	-	59,59,59,59	0
54	MG	BA	3186	1/1	0.98	0.35	-	26,26,26,26	0
54	MG	DA	3256	1/1	0.93	0.24	-	52,52,52,52	0
54	MG	BA	3242	1/1	0.94	0.20	-	38,38,38,38	0
54	MG	DA	3560	1/1	0.95	0.14	-	57,57,57,57	0
54	MG	DA	3416	1/1	0.89	0.13	-	66,66,66,66	0
54	MG	DA	3481	1/1	0.93	0.44	-	61,61,61,61	0
54	MG	DA	3492	1/1	0.89	0.07	-	56,56,56,56	0
54	MG	BA	3589	1/1	0.90	0.18	-	94,94,94,94	0
54	MG	DA	3381	1/1	0.95	0.05	-	42,42,42,42	0
54	MG	CA	1643	1/1	0.93	0.22	-	70,70,70,70	0
54	MG	DA	3507	1/1	0.98	0.12	-	80,80,80,80	0
54	MG	BA	3342	1/1	0.89	0.15	-	32,32,32,32	0
54	MG	CA	1668	1/1	0.90	0.55	-	87,87,87,87	0
54	MG	DA	3525	1/1	0.81	0.16	-	106,106,106,106	0
54	MG	AA	1645	1/1	0.91	0.26	-	60,60,60,60	0
54	MG	BA	3362	1/1	0.96	0.11	-	43,43,43,43	0
54	MG	CA	1637	1/1	0.69	0.42	-	73,73,73,73	0
54	MG	CA	1617	1/1	0.88	0.13	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3123	1/1	0.85	0.27	-	43,43,43,43	0
54	MG	DB	202	1/1	0.92	0.21	-	50,50,50,50	0
54	MG	CA	1752	1/1	0.94	0.13	-	71,71,71,71	0
54	MG	DA	3443	1/1	0.93	0.11	-	75,75,75,75	0
54	MG	BA	3094	1/1	0.90	0.21	-	54,54,54,54	0
54	MG	AA	1722	1/1	0.94	0.18	-	66,66,66,66	0
54	MG	DA	3413	1/1	0.89	0.12	-	56,56,56,56	0
54	MG	DA	3109	1/1	0.89	0.17	-	59,59,59,59	0
54	MG	DA	3174	1/1	0.90	0.19	-	51,51,51,51	0
54	MG	CA	1651	1/1	0.87	0.35	-	46,46,46,46	0
54	MG	BA	3321	1/1	0.96	0.06	-	32,32,32,32	0
54	MG	DA	3001	1/1	0.87	0.31	-	48,48,48,48	0
54	MG	BA	3088	1/1	0.94	0.19	-	33,33,33,33	0
54	MG	BA	3243	1/1	0.89	0.30	-	42,42,42,42	0
54	MG	CA	1708	1/1	0.88	0.07	-	80,80,80,80	0
54	MG	DA	3323	1/1	0.95	0.13	-	40,40,40,40	0
54	MG	BA	3409	1/1	0.95	0.07	-	68,68,68,68	0
54	MG	DA	3098	1/1	0.90	0.19	-	37,37,37,37	0
54	MG	BA	3529	1/1	0.95	0.07	-	65,65,65,65	0
54	MG	BA	3550	1/1	0.91	0.06	-	87,87,87,87	0
54	MG	BA	3547	1/1	0.80	0.25	-	105,105,105,105	0
54	MG	BA	3588	1/1	0.95	0.12	-	64,64,64,64	0
54	MG	DA	3179	1/1	0.77	0.21	-	68,68,68,68	0
54	MG	BA	3624	1/1	0.97	0.11	-	36,36,36,36	0
54	MG	CA	1694	1/1	0.89	0.17	-	62,62,62,62	0
54	MG	BA	3053	1/1	0.93	0.44	-	57,57,57,57	0
54	MG	BA	3142	1/1	0.85	0.26	-	42,42,42,42	0
54	MG	BA	3198	1/1	0.98	0.12	-	44,44,44,44	0
54	MG	BA	3043	1/1	0.86	0.12	-	39,39,39,39	0
54	MG	DA	3265	1/1	0.94	0.32	-	44,44,44,44	0
54	MG	DA	3341	1/1	0.97	0.14	-	43,43,43,43	0
54	MG	BA	3582	1/1	0.80	0.23	-	79,79,79,79	0
54	MG	DA	3517	1/1	0.88	0.24	-	66,66,66,66	0
54	MG	CA	1650	1/1	0.91	0.21	-	60,60,60,60	0
54	MG	CA	1693	1/1	0.87	0.85	-	59,59,59,59	0
54	MG	BA	3621	1/1	0.88	0.30	-	52,52,52,52	0
54	MG	CA	1629	1/1	0.90	0.20	-	87,87,87,87	0
54	MG	DA	3049	1/1	0.88	0.19	-	49,49,49,49	0
54	MG	CA	1626	1/1	0.82	0.39	-	62,62,62,62	0
54	MG	DA	3292	1/1	0.94	0.27	-	33,33,33,33	0
54	MG	BA	3359	1/1	0.93	0.11	-	70,70,70,70	0
54	MG	DA	3270	1/1	0.91	0.17	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3208	1/1	0.96	0.39	-	53,53,53,53	0
54	MG	DA	3089	1/1	0.89	0.11	-	52,52,52,52	0
54	MG	CA	1721	1/1	0.97	0.21	-	64,64,64,64	0
54	MG	BA	3049	1/1	0.95	0.37	-	53,53,53,53	0
54	MG	BA	3427	1/1	0.87	0.14	-	89,89,89,89	0
54	MG	DA	3074	1/1	0.92	0.19	-	54,54,54,54	0
54	MG	CA	1601	1/1	0.96	0.21	-	45,45,45,45	0
54	MG	BA	3443	1/1	0.98	0.21	-	47,47,47,47	0
54	MG	CA	1669	1/1	0.94	0.31	-	76,76,76,76	0
54	MG	BA	3572	1/1	0.88	0.17	-	63,63,63,63	0
54	MG	BA	3148	1/1	0.96	0.23	-	47,47,47,47	0
54	MG	BA	3478	1/1	0.93	0.16	-	41,41,41,41	0
54	MG	AA	1710	1/1	0.97	0.07	-	79,79,79,79	0
54	MG	B1	101	1/1	0.95	0.18	-	45,45,45,45	0
54	MG	DA	3339	1/1	0.93	0.07	-	44,44,44,44	0
54	MG	BA	3567	1/1	0.83	0.10	-	54,54,54,54	0
54	MG	DA	3002	1/1	0.93	0.12	-	69,69,69,69	0
54	MG	BB	203	1/1	0.96	0.23	-	70,70,70,70	0
54	MG	DA	3297	1/1	0.82	0.22	-	78,78,78,78	0
54	MG	BA	3528	1/1	0.94	0.17	-	39,39,39,39	0
54	MG	BA	3526	1/1	0.92	0.13	-	22,22,22,22	0
54	MG	DA	3175	1/1	0.92	0.37	-	44,44,44,44	0
54	MG	BB	208	1/1	0.90	0.23	-	43,43,43,43	0
54	MG	AA	1730	1/1	0.90	0.10	-	51,51,51,51	0
54	MG	BA	3136	1/1	0.94	0.36	-	45,45,45,45	0
54	MG	BA	3426	1/1	0.94	0.08	-	37,37,37,37	0
54	MG	AA	1664	1/1	0.92	0.15	-	57,57,57,57	0
54	MG	DA	3460	1/1	0.92	0.19	-	65,65,65,65	0
54	MG	AA	1630	1/1	0.97	0.26	-	39,39,39,39	0
54	MG	BA	3406	1/1	0.94	0.06	-	66,66,66,66	0
54	MG	BA	3013	1/1	0.89	0.25	-	49,49,49,49	0
54	MG	BA	3101	1/1	0.91	0.11	-	37,37,37,37	0
54	MG	CA	1687	1/1	0.96	0.22	-	62,62,62,62	0
54	MG	BA	3418	1/1	0.91	0.12	-	49,49,49,49	0
54	MG	DA	3259	1/1	0.93	0.18	-	43,43,43,43	0
54	MG	DA	3087	1/1	0.88	0.09	-	54,54,54,54	0
54	MG	DA	3394	1/1	0.98	0.06	-	47,47,47,47	0
54	MG	DA	3187	1/1	0.74	0.14	-	71,71,71,71	0
54	MG	AA	1614	1/1	0.69	0.50	-	56,56,56,56	0
54	MG	DA	3291	1/1	0.94	0.32	-	53,53,53,53	0
54	MG	BA	3099	1/1	0.98	0.16	-	46,46,46,46	0
54	MG	DA	3437	1/1	0.89	0.16	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3451	1/1	0.82	0.14	-	103,103,103,103	0
54	MG	BA	3092	1/1	0.97	0.40	-	26,26,26,26	0
54	MG	DA	3399	1/1	0.97	0.11	-	51,51,51,51	0
54	MG	AA	1603	1/1	0.67	0.36	-	79,79,79,79	0
54	MG	AA	1656	1/1	0.91	0.58	-	59,59,59,59	0
54	MG	BA	3223	1/1	0.96	0.51	-	60,60,60,60	0
54	MG	BA	3228	1/1	0.95	0.40	-	37,37,37,37	0
54	MG	AA	1617	1/1	0.91	0.17	-	45,45,45,45	0
54	MG	AA	1678	1/1	0.74	0.53	-	74,74,74,74	0
54	MG	BA	3241	1/1	0.80	0.23	-	65,65,65,65	0
54	MG	DA	3534	1/1	0.96	0.14	-	28,28,28,28	0
54	MG	BA	3479	1/1	0.93	0.18	-	32,32,32,32	0
54	MG	CA	1606	1/1	0.86	0.24	-	59,59,59,59	0
54	MG	BA	3180	1/1	0.93	0.29	-	41,41,41,41	0
54	MG	BA	3229	1/1	0.90	0.22	-	41,41,41,41	0
54	MG	BD	302	1/1	0.90	0.21	-	28,28,28,28	0
54	MG	BA	3165	1/1	0.94	0.28	-	51,51,51,51	0
54	MG	DA	3464	1/1	0.89	0.10	-	89,89,89,89	0
54	MG	DA	3056	1/1	0.95	0.18	-	43,43,43,43	0
54	MG	DA	3235	1/1	0.88	0.37	-	54,54,54,54	0
54	MG	BA	3329	1/1	0.85	0.19	-	74,74,74,74	0
54	MG	BA	3260	1/1	0.97	0.39	-	30,30,30,30	0
54	MG	BA	3138	1/1	0.91	0.35	-	42,42,42,42	0
54	MG	AA	1638	1/1	0.88	0.13	-	53,53,53,53	0
54	MG	DA	3117	1/1	0.93	0.17	-	47,47,47,47	0
54	MG	DA	3557	1/1	0.83	0.16	-	103,103,103,103	0
54	MG	DA	3523	1/1	0.84	0.07	-	74,74,74,74	0
54	MG	BA	3434	1/1	0.97	0.11	-	62,62,62,62	0
54	MG	DA	3446	1/1	0.98	0.24	-	42,42,42,42	0
54	MG	BA	3343	1/1	0.83	0.09	-	73,73,73,73	0
54	MG	DA	3103	1/1	0.92	0.17	-	54,54,54,54	0
54	MG	BA	3536	1/1	0.92	0.08	-	68,68,68,68	0
54	MG	BA	3055	1/1	0.91	0.20	-	53,53,53,53	0
54	MG	BA	3214	1/1	0.88	0.22	-	52,52,52,52	0
54	MG	CA	1702	1/1	0.82	0.12	-	64,64,64,64	0
54	MG	DA	3409	1/1	0.92	0.09	-	73,73,73,73	0
54	MG	BB	209	1/1	0.87	0.11	-	60,60,60,60	0
54	MG	BB	210	1/1	0.90	0.15	-	60,60,60,60	0
54	MG	BQ	201	1/1	0.86	0.19	-	51,51,51,51	0
54	MG	DA	3594	1/1	0.99	0.18	-	58,58,58,58	0
54	MG	CA	1609	1/1	0.90	0.24	-	70,70,70,70	0
54	MG	DA	3597	1/1	0.90	0.11	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3379	1/1	0.94	0.09	-	22,22,22,22	0
54	MG	BA	3163	1/1	0.97	0.28	-	23,23,23,23	0
54	MG	CA	1604	1/1	0.71	0.51	-	81,81,81,81	0
54	MG	CA	1677	1/1	0.85	0.15	-	64,64,64,64	0
54	MG	BA	3111	1/1	0.93	0.20	-	56,56,56,56	0
54	MG	DA	3102	1/1	0.97	0.47	-	40,40,40,40	0
54	MG	BA	3422	1/1	0.92	0.17	-	76,76,76,76	0
54	MG	DA	3589	1/1	0.87	0.12	-	75,75,75,75	0
54	MG	DA	3546	1/1	0.95	0.11	-	64,64,64,64	0
54	MG	BA	3639	1/1	0.95	0.20	-	65,65,65,65	0
54	MG	DA	3246	1/1	0.82	0.38	-	68,68,68,68	0
54	MG	BA	3465	1/1	0.98	0.15	-	44,44,44,44	0
54	MG	DA	3478	1/1	0.81	0.17	-	87,87,87,87	0
54	MG	DA	3463	1/1	0.98	0.09	-	69,69,69,69	0
54	MG	DA	3264	1/1	0.93	0.46	-	61,61,61,61	0
54	MG	DA	3019	1/1	0.93	0.16	-	40,40,40,40	0
54	MG	BA	3152	1/1	0.90	0.37	-	54,54,54,54	0
54	MG	BA	3041	1/1	0.93	0.26	-	40,40,40,40	0
54	MG	BA	3564	1/1	0.92	0.11	-	59,59,59,59	0
54	MG	CA	1656	1/1	0.90	0.31	-	86,86,86,86	0
54	MG	DA	3273	1/1	0.88	0.33	-	50,50,50,50	0
54	MG	BA	3090	1/1	0.84	0.12	-	62,62,62,62	0
54	MG	DA	3245	1/1	0.87	0.28	-	57,57,57,57	0
54	MG	BA	3289	1/1	0.97	0.34	-	34,34,34,34	0
54	MG	DA	3334	1/1	0.98	0.12	-	52,52,52,52	0
54	MG	DA	3188	1/1	0.87	0.11	-	69,69,69,69	0
54	MG	AA	1667	1/1	0.95	0.19	-	38,38,38,38	0
54	MG	CA	1701	1/1	0.89	0.08	-	72,72,72,72	0
54	MG	CA	1660	1/1	0.51	0.41	-	70,70,70,70	0
54	MG	BA	3303	1/1	0.88	0.11	-	64,64,64,64	0
54	MG	CA	1697	1/1	0.77	0.13	-	57,57,57,57	0
54	MG	DA	3340	1/1	0.93	0.12	-	45,45,45,45	0
54	MG	BA	3470	1/1	0.88	0.27	-	60,60,60,60	0
54	MG	BA	3637	1/1	0.83	0.18	-	108,108,108,108	0
54	MG	BA	3239	1/1	0.67	0.14	-	67,67,67,67	0
54	MG	BA	3518	1/1	0.96	0.10	-	50,50,50,50	0
54	MG	DA	3483	1/1	0.98	0.26	-	59,59,59,59	0
54	MG	BA	3204	1/1	0.93	0.13	-	38,38,38,38	0
54	MG	DA	3261	1/1	0.90	0.32	-	44,44,44,44	0
54	MG	DA	3475	1/1	0.96	0.11	-	30,30,30,30	0
54	MG	BA	3489	1/1	0.97	0.15	-	23,23,23,23	0
54	MG	CA	1664	1/1	0.83	0.08	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3449	1/1	0.94	0.30	-	29,29,29,29	0
54	MG	DA	3134	1/1	0.81	0.28	-	62,62,62,62	0
54	MG	BA	3437	1/1	0.86	0.11	-	49,49,49,49	0
54	MG	AA	1653	1/1	0.98	0.08	-	49,49,49,49	0
54	MG	DA	3561	1/1	0.94	0.19	-	71,71,71,71	0
54	MG	BA	3096	1/1	0.92	0.44	-	47,47,47,47	0
54	MG	DA	3410	1/1	0.61	0.12	-	86,86,86,86	0
54	MG	DA	3368	1/1	0.86	0.16	-	52,52,52,52	0
54	MG	DA	3468	1/1	0.94	0.07	-	53,53,53,53	0
54	MG	AA	1647	1/1	0.86	0.23	-	55,55,55,55	0
54	MG	AA	1688	1/1	0.76	0.15	-	96,96,96,96	0
54	MG	BA	3597	1/1	0.96	0.24	-	84,84,84,84	0
54	MG	DA	3161	1/1	0.95	0.34	-	39,39,39,39	0
54	MG	BA	3575	1/1	0.98	0.08	-	41,41,41,41	0
54	MG	BS	201	1/1	0.83	0.54	-	49,49,49,49	0
54	MG	DA	3435	1/1	0.88	0.45	-	57,57,57,57	0
54	MG	BA	3272	1/1	0.94	0.38	-	31,31,31,31	0
54	MG	BA	3320	1/1	0.98	0.17	-	42,42,42,42	0
54	MG	BA	3429	1/1	0.96	0.21	-	47,47,47,47	0
54	MG	DA	3142	1/1	0.92	0.21	-	37,37,37,37	0
54	MG	BA	3238	1/1	0.79	0.36	-	53,53,53,53	0
54	MG	DA	3057	1/1	0.94	0.15	-	35,35,35,35	0
54	MG	CA	1646	1/1	0.89	0.38	-	59,59,59,59	0
54	MG	BA	3354	1/1	0.94	0.09	-	37,37,37,37	0
54	MG	DA	3147	1/1	0.89	0.42	-	54,54,54,54	0
54	MG	DA	3240	1/1	0.98	0.15	-	53,53,53,53	0
54	MG	BA	3644	1/1	0.97	0.08	-	88,88,88,88	0
54	MG	BA	3232	1/1	0.53	0.18	-	64,64,64,64	0
54	MG	CA	1610	1/1	0.93	0.29	-	60,60,60,60	0
54	MG	DA	3031	1/1	0.92	0.23	-	53,53,53,53	0
54	MG	DA	3331	1/1	0.76	0.13	-	71,71,71,71	0
54	MG	BA	3373	1/1	0.93	0.08	-	44,44,44,44	0
54	MG	AA	1621	1/1	0.89	0.29	-	62,62,62,62	0
54	MG	DA	3365	1/1	0.97	0.08	-	40,40,40,40	0
54	MG	CA	1691	1/1	0.95	0.43	-	51,51,51,51	0
54	MG	DA	3521	1/1	0.86	0.12	-	86,86,86,86	0
54	MG	DA	3391	1/1	0.87	0.09	-	37,37,37,37	0
54	MG	DA	3407	1/1	0.93	0.06	-	70,70,70,70	0
54	MG	DA	3233	1/1	0.95	0.14	-	38,38,38,38	0
54	MG	BA	3299	1/1	0.97	0.27	-	66,66,66,66	0
54	MG	BA	3655	1/1	0.88	0.18	-	104,104,104,104	0
54	MG	BA	3557	1/1	0.86	0.15	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1652	1/1	0.97	0.25	-	49,49,49,49	0
54	MG	BA	3460	1/1	0.95	0.30	-	61,61,61,61	0
54	MG	BA	3051	1/1	0.97	0.17	-	48,48,48,48	0
54	MG	CA	1730	1/1	0.96	0.10	-	62,62,62,62	0
54	MG	BA	3112	1/1	0.96	0.19	-	55,55,55,55	0
54	MG	DA	3140	1/1	0.95	0.33	-	64,64,64,64	0
54	MG	DA	3505	1/1	0.93	0.12	-	91,91,91,91	0
54	MG	BA	3156	1/1	0.97	0.27	-	39,39,39,39	0
54	MG	BA	3519	1/1	0.94	0.05	-	64,64,64,64	0
54	MG	DA	3282	1/1	0.83	0.14	-	64,64,64,64	0
54	MG	DA	3003	1/1	0.88	0.22	-	46,46,46,46	0
54	MG	DA	3316	1/1	0.93	0.73	-	69,69,69,69	0
54	MG	DA	3490	1/1	0.97	0.12	-	33,33,33,33	0
54	MG	DA	3026	1/1	0.95	0.08	-	39,39,39,39	0
54	MG	BA	3417	1/1	0.93	0.08	-	48,48,48,48	0
54	MG	DA	3415	1/1	0.97	0.11	-	43,43,43,43	0
54	MG	DA	3149	1/1	0.81	0.37	-	53,53,53,53	0
54	MG	DA	3551	1/1	0.94	0.19	-	62,62,62,62	0
54	MG	DA	3328	1/1	0.87	0.40	-	57,57,57,57	0
54	MG	DA	3344	1/1	0.94	0.09	-	30,30,30,30	0
54	MG	DA	3479	1/1	0.90	0.15	-	62,62,62,62	0
54	MG	DA	3461	1/1	0.93	0.15	-	41,41,41,41	0
54	MG	BA	3093	1/1	0.95	0.19	-	42,42,42,42	0
54	MG	DQ	201	1/1	0.94	0.15	-	40,40,40,40	0
54	MG	BA	3658	1/1	0.84	0.14	-	114,114,114,114	0
54	MG	DA	3313	1/1	0.95	0.36	-	29,29,29,29	0
54	MG	BA	3654	1/1	0.57	0.15	-	126,126,126,126	0
54	MG	BA	3542	1/1	0.94	0.11	-	83,83,83,83	0
54	MG	CA	1714	1/1	0.82	0.15	-	87,87,87,87	0
54	MG	DB	206	1/1	0.97	0.26	-	58,58,58,58	0
54	MG	BA	3440	1/1	0.96	0.07	-	46,46,46,46	0
54	MG	AA	1642	1/1	0.88	0.82	-	54,54,54,54	0
54	MG	BA	3476	1/1	0.95	0.18	-	49,49,49,49	0
54	MG	BA	3286	1/1	0.95	0.46	-	52,52,52,52	0
54	MG	DA	3072	1/1	0.94	0.49	-	50,50,50,50	0
54	MG	BR	201	1/1	0.96	0.17	-	29,29,29,29	0
54	MG	DA	3586	1/1	0.93	0.14	-	49,49,49,49	0
54	MG	CA	1756	1/1	0.82	0.19	-	80,80,80,80	0
54	MG	AA	1627	1/1	0.86	0.33	-	59,59,59,59	0
54	MG	DA	3132	1/1	0.89	0.42	-	49,49,49,49	0
54	MG	DA	3121	1/1	0.97	0.13	-	34,34,34,34	0
54	MG	BA	3376	1/1	0.96	0.11	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	223	1/1	0.75	0.14	-	133,133,133,133	0
54	MG	DA	3085	1/1	0.93	0.22	-	43,43,43,43	0
54	MG	BA	3203	1/1	0.87	0.50	-	55,55,55,55	0
54	MG	BQ	202	1/1	0.93	0.21	-	34,34,34,34	0
54	MG	AA	1676	1/1	0.85	0.30	-	59,59,59,59	0
54	MG	AA	1669	1/1	0.15	0.17	-	103,103,103,103	0
54	MG	BB	204	1/1	0.86	0.21	-	52,52,52,52	0
54	MG	DA	3111	1/1	0.90	0.17	-	50,50,50,50	0
54	MG	DB	208	1/1	0.96	0.10	-	104,104,104,104	0
54	MG	BA	3017	1/1	0.91	0.14	-	31,31,31,31	0
54	MG	DA	3129	1/1	0.92	0.13	-	61,61,61,61	0
54	MG	DA	3343	1/1	0.92	0.06	-	37,37,37,37	0
54	MG	DA	3194	1/1	0.93	0.23	-	37,37,37,37	0
54	MG	CA	1648	1/1	0.89	0.41	-	60,60,60,60	0
54	MG	DA	3210	1/1	0.95	0.26	-	53,53,53,53	0
54	MG	BA	3656	1/1	0.92	0.16	-	68,68,68,68	0
54	MG	BA	3162	1/1	0.92	0.35	-	42,42,42,42	0
54	MG	BE	302	1/1	0.93	0.20	-	41,41,41,41	0
54	MG	BA	3367	1/1	0.67	0.20	-	71,71,71,71	0
54	MG	BA	3522	1/1	0.93	0.11	-	74,74,74,74	0
54	MG	DA	3181	1/1	0.98	0.28	-	49,49,49,49	0
54	MG	DA	3166	1/1	0.91	0.29	-	45,45,45,45	0
54	MG	DA	3021	1/1	0.93	0.13	-	51,51,51,51	0
54	MG	BA	3501	1/1	0.99	0.10	-	29,29,29,29	0
54	MG	DA	3018	1/1	0.96	0.20	-	54,54,54,54	0
54	MG	DA	3588	1/1	0.93	0.18	-	34,34,34,34	0
54	MG	DA	3542	1/1	0.91	0.07	-	83,83,83,83	0
54	MG	DA	3158	1/1	0.96	0.30	-	46,46,46,46	0
54	MG	BA	3066	1/1	0.97	0.35	-	39,39,39,39	0
54	MG	DA	3462	1/1	0.94	0.12	-	51,51,51,51	0
54	MG	BA	3307	1/1	0.97	0.11	-	44,44,44,44	0
54	MG	DA	3482	1/1	0.94	0.19	-	56,56,56,56	0
54	MG	BA	3533	1/1	0.95	0.14	-	61,61,61,61	0
54	MG	BA	3626	1/1	0.91	0.09	-	64,64,64,64	0
54	MG	DA	3028	1/1	0.85	0.31	-	67,67,67,67	0
54	MG	BB	216	1/1	0.89	0.10	-	82,82,82,82	0
54	MG	DA	3500	1/1	0.90	0.12	-	74,74,74,74	0
54	MG	DA	3547	1/1	0.96	0.17	-	29,29,29,29	0
54	MG	BA	3602	1/1	0.97	0.05	-	56,56,56,56	0
54	MG	AA	1735	1/1	0.93	0.16	-	110,110,110,110	0
54	MG	BA	3153	1/1	0.88	0.37	-	51,51,51,51	0
54	MG	BA	3201	1/1	0.93	0.33	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1743	1/1	0.97	0.08	-	61,61,61,61	0
54	MG	AA	1733	1/1	0.94	0.07	-	78,78,78,78	0
54	MG	CA	1753	1/1	0.81	0.14	-	86,86,86,86	0
54	MG	BQ	203	1/1	0.96	0.12	-	73,73,73,73	0
54	MG	BA	3133	1/1	0.78	0.26	-	53,53,53,53	0
54	MG	CA	1653	1/1	0.94	0.81	-	57,57,57,57	0
54	MG	BA	3184	1/1	0.97	0.22	-	40,40,40,40	0
54	MG	DB	205	1/1	0.97	0.16	-	55,55,55,55	0
54	MG	DA	3427	1/1	0.92	0.06	-	59,59,59,59	0
54	MG	DA	3094	1/1	0.90	0.16	-	56,56,56,56	0
54	MG	BA	3297	1/1	0.89	0.26	-	46,46,46,46	0
54	MG	BA	3383	1/1	0.94	0.13	-	70,70,70,70	0
54	MG	BA	3219	1/1	0.88	0.15	-	46,46,46,46	0
54	MG	DA	3201	1/1	0.88	0.30	-	49,49,49,49	0
54	MG	DA	3439	1/1	0.95	0.07	-	57,57,57,57	0
54	MG	DA	3567	1/1	0.85	0.24	-	46,46,46,46	0
54	MG	BA	3038	1/1	0.76	0.26	-	76,76,76,76	0
54	MG	BA	3080	1/1	0.89	0.23	-	39,39,39,39	0
54	MG	BW	202	1/1	0.95	0.12	-	33,33,33,33	0
54	MG	DA	3271	1/1	0.84	0.38	-	57,57,57,57	0
54	MG	BA	3291	1/1	0.93	0.13	-	39,39,39,39	0
54	MG	DA	3390	1/1	0.96	0.07	-	47,47,47,47	0
54	MG	AA	1651	1/1	0.70	0.31	-	60,60,60,60	0
54	MG	DA	3518	1/1	0.97	0.09	-	69,69,69,69	0
54	MG	CA	1738	1/1	0.86	0.08	-	112,112,112,112	0
54	MG	DA	3046	1/1	0.93	0.19	-	42,42,42,42	0
54	MG	BA	3095	1/1	0.93	0.19	-	48,48,48,48	0
54	MG	DA	3583	1/1	0.88	0.10	-	65,65,65,65	0
54	MG	BA	3570	1/1	0.55	0.12	-	78,78,78,78	0
54	MG	CA	1662	1/1	0.93	0.40	-	75,75,75,75	0
54	MG	BA	3625	1/1	0.96	0.06	-	53,53,53,53	0
54	MG	CA	1640	1/1	0.75	0.23	-	82,82,82,82	0
54	MG	CA	1712	1/1	0.93	0.28	-	87,87,87,87	0
54	MG	BA	3540	1/1	0.97	0.14	-	35,35,35,35	0
54	MG	BA	3199	1/1	0.96	0.14	-	41,41,41,41	0
54	MG	AA	1731	1/1	0.81	0.17	-	119,119,119,119	0
54	MG	AA	1683	1/1	0.90	0.65	-	58,58,58,58	0
54	MG	DA	3218	1/1	0.90	0.65	-	62,62,62,62	0
54	MG	DA	3258	1/1	0.85	0.45	-	52,52,52,52	0
54	MG	DA	3348	1/1	0.96	0.15	-	41,41,41,41	0
54	MG	BA	3137	1/1	0.92	0.23	-	38,38,38,38	0
54	MG	BA	3404	1/1	0.93	0.10	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BW	201	1/1	0.98	0.12	-	32,32,32,32	0
54	MG	BA	3181	1/1	0.93	0.20	-	38,38,38,38	0
54	MG	DA	3430	1/1	0.96	0.12	-	30,30,30,30	0
54	MG	DA	3569	1/1	0.83	0.12	-	104,104,104,104	0
54	MG	DA	3432	1/1	0.92	0.10	-	70,70,70,70	0
54	MG	DA	3113	1/1	0.93	0.42	-	59,59,59,59	0
54	MG	BA	3520	1/1	0.94	0.14	-	95,95,95,95	0
54	MG	BA	3613	1/1	0.94	0.07	-	65,65,65,65	0
54	MG	DA	3095	1/1	0.93	0.24	-	53,53,53,53	0
54	MG	BA	3113	1/1	0.77	0.09	-	60,60,60,60	0
54	MG	DA	3508	1/1	0.89	0.10	-	60,60,60,60	0
54	MG	BA	3059	1/1	0.96	0.12	-	48,48,48,48	0
54	MG	BT	202	1/1	0.89	0.28	-	52,52,52,52	0
54	MG	BA	3032	1/1	0.98	0.09	-	40,40,40,40	0
54	MG	BA	3561	1/1	0.96	0.09	-	54,54,54,54	0
54	MG	DA	3180	1/1	0.82	0.24	-	49,49,49,49	0
54	MG	B0	102	1/1	0.96	0.16	-	54,54,54,54	0
54	MG	DQ	202	1/1	0.89	0.17	-	33,33,33,33	0
54	MG	BA	3120	1/1	0.87	0.13	-	51,51,51,51	0
54	MG	BA	3375	1/1	0.98	0.16	-	34,34,34,34	0
54	MG	BA	3493	1/1	0.97	0.20	-	40,40,40,40	0
54	MG	BA	3173	1/1	0.98	0.40	-	32,32,32,32	0
54	MG	BA	3118	1/1	0.97	0.22	-	44,44,44,44	0
54	MG	CA	1745	1/1	0.91	0.34	-	116,116,116,116	0
54	MG	AA	1690	1/1	0.80	0.09	-	72,72,72,72	0
54	MG	DA	3176	1/1	0.87	0.42	-	70,70,70,70	0
54	MG	AA	1717	1/1	0.46	0.14	-	93,93,93,93	0
54	MG	BA	3091	1/1	0.91	0.35	-	40,40,40,40	0
54	MG	BA	3539	1/1	0.89	0.08	-	47,47,47,47	0
54	MG	BA	3258	1/1	0.92	0.38	-	55,55,55,55	0
54	MG	DA	3097	1/1	0.97	0.27	-	23,23,23,23	0
54	MG	DA	3497	1/1	0.84	0.26	-	83,83,83,83	0
54	MG	DA	3426	1/1	0.93	0.07	-	81,81,81,81	0
54	MG	BA	3330	1/1	0.92	0.13	-	34,34,34,34	0
54	MG	AA	1719	1/1	0.78	0.17	-	144,144,144,144	0
54	MG	BA	3183	1/1	0.91	0.34	-	29,29,29,29	0
54	MG	CA	1670	1/1	0.77	0.64	-	73,73,73,73	0
54	MG	CA	1663	1/1	0.93	0.34	-	64,64,64,64	0
54	MG	DA	3204	1/1	0.94	0.44	-	43,43,43,43	0
54	MG	DA	3122	1/1	0.84	0.20	-	49,49,49,49	0
54	MG	CA	1672	1/1	0.89	0.20	-	66,66,66,66	0
54	MG	DA	3538	1/1	0.92	0.13	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3071	1/1	0.95	0.17	-	34,34,34,34	0
54	MG	BA	3009	1/1	0.93	0.29	-	45,45,45,45	0
54	MG	DA	3433	1/1	0.86	0.12	-	47,47,47,47	0
54	MG	BA	3014	1/1	0.80	0.55	-	65,65,65,65	0
54	MG	BA	3211	1/1	0.96	0.09	-	26,26,26,26	0
54	MG	AA	1613	1/1	0.92	0.19	-	65,65,65,65	0
54	MG	AA	1714	1/1	0.92	0.25	-	57,57,57,57	0
54	MG	BA	3196	1/1	0.93	0.17	-	46,46,46,46	0
54	MG	BA	3643	1/1	0.94	0.10	-	59,59,59,59	0
54	MG	AA	1673	1/1	0.94	0.59	-	60,60,60,60	0
54	MG	BA	3149	1/1	0.84	0.28	-	57,57,57,57	0
54	MG	DA	3084	1/1	0.95	0.25	-	37,37,37,37	0
54	MG	DA	3274	1/1	0.90	0.41	-	61,61,61,61	0
54	MG	CA	1761	1/1	0.98	0.18	-	65,65,65,65	0
54	MG	AA	1632	1/1	0.92	0.21	-	71,71,71,71	0
54	MG	BA	3308	1/1	0.92	0.17	-	52,52,52,52	0
54	MG	BA	3122	1/1	0.94	0.31	-	49,49,49,49	0
54	MG	DA	3226	1/1	0.94	0.50	-	55,55,55,55	0
54	MG	BA	3114	1/1	0.85	0.32	-	63,63,63,63	0
54	MG	AA	1734	1/1	0.87	0.11	-	96,96,96,96	0
54	MG	BA	3494	1/1	0.97	0.13	-	34,34,34,34	0
54	MG	BA	3394	1/1	0.81	0.14	-	50,50,50,50	0
54	MG	DA	3192	1/1	0.93	0.17	-	50,50,50,50	0
54	MG	BA	3317	1/1	0.76	0.17	-	34,34,34,34	0
54	MG	AA	1716	1/1	0.89	0.08	-	116,116,116,116	0
54	MG	DB	207	1/1	0.96	0.24	-	57,57,57,57	0
54	MG	BA	3554	1/1	0.69	0.10	-	88,88,88,88	0
54	MG	DA	3065	1/1	0.84	0.14	-	53,53,53,53	0
54	MG	BA	3220	1/1	0.94	0.28	-	31,31,31,31	0
54	MG	DA	3349	1/1	0.95	0.15	-	35,35,35,35	0
54	MG	BA	3407	1/1	0.89	0.17	-	47,47,47,47	0
54	MG	DA	3512	1/1	0.89	0.13	-	42,42,42,42	0
54	MG	DA	3067	1/1	0.95	0.23	-	49,49,49,49	0
54	MG	BA	3641	1/1	0.92	0.21	-	72,72,72,72	0
54	MG	DA	3199	1/1	0.93	0.18	-	44,44,44,44	0
54	MG	DA	3467	1/1	0.97	0.11	-	43,43,43,43	0
54	MG	BA	3352	1/1	0.97	0.14	-	81,81,81,81	0
54	MG	DA	3367	1/1	0.96	0.24	-	30,30,30,30	0
54	MG	AA	1732	1/1	0.94	0.10	-	94,94,94,94	0
54	MG	DA	3250	1/1	0.94	0.17	-	49,49,49,49	0
54	MG	DA	3088	1/1	0.97	0.39	-	55,55,55,55	0
54	MG	AA	1628	1/1	0.78	0.25	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3057	1/1	0.97	0.24	-	51,51,51,51	0
54	MG	BA	3361	1/1	0.98	0.04	-	59,59,59,59	0
54	MG	AA	1637	1/1	0.69	0.24	-	84,84,84,84	0
54	MG	CA	1717	1/1	0.82	0.14	-	110,110,110,110	0
54	MG	BA	3532	1/1	0.74	0.23	-	79,79,79,79	0
54	MG	CA	1734	1/1	0.95	0.23	-	66,66,66,66	0
54	MG	BA	3390	1/1	0.92	0.08	-	62,62,62,62	0
54	MG	DA	3081	1/1	0.70	0.59	-	58,58,58,58	0
54	MG	DA	3553	1/1	0.95	0.08	-	54,54,54,54	0
54	MG	BA	3178	1/1	0.97	0.29	-	43,43,43,43	0
54	MG	DA	3488	1/1	0.85	0.17	-	58,58,58,58	0
54	MG	CA	1671	1/1	0.94	0.43	-	49,49,49,49	0
54	MG	BA	3357	1/1	0.99	0.16	-	25,25,25,25	0
54	MG	BA	3549	1/1	0.98	0.05	-	55,55,55,55	0
54	MG	DA	3299	1/1	0.95	0.43	-	65,65,65,65	0
54	MG	DA	3212	1/1	0.72	0.27	-	75,75,75,75	0
54	MG	BA	3230	1/1	0.91	0.20	-	30,30,30,30	0
54	MG	AA	1643	1/1	0.93	0.59	-	47,47,47,47	0
54	MG	CA	1679	1/1	0.86	0.51	-	59,59,59,59	0
54	MG	BA	3660	1/1	0.93	0.13	-	104,104,104,104	0
54	MG	DA	3577	1/1	0.98	0.09	-	57,57,57,57	0
54	MG	AA	1721	1/1	0.97	0.06	-	62,62,62,62	0
54	MG	DA	3436	1/1	0.85	0.14	-	81,81,81,81	0
54	MG	BA	3292	1/1	0.88	0.32	-	70,70,70,70	0
54	MG	DA	3318	1/1	0.87	0.14	-	58,58,58,58	0
54	MG	BA	3235	1/1	0.94	0.20	-	50,50,50,50	0
54	MG	DE	303	1/1	0.89	0.12	-	45,45,45,45	0
54	MG	DA	3035	1/1	0.94	0.17	-	60,60,60,60	0
54	MG	BA	3121	1/1	0.98	0.33	-	36,36,36,36	0
54	MG	BA	3131	1/1	0.89	0.82	-	62,62,62,62	0
54	MG	DA	3498	1/1	0.96	0.10	-	28,28,28,28	0
54	MG	BA	3318	1/1	0.92	0.20	-	35,35,35,35	0
54	MG	CA	1688	1/1	0.97	0.35	-	54,54,54,54	0
54	MG	BA	3125	1/1	0.95	0.31	-	45,45,45,45	0
54	MG	DA	3154	1/1	0.95	0.33	-	26,26,26,26	0
54	MG	BA	3388	1/1	0.85	0.10	-	47,47,47,47	0
54	MG	BA	3077	1/1	0.84	0.27	-	42,42,42,42	0
54	MG	BA	3191	1/1	0.92	0.27	-	40,40,40,40	0
54	MG	BA	3604	1/1	0.96	0.07	-	50,50,50,50	0
54	MG	DA	3524	1/1	0.73	0.17	-	79,79,79,79	0
54	MG	BA	3072	1/1	0.93	0.10	-	59,59,59,59	0
54	MG	DA	3385	1/1	0.96	0.09	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3012	1/1	0.91	0.34	-	27,27,27,27	0
54	MG	DA	3576	1/1	0.89	0.10	-	48,48,48,48	0
54	MG	DA	3584	1/1	0.94	0.30	-	48,48,48,48	0
54	MG	CA	1746	1/1	0.90	0.11	-	97,97,97,97	0
54	MG	BA	3592	1/1	0.90	0.13	-	47,47,47,47	0
54	MG	CA	1624	1/1	0.96	0.54	-	63,63,63,63	0
54	MG	BA	3116	1/1	0.95	0.17	-	53,53,53,53	0
54	MG	DD	301	1/1	0.92	0.22	-	47,47,47,47	0
54	MG	DA	3127	1/1	0.91	0.25	-	56,56,56,56	0
54	MG	BA	3325	1/1	0.96	0.11	-	40,40,40,40	0
54	MG	DA	3332	1/1	0.92	0.23	-	53,53,53,53	0
54	MG	AA	1626	1/1	0.94	0.43	-	71,71,71,71	0
54	MG	DA	3455	1/1	0.95	0.05	-	68,68,68,68	0
54	MG	BA	3577	1/1	0.82	0.13	-	77,77,77,77	0
54	MG	BA	3240	1/1	0.64	0.28	-	71,71,71,71	0
54	MG	DA	3033	1/1	0.91	0.16	-	66,66,66,66	0
54	MG	DA	3136	1/1	0.91	0.33	-	62,62,62,62	0
54	MG	AA	1666	1/1	0.94	0.13	-	74,74,74,74	0
54	MG	D0	101	1/1	0.95	0.09	-	41,41,41,41	0
54	MG	DA	3112	1/1	0.98	0.24	-	51,51,51,51	0
54	MG	BB	219	1/1	0.91	0.06	-	105,105,105,105	0
54	MG	DA	3402	1/1	0.87	0.13	-	44,44,44,44	0
54	MG	DA	3004	1/1	0.93	0.07	-	88,88,88,88	0
54	MG	BF	302	1/1	0.87	0.24	-	42,42,42,42	0
54	MG	BA	3620	1/1	0.95	0.05	-	68,68,68,68	0
54	MG	AA	1693	1/1	0.96	0.11	-	51,51,51,51	0
54	MG	BA	3364	1/1	0.95	0.07	-	81,81,81,81	0
54	MG	BA	3459	1/1	0.87	0.17	-	38,38,38,38	0
54	MG	BA	3605	1/1	0.96	0.07	-	55,55,55,55	0
54	MG	DA	3107	1/1	0.98	0.08	-	54,54,54,54	0
54	MG	CA	1642	1/1	0.89	0.17	-	87,87,87,87	0
54	MG	BA	3054	1/1	0.90	0.17	-	34,34,34,34	0
54	MG	DA	3465	1/1	0.86	0.08	-	75,75,75,75	0
54	MG	BA	3534	1/1	0.84	0.19	-	25,25,25,25	0
54	MG	AA	1705	1/1	0.55	0.39	-	97,97,97,97	0
54	MG	DA	3190	1/1	0.94	0.10	-	59,59,59,59	0
54	MG	BA	3503	1/1	0.86	0.10	-	64,64,64,64	0
54	MG	BA	3146	1/1	0.70	0.60	-	65,65,65,65	0
54	MG	AA	1623	1/1	0.93	0.17	-	74,74,74,74	0
54	MG	BA	3488	1/1	0.94	0.17	-	24,24,24,24	0
54	MG	BA	3420	1/1	0.97	0.19	-	61,61,61,61	0
54	MG	BA	3324	1/1	0.96	0.10	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3021	1/1	0.88	0.20	-	44,44,44,44	0
54	MG	DA	3126	1/1	0.94	0.60	-	63,63,63,63	0
54	MG	BA	3386	1/1	0.96	0.09	-	40,40,40,40	0
54	MG	BA	3408	1/1	0.86	0.22	-	50,50,50,50	0
54	MG	DA	3485	1/1	0.95	0.26	-	58,58,58,58	0
54	MG	BA	3399	1/1	0.83	0.13	-	43,43,43,43	0
54	MG	DA	3141	1/1	0.88	0.52	-	60,60,60,60	0
54	MG	BA	3108	1/1	0.91	0.23	-	51,51,51,51	0
54	MG	BA	3335	1/1	0.88	0.10	-	66,66,66,66	0
54	MG	BA	3141	1/1	0.83	0.30	-	36,36,36,36	0
54	MG	CA	1725	1/1	0.95	0.18	-	65,65,65,65	0
54	MG	DA	3104	1/1	0.95	0.22	-	34,34,34,34	0
54	MG	DA	3236	1/1	0.92	0.30	-	47,47,47,47	0
54	MG	CA	1678	1/1	0.96	0.24	-	55,55,55,55	0
54	MG	DA	3062	1/1	0.97	0.37	-	49,49,49,49	0
54	MG	DA	3106	1/1	0.96	0.41	-	37,37,37,37	0
54	MG	DA	3148	1/1	0.90	0.16	-	48,48,48,48	0
54	MG	BB	222	1/1	0.95	0.18	-	80,80,80,80	0
54	MG	BA	3098	1/1	0.94	0.24	-	40,40,40,40	0
54	MG	DA	3251	1/1	0.89	0.18	-	40,40,40,40	0
54	MG	BA	3642	1/1	0.72	0.15	-	139,139,139,139	0
54	MG	BE	304	1/1	1.00	0.19	-	25,25,25,25	0
54	MG	BA	3007	1/1	0.90	0.30	-	28,28,28,28	0
54	MG	DA	3493	1/1	0.96	0.04	-	63,63,63,63	0
54	MG	DA	3144	1/1	0.92	0.47	-	42,42,42,42	0
54	MG	DA	3013	1/1	0.95	0.12	-	37,37,37,37	0
54	MG	DA	3544	1/1	0.92	0.06	-	72,72,72,72	0
54	MG	DA	3522	1/1	0.87	0.23	-	61,61,61,61	0
54	MG	DA	3173	1/1	0.95	0.13	-	52,52,52,52	0
54	MG	DA	3386	1/1	0.96	0.08	-	39,39,39,39	0
54	MG	DA	3494	1/1	0.94	0.14	-	37,37,37,37	0
54	MG	DA	3587	1/1	0.84	0.24	-	95,95,95,95	0
54	MG	AA	1707	1/1	0.86	0.17	-	102,102,102,102	0
54	MG	AA	1654	1/1	0.86	0.52	-	59,59,59,59	0
54	MG	BA	3608	1/1	0.95	0.26	-	71,71,71,71	0
54	MG	BA	3576	1/1	0.97	0.19	-	21,21,21,21	0
54	MG	AA	1635	1/1	0.84	0.15	-	61,61,61,61	0
54	MG	BB	217	1/1	0.95	0.11	-	67,67,67,67	0
54	MG	CA	1618	1/1	0.83	0.40	-	64,64,64,64	0
54	MG	DA	3120	1/1	0.92	0.26	-	43,43,43,43	0
54	MG	BA	3140	1/1	0.96	0.56	-	36,36,36,36	0
54	MG	DA	3405	1/1	0.96	0.15	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1723	1/1	0.65	0.12	-	112,112,112,112	0
54	MG	AA	1726	1/1	0.97	0.14	-	86,86,86,86	0
54	MG	DA	3145	1/1	0.89	0.23	-	61,61,61,61	0
54	MG	DA	3076	1/1	0.96	0.15	-	42,42,42,42	0
54	MG	BA	3615	1/1	0.94	0.12	-	52,52,52,52	0
54	MG	DA	3215	1/1	0.88	0.09	-	49,49,49,49	0
54	MG	DA	3228	1/1	0.92	0.48	-	40,40,40,40	0
54	MG	DA	3342	1/1	0.76	0.18	-	38,38,38,38	0
54	MG	DA	3061	1/1	0.93	0.17	-	32,32,32,32	0
54	MG	DA	3115	1/1	0.78	0.42	-	59,59,59,59	0
54	MG	BA	3569	1/1	0.88	0.08	-	69,69,69,69	0
54	MG	BA	3147	1/1	0.93	0.11	-	55,55,55,55	0
54	MG	DA	3064	1/1	0.94	0.36	-	48,48,48,48	0
54	MG	BA	3283	1/1	0.97	0.45	-	21,21,21,21	0
54	MG	BA	3087	1/1	0.98	0.20	-	46,46,46,46	0
54	MG	DA	3380	1/1	0.89	0.10	-	42,42,42,42	0
54	MG	BA	3372	1/1	0.98	0.07	-	49,49,49,49	0
54	MG	DA	3486	1/1	0.89	0.21	-	64,64,64,64	0
54	MG	DA	3442	1/1	0.87	0.12	-	82,82,82,82	0
54	MG	DA	3535	1/1	0.96	0.15	-	64,64,64,64	0
54	MG	BA	3221	1/1	0.89	0.34	-	57,57,57,57	0
54	MG	BA	3062	1/1	0.82	0.34	-	45,45,45,45	0
54	MG	DA	3329	1/1	0.92	0.13	-	41,41,41,41	0
54	MG	BA	3266	1/1	0.98	0.46	-	22,22,22,22	0
54	MG	BA	3209	1/1	0.95	0.21	-	56,56,56,56	0
54	MG	DA	3515	1/1	0.83	0.28	-	37,37,37,37	0
54	MG	DA	3480	1/1	0.98	0.18	-	52,52,52,52	0
54	MG	DA	3253	1/1	0.96	0.09	-	50,50,50,50	0
54	MG	DA	3172	1/1	0.79	0.29	-	64,64,64,64	0
54	MG	DA	3202	1/1	0.60	0.33	-	66,66,66,66	0
54	MG	CA	1740	1/1	0.93	0.40	-	68,68,68,68	0
54	MG	DA	3275	1/1	0.88	0.36	-	47,47,47,47	0
54	MG	DA	3529	1/1	0.97	0.09	-	56,56,56,56	0
54	MG	DA	3189	1/1	0.83	0.19	-	84,84,84,84	0
54	MG	DA	3171	1/1	0.93	0.17	-	61,61,61,61	0
54	MG	DA	3425	1/1	0.98	0.07	-	47,47,47,47	0
54	MG	DA	3531	1/1	0.95	0.18	-	91,91,91,91	0
54	MG	DA	3552	1/1	0.95	0.39	-	35,35,35,35	0
54	MG	BA	3268	1/1	0.94	0.37	-	27,27,27,27	0
54	MG	AA	1677	1/1	0.92	0.32	-	62,62,62,62	0
54	MG	DA	3554	1/1	0.98	0.09	-	47,47,47,47	0
54	MG	BA	3004	1/1	0.94	0.08	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3324	1/1	0.86	0.12	-	51,51,51,51	0
54	MG	DA	3030	1/1	0.90	0.28	-	55,55,55,55	0
54	MG	BA	3078	1/1	0.96	0.27	-	30,30,30,30	0
54	MG	BA	3505	1/1	0.97	0.20	-	41,41,41,41	0
54	MG	BA	3651	1/1	0.95	0.21	-	87,87,87,87	0
54	MG	BA	3506	1/1	0.99	0.11	-	30,30,30,30	0
54	MG	BA	3301	1/1	0.88	0.66	-	75,75,75,75	0
54	MG	BA	3081	1/1	0.94	0.36	-	42,42,42,42	0
54	MG	DA	3155	1/1	0.95	0.36	-	64,64,64,64	0
54	MG	CA	1625	1/1	0.89	0.36	-	63,63,63,63	0
54	MG	BA	3395	1/1	0.96	0.11	-	60,60,60,60	0
54	MG	DA	3484	1/1	0.94	0.07	-	64,64,64,64	0
54	MG	DA	3351	1/1	0.96	0.12	-	40,40,40,40	0
54	MG	CA	1715	1/1	0.95	0.05	-	103,103,103,103	0
54	MG	DA	3288	1/1	0.91	0.25	-	39,39,39,39	0
54	MG	BA	3192	1/1	0.96	0.10	-	51,51,51,51	0
54	MG	BA	3616	1/1	0.80	0.28	-	131,131,131,131	0
54	MG	DA	3099	1/1	0.94	0.23	-	36,36,36,36	0
54	MG	BA	3315	1/1	0.97	0.15	-	31,31,31,31	0
54	MG	DA	3306	1/1	0.92	0.35	-	29,29,29,29	0
54	MG	CA	1759	1/1	0.92	0.22	-	69,69,69,69	0
54	MG	DA	3509	1/1	0.91	0.19	-	37,37,37,37	0
54	MG	BA	3510	1/1	0.74	0.11	-	56,56,56,56	0
54	MG	DA	3177	1/1	0.64	0.13	-	88,88,88,88	0
54	MG	DA	3537	1/1	0.86	0.09	-	63,63,63,63	0
54	MG	AA	1601	1/1	0.93	0.29	-	55,55,55,55	0
54	MG	CA	1652	1/1	0.73	0.50	-	76,76,76,76	0
54	MG	BA	3117	1/1	0.89	0.28	-	39,39,39,39	0
54	MG	DA	3565	1/1	0.93	0.20	-	34,34,34,34	0
54	MG	BA	3507	1/1	0.91	0.28	-	41,41,41,41	0
54	MG	AA	1658	1/1	0.88	0.51	-	57,57,57,57	0
54	MG	DA	3548	1/1	0.84	0.12	-	89,89,89,89	0
54	MG	DA	3459	1/1	0.90	0.07	-	53,53,53,53	0
54	MG	DA	3124	1/1	0.97	0.38	-	37,37,37,37	0
54	MG	CA	1733	1/1	0.97	0.14	-	82,82,82,82	0
54	MG	DA	3379	1/1	0.95	0.12	-	59,59,59,59	0
54	MG	BA	3653	1/1	0.94	0.15	-	104,104,104,104	0
54	MG	BA	3579	1/1	0.87	0.09	-	100,100,100,100	0
54	MG	DA	3335	1/1	0.98	0.10	-	36,36,36,36	0
54	MG	BA	3509	1/1	0.96	0.15	-	50,50,50,50	0
54	MG	B2	101	1/1	0.95	0.17	-	45,45,45,45	0
54	MG	CA	1667	1/1	0.80	0.33	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3294	1/1	0.94	0.15	-	42,42,42,42	0
54	MG	BA	3535	1/1	0.94	0.11	-	55,55,55,55	0
54	MG	CA	1704	1/1	0.77	0.15	-	92,92,92,92	0
54	MG	DA	3327	1/1	0.96	0.49	-	52,52,52,52	0
54	MG	DA	3506	1/1	0.67	0.11	-	96,96,96,96	0
54	MG	CA	1720	1/1	0.80	0.14	-	89,89,89,89	0
54	MG	BA	3135	1/1	0.96	0.41	-	45,45,45,45	0
54	MG	BA	3491	1/1	0.97	0.10	-	28,28,28,28	0
54	MG	CA	1682	1/1	0.94	0.14	-	58,58,58,58	0
54	MG	BA	3461	1/1	0.88	0.17	-	79,79,79,79	0
54	MG	DA	3357	1/1	0.94	0.19	-	36,36,36,36	0
54	MG	BA	3233	1/1	0.92	0.45	-	41,41,41,41	0
54	MG	BA	3497	1/1	0.97	0.26	-	61,61,61,61	0
54	MG	DA	3252	1/1	0.90	0.54	-	59,59,59,59	0
54	MG	BA	3060	1/1	0.89	0.14	-	54,54,54,54	0
54	MG	BE	305	1/1	0.82	0.16	-	60,60,60,60	0
54	MG	BA	3521	1/1	0.95	0.09	-	40,40,40,40	0
54	MG	BA	3045	1/1	0.90	0.23	-	45,45,45,45	0
54	MG	BA	3544	1/1	0.81	0.15	-	46,46,46,46	0
54	MG	BA	3552	1/1	0.87	0.22	-	82,82,82,82	0
54	MG	AQ	201	1/1	0.89	0.25	-	58,58,58,58	0
54	MG	BA	3627	1/1	0.81	0.10	-	50,50,50,50	0
54	MG	CA	1736	1/1	0.97	0.18	-	70,70,70,70	0
54	MG	BA	3598	1/1	0.88	0.11	-	65,65,65,65	0
54	MG	BA	3076	1/1	0.90	0.22	-	44,44,44,44	0
54	MG	BA	3363	1/1	0.91	0.14	-	64,64,64,64	0
54	MG	BA	3298	1/1	0.90	0.55	-	54,54,54,54	0
54	MG	AA	1700	1/1	0.95	0.09	-	42,42,42,42	0
54	MG	DA	3360	1/1	0.91	0.20	-	37,37,37,37	0
54	MG	DA	3408	1/1	0.90	0.15	-	51,51,51,51	0
54	MG	BA	3474	1/1	0.93	0.08	-	37,37,37,37	0
54	MG	AA	1674	1/1	0.86	0.32	-	63,63,63,63	0
54	MG	CA	1658	1/1	0.93	0.34	-	58,58,58,58	0
54	MG	BA	3215	1/1	0.85	0.22	-	50,50,50,50	0
54	MG	DA	3530	1/1	0.61	0.24	-	132,132,132,132	0
54	MG	BA	3524	1/1	0.76	0.12	-	38,38,38,38	0
54	MG	DA	3191	1/1	0.88	0.19	-	51,51,51,51	0
54	MG	BA	3344	1/1	0.95	0.31	-	61,61,61,61	0
54	MG	BB	221	1/1	0.94	0.06	-	50,50,50,50	0
54	MG	CA	1654	1/1	0.96	0.13	-	65,65,65,65	0
54	MG	BA	3438	1/1	0.91	0.20	-	65,65,65,65	0
54	MG	BA	3371	1/1	0.96	0.12	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3195	1/1	0.94	0.22	-	60,60,60,60	0
54	MG	BA	3176	1/1	0.94	0.16	-	60,60,60,60	0
54	MG	CA	1666	1/1	0.94	0.37	-	64,64,64,64	0
54	MG	BZ	301	1/1	0.94	0.17	-	55,55,55,55	0
54	MG	DA	3354	1/1	0.90	0.09	-	49,49,49,49	0
54	MG	CA	1705	1/1	0.80	0.14	-	96,96,96,96	0
54	MG	DA	3448	1/1	0.96	0.10	-	42,42,42,42	0
54	MG	BA	3551	1/1	0.97	0.11	-	82,82,82,82	0
54	MG	AA	1686	1/1	0.83	0.11	-	68,68,68,68	0
54	MG	DA	3520	1/1	0.95	0.12	-	56,56,56,56	0
54	MG	AA	1670	1/1	0.91	0.32	-	53,53,53,53	0
54	MG	BA	3168	1/1	0.96	0.26	-	28,28,28,28	0
54	MG	DA	3422	1/1	0.97	0.18	-	43,43,43,43	0
54	MG	BA	3400	1/1	0.92	0.22	-	47,47,47,47	0
54	MG	AA	1616	1/1	0.88	0.14	-	92,92,92,92	0
54	MG	CA	1742	1/1	0.95	0.07	-	113,113,113,113	0
54	MG	BA	3636	1/1	0.97	0.06	-	28,28,28,28	0
54	MG	BA	3628	1/1	0.96	0.15	-	35,35,35,35	0
54	MG	CA	1657	1/1	0.79	0.41	-	61,61,61,61	0
54	MG	DA	3220	1/1	0.82	0.24	-	51,51,51,51	0
54	MG	DA	3165	1/1	0.69	0.41	-	60,60,60,60	0
54	MG	BA	3177	1/1	0.91	0.10	-	57,57,57,57	0
54	MG	BA	3070	1/1	0.95	0.20	-	37,37,37,37	0
54	MG	DO	202	1/1	0.90	0.17	-	39,39,39,39	0
54	MG	DA	3263	1/1	0.93	0.20	-	40,40,40,40	0
54	MG	DA	3595	1/1	0.93	0.12	-	58,58,58,58	0
54	MG	AA	1696	1/1	0.97	0.16	-	66,66,66,66	0
54	MG	BA	3261	1/1	0.77	0.36	-	34,34,34,34	0
54	MG	DA	3237	1/1	0.87	0.29	-	62,62,62,62	0
54	MG	BA	3556	1/1	0.96	0.20	-	57,57,57,57	0
54	MG	BA	3403	1/1	0.81	0.15	-	67,67,67,67	0
54	MG	DA	3346	1/1	0.90	0.12	-	35,35,35,35	0
54	MG	BA	3586	1/1	0.90	0.10	-	63,63,63,63	0
54	MG	BA	3340	1/1	0.72	0.14	-	79,79,79,79	0
54	MG	DA	3195	1/1	0.84	0.24	-	48,48,48,48	0
54	MG	BA	3623	1/1	0.94	0.12	-	73,73,73,73	0
54	MG	DA	3268	1/1	0.82	0.58	-	54,54,54,54	0
54	MG	BA	3313	1/1	0.96	0.08	-	37,37,37,37	0
54	MG	BA	3126	1/1	0.96	0.22	-	41,41,41,41	0
54	MG	DA	3581	1/1	0.96	0.09	-	52,52,52,52	0
54	MG	CA	1683	1/1	0.84	0.21	-	100,100,100,100	0
54	MG	CA	1731	1/1	0.89	0.12	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3079	1/1	0.96	0.18	-	47,47,47,47	0
54	MG	BA	3166	1/1	0.96	0.29	-	36,36,36,36	0
54	MG	DA	3080	1/1	0.96	0.17	-	44,44,44,44	0
54	MG	BA	3280	1/1	0.93	0.30	-	46,46,46,46	0
54	MG	BA	3306	1/1	0.92	0.18	-	55,55,55,55	0
54	MG	BA	3185	1/1	0.87	0.51	-	51,51,51,51	0
54	MG	BA	3622	1/1	0.93	0.11	-	45,45,45,45	0
54	MG	BA	3356	1/1	0.92	0.17	-	29,29,29,29	0
54	MG	AA	1622	1/1	0.68	0.19	-	81,81,81,81	0
54	MG	DA	3277	1/1	0.86	0.17	-	77,77,77,77	0
54	MG	DA	3066	1/1	0.91	0.20	-	62,62,62,62	0
54	MG	BA	3236	1/1	0.79	0.23	-	66,66,66,66	0
54	MG	BA	3649	1/1	0.83	0.22	-	125,125,125,125	0
54	MG	DA	3592	1/1	0.93	0.06	-	83,83,83,83	0
54	MG	DA	3279	1/1	0.97	0.12	-	44,44,44,44	0
54	MG	BA	3614	1/1	0.97	0.04	-	66,66,66,66	0
54	MG	AA	1692	1/1	0.79	0.57	-	144,144,144,144	0
54	MG	DA	3499	1/1	0.91	0.14	-	67,67,67,67	0
54	MG	BA	3063	1/1	0.93	0.13	-	54,54,54,54	0
54	MG	CA	1631	1/1	0.88	0.45	-	48,48,48,48	0
54	MG	CA	1696	1/1	0.95	0.43	-	61,61,61,61	0
54	MG	DA	3527	1/1	0.94	0.15	-	91,91,91,91	0
54	MG	DA	3036	1/1	0.96	0.29	-	44,44,44,44	0
54	MG	DA	3071	1/1	0.95	0.19	-	44,44,44,44	0
54	MG	BA	3645	1/1	0.81	0.08	-	102,102,102,102	0
54	MG	BA	3346	1/1	0.90	0.12	-	52,52,52,52	0
54	MG	BA	3374	1/1	0.93	0.08	-	34,34,34,34	0
54	MG	DA	3034	1/1	0.97	0.10	-	32,32,32,32	0
54	MG	BA	3326	1/1	0.97	0.11	-	49,49,49,49	0
54	MG	AF	201	1/1	0.88	0.20	-	62,62,62,62	0
54	MG	DA	3398	1/1	0.84	0.26	-	88,88,88,88	0
54	MG	B5	102	1/1	0.97	0.10	-	52,52,52,52	0
54	MG	DB	204	1/1	0.71	0.70	-	74,74,74,74	0
54	MG	BA	3421	1/1	0.90	0.07	-	68,68,68,68	0
54	MG	BA	3058	1/1	0.95	0.14	-	32,32,32,32	0
54	MG	AA	1697	1/1	0.80	0.20	-	106,106,106,106	0
54	MG	DA	3086	1/1	0.90	0.21	-	48,48,48,48	0
54	MG	CA	1615	1/1	0.91	0.12	-	65,65,65,65	0
54	MG	DA	3591	1/1	0.81	0.11	-	66,66,66,66	0
54	MG	BA	3650	1/1	0.91	0.16	-	88,88,88,88	0
54	MG	BA	3305	1/1	0.91	0.26	-	69,69,69,69	0
54	MG	AA	1602	1/1	0.97	0.29	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3428	1/1	0.95	0.09	-	56,56,56,56	0
54	MG	CA	1719	1/1	0.98	0.07	-	54,54,54,54	0
54	MG	BA	3393	1/1	0.90	0.19	-	37,37,37,37	0
54	MG	CA	1661	1/1	0.85	0.64	-	67,67,67,67	0
54	MG	BA	3472	1/1	0.97	0.27	-	26,26,26,26	0
54	MG	DA	3310	1/1	0.96	0.37	-	28,28,28,28	0
54	MG	CA	1706	1/1	0.80	0.10	-	103,103,103,103	0
54	MG	DA	3395	1/1	0.96	0.11	-	39,39,39,39	0
54	MG	DA	3227	1/1	0.89	0.28	-	52,52,52,52	0
54	MG	DA	3020	1/1	0.90	0.18	-	56,56,56,56	0
54	MG	DA	3590	1/1	0.82	0.24	-	82,82,82,82	0
54	MG	BA	3600	1/1	0.69	0.07	-	81,81,81,81	0
54	MG	BA	3634	1/1	0.99	0.11	-	53,53,53,53	0
54	MG	BB	205	1/1	0.92	0.38	-	45,45,45,45	0
54	MG	DA	3536	1/1	0.93	0.16	-	51,51,51,51	0
54	MG	BA	3169	1/1	0.94	0.23	-	31,31,31,31	0
54	MG	AA	1679	1/1	0.92	0.22	-	44,44,44,44	0
54	MG	DA	3593	1/1	0.90	0.15	-	83,83,83,83	0
54	MG	DA	3283	1/1	0.93	0.18	-	61,61,61,61	0
54	MG	CA	1603	1/1	0.83	0.30	-	56,56,56,56	0
54	MG	DA	3314	1/1	0.93	0.39	-	43,43,43,43	0
54	MG	DO	201	1/1	0.95	0.09	-	120,120,120,120	0
54	MG	AA	1625	1/1	0.62	0.40	-	79,79,79,79	0
54	MG	CA	1757	1/1	0.69	0.26	-	80,80,80,80	0
54	MG	CA	1630	1/1	0.94	0.62	-	72,72,72,72	0
54	MG	BA	3530	1/1	0.96	0.14	-	56,56,56,56	0
54	MG	BA	3107	1/1	0.86	0.20	-	60,60,60,60	0
54	MG	DE	304	1/1	0.96	0.21	-	42,42,42,42	0
54	MG	DA	3060	1/1	0.92	0.34	-	41,41,41,41	0
54	MG	DA	3016	1/1	0.84	0.22	-	62,62,62,62	0
54	MG	BA	3207	1/1	0.94	0.13	-	33,33,33,33	0
54	MG	DA	3153	1/1	0.86	0.42	-	58,58,58,58	0
54	MG	AA	1699	1/1	0.80	0.20	-	99,99,99,99	0
54	MG	DA	3198	1/1	0.82	0.79	-	57,57,57,57	0
54	MG	CA	1620	1/1	0.89	0.12	-	58,58,58,58	0
54	MG	DA	3213	1/1	0.90	0.33	-	48,48,48,48	0
54	MG	CA	1676	1/1	0.88	0.24	-	73,73,73,73	0
54	MG	CA	1621	1/1	0.86	0.56	-	64,64,64,64	0
54	MG	BA	3584	1/1	0.92	0.11	-	42,42,42,42	0
54	MG	DA	3139	1/1	0.87	0.50	-	59,59,59,59	0
54	MG	DA	3317	1/1	0.94	0.23	-	47,47,47,47	0
54	MG	DA	3325	1/1	0.88	0.19	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3034	1/1	0.99	0.10	-	41,41,41,41	0
54	MG	CA	1674	1/1	0.88	0.11	-	74,74,74,74	0
54	MG	CA	1633	1/1	0.64	0.57	-	77,77,77,77	0
54	MG	BA	3208	1/1	0.95	0.29	-	38,38,38,38	0
54	MG	BA	3164	1/1	0.83	0.35	-	50,50,50,50	0
54	MG	BA	3287	1/1	0.80	0.42	-	44,44,44,44	0
54	MG	DA	3207	1/1	0.84	0.28	-	54,54,54,54	0
54	MG	BA	3648	1/1	0.81	0.12	-	91,91,91,91	0
54	MG	AA	1648	1/1	0.96	0.44	-	44,44,44,44	0
54	MG	DA	3596	1/1	0.89	0.19	-	125,125,125,125	0
54	MG	BA	3347	1/1	0.76	0.16	-	94,94,94,94	0
54	MG	DA	3347	1/1	0.96	0.17	-	35,35,35,35	0
54	MG	DA	3312	1/1	0.86	0.52	-	29,29,29,29	0
54	MG	CA	1699	1/1	0.95	0.15	-	83,83,83,83	0
54	MG	DA	3267	1/1	0.91	0.28	-	54,54,54,54	0
54	MG	AA	1636	1/1	0.84	0.27	-	79,79,79,79	0
54	MG	BA	3633	1/1	0.95	0.12	-	43,43,43,43	0
54	MG	AC	301	1/1	0.94	0.14	-	57,57,57,57	0
54	MG	CA	1755	1/1	0.50	0.12	-	129,129,129,129	0
54	MG	DA	3214	1/1	0.90	0.24	-	37,37,37,37	0
54	MG	BA	3405	1/1	0.93	0.15	-	61,61,61,61	0
54	MG	DA	3037	1/1	0.96	0.12	-	43,43,43,43	0
54	MG	BA	3187	1/1	0.97	0.59	-	42,42,42,42	0
54	MG	DA	3193	1/1	0.84	0.58	-	40,40,40,40	0
54	MG	DA	3528	1/1	0.85	0.17	-	124,124,124,124	0
54	MG	CA	1622	1/1	0.94	0.28	-	47,47,47,47	0
54	MG	DA	3185	1/1	0.85	0.16	-	57,57,57,57	0
54	MG	AA	1706	1/1	0.67	0.10	-	91,91,91,91	0
54	MG	AA	1708	1/1	0.88	0.29	-	91,91,91,91	0
54	MG	D0	102	1/1	0.97	0.16	-	72,72,72,72	0
54	MG	DA	3143	1/1	0.97	0.19	-	60,60,60,60	0
54	MG	DA	3077	1/1	0.93	0.17	-	49,49,49,49	0
54	MG	DA	3559	1/1	0.85	0.06	-	79,79,79,79	0
54	MG	DA	3249	1/1	0.95	0.29	-	49,49,49,49	0
54	MG	BA	3085	1/1	0.89	0.49	-	52,52,52,52	0
54	MG	DA	3541	1/1	0.76	0.12	-	130,130,130,130	0
54	MG	DA	3300	1/1	0.95	0.14	-	41,41,41,41	0
54	MG	BA	3396	1/1	0.91	0.17	-	29,29,29,29	0
54	MG	BA	3100	1/1	0.86	0.20	-	42,42,42,42	0
54	MG	DA	3186	1/1	0.93	0.13	-	54,54,54,54	0
54	MG	BA	3029	1/1	0.87	0.18	-	32,32,32,32	0
54	MG	BA	3139	1/1	0.84	0.28	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3452	1/1	0.91	0.13	-	64,64,64,64	0
54	MG	BA	3316	1/1	0.97	0.13	-	45,45,45,45	0
54	MG	AA	1649	1/1	0.89	0.31	-	43,43,43,43	0
54	MG	CA	1644	1/1	0.97	0.26	-	53,53,53,53	0
54	MG	DA	3110	1/1	0.82	0.31	-	53,53,53,53	0
54	MG	BA	3048	1/1	0.87	0.18	-	68,68,68,68	0
54	MG	CA	1762	1/1	0.88	0.07	-	156,156,156,156	0
54	MG	CA	1692	1/1	0.50	0.51	-	86,86,86,86	0
54	MG	BB	213	1/1	0.88	0.14	-	38,38,38,38	0
54	MG	DA	3009	1/1	0.96	0.28	-	46,46,46,46	0
54	MG	DA	3070	1/1	0.89	0.36	-	57,57,57,57	0
54	MG	BA	3537	1/1	0.98	0.17	-	31,31,31,31	0
54	MG	DA	3401	1/1	0.71	0.29	-	108,108,108,108	0
54	MG	DA	3225	1/1	0.92	0.50	-	51,51,51,51	0
54	MG	BA	3431	1/1	0.92	0.08	-	71,71,71,71	0
54	MG	AA	1675	1/1	0.90	0.23	-	76,76,76,76	0
54	MG	BA	3097	1/1	0.68	0.54	-	47,47,47,47	0
54	MG	DA	3262	1/1	0.85	0.33	-	53,53,53,53	0
54	MG	BT	201	1/1	0.92	0.15	-	53,53,53,53	0
54	MG	DA	3315	1/1	0.96	0.11	-	31,31,31,31	0
54	MG	BA	3349	1/1	0.94	0.10	-	36,36,36,36	0
54	MG	DA	3320	1/1	0.95	0.14	-	38,38,38,38	0
54	MG	DA	3545	1/1	0.92	0.08	-	82,82,82,82	0
54	MG	DA	3114	1/1	0.97	0.39	-	30,30,30,30	0
54	MG	BA	3515	1/1	0.91	0.16	-	72,72,72,72	0
54	MG	BA	3079	1/1	0.95	0.20	-	50,50,50,50	0
54	MG	CA	1681	1/1	0.82	0.41	-	82,82,82,82	0
54	MG	DA	3184	1/1	0.94	0.15	-	46,46,46,46	0
54	MG	BA	3213	1/1	0.98	0.10	-	43,43,43,43	0
54	MG	DA	3575	1/1	0.96	0.21	-	35,35,35,35	0
54	MG	DA	3585	1/1	0.99	0.13	-	33,33,33,33	0
54	MG	CA	1636	1/1	0.90	0.36	-	59,59,59,59	0
54	MG	BF	301	1/1	0.95	0.21	-	33,33,33,33	0
54	MG	AA	1657	1/1	0.93	0.39	-	58,58,58,58	0
54	MG	BA	3237	1/1	0.51	0.32	-	71,71,71,71	0
54	MG	BA	3293	1/1	0.97	0.18	-	48,48,48,48	0
54	MG	BA	3182	1/1	0.94	0.41	-	37,37,37,37	0
54	MG	CA	1627	1/1	0.86	0.37	-	55,55,55,55	0
54	MG	DA	3319	1/1	0.87	0.32	-	57,57,57,57	0
54	MG	AA	1611	1/1	0.91	0.28	-	83,83,83,83	0
54	MG	CA	1710	1/1	0.94	0.09	-	48,48,48,48	0
54	MG	DA	3532	1/1	0.54	0.23	-	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3504	1/1	0.89	0.07	-	63,63,63,63	0
54	MG	DA	3447	1/1	0.89	0.27	-	74,74,74,74	0
54	MG	BA	3563	1/1	0.91	0.09	-	70,70,70,70	0
54	MG	BA	3571	1/1	0.91	0.17	-	44,44,44,44	0
54	MG	BA	3110	1/1	0.93	0.20	-	66,66,66,66	0
54	MG	CA	1758	1/1	0.87	0.22	-	84,84,84,84	0
54	MG	BA	3450	1/1	0.93	0.10	-	38,38,38,38	0
54	MG	BA	3512	1/1	0.59	0.28	-	109,109,109,109	0
54	MG	AA	1713	1/1	0.91	0.10	-	91,91,91,91	0
54	MG	BA	3496	1/1	0.92	0.17	-	39,39,39,39	0
54	MG	BA	3281	1/1	0.94	0.25	-	24,24,24,24	0
54	MG	DA	3206	1/1	0.96	0.60	-	52,52,52,52	0
54	MG	BA	3300	1/1	0.89	0.42	-	48,48,48,48	0
54	MG	CA	1608	1/1	0.81	0.53	-	93,93,93,93	0
54	MG	DA	3138	1/1	0.97	0.31	-	41,41,41,41	0
54	MG	BA	3082	1/1	0.99	0.12	-	36,36,36,36	0
54	MG	BA	3553	1/1	0.87	0.11	-	89,89,89,89	0
54	MG	BA	3267	1/1	0.90	0.33	-	36,36,36,36	0
54	MG	CA	1713	1/1	0.89	0.14	-	73,73,73,73	0
54	MG	BA	3612	1/1	0.91	0.07	-	59,59,59,59	0
54	MG	BA	3370	1/1	0.83	0.23	-	41,41,41,41	0
54	MG	BA	3074	1/1	0.81	0.44	-	53,53,53,53	0
54	MG	BA	3659	1/1	0.88	0.07	-	81,81,81,81	0
54	MG	AA	1608	1/1	0.97	0.33	-	67,67,67,67	0
54	MG	BA	3391	1/1	0.96	0.11	-	39,39,39,39	0
54	MG	AA	1663	1/1	0.84	0.52	-	64,64,64,64	0
54	MG	BA	3398	1/1	0.93	0.14	-	52,52,52,52	0
54	MG	DA	3211	1/1	0.90	0.23	-	48,48,48,48	0
54	MG	DA	3135	1/1	0.95	0.32	-	47,47,47,47	0
54	MG	DA	3119	1/1	0.89	0.33	-	48,48,48,48	0
54	MG	DA	3556	1/1	0.92	0.06	-	56,56,56,56	0
54	MG	DA	3255	1/1	0.88	0.20	-	58,58,58,58	0
54	MG	BA	3432	1/1	0.93	0.04	-	67,67,67,67	0
54	MG	BA	3206	1/1	0.97	0.26	-	49,49,49,49	0
54	MG	BA	3545	1/1	0.96	0.07	-	43,43,43,43	0
54	MG	DA	3168	1/1	0.96	0.20	-	42,42,42,42	0
54	MG	DA	3428	1/1	0.98	0.05	-	68,68,68,68	0
54	MG	BA	3285	1/1	0.89	0.57	-	38,38,38,38	0
54	MG	BA	3254	1/1	0.91	0.35	-	25,25,25,25	0
54	MG	DA	3054	1/1	0.95	0.12	-	46,46,46,46	0
54	MG	DA	3012	1/1	0.88	0.19	-	30,30,30,30	0
54	MG	DA	3286	1/1	0.98	0.20	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3294	1/1	0.97	0.19	-	39,39,39,39	0
54	MG	BA	3543	1/1	0.78	0.19	-	119,119,119,119	0
54	MG	BA	3134	1/1	0.92	0.43	-	41,41,41,41	0
54	MG	DA	3371	1/1	0.83	0.25	-	43,43,43,43	0
54	MG	DA	3440	1/1	0.96	0.28	-	42,42,42,42	0
54	MG	BA	3523	1/1	0.86	0.10	-	110,110,110,110	0
54	MG	BA	3568	1/1	0.97	0.12	-	39,39,39,39	0
54	MG	DA	3280	1/1	0.77	0.44	-	58,58,58,58	0
54	MG	CA	1616	1/1	0.88	0.26	-	58,58,58,58	0
54	MG	DA	3582	1/1	0.89	0.25	-	63,63,63,63	0
54	MG	BA	3311	1/1	0.93	0.17	-	24,24,24,24	0
54	MG	AA	1695	1/1	0.95	0.11	-	74,74,74,74	0
54	MG	CA	1711	1/1	0.66	0.11	-	103,103,103,103	0
54	MG	BA	3638	1/1	0.75	0.13	-	67,67,67,67	0
54	MG	BA	3499	1/1	0.97	0.12	-	60,60,60,60	0
54	MG	DA	3400	1/1	0.90	0.17	-	66,66,66,66	0
54	MG	BA	3531	1/1	0.83	0.09	-	89,89,89,89	0
54	MG	DA	3048	1/1	0.91	0.25	-	40,40,40,40	0
54	MG	DA	3078	1/1	0.97	0.17	-	48,48,48,48	0
54	MG	AA	1640	1/1	0.90	0.19	-	58,58,58,58	0
54	MG	BA	3587	1/1	0.86	0.14	-	60,60,60,60	0
54	MG	BA	3402	1/1	0.98	0.06	-	54,54,54,54	0
54	MG	BA	3104	1/1	0.85	0.23	-	63,63,63,63	0
54	MG	BA	3020	1/1	0.92	0.09	-	82,82,82,82	0
54	MG	BA	3151	1/1	0.98	0.35	-	33,33,33,33	0
54	MG	BA	3610	1/1	0.95	0.08	-	63,63,63,63	0
54	MG	DA	3093	1/1	0.92	0.27	-	56,56,56,56	0
54	MG	DA	3296	1/1	0.93	0.09	-	67,67,67,67	0
54	MG	BA	3618	1/1	0.95	0.08	-	52,52,52,52	0
54	MG	DA	3222	1/1	0.85	0.23	-	68,68,68,68	0
54	MG	BA	3193	1/1	0.92	0.67	-	35,35,35,35	0
54	MG	BA	3008	1/1	0.89	0.23	-	28,28,28,28	0
54	MG	DA	3580	1/1	0.98	0.17	-	52,52,52,52	0
54	MG	BA	3439	1/1	0.90	0.16	-	59,59,59,59	0
54	MG	BA	3171	1/1	0.92	0.32	-	31,31,31,31	0
54	MG	DA	3059	1/1	0.86	0.21	-	45,45,45,45	0
54	MG	DA	3543	1/1	0.90	0.09	-	53,53,53,53	0
54	MG	BA	3290	1/1	0.92	0.17	-	63,63,63,63	0
54	MG	BA	3084	1/1	0.87	0.11	-	59,59,59,59	0
54	MG	DA	3217	1/1	0.99	0.49	-	32,32,32,32	0
54	MG	AA	1606	1/1	0.86	0.19	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.