



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 09:40 pm BST

PDB ID : 4V6G  
Title : Initiation complex of 70S ribosome with two tRNAs and mRNA.  
Authors : Jenner, L.B.; Yusupova, G.; Yusupov, M.  
Deposited on : 2009-07-10  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

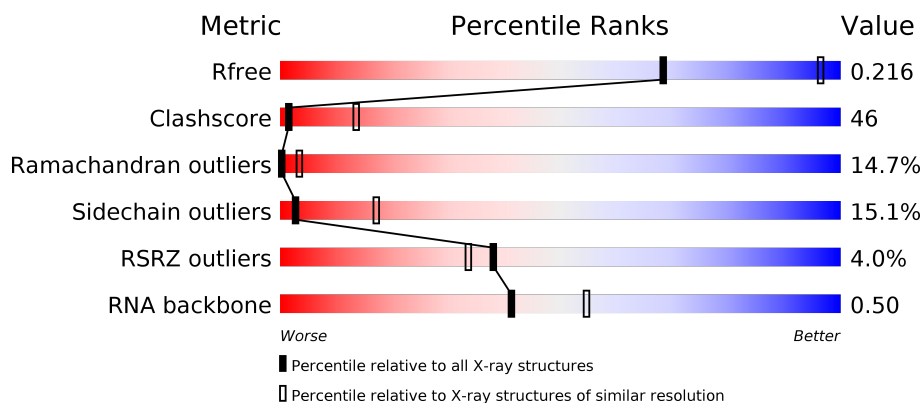
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	1517	<div> <div>25%</div> <div>50%</div> <div>22%</div> <div>•</div> </div>
1	CA	1517	<div> <div>25%</div> <div>52%</div> <div>20%</div> <div>•</div> </div>
2	AE	256	<div> <div>17%</div> <div>9%</div> <div>57%</div> <div>23%</div> <div>•</div> <div>8%</div> </div>
2	CE	256	<div> <div>18%</div> <div>17%</div> <div>59%</div> <div>16%</div> <div>•</div> <div>7%</div> </div>


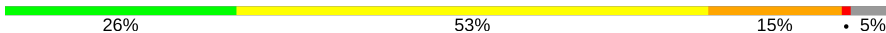
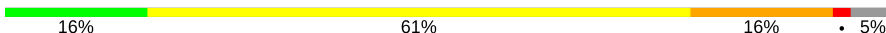


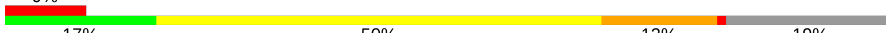
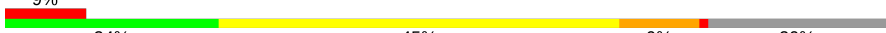




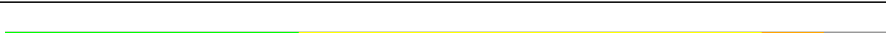


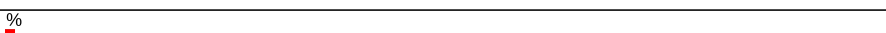




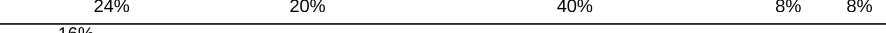

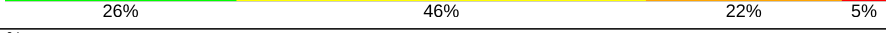
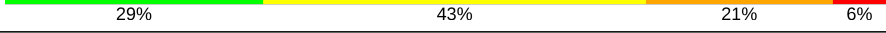
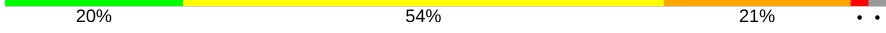

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	209	
4	CG	209	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126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

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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AC	77	
22	AD	77	
22	CB	77	
22	CC	77	
22	CD	77	
23	A1	25	
23	C1	25	
24	BA	2898	
24	DA	2898	
25	BB	122	
25	DB	122	
26	BD	276	

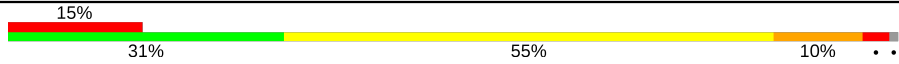

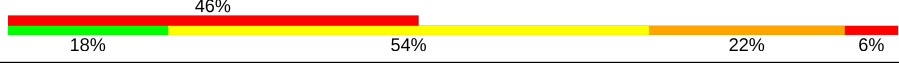
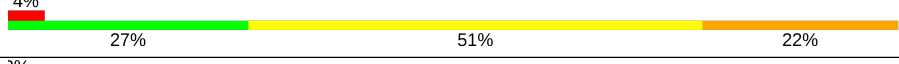
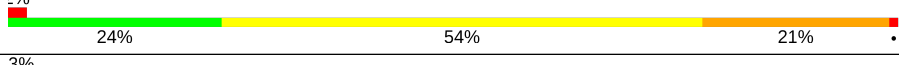
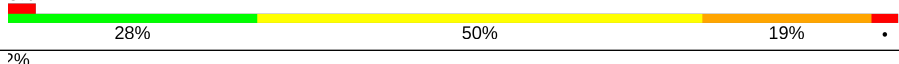
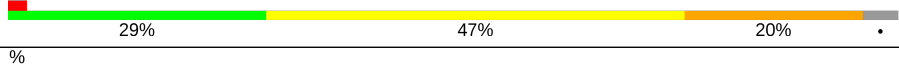


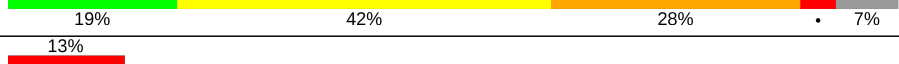

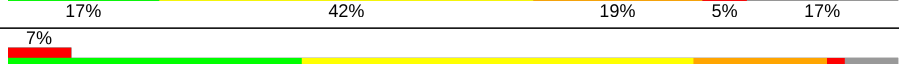
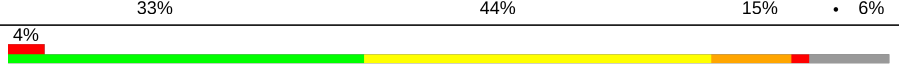
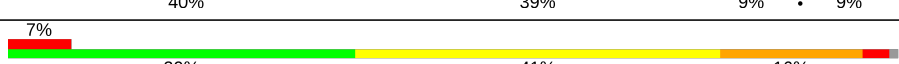
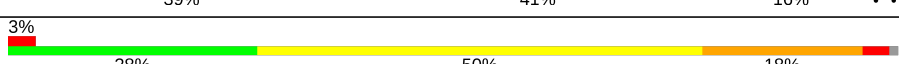
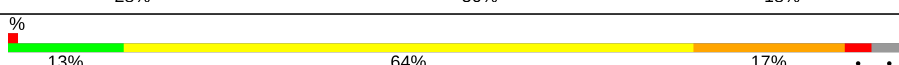
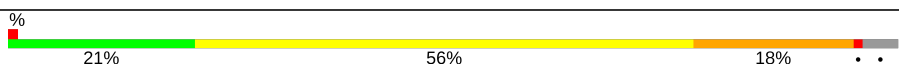
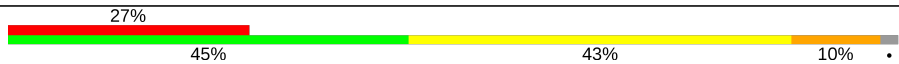
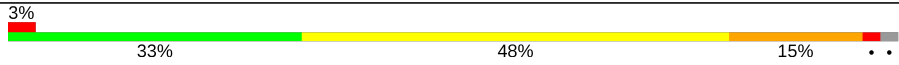


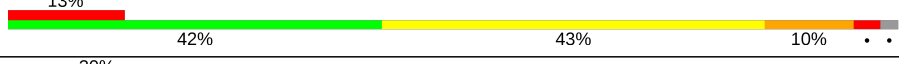
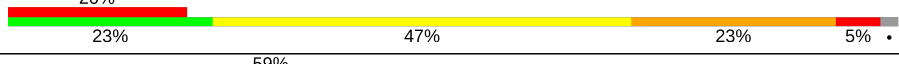
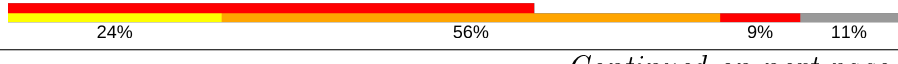

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Mol	Chain	Length	Quality of chain
26	DD	276	
27	BE	206	
27	DE	206	
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0	118	
37	BQ	112	
37	DQ	112	
38	BR	146	
38	DR	146	

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Mol	Chain	Length	Quality of chain
39	B1	118	
39	D1	118	
40	B2	101	
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
51	B6	54	

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Mol	Chain	Length	Quality of chain
51	D6	54	
52	B7	49	
52	D7	49	
53	B8	65	
53	D8	65	

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	1647	-	-	-	X
54	MG	AA	1668	-	-	-	X
54	MG	AA	1687	-	-	-	X
54	MG	AA	1730	-	-	-	X
54	MG	AA	1761	-	-	-	X
54	MG	AA	1767	-	-	-	X
54	MG	AA	1840	-	-	-	X
54	MG	AA	1850	-	-	-	X
54	MG	AA	1863	-	-	-	X
54	MG	AA	1909	-	-	-	X
54	MG	AA	1917	-	-	-	X
54	MG	AA	2014	-	-	-	X
54	MG	AA	2030	-	-	-	X
54	MG	AC	107	-	-	-	X
54	MG	BA	3018	-	-	-	X
54	MG	BA	3360	-	-	-	X
54	MG	BF	302	-	-	-	X
54	MG	BH	201	-	-	-	X
54	MG	CA	1741	-	-	-	X
54	MG	CA	1815	-	-	-	X
54	MG	CA	1860	-	-	-	X
54	MG	CA	1952	-	-	-	X
54	MG	CA	1955	-	-	-	X
54	MG	CG	301	-	-	-	X
54	MG	CL	201	-	-	-	X
54	MG	CR	101	-	-	-	X
54	MG	D0	205	-	-	-	X
54	MG	DA	3018	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3049	-	-	-	X
54	MG	DA	3091	-	-	-	X
54	MG	DA	3109	-	-	-	X
54	MG	DA	3188	-	-	-	X
54	MG	DA	3293	-	-	-	X
54	MG	DA	3326	-	-	-	X
54	MG	DA	3336	-	-	-	X
54	MG	DA	3347	-	-	-	X
54	MG	DA	3379	-	-	-	X
54	MG	DA	3398	-	-	-	X
54	MG	DA	3437	-	-	-	X
54	MG	DA	3439	-	-	-	X
54	MG	DA	3472	-	-	-	X
54	MG	DA	3487	-	-	-	X
54	MG	DA	3512	-	-	-	X
54	MG	DA	3527	-	-	-	X
54	MG	DA	3570	-	-	-	X
54	MG	DA	3573	-	-	-	X
54	MG	DA	3589	-	-	-	X
54	MG	DA	3597	-	-	-	X
54	MG	DA	3611	-	-	-	X
54	MG	DA	3656	-	-	-	X
54	MG	DA	3682	-	-	-	X
54	MG	DA	3704	-	-	-	X
54	MG	DA	3710	-	-	-	X
54	MG	DA	3712	-	-	-	X
54	MG	DA	3754	-	-	-	X
54	MG	DA	3759	-	-	-	X
54	MG	DA	3789	-	-	-	X
54	MG	DA	3795	-	-	-	X
54	MG	DA	3801	-	-	-	X
54	MG	DA	3802	-	-	-	X
54	MG	DB	213	-	-	-	X
54	MG	DS	201	-	-	-	X
54	MG	DU	202	-	-	-	X
55	ZN	AA	2040	-	-	-	X



## 2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 298428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RRNA (E.COLI NUMBERING).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1517	Total	C	N	O	P	0	0	0
			32600	14510	6032	10541	1517			
1	CA	1515	Total	C	N	O	P	0	0	0
			32554	14491	6025	10524	1514			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1542	G	U	CONFLICT	GB M26923.1
CA	1542	G	U	CONFLICT	GB M26923.1

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	CF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AH	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AL	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			
9	CL	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			
11	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
13	CP	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	71	Total	C	N	O	0	0	0
			585	373	116	96			
18	CU	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			
19	CV	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA FMET (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	AD	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CD	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CB	65	Total	C	N	O	P	0	0	0
			1385	618	250	453	64			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	23	Total	C	N	O	P	0	0	0
			502	227	107	146	22			
23	C1	23	Total	C	N	O	P	0	0	0
			502	227	107	146	22			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2885	Total	C	N	O	P	0	0	0
			62134	27656	11622	19972	2884			
24	DA	2886	Total	C	N	O	P	0	0	0
			62151	27664	11620	19982	2885			

There are 29 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
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	161	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	?	-	G	DELETION	GB AP008226.1
DA	?	-	G	DELETION	GB AP008226.1
DA	?	-	C	DELETION	GB AP008226.1
DA	?	-	A	DELETION	GB AP008226.1
DA	654L	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
25	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	1M	A	-	INSERTION	GB X01554.1

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
26	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			
28	DF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
30	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
31	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
33	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
35	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B0	117	Total	C	N	O		0	0	0
			960	599	202	159				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	D0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	111	Total	C	N	O		0	0	0
			882	556	176	150				
37	DQ	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
42	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
43	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			
44	DV	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B3	80	Total	C	N	O	S	0	0	0
			629	389	132	107	1			
45	D3	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
47	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BX	59	Total	C	N	O	S	0	0	0
			469	298	90	81				
48	DX	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
49	D4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
50	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			
51	D6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
53	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AP	1	Total	Mg	0	0
			1	1		
54	CR	1	Total	Mg	0	0
			1	1		
54	B4	1	Total	Mg	0	0
			1	1		
54	BA	683	Total	Mg	0	0
			683	683		
54	AK	1	Total	Mg	0	0
			1	1		
54	CH	2	Total	Mg	0	0
			2	2		
54	DF	1	Total	Mg	0	0
			1	1		
54	B8	1	Total	Mg	0	0
			1	1		
54	BE	7	Total	Mg	0	0
			7	7		
54	AW	4	Total	Mg	0	0
			4	4		
54	DU	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	C1	1	Total	Mg	0	0
			1	1		
54	CD	26	Total	Mg	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DZ	2	Total 2	Mg 2	0	0
54	AX	1	Total 1	Mg 1	0	0
54	D6	2	Total 2	Mg 2	0	0
54	AS	2	Total 2	Mg 2	0	0
54	CA	384	Total 384	Mg 384	0	0
54	B5	1	Total 1	Mg 1	0	0
54	BB	26	Total 26	Mg 26	0	0
54	AJ	1	Total 1	Mg 1	0	0
54	BT	2	Total 2	Mg 2	0	0
54	CC	13	Total 13	Mg 13	0	0
54	DB	29	Total 29	Mg 29	0	0
54	D3	4	Total 4	Mg 4	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	2	Total 2	Mg 2	0	0
54	DA	905	Total 905	Mg 905	0	0
54	AA	440	Total 440	Mg 440	0	0
54	BQ	1	Total 1	Mg 1	0	0
54	CQ	3	Total 3	Mg 3	0	0
54	D7	1	Total 1	Mg 1	0	0
54	CX	2	Total 2	Mg 2	0	0
54	B6	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CG	1	Total 1	Mg 1	0	0
54	BU	5	Total 5	Mg 5	0	0
54	A1	1	Total 1	Mg 1	0	0
54	AD	3	Total 3	Mg 3	0	0
54	DD	3	Total 3	Mg 3	0	0
54	CT	1	Total 1	Mg 1	0	0
54	DH	4	Total 4	Mg 4	0	0
54	D0	5	Total 5	Mg 5	0	0
54	BG	1	Total 1	Mg 1	0	0
54	AI	1	Total 1	Mg 1	0	0
54	DS	1	Total 1	Mg 1	0	0
54	DE	3	Total 3	Mg 3	0	0
54	B3	2	Total 2	Mg 2	0	0
54	BR	2	Total 2	Mg 2	0	0
54	CP	4	Total 4	Mg 4	0	0
54	BK	1	Total 1	Mg 1	0	0
54	DW	2	Total 2	Mg 2	0	0
54	D2	1	Total 1	Mg 1	0	0
54	AL	2	Total 2	Mg 2	0	0
54	CM	1	Total 1	Mg 1	0	0
54	BO	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AQ	1	Total 1	Mg 1	0	0
54	D1	6	Total 6	Mg 6	0	0
54	AH	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	DO	5	Total 5	Mg 5	0	0
54	AC	8	Total 8	Mg 8	0	0
54	CW	5	Total 5	Mg 5	0	0
54	DG	3	Total 3	Mg 3	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	2	Total 2	Mg 2	0	0
54	AT	2	Total 2	Mg 2	0	0
54	DT	2	Total 2	Mg 2	0	0
54	B0	2	Total 2	Mg 2	0	0
54	AO	1	Total 1	Mg 1	0	0
54	BW	1	Total 1	Mg 1	0	0
54	CS	2	Total 2	Mg 2	0	0
54	CK	2	Total 2	Mg 2	0	0
54	CL	1	Total 1	Mg 1	0	0
54	BH	1	Total 1	Mg 1	0	0

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

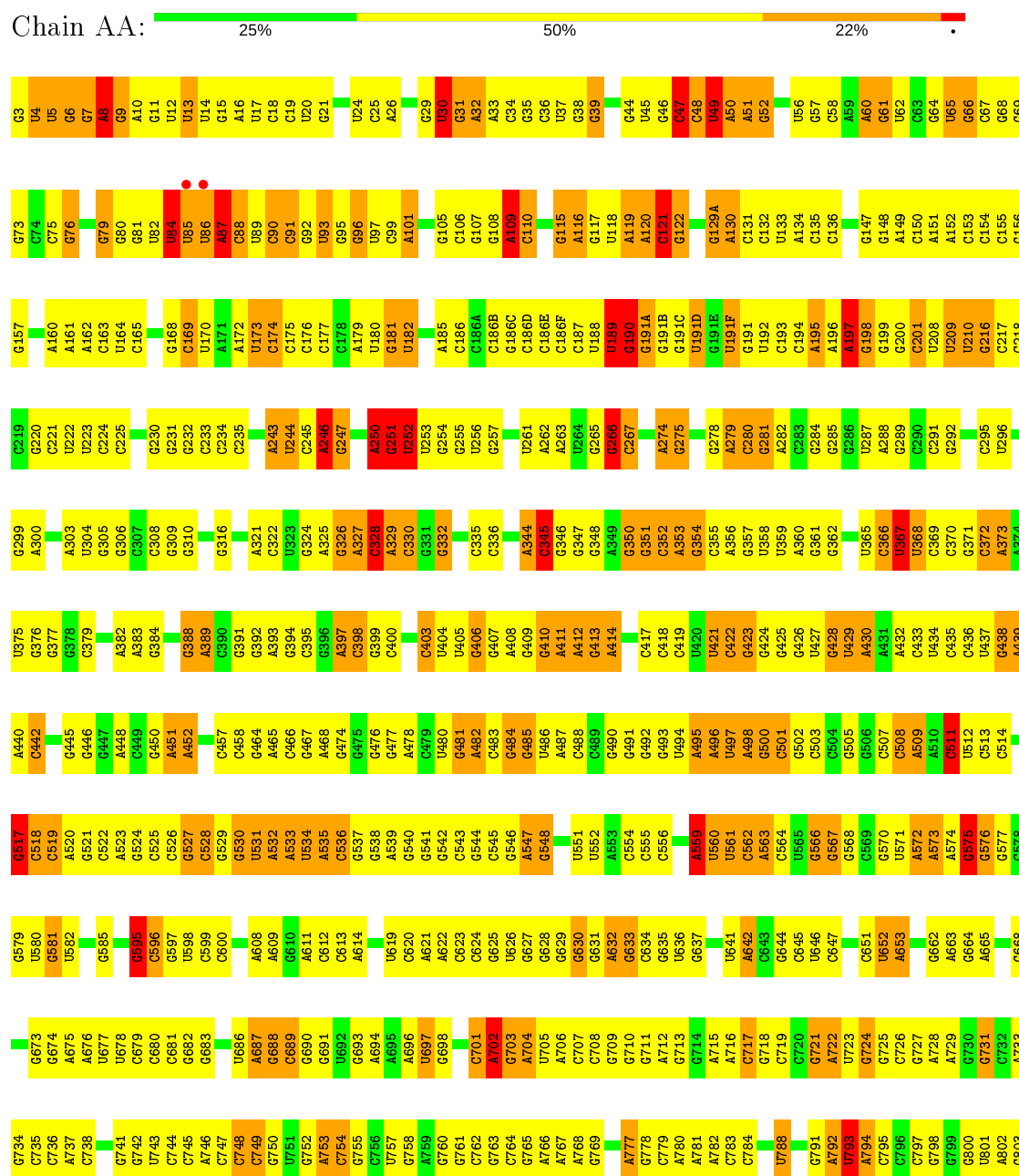
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	Zn 1	0	0
55	AG	1	Total 1	Zn 1	0	0
55	AA	2	Total 2	Zn 2	0	0
55	AQ	1	Total 1	Zn 1	0	0
55	CG	1	Total 1	Zn 1	0	0

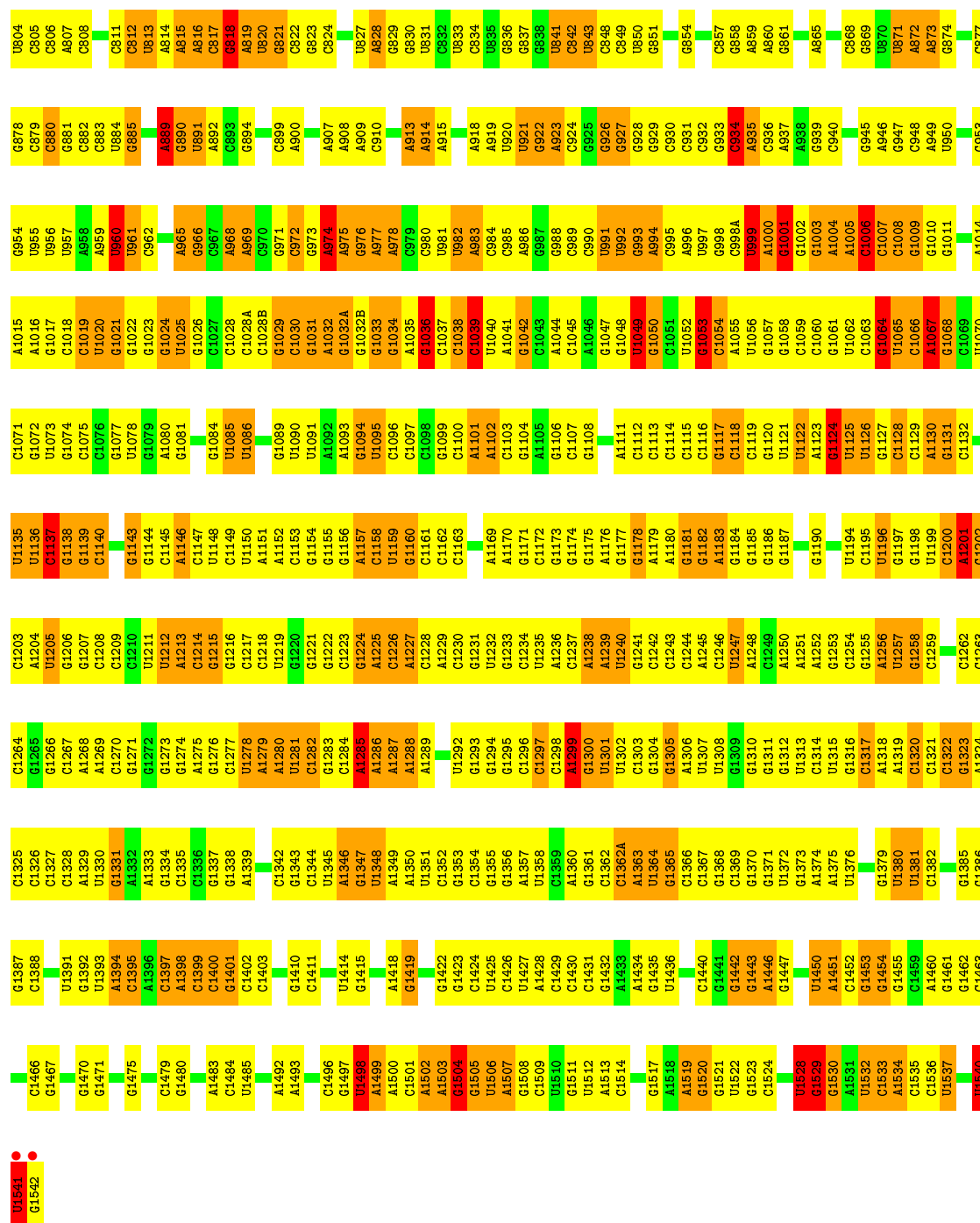


### 3 Residue-property plots

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

- Molecule 1: 16S rRNA (E.COLI NUMBERING)

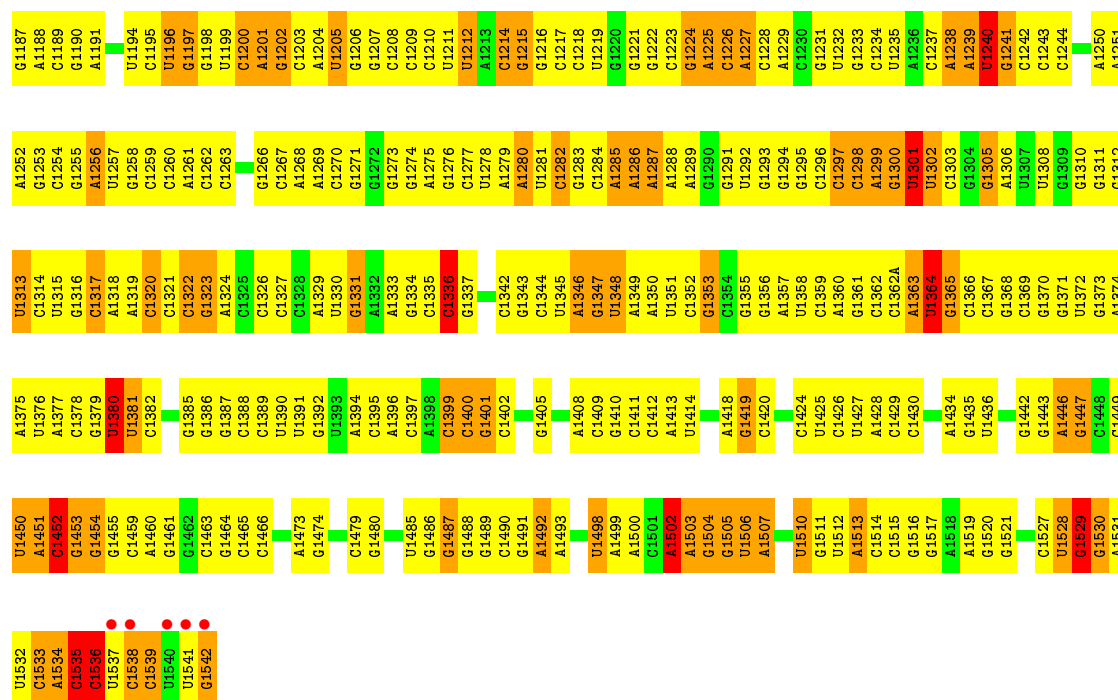




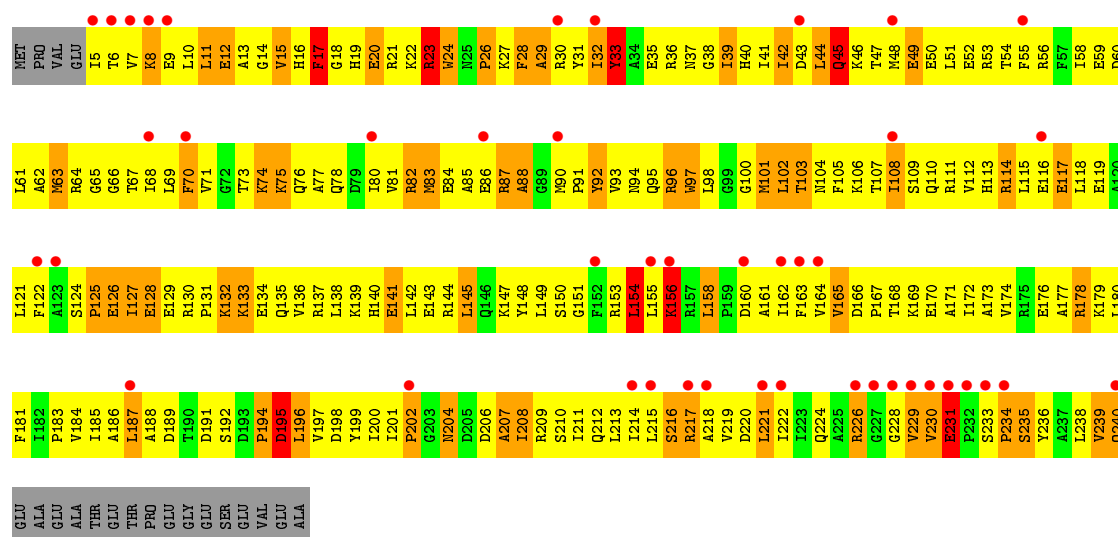
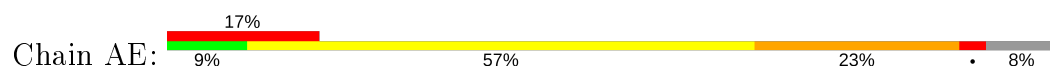
• Molecule 1: 16S rRNA (E.COLI NUMBERING)



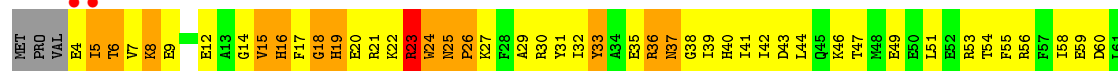
G1124	U1062	U999	A935	U863	A777	C707	G633	G558	G490	A414	A349	A278	G198	G147
U1125	C1063	A1000	C936	A864	G778	C708	A640	A559	G491	A415	G350	C280	G199	G148
U1126	G1064	G1001	A937	A865	C779	G709	G641	A560	G492	G416	G351	G281	G200	A149
G1127	G1065	G1002	A938	A866	A780	G710	A642	A561	G493	C417	C352	C201	C201	C150
G1128	C1066	G1003	C939	C866	G788	G713	A643	A562	U494	C418	G353	U208	U208	A151
G1129	A1067	A1004	C940	G867	U789	G714	C644	A563	A495	C419	G354	U209	U209	A152
A1130	G1068	A1005	C941	U870	A790	A715	G644	A564	A496	G422	C355	C291	C217	G156
G1131	C1067	C1006	G942	U871	C791	A716	C645	A565	U497	G423	A356	C292	C218	G157
G1132	G1071	G1007	U950	U872	A792	C717	G649	G566	A498	G423	G357	G295	C219	G158
G1133	G1072	C1008	A946	A873	G718	G718	G650	G567	C501	G428	U358	U296	C220	G159
G1134	U1073	G1009	G947	A793	C719	G719	G651	G568	G502	U429	U359	U296	C221	A160
U1135	G1074	G1010	G948	G874	A794	C720	G652	G569	G503	A430	G361	U297	C222	A161
U1136	C1075	G1011	A949	U875	G721	G721	U852	A572	C504	A431	A362	U298	U223	A162
G1137	G1076	A1014	U950	C877	C796	A722	A853	A573	C505	A432	G362	G299	U224	A163
G1138	U1077	A1015	G951	G878	C797	U723	G854	A574	C506	A433	C358	A300	C224	C163
G1139	U1078	A1016	U952	C879	A807	G727	A855	G575	A509	A434	U365	G301	G229	C164
C1140	G1079	G1017	G953	G880	A728	A728	G856	G576	A510	C435	C366	G302	U229	C165
C1141	A1080	C1018	G954	G881	C808	G729	G857	G577	C511	C436	U367	G230	G230	G166
G1142	G1081	C1019	U955	C882	G730	G730	G858	G578	U512	C437	U368	G305	G233	G167
G1143	G1082	U1020	U956	C883	G731	G731	G859	G579	G517	U438	C372	G306	C234	U170
G1144	U1083	G1021	U957	C884	U813	G732	G860	G580	C518	A439	A373	G310	C235	A171
G1145	G1084	G1022	G885	A814	A733	A733	A663	G581	C519	A440	A374	C311	C236	A172
U1146	U1085	G1023	G886	A815	G734	G734	A664	G582	A520	C442	U375	C312	U173	U173
G1147	G1147	U1024	U960	A816	G735	G735	A665	G583	G521	C443	G376	A313	C240	C174
U1148	U1025	U1025	U961	C817	C736	C736	G866	G584	C522	C444	G377	C314	G175	C175
C1149	G1026	G1026	G862	G818	A737	A737	G867	G585	A523	G447	G378	A315	A243	C176
U1150	C1027	C1027	G963	A819	C738	C738	G868	G586	G524	G448	U244	A316	U244	C177
A1151	U1028	G1028	A964	A820	C739	C739	G869	G587	C525	A449	G380	G317	U245	G178
A1152	A1029	C1028A	G965	G821	G740	G740	G871	G588	C526	C449	G381	C449	A246	A179
C1153	A103	C1028B	G966	G822	U740	U740	G672	G589	C527	G450	A382	G319	G247	U180
G1094	G1029	G1029	C967	G823	G741	G741	G673	G590	G528	A451	A383	C320	G247	U181
U1095	U1095	U1095	A968	C824	G742	G742	G674	G591	G529	A452	G384	A321	A250	U182
G1156	C1096	A1032	A969	G825	U743	U743	A675	G592	G530	A453	C385	C322	G251	G183
A1157	C1097	G1032A	C970	G826	C744	C744	A676	G593	U531	C454	U323	U323	G252	G184
C1158	C1098	G1032B	C971	G827	C745	C745	U677	C596	U532	C455	G324	U253	U253	A185
U1159	G1099	G1033	G972	G828	A746	A746	U678	G597	A533	C456	A389	G325	G254	C186
G1160	C1100	U1034	G973	G829	C747	C747	U679	G598	U534	C457	C390	G326	G255	C186A
C1161	A1101	A1035	A974	G830	C748	C748	A684	G599	A535	C458	G391	A327	U256	C186B
C1162	C1102	G1036	A975	G831	C749	C749	G885	C600	C536	G464	G392	C328	G257	G186C
G1163	G1103	C1037	G976	U832	G752	G752	U686	G601	G537	A465	A393	A329	G260	C186D
G1164	C1104	C1038	A977	U833	A753	A753	U687	A602	G538	C466	G394	G331	U261	C186E
C1165	A1105	C1039	A978	U834	C754	C754	G688	U603	A539	C467	G397	G332	A262	C186F
G1166	G1106	U1040	C979	U835	G755	G755	G689	G604	G540	A468	A397	G333	A263	C187
A1169	C1107	A1041	C980	G836	C756	C756	G690	U605	G541	G474	C396	G334	A264	U188
A1170	G1108	G1042	U981	G837	U757	U757	G691	G606	C542	G475	G399	C334	U264	U189
G1171	C1109	C1043	U982	G838	U758	G758	U692	G607	C543	G476	G400	C335	G265	G190
C1172	A1110	G1043	U983	U841	A759	A759	G693	A607	G544	G477	G401	C336	G266	G191A
G1173	G1111	G1047	C984	C842	A759	A759	A694	G608	C545	A478	G402	C337	G267	G191B
A1176	C1112	U1049	U985	U843	G760	G760	A695	G609	G546	C479	O403	A338	C268	G191C
G1177	G1113	G1050	G987	C848	G763	G763	A696	A621	A547	U480	U404	C339	C269	U191D
G1178	C1114	C1051	G922	C849	C764	C764	A697	G623	G548	G481	U405	U340	A270	G191E
A1179	G1115	U1052	A923	U850	G765	G765	G698	G624	C549	A482	G406	C341	C271	U191F
A1180	C1116	U1053	G924	G851	A766	A766	U626	G625	C549	C483	G407	C342	C272	G191G
G1181	G1117	G1054	G925	G852	A767	A767	G627	U626	U552	G484	A408	U343	A273	U192
G1182	C1118	C1054	G926	G853	A768	A768	A702	G628	C553	G485	G409	A344	A274	C193
C1183	C1119	A1055	G927	G854	G769	G769	G703	G629	C554	U486	G410	C345	G275	C194
G1184	G1120	G932	C922	G855	G775	G775	U704	G630	C555	A487	A411	G346	G276	A195
G1185	U1121	C1059	G933	A858	G776	G776	A705	G631	C556	C488	A412	G347	G277	A196
C1186	C1060	G1061	C934	A860	G776	G776	A706	A632	G557	C489	G413	G348	G278	A197

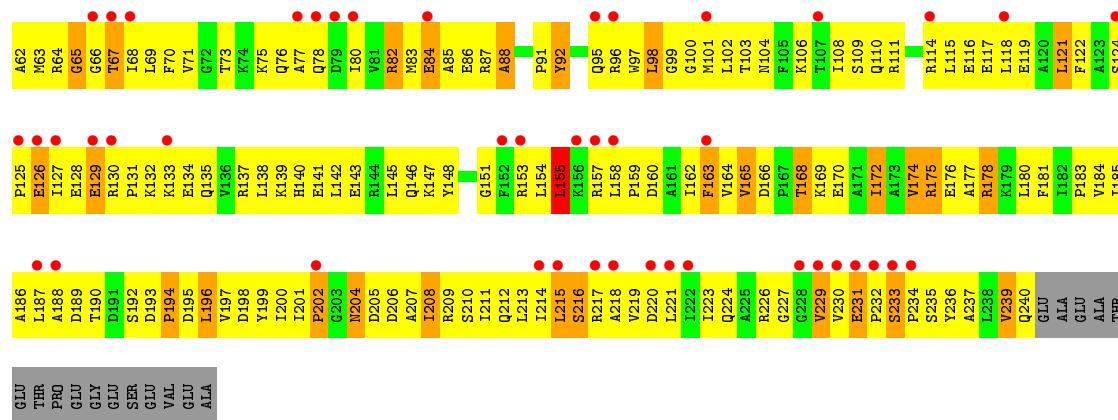


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

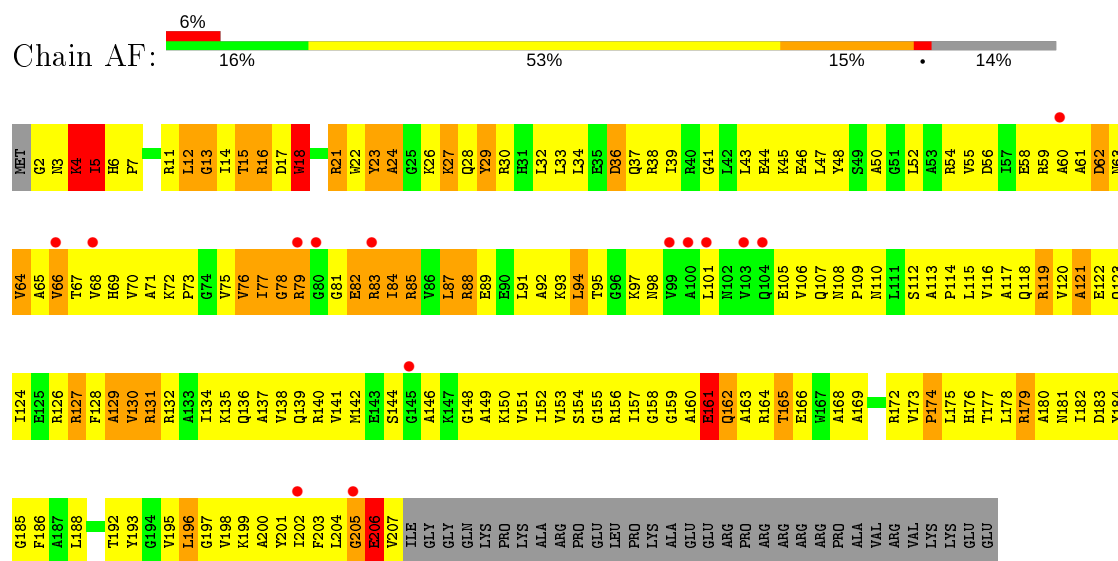


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

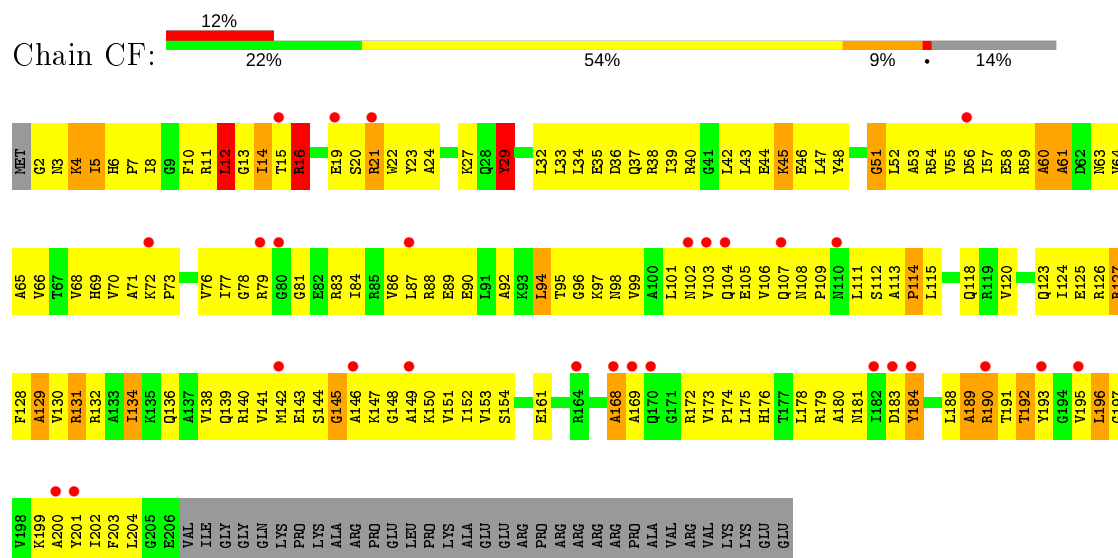




• Molecule 3: 30S RIBOSOMAL PROTEIN S3

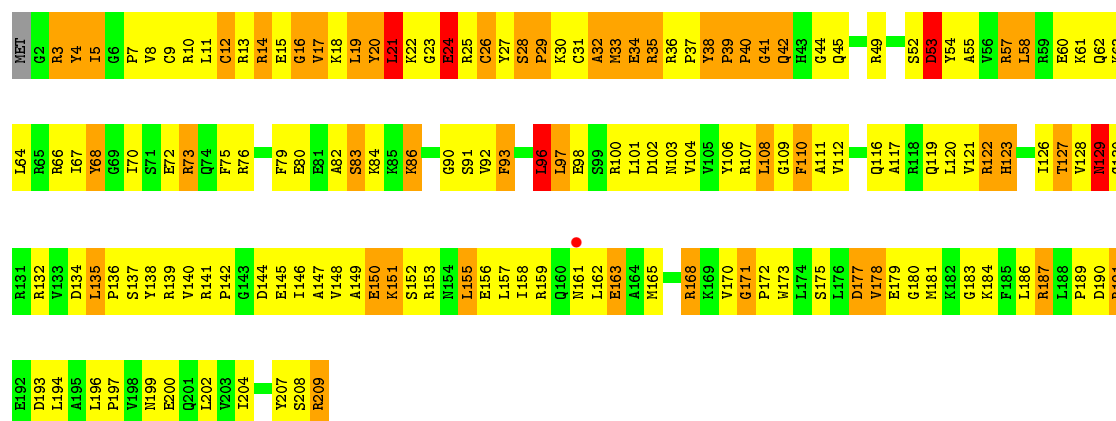


• Molecule 3: 30S RIBOSOMAL PROTEIN S3



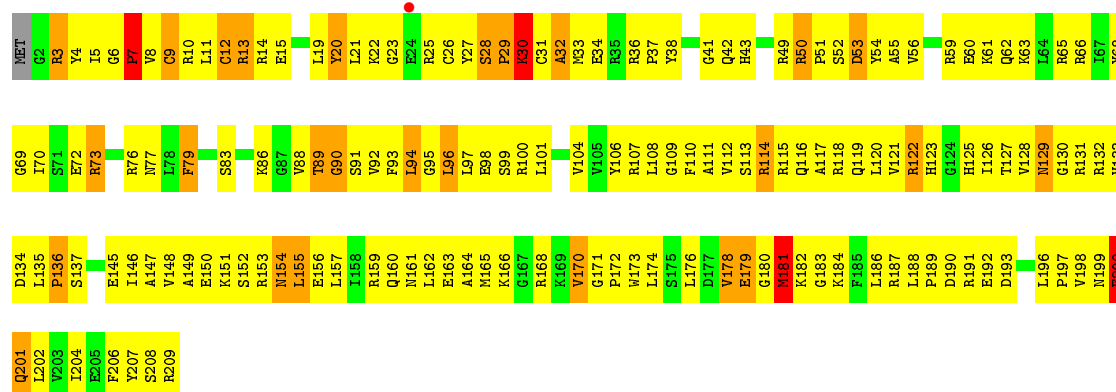
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG: 



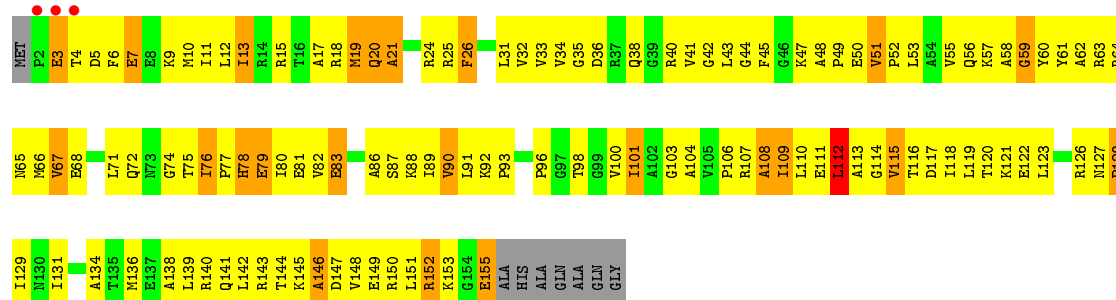
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG: 



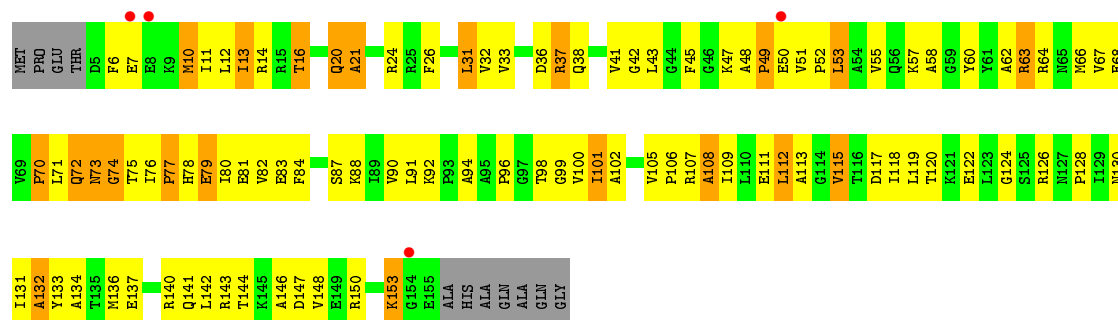
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH: 

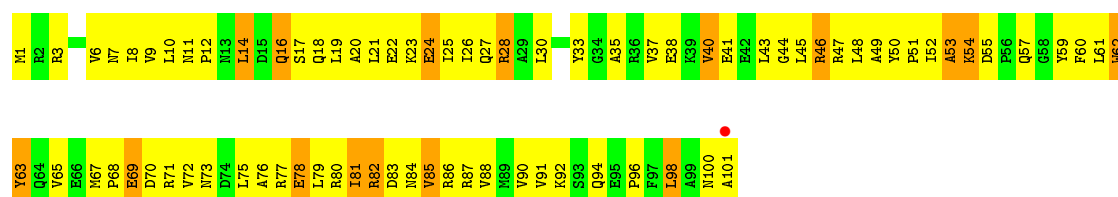


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

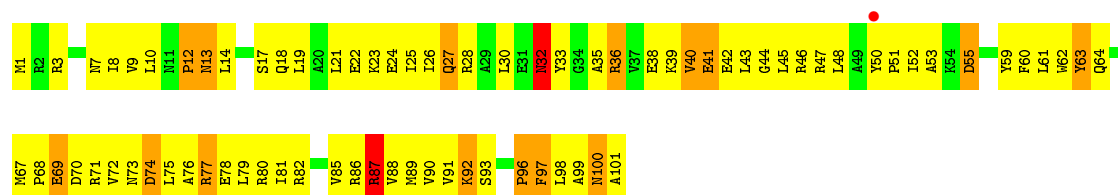
Chain CH: 



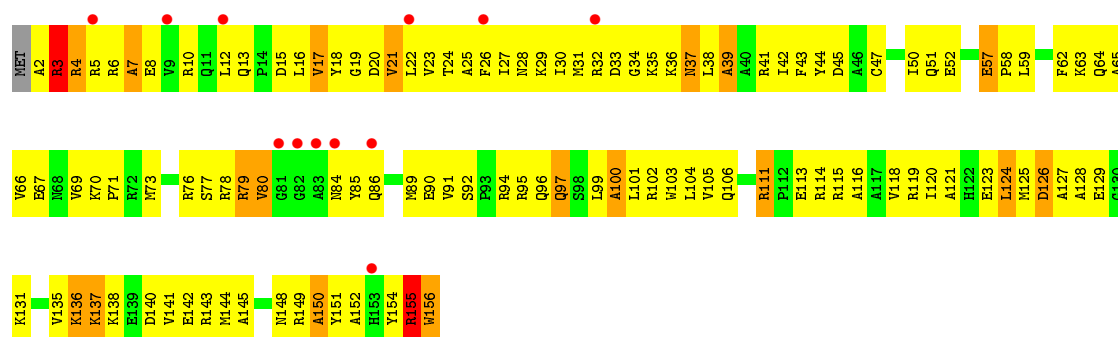
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

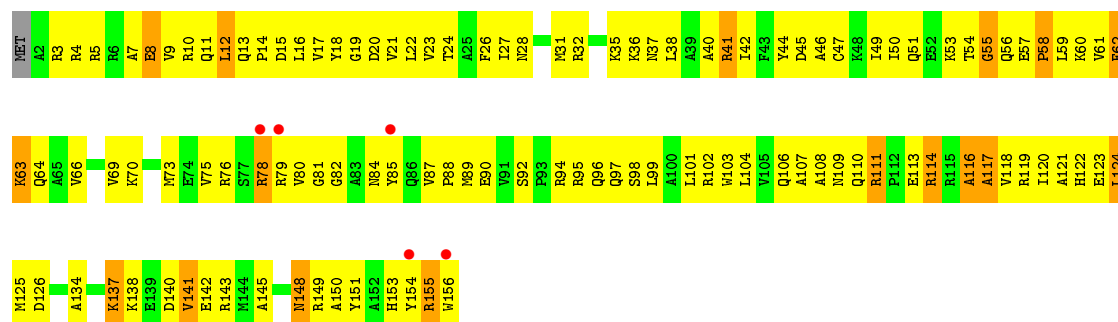


• Molecule 7: 30S RIBOSOMAL PROTEIN S7



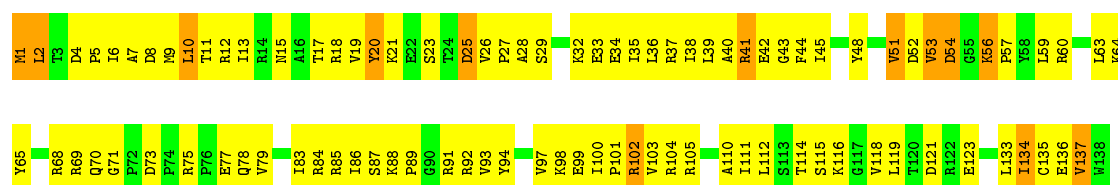
• Molecule 7: 30S RIBOSOMAL PROTEIN S7





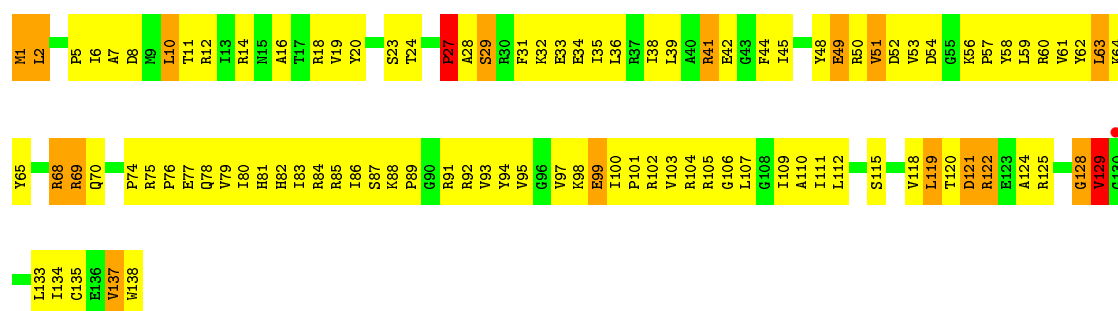
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK: 32% 59% 9%



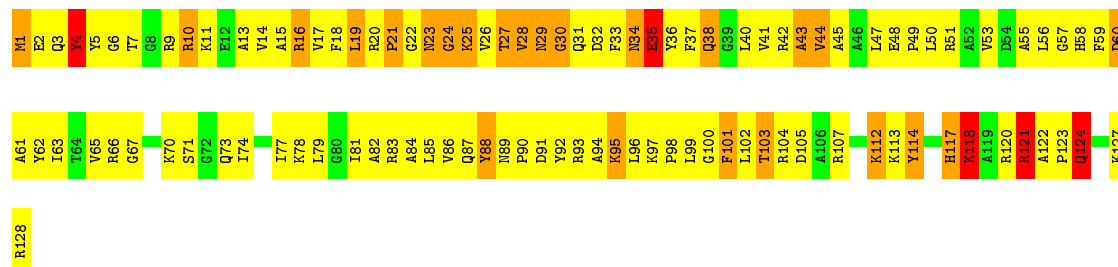
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK: 26% 61% 12%



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

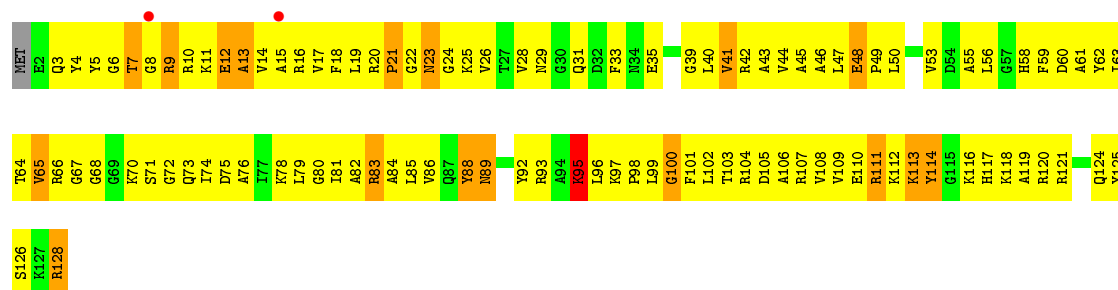
Chain AL: 18% 59% 19%



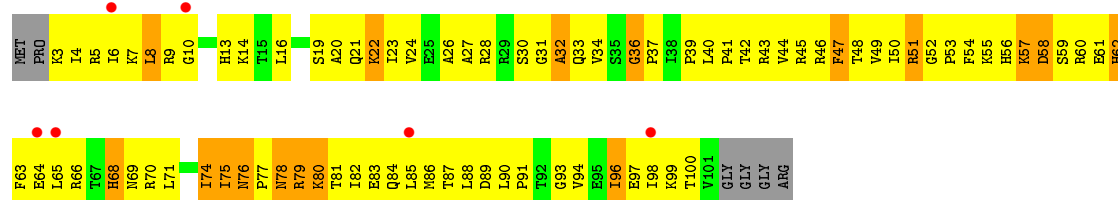
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL: 2% 17% 68% 13%

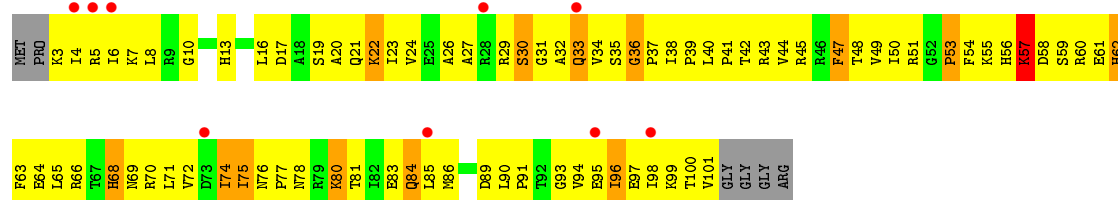




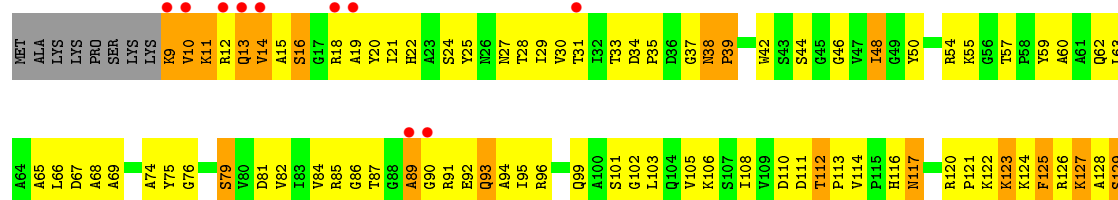
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

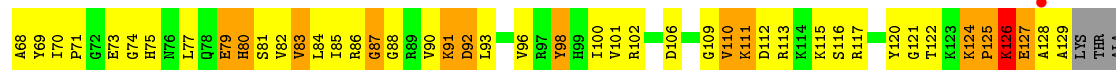
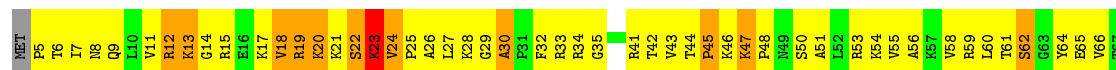


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

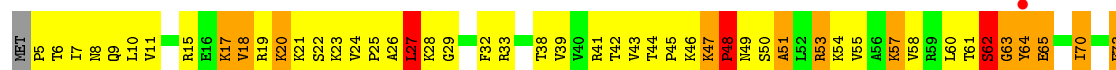




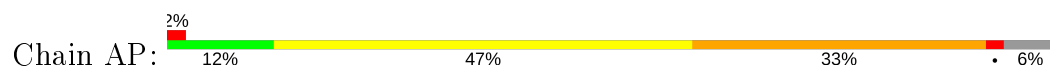
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



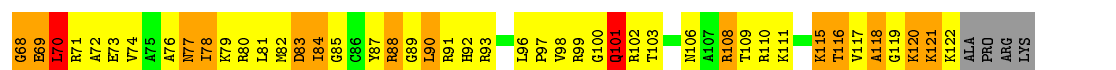
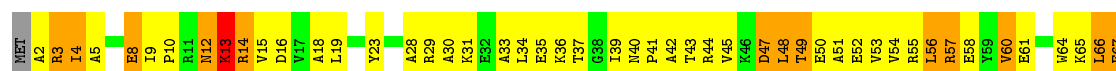
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:  28% 59% 8% . .



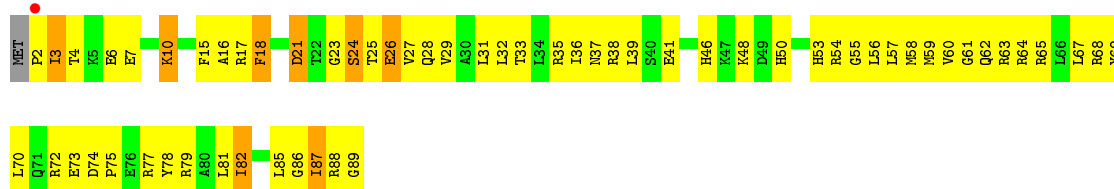
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:  18% 57% 16% 7% .



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:  30% 60% 9% .



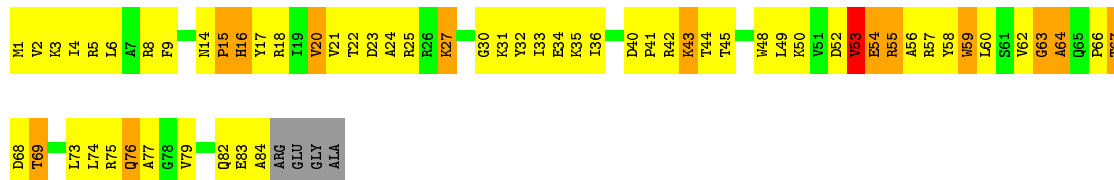
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:  29% 58% 11% .



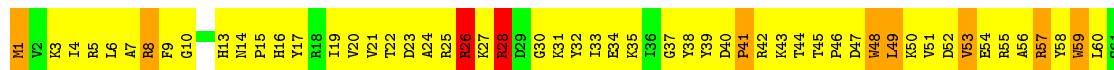
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

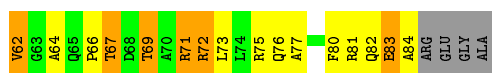
Chain AS:  26% 53% 15% 5% .



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:  16% 61% 16% 5% .





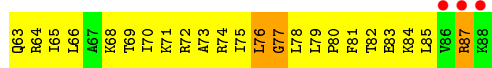
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



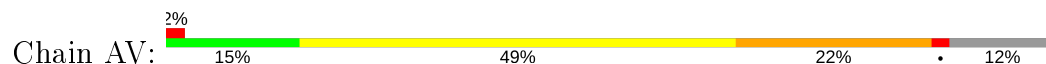
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

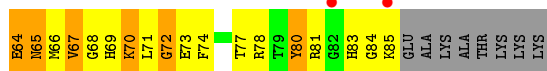
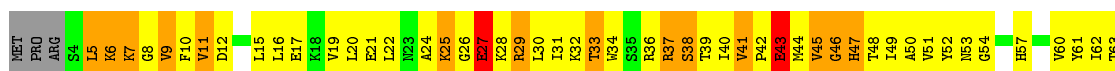


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

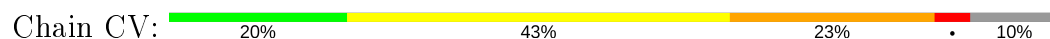


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

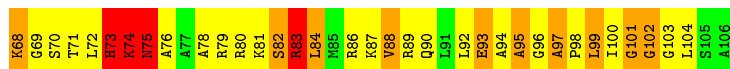




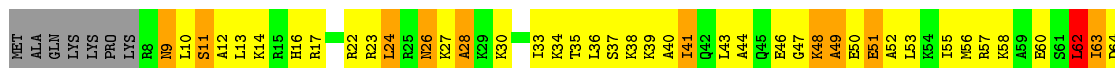
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



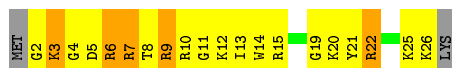
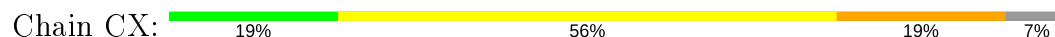
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

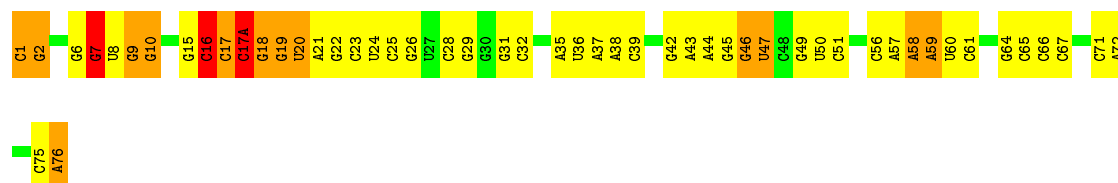


• Molecule 21: 30S RIBOSOMAL PROTEIN THX




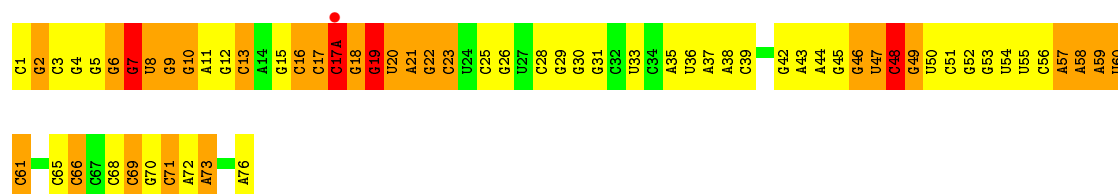
- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain AC:  32% 47% 17% 4%



- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain AD: 



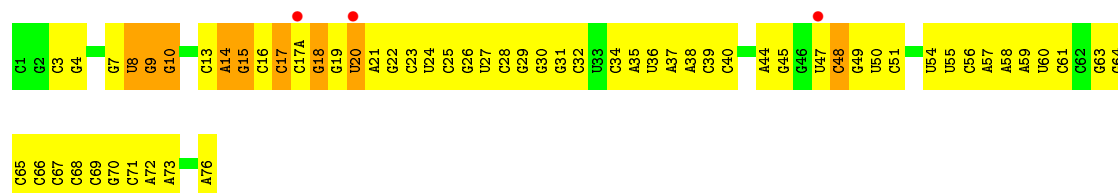
- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain CC: 




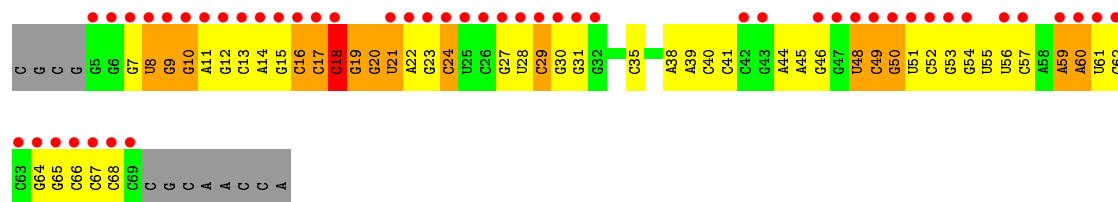
- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain CD: 

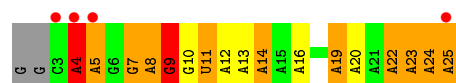


- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain CB: 



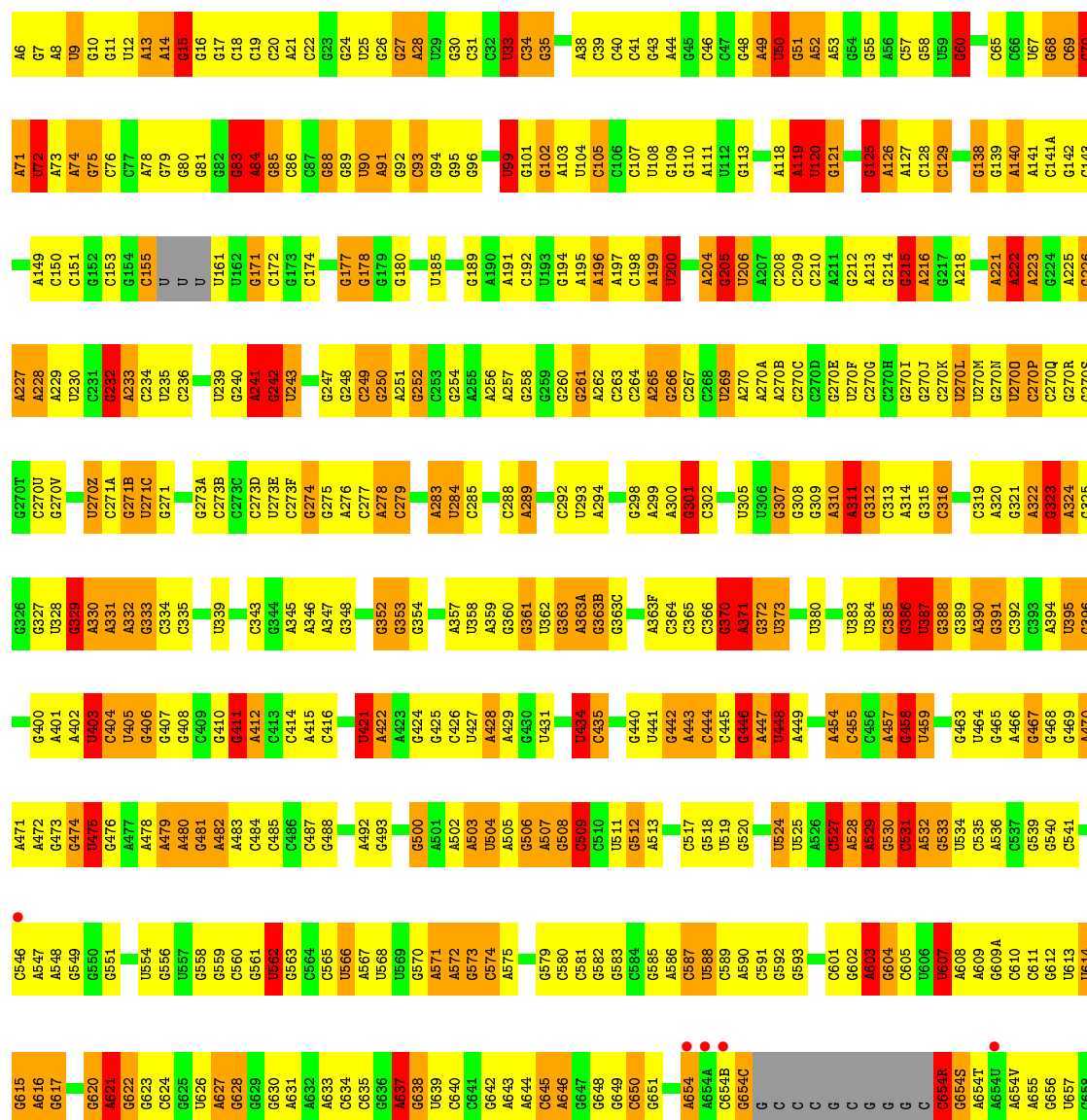
- Molecule 23: mRNA



• Molecule 23: MRNA



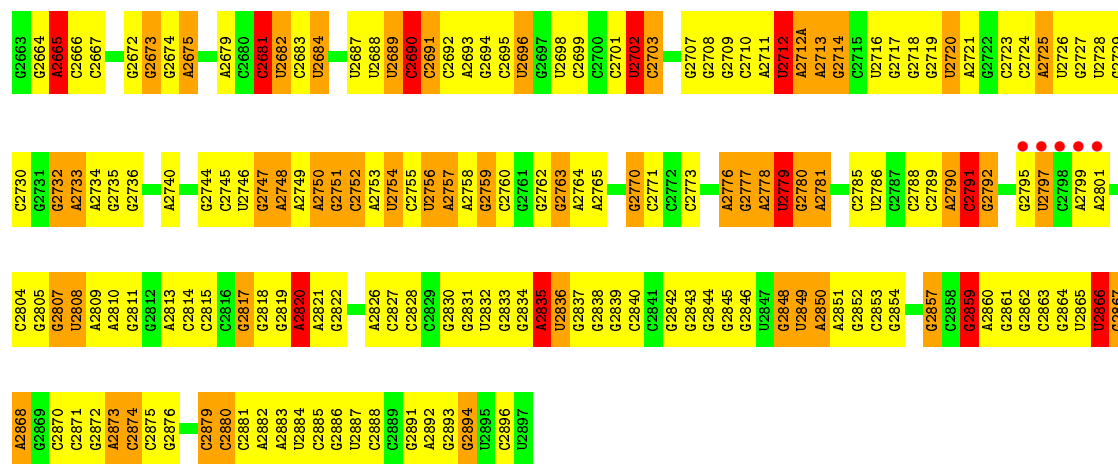
• Molecule 24: 23S ribosomal RNA



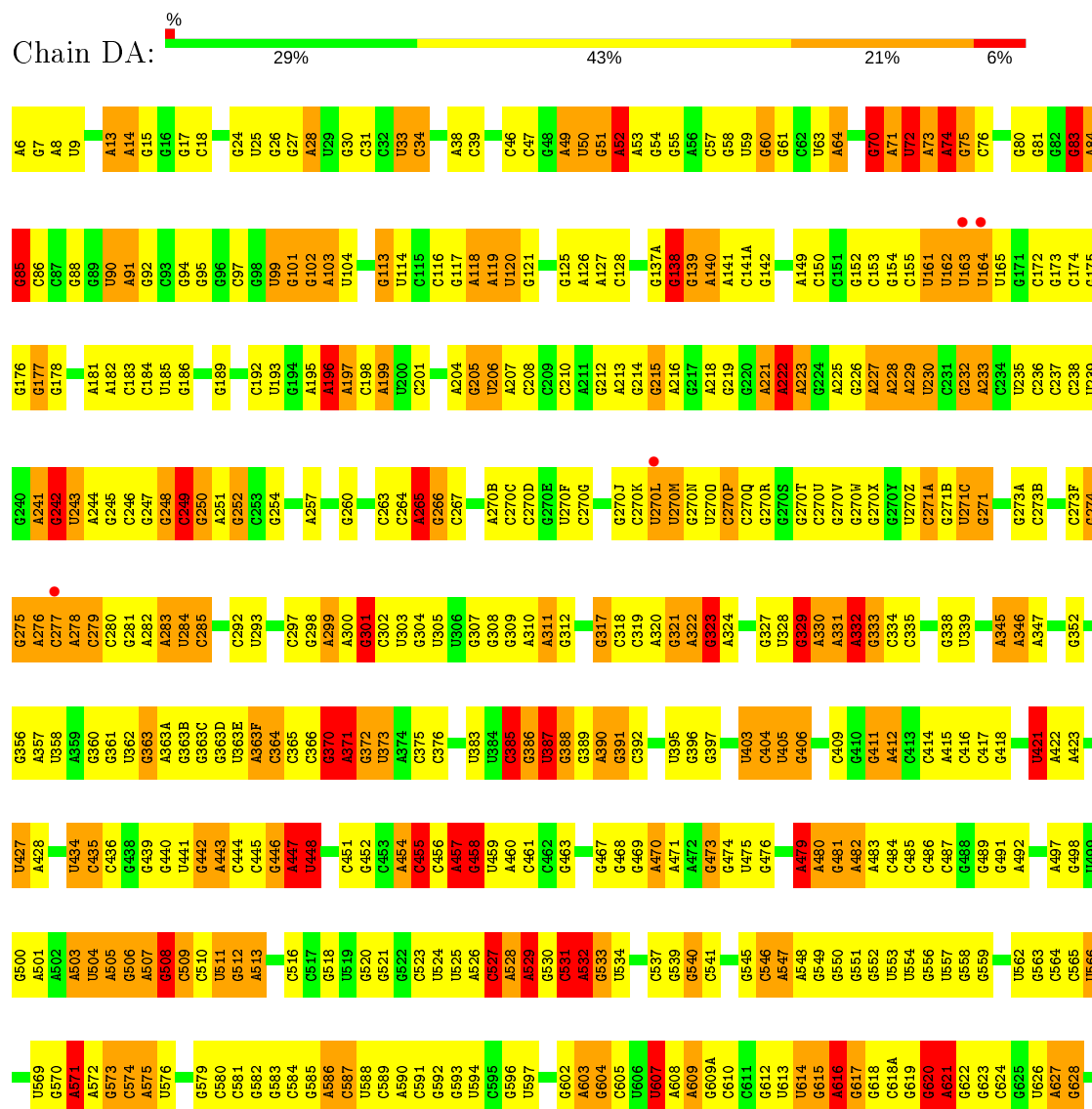
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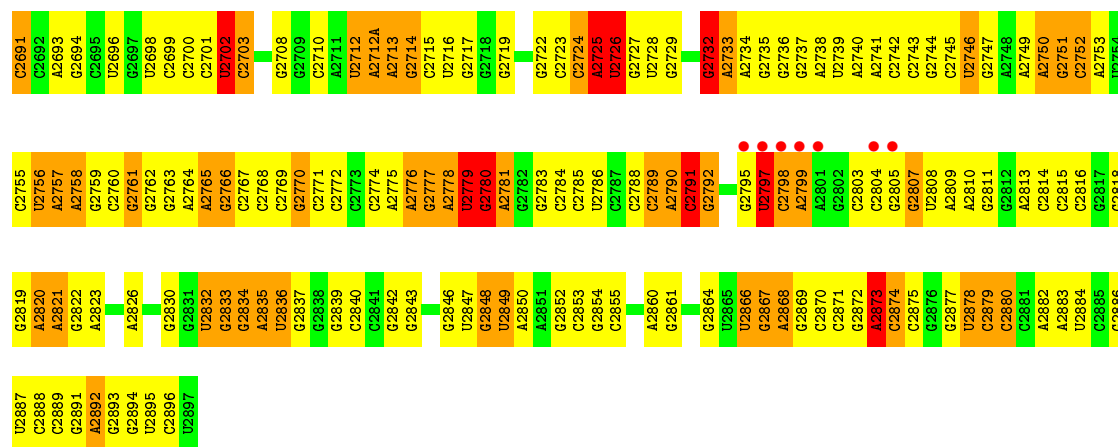


• Molecule 24: 23S ribosomal RNA



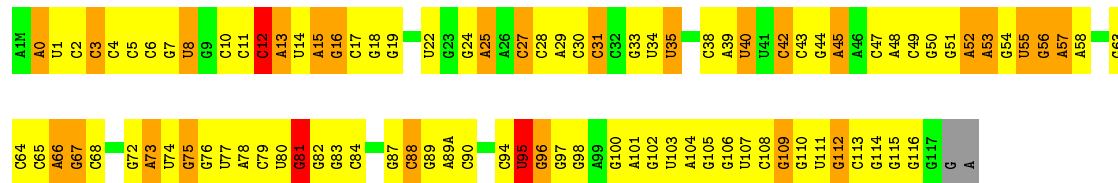
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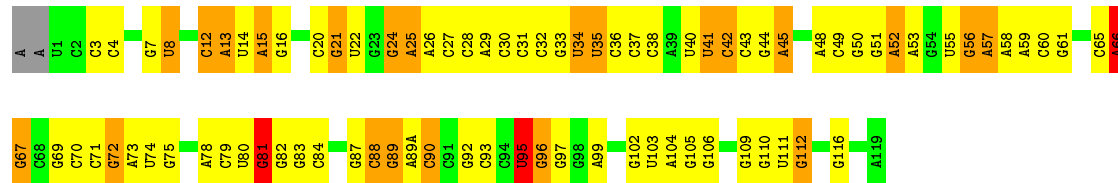
• Molecule 25: 5S ribosomal RNA

Chain BB: 20% 54% 21% . .



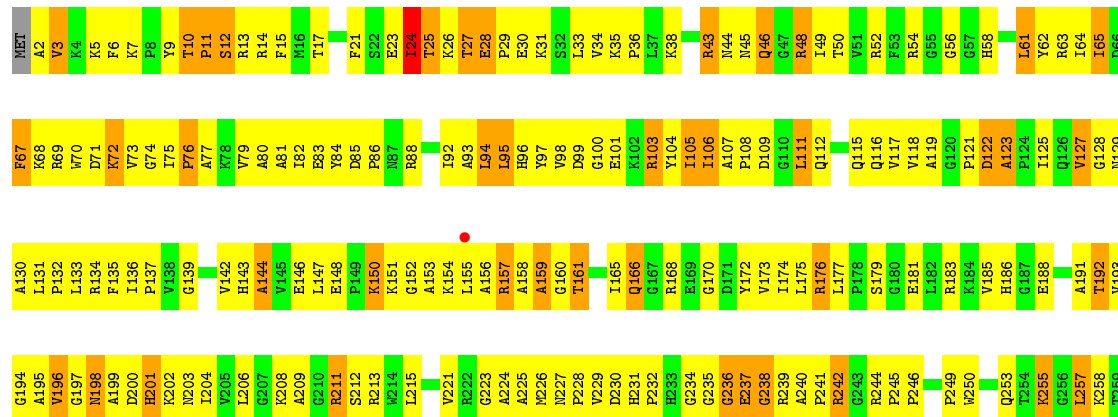
• Molecule 25: 5S ribosomal RNA

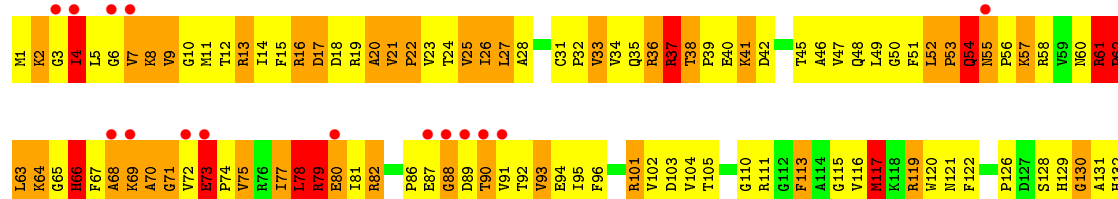
Chain DB: 30% 48% 18% . .

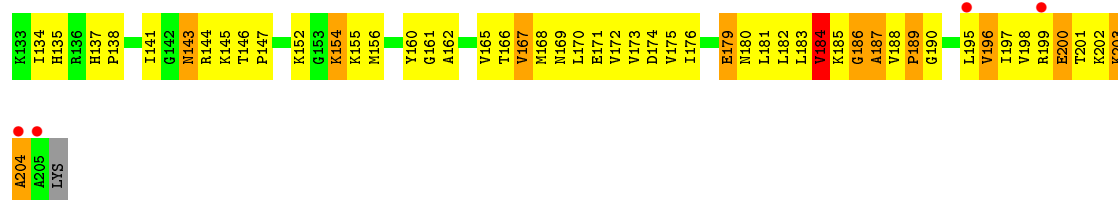


• Molecule 26: 50S ribosomal protein L2

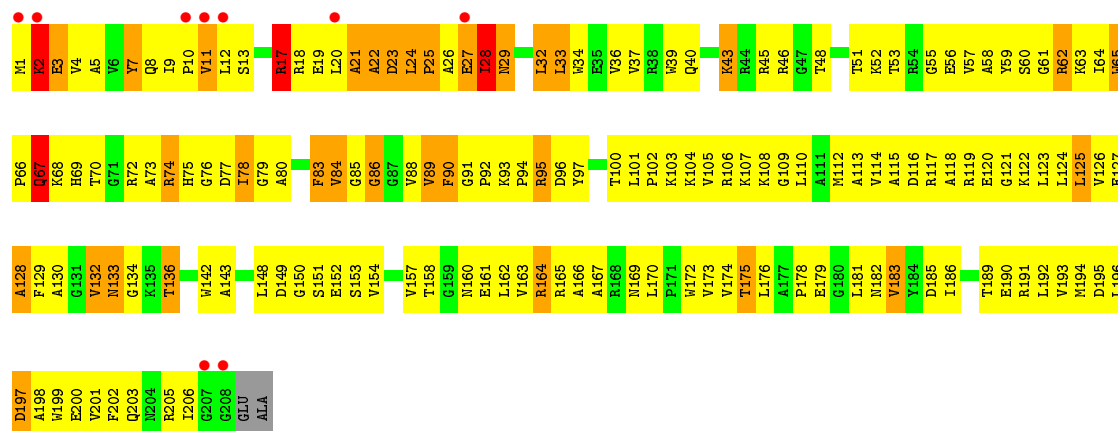
Chain BD: 26% 55% 17% .



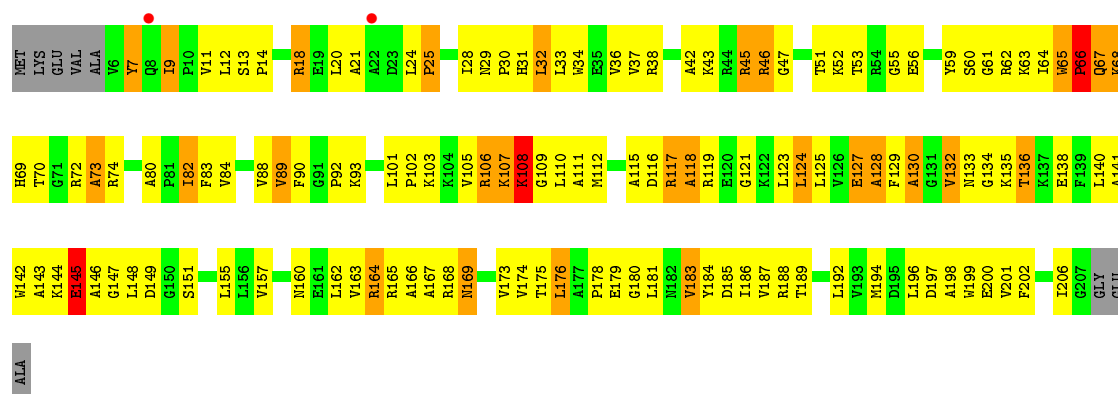




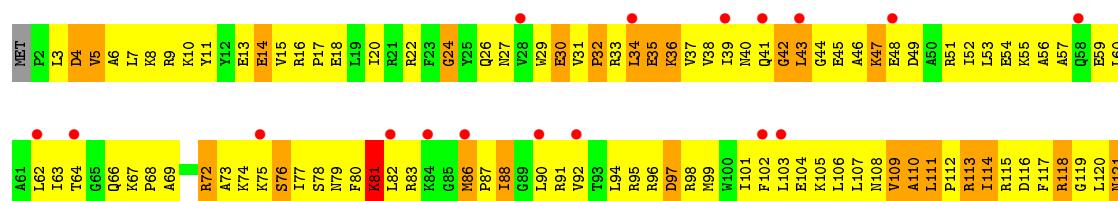
● Molecule 28: 50S ribosomal protein L4



● Molecule 28: 50S ribosomal protein L4

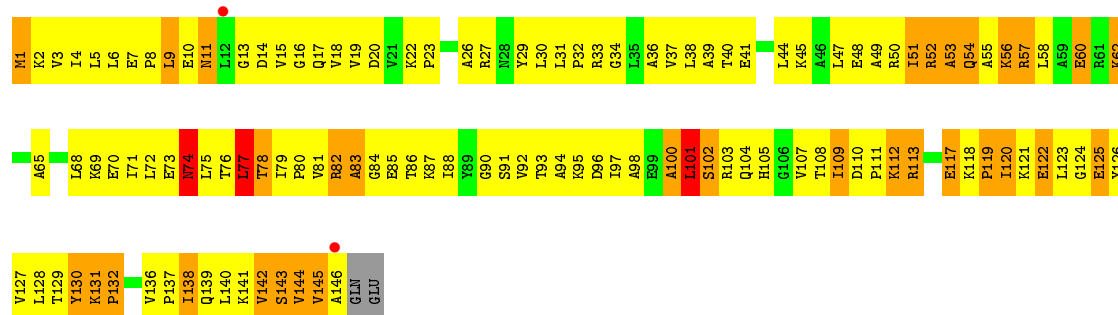


● Molecule 29: 50S ribosomal protein L5

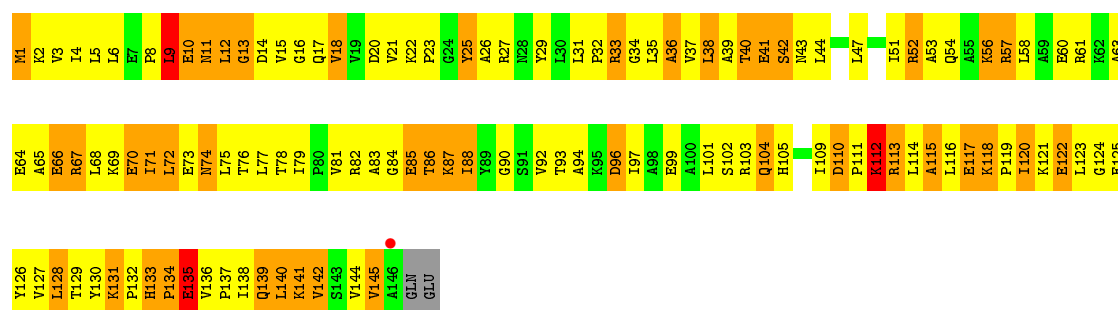
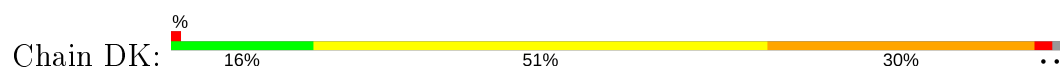




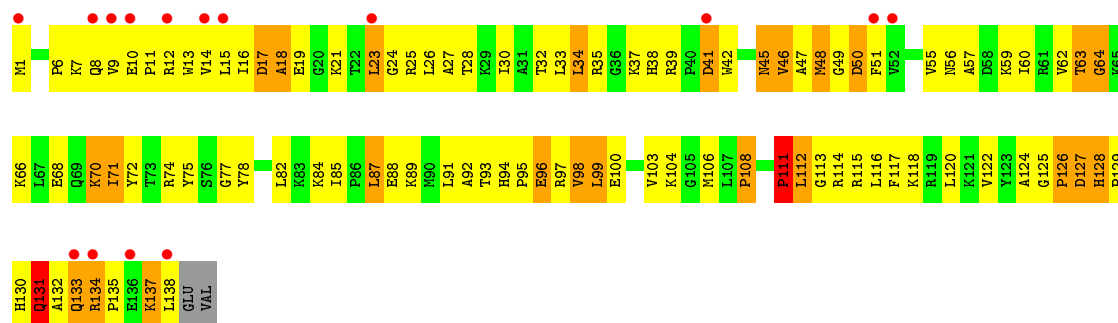




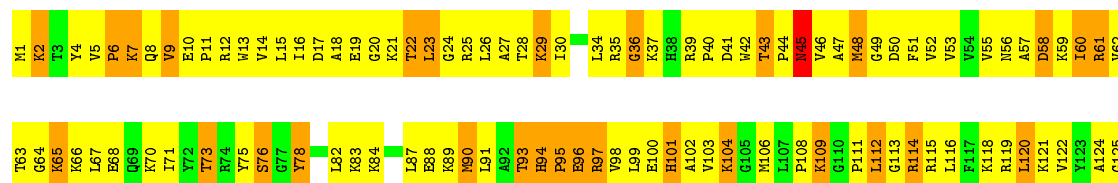
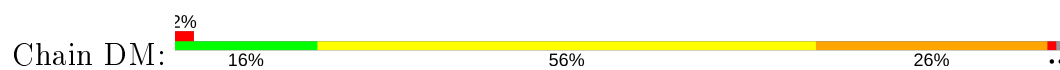
- Molecule 31: 50S ribosomal protein L9

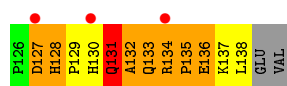


- Molecule 32: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L13

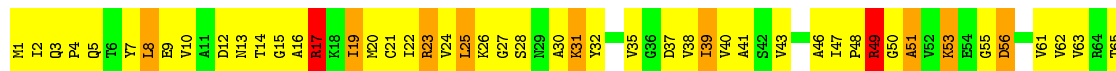




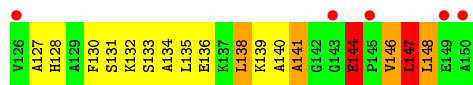
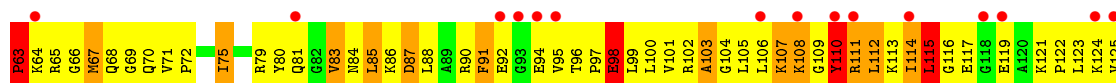
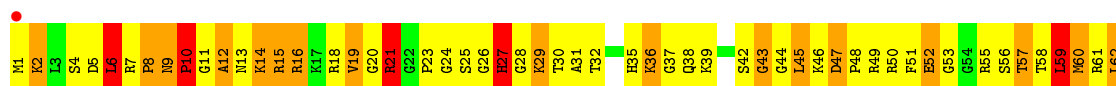
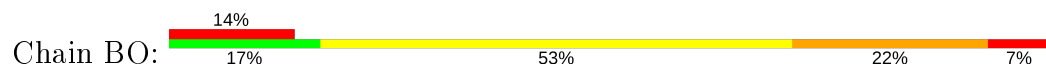
• Molecule 33: 50S ribosomal protein L14



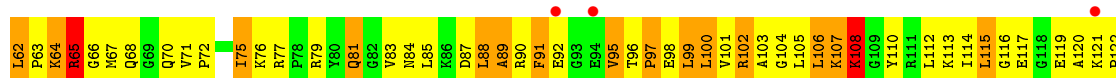
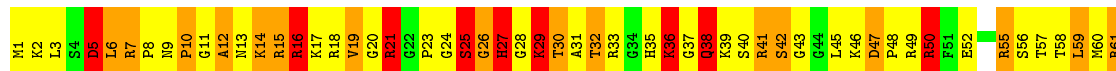
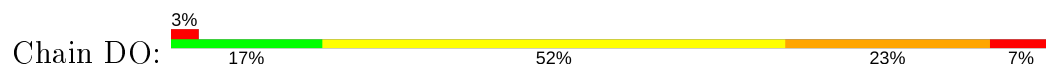
• Molecule 33: 50S ribosomal protein L14

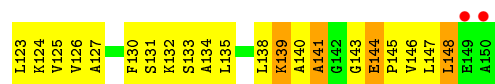


• Molecule 34: 50S ribosomal protein L15

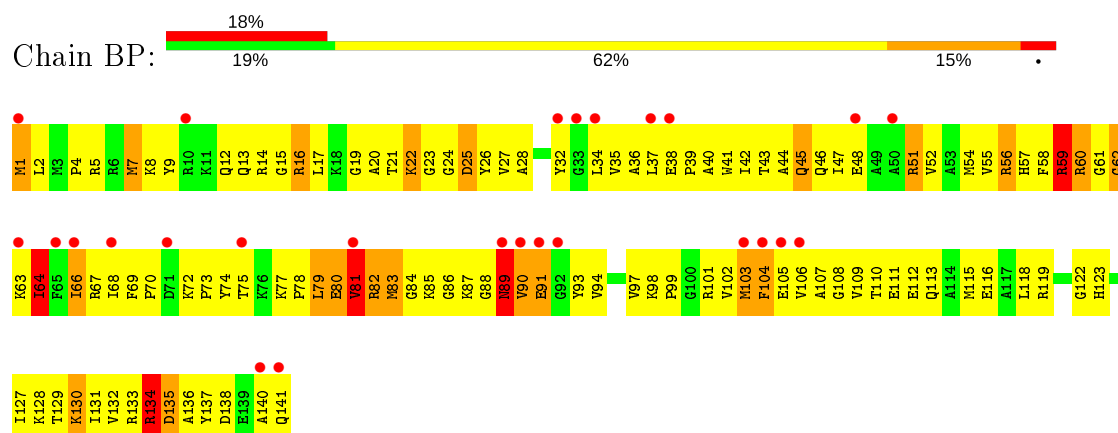


• Molecule 34: 50S ribosomal protein L15

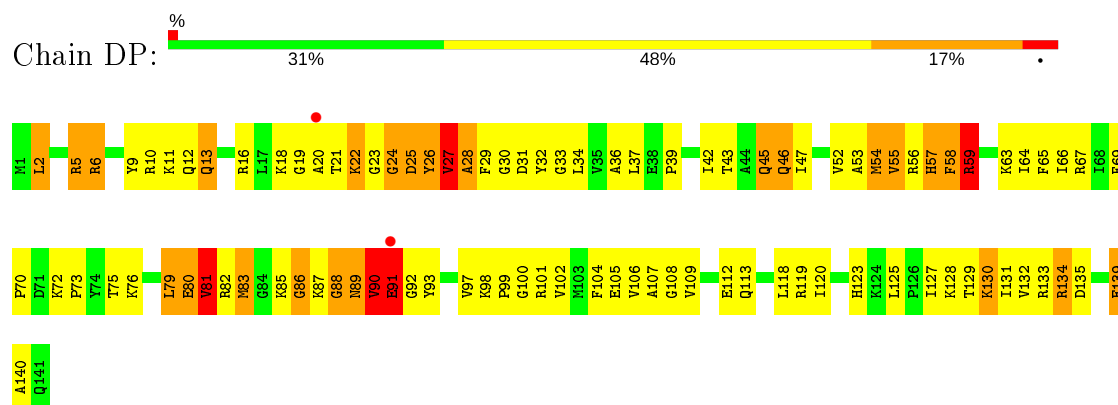




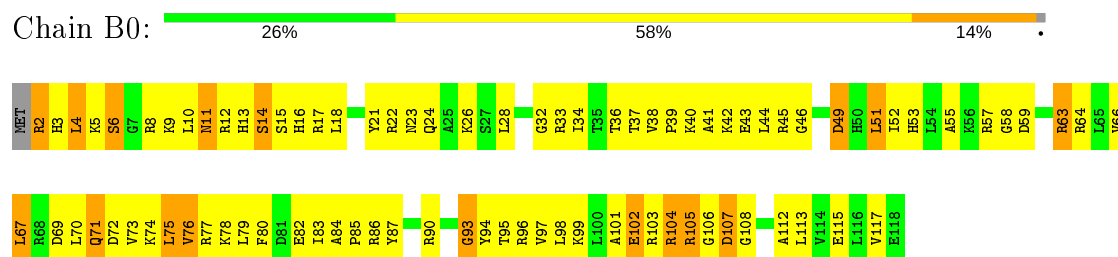
• Molecule 35: 50S ribosomal protein L16



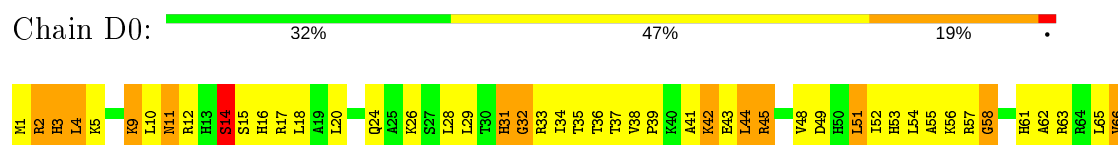
• Molecule 35: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L17



• Molecule 36: 50S ribosomal protein L17

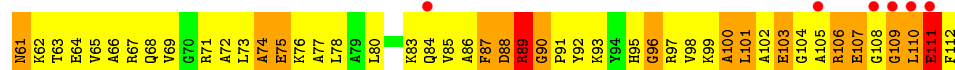
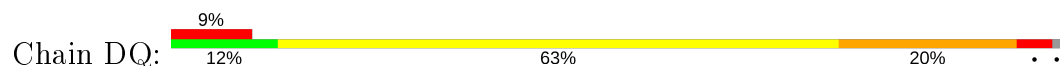




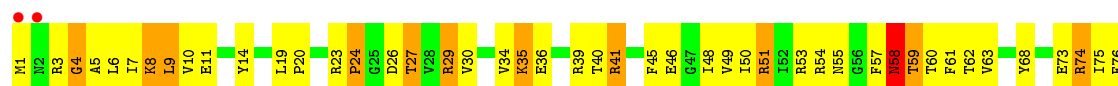
- Molecule 37: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L18

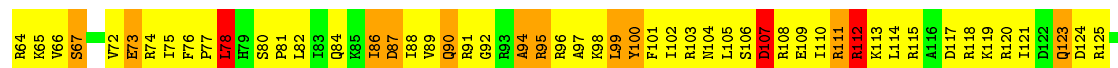


- Molecule 38: 50S ribosomal protein L19



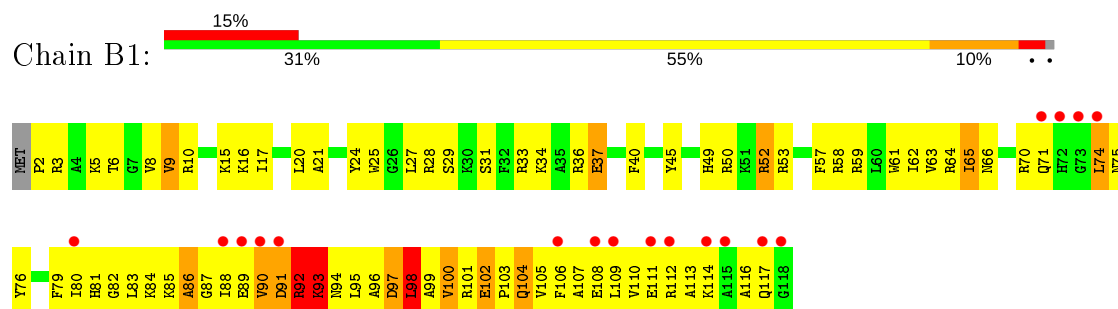
LYS  
ALA  
SER  
GLN  
GLU

- Molecule 38: 50S ribosomal protein L19

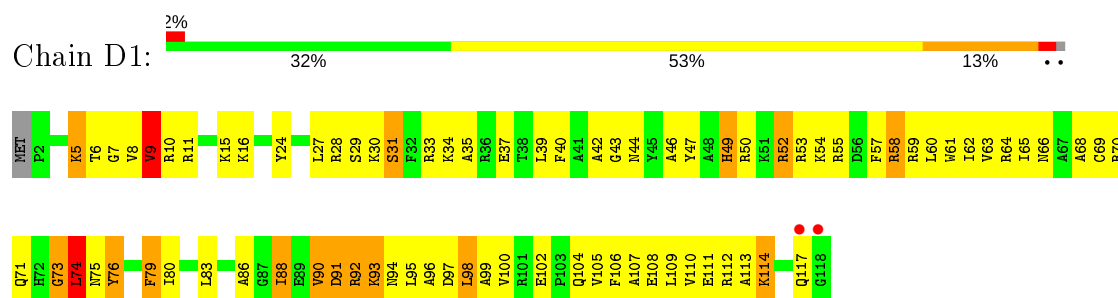




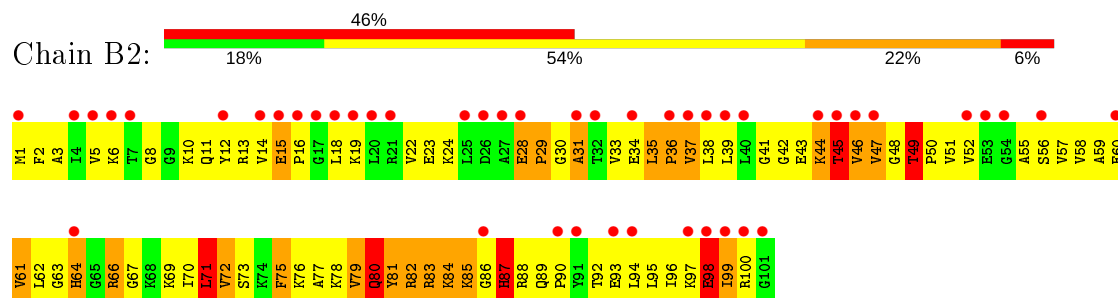
- Molecule 39: 50S ribosomal protein L20



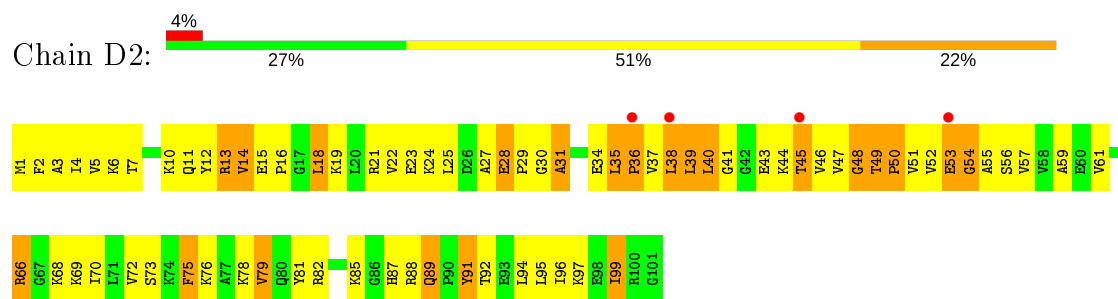
- Molecule 39: 50S ribosomal protein L20



- Molecule 40: 50S ribosomal protein L21

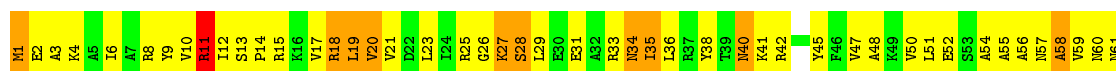


- Molecule 40: 50S ribosomal protein L21

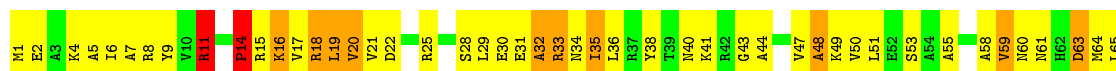


- Molecule 41: 50S ribosomal protein L22





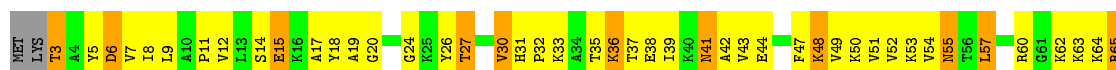
- Molecule 41: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L23



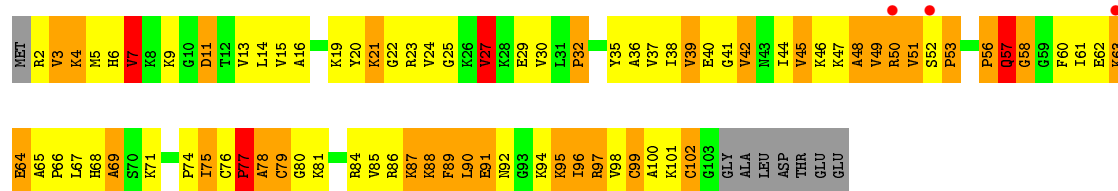
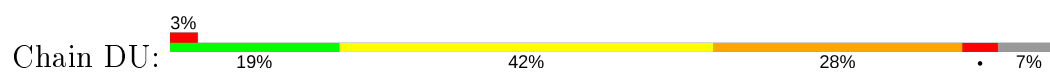
- Molecule 42: 50S ribosomal protein L23



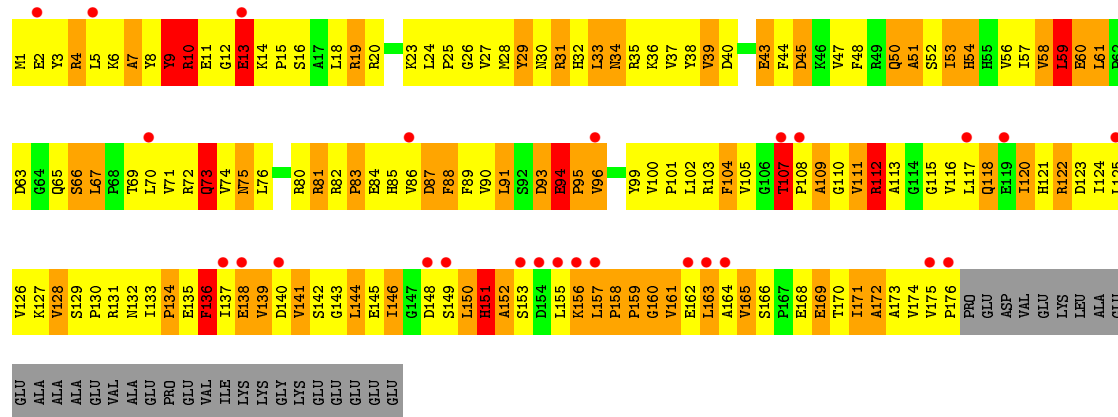
- Molecule 43: 50S ribosomal protein L24



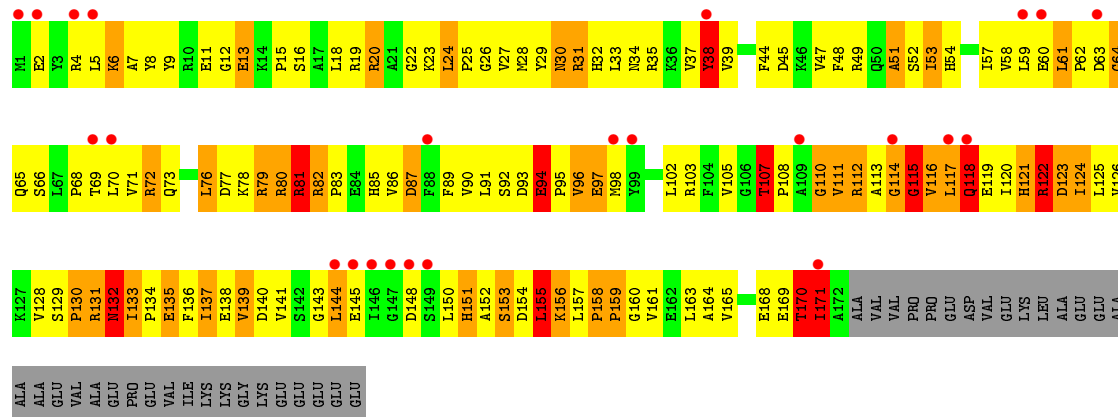
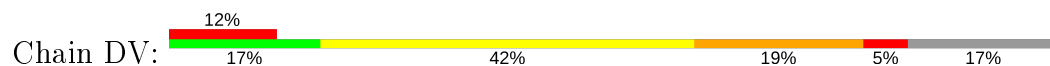
- Molecule 43: 50S ribosomal protein L24



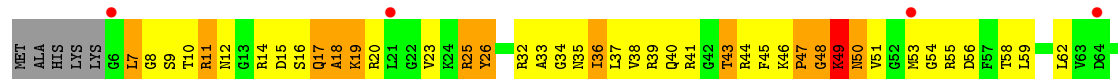
• Molecule 44: 50S ribosomal protein L25



• Molecule 44: 50S ribosomal protein L25

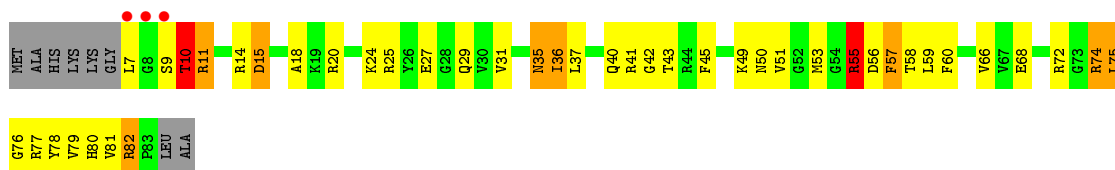


• Molecule 45: 50S ribosomal protein L27

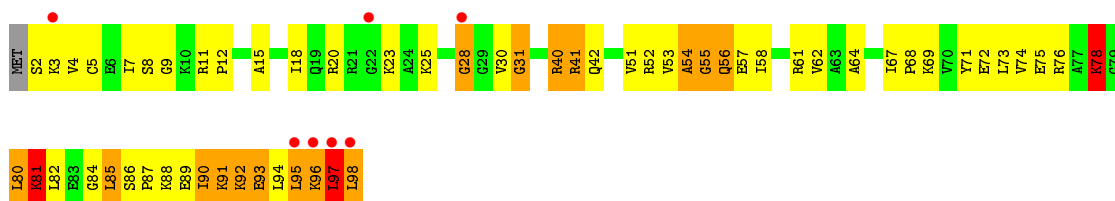




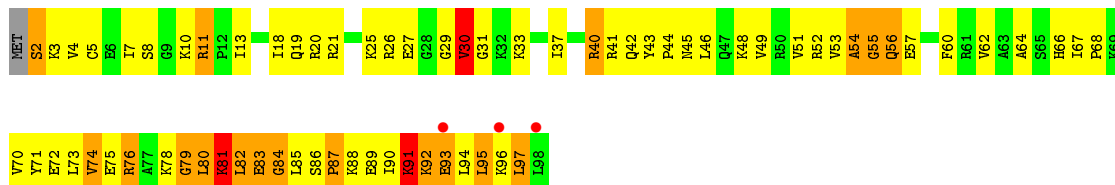
- Molecule 45: 50S ribosomal protein L27



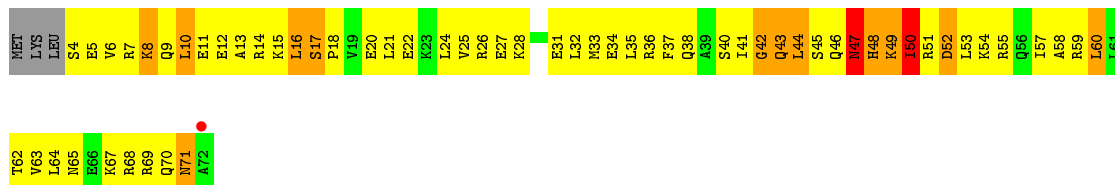
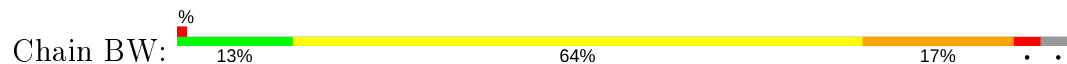
- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29



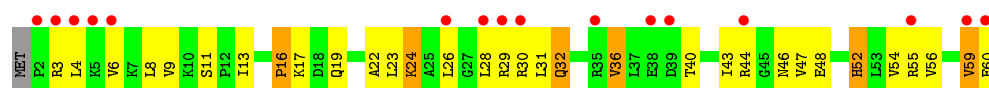
- Molecule 47: 50S ribosomal protein L29



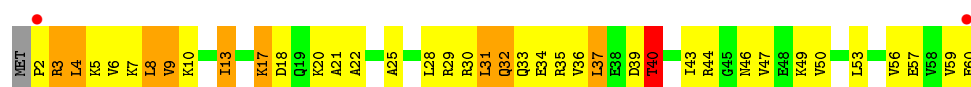




- Molecule 48: 50S ribosomal protein L30



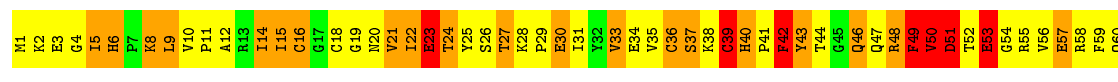
- Molecule 48: 50S ribosomal protein L30



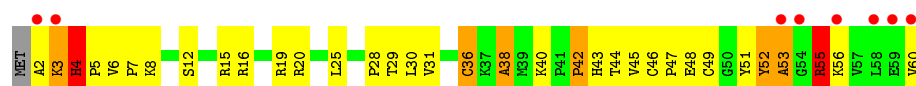
- Molecule 49: 50S ribosomal protein L31



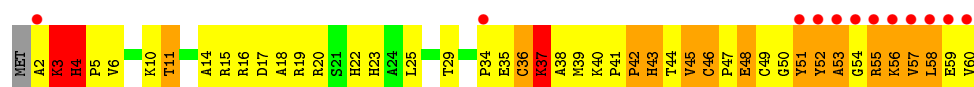
- Molecule 49: 50S ribosomal protein L31



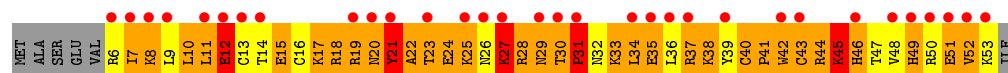
- Molecule 50: 50S ribosomal protein L32



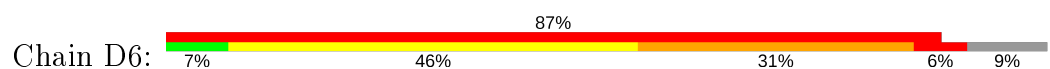
- Molecule 50: 50S ribosomal protein L32



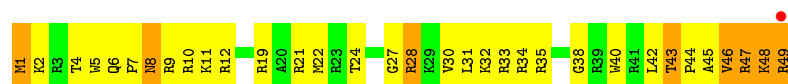
- Molecule 51: 50S ribosomal protein L33



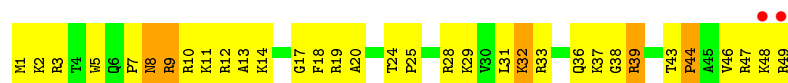
- Molecule 51: 50S ribosomal protein L33



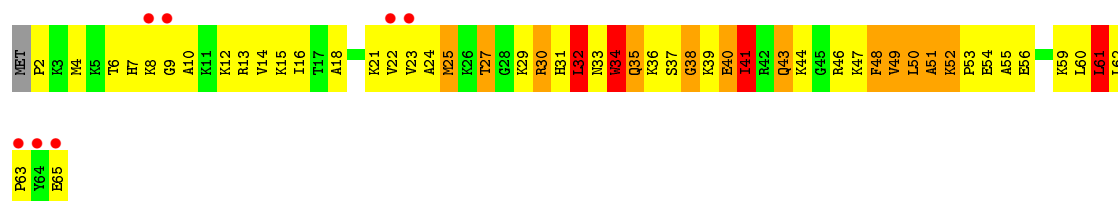
- Molecule 52: 50S ribosomal protein L34



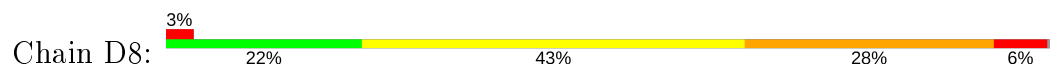
- Molecule 52: 50S ribosomal protein L34

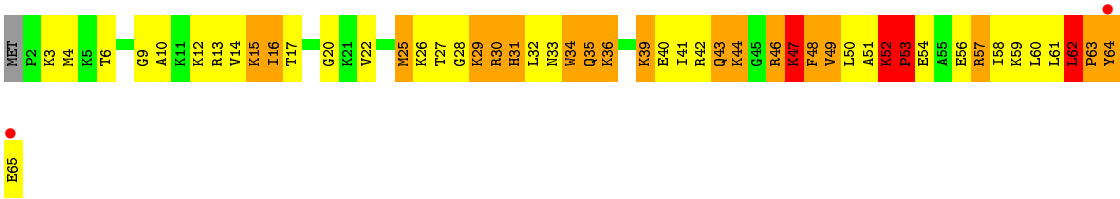


- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.46Å 452.18Å 626.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 3.50 226.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-3.50) 100.0 (226.09-3.00)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.252 0.214 , 0.216	Depositor DCC
$R_{free}$ test set	22133 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 63.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	298428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	1/36490 (0.0%)	0.80	49/56951 (0.1%)
1	CA	0.49	9/36439 (0.0%)	0.82	73/56872 (0.1%)
2	AE	0.34	0/1950	0.66	0/2630
2	CE	0.35	0/1959	0.64	0/2642
3	AF	0.36	0/1636	0.65	0/2205
3	CF	0.36	0/1629	0.60	0/2195
4	AG	0.44	0/1733	0.78	4/2318 (0.2%)
4	CG	0.41	0/1733	0.69	1/2318 (0.0%)
5	AH	0.40	0/1195	0.68	0/1609
5	CH	0.37	0/1171	0.66	0/1576
6	AI	0.38	0/856	0.67	0/1154
6	CI	0.42	0/856	0.67	0/1154
7	AJ	0.36	0/1276	0.66	0/1709
7	CJ	0.36	0/1276	0.60	0/1709
8	AK	0.35	0/1136	0.65	0/1527
8	CK	0.40	0/1136	0.69	0/1527
9	AL	0.35	0/1037	0.70	0/1389
9	CL	0.35	0/1029	0.67	0/1379
10	AM	0.34	0/814	0.65	0/1095
10	CM	0.35	0/814	0.61	0/1095
11	AN	0.38	0/916	0.72	0/1234
11	CN	0.39	0/900	0.67	0/1213
12	AO	0.42	0/991	0.74	0/1327
12	CO	0.45	0/991	1.00	4/1327 (0.3%)
13	AP	0.47	1/947 (0.1%)	0.72	0/1270
13	CP	0.34	0/974	0.66	0/1303
14	AQ	0.36	0/501	0.64	0/664
14	CQ	0.42	0/501	0.70	1/664 (0.2%)
15	AR	0.39	0/745	0.61	0/992
15	CR	0.39	0/745	0.66	0/992
16	AS	0.38	0/721	0.67	0/970
16	CS	0.36	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.38	0/847	0.67	0/1131
17	CT	0.37	0/847	0.68	0/1131
18	AU	0.40	0/590	0.68	0/782
18	CU	0.39	0/579	0.72	0/768
19	AV	0.37	0/670	0.68	0/901
19	CV	0.35	0/689	0.84	2/926 (0.2%)
20	AW	0.37	0/765	0.71	0/1007
20	CW	0.33	0/765	0.69	0/1007
21	AX	0.37	0/221	0.54	0/288
21	CX	0.36	0/221	0.63	0/288
22	AC	0.54	2/1832 (0.1%)	0.92	7/2855 (0.2%)
22	AD	0.48	2/1832 (0.1%)	0.91	6/2855 (0.2%)
22	CB	0.49	2/1547 (0.1%)	0.94	5/2411 (0.2%)
22	CC	0.58	2/1832 (0.1%)	0.94	6/2855 (0.2%)
22	CD	0.45	2/1832 (0.1%)	0.87	5/2855 (0.2%)
23	A1	0.50	0/567	0.88	0/884
23	C1	0.46	0/567	0.83	2/884 (0.2%)
24	BA	0.59	15/69594 (0.0%)	0.89	199/108647 (0.2%)
24	DA	0.64	12/69611 (0.0%)	0.93	232/108670 (0.2%)
25	BB	0.46	3/2877 (0.1%)	0.79	3/4488 (0.1%)
25	DB	0.56	3/2878 (0.1%)	0.84	6/4490 (0.1%)
26	BD	0.48	0/2165	0.82	1/2919 (0.0%)
26	DD	0.61	2/2165 (0.1%)	0.89	3/2919 (0.1%)
27	BE	0.44	0/1601	0.81	2/2160 (0.1%)
27	DE	0.52	0/1601	0.91	2/2160 (0.1%)
28	BF	0.43	0/1662	0.76	0/2249
28	DF	0.49	0/1620	0.76	0/2194
29	BG	0.36	0/1499	0.64	0/2016
29	DG	0.39	0/1499	0.66	0/2016
30	BH	0.35	0/1332	0.75	1/1802 (0.1%)
30	DH	0.45	0/1332	0.85	4/1802 (0.2%)
31	BK	0.35	0/1151	0.77	0/1558
31	DK	0.41	0/1151	0.81	1/1558 (0.1%)
32	BM	0.39	0/1131	0.70	0/1525
32	DM	0.45	0/1131	0.77	1/1525 (0.1%)
33	BN	0.47	0/943	0.76	1/1269 (0.1%)
33	DN	0.53	0/943	0.71	0/1269
34	BO	0.44	0/1162	0.85	1/1544 (0.1%)
34	DO	0.49	0/1162	0.94	3/1544 (0.2%)
35	BP	0.41	0/1143	0.70	0/1527
35	DP	0.53	0/1143	0.89	3/1527 (0.2%)
36	B0	0.43	0/974	0.71	0/1302
36	D0	0.44	0/982	0.80	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	BQ	0.36	0/892	0.67	0/1187
37	DQ	0.45	0/892	0.82	1/1187 (0.1%)
38	BR	0.43	0/1155	0.73	0/1542
38	DR	0.46	0/1155	0.73	2/1542 (0.1%)
39	B1	0.41	0/982	0.70	0/1306
39	D1	0.48	0/982	0.77	0/1306
40	B2	0.45	0/790	0.83	1/1057 (0.1%)
40	D2	0.46	0/790	0.82	0/1057
41	BS	0.47	0/911	0.71	0/1220
41	DS	0.45	0/911	0.75	0/1220
42	BT	0.49	0/739	0.71	0/993
42	DT	0.56	0/739	0.77	0/993
43	BU	0.50	0/798	0.85	1/1064 (0.1%)
43	DU	0.52	0/798	0.80	0/1064
44	BV	0.39	0/1435	0.77	1/1947 (0.1%)
44	DV	0.47	0/1408	0.77	1/1908 (0.1%)
45	B3	0.44	0/637	0.74	1/848 (0.1%)
45	D3	0.44	0/619	0.78	0/825
46	BZ	0.44	0/770	0.78	0/1022
46	DZ	0.49	0/770	0.85	1/1022 (0.1%)
47	BW	0.45	0/583	0.75	0/771
47	DW	0.50	0/583	0.83	1/771 (0.1%)
48	BX	0.37	0/474	0.68	0/635
48	DX	0.43	0/474	0.71	0/635
49	B4	0.43	0/594	0.81	0/795
49	D4	0.38	0/594	0.78	1/795 (0.1%)
50	B5	0.41	0/473	0.70	0/639
50	D5	0.51	0/473	0.74	0/639
51	B6	0.37	0/424	0.82	0/565
51	D6	0.42	0/431	0.76	0/575
52	B7	0.48	0/438	0.72	0/575
52	D7	0.56	0/438	0.76	0/575
53	B8	0.50	0/525	0.95	2/691 (0.3%)
53	D8	0.62	0/525	0.93	1/691 (0.1%)
All	All	0.53	56/321675 (0.0%)	0.84	643/481462 (0.1%)

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
1	AA	0	54

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	53
22	AC	0	2
22	AD	0	2
22	CD	0	1
23	A1	0	3
23	C1	0	3
24	BA	0	136
24	DA	0	153
25	BB	0	4
25	DB	0	5
All	All	0	416

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	654(R)	C	N1-C2	28.46	1.68	1.40
24	BA	654(R)	C	O5'-C5'	21.81	1.79	1.44
24	BA	654(R)	C	N3-C4	16.66	1.45	1.33
24	BA	654(R)	C	C2-N3	16.59	1.49	1.35
24	BA	654(R)	C	N1-C6	16.36	1.47	1.37

The worst 5 of 643 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	945	A	C1'-O4'-C4'	-24.45	90.34	109.90
24	DA	1379	A	C1'-O4'-C4'	-24.15	90.58	109.90
24	DA	945	A	C1'-O4'-C4'	-23.55	91.06	109.90
24	DA	2286	A	C1'-O4'-C4'	-20.78	93.27	109.90
12	CO	47	LYS	C-N-CD	-20.50	75.50	120.60

There are no chirality outliers.

5 of 416 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	30	U	Sidechain
1	AA	47	C	Sidechain
1	AA	49	U	Sidechain
1	AA	51	A	Sidechain
1	AA	82	U	Sidechain



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32600	0	16446	1807	2
1	CA	32554	0	16428	1770	14
2	AE	1915	0	1969	380	0
2	CE	1924	0	1975	293	0
3	AF	1612	0	1677	307	0
3	CF	1605	0	1668	219	0
4	AG	1703	0	1764	262	0
4	CG	1703	0	1763	241	0
5	AH	1178	0	1233	148	0
5	CH	1155	0	1213	135	0
6	AI	843	0	857	109	0
6	CI	843	0	857	101	0
7	AJ	1257	0	1296	178	0
7	CJ	1257	0	1296	156	0
8	AK	1116	0	1177	151	0
8	CK	1116	0	1177	151	0
9	AL	1018	0	1049	212	0
9	CL	1010	0	1037	161	0
10	AM	801	0	849	152	0
10	CM	801	0	849	149	0
11	AN	901	0	926	123	0
11	CN	885	0	904	108	0
12	AO	975	0	1062	135	0
12	CO	975	0	1062	111	0
13	AP	937	0	995	203	0
13	CP	964	0	1034	154	0
14	AQ	492	0	529	69	0
14	CQ	492	0	529	95	0
15	AR	734	0	771	102	0
15	CR	734	0	771	79	0
16	AS	705	0	725	75	0
16	CS	705	0	725	130	0
17	AT	834	0	904	64	0
17	CT	834	0	904	84	0
18	AU	585	0	657	99	0
18	CU	574	0	644	73	0
19	AV	656	0	678	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CV	674	0	699	141	0
20	AW	763	0	861	84	0
20	CW	763	0	861	117	0
21	AX	217	0	234	35	0
21	CX	217	0	234	33	0
22	AC	1640	0	836	72	0
22	AD	1640	0	836	121	0
22	CB	1385	0	704	64	0
22	CC	1640	0	836	41	0
22	CD	1640	0	834	93	0
23	A1	502	0	253	40	0
23	C1	502	0	253	38	0
24	BA	62134	0	31302	3009	2
24	DA	62151	0	31309	2760	0
25	BB	2572	0	1305	184	0
25	DB	2573	0	1305	137	0
26	BD	2115	0	2195	297	0
26	DD	2115	0	2195	344	0
27	BE	1568	0	1634	286	0
27	DE	1568	0	1634	286	0
28	BF	1627	0	1680	255	0
28	DF	1585	0	1632	189	0
29	BG	1474	0	1535	262	0
29	DG	1474	0	1535	209	0
30	BH	1307	0	1382	320	14
30	DH	1307	0	1382	232	0
31	BK	1136	0	1223	201	0
31	DK	1136	0	1223	206	0
32	BM	1104	0	1180	135	0
32	DM	1104	0	1180	200	0
33	BN	933	0	996	114	0
33	DN	933	0	996	128	0
34	BO	1145	0	1228	260	0
34	DO	1145	0	1228	262	0
35	BP	1122	0	1179	237	0
35	DP	1122	0	1179	153	0
36	B0	960	0	1021	123	0
36	D0	968	0	1033	117	0
37	BQ	882	0	943	162	0
37	DQ	882	0	943	167	0
38	BR	1141	0	1202	154	0
38	DR	1141	0	1202	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B1	964	0	1022	163	0
39	D1	964	0	1022	131	0
40	B2	779	0	852	198	0
40	D2	779	0	851	136	0
41	BS	900	0	964	112	0
41	DS	900	0	964	105	0
42	BT	725	0	778	88	0
42	DT	725	0	778	75	0
43	BU	785	0	878	209	0
43	DU	785	0	878	162	0
44	BV	1404	0	1437	309	0
44	DV	1378	0	1407	234	0
45	B3	629	0	650	73	0
45	D3	611	0	631	61	0
46	BZ	763	0	848	104	0
46	DZ	763	0	848	141	0
47	BW	581	0	629	107	0
47	DW	581	0	629	85	0
48	BX	469	0	518	40	0
48	DX	469	0	518	43	0
49	B4	581	0	573	167	0
49	D4	581	0	574	164	0
50	B5	459	0	480	51	0
50	D5	459	0	480	79	0
51	B6	417	0	441	91	0
51	D6	424	0	450	99	0
52	B7	430	0	480	57	0
52	D7	430	0	480	50	0
53	B8	517	0	582	138	0
53	D8	517	0	582	112	0
54	A1	1	0	0	0	0
54	AA	440	0	0	0	0
54	AC	8	0	0	0	0
54	AD	3	0	0	0	0
54	AH	2	0	0	0	0
54	AI	1	0	0	0	0
54	AJ	1	0	0	0	0
54	AK	1	0	0	0	0
54	AL	2	0	0	0	0
54	AO	1	0	0	0	0
54	AP	1	0	0	0	0
54	AQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AS	2	0	0	0	0
54	AT	2	0	0	0	0
54	AW	4	0	0	0	0
54	AX	1	0	0	0	0
54	B0	2	0	0	0	0
54	B1	1	0	0	0	0
54	B3	2	0	0	0	0
54	B4	1	0	0	0	0
54	B5	1	0	0	0	0
54	B6	1	0	0	0	0
54	B8	1	0	0	0	0
54	BA	683	0	0	0	0
54	BB	26	0	0	0	0
54	BD	2	0	0	0	0
54	BE	7	0	0	0	0
54	BF	2	0	0	0	0
54	BG	1	0	0	0	0
54	BH	1	0	0	0	0
54	BK	1	0	0	0	0
54	BO	1	0	0	0	0
54	BQ	1	0	0	0	0
54	BR	2	0	0	0	0
54	BT	2	0	0	0	0
54	BU	5	0	0	0	0
54	BW	1	0	0	0	0
54	BZ	1	0	0	0	0
54	C1	1	0	0	0	0
54	CA	384	0	0	0	0
54	CC	13	0	0	0	0
54	CD	26	0	0	0	0
54	CG	1	0	0	0	0
54	CH	2	0	0	0	0
54	CK	2	0	0	0	0
54	CL	1	0	0	0	0
54	CM	1	0	0	0	0
54	CP	4	0	0	0	0
54	CQ	3	0	0	0	0
54	CR	1	0	0	0	0
54	CS	2	0	0	0	0
54	CT	1	0	0	0	0
54	CW	5	0	0	0	0
54	CX	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	D0	5	0	0	0	0
54	D1	6	0	0	0	0
54	D2	1	0	0	0	0
54	D3	4	0	0	0	0
54	D5	1	0	0	0	0
54	D6	2	0	0	0	0
54	D7	1	0	0	0	0
54	DA	905	0	0	0	0
54	DB	29	0	0	0	0
54	DD	3	0	0	0	0
54	DE	3	0	0	0	0
54	DF	1	0	0	0	0
54	DG	3	0	0	0	0
54	DH	4	0	0	0	0
54	DO	5	0	0	0	0
54	DR	2	0	0	0	0
54	DS	1	0	0	0	0
54	DT	2	0	0	0	0
54	DU	6	0	0	0	0
54	DW	2	0	0	0	0
54	DZ	2	0	0	0	0
55	AA	2	0	0	0	0
55	AG	1	0	0	0	0
55	AQ	1	0	0	0	0
55	CG	1	0	0	0	0
55	CQ	1	0	0	0	0
All	All	298428	0	200046	22780	16

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 46.

The worst 5 of 22780 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)
30:DH:127:GLU:CG	30:DH:128:PRO:HD3	1.36	1.52
24:BA:654(R):C:C5'	24:BA:654(R):C:C2	1.96	1.45
24:DA:1378:A:O2'	24:DA:1379:A:C5'	1.64	1.44
49:B4:12:ALA:CB	49:B4:23:GLU:O	1.68	1.41
24:BA:654(R):C:C5'	24:BA:654(R):C:C4	2.07	1.38

The worst 5 of 16 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)
30:BH:125:VAL:CG2	1:CA:84:U:N1[3_545]	1.00	1.20
30:BH:126:PRO:CG	1:CA:84:U:O5'[3_545]	1.57	0.63
30:BH:126:PRO:CG	1:CA:84:U:P[3_545]	1.60	0.60
30:BH:126:PRO:CG	1:CA:84:U:C5'[3_545]	1.66	0.54
30:BH:126:PRO:CG	1:CA:82:U:O3'[3_545]	1.70	0.50

## 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	AE	234/256 (91%)	128 (55%)	55 (24%)	51 (22%)	0	1
2	CE	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	4
3	AF	204/239 (85%)	119 (58%)	49 (24%)	36 (18%)	0	2
3	CF	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	8
4	AG	206/209 (99%)	117 (57%)	56 (27%)	33 (16%)	0	2
4	CG	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	0	6
5	AH	152/162 (94%)	103 (68%)	34 (22%)	15 (10%)	0	7
5	CH	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	7
6	AI	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	12
6	CI	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	8
7	AJ	153/156 (98%)	95 (62%)	42 (28%)	16 (10%)	0	7
7	CJ	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	7
8	AK	136/138 (99%)	98 (72%)	29 (21%)	9 (7%)	1	13
8	CK	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	6
9	AL	126/128 (98%)	71 (56%)	36 (29%)	19 (15%)	0	3
9	CL	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
10	AM	97/105 (92%)	67 (69%)	20 (21%)	10 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CM	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	7
11	AN	119/129 (92%)	76 (64%)	29 (24%)	14 (12%)	0	5
11	CN	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	10
12	AO	123/132 (93%)	80 (65%)	22 (18%)	21 (17%)	0	2
12	CO	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
13	AP	116/126 (92%)	62 (53%)	23 (20%)	31 (27%)	0	0
13	CP	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	2
14	AQ	58/61 (95%)	37 (64%)	15 (26%)	6 (10%)	0	7
14	CQ	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
15	AR	86/89 (97%)	55 (64%)	27 (31%)	4 (5%)	2	20
15	CR	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	12
16	AS	82/88 (93%)	57 (70%)	16 (20%)	9 (11%)	0	6
16	CS	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
17	AT	98/105 (93%)	75 (76%)	17 (17%)	6 (6%)	1	15
17	CT	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	9
18	AU	69/88 (78%)	42 (61%)	21 (30%)	6 (9%)	1	9
18	CU	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
19	AV	80/93 (86%)	43 (54%)	20 (25%)	17 (21%)	0	1
19	CV	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	AW	97/106 (92%)	54 (56%)	26 (27%)	17 (18%)	0	2
20	CW	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
21	AX	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	2	22
21	CX	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
26	BD	270/276 (98%)	193 (72%)	46 (17%)	31 (12%)	0	6
26	DD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	11
27	BE	203/206 (98%)	114 (56%)	46 (23%)	43 (21%)	0	1
27	DE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	BF	206/210 (98%)	137 (66%)	45 (22%)	24 (12%)	0	5
28	DF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	7
29	BG	179/182 (98%)	114 (64%)	39 (22%)	26 (14%)	0	3
29	DG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	168/180 (93%)	60 (36%)	54 (32%)	54 (32%)	0	0
30	DH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	BK	144/148 (97%)	77 (54%)	45 (31%)	22 (15%)	0	3
31	DK	144/148 (97%)	80 (56%)	36 (25%)	28 (19%)	0	2
32	BM	136/140 (97%)	88 (65%)	29 (21%)	19 (14%)	0	3
32	DM	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	BN	120/122 (98%)	96 (80%)	17 (14%)	7 (6%)	1	16
33	DN	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	11
34	BO	148/150 (99%)	80 (54%)	32 (22%)	36 (24%)	0	0
34	DO	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	BP	139/141 (99%)	96 (69%)	24 (17%)	19 (14%)	0	4
35	DP	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	6
36	B0	115/118 (98%)	73 (64%)	31 (27%)	11 (10%)	0	8
36	D0	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	5
37	BQ	109/112 (97%)	58 (53%)	32 (29%)	19 (17%)	0	2
37	DQ	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
38	BR	135/146 (92%)	94 (70%)	31 (23%)	10 (7%)	1	11
38	DR	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
39	B1	115/118 (98%)	81 (70%)	22 (19%)	12 (10%)	0	7
39	D1	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	10
40	B2	99/101 (98%)	67 (68%)	12 (12%)	20 (20%)	0	1
40	D2	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	7
41	BS	111/113 (98%)	79 (71%)	20 (18%)	12 (11%)	0	6
41	DS	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
42	BT	90/96 (94%)	63 (70%)	18 (20%)	9 (10%)	0	7
42	DT	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	17
43	BU	100/110 (91%)	37 (37%)	29 (29%)	34 (34%)	0	0
43	DU	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
44	BV	174/206 (84%)	85 (49%)	43 (25%)	46 (26%)	0	0
44	DV	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
45	B3	78/85 (92%)	54 (69%)	13 (17%)	11 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	D3	75/85 (88%)	56 (75%)	13 (17%)	6 (8%)	1	10
46	BZ	95/98 (97%)	66 (70%)	17 (18%)	12 (13%)	0	5
46	DZ	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
47	BW	67/72 (93%)	43 (64%)	12 (18%)	12 (18%)	0	2
47	DW	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
48	BX	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	3	27
48	DX	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	17
49	B4	69/71 (97%)	33 (48%)	10 (14%)	26 (38%)	0	0
49	D4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	B5	57/60 (95%)	37 (65%)	14 (25%)	6 (10%)	0	7
50	D5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	B6	46/54 (85%)	9 (20%)	11 (24%)	26 (56%)	0	0
51	D6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	B7	47/49 (96%)	36 (77%)	9 (19%)	2 (4%)	2	22
52	D7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	14
53	B8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	2
53	D8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
All	All	11381/12054 (94%)	7244 (64%)	2468 (22%)	1669 (15%)	0	3

5 of 1669 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	8	LYS
2	AE	17	PHE
2	AE	20	GLU
2	AE	23	ARG
2	AE	29	ALA

### 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	AE	204/220 (93%)	169 (83%)	35 (17%)	2	11
2	CE	205/220 (93%)	181 (88%)	24 (12%)	5	26
3	AF	160/188 (85%)	141 (88%)	19 (12%)	5	25
3	CF	159/188 (85%)	145 (91%)	14 (9%)	10	38
4	AG	180/181 (99%)	152 (84%)	28 (16%)	2	16
4	CG	180/181 (99%)	163 (91%)	17 (9%)	8	35
5	AH	119/123 (97%)	102 (86%)	17 (14%)	3	19
5	CH	116/123 (94%)	106 (91%)	10 (9%)	10	38
6	AI	90/90 (100%)	80 (89%)	10 (11%)	6	28
6	CI	90/90 (100%)	76 (84%)	14 (16%)	2	16
7	AJ	126/127 (99%)	114 (90%)	12 (10%)	8	34
7	CJ	126/127 (99%)	115 (91%)	11 (9%)	10	38
8	AK	119/119 (100%)	112 (94%)	7 (6%)	19	53
8	CK	119/119 (100%)	106 (89%)	13 (11%)	6	29
9	AL	99/99 (100%)	80 (81%)	19 (19%)	1	7
9	CL	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	AM	89/92 (97%)	80 (90%)	9 (10%)	7	32
10	CM	89/92 (97%)	81 (91%)	8 (9%)	9	37
11	AN	92/99 (93%)	83 (90%)	9 (10%)	8	33
11	CN	90/99 (91%)	81 (90%)	9 (10%)	7	32
12	AO	104/109 (95%)	92 (88%)	12 (12%)	5	26
12	CO	104/109 (95%)	90 (86%)	14 (14%)	4	21
13	AP	94/101 (93%)	75 (80%)	19 (20%)	1	6
13	CP	97/101 (96%)	81 (84%)	16 (16%)	2	13
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	7	32
14	CQ	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	AR	79/80 (99%)	74 (94%)	5 (6%)	18	51
15	CR	79/80 (99%)	73 (92%)	6 (8%)	13	43
16	AS	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	CS	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	AT	95/97 (98%)	87 (92%)	8 (8%)	11	40
17	CT	95/97 (98%)	89 (94%)	6 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	62/77 (80%)	53 (86%)	9 (14%)	3	18
18	CU	61/77 (79%)	55 (90%)	6 (10%)	8	33
19	AV	71/80 (89%)	63 (89%)	8 (11%)	6	27
19	CV	73/80 (91%)	61 (84%)	12 (16%)	2	13
20	AW	76/82 (93%)	65 (86%)	11 (14%)	3	18
20	CW	76/82 (93%)	67 (88%)	9 (12%)	5	25
21	AX	20/22 (91%)	18 (90%)	2 (10%)	7	32
21	CX	20/22 (91%)	19 (95%)	1 (5%)	24	58
26	BD	214/218 (98%)	183 (86%)	31 (14%)	3	18
26	DD	214/218 (98%)	176 (82%)	38 (18%)	2	10
27	BE	165/166 (99%)	137 (83%)	28 (17%)	2	12
27	DE	165/166 (99%)	127 (77%)	38 (23%)	1	4
28	BF	165/166 (99%)	142 (86%)	23 (14%)	3	20
28	DF	161/166 (97%)	139 (86%)	22 (14%)	3	20
29	BG	155/156 (99%)	139 (90%)	16 (10%)	7	32
29	DG	155/156 (99%)	130 (84%)	25 (16%)	2	14
30	BH	142/148 (96%)	111 (78%)	31 (22%)	1	5
30	DH	142/148 (96%)	115 (81%)	27 (19%)	1	8
31	BK	122/124 (98%)	105 (86%)	17 (14%)	3	20
31	DK	122/124 (98%)	95 (78%)	27 (22%)	1	5
32	BM	117/119 (98%)	101 (86%)	16 (14%)	3	20
32	DM	117/119 (98%)	97 (83%)	20 (17%)	2	12
33	BN	100/100 (100%)	88 (88%)	12 (12%)	5	24
33	DN	100/100 (100%)	90 (90%)	10 (10%)	7	32
34	BO	116/116 (100%)	86 (74%)	30 (26%)	0	3
34	DO	116/116 (100%)	89 (77%)	27 (23%)	1	4
35	BP	111/111 (100%)	92 (83%)	19 (17%)	2	12
35	DP	111/111 (100%)	92 (83%)	19 (17%)	2	12
36	B0	100/101 (99%)	87 (87%)	13 (13%)	4	21
36	D0	101/101 (100%)	83 (82%)	18 (18%)	2	10
37	BQ	87/88 (99%)	74 (85%)	13 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DQ	87/88 (99%)	74 (85%)	13 (15%)	3	17
38	BR	120/127 (94%)	99 (82%)	21 (18%)	2	10
38	DR	120/127 (94%)	96 (80%)	24 (20%)	1	7
39	B1	93/94 (99%)	82 (88%)	11 (12%)	5	25
39	D1	93/94 (99%)	79 (85%)	14 (15%)	3	17
40	B2	82/82 (100%)	67 (82%)	15 (18%)	1	8
40	D2	82/82 (100%)	70 (85%)	12 (15%)	3	18
41	BS	92/92 (100%)	76 (83%)	16 (17%)	2	11
41	DS	92/92 (100%)	77 (84%)	15 (16%)	2	13
42	BT	74/78 (95%)	61 (82%)	13 (18%)	2	10
42	DT	74/78 (95%)	62 (84%)	12 (16%)	2	14
43	BU	85/91 (93%)	61 (72%)	24 (28%)	0	3
43	DU	85/91 (93%)	70 (82%)	15 (18%)	2	10
44	BV	155/179 (87%)	120 (77%)	35 (23%)	1	4
44	DV	152/179 (85%)	124 (82%)	28 (18%)	1	8
45	B3	63/67 (94%)	55 (87%)	8 (13%)	4	22
45	D3	62/67 (92%)	54 (87%)	8 (13%)	4	22
46	BZ	82/83 (99%)	69 (84%)	13 (16%)	2	14
46	DZ	82/83 (99%)	67 (82%)	15 (18%)	1	8
47	BW	64/67 (96%)	57 (89%)	7 (11%)	6	29
47	DW	64/67 (96%)	57 (89%)	7 (11%)	6	29
48	BX	51/52 (98%)	43 (84%)	8 (16%)	2	15
48	DX	51/52 (98%)	40 (78%)	11 (22%)	1	5
49	B4	63/63 (100%)	43 (68%)	20 (32%)	0	2
49	D4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	B5	51/52 (98%)	46 (90%)	5 (10%)	8	33
50	D5	51/52 (98%)	40 (78%)	11 (22%)	1	5
51	B6	47/52 (90%)	30 (64%)	17 (36%)	0	1
51	D6	48/52 (92%)	38 (79%)	10 (21%)	1	6
52	B7	42/42 (100%)	33 (79%)	9 (21%)	1	5
52	D7	42/42 (100%)	38 (90%)	4 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	B8	54/55 (98%)	43 (80%)	11 (20%)	<b>1</b> <b>6</b>
53	D8	54/55 (98%)	39 (72%)	15 (28%)	<b>0</b> <b>3</b>
All	All	9616/9998 (96%)	8160 (85%)	1456 (15%)	<b>3</b> <b>17</b>

5 of 1456 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BW	9	GLN
7	CJ	12	LEU
44	DV	121	HIS
49	B4	10	VAL
2	CE	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 298 such sidechains are listed below:

Mol	Chain	Res	Type
48	BX	46	ASN
6	CI	7	ASN
42	DT	55	ASN
50	B5	43	HIS
3	CF	37	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1516/1517 (99%)	341 (22%)	139 (9%)
1	CA	1514/1517 (99%)	316 (20%)	133 (8%)
22	AC	77/77 (100%)	15 (19%)	5 (6%)
22	AD	76/77 (98%)	28 (36%)	6 (7%)
22	CB	64/77 (83%)	15 (23%)	3 (4%)
22	CC	76/77 (98%)	15 (19%)	8 (10%)
22	CD	76/77 (98%)	11 (14%)	1 (1%)
23	A1	22/25 (88%)	10 (45%)	3 (13%)
23	C1	22/25 (88%)	9 (40%)	5 (22%)
24	BA	2884/2898 (99%)	762 (26%)	325 (11%)
24	DA	2884/2898 (99%)	776 (26%)	354 (12%)
25	BB	119/122 (97%)	25 (21%)	3 (2%)
25	DB	119/122 (97%)	21 (17%)	6 (5%)
All	All	9449/9509 (99%)	2344 (24%)	991 (10%)

5 of 2344 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	8	A
1	AA	9	G

5 of 991 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2517	C
1	CA	792	A
24	DA	2266	A
24	BA	2689	U
1	CA	246	A

## 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 2659 ligands modelled in this entry, 2659 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1517/1517 (100%)	-0.79	4 (0%) 94 91	66, 113, 195, 251	0
1	CA	1515/1517 (99%)	-0.77	10 (0%) 87 83	47, 111, 193, 247	0
2	AE	236/256 (92%)	0.94	44 (18%) 1 1	111, 152, 183, 188	0
2	CE	237/256 (92%)	0.86	46 (19%) 1 1	108, 138, 175, 185	0
3	AF	206/239 (86%)	0.31	14 (6%) 17 16	116, 134, 171, 178	0
3	CF	205/239 (85%)	0.73	28 (13%) 3 4	98, 128, 150, 160	0
4	AG	208/209 (99%)	-0.49	1 (0%) 91 88	72, 106, 128, 137	0
4	CG	208/209 (99%)	-0.11	1 (0%) 91 88	95, 116, 136, 143	0
5	AH	154/162 (95%)	-0.35	3 (1%) 66 61	89, 109, 139, 163	0
5	CH	151/162 (93%)	0.08	4 (2%) 56 49	84, 105, 132, 157	0
6	AI	101/101 (100%)	0.07	1 (0%) 82 77	85, 106, 121, 138	0
6	CI	101/101 (100%)	0.07	1 (0%) 82 77	80, 109, 119, 139	0
7	AJ	155/156 (99%)	0.24	12 (7%) 13 13	105, 129, 150, 160	0
7	CJ	155/156 (99%)	-0.10	5 (3%) 47 42	98, 121, 141, 157	0
8	AK	138/138 (100%)	-0.77	0 100 100	91, 114, 126, 131	0
8	CK	138/138 (100%)	-0.39	1 (0%) 87 83	83, 109, 121, 123	0
9	AL	128/128 (100%)	-0.31	0 100 100	109, 150, 168, 173	0
9	CL	127/128 (99%)	-0.31	2 (1%) 72 66	98, 138, 160, 169	0
10	AM	99/105 (94%)	0.19	6 (6%) 21 19	118, 152, 168, 172	0
10	CM	99/105 (94%)	0.41	9 (9%) 9 9	111, 147, 168, 175	0
11	AN	121/129 (93%)	0.54	10 (8%) 11 12	88, 110, 140, 155	0
11	CN	119/129 (92%)	0.63	7 (5%) 22 20	79, 102, 128, 146	0
12	AO	125/132 (94%)	-0.24	1 (0%) 86 81	77, 96, 115, 148	0
12	CO	125/132 (94%)	0.06	1 (0%) 86 81	72, 90, 115, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	118/126 (93%)	-0.23	3 (2%) 57 51	114, 146, 169, 172	0
13	CP	121/126 (96%)	-0.70	0 100 100	95, 132, 150, 153	0
14	AQ	60/61 (98%)	-0.40	0 100 100	119, 134, 148, 152	0
14	CQ	60/61 (98%)	-0.47	0 100 100	97, 116, 127, 129	0
15	AR	88/89 (98%)	-0.35	1 (1%) 80 75	80, 102, 125, 136	0
15	CR	88/89 (98%)	-0.66	0 100 100	77, 103, 122, 127	0
16	AS	84/88 (95%)	-0.93	0 100 100	86, 97, 118, 150	0
16	CS	84/88 (95%)	-0.91	0 100 100	95, 112, 140, 156	0
17	AT	100/105 (95%)	-0.66	1 (1%) 82 77	81, 104, 130, 155	0
17	CT	100/105 (95%)	-0.66	0 100 100	82, 109, 125, 144	0
18	AU	71/88 (80%)	0.21	8 (11%) 5 6	87, 107, 135, 141	0
18	CU	70/88 (79%)	0.68	8 (11%) 5 6	84, 107, 125, 125	0
19	AV	82/93 (88%)	-0.13	2 (2%) 59 53	130, 159, 169, 170	0
19	CV	84/93 (90%)	-0.48	0 100 100	118, 134, 149, 152	0
20	AW	99/106 (93%)	-0.70	0 100 100	88, 106, 149, 157	0
20	CW	99/106 (93%)	-0.87	0 100 100	96, 119, 148, 155	0
21	AX	25/27 (92%)	-0.43	0 100 100	143, 151, 161, 165	0
21	CX	25/27 (92%)	-0.94	0 100 100	101, 131, 147, 158	0
22	AC	77/77 (100%)	-0.47	0 100 100	76, 119, 153, 162	0
22	AD	77/77 (100%)	0.14	1 (1%) 77 71	111, 217, 236, 246	0
22	CB	65/77 (84%)	3.37	50 (76%) 0 0	133, 199, 226, 234	0
22	CC	77/77 (100%)	-0.60	0 100 100	68, 99, 133, 139	0
22	CD	77/77 (100%)	0.09	3 (3%) 39 35	105, 210, 222, 228	0
23	A1	23/25 (92%)	0.70	4 (17%) 1 1	101, 193, 235, 240	0
23	C1	23/25 (92%)	1.10	4 (17%) 1 1	87, 180, 239, 241	0
24	BA	2885/2898 (99%)	-0.69	20 (0%) 87 83	53, 90, 211, 243	0
24	DA	2886/2898 (99%)	-0.57	15 (0%) 91 88	35, 74, 192, 231	0
25	BB	120/122 (98%)	-0.72	0 100 100	103, 144, 169, 214	0
25	DB	120/122 (98%)	-0.72	0 100 100	77, 106, 126, 157	0
26	BD	272/276 (98%)	-0.11	1 (0%) 92 90	50, 78, 97, 112	0
26	DD	272/276 (98%)	-0.30	1 (0%) 92 90	44, 63, 84, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	BE	205/206 (99%)	-0.19	5 (2%) 59 53	60, 93, 138, 151	0
27	DE	205/206 (99%)	0.31	19 (9%) 8 9	48, 84, 123, 139	0
28	BF	208/210 (99%)	0.26	9 (4%) 35 31	62, 98, 158, 176	0
28	DF	202/210 (96%)	-0.41	2 (0%) 82 77	40, 74, 112, 125	0
29	BG	181/182 (99%)	0.75	29 (16%) 1 2	120, 144, 163, 175	0
29	DG	181/182 (99%)	-0.50	0 100 100	86, 109, 136, 146	0
30	BH	170/180 (94%)	0.69	34 (20%) 1 1	121, 169, 203, 209	0
30	DH	170/180 (94%)	-0.31	1 (0%) 89 86	75, 101, 123, 131	0
31	BK	146/148 (98%)	-0.02	2 (1%) 75 69	82, 122, 143, 151	0
31	DK	146/148 (98%)	-0.38	1 (0%) 87 83	68, 112, 127, 142	0
32	BM	138/140 (98%)	0.60	15 (10%) 5 6	80, 105, 124, 129	0
32	DM	138/140 (98%)	-0.12	3 (2%) 62 56	66, 84, 116, 123	0
33	BN	122/122 (100%)	0.09	1 (0%) 86 81	69, 86, 99, 105	0
33	DN	122/122 (100%)	0.12	1 (0%) 86 81	50, 77, 90, 95	0
34	BO	150/150 (100%)	0.72	21 (14%) 2 3	67, 106, 135, 158	0
34	DO	150/150 (100%)	0.08	5 (3%) 46 41	45, 88, 114, 138	0
35	BP	141/141 (100%)	0.98	26 (18%) 1 1	82, 105, 134, 178	0
35	DP	141/141 (100%)	-0.01	2 (1%) 75 69	62, 86, 107, 131	0
36	B0	117/118 (99%)	-0.75	0 100 100	54, 80, 102, 119	0
36	D0	118/118 (100%)	-0.22	0 100 100	54, 80, 98, 107	0
37	BQ	111/112 (99%)	0.22	7 (6%) 20 18	113, 132, 155, 167	0
37	DQ	111/112 (99%)	0.54	10 (9%) 9 10	82, 97, 130, 139	0
38	BR	137/146 (93%)	-0.58	2 (1%) 73 68	77, 93, 148, 177	0
38	DR	137/146 (93%)	-0.28	2 (1%) 73 68	71, 89, 136, 157	0
39	B1	117/118 (99%)	0.90	18 (15%) 2 2	68, 94, 135, 155	0
39	D1	117/118 (99%)	-0.48	2 (1%) 70 64	53, 69, 104, 130	0
40	B2	101/101 (100%)	2.09	46 (45%) 0 0	64, 118, 132, 136	0
40	D2	101/101 (100%)	0.05	4 (3%) 38 33	52, 97, 117, 126	0
41	BS	113/113 (100%)	-0.27	2 (1%) 68 62	67, 80, 101, 141	0
41	DS	113/113 (100%)	-0.13	3 (2%) 54 48	53, 70, 100, 142	0
42	BT	92/96 (95%)	-0.36	2 (2%) 62 56	73, 89, 111, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
42	DT	92/96 (95%)	-0.47	1 (1%) 80 75	54, 70, 91, 103	0
43	BU	102/110 (92%)	0.39	10 (9%) 7 8	79, 106, 161, 172	0
43	DU	102/110 (92%)	-0.42	3 (2%) 51 45	67, 93, 134, 144	0
44	BV	176/206 (85%)	0.99	26 (14%) 2 3	113, 142, 185, 190	0
44	DV	172/206 (83%)	0.92	24 (13%) 2 3	90, 126, 184, 190	0
45	B3	80/85 (94%)	0.87	6 (7%) 14 14	84, 99, 113, 119	0
45	D3	77/85 (90%)	0.16	3 (3%) 39 35	67, 81, 100, 115	0
46	BZ	97/98 (98%)	0.17	7 (7%) 15 15	67, 91, 149, 174	0
46	DZ	97/98 (98%)	-0.27	3 (3%) 49 43	48, 78, 141, 158	0
47	BW	69/72 (95%)	-0.28	1 (1%) 75 69	80, 105, 125, 140	0
47	DW	69/72 (95%)	-0.38	1 (1%) 75 69	60, 83, 105, 122	0
48	BX	59/60 (98%)	1.50	16 (27%) 0 0	83, 107, 129, 134	0
48	DX	59/60 (98%)	0.19	2 (3%) 45 40	64, 84, 110, 124	0
49	B4	71/71 (100%)	1.80	27 (38%) 0 0	164, 193, 208, 211	0
49	D4	71/71 (100%)	-0.25	0 100 100	128, 160, 185, 188	0
50	B5	59/60 (98%)	0.19	8 (13%) 3 4	57, 91, 168, 177	0
50	D5	59/60 (98%)	0.64	12 (20%) 1 1	46, 86, 186, 190	0
51	B6	48/54 (88%)	2.68	32 (66%) 0 0	138, 153, 169, 175	0
51	D6	49/54 (90%)	4.63	47 (95%) 0 0	132, 146, 156, 162	0
52	B7	49/49 (100%)	-0.21	1 (2%) 65 60	51, 68, 116, 148	0
52	D7	49/49 (100%)	-0.44	2 (4%) 37 33	40, 49, 109, 135	0
53	B8	64/65 (98%)	1.02	7 (10%) 5 6	77, 93, 114, 152	0
53	D8	64/65 (98%)	0.16	2 (3%) 49 43	53, 72, 100, 127	0
All	All	21035/21563 (97%)	-0.24	848 (4%) 38 33	35, 102, 179, 251	0

The worst 5 of 848 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	B8	65	GLU	14.5
24	BA	1176	G	12.2
41	DS	113	LYS	11.2
24	BA	2798	C	9.7
39	B1	118	GLY	9.6

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3589	1/1	-0.28	0.77	136,136,136,136	0
54	MG	BF	302	1/1	-0.23	0.42	117,117,117,117	0
54	MG	AA	1985	1/1	0.03	0.31	131,131,131,131	0
54	MG	AA	1971	1/1	0.06	0.27	123,123,123,123	0
54	MG	DA	3527	1/1	0.10	0.55	127,127,127,127	0
54	MG	DU	202	1/1	0.20	0.60	139,139,139,139	0
54	MG	BA	3572	1/1	0.21	0.32	106,106,106,106	0
54	MG	AA	1875	1/1	0.22	0.13	113,113,113,113	0
54	MG	BA	2912	1/1	0.24	0.17	138,138,138,138	0
54	MG	BA	3582	1/1	0.25	0.19	133,133,133,133	0
54	MG	DA	3784	1/1	0.25	0.35	106,106,106,106	0
54	MG	BA	3076	1/1	0.27	0.12	88,88,88,88	0
54	MG	DA	3611	1/1	0.28	0.54	112,112,112,112	0
54	MG	BA	3378	1/1	0.29	0.26	129,129,129,129	0
54	MG	AA	1904	1/1	0.29	0.24	121,121,121,121	0
54	MG	AA	1956	1/1	0.30	0.24	118,118,118,118	0
54	MG	BA	3581	1/1	0.30	0.29	125,125,125,125	0
54	MG	CA	1878	1/1	0.30	0.29	133,133,133,133	0
54	MG	BA	3550	1/1	0.31	0.21	102,102,102,102	0
54	MG	DA	3704	1/1	0.33	0.52	134,134,134,134	0
54	MG	BA	3459	1/1	0.34	0.24	110,110,110,110	0
54	MG	AA	1800	1/1	0.35	0.36	117,117,117,117	0
54	MG	DA	3754	1/1	0.35	0.57	99,99,99,99	0
54	MG	AA	2014	1/1	0.35	0.53	175,175,175,175	0
54	MG	CA	1824	1/1	0.35	0.38	156,156,156,156	0
54	MG	CA	1760	1/1	0.36	0.08	118,118,118,118	0
54	MG	BA	3394	1/1	0.37	0.13	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3554	1/1	0.37	0.18	122,122,122,122	0
54	MG	AA	1840	1/1	0.38	0.54	132,132,132,132	0
54	MG	DA	3802	1/1	0.39	0.53	138,138,138,138	0
54	MG	DA	3579	1/1	0.40	0.38	94,94,94,94	0
54	MG	CA	1852	1/1	0.41	0.33	111,111,111,111	0
54	MG	CA	1984	1/1	0.41	0.18	106,106,106,106	0
54	MG	BA	3490	1/1	0.42	0.19	107,107,107,107	0
54	MG	AA	1955	1/1	0.42	0.29	103,103,103,103	0
54	MG	DA	3673	1/1	0.42	0.32	94,94,94,94	0
54	MG	BA	3571	1/1	0.42	0.22	94,94,94,94	0
54	MG	BR	201	1/1	0.42	0.15	103,103,103,103	0
54	MG	BH	201	1/1	0.43	0.64	193,193,193,193	0
54	MG	CA	1811	1/1	0.43	0.27	108,108,108,108	0
54	MG	AA	1850	1/1	0.44	0.44	112,112,112,112	0
54	MG	CG	301	1/1	0.44	0.53	113,113,113,113	0
54	MG	DA	3570	1/1	0.45	0.66	152,152,152,152	0
54	MG	CA	1898	1/1	0.46	0.29	122,122,122,122	0
54	MG	BA	3297	1/1	0.46	0.24	131,131,131,131	0
54	MG	BA	3154	1/1	0.46	0.25	117,117,117,117	0
54	MG	BA	3499	1/1	0.46	0.25	114,114,114,114	0
54	MG	AA	1882	1/1	0.46	0.30	134,134,134,134	0
54	MG	BA	3205	1/1	0.47	0.20	92,92,92,92	0
54	MG	AA	1835	1/1	0.47	0.33	109,109,109,109	0
54	MG	DA	3546	1/1	0.49	0.28	68,68,68,68	0
54	MG	AD	103	1/1	0.49	0.14	101,101,101,101	0
54	MG	AA	1833	1/1	0.50	0.23	88,88,88,88	0
54	MG	DA	3765	1/1	0.50	0.29	110,110,110,110	0
54	MG	DA	3800	1/1	0.50	0.21	86,86,86,86	0
54	MG	AA	1767	1/1	0.51	0.43	110,110,110,110	0
54	MG	DA	3781	1/1	0.52	0.23	97,97,97,97	0
54	MG	DA	3652	1/1	0.52	0.23	83,83,83,83	0
54	MG	DA	3738	1/1	0.52	0.14	114,114,114,114	0
54	MG	DA	3793	1/1	0.52	0.14	108,108,108,108	0
54	MG	CA	1923	1/1	0.53	0.15	104,104,104,104	0
54	MG	DA	3109	1/1	0.53	0.60	103,103,103,103	0
54	MG	BA	3518	1/1	0.53	0.34	134,134,134,134	0
54	MG	CA	1840	1/1	0.53	0.25	113,113,113,113	0
54	MG	BA	3419	1/1	0.54	0.08	101,101,101,101	0
54	MG	AA	1929	1/1	0.54	0.21	124,124,124,124	0
54	MG	BA	3574	1/1	0.54	0.12	86,86,86,86	0
54	MG	CA	1862	1/1	0.54	0.27	112,112,112,112	0
54	MG	DA	3783	1/1	0.54	0.27	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	2012	1/1	0.54	0.20	117,117,117,117	0
54	MG	BA	3483	1/1	0.55	0.21	103,103,103,103	0
54	MG	CA	1813	1/1	0.55	0.16	127,127,127,127	0
54	MG	CC	112	1/1	0.55	0.15	88,88,88,88	0
54	MG	BA	3201	1/1	0.55	0.27	97,97,97,97	0
54	MG	DA	3694	1/1	0.55	0.36	110,110,110,110	0
54	MG	CA	1903	1/1	0.55	0.33	134,134,134,134	0
54	MG	BA	3242	1/1	0.55	0.18	82,82,82,82	0
54	MG	CD	107	1/1	0.55	0.25	122,122,122,122	0
54	MG	BA	3437	1/1	0.55	0.18	88,88,88,88	0
54	MG	AA	1917	1/1	0.56	0.45	132,132,132,132	0
54	MG	DA	3091	1/1	0.56	0.44	92,92,92,92	0
54	MG	AA	1812	1/1	0.56	0.27	110,110,110,110	0
54	MG	DA	3719	1/1	0.56	0.31	116,116,116,116	0
54	MG	AA	1725	1/1	0.56	0.33	92,92,92,92	0
54	MG	DA	3501	1/1	0.56	0.24	84,84,84,84	0
54	MG	AA	1965	1/1	0.56	0.19	117,117,117,117	0
54	MG	BA	3510	1/1	0.56	0.18	91,91,91,91	0
54	MG	CA	1897	1/1	0.57	0.30	105,105,105,105	0
54	MG	DA	3336	1/1	0.57	0.69	127,127,127,127	0
54	MG	DA	3610	1/1	0.57	0.31	99,99,99,99	0
54	MG	DA	3671	1/1	0.57	0.40	102,102,102,102	0
54	MG	CA	1833	1/1	0.57	0.12	70,70,70,70	0
54	MG	BA	3450	1/1	0.57	0.14	90,90,90,90	0
54	MG	B0	202	1/1	0.57	0.34	111,111,111,111	0
54	MG	DB	222	1/1	0.58	0.20	92,92,92,92	0
54	MG	DA	3078	1/1	0.58	0.22	77,77,77,77	0
54	MG	AA	2030	1/1	0.58	0.67	188,188,188,188	0
54	MG	BA	3501	1/1	0.58	0.21	80,80,80,80	0
54	MG	DA	3493	1/1	0.58	0.19	78,78,78,78	0
54	MG	DA	3656	1/1	0.58	0.77	136,136,136,136	0
54	MG	DA	3505	1/1	0.58	0.29	88,88,88,88	0
54	MG	DA	3188	1/1	0.59	0.42	96,96,96,96	0
54	MG	CA	1730	1/1	0.59	0.21	66,66,66,66	0
54	MG	CA	1782	1/1	0.59	0.36	123,123,123,123	0
54	MG	CS	102	1/1	0.59	0.10	119,119,119,119	0
54	MG	DA	3712	1/1	0.59	0.78	138,138,138,138	0
54	MG	DA	3624	1/1	0.59	0.21	82,82,82,82	0
54	MG	AA	1919	1/1	0.59	0.30	117,117,117,117	0
54	MG	DA	3768	1/1	0.59	0.30	92,92,92,92	0
54	MG	CA	1960	1/1	0.59	0.26	108,108,108,108	0
54	MG	DA	3660	1/1	0.59	0.29	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3573	1/1	0.60	0.67	124,124,124,124	0
54	MG	BA	3448	1/1	0.60	0.23	95,95,95,95	0
54	MG	AA	1868	1/1	0.60	0.19	103,103,103,103	0
54	MG	BA	3504	1/1	0.60	0.07	115,115,115,115	0
54	MG	CA	1919	1/1	0.60	0.31	112,112,112,112	0
54	MG	DA	3559	1/1	0.60	0.33	103,103,103,103	0
54	MG	AA	1911	1/1	0.60	0.29	104,104,104,104	0
54	MG	AA	1789	1/1	0.61	0.18	128,128,128,128	0
54	MG	BA	3137	1/1	0.61	0.31	88,88,88,88	0
54	MG	CC	107	1/1	0.61	0.12	102,102,102,102	0
54	MG	AA	1973	1/1	0.61	0.10	84,84,84,84	0
54	MG	BA	3167	1/1	0.61	0.38	91,91,91,91	0
54	MG	DA	3771	1/1	0.61	0.33	97,97,97,97	0
54	MG	AA	1754	1/1	0.61	0.31	96,96,96,96	0
54	MG	DA	3313	1/1	0.61	0.20	71,71,71,71	0
54	MG	BB	222	1/1	0.61	0.17	93,93,93,93	0
54	MG	DA	3451	1/1	0.62	0.26	80,80,80,80	0
54	MG	D1	205	1/1	0.62	0.27	110,110,110,110	0
54	MG	BA	3393	1/1	0.62	0.12	82,82,82,82	0
54	MG	AA	1913	1/1	0.62	0.37	114,114,114,114	0
54	MG	DA	3759	1/1	0.62	0.50	84,84,84,84	0
54	MG	AA	1959	1/1	0.62	0.40	104,104,104,104	0
54	MG	DA	3293	1/1	0.63	0.65	134,134,134,134	0
54	MG	AA	1909	1/1	0.63	0.55	128,128,128,128	0
54	MG	BR	202	1/1	0.63	0.20	105,105,105,105	0
54	MG	CA	1828	1/1	0.63	0.19	89,89,89,89	0
54	MG	AA	2004	1/1	0.63	0.36	124,124,124,124	0
54	MG	AA	2020	1/1	0.63	0.20	103,103,103,103	0
54	MG	DA	3791	1/1	0.63	0.22	114,114,114,114	0
54	MG	AA	1622	1/1	0.63	0.17	78,78,78,78	0
54	MG	BA	3476	1/1	0.63	0.24	97,97,97,97	0
54	MG	DB	213	1/1	0.63	0.65	133,133,133,133	0
54	MG	AH	201	1/1	0.63	0.28	103,103,103,103	0
54	MG	BA	3512	1/1	0.63	0.22	113,113,113,113	0
54	MG	AA	1687	1/1	0.63	0.51	138,138,138,138	0
54	MG	DA	3467	1/1	0.63	0.21	61,61,61,61	0
54	MG	DA	3049	1/1	0.63	0.48	114,114,114,114	0
54	MG	CA	1763	1/1	0.63	0.22	72,72,72,72	0
54	MG	AL	202	1/1	0.63	0.26	129,129,129,129	0
54	MG	BA	3199	1/1	0.64	0.24	84,84,84,84	0
54	MG	AA	2024	1/1	0.64	0.25	75,75,75,75	0
54	MG	BA	3325	1/1	0.64	0.15	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	ZN	AA	2040	1/1	0.64	0.49	300,300,300,300	0
54	MG	DA	3548	1/1	0.64	0.23	86,86,86,86	0
54	MG	BA	3561	1/1	0.64	0.36	117,117,117,117	0
54	MG	DU	206	1/1	0.64	0.16	83,83,83,83	0
54	MG	DA	3417	1/1	0.64	0.08	120,120,120,120	0
54	MG	DA	3159	1/1	0.64	0.14	77,77,77,77	0
54	MG	CA	1971	1/1	0.64	0.25	116,116,116,116	0
54	MG	DA	3667	1/1	0.64	0.34	112,112,112,112	0
54	MG	DA	3416	1/1	0.64	0.35	94,94,94,94	0
54	MG	B3	101	1/1	0.65	0.15	72,72,72,72	0
54	MG	AA	1720	1/1	0.65	0.15	76,76,76,76	0
54	MG	BA	3328	1/1	0.65	0.20	105,105,105,105	0
54	MG	AC	107	1/1	0.65	0.51	114,114,114,114	0
54	MG	BA	3151	1/1	0.65	0.38	114,114,114,114	0
55	ZN	AA	2041	1/1	0.65	0.19	262,262,262,262	0
54	MG	DA	3382	1/1	0.65	0.28	91,91,91,91	0
54	MG	CA	1860	1/1	0.65	0.42	127,127,127,127	0
54	MG	BA	3283	1/1	0.65	0.39	126,126,126,126	0
54	MG	AA	1899	1/1	0.66	0.17	112,112,112,112	0
54	MG	CR	101	1/1	0.66	0.43	117,117,117,117	0
54	MG	BA	3503	1/1	0.66	0.14	66,66,66,66	0
54	MG	AA	1972	1/1	0.66	0.18	78,78,78,78	0
54	MG	DF	301	1/1	0.66	0.15	82,82,82,82	0
54	MG	BA	3479	1/1	0.66	0.21	119,119,119,119	0
54	MG	BA	3569	1/1	0.66	0.17	137,137,137,137	0
54	MG	AA	1826	1/1	0.66	0.39	108,108,108,108	0
54	MG	DA	3205	1/1	0.66	0.33	115,115,115,115	0
54	MG	CA	1977	1/1	0.66	0.18	100,100,100,100	0
54	MG	DA	3487	1/1	0.66	0.41	96,96,96,96	0
54	MG	CA	1942	1/1	0.66	0.14	101,101,101,101	0
54	MG	D0	204	1/1	0.67	0.32	95,95,95,95	0
54	MG	AA	1927	1/1	0.67	0.34	98,98,98,98	0
54	MG	DA	3509	1/1	0.67	0.33	94,94,94,94	0
54	MG	BA	3559	1/1	0.67	0.26	104,104,104,104	0
54	MG	AA	1999	1/1	0.67	0.17	100,100,100,100	0
54	MG	DA	3472	1/1	0.67	0.49	111,111,111,111	0
54	MG	AA	1730	1/1	0.67	0.40	85,85,85,85	0
54	MG	CA	1952	1/1	0.67	0.45	134,134,134,134	0
54	MG	AA	1776	1/1	0.67	0.35	110,110,110,110	0
54	MG	DA	3597	1/1	0.67	1.04	168,168,168,168	0
54	MG	BA	3266	1/1	0.67	0.30	97,97,97,97	0
54	MG	AA	1719	1/1	0.67	0.37	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3642	1/1	0.67	0.27	81,81,81,81	0
54	MG	CA	1761	1/1	0.68	0.11	129,129,129,129	0
54	MG	DA	3306	1/1	0.68	0.19	65,65,65,65	0
54	MG	CA	1752	1/1	0.68	0.27	90,90,90,90	0
54	MG	DA	3674	1/1	0.68	0.12	83,83,83,83	0
54	MG	BA	3342	1/1	0.68	0.25	90,90,90,90	0
54	MG	BA	3402	1/1	0.68	0.17	96,96,96,96	0
54	MG	CA	1962	1/1	0.68	0.12	90,90,90,90	0
54	MG	BB	226	1/1	0.68	0.18	146,146,146,146	0
54	MG	BA	3117	1/1	0.68	0.10	93,93,93,93	0
54	MG	BA	3484	1/1	0.68	0.17	106,106,106,106	0
54	MG	DA	3594	1/1	0.68	0.32	123,123,123,123	0
54	MG	DA	3519	1/1	0.68	0.32	87,87,87,87	0
54	MG	BA	3376	1/1	0.68	0.18	121,121,121,121	0
54	MG	CA	1920	1/1	0.69	0.21	81,81,81,81	0
54	MG	AA	1713	1/1	0.69	0.31	94,94,94,94	0
54	MG	DA	3198	1/1	0.69	0.24	82,82,82,82	0
54	MG	CC	110	1/1	0.69	0.12	110,110,110,110	0
54	MG	DA	3446	1/1	0.69	0.27	86,86,86,86	0
54	MG	AJ	201	1/1	0.69	0.17	116,116,116,116	0
54	MG	BA	3223	1/1	0.69	0.19	88,88,88,88	0
54	MG	DU	205	1/1	0.69	0.17	75,75,75,75	0
54	MG	CA	1788	1/1	0.69	0.23	86,86,86,86	0
54	MG	CA	1718	1/1	0.69	0.34	96,96,96,96	0
54	MG	AA	1891	1/1	0.69	0.20	93,93,93,93	0
54	MG	BA	3468	1/1	0.69	0.29	110,110,110,110	0
54	MG	CA	1803	1/1	0.69	0.22	100,100,100,100	0
54	MG	BA	3474	1/1	0.70	0.21	78,78,78,78	0
54	MG	AA	1636	1/1	0.70	0.34	71,71,71,71	0
54	MG	BA	3124	1/1	0.70	0.30	75,75,75,75	0
54	MG	BE	301	1/1	0.70	0.10	60,60,60,60	0
54	MG	DA	3295	1/1	0.70	0.17	104,104,104,104	0
54	MG	AA	1932	1/1	0.70	0.28	122,122,122,122	0
54	MG	CA	1937	1/1	0.70	0.21	81,81,81,81	0
54	MG	AA	1986	1/1	0.70	0.12	96,96,96,96	0
54	MG	CA	1742	1/1	0.70	0.15	124,124,124,124	0
54	MG	BA	3018	1/1	0.70	0.44	109,109,109,109	0
54	MG	BA	3221	1/1	0.70	0.26	82,82,82,82	0
54	MG	CA	1908	1/1	0.70	0.38	128,128,128,128	0
54	MG	BB	204	1/1	0.70	0.26	97,97,97,97	0
54	MG	BA	3206	1/1	0.71	0.16	67,67,67,67	0
54	MG	AD	102	1/1	0.71	0.18	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3539	1/1	0.71	0.19	100,100,100,100	0
54	MG	DA	3653	1/1	0.71	0.28	88,88,88,88	0
54	MG	DB	214	1/1	0.71	0.13	85,85,85,85	0
54	MG	AA	1828	1/1	0.71	0.09	98,98,98,98	0
54	MG	DA	3608	1/1	0.71	0.32	74,74,74,74	0
54	MG	AA	2034	1/1	0.71	0.37	94,94,94,94	0
54	MG	CA	1922	1/1	0.71	0.34	116,116,116,116	0
54	MG	B1	201	1/1	0.71	0.25	80,80,80,80	0
54	MG	BA	3261	1/1	0.71	0.20	99,99,99,99	0
54	MG	CA	1723	1/1	0.71	0.12	111,111,111,111	0
54	MG	CD	121	1/1	0.71	0.14	112,112,112,112	0
54	MG	BA	3463	1/1	0.71	0.23	69,69,69,69	0
54	MG	BA	3105	1/1	0.71	0.28	87,87,87,87	0
54	MG	DA	3733	1/1	0.71	0.25	75,75,75,75	0
54	MG	DA	3631	1/1	0.71	0.39	118,118,118,118	0
54	MG	CA	1817	1/1	0.71	0.33	105,105,105,105	0
54	MG	AA	1947	1/1	0.72	0.17	119,119,119,119	0
54	MG	DA	3625	1/1	0.72	0.20	99,99,99,99	0
54	MG	DA	3477	1/1	0.72	0.15	83,83,83,83	0
54	MG	AA	1804	1/1	0.72	0.37	88,88,88,88	0
54	MG	DA	3439	1/1	0.72	0.58	104,104,104,104	0
54	MG	DB	229	1/1	0.72	0.17	78,78,78,78	0
54	MG	BA	3334	1/1	0.72	0.20	75,75,75,75	0
54	MG	AA	1629	1/1	0.72	0.28	74,74,74,74	0
54	MG	AA	1654	1/1	0.72	0.21	54,54,54,54	0
54	MG	DA	3099	1/1	0.72	0.40	60,60,60,60	0
54	MG	DA	3620	1/1	0.72	0.29	98,98,98,98	0
54	MG	CA	1753	1/1	0.72	0.14	114,114,114,114	0
54	MG	AA	1661	1/1	0.72	0.39	93,93,93,93	0
54	MG	AA	1924	1/1	0.72	0.29	114,114,114,114	0
54	MG	DA	3789	1/1	0.72	0.43	118,118,118,118	0
54	MG	DA	3506	1/1	0.72	0.32	63,63,63,63	0
54	MG	DA	3804	1/1	0.72	0.17	94,94,94,94	0
54	MG	DA	3028	1/1	0.72	0.23	59,59,59,59	0
54	MG	CA	1882	1/1	0.72	0.31	106,106,106,106	0
54	MG	AA	1655	1/1	0.72	0.24	91,91,91,91	0
54	MG	CA	1676	1/1	0.72	0.34	83,83,83,83	0
54	MG	BA	3520	1/1	0.72	0.22	55,55,55,55	0
54	MG	DW	101	1/1	0.72	0.20	75,75,75,75	0
54	MG	AA	1970	1/1	0.72	0.17	98,98,98,98	0
54	MG	CA	1765	1/1	0.73	0.36	118,118,118,118	0
54	MG	DA	3281	1/1	0.73	0.25	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3573	1/1	0.73	0.18	86,86,86,86	0
54	MG	DA	3703	1/1	0.73	0.23	99,99,99,99	0
54	MG	AA	1704	1/1	0.73	0.30	88,88,88,88	0
54	MG	CA	1739	1/1	0.73	0.09	80,80,80,80	0
54	MG	DG	203	1/1	0.73	0.38	112,112,112,112	0
54	MG	DA	3714	1/1	0.73	0.33	92,92,92,92	0
54	MG	DA	3715	1/1	0.73	0.39	91,91,91,91	0
54	MG	BA	3217	1/1	0.73	0.25	86,86,86,86	0
54	MG	DA	3560	1/1	0.73	0.23	79,79,79,79	0
54	MG	CA	1820	1/1	0.73	0.24	102,102,102,102	0
54	MG	DA	3799	1/1	0.73	0.26	92,92,92,92	0
54	MG	BA	3130	1/1	0.73	0.26	75,75,75,75	0
54	MG	CA	1895	1/1	0.73	0.10	87,87,87,87	0
54	MG	CA	1771	1/1	0.73	0.26	101,101,101,101	0
54	MG	AA	1680	1/1	0.73	0.21	70,70,70,70	0
54	MG	CA	1976	1/1	0.73	0.17	103,103,103,103	0
54	MG	AA	1934	1/1	0.73	0.14	88,88,88,88	0
54	MG	BB	213	1/1	0.73	0.14	122,122,122,122	0
54	MG	CA	1706	1/1	0.73	0.20	61,61,61,61	0
54	MG	AA	1799	1/1	0.73	0.12	91,91,91,91	0
54	MG	CA	1720	1/1	0.73	0.15	94,94,94,94	0
54	MG	AA	2018	1/1	0.73	0.24	117,117,117,117	0
54	MG	DA	3801	1/1	0.73	0.52	101,101,101,101	0
54	MG	DA	3710	1/1	0.73	0.71	106,106,106,106	0
54	MG	CD	116	1/1	0.73	0.13	90,90,90,90	0
54	MG	CA	1851	1/1	0.74	0.31	87,87,87,87	0
54	MG	BA	3570	1/1	0.74	0.17	104,104,104,104	0
54	MG	CA	1741	1/1	0.74	0.41	123,123,123,123	0
54	MG	DA	3437	1/1	0.74	0.49	107,107,107,107	0
54	MG	CC	111	1/1	0.74	0.23	99,99,99,99	0
54	MG	BA	3495	1/1	0.74	0.18	97,97,97,97	0
54	MG	AA	1813	1/1	0.74	0.30	93,93,93,93	0
54	MG	CA	1918	1/1	0.74	0.07	93,93,93,93	0
54	MG	AA	1652	1/1	0.74	0.19	82,82,82,82	0
54	MG	DA	3132	1/1	0.74	0.32	76,76,76,76	0
54	MG	CA	1847	1/1	0.74	0.31	133,133,133,133	0
54	MG	DA	3227	1/1	0.74	0.25	66,66,66,66	0
54	MG	DA	3351	1/1	0.74	0.15	88,88,88,88	0
54	MG	DA	3319	1/1	0.74	0.17	71,71,71,71	0
54	MG	DA	3794	1/1	0.74	0.18	142,142,142,142	0
54	MG	AA	2026	1/1	0.74	0.30	90,90,90,90	0
54	MG	AA	1852	1/1	0.74	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	217	1/1	0.74	0.36	102,102,102,102	0
54	MG	BA	3278	1/1	0.74	0.23	119,119,119,119	0
54	MG	DA	3217	1/1	0.74	0.37	79,79,79,79	0
54	MG	BA	3417	1/1	0.75	0.11	97,97,97,97	0
54	MG	BA	3179	1/1	0.75	0.15	51,51,51,51	0
54	MG	AA	1945	1/1	0.75	0.29	67,67,67,67	0
54	MG	BA	3281	1/1	0.75	0.27	113,113,113,113	0
54	MG	AA	2031	1/1	0.75	0.34	86,86,86,86	0
54	MG	AW	204	1/1	0.75	0.13	105,105,105,105	0
54	MG	BA	3464	1/1	0.75	0.20	102,102,102,102	0
54	MG	D1	201	1/1	0.75	0.34	83,83,83,83	0
54	MG	CA	1968	1/1	0.75	0.29	90,90,90,90	0
54	MG	CD	106	1/1	0.75	0.18	94,94,94,94	0
54	MG	DA	3445	1/1	0.75	0.32	95,95,95,95	0
54	MG	CA	1955	1/1	0.75	0.49	102,102,102,102	0
54	MG	DA	3539	1/1	0.75	0.23	76,76,76,76	0
54	MG	CA	1781	1/1	0.75	0.39	118,118,118,118	0
54	MG	DA	3761	1/1	0.75	0.30	112,112,112,112	0
54	MG	BA	3315	1/1	0.75	0.16	84,84,84,84	0
54	MG	AA	1953	1/1	0.75	0.14	94,94,94,94	0
54	MG	CM	201	1/1	0.75	0.22	91,91,91,91	0
54	MG	BA	3447	1/1	0.76	0.14	109,109,109,109	0
54	MG	AI	201	1/1	0.76	0.12	72,72,72,72	0
54	MG	DA	3518	1/1	0.76	0.22	78,78,78,78	0
54	MG	CA	1748	1/1	0.76	0.12	71,71,71,71	0
54	MG	BU	205	1/1	0.76	0.18	55,55,55,55	0
54	MG	BA	3347	1/1	0.76	0.21	99,99,99,99	0
54	MG	DA	3706	1/1	0.76	0.21	78,78,78,78	0
54	MG	AA	1863	1/1	0.76	0.42	92,92,92,92	0
54	MG	DA	3261	1/1	0.76	0.29	102,102,102,102	0
54	MG	AA	2007	1/1	0.76	0.29	119,119,119,119	0
54	MG	DA	3617	1/1	0.76	0.30	91,91,91,91	0
54	MG	DA	3369	1/1	0.76	0.31	90,90,90,90	0
54	MG	AT	201	1/1	0.76	0.16	101,101,101,101	0
54	MG	DA	3398	1/1	0.76	0.46	100,100,100,100	0
54	MG	DA	3584	1/1	0.76	0.25	86,86,86,86	0
54	MG	DA	3553	1/1	0.76	0.23	74,74,74,74	0
54	MG	DA	3320	1/1	0.76	0.17	131,131,131,131	0
54	MG	DA	3654	1/1	0.76	0.10	105,105,105,105	0
54	MG	DA	3614	1/1	0.76	0.18	67,67,67,67	0
54	MG	BA	3478	1/1	0.76	0.39	127,127,127,127	0
54	MG	AA	1647	1/1	0.76	0.43	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3716	1/1	0.76	0.28	86,86,86,86	0
54	MG	AA	1668	1/1	0.76	0.61	107,107,107,107	0
54	MG	AW	203	1/1	0.76	0.21	114,114,114,114	0
54	MG	AA	1905	1/1	0.76	0.16	96,96,96,96	0
54	MG	DA	3142	1/1	0.76	0.28	61,61,61,61	0
54	MG	CD	103	1/1	0.76	0.14	113,113,113,113	0
54	MG	CC	113	1/1	0.76	0.18	67,67,67,67	0
54	MG	CA	1975	1/1	0.76	0.27	110,110,110,110	0
54	MG	AA	1761	1/1	0.76	0.51	136,136,136,136	0
54	MG	CP	201	1/1	0.77	0.32	118,118,118,118	0
54	MG	DA	3690	1/1	0.77	0.32	83,83,83,83	0
54	MG	BA	3264	1/1	0.77	0.12	64,64,64,64	0
54	MG	CX	101	1/1	0.77	0.09	90,90,90,90	0
54	MG	CA	1697	1/1	0.77	0.28	98,98,98,98	0
54	MG	DA	3409	1/1	0.77	0.32	70,70,70,70	0
54	MG	CA	1954	1/1	0.77	0.12	95,95,95,95	0
54	MG	DS	201	1/1	0.77	0.54	104,104,104,104	0
54	MG	BA	3319	1/1	0.77	0.34	108,108,108,108	0
54	MG	BA	3358	1/1	0.77	0.15	101,101,101,101	0
54	MG	BA	3298	1/1	0.77	0.17	95,95,95,95	0
54	MG	CA	1861	1/1	0.77	0.15	109,109,109,109	0
54	MG	CS	101	1/1	0.77	0.24	82,82,82,82	0
54	MG	DA	3219	1/1	0.77	0.38	80,80,80,80	0
54	MG	AA	1984	1/1	0.77	0.11	80,80,80,80	0
54	MG	AT	202	1/1	0.77	0.25	111,111,111,111	0
54	MG	AA	1825	1/1	0.77	0.09	95,95,95,95	0
54	MG	DA	3226	1/1	0.77	0.13	74,74,74,74	0
54	MG	BA	3125	1/1	0.78	0.14	94,94,94,94	0
54	MG	BA	3428	1/1	0.78	0.14	93,93,93,93	0
54	MG	BA	3535	1/1	0.78	0.13	94,94,94,94	0
54	MG	D0	205	1/1	0.78	0.85	95,95,95,95	0
54	MG	CL	201	1/1	0.78	0.40	81,81,81,81	0
54	MG	DA	3795	1/1	0.78	0.54	112,112,112,112	0
54	MG	DA	3181	1/1	0.78	0.15	48,48,48,48	0
54	MG	BA	3335	1/1	0.78	0.36	86,86,86,86	0
54	MG	BA	3063	1/1	0.78	0.27	63,63,63,63	0
54	MG	AA	1879	1/1	0.78	0.04	85,85,85,85	0
54	MG	BA	3232	1/1	0.78	0.15	99,99,99,99	0
54	MG	BA	3370	1/1	0.78	0.11	70,70,70,70	0
54	MG	B4	101	1/1	0.78	0.12	85,85,85,85	0
54	MG	CA	1808	1/1	0.78	0.28	98,98,98,98	0
54	MG	CA	1875	1/1	0.78	0.18	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1996	1/1	0.78	0.26	106,106,106,106	0
54	MG	BA	3267	1/1	0.78	0.29	102,102,102,102	0
54	MG	AA	1855	1/1	0.78	0.23	101,101,101,101	0
54	MG	BA	3254	1/1	0.78	0.22	101,101,101,101	0
54	MG	BA	3276	1/1	0.78	0.13	79,79,79,79	0
54	MG	BA	3032	1/1	0.78	0.38	66,66,66,66	0
54	MG	CA	1626	1/1	0.78	0.31	68,68,68,68	0
54	MG	DA	3583	1/1	0.78	0.26	99,99,99,99	0
54	MG	BA	3212	1/1	0.78	0.20	87,87,87,87	0
54	MG	CA	1797	1/1	0.78	0.20	77,77,77,77	0
54	MG	DA	3379	1/1	0.78	0.50	100,100,100,100	0
54	MG	CC	103	1/1	0.78	0.21	86,86,86,86	0
54	MG	BA	3049	1/1	0.78	0.19	71,71,71,71	0
54	MG	BA	3489	1/1	0.78	0.12	93,93,93,93	0
54	MG	DA	3326	1/1	0.78	0.59	105,105,105,105	0
54	MG	DA	3484	1/1	0.78	0.18	72,72,72,72	0
54	MG	DA	3554	1/1	0.78	0.33	72,72,72,72	0
54	MG	D3	104	1/1	0.79	0.27	75,75,75,75	0
54	MG	DA	3512	1/1	0.79	0.56	96,96,96,96	0
54	MG	BA	3066	1/1	0.79	0.34	99,99,99,99	0
54	MG	DA	3569	1/1	0.79	0.36	92,92,92,92	0
54	MG	AA	1883	1/1	0.79	0.15	64,64,64,64	0
54	MG	DA	3228	1/1	0.79	0.29	77,77,77,77	0
54	MG	CA	1775	1/1	0.79	0.25	99,99,99,99	0
54	MG	CA	1821	1/1	0.79	0.30	104,104,104,104	0
54	MG	DA	3018	1/1	0.79	0.40	83,83,83,83	0
54	MG	DU	201	1/1	0.79	0.15	60,60,60,60	0
54	MG	BA	3544	1/1	0.79	0.14	71,71,71,71	0
54	MG	DA	3335	1/1	0.79	0.38	93,93,93,93	0
54	MG	AA	1635	1/1	0.79	0.16	54,54,54,54	0
54	MG	DA	3644	1/1	0.79	0.26	106,106,106,106	0
54	MG	BA	3567	1/1	0.79	0.11	69,69,69,69	0
54	MG	CA	1933	1/1	0.79	0.10	69,69,69,69	0
54	MG	DA	3534	1/1	0.79	0.24	86,86,86,86	0
54	MG	CA	1680	1/1	0.79	0.26	99,99,99,99	0
54	MG	BZ	101	1/1	0.79	0.14	92,92,92,92	0
54	MG	DA	3347	1/1	0.79	0.51	98,98,98,98	0
54	MG	CA	1921	1/1	0.79	0.24	70,70,70,70	0
54	MG	DA	3492	1/1	0.79	0.28	95,95,95,95	0
54	MG	BA	3272	1/1	0.79	0.16	66,66,66,66	0
54	MG	DA	3775	1/1	0.79	0.24	90,90,90,90	0
54	MG	BQ	201	1/1	0.79	0.19	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3397	1/1	0.79	0.23	77,77,77,77	0
54	MG	AA	1908	1/1	0.79	0.28	95,95,95,95	0
54	MG	AA	1675	1/1	0.79	0.18	62,62,62,62	0
54	MG	BA	3547	1/1	0.79	0.15	74,74,74,74	0
54	MG	BA	3491	1/1	0.79	0.19	104,104,104,104	0
54	MG	DA	3773	1/1	0.79	0.25	89,89,89,89	0
54	MG	DA	3355	1/1	0.79	0.17	60,60,60,60	0
54	MG	CA	1707	1/1	0.79	0.22	106,106,106,106	0
54	MG	CA	1885	1/1	0.79	0.18	74,74,74,74	0
54	MG	BA	3443	1/1	0.79	0.09	79,79,79,79	0
54	MG	BA	3365	1/1	0.79	0.15	77,77,77,77	0
54	MG	BA	2906	1/1	0.79	0.14	101,101,101,101	0
54	MG	AA	2028	1/1	0.79	0.15	102,102,102,102	0
54	MG	AA	1841	1/1	0.79	0.26	100,100,100,100	0
54	MG	AA	1858	1/1	0.79	0.08	83,83,83,83	0
54	MG	BA	3055	1/1	0.79	0.16	58,58,58,58	0
54	MG	DO	204	1/1	0.79	0.16	65,65,65,65	0
54	MG	BA	3180	1/1	0.79	0.16	72,72,72,72	0
54	MG	BA	3184	1/1	0.79	0.32	116,116,116,116	0
54	MG	AA	1861	1/1	0.79	0.11	120,120,120,120	0
54	MG	AA	1978	1/1	0.80	0.06	99,99,99,99	0
54	MG	AA	1878	1/1	0.80	0.15	99,99,99,99	0
54	MG	BA	3377	1/1	0.80	0.11	67,67,67,67	0
54	MG	CA	1911	1/1	0.80	0.09	123,123,123,123	0
54	MG	DA	3480	1/1	0.80	0.23	76,76,76,76	0
54	MG	DA	3107	1/1	0.80	0.33	91,91,91,91	0
54	MG	BA	3389	1/1	0.80	0.17	89,89,89,89	0
54	MG	AA	1903	1/1	0.80	0.20	95,95,95,95	0
54	MG	DA	3764	1/1	0.80	0.32	108,108,108,108	0
54	MG	DA	3682	1/1	0.80	0.61	141,141,141,141	0
54	MG	DA	3317	1/1	0.80	0.16	91,91,91,91	0
54	MG	DA	3697	1/1	0.80	0.29	89,89,89,89	0
54	MG	DA	3327	1/1	0.80	0.38	100,100,100,100	0
54	MG	BE	305	1/1	0.80	0.15	68,68,68,68	0
54	MG	DA	3251	1/1	0.80	0.42	83,83,83,83	0
54	MG	AA	1872	1/1	0.80	0.16	108,108,108,108	0
54	MG	DA	3243	1/1	0.80	0.20	65,65,65,65	0
54	MG	CA	1899	1/1	0.80	0.26	66,66,66,66	0
54	MG	DA	3727	1/1	0.80	0.51	106,106,106,106	0
54	MG	CD	110	1/1	0.80	0.26	102,102,102,102	0
54	MG	BA	3150	1/1	0.80	0.28	72,72,72,72	0
54	MG	BA	3316	1/1	0.80	0.40	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3747	1/1	0.80	0.11	90,90,90,90	0
54	MG	DA	3127	1/1	0.80	0.27	78,78,78,78	0
54	MG	AA	1910	1/1	0.80	0.13	103,103,103,103	0
54	MG	DA	3533	1/1	0.80	0.08	91,91,91,91	0
54	MG	CA	1750	1/1	0.80	0.12	80,80,80,80	0
54	MG	DA	3114	1/1	0.80	0.38	72,72,72,72	0
54	MG	DA	3279	1/1	0.80	0.33	98,98,98,98	0
54	MG	AA	1960	1/1	0.80	0.17	98,98,98,98	0
54	MG	CC	102	1/1	0.80	0.16	87,87,87,87	0
54	MG	CA	1641	1/1	0.80	0.20	72,72,72,72	0
54	MG	DA	3797	1/1	0.80	0.80	85,85,85,85	0
54	MG	CA	1728	1/1	0.80	0.33	85,85,85,85	0
54	MG	BA	3360	1/1	0.80	0.41	117,117,117,117	0
54	MG	DA	3609	1/1	0.80	0.26	86,86,86,86	0
54	MG	BA	3558	1/1	0.80	0.13	108,108,108,108	0
54	MG	AA	1844	1/1	0.80	0.20	108,108,108,108	0
54	MG	DA	3689	1/1	0.80	0.16	63,63,63,63	0
54	MG	DA	3723	1/1	0.80	0.27	106,106,106,106	0
54	MG	BG	201	1/1	0.80	0.22	117,117,117,117	0
54	MG	CA	1704	1/1	0.80	0.17	88,88,88,88	0
54	MG	CA	1964	1/1	0.80	0.12	94,94,94,94	0
54	MG	CA	1815	1/1	0.80	0.44	105,105,105,105	0
54	MG	DA	3790	1/1	0.80	0.16	109,109,109,109	0
54	MG	BA	3293	1/1	0.80	0.29	111,111,111,111	0
54	MG	DA	3265	1/1	0.80	0.24	84,84,84,84	0
54	MG	BA	2903	1/1	0.80	0.10	82,82,82,82	0
54	MG	AA	1759	1/1	0.80	0.26	77,77,77,77	0
54	MG	BA	3341	1/1	0.81	0.05	119,119,119,119	0
54	MG	DA	3380	1/1	0.81	0.28	78,78,78,78	0
54	MG	DA	3376	1/1	0.81	0.30	93,93,93,93	0
54	MG	AA	2019	1/1	0.81	0.07	104,104,104,104	0
54	MG	BA	3379	1/1	0.81	0.25	98,98,98,98	0
54	MG	DA	3072	1/1	0.81	0.25	66,66,66,66	0
54	MG	BA	3416	1/1	0.81	0.21	74,74,74,74	0
54	MG	DA	3190	1/1	0.81	0.13	50,50,50,50	0
54	MG	DA	3536	1/1	0.81	0.26	94,94,94,94	0
54	MG	BA	2910	1/1	0.81	0.18	149,149,149,149	0
54	MG	BA	3423	1/1	0.81	0.12	85,85,85,85	0
54	MG	AA	1851	1/1	0.81	0.28	97,97,97,97	0
54	MG	DA	3134	1/1	0.81	0.52	111,111,111,111	0
54	MG	BA	3568	1/1	0.81	0.12	123,123,123,123	0
54	MG	DA	2981	1/1	0.81	0.30	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3167	1/1	0.81	0.34	68,68,68,68	0
54	MG	DA	3098	1/1	0.81	0.38	65,65,65,65	0
54	MG	BA	3291	1/1	0.81	0.17	86,86,86,86	0
54	MG	CC	109	1/1	0.81	0.36	99,99,99,99	0
54	MG	DA	3470	1/1	0.81	0.35	79,79,79,79	0
54	MG	BA	3375	1/1	0.81	0.16	112,112,112,112	0
54	MG	AA	2038	1/1	0.81	0.35	116,116,116,116	0
54	MG	AA	1866	1/1	0.81	0.35	117,117,117,117	0
54	MG	BA	3348	1/1	0.81	0.25	99,99,99,99	0
54	MG	BA	3439	1/1	0.81	0.19	73,73,73,73	0
54	MG	BA	3123	1/1	0.81	0.33	71,71,71,71	0
54	MG	BA	3533	1/1	0.81	0.08	81,81,81,81	0
54	MG	BA	3244	1/1	0.81	0.08	67,67,67,67	0
54	MG	DA	3672	1/1	0.81	0.39	87,87,87,87	0
54	MG	CA	1628	1/1	0.81	0.40	87,87,87,87	0
54	MG	CA	1749	1/1	0.81	0.20	69,69,69,69	0
54	MG	DA	3185	1/1	0.81	0.33	75,75,75,75	0
54	MG	DA	3752	1/1	0.81	0.19	74,74,74,74	0
54	MG	BA	3523	1/1	0.81	0.11	104,104,104,104	0
54	MG	BA	3524	1/1	0.81	0.19	52,52,52,52	0
54	MG	DA	3547	1/1	0.81	0.19	91,91,91,91	0
54	MG	CA	1732	1/1	0.81	0.25	82,82,82,82	0
54	MG	CA	1722	1/1	0.81	0.17	99,99,99,99	0
54	MG	AA	1937	1/1	0.81	0.25	95,95,95,95	0
54	MG	AA	1930	1/1	0.81	0.38	82,82,82,82	0
54	MG	BA	2908	1/1	0.81	0.12	102,102,102,102	0
54	MG	DA	3413	1/1	0.81	0.48	99,99,99,99	0
54	MG	CD	122	1/1	0.81	0.18	97,97,97,97	0
54	MG	BA	3340	1/1	0.81	0.08	77,77,77,77	0
54	MG	AA	1857	1/1	0.81	0.36	88,88,88,88	0
54	MG	AP	201	1/1	0.81	0.12	82,82,82,82	0
54	MG	AA	1795	1/1	0.81	0.21	70,70,70,70	0
54	MG	DA	3496	1/1	0.81	0.25	69,69,69,69	0
54	MG	CA	1799	1/1	0.81	0.30	86,86,86,86	0
54	MG	DA	3557	1/1	0.81	0.18	97,97,97,97	0
54	MG	DA	3785	1/1	0.81	0.30	117,117,117,117	0
54	MG	DA	3680	1/1	0.82	0.17	75,75,75,75	0
54	MG	DA	3239	1/1	0.82	0.17	67,67,67,67	0
54	MG	DA	3377	1/1	0.82	0.31	111,111,111,111	0
54	MG	CA	1700	1/1	0.82	0.30	107,107,107,107	0
54	MG	AA	1699	1/1	0.82	0.22	95,95,95,95	0
54	MG	BA	3249	1/1	0.82	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3534	1/1	0.82	0.13	93,93,93,93	0
54	MG	DA	3120	1/1	0.82	0.51	74,74,74,74	0
54	MG	DA	3648	1/1	0.82	0.24	63,63,63,63	0
54	MG	AA	1884	1/1	0.82	0.10	86,86,86,86	0
54	MG	CD	124	1/1	0.82	0.25	109,109,109,109	0
54	MG	BA	3270	1/1	0.82	0.42	98,98,98,98	0
54	MG	CA	1848	1/1	0.82	0.30	130,130,130,130	0
54	MG	BB	225	1/1	0.82	0.16	90,90,90,90	0
54	MG	BA	3472	1/1	0.82	0.14	125,125,125,125	0
54	MG	CA	1793	1/1	0.82	0.22	66,66,66,66	0
54	MG	DA	3230	1/1	0.82	0.15	63,63,63,63	0
54	MG	BA	3396	1/1	0.82	0.22	63,63,63,63	0
54	MG	DA	3328	1/1	0.82	0.38	93,93,93,93	0
54	MG	AA	1640	1/1	0.82	0.21	75,75,75,75	0
54	MG	CA	1872	1/1	0.82	0.23	84,84,84,84	0
54	MG	DA	3115	1/1	0.82	0.32	55,55,55,55	0
54	MG	DA	3182	1/1	0.82	0.23	71,71,71,71	0
54	MG	DO	203	1/1	0.82	0.23	100,100,100,100	0
54	MG	DB	204	1/1	0.82	0.14	94,94,94,94	0
54	MG	CA	1735	1/1	0.82	0.45	108,108,108,108	0
54	MG	DA	3511	1/1	0.82	0.33	82,82,82,82	0
54	MG	AA	1963	1/1	0.82	0.48	103,103,103,103	0
54	MG	CA	1888	1/1	0.82	0.12	112,112,112,112	0
54	MG	BA	3177	1/1	0.82	0.24	89,89,89,89	0
54	MG	DA	3602	1/1	0.82	0.09	116,116,116,116	0
54	MG	BA	3226	1/1	0.82	0.22	88,88,88,88	0
54	MG	DA	3735	1/1	0.82	0.16	82,82,82,82	0
54	MG	DA	3358	1/1	0.82	0.26	78,78,78,78	0
54	MG	BA	2911	1/1	0.82	0.12	120,120,120,120	0
54	MG	CW	205	1/1	0.82	0.27	143,143,143,143	0
54	MG	BA	3152	1/1	0.82	0.29	72,72,72,72	0
54	MG	AA	1762	1/1	0.82	0.28	104,104,104,104	0
54	MG	BA	3424	1/1	0.82	0.25	107,107,107,107	0
54	MG	BA	3275	1/1	0.82	0.24	77,77,77,77	0
54	MG	CA	1880	1/1	0.82	0.16	130,130,130,130	0
54	MG	DB	227	1/1	0.82	0.32	105,105,105,105	0
54	MG	CA	1894	1/1	0.82	0.10	61,61,61,61	0
54	MG	BA	2987	1/1	0.83	0.27	57,57,57,57	0
54	MG	BA	3456	1/1	0.83	0.10	86,86,86,86	0
54	MG	D3	102	1/1	0.83	0.10	72,72,72,72	0
54	MG	BA	3517	1/1	0.83	0.10	93,93,93,93	0
54	MG	DT	101	1/1	0.83	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3433	1/1	0.83	0.25	109,109,109,109	0
54	MG	DA	3709	1/1	0.83	0.18	84,84,84,84	0
54	MG	AA	1843	1/1	0.83	0.33	93,93,93,93	0
54	MG	AA	1737	1/1	0.83	0.08	97,97,97,97	0
54	MG	BA	3253	1/1	0.83	0.16	70,70,70,70	0
54	MG	AA	1634	1/1	0.83	0.40	97,97,97,97	0
54	MG	AA	1842	1/1	0.83	0.14	72,72,72,72	0
54	MG	BA	3385	1/1	0.83	0.19	64,64,64,64	0
54	MG	DA	3529	1/1	0.83	0.23	94,94,94,94	0
54	MG	DB	212	1/1	0.83	0.35	75,75,75,75	0
54	MG	BA	3366	1/1	0.83	0.13	69,69,69,69	0
54	MG	AA	2029	1/1	0.83	0.29	127,127,127,127	0
54	MG	BA	3514	1/1	0.83	0.21	102,102,102,102	0
54	MG	CD	125	1/1	0.83	0.21	83,83,83,83	0
54	MG	AA	1740	1/1	0.83	0.15	69,69,69,69	0
54	MG	BA	3282	1/1	0.83	0.15	103,103,103,103	0
54	MG	DA	3688	1/1	0.83	0.34	111,111,111,111	0
54	MG	CP	204	1/1	0.83	0.31	137,137,137,137	0
54	MG	DA	3287	1/1	0.83	0.18	63,63,63,63	0
54	MG	BA	2907	1/1	0.83	0.23	106,106,106,106	0
54	MG	BA	3526	1/1	0.83	0.09	100,100,100,100	0
54	MG	BA	3006	1/1	0.83	0.15	54,54,54,54	0
54	MG	CA	1866	1/1	0.83	0.19	118,118,118,118	0
54	MG	BA	3536	1/1	0.83	0.19	89,89,89,89	0
54	MG	BA	3412	1/1	0.83	0.18	94,94,94,94	0
54	MG	DA	3600	1/1	0.83	0.27	107,107,107,107	0
54	MG	BA	3020	1/1	0.83	0.21	72,72,72,72	0
54	MG	DA	3373	1/1	0.83	0.13	75,75,75,75	0
54	MG	CA	1759	1/1	0.83	0.36	113,113,113,113	0
54	MG	DA	3568	1/1	0.83	0.16	93,93,93,93	0
54	MG	CA	1838	1/1	0.83	0.26	83,83,83,83	0
54	MG	CA	1950	1/1	0.83	0.38	121,121,121,121	0
54	MG	AA	1897	1/1	0.83	0.10	56,56,56,56	0
54	MG	DA	3545	1/1	0.83	0.27	74,74,74,74	0
54	MG	CA	1983	1/1	0.83	0.11	92,92,92,92	0
54	MG	BA	3390	1/1	0.83	0.11	77,77,77,77	0
54	MG	DB	215	1/1	0.83	0.20	99,99,99,99	0
54	MG	CA	1887	1/1	0.83	0.13	82,82,82,82	0
54	MG	DA	3259	1/1	0.83	0.35	71,71,71,71	0
54	MG	BA	3229	1/1	0.83	0.22	77,77,77,77	0
54	MG	BA	3019	1/1	0.83	0.10	67,67,67,67	0
54	MG	AA	2011	1/1	0.83	0.35	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3384	1/1	0.83	0.18	62,62,62,62	0
54	MG	CA	1929	1/1	0.83	0.26	92,92,92,92	0
54	MG	AA	1819	1/1	0.83	0.25	98,98,98,98	0
54	MG	AA	1958	1/1	0.83	0.32	93,93,93,93	0
54	MG	AA	2013	1/1	0.84	0.17	94,94,94,94	0
54	MG	DA	3381	1/1	0.84	0.19	73,73,73,73	0
54	MG	AA	2027	1/1	0.84	0.17	81,81,81,81	0
54	MG	CA	1751	1/1	0.84	0.16	96,96,96,96	0
54	MG	AC	105	1/1	0.84	0.17	88,88,88,88	0
54	MG	DA	3389	1/1	0.84	0.29	70,70,70,70	0
54	MG	CA	1635	1/1	0.84	0.33	86,86,86,86	0
54	MG	AX	101	1/1	0.84	0.14	107,107,107,107	0
54	MG	AA	1831	1/1	0.84	0.15	76,76,76,76	0
54	MG	AA	1805	1/1	0.84	0.45	109,109,109,109	0
54	MG	DA	3447	1/1	0.84	0.14	84,84,84,84	0
54	MG	DA	3630	1/1	0.84	0.21	67,67,67,67	0
54	MG	CA	1653	1/1	0.84	0.37	86,86,86,86	0
54	MG	BA	3191	1/1	0.84	0.35	79,79,79,79	0
54	MG	CA	1967	1/1	0.84	0.08	113,113,113,113	0
54	MG	BA	3386	1/1	0.84	0.13	85,85,85,85	0
54	MG	DA	3670	1/1	0.84	0.36	98,98,98,98	0
54	MG	CA	1951	1/1	0.84	0.16	74,74,74,74	0
54	MG	DA	3628	1/1	0.84	0.12	70,70,70,70	0
54	MG	BA	3414	1/1	0.84	0.18	105,105,105,105	0
54	MG	DA	3740	1/1	0.84	0.28	88,88,88,88	0
54	MG	BA	3541	1/1	0.84	0.22	79,79,79,79	0
54	MG	DA	3081	1/1	0.84	0.34	84,84,84,84	0
54	MG	DA	3085	1/1	0.84	0.40	67,67,67,67	0
54	MG	CA	1717	1/1	0.84	0.24	76,76,76,76	0
54	MG	AA	1824	1/1	0.84	0.21	85,85,85,85	0
54	MG	BA	3051	1/1	0.84	0.24	74,74,74,74	0
54	MG	DA	3296	1/1	0.84	0.44	82,82,82,82	0
54	MG	DA	3563	1/1	0.84	0.12	76,76,76,76	0
54	MG	BA	3262	1/1	0.84	0.11	58,58,58,58	0
54	MG	BA	2967	1/1	0.84	0.30	60,60,60,60	0
54	MG	BA	3537	1/1	0.84	0.24	108,108,108,108	0
54	MG	BW	101	1/1	0.84	0.11	65,65,65,65	0
54	MG	BA	3497	1/1	0.84	0.16	72,72,72,72	0
54	MG	BA	3161	1/1	0.84	0.42	96,96,96,96	0
54	MG	CA	1663	1/1	0.84	0.36	81,81,81,81	0
54	MG	DA	3130	1/1	0.84	0.45	89,89,89,89	0
54	MG	BU	204	1/1	0.84	0.23	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3666	1/1	0.84	0.14	78,78,78,78	0
54	MG	DA	3443	1/1	0.84	0.36	86,86,86,86	0
54	MG	AA	1988	1/1	0.84	0.10	93,93,93,93	0
54	MG	AA	1657	1/1	0.84	0.40	83,83,83,83	0
54	MG	DA	3110	1/1	0.84	0.23	54,54,54,54	0
54	MG	CA	1647	1/1	0.84	0.25	81,81,81,81	0
54	MG	DA	3404	1/1	0.84	0.24	94,94,94,94	0
54	MG	BA	2904	1/1	0.84	0.10	101,101,101,101	0
54	MG	CA	1876	1/1	0.84	0.15	83,83,83,83	0
54	MG	DA	3405	1/1	0.84	0.16	91,91,91,91	0
54	MG	AA	1674	1/1	0.84	0.19	74,74,74,74	0
54	MG	BA	3069	1/1	0.84	0.09	48,48,48,48	0
54	MG	BA	3129	1/1	0.84	0.23	72,72,72,72	0
54	MG	CA	1904	1/1	0.84	0.32	117,117,117,117	0
54	MG	DA	3565	1/1	0.84	0.20	100,100,100,100	0
54	MG	BE	304	1/1	0.84	0.31	86,86,86,86	0
54	MG	DA	3542	1/1	0.84	0.17	92,92,92,92	0
54	MG	BA	3080	1/1	0.84	0.14	69,69,69,69	0
54	MG	DA	3007	1/1	0.84	0.22	48,48,48,48	0
54	MG	DA	3455	1/1	0.84	0.10	80,80,80,80	0
54	MG	CA	1868	1/1	0.84	0.24	72,72,72,72	0
54	MG	BA	3575	1/1	0.85	0.15	82,82,82,82	0
54	MG	BA	3207	1/1	0.85	0.11	67,67,67,67	0
54	MG	AA	1768	1/1	0.85	0.20	67,67,67,67	0
54	MG	BA	2913	1/1	0.85	0.26	115,115,115,115	0
54	MG	CA	1794	1/1	0.85	0.27	80,80,80,80	0
54	MG	CA	1661	1/1	0.85	0.16	64,64,64,64	0
54	MG	BA	3057	1/1	0.85	0.15	65,65,65,65	0
54	MG	DA	3357	1/1	0.85	0.20	77,77,77,77	0
54	MG	BA	3286	1/1	0.85	0.23	80,80,80,80	0
54	MG	DA	3211	1/1	0.85	0.10	71,71,71,71	0
54	MG	AA	1774	1/1	0.85	0.23	75,75,75,75	0
54	MG	DA	3061	1/1	0.85	0.29	52,52,52,52	0
54	MG	CA	1608	1/1	0.85	0.14	53,53,53,53	0
54	MG	BA	2994	1/1	0.85	0.27	60,60,60,60	0
54	MG	BA	3120	1/1	0.85	0.18	75,75,75,75	0
54	MG	BA	3092	1/1	0.85	0.10	58,58,58,58	0
54	MG	DA	3323	1/1	0.85	0.17	105,105,105,105	0
54	MG	CD	115	1/1	0.85	0.26	106,106,106,106	0
54	MG	CA	1959	1/1	0.85	0.12	84,84,84,84	0
54	MG	BA	3563	1/1	0.85	0.15	74,74,74,74	0
54	MG	B6	101	1/1	0.85	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1663	1/1	0.85	0.19	71,71,71,71	0
54	MG	BA	3337	1/1	0.85	0.12	73,73,73,73	0
54	MG	BA	3277	1/1	0.85	0.12	73,73,73,73	0
54	MG	DA	3422	1/1	0.85	0.40	82,82,82,82	0
54	MG	BA	3146	1/1	0.85	0.14	78,78,78,78	0
54	MG	CA	1965	1/1	0.85	0.30	92,92,92,92	0
54	MG	DA	3686	1/1	0.85	0.14	93,93,93,93	0
54	MG	AA	1685	1/1	0.85	0.21	96,96,96,96	0
54	MG	DA	3162	1/1	0.85	0.27	55,55,55,55	0
54	MG	AA	1698	1/1	0.85	0.37	79,79,79,79	0
54	MG	DA	3180	1/1	0.85	0.10	102,102,102,102	0
54	MG	DA	2980	1/1	0.85	0.30	44,44,44,44	0
54	MG	DA	3184	1/1	0.85	0.26	66,66,66,66	0
54	MG	BA	3373	1/1	0.85	0.36	105,105,105,105	0
54	MG	AA	1895	1/1	0.85	0.14	133,133,133,133	0
54	MG	BA	3198	1/1	0.85	0.08	58,58,58,58	0
54	MG	DA	3770	1/1	0.85	0.35	87,87,87,87	0
54	MG	CA	1689	1/1	0.85	0.17	62,62,62,62	0
54	MG	DA	3488	1/1	0.85	0.21	66,66,66,66	0
54	MG	CA	1826	1/1	0.85	0.21	107,107,107,107	0
54	MG	DA	3148	1/1	0.85	0.35	76,76,76,76	0
54	MG	DA	3668	1/1	0.85	0.51	117,117,117,117	0
54	MG	CA	1941	1/1	0.85	0.11	88,88,88,88	0
54	MG	DA	3748	1/1	0.85	0.57	71,71,71,71	0
54	MG	BU	202	1/1	0.85	0.16	73,73,73,73	0
54	MG	DA	3588	1/1	0.85	0.14	91,91,91,91	0
54	MG	BB	210	1/1	0.85	0.17	62,62,62,62	0
54	MG	DA	3349	1/1	0.85	0.20	56,56,56,56	0
54	MG	AK	201	1/1	0.85	0.17	90,90,90,90	0
54	MG	AA	1849	1/1	0.85	0.28	92,92,92,92	0
54	MG	DA	3124	1/1	0.85	0.18	66,66,66,66	0
54	MG	AA	1830	1/1	0.85	0.27	88,88,88,88	0
54	MG	CA	1970	1/1	0.85	0.17	87,87,87,87	0
54	MG	DA	3410	1/1	0.85	0.35	95,95,95,95	0
54	MG	BA	3156	1/1	0.85	0.33	68,68,68,68	0
54	MG	BA	3310	1/1	0.85	0.13	80,80,80,80	0
54	MG	AA	1998	1/1	0.85	0.26	98,98,98,98	0
54	MG	DA	3150	1/1	0.85	0.31	54,54,54,54	0
54	MG	DA	3272	1/1	0.85	0.32	66,66,66,66	0
54	MG	AA	1646	1/1	0.85	0.21	66,66,66,66	0
54	MG	BB	209	1/1	0.85	0.13	59,59,59,59	0
54	MG	DA	3193	1/1	0.85	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1790	1/1	0.85	0.14	76,76,76,76	0
54	MG	CA	1944	1/1	0.85	0.13	99,99,99,99	0
54	MG	AA	1756	1/1	0.85	0.17	68,68,68,68	0
54	MG	BO	201	1/1	0.85	0.14	50,50,50,50	0
54	MG	DA	3284	1/1	0.85	0.21	75,75,75,75	0
54	MG	BA	3320	1/1	0.85	0.33	101,101,101,101	0
54	MG	BB	215	1/1	0.85	0.10	65,65,65,65	0
54	MG	DA	3658	1/1	0.85	0.46	88,88,88,88	0
54	MG	DA	3581	1/1	0.85	0.20	139,139,139,139	0
54	MG	DA	3657	1/1	0.85	0.12	88,88,88,88	0
54	MG	CC	105	1/1	0.85	0.34	88,88,88,88	0
54	MG	CD	117	1/1	0.85	0.09	85,85,85,85	0
54	MG	BA	3052	1/1	0.86	0.14	63,63,63,63	0
54	MG	BB	202	1/1	0.86	0.13	59,59,59,59	0
54	MG	BA	3368	1/1	0.86	0.43	113,113,113,113	0
54	MG	CA	1957	1/1	0.86	0.10	90,90,90,90	0
54	MG	BA	3380	1/1	0.86	0.17	71,71,71,71	0
54	MG	BB	216	1/1	0.86	0.11	83,83,83,83	0
54	MG	DB	216	1/1	0.86	0.17	94,94,94,94	0
54	MG	BA	3196	1/1	0.86	0.43	89,89,89,89	0
54	MG	CA	1953	1/1	0.86	0.45	103,103,103,103	0
54	MG	BA	3116	1/1	0.86	0.26	64,64,64,64	0
54	MG	DA	2989	1/1	0.86	0.24	42,42,42,42	0
54	MG	CA	1850	1/1	0.86	0.11	96,96,96,96	0
54	MG	DA	3550	1/1	0.86	0.30	76,76,76,76	0
54	MG	BA	3438	1/1	0.86	0.19	54,54,54,54	0
54	MG	CA	1831	1/1	0.86	0.37	95,95,95,95	0
54	MG	AA	1695	1/1	0.86	0.34	73,73,73,73	0
54	MG	BA	3521	1/1	0.86	0.22	109,109,109,109	0
54	MG	DA	3362	1/1	0.86	0.13	58,58,58,58	0
54	MG	DA	3101	1/1	0.86	0.33	52,52,52,52	0
54	MG	BA	3121	1/1	0.86	0.24	76,76,76,76	0
54	MG	AQ	101	1/1	0.86	0.06	83,83,83,83	0
54	MG	CD	108	1/1	0.86	0.11	174,174,174,174	0
54	MG	BT	102	1/1	0.86	0.10	100,100,100,100	0
54	MG	AA	1779	1/1	0.86	0.11	114,114,114,114	0
54	MG	DA	3805	1/1	0.86	0.26	90,90,90,90	0
54	MG	CA	1835	1/1	0.86	0.15	74,74,74,74	0
54	MG	BA	3515	1/1	0.86	0.20	80,80,80,80	0
54	MG	CA	1839	1/1	0.86	0.14	65,65,65,65	0
54	MG	BA	3354	1/1	0.86	0.09	57,57,57,57	0
54	MG	DA	3089	1/1	0.86	0.37	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3241	1/1	0.86	0.30	92,92,92,92	0
54	MG	CA	1715	1/1	0.86	0.33	101,101,101,101	0
54	MG	DA	3440	1/1	0.86	0.58	118,118,118,118	0
54	MG	CC	108	1/1	0.86	0.13	75,75,75,75	0
54	MG	DA	3308	1/1	0.86	0.25	49,49,49,49	0
54	MG	AA	1696	1/1	0.86	0.27	134,134,134,134	0
54	MG	BA	3351	1/1	0.86	0.08	69,69,69,69	0
54	MG	BA	3118	1/1	0.86	0.20	82,82,82,82	0
54	MG	CP	203	1/1	0.86	0.09	93,93,93,93	0
54	MG	DA	3364	1/1	0.86	0.37	79,79,79,79	0
54	MG	DA	3303	1/1	0.86	0.57	113,113,113,113	0
54	MG	AA	2015	1/1	0.86	0.27	106,106,106,106	0
54	MG	AA	1876	1/1	0.86	0.24	78,78,78,78	0
54	MG	BA	3460	1/1	0.86	0.15	90,90,90,90	0
54	MG	DA	3276	1/1	0.86	0.26	70,70,70,70	0
54	MG	BA	3002	1/1	0.86	0.23	62,62,62,62	0
54	MG	DA	3699	1/1	0.86	0.45	102,102,102,102	0
54	MG	DA	3314	1/1	0.86	0.15	107,107,107,107	0
54	MG	DB	218	1/1	0.86	0.39	84,84,84,84	0
54	MG	DA	3126	1/1	0.86	0.28	65,65,65,65	0
54	MG	DA	3788	1/1	0.86	0.34	111,111,111,111	0
54	MG	BA	3391	1/1	0.86	0.20	86,86,86,86	0
54	MG	DA	3178	1/1	0.86	0.30	72,72,72,72	0
54	MG	DB	220	1/1	0.86	0.30	122,122,122,122	0
54	MG	DA	3374	1/1	0.86	0.19	75,75,75,75	0
54	MG	AA	1726	1/1	0.86	0.14	68,68,68,68	0
54	MG	AA	1936	1/1	0.86	0.07	74,74,74,74	0
54	MG	DA	3465	1/1	0.86	0.51	104,104,104,104	0
54	MG	DA	3772	1/1	0.86	0.18	76,76,76,76	0
54	MG	DA	3424	1/1	0.86	0.15	77,77,77,77	0
54	MG	BA	3015	1/1	0.86	0.24	70,70,70,70	0
54	MG	BA	3112	1/1	0.87	0.21	64,64,64,64	0
54	MG	DA	3414	1/1	0.87	0.35	70,70,70,70	0
54	MG	BA	3357	1/1	0.87	0.15	66,66,66,66	0
54	MG	DA	2991	1/1	0.87	0.45	75,75,75,75	0
54	MG	DA	3290	1/1	0.87	0.43	81,81,81,81	0
54	MG	CA	1926	1/1	0.87	0.22	81,81,81,81	0
54	MG	DA	3441	1/1	0.87	0.68	116,116,116,116	0
54	MG	AA	1693	1/1	0.87	0.09	95,95,95,95	0
54	MG	BA	3248	1/1	0.87	0.08	81,81,81,81	0
54	MG	DH	201	1/1	0.87	0.15	77,77,77,77	0
54	MG	DA	3168	1/1	0.87	0.60	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3273	1/1	0.87	0.10	72,72,72,72	0
54	MG	AA	1660	1/1	0.87	0.10	60,60,60,60	0
54	MG	DB	225	1/1	0.87	0.32	84,84,84,84	0
54	MG	DA	3204	1/1	0.87	0.44	62,62,62,62	0
54	MG	DA	3613	1/1	0.87	0.11	70,70,70,70	0
54	MG	DA	3195	1/1	0.87	0.34	77,77,77,77	0
54	MG	BA	3240	1/1	0.87	0.33	71,71,71,71	0
54	MG	BA	3081	1/1	0.87	0.29	72,72,72,72	0
54	MG	BA	3507	1/1	0.87	0.16	80,80,80,80	0
54	MG	CA	1946	1/1	0.87	0.06	91,91,91,91	0
54	MG	AA	1742	1/1	0.87	0.24	83,83,83,83	0
54	MG	DA	3755	1/1	0.87	0.18	67,67,67,67	0
54	MG	DA	3645	1/1	0.87	0.49	88,88,88,88	0
54	MG	DA	3478	1/1	0.87	0.28	71,71,71,71	0
54	MG	DA	3294	1/1	0.87	0.27	78,78,78,78	0
54	MG	BA	3313	1/1	0.87	0.17	102,102,102,102	0
54	MG	CD	114	1/1	0.87	0.07	109,109,109,109	0
54	MG	AA	1738	1/1	0.87	0.32	84,84,84,84	0
54	MG	DA	3471	1/1	0.87	0.17	94,94,94,94	0
54	MG	DA	3138	1/1	0.87	0.35	56,56,56,56	0
54	MG	BA	3321	1/1	0.87	0.16	64,64,64,64	0
54	MG	AA	1888	1/1	0.87	0.11	114,114,114,114	0
54	MG	CQ	102	1/1	0.87	0.19	111,111,111,111	0
54	MG	DA	3164	1/1	0.87	0.39	72,72,72,72	0
54	MG	DA	3238	1/1	0.87	0.36	100,100,100,100	0
54	MG	CA	1925	1/1	0.87	0.18	90,90,90,90	0
54	MG	CA	1634	1/1	0.87	0.20	54,54,54,54	0
54	MG	AA	1700	1/1	0.87	0.22	62,62,62,62	0
54	MG	DA	3074	1/1	0.87	0.14	52,52,52,52	0
54	MG	AA	1993	1/1	0.87	0.20	134,134,134,134	0
54	MG	DA	3598	1/1	0.87	0.18	79,79,79,79	0
54	MG	DA	3385	1/1	0.87	0.47	99,99,99,99	0
54	MG	BA	3064	1/1	0.87	0.24	76,76,76,76	0
54	MG	BA	2988	1/1	0.87	0.14	46,46,46,46	0
54	MG	CA	1780	1/1	0.87	0.15	78,78,78,78	0
54	MG	CA	1692	1/1	0.87	0.12	79,79,79,79	0
54	MG	BA	3549	1/1	0.87	0.33	110,110,110,110	0
54	MG	DA	3237	1/1	0.87	0.27	68,68,68,68	0
54	MG	BA	3470	1/1	0.87	0.15	79,79,79,79	0
54	MG	DA	3348	1/1	0.87	0.13	58,58,58,58	0
54	MG	BA	3445	1/1	0.87	0.36	96,96,96,96	0
54	MG	DA	3531	1/1	0.87	0.31	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1645	1/1	0.87	0.33	79,79,79,79	0
54	MG	DA	3647	1/1	0.87	0.23	98,98,98,98	0
54	MG	BA	3343	1/1	0.87	0.22	73,73,73,73	0
54	MG	AA	1845	1/1	0.87	0.15	88,88,88,88	0
54	MG	DA	3387	1/1	0.87	0.31	83,83,83,83	0
54	MG	DA	3778	1/1	0.87	0.13	97,97,97,97	0
54	MG	AA	1975	1/1	0.87	0.15	86,86,86,86	0
54	MG	DA	3549	1/1	0.87	0.44	70,70,70,70	0
54	MG	AA	1931	1/1	0.87	0.31	98,98,98,98	0
54	MG	AA	1950	1/1	0.87	0.15	90,90,90,90	0
54	MG	CA	1633	1/1	0.87	0.27	70,70,70,70	0
54	MG	CA	1754	1/1	0.87	0.17	82,82,82,82	0
54	MG	DA	3071	1/1	0.87	0.21	60,60,60,60	0
54	MG	DA	3304	1/1	0.87	0.09	41,41,41,41	0
54	MG	AA	1818	1/1	0.87	0.09	64,64,64,64	0
54	MG	DA	3523	1/1	0.87	0.07	64,64,64,64	0
54	MG	BB	208	1/1	0.87	0.12	91,91,91,91	0
54	MG	DA	3125	1/1	0.87	0.20	48,48,48,48	0
54	MG	DA	3432	1/1	0.87	0.26	66,66,66,66	0
54	MG	DA	3526	1/1	0.87	0.20	74,74,74,74	0
54	MG	BA	3467	1/1	0.87	0.06	81,81,81,81	0
54	MG	CA	1631	1/1	0.87	0.28	68,68,68,68	0
54	MG	BA	3434	1/1	0.87	0.23	88,88,88,88	0
54	MG	BA	3400	1/1	0.87	0.16	117,117,117,117	0
54	MG	DA	3299	1/1	0.87	0.34	84,84,84,84	0
54	MG	AA	1639	1/1	0.87	0.43	73,73,73,73	0
54	MG	AA	1854	1/1	0.87	0.13	97,97,97,97	0
54	MG	CA	1755	1/1	0.87	0.27	70,70,70,70	0
54	MG	BA	3545	1/1	0.87	0.20	82,82,82,82	0
54	MG	CA	1773	1/1	0.87	0.05	87,87,87,87	0
54	MG	DA	3495	1/1	0.87	0.29	92,92,92,92	0
54	MG	DA	3400	1/1	0.87	0.23	73,73,73,73	0
54	MG	AA	1856	1/1	0.87	0.22	71,71,71,71	0
54	MG	AA	1645	1/1	0.88	0.20	55,55,55,55	0
54	MG	DA	3537	1/1	0.88	0.32	73,73,73,73	0
54	MG	CA	1638	1/1	0.88	0.28	60,60,60,60	0
54	MG	BB	201	1/1	0.88	0.17	69,69,69,69	0
54	MG	CA	1814	1/1	0.88	0.29	84,84,84,84	0
54	MG	DA	3685	1/1	0.88	0.14	66,66,66,66	0
54	MG	DA	3751	1/1	0.88	0.30	101,101,101,101	0
54	MG	BA	3473	1/1	0.88	0.17	93,93,93,93	0
54	MG	DA	3288	1/1	0.88	0.39	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1746	1/1	0.88	0.51	86,86,86,86	0
54	MG	CA	1695	1/1	0.88	0.21	62,62,62,62	0
54	MG	AA	2033	1/1	0.88	0.29	106,106,106,106	0
54	MG	AA	2016	1/1	0.88	0.36	102,102,102,102	0
54	MG	DA	3601	1/1	0.88	0.36	95,95,95,95	0
54	MG	DA	3627	1/1	0.88	0.09	87,87,87,87	0
54	MG	DA	3742	1/1	0.88	0.21	58,58,58,58	0
54	MG	BA	3387	1/1	0.88	0.12	67,67,67,67	0
54	MG	DA	3774	1/1	0.88	0.36	76,76,76,76	0
54	MG	DA	3636	1/1	0.88	0.17	66,66,66,66	0
54	MG	BA	3255	1/1	0.88	0.22	93,93,93,93	0
54	MG	DA	3163	1/1	0.88	0.33	60,60,60,60	0
54	MG	AA	1710	1/1	0.88	0.12	78,78,78,78	0
54	MG	BA	3228	1/1	0.88	0.17	83,83,83,83	0
54	MG	CA	1938	1/1	0.88	0.26	85,85,85,85	0
54	MG	AA	1977	1/1	0.88	0.30	86,86,86,86	0
54	MG	DA	3430	1/1	0.88	0.48	95,95,95,95	0
54	MG	DA	3191	1/1	0.88	0.41	89,89,89,89	0
54	MG	DA	3720	1/1	0.88	0.43	82,82,82,82	0
54	MG	CA	1674	1/1	0.88	0.19	73,73,73,73	0
54	MG	BA	3388	1/1	0.88	0.30	95,95,95,95	0
54	MG	D0	202	1/1	0.88	0.20	51,51,51,51	0
54	MG	DA	3043	1/1	0.88	0.17	59,59,59,59	0
54	MG	CA	1668	1/1	0.88	0.30	62,62,62,62	0
54	MG	DA	3131	1/1	0.88	0.30	63,63,63,63	0
54	MG	BA	3345	1/1	0.88	0.12	80,80,80,80	0
54	MG	BA	3299	1/1	0.88	0.23	94,94,94,94	0
54	MG	BA	3185	1/1	0.88	0.14	84,84,84,84	0
54	MG	AA	1806	1/1	0.88	0.24	118,118,118,118	0
54	MG	AC	101	1/1	0.88	0.07	88,88,88,88	0
54	MG	BA	3039	1/1	0.88	0.17	58,58,58,58	0
54	MG	DA	3435	1/1	0.88	0.19	90,90,90,90	0
54	MG	DA	3490	1/1	0.88	0.28	90,90,90,90	0
54	MG	DA	3052	1/1	0.88	0.09	42,42,42,42	0
54	MG	DA	3396	1/1	0.88	0.20	85,85,85,85	0
54	MG	DA	3743	1/1	0.88	0.39	111,111,111,111	0
54	MG	CA	1684	1/1	0.88	0.15	60,60,60,60	0
54	MG	BA	3218	1/1	0.88	0.10	70,70,70,70	0
54	MG	DA	3622	1/1	0.88	0.38	84,84,84,84	0
54	MG	B8	101	1/1	0.88	0.17	76,76,76,76	0
54	MG	DA	3224	1/1	0.88	0.23	55,55,55,55	0
54	MG	CA	1690	1/1	0.88	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3513	1/1	0.88	0.81	82,82,82,82	0
54	MG	BK	201	1/1	0.88	0.11	68,68,68,68	0
54	MG	AA	1664	1/1	0.88	0.33	69,69,69,69	0
54	MG	DA	3291	1/1	0.88	0.25	76,76,76,76	0
54	MG	BA	3245	1/1	0.88	0.15	128,128,128,128	0
54	MG	AA	1773	1/1	0.88	0.14	81,81,81,81	0
54	MG	AA	1734	1/1	0.88	0.23	60,60,60,60	0
54	MG	DA	3591	1/1	0.88	0.14	81,81,81,81	0
54	MG	DA	3256	1/1	0.88	0.28	55,55,55,55	0
54	MG	CA	1949	1/1	0.88	0.21	91,91,91,91	0
54	MG	AA	1918	1/1	0.88	0.11	84,84,84,84	0
54	MG	DA	3450	1/1	0.88	0.25	98,98,98,98	0
54	MG	DA	3538	1/1	0.88	0.14	91,91,91,91	0
54	MG	DA	3491	1/1	0.88	0.47	102,102,102,102	0
54	MG	AA	1644	1/1	0.88	0.43	90,90,90,90	0
54	MG	CA	1961	1/1	0.88	0.21	78,78,78,78	0
54	MG	BA	3230	1/1	0.88	0.10	67,67,67,67	0
54	MG	CA	1869	1/1	0.88	0.11	98,98,98,98	0
54	MG	DA	3316	1/1	0.88	0.22	88,88,88,88	0
54	MG	AO	201	1/1	0.88	0.15	70,70,70,70	0
54	MG	CA	1883	1/1	0.88	0.09	80,80,80,80	0
54	MG	AA	1616	1/1	0.88	0.14	76,76,76,76	0
54	MG	DA	3640	1/1	0.88	0.26	82,82,82,82	0
54	MG	BA	2992	1/1	0.88	0.26	63,63,63,63	0
54	MG	DA	3354	1/1	0.88	0.12	55,55,55,55	0
54	MG	DA	3235	1/1	0.88	0.31	71,71,71,71	0
54	MG	AA	1618	1/1	0.88	0.25	39,39,39,39	0
54	MG	AA	1711	1/1	0.88	0.37	86,86,86,86	0
54	MG	AA	1682	1/1	0.88	0.37	87,87,87,87	0
54	MG	DU	203	1/1	0.88	0.16	94,94,94,94	0
54	MG	BA	3349	1/1	0.88	0.10	82,82,82,82	0
54	MG	B0	201	1/1	0.88	0.16	74,74,74,74	0
54	MG	CD	118	1/1	0.88	0.08	60,60,60,60	0
54	MG	CA	1612	1/1	0.88	0.12	37,37,37,37	0
54	MG	CA	1879	1/1	0.88	0.31	90,90,90,90	0
54	MG	DA	3798	1/1	0.88	0.68	78,78,78,78	0
54	MG	BA	3505	1/1	0.88	0.22	114,114,114,114	0
54	MG	BA	3509	1/1	0.88	0.21	107,107,107,107	0
54	MG	BA	3056	1/1	0.88	0.26	71,71,71,71	0
54	MG	DA	3605	1/1	0.88	0.19	80,80,80,80	0
54	MG	CA	1912	1/1	0.88	0.14	127,127,127,127	0
54	MG	AA	1796	1/1	0.88	0.33	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3681	1/1	0.88	0.26	92,92,92,92	0
54	MG	BA	2959	1/1	0.88	0.13	36,36,36,36	0
54	MG	BA	3068	1/1	0.88	0.18	72,72,72,72	0
54	MG	AA	1641	1/1	0.88	0.13	76,76,76,76	0
54	MG	CA	1981	1/1	0.88	0.08	65,65,65,65	0
54	MG	AA	2042	1/1	0.88	0.10	66,66,66,66	0
54	MG	AA	1721	1/1	0.88	0.39	72,72,72,72	0
54	MG	CA	1769	1/1	0.89	0.18	81,81,81,81	0
54	MG	BA	3164	1/1	0.89	0.08	70,70,70,70	0
54	MG	DA	3626	1/1	0.89	0.49	109,109,109,109	0
54	MG	DB	221	1/1	0.89	0.24	94,94,94,94	0
54	MG	DA	2992	1/1	0.89	0.26	43,43,43,43	0
54	MG	DA	3502	1/1	0.89	0.38	112,112,112,112	0
54	MG	DA	3606	1/1	0.89	0.23	72,72,72,72	0
54	MG	DA	2996	1/1	0.89	0.32	40,40,40,40	0
54	MG	DA	3247	1/1	0.89	0.14	45,45,45,45	0
54	MG	BA	3216	1/1	0.89	0.21	86,86,86,86	0
54	MG	DA	3454	1/1	0.89	0.36	69,69,69,69	0
54	MG	DA	3199	1/1	0.89	0.12	39,39,39,39	0
54	MG	CA	1758	1/1	0.89	0.08	90,90,90,90	0
54	MG	DA	3202	1/1	0.89	0.17	49,49,49,49	0
54	MG	AA	1938	1/1	0.89	0.33	89,89,89,89	0
54	MG	AA	1716	1/1	0.89	0.11	66,66,66,66	0
54	MG	CA	1658	1/1	0.89	0.28	76,76,76,76	0
54	MG	BA	3410	1/1	0.89	0.11	82,82,82,82	0
54	MG	AA	1933	1/1	0.89	0.35	98,98,98,98	0
54	MG	AA	1870	1/1	0.89	0.09	92,92,92,92	0
54	MG	DA	3252	1/1	0.89	0.28	65,65,65,65	0
54	MG	DA	3370	1/1	0.89	0.38	79,79,79,79	0
54	MG	CA	1698	1/1	0.89	0.22	101,101,101,101	0
54	MG	AA	1617	1/1	0.89	0.41	77,77,77,77	0
54	MG	DA	3318	1/1	0.89	0.46	87,87,87,87	0
54	MG	DB	228	1/1	0.89	0.38	116,116,116,116	0
54	MG	AA	1765	1/1	0.89	0.21	83,83,83,83	0
54	MG	DA	3236	1/1	0.89	0.32	60,60,60,60	0
54	MG	DA	3730	1/1	0.89	0.16	79,79,79,79	0
54	MG	DA	3753	1/1	0.89	0.32	92,92,92,92	0
54	MG	AS	101	1/1	0.89	0.35	84,84,84,84	0
54	MG	CA	1736	1/1	0.89	0.17	89,89,89,89	0
54	MG	BA	3364	1/1	0.89	0.12	77,77,77,77	0
54	MG	DA	3803	1/1	0.89	0.05	99,99,99,99	0
54	MG	CA	1800	1/1	0.89	0.15	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3399	1/1	0.89	0.28	86,86,86,86	0
54	MG	AD	101	1/1	0.89	0.26	85,85,85,85	0
54	MG	AA	1735	1/1	0.89	0.41	108,108,108,108	0
54	MG	CA	1724	1/1	0.89	0.18	66,66,66,66	0
54	MG	BA	3532	1/1	0.89	0.13	83,83,83,83	0
54	MG	CA	1630	1/1	0.89	0.30	59,59,59,59	0
54	MG	CA	1708	1/1	0.89	0.16	77,77,77,77	0
54	MG	DA	3271	1/1	0.89	0.56	87,87,87,87	0
54	MG	BA	3318	1/1	0.89	0.18	76,76,76,76	0
54	MG	BA	3227	1/1	0.89	0.24	82,82,82,82	0
54	MG	AA	1881	1/1	0.89	0.16	77,77,77,77	0
54	MG	BA	3538	1/1	0.89	0.14	65,65,65,65	0
54	MG	DA	3616	1/1	0.89	0.15	59,59,59,59	0
54	MG	AA	1736	1/1	0.89	0.16	53,53,53,53	0
54	MG	DA	3641	1/1	0.89	0.22	76,76,76,76	0
54	MG	DA	3734	1/1	0.89	0.19	69,69,69,69	0
54	MG	DA	3359	1/1	0.89	0.31	70,70,70,70	0
54	MG	DA	3037	1/1	0.89	0.25	58,58,58,58	0
54	MG	DA	3218	1/1	0.89	0.33	61,61,61,61	0
54	MG	DA	3632	1/1	0.89	0.07	73,73,73,73	0
54	MG	BA	3183	1/1	0.89	0.11	80,80,80,80	0
54	MG	CA	1673	1/1	0.89	0.19	63,63,63,63	0
54	MG	AA	1604	1/1	0.89	0.27	53,53,53,53	0
54	MG	BA	3143	1/1	0.89	0.32	74,74,74,74	0
54	MG	AA	1802	1/1	0.89	0.23	98,98,98,98	0
54	MG	CA	1801	1/1	0.89	0.27	88,88,88,88	0
54	MG	AA	1846	1/1	0.89	0.43	97,97,97,97	0
54	MG	BA	3074	1/1	0.89	0.22	41,41,41,41	0
54	MG	DA	3612	1/1	0.89	0.15	99,99,99,99	0
54	MG	BA	3403	1/1	0.89	0.22	89,89,89,89	0
54	MG	CA	1774	1/1	0.89	0.17	66,66,66,66	0
54	MG	AA	1957	1/1	0.89	0.15	82,82,82,82	0
54	MG	DA	3206	1/1	0.89	0.33	59,59,59,59	0
54	MG	DA	3402	1/1	0.89	0.11	70,70,70,70	0
54	MG	CA	1601	1/1	0.89	0.22	50,50,50,50	0
54	MG	BA	3300	1/1	0.89	0.12	87,87,87,87	0
54	MG	BA	3114	1/1	0.89	0.18	67,67,67,67	0
54	MG	BF	301	1/1	0.89	0.13	80,80,80,80	0
54	MG	DA	3084	1/1	0.89	0.28	47,47,47,47	0
54	MG	DA	3669	1/1	0.89	0.19	70,70,70,70	0
54	MG	AA	1648	1/1	0.89	0.35	68,68,68,68	0
54	MG	BA	3407	1/1	0.89	0.34	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1886	1/1	0.89	0.20	120,120,120,120	0
54	MG	DA	3457	1/1	0.89	0.14	74,74,74,74	0
54	MG	CA	1762	1/1	0.89	0.24	110,110,110,110	0
54	MG	DA	3481	1/1	0.89	0.27	91,91,91,91	0
54	MG	CA	1980	1/1	0.89	0.16	50,50,50,50	0
54	MG	AA	1728	1/1	0.89	0.21	77,77,77,77	0
54	MG	AA	1893	1/1	0.89	0.14	95,95,95,95	0
54	MG	BA	3144	1/1	0.89	0.14	68,68,68,68	0
54	MG	DA	3453	1/1	0.89	0.43	81,81,81,81	0
54	MG	BA	3065	1/1	0.89	0.18	51,51,51,51	0
54	MG	AA	1666	1/1	0.89	0.27	95,95,95,95	0
54	MG	CA	1827	1/1	0.89	0.06	100,100,100,100	0
54	MG	AA	1827	1/1	0.89	0.21	88,88,88,88	0
54	MG	DA	3231	1/1	0.89	0.40	78,78,78,78	0
54	MG	AA	1784	1/1	0.89	0.05	76,76,76,76	0
54	MG	DA	3275	1/1	0.89	0.17	62,62,62,62	0
54	MG	CA	1664	1/1	0.89	0.17	87,87,87,87	0
54	MG	AA	1814	1/1	0.89	0.20	63,63,63,63	0
54	MG	CA	1609	1/1	0.89	0.33	54,54,54,54	0
54	MG	BA	3139	1/1	0.89	0.09	40,40,40,40	0
54	MG	DA	3050	1/1	0.89	0.35	56,56,56,56	0
54	MG	BA	3295	1/1	0.89	0.09	55,55,55,55	0
54	MG	DB	203	1/1	0.89	0.35	67,67,67,67	0
54	MG	DA	3208	1/1	0.89	0.19	57,57,57,57	0
54	MG	DA	3213	1/1	0.89	0.20	40,40,40,40	0
54	MG	BA	3462	1/1	0.89	0.26	77,77,77,77	0
54	MG	DA	3283	1/1	0.89	0.10	81,81,81,81	0
54	MG	AA	1823	1/1	0.89	0.42	104,104,104,104	0
54	MG	DA	3186	1/1	0.89	0.11	23,23,23,23	0
54	MG	BA	3477	1/1	0.89	0.12	60,60,60,60	0
54	MG	BA	3071	1/1	0.89	0.19	74,74,74,74	0
54	MG	CD	119	1/1	0.89	0.05	95,95,95,95	0
54	MG	CD	113	1/1	0.89	0.14	80,80,80,80	0
54	MG	CA	1702	1/1	0.89	0.20	71,71,71,71	0
54	MG	BA	3181	1/1	0.89	0.30	97,97,97,97	0
54	MG	DA	3363	1/1	0.89	0.35	113,113,113,113	0
54	MG	DA	3474	1/1	0.90	0.49	89,89,89,89	0
54	MG	CA	1810	1/1	0.90	0.16	92,92,92,92	0
54	MG	BA	3309	1/1	0.90	0.11	61,61,61,61	0
54	MG	CA	1784	1/1	0.90	0.31	85,85,85,85	0
54	MG	AA	1608	1/1	0.90	0.42	67,67,67,67	0
54	MG	DA	3691	1/1	0.90	0.29	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	206	1/1	0.90	0.17	57,57,57,57	0
54	MG	CA	1864	1/1	0.90	0.30	90,90,90,90	0
54	MG	BA	3147	1/1	0.90	0.38	83,83,83,83	0
54	MG	AA	1964	1/1	0.90	0.43	103,103,103,103	0
54	MG	BA	3033	1/1	0.90	0.19	45,45,45,45	0
54	MG	BB	214	1/1	0.90	0.26	91,91,91,91	0
54	MG	BB	211	1/1	0.90	0.14	80,80,80,80	0
54	MG	CA	1870	1/1	0.90	0.20	69,69,69,69	0
54	MG	BA	3263	1/1	0.90	0.24	65,65,65,65	0
54	MG	CA	1712	1/1	0.90	0.11	65,65,65,65	0
54	MG	CA	1825	1/1	0.90	0.08	106,106,106,106	0
54	MG	DA	3498	1/1	0.90	0.17	107,107,107,107	0
54	MG	BA	3247	1/1	0.90	0.17	63,63,63,63	0
54	MG	DA	3019	1/1	0.90	0.26	68,68,68,68	0
54	MG	BA	3560	1/1	0.90	0.18	48,48,48,48	0
54	MG	DA	2988	1/1	0.90	0.24	42,42,42,42	0
54	MG	AS	102	1/1	0.90	0.22	90,90,90,90	0
54	MG	AA	1928	1/1	0.90	0.35	117,117,117,117	0
54	MG	AA	1834	1/1	0.90	0.49	183,183,183,183	0
54	MG	AA	1706	1/1	0.90	0.34	143,143,143,143	0
54	MG	CA	1907	1/1	0.90	0.09	83,83,83,83	0
54	MG	AA	1896	1/1	0.90	0.28	93,93,93,93	0
54	MG	BA	3010	1/1	0.90	0.27	55,55,55,55	0
54	MG	DA	2955	1/1	0.90	0.32	39,39,39,39	0
54	MG	DA	3464	1/1	0.90	0.49	93,93,93,93	0
54	MG	AA	1848	1/1	0.90	0.12	70,70,70,70	0
54	MG	AA	1724	1/1	0.90	0.43	82,82,82,82	0
54	MG	DA	3274	1/1	0.90	0.20	82,82,82,82	0
54	MG	AA	1619	1/1	0.90	0.41	55,55,55,55	0
54	MG	DA	3305	1/1	0.90	0.11	63,63,63,63	0
54	MG	DA	3776	1/1	0.90	0.12	71,71,71,71	0
54	MG	CA	1683	1/1	0.90	0.21	70,70,70,70	0
54	MG	CA	1786	1/1	0.90	0.20	86,86,86,86	0
54	MG	DA	3383	1/1	0.90	0.16	32,32,32,32	0
54	MG	DA	3718	1/1	0.90	0.23	88,88,88,88	0
54	MG	DA	3578	1/1	0.90	0.23	89,89,89,89	0
54	MG	BA	3301	1/1	0.90	0.23	92,92,92,92	0
54	MG	DA	3338	1/1	0.90	0.16	52,52,52,52	0
54	MG	CK	201	1/1	0.90	0.24	90,90,90,90	0
54	MG	DA	3116	1/1	0.90	0.46	93,93,93,93	0
54	MG	AA	1991	1/1	0.90	0.07	70,70,70,70	0
54	MG	DA	3060	1/1	0.90	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1781	1/1	0.90	0.36	98,98,98,98	0
54	MG	A1	101	1/1	0.90	0.11	102,102,102,102	0
54	MG	AA	1877	1/1	0.90	0.30	80,80,80,80	0
54	MG	DA	3289	1/1	0.90	0.24	63,63,63,63	0
54	MG	DA	3367	1/1	0.90	0.06	60,60,60,60	0
54	MG	AA	1751	1/1	0.90	0.21	73,73,73,73	0
54	MG	AA	1922	1/1	0.90	0.27	94,94,94,94	0
54	MG	BA	3089	1/1	0.90	0.32	74,74,74,74	0
54	MG	AA	1691	1/1	0.90	0.27	62,62,62,62	0
54	MG	DA	3350	1/1	0.90	0.33	109,109,109,109	0
54	MG	CA	1818	1/1	0.90	0.26	92,92,92,92	0
54	MG	DA	3769	1/1	0.90	0.21	73,73,73,73	0
54	MG	DA	3419	1/1	0.90	0.49	92,92,92,92	0
54	MG	DB	207	1/1	0.90	0.17	99,99,99,99	0
54	MG	BA	3353	1/1	0.90	0.20	75,75,75,75	0
54	MG	CA	1854	1/1	0.90	0.27	79,79,79,79	0
54	MG	BA	3220	1/1	0.90	0.16	59,59,59,59	0
54	MG	AA	2023	1/1	0.90	0.06	112,112,112,112	0
54	MG	CA	1974	1/1	0.90	0.09	88,88,88,88	0
54	MG	CA	1805	1/1	0.90	0.07	89,89,89,89	0
54	MG	DA	3169	1/1	0.90	0.35	59,59,59,59	0
54	MG	CA	1623	1/1	0.90	0.40	71,71,71,71	0
54	MG	AA	1637	1/1	0.90	0.51	82,82,82,82	0
54	MG	BA	3100	1/1	0.90	0.15	70,70,70,70	0
54	MG	BA	3209	1/1	0.90	0.18	58,58,58,58	0
54	MG	BA	3436	1/1	0.90	0.18	66,66,66,66	0
54	MG	AA	1638	1/1	0.90	0.24	61,61,61,61	0
54	MG	DA	3065	1/1	0.90	0.08	46,46,46,46	0
54	MG	DA	3322	1/1	0.90	0.30	79,79,79,79	0
54	MG	BA	3302	1/1	0.90	0.07	61,61,61,61	0
54	MG	BA	3173	1/1	0.90	0.10	68,68,68,68	0
54	MG	BA	3440	1/1	0.90	0.15	100,100,100,100	0
54	MG	DA	3593	1/1	0.90	0.16	97,97,97,97	0
54	MG	CA	1973	1/1	0.90	0.10	116,116,116,116	0
54	MG	DA	3339	1/1	0.90	0.29	67,67,67,67	0
54	MG	CA	1726	1/1	0.90	0.14	54,54,54,54	0
54	MG	DA	3172	1/1	0.90	0.19	53,53,53,53	0
54	MG	DA	3024	1/1	0.90	0.10	39,39,39,39	0
54	MG	DA	3473	1/1	0.90	0.33	87,87,87,87	0
54	MG	BA	2905	1/1	0.90	0.08	136,136,136,136	0
54	MG	AA	1886	1/1	0.90	0.25	102,102,102,102	0
54	MG	AA	1997	1/1	0.90	0.30	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AC	103	1/1	0.90	0.10	86,86,86,86	0
54	MG	DA	3595	1/1	0.90	0.11	80,80,80,80	0
54	MG	CA	1777	1/1	0.90	0.20	71,71,71,71	0
54	MG	DA	3262	1/1	0.90	0.20	84,84,84,84	0
54	MG	CA	1945	1/1	0.90	0.09	77,77,77,77	0
54	MG	CA	1696	1/1	0.90	0.22	84,84,84,84	0
54	MG	CA	1687	1/1	0.90	0.09	76,76,76,76	0
54	MG	BA	3409	1/1	0.90	0.16	100,100,100,100	0
54	MG	BA	3131	1/1	0.90	0.32	76,76,76,76	0
54	MG	DA	2925	1/1	0.90	0.41	38,38,38,38	0
54	MG	AA	1731	1/1	0.90	0.30	63,63,63,63	0
54	MG	BA	3404	1/1	0.90	0.07	82,82,82,82	0
54	MG	BA	3451	1/1	0.91	0.16	64,64,64,64	0
54	MG	CA	1721	1/1	0.91	0.18	60,60,60,60	0
54	MG	AA	1797	1/1	0.91	0.18	75,75,75,75	0
54	MG	AC	104	1/1	0.91	0.09	85,85,85,85	0
54	MG	BA	3145	1/1	0.91	0.18	74,74,74,74	0
54	MG	CA	1747	1/1	0.91	0.33	93,93,93,93	0
54	MG	DA	3345	1/1	0.91	0.29	80,80,80,80	0
54	MG	DA	3311	1/1	0.91	0.31	100,100,100,100	0
54	MG	DA	3292	1/1	0.91	0.22	83,83,83,83	0
54	MG	DA	3556	1/1	0.91	0.28	183,183,183,183	0
54	MG	BA	3551	1/1	0.91	0.10	98,98,98,98	0
54	MG	DA	3543	1/1	0.91	0.18	96,96,96,96	0
54	MG	AA	1867	1/1	0.91	0.36	85,85,85,85	0
54	MG	AA	2006	1/1	0.91	0.09	86,86,86,86	0
54	MG	AA	2025	1/1	0.91	0.35	71,71,71,71	0
54	MG	AA	1632	1/1	0.91	0.21	72,72,72,72	0
54	MG	CA	1738	1/1	0.91	0.16	88,88,88,88	0
54	MG	DA	3022	1/1	0.91	0.25	36,36,36,36	0
54	MG	CA	1930	1/1	0.91	0.19	96,96,96,96	0
54	MG	DA	3483	1/1	0.91	0.14	66,66,66,66	0
54	MG	CA	1649	1/1	0.91	0.45	86,86,86,86	0
54	MG	AA	1935	1/1	0.91	0.21	94,94,94,94	0
54	MG	AA	1651	1/1	0.91	0.33	60,60,60,60	0
54	MG	CA	1892	1/1	0.91	0.07	99,99,99,99	0
54	MG	BA	3231	1/1	0.91	0.12	68,68,68,68	0
54	MG	DA	3331	1/1	0.91	0.14	70,70,70,70	0
54	MG	DA	3268	1/1	0.91	0.46	73,73,73,73	0
54	MG	DA	3087	1/1	0.91	0.23	41,41,41,41	0
54	MG	AA	1772	1/1	0.91	0.28	71,71,71,71	0
54	MG	DA	3745	1/1	0.91	0.21	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	2922	1/1	0.91	0.20	46,46,46,46	0
54	MG	BA	3054	1/1	0.91	0.15	66,66,66,66	0
54	MG	DA	3649	1/1	0.91	0.16	62,62,62,62	0
54	MG	BA	3012	1/1	0.91	0.16	56,56,56,56	0
54	MG	DA	3137	1/1	0.91	0.15	51,51,51,51	0
54	MG	AA	1995	1/1	0.91	0.20	142,142,142,142	0
54	MG	BA	3323	1/1	0.91	0.10	58,58,58,58	0
54	MG	DH	204	1/1	0.91	0.22	77,77,77,77	0
54	MG	DA	3034	1/1	0.91	0.28	75,75,75,75	0
54	MG	DA	3758	1/1	0.91	0.10	65,65,65,65	0
54	MG	CA	1889	1/1	0.91	0.25	89,89,89,89	0
54	MG	AA	1890	1/1	0.91	0.10	72,72,72,72	0
54	MG	BA	3127	1/1	0.91	0.29	64,64,64,64	0
54	MG	BD	302	1/1	0.91	0.11	69,69,69,69	0
54	MG	DA	3500	1/1	0.91	0.12	60,60,60,60	0
54	MG	AA	1816	1/1	0.91	0.26	107,107,107,107	0
54	MG	CD	120	1/1	0.91	0.09	110,110,110,110	0
54	MG	CT	201	1/1	0.91	0.21	76,76,76,76	0
54	MG	CC	104	1/1	0.91	0.10	65,65,65,65	0
54	MG	BA	3415	1/1	0.91	0.22	89,89,89,89	0
54	MG	AA	1948	1/1	0.91	0.08	82,82,82,82	0
54	MG	BA	3099	1/1	0.91	0.05	42,42,42,42	0
54	MG	DA	3596	1/1	0.91	0.28	110,110,110,110	0
54	MG	BA	3017	1/1	0.91	0.16	48,48,48,48	0
54	MG	CA	1978	1/1	0.91	0.19	73,73,73,73	0
54	MG	BA	3339	1/1	0.91	0.07	74,74,74,74	0
54	MG	DA	3746	1/1	0.91	0.09	64,64,64,64	0
54	MG	BA	3094	1/1	0.91	0.14	84,84,84,84	0
54	MG	BA	3367	1/1	0.91	0.27	111,111,111,111	0
54	MG	BA	3564	1/1	0.91	0.07	77,77,77,77	0
54	MG	CA	1842	1/1	0.91	0.09	112,112,112,112	0
54	MG	DA	3415	1/1	0.91	0.24	77,77,77,77	0
54	MG	CH	202	1/1	0.91	0.17	72,72,72,72	0
54	MG	AA	2008	1/1	0.91	0.10	69,69,69,69	0
54	MG	AA	1702	1/1	0.91	0.20	71,71,71,71	0
54	MG	DA	3650	1/1	0.91	0.15	76,76,76,76	0
54	MG	BA	3091	1/1	0.91	0.16	59,59,59,59	0
54	MG	AA	1782	1/1	0.91	0.24	106,106,106,106	0
54	MG	BA	3408	1/1	0.91	0.08	75,75,75,75	0
54	MG	BA	3034	1/1	0.91	0.19	61,61,61,61	0
54	MG	DA	3792	1/1	0.91	0.22	157,157,157,157	0
54	MG	CC	101	1/1	0.91	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1916	1/1	0.91	0.17	114,114,114,114	0
54	MG	BA	3543	1/1	0.91	0.09	72,72,72,72	0
54	MG	AA	1898	1/1	0.91	0.18	102,102,102,102	0
54	MG	CA	1927	1/1	0.91	0.27	86,86,86,86	0
54	MG	CA	1662	1/1	0.91	0.18	61,61,61,61	0
54	MG	DA	3489	1/1	0.91	0.52	79,79,79,79	0
54	MG	BA	3136	1/1	0.91	0.38	111,111,111,111	0
54	MG	CW	203	1/1	0.91	0.13	111,111,111,111	0
54	MG	DA	3528	1/1	0.91	0.37	80,80,80,80	0
54	MG	DA	2972	1/1	0.91	0.30	41,41,41,41	0
54	MG	DA	3766	1/1	0.91	0.16	81,81,81,81	0
54	MG	DA	3466	1/1	0.91	0.33	85,85,85,85	0
54	MG	CA	1756	1/1	0.91	0.09	57,57,57,57	0
54	MG	BA	3174	1/1	0.91	0.29	90,90,90,90	0
54	MG	BA	3331	1/1	0.91	0.27	80,80,80,80	0
54	MG	DA	3112	1/1	0.91	0.19	55,55,55,55	0
54	MG	DA	3212	1/1	0.91	0.16	113,113,113,113	0
54	MG	DE	302	1/1	0.91	0.10	51,51,51,51	0
54	MG	DA	3634	1/1	0.91	0.44	63,63,63,63	0
54	MG	AA	1829	1/1	0.91	0.19	109,109,109,109	0
54	MG	DA	3724	1/1	0.91	0.37	106,106,106,106	0
54	MG	CA	1691	1/1	0.91	0.16	56,56,56,56	0
54	MG	CA	1604	1/1	0.91	0.27	66,66,66,66	0
54	MG	DA	3145	1/1	0.91	0.32	64,64,64,64	0
54	MG	BA	3399	1/1	0.91	0.12	82,82,82,82	0
54	MG	BA	3452	1/1	0.91	0.15	57,57,57,57	0
54	MG	BA	3395	1/1	0.91	0.07	60,60,60,60	0
54	MG	BA	2982	1/1	0.91	0.34	61,61,61,61	0
54	MG	DA	3375	1/1	0.91	0.09	57,57,57,57	0
54	MG	AA	1709	1/1	0.91	0.34	130,130,130,130	0
54	MG	DA	3462	1/1	0.91	0.25	80,80,80,80	0
54	MG	DG	201	1/1	0.91	0.17	76,76,76,76	0
54	MG	BA	3411	1/1	0.91	0.15	71,71,71,71	0
54	MG	BA	3306	1/1	0.91	0.50	105,105,105,105	0
54	MG	AA	2017	1/1	0.91	0.15	92,92,92,92	0
54	MG	CA	1650	1/1	0.91	0.13	52,52,52,52	0
54	MG	DA	3263	1/1	0.91	0.37	78,78,78,78	0
54	MG	DA	3520	1/1	0.91	0.22	90,90,90,90	0
54	MG	AA	1885	1/1	0.91	0.15	113,113,113,113	0
54	MG	CA	1877	1/1	0.91	0.21	62,62,62,62	0
54	MG	AA	1987	1/1	0.91	0.10	86,86,86,86	0
54	MG	AA	1747	1/1	0.91	0.29	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3392	1/1	0.91	0.15	66,66,66,66	0
54	MG	AA	1966	1/1	0.91	0.24	85,85,85,85	0
54	MG	DA	3692	1/1	0.91	0.11	60,60,60,60	0
54	MG	AA	1694	1/1	0.91	0.27	66,66,66,66	0
54	MG	BA	3383	1/1	0.91	0.17	63,63,63,63	0
54	MG	DA	3006	1/1	0.91	0.29	51,51,51,51	0
54	MG	DA	3094	1/1	0.91	0.22	49,49,49,49	0
54	MG	BA	3189	1/1	0.91	0.28	76,76,76,76	0
54	MG	AA	1865	1/1	0.91	0.53	140,140,140,140	0
54	MG	DA	3700	1/1	0.91	0.14	75,75,75,75	0
54	MG	DA	2984	1/1	0.91	0.40	46,46,46,46	0
54	MG	DA	3763	1/1	0.91	0.14	71,71,71,71	0
54	MG	DA	3687	1/1	0.91	0.23	78,78,78,78	0
54	MG	DA	3494	1/1	0.91	0.11	110,110,110,110	0
54	MG	D7	101	1/1	0.91	0.16	55,55,55,55	0
54	MG	AA	1894	1/1	0.91	0.42	103,103,103,103	0
54	MG	BA	3168	1/1	0.91	0.18	65,65,65,65	0
54	MG	AA	1743	1/1	0.91	0.08	75,75,75,75	0
54	MG	AA	1746	1/1	0.91	0.24	81,81,81,81	0
54	MG	CA	1792	1/1	0.91	0.30	84,84,84,84	0
54	MG	DA	3075	1/1	0.91	0.13	43,43,43,43	0
54	MG	DA	3739	1/1	0.91	0.17	127,127,127,127	0
54	MG	CA	1910	1/1	0.91	0.21	130,130,130,130	0
54	MG	DB	202	1/1	0.92	0.09	87,87,87,87	0
54	MG	DA	3080	1/1	0.92	0.08	23,23,23,23	0
54	MG	BA	3498	1/1	0.92	0.21	59,59,59,59	0
54	MG	CA	1694	1/1	0.92	0.20	55,55,55,55	0
54	MG	BA	3208	1/1	0.92	0.16	68,68,68,68	0
54	MG	BA	3284	1/1	0.92	0.14	74,74,74,74	0
54	MG	BA	3250	1/1	0.92	0.29	93,93,93,93	0
54	MG	DA	3056	1/1	0.92	0.32	71,71,71,71	0
54	MG	CA	1931	1/1	0.92	0.20	84,84,84,84	0
54	MG	DA	3176	1/1	0.92	0.31	57,57,57,57	0
54	MG	BA	3222	1/1	0.92	0.31	88,88,88,88	0
54	MG	BA	3186	1/1	0.92	0.14	83,83,83,83	0
54	MG	AA	2003	1/1	0.92	0.15	128,128,128,128	0
54	MG	DA	3744	1/1	0.92	0.15	68,68,68,68	0
54	MG	DA	3064	1/1	0.92	0.31	72,72,72,72	0
54	MG	DA	3403	1/1	0.92	0.23	69,69,69,69	0
54	MG	DA	3499	1/1	0.92	0.30	87,87,87,87	0
54	MG	DA	3693	1/1	0.92	0.21	56,56,56,56	0
54	MG	DA	3100	1/1	0.92	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3004	1/1	0.92	0.29	52,52,52,52	0
54	MG	DA	3298	1/1	0.92	0.23	70,70,70,70	0
54	MG	DA	3366	1/1	0.92	0.14	50,50,50,50	0
54	MG	CA	1660	1/1	0.92	0.25	74,74,74,74	0
54	MG	DA	3067	1/1	0.92	0.29	47,47,47,47	0
54	MG	BA	3271	1/1	0.92	0.11	59,59,59,59	0
54	MG	AA	1769	1/1	0.92	0.22	80,80,80,80	0
54	MG	BA	3442	1/1	0.92	0.06	89,89,89,89	0
54	MG	BA	3427	1/1	0.92	0.07	80,80,80,80	0
54	MG	AA	1847	1/1	0.92	0.18	91,91,91,91	0
54	MG	AA	1602	1/1	0.92	0.26	53,53,53,53	0
54	MG	DA	3020	1/1	0.92	0.28	58,58,58,58	0
54	MG	BA	3215	1/1	0.92	0.16	58,58,58,58	0
54	MG	AA	1951	1/1	0.92	0.18	79,79,79,79	0
54	MG	BA	2975	1/1	0.92	0.20	40,40,40,40	0
54	MG	CK	202	1/1	0.92	0.12	87,87,87,87	0
54	MG	BA	3021	1/1	0.92	0.13	35,35,35,35	0
54	MG	DA	3092	1/1	0.92	0.16	39,39,39,39	0
54	MG	CH	201	1/1	0.92	0.16	82,82,82,82	0
54	MG	DA	3736	1/1	0.92	0.14	76,76,76,76	0
54	MG	DA	3258	1/1	0.92	0.11	76,76,76,76	0
54	MG	DA	3619	1/1	0.92	0.12	52,52,52,52	0
54	MG	BA	3492	1/1	0.92	0.07	86,86,86,86	0
54	MG	AA	1631	1/1	0.92	0.29	60,60,60,60	0
54	MG	DA	3223	1/1	0.92	0.16	64,64,64,64	0
54	MG	BA	3203	1/1	0.92	0.21	64,64,64,64	0
54	MG	BA	3237	1/1	0.92	0.13	82,82,82,82	0
54	MG	BA	3352	1/1	0.92	0.13	112,112,112,112	0
54	MG	AA	1926	1/1	0.92	0.16	102,102,102,102	0
54	MG	AA	1671	1/1	0.92	0.16	66,66,66,66	0
54	MG	DA	3411	1/1	0.92	0.29	86,86,86,86	0
54	MG	CA	1834	1/1	0.92	0.27	103,103,103,103	0
54	MG	BA	3363	1/1	0.92	0.16	79,79,79,79	0
54	MG	DA	3171	1/1	0.92	0.16	45,45,45,45	0
54	MG	CA	1757	1/1	0.92	0.12	79,79,79,79	0
54	MG	BA	3233	1/1	0.92	0.13	84,84,84,84	0
54	MG	CA	1871	1/1	0.92	0.08	73,73,73,73	0
54	MG	BA	3279	1/1	0.92	0.27	85,85,85,85	0
54	MG	AA	1749	1/1	0.92	0.28	72,72,72,72	0
54	MG	BA	3087	1/1	0.92	0.20	72,72,72,72	0
54	MG	AC	102	1/1	0.92	0.35	85,85,85,85	0
54	MG	BB	205	1/1	0.92	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3060	1/1	0.92	0.09	35,35,35,35	0
54	MG	AL	201	1/1	0.92	0.15	79,79,79,79	0
54	MG	BA	3073	1/1	0.92	0.29	71,71,71,71	0
54	MG	DA	3014	1/1	0.92	0.44	68,68,68,68	0
54	MG	DA	3525	1/1	0.92	0.24	78,78,78,78	0
54	MG	DA	3156	1/1	0.92	0.56	95,95,95,95	0
54	MG	DA	2993	1/1	0.92	0.40	57,57,57,57	0
54	MG	DA	3194	1/1	0.92	0.29	65,65,65,65	0
54	MG	AA	1673	1/1	0.92	0.09	91,91,91,91	0
54	MG	BA	3289	1/1	0.92	0.25	71,71,71,71	0
54	MG	DA	3035	1/1	0.92	0.26	55,55,55,55	0
54	MG	DA	3173	1/1	0.92	0.11	57,57,57,57	0
54	MG	DA	3097	1/1	0.92	0.31	63,63,63,63	0
54	MG	DA	3044	1/1	0.92	0.17	61,61,61,61	0
54	MG	BA	3500	1/1	0.92	0.07	64,64,64,64	0
54	MG	BA	3194	1/1	0.92	0.25	87,87,87,87	0
54	MG	DA	3076	1/1	0.92	0.19	38,38,38,38	0
54	MG	BA	3406	1/1	0.92	0.10	68,68,68,68	0
54	MG	DA	2963	1/1	0.92	0.35	45,45,45,45	0
54	MG	CA	1906	1/1	0.92	0.13	107,107,107,107	0
54	MG	DA	3264	1/1	0.92	0.37	73,73,73,73	0
54	MG	CQ	101	1/1	0.92	0.06	71,71,71,71	0
54	MG	CA	1822	1/1	0.92	0.12	92,92,92,92	0
54	MG	CA	1644	1/1	0.92	0.20	52,52,52,52	0
54	MG	DA	3571	1/1	0.92	0.24	81,81,81,81	0
54	MG	DA	3456	1/1	0.92	0.45	92,92,92,92	0
54	MG	CA	1621	1/1	0.92	0.21	49,49,49,49	0
54	MG	DB	209	1/1	0.92	0.43	81,81,81,81	0
54	MG	AA	1860	1/1	0.92	0.28	93,93,93,93	0
54	MG	DA	3315	1/1	0.92	0.40	81,81,81,81	0
54	MG	DA	3599	1/1	0.92	0.47	80,80,80,80	0
54	MG	DA	3662	1/1	0.92	0.29	78,78,78,78	0
54	MG	DA	3762	1/1	0.92	0.14	119,119,119,119	0
54	MG	BA	3384	1/1	0.92	0.13	76,76,76,76	0
54	MG	BA	3548	1/1	0.92	0.20	81,81,81,81	0
54	MG	AA	1609	1/1	0.92	0.40	71,71,71,71	0
54	MG	AA	1611	1/1	0.92	0.34	63,63,63,63	0
54	MG	DA	3717	1/1	0.92	0.22	88,88,88,88	0
54	MG	BA	3095	1/1	0.92	0.16	52,52,52,52	0
54	MG	DA	3005	1/1	0.92	0.43	69,69,69,69	0
54	MG	AH	202	1/1	0.92	0.06	80,80,80,80	0
54	MG	CA	1804	1/1	0.92	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3448	1/1	0.92	0.38	103,103,103,103	0
54	MG	BA	3238	1/1	0.92	0.24	85,85,85,85	0
54	MG	BA	3336	1/1	0.92	0.20	88,88,88,88	0
54	MG	BA	3235	1/1	0.92	0.10	59,59,59,59	0
54	MG	DA	3503	1/1	0.92	0.18	74,74,74,74	0
54	MG	BA	3511	1/1	0.92	0.10	140,140,140,140	0
54	MG	DA	3144	1/1	0.92	0.15	43,43,43,43	0
54	MG	DA	3486	1/1	0.92	0.18	90,90,90,90	0
54	MG	DA	3161	1/1	0.92	0.29	60,60,60,60	0
54	MG	CA	1779	1/1	0.92	0.20	104,104,104,104	0
54	MG	AA	1690	1/1	0.92	0.12	91,91,91,91	0
54	MG	DA	3535	1/1	0.92	0.26	79,79,79,79	0
54	MG	BA	3485	1/1	0.92	0.16	69,69,69,69	0
54	MG	DA	3240	1/1	0.92	0.18	58,58,58,58	0
54	MG	CD	112	1/1	0.93	0.09	85,85,85,85	0
54	MG	DA	3637	1/1	0.93	0.18	74,74,74,74	0
54	MG	BA	3392	1/1	0.93	0.11	70,70,70,70	0
54	MG	DA	3393	1/1	0.93	0.15	60,60,60,60	0
54	MG	BA	3449	1/1	0.93	0.13	76,76,76,76	0
54	MG	BA	3193	1/1	0.93	0.25	80,80,80,80	0
54	MG	DA	3665	1/1	0.93	0.32	88,88,88,88	0
54	MG	AA	2010	1/1	0.93	0.12	83,83,83,83	0
54	MG	BA	3178	1/1	0.93	0.21	60,60,60,60	0
54	MG	BA	3355	1/1	0.93	0.13	64,64,64,64	0
54	MG	DA	2951	1/1	0.93	0.34	54,54,54,54	0
54	MG	DA	3248	1/1	0.93	0.28	56,56,56,56	0
54	MG	AA	1869	1/1	0.93	0.10	83,83,83,83	0
54	MG	DA	3083	1/1	0.93	0.18	56,56,56,56	0
54	MG	BE	307	1/1	0.93	0.17	84,84,84,84	0
54	MG	CA	1656	1/1	0.93	0.27	98,98,98,98	0
54	MG	CA	1667	1/1	0.93	0.04	93,93,93,93	0
54	MG	DA	3728	1/1	0.93	0.51	123,123,123,123	0
54	MG	BA	3430	1/1	0.93	0.11	90,90,90,90	0
54	MG	CA	1605	1/1	0.93	0.18	39,39,39,39	0
54	MG	CA	1934	1/1	0.93	0.30	94,94,94,94	0
54	MG	BA	2958	1/1	0.93	0.20	44,44,44,44	0
54	MG	DA	3749	1/1	0.93	0.17	102,102,102,102	0
54	MG	BA	2971	1/1	0.93	0.13	57,57,57,57	0
54	MG	DA	2949	1/1	0.93	0.21	35,35,35,35	0
54	MG	AA	1626	1/1	0.93	0.14	55,55,55,55	0
54	MG	AA	1793	1/1	0.93	0.13	73,73,73,73	0
54	MG	DA	3337	1/1	0.93	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3401	1/1	0.93	0.08	182,182,182,182	0
54	MG	BA	3361	1/1	0.93	0.12	72,72,72,72	0
54	MG	BA	3469	1/1	0.93	0.22	70,70,70,70	0
54	MG	DA	3698	1/1	0.93	0.32	89,89,89,89	0
54	MG	DR	202	1/1	0.93	0.15	102,102,102,102	0
54	MG	DA	3504	1/1	0.93	0.09	81,81,81,81	0
54	MG	AA	2009	1/1	0.93	0.08	71,71,71,71	0
54	MG	BA	3132	1/1	0.93	0.34	90,90,90,90	0
54	MG	DA	3756	1/1	0.93	0.15	57,57,57,57	0
54	MG	BA	3013	1/1	0.93	0.22	60,60,60,60	0
54	MG	DA	3241	1/1	0.93	0.16	56,56,56,56	0
54	MG	CA	1767	1/1	0.93	0.23	68,68,68,68	0
54	MG	DA	3562	1/1	0.93	0.32	75,75,75,75	0
54	MG	CA	1657	1/1	0.93	0.32	96,96,96,96	0
54	MG	AA	1780	1/1	0.93	0.29	95,95,95,95	0
54	MG	DA	3639	1/1	0.93	0.28	71,71,71,71	0
54	MG	BA	3290	1/1	0.93	0.10	91,91,91,91	0
54	MG	BA	3213	1/1	0.93	0.10	61,61,61,61	0
54	MG	CA	1785	1/1	0.93	0.21	69,69,69,69	0
54	MG	DA	3552	1/1	0.93	0.12	130,130,130,130	0
54	MG	BA	3260	1/1	0.93	0.21	77,77,77,77	0
54	MG	CA	1809	1/1	0.93	0.20	78,78,78,78	0
54	MG	BA	3307	1/1	0.93	0.17	79,79,79,79	0
54	MG	BA	3488	1/1	0.93	0.24	96,96,96,96	0
54	MG	BA	3070	1/1	0.93	0.19	53,53,53,53	0
54	MG	AA	1684	1/1	0.93	0.24	74,74,74,74	0
54	MG	DA	3200	1/1	0.93	0.27	52,52,52,52	0
54	MG	CA	1632	1/1	0.93	0.28	62,62,62,62	0
54	MG	DA	3090	1/1	0.93	0.13	43,43,43,43	0
54	MG	CA	1816	1/1	0.93	0.26	65,65,65,65	0
54	MG	DA	3517	1/1	0.93	0.18	81,81,81,81	0
54	MG	DA	3197	1/1	0.93	0.29	64,64,64,64	0
54	MG	DA	3429	1/1	0.93	0.16	83,83,83,83	0
54	MG	BA	3429	1/1	0.93	0.15	56,56,56,56	0
54	MG	BA	3527	1/1	0.93	0.08	63,63,63,63	0
54	MG	AA	1889	1/1	0.93	0.08	68,68,68,68	0
54	MG	DA	3045	1/1	0.93	0.34	57,57,57,57	0
54	MG	CA	1614	1/1	0.93	0.10	67,67,67,67	0
54	MG	DA	3332	1/1	0.93	0.26	67,67,67,67	0
54	MG	CA	1791	1/1	0.93	0.10	85,85,85,85	0
54	MG	DA	3544	1/1	0.93	0.23	87,87,87,87	0
54	MG	CA	1776	1/1	0.93	0.17	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3438	1/1	0.93	0.18	83,83,83,83	0
54	MG	DA	2964	1/1	0.93	0.17	21,21,21,21	0
54	MG	DA	3209	1/1	0.93	0.13	57,57,57,57	0
54	MG	BA	3023	1/1	0.93	0.22	52,52,52,52	0
54	MG	BB	221	1/1	0.93	0.11	106,106,106,106	0
54	MG	DA	3215	1/1	0.93	0.26	58,58,58,58	0
54	MG	BB	212	1/1	0.93	0.20	81,81,81,81	0
54	MG	DA	2958	1/1	0.93	0.11	46,46,46,46	0
54	MG	DA	3302	1/1	0.93	0.30	76,76,76,76	0
54	MG	AA	1871	1/1	0.93	0.07	117,117,117,117	0
54	MG	BA	3103	1/1	0.93	0.18	53,53,53,53	0
54	MG	AA	1820	1/1	0.93	0.13	98,98,98,98	0
54	MG	CA	1845	1/1	0.93	0.27	82,82,82,82	0
54	MG	DA	3244	1/1	0.93	0.30	64,64,64,64	0
54	MG	BB	207	1/1	0.93	0.21	69,69,69,69	0
54	MG	DA	3297	1/1	0.93	0.25	54,54,54,54	0
54	MG	CA	1979	1/1	0.93	0.13	104,104,104,104	0
54	MG	BA	3268	1/1	0.93	0.33	87,87,87,87	0
54	MG	BA	3086	1/1	0.93	0.22	50,50,50,50	0
54	MG	CA	1772	1/1	0.93	0.20	82,82,82,82	0
54	MG	AA	1969	1/1	0.93	0.11	89,89,89,89	0
54	MG	DB	217	1/1	0.93	0.32	122,122,122,122	0
54	MG	DA	3146	1/1	0.93	0.15	54,54,54,54	0
54	MG	AA	1809	1/1	0.93	0.30	85,85,85,85	0
54	MG	BA	3475	1/1	0.93	0.11	73,73,73,73	0
54	MG	DA	3541	1/1	0.93	0.23	54,54,54,54	0
54	MG	DA	3725	1/1	0.93	0.24	132,132,132,132	0
54	MG	BA	3552	1/1	0.93	0.13	76,76,76,76	0
54	MG	CA	1969	1/1	0.93	0.20	86,86,86,86	0
54	MG	DA	3246	1/1	0.93	0.51	101,101,101,101	0
54	MG	CA	1729	1/1	0.93	0.15	61,61,61,61	0
54	MG	BA	3078	1/1	0.93	0.23	57,57,57,57	0
54	MG	BA	3016	1/1	0.93	0.23	63,63,63,63	0
54	MG	CA	1982	1/1	0.93	0.06	80,80,80,80	0
54	MG	AA	1949	1/1	0.93	0.20	122,122,122,122	0
54	MG	CD	123	1/1	0.93	0.09	81,81,81,81	0
54	MG	DA	3516	1/1	0.93	0.18	99,99,99,99	0
54	MG	CA	1669	1/1	0.93	0.30	71,71,71,71	0
54	MG	BA	2996	1/1	0.93	0.28	68,68,68,68	0
54	MG	CA	1627	1/1	0.93	0.28	50,50,50,50	0
54	MG	BA	3529	1/1	0.93	0.12	88,88,88,88	0
54	MG	AA	1839	1/1	0.93	0.09	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1764	1/1	0.93	0.11	83,83,83,83	0
54	MG	BA	3210	1/1	0.93	0.05	54,54,54,54	0
54	MG	AA	1783	1/1	0.93	0.39	90,90,90,90	0
54	MG	CA	1858	1/1	0.93	0.26	109,109,109,109	0
54	MG	CA	1855	1/1	0.93	0.17	99,99,99,99	0
54	MG	AA	1873	1/1	0.93	0.09	80,80,80,80	0
54	MG	AA	1923	1/1	0.93	0.16	85,85,85,85	0
54	MG	DA	3093	1/1	0.93	0.33	53,53,53,53	0
54	MG	DA	3015	1/1	0.93	0.17	41,41,41,41	0
54	MG	DA	3420	1/1	0.93	0.10	91,91,91,91	0
54	MG	AA	1733	1/1	0.93	0.21	102,102,102,102	0
54	MG	DA	3683	1/1	0.93	0.25	100,100,100,100	0
54	MG	BA	3397	1/1	0.93	0.16	47,47,47,47	0
54	MG	DA	3079	1/1	0.93	0.37	59,59,59,59	0
54	MG	DA	3222	1/1	0.93	0.50	83,83,83,83	0
54	MG	CA	1719	1/1	0.93	0.17	56,56,56,56	0
54	MG	BA	3101	1/1	0.93	0.18	56,56,56,56	0
54	MG	BA	3506	1/1	0.93	0.10	77,77,77,77	0
54	MG	CA	1795	1/1	0.93	0.08	78,78,78,78	0
54	MG	DA	3214	1/1	0.93	0.37	72,72,72,72	0
54	MG	AA	1801	1/1	0.93	0.47	94,94,94,94	0
54	MG	BA	3486	1/1	0.93	0.24	90,90,90,90	0
54	MG	BU	201	1/1	0.93	0.37	75,75,75,75	0
54	MG	AA	1689	1/1	0.93	0.16	93,93,93,93	0
54	MG	DA	3433	1/1	0.93	0.24	87,87,87,87	0
54	MG	DA	3368	1/1	0.93	0.34	87,87,87,87	0
54	MG	AA	1914	1/1	0.93	0.18	109,109,109,109	0
54	MG	BA	3350	1/1	0.93	0.15	63,63,63,63	0
54	MG	CA	1928	1/1	0.93	0.06	122,122,122,122	0
54	MG	DA	3003	1/1	0.93	0.28	62,62,62,62	0
54	MG	DA	3048	1/1	0.93	0.21	67,67,67,67	0
54	MG	DA	3174	1/1	0.93	0.10	66,66,66,66	0
54	MG	DA	3095	1/1	0.93	0.15	46,46,46,46	0
54	MG	BA	3005	1/1	0.93	0.28	70,70,70,70	0
54	MG	CA	1648	1/1	0.93	0.37	79,79,79,79	0
54	MG	AA	1760	1/1	0.93	0.37	91,91,91,91	0
54	MG	CA	1972	1/1	0.93	0.15	61,61,61,61	0
54	MG	BA	3540	1/1	0.93	0.14	69,69,69,69	0
54	MG	BA	2991	1/1	0.93	0.26	76,76,76,76	0
54	MG	BA	2998	1/1	0.94	0.09	51,51,51,51	0
54	MG	BA	3106	1/1	0.94	0.34	80,80,80,80	0
54	MG	BA	3126	1/1	0.94	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3059	1/1	0.94	0.34	58,58,58,58	0
54	MG	DA	3232	1/1	0.94	0.22	67,67,67,67	0
54	MG	AA	1656	1/1	0.94	0.13	71,71,71,71	0
54	MG	CA	1881	1/1	0.94	0.14	105,105,105,105	0
54	MG	CA	1716	1/1	0.94	0.13	110,110,110,110	0
54	MG	CA	1603	1/1	0.94	0.35	56,56,56,56	0
54	MG	DA	3449	1/1	0.94	0.16	95,95,95,95	0
54	MG	DA	3561	1/1	0.94	0.25	59,59,59,59	0
54	MG	CA	1865	1/1	0.94	0.10	85,85,85,85	0
54	MG	CA	1836	1/1	0.94	0.24	58,58,58,58	0
54	MG	CA	1844	1/1	0.94	0.21	76,76,76,76	0
54	MG	BA	3200	1/1	0.94	0.26	90,90,90,90	0
54	MG	DB	226	1/1	0.94	0.11	84,84,84,84	0
54	MG	CD	111	1/1	0.94	0.10	87,87,87,87	0
54	MG	AA	1766	1/1	0.94	0.08	69,69,69,69	0
54	MG	CA	1863	1/1	0.94	0.09	121,121,121,121	0
54	MG	DA	3476	1/1	0.94	0.11	68,68,68,68	0
54	MG	DA	3153	1/1	0.94	0.12	51,51,51,51	0
54	MG	BA	3372	1/1	0.94	0.16	53,53,53,53	0
54	MG	DA	3189	1/1	0.94	0.20	68,68,68,68	0
54	MG	BA	2945	1/1	0.94	0.20	39,39,39,39	0
54	MG	DO	205	1/1	0.94	0.19	90,90,90,90	0
54	MG	DA	3310	1/1	0.94	0.36	66,66,66,66	0
54	MG	AA	1677	1/1	0.94	0.34	63,63,63,63	0
54	MG	AA	1837	1/1	0.94	0.13	59,59,59,59	0
54	MG	D1	202	1/1	0.94	0.13	75,75,75,75	0
54	MG	BA	3454	1/1	0.94	0.10	100,100,100,100	0
54	MG	DB	205	1/1	0.94	0.21	69,69,69,69	0
54	MG	DA	3220	1/1	0.94	0.17	59,59,59,59	0
54	MG	CA	1678	1/1	0.94	0.15	66,66,66,66	0
54	MG	BA	3531	1/1	0.94	0.07	75,75,75,75	0
54	MG	DA	3522	1/1	0.94	0.08	66,66,66,66	0
54	MG	DA	3707	1/1	0.94	0.12	64,64,64,64	0
54	MG	CA	1646	1/1	0.94	0.11	53,53,53,53	0
54	MG	DA	3558	1/1	0.94	0.24	65,65,65,65	0
54	MG	AA	1916	1/1	0.94	0.15	93,93,93,93	0
54	MG	DA	3082	1/1	0.94	0.44	67,67,67,67	0
54	MG	AA	1981	1/1	0.94	0.06	115,115,115,115	0
54	MG	CA	1819	1/1	0.94	0.11	61,61,61,61	0
54	MG	AA	1708	1/1	0.94	0.25	70,70,70,70	0
54	MG	D6	101	1/1	0.94	0.70	98,98,98,98	0
54	MG	AA	1901	1/1	0.94	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1941	1/1	0.94	0.09	93,93,93,93	0
54	MG	AA	1907	1/1	0.94	0.12	106,106,106,106	0
54	MG	BA	3455	1/1	0.94	0.20	78,78,78,78	0
54	MG	AA	1982	1/1	0.94	0.20	126,126,126,126	0
54	MG	AA	1620	1/1	0.94	0.25	67,67,67,67	0
54	MG	DA	2910	1/1	0.94	0.26	25,25,25,25	0
54	MG	DA	3580	1/1	0.94	0.24	96,96,96,96	0
54	MG	AA	1790	1/1	0.94	0.20	53,53,53,53	0
54	MG	CA	1725	1/1	0.94	0.26	54,54,54,54	0
54	MG	CA	1606	1/1	0.94	0.26	70,70,70,70	0
54	MG	AA	1968	1/1	0.94	0.07	80,80,80,80	0
54	MG	BA	2909	1/1	0.94	0.07	66,66,66,66	0
54	MG	AA	1722	1/1	0.94	0.39	68,68,68,68	0
54	MG	AA	1601	1/1	0.94	0.20	42,42,42,42	0
54	MG	DA	3225	1/1	0.94	0.17	45,45,45,45	0
54	MG	BA	3305	1/1	0.94	0.12	62,62,62,62	0
54	MG	BA	3369	1/1	0.94	0.07	73,73,73,73	0
54	MG	BA	3426	1/1	0.94	0.07	43,43,43,43	0
54	MG	CA	1740	1/1	0.94	0.11	104,104,104,104	0
54	MG	DT	102	1/1	0.94	0.16	64,64,64,64	0
54	MG	DA	3555	1/1	0.94	0.28	81,81,81,81	0
54	MG	BA	3009	1/1	0.94	0.19	57,57,57,57	0
54	MG	BA	3435	1/1	0.94	0.09	59,59,59,59	0
54	MG	BA	3159	1/1	0.94	0.24	61,61,61,61	0
54	MG	DA	2952	1/1	0.94	0.35	39,39,39,39	0
54	MG	AA	1649	1/1	0.94	0.18	84,84,84,84	0
54	MG	CA	1963	1/1	0.94	0.24	145,145,145,145	0
54	MG	DA	3253	1/1	0.94	0.34	67,67,67,67	0
54	MG	C1	101	1/1	0.94	0.08	65,65,65,65	0
54	MG	AA	1723	1/1	0.94	0.14	89,89,89,89	0
54	MG	CA	1745	1/1	0.94	0.13	74,74,74,74	0
54	MG	DA	3183	1/1	0.94	0.29	56,56,56,56	0
54	MG	DA	3406	1/1	0.94	0.17	82,82,82,82	0
54	MG	CA	1812	1/1	0.94	0.14	86,86,86,86	0
54	MG	BA	3314	1/1	0.94	0.20	76,76,76,76	0
54	MG	CA	1620	1/1	0.94	0.30	69,69,69,69	0
54	MG	BA	3225	1/1	0.94	0.09	49,49,49,49	0
54	MG	CW	202	1/1	0.94	0.10	108,108,108,108	0
54	MG	DA	3250	1/1	0.94	0.18	44,44,44,44	0
54	MG	BA	3204	1/1	0.94	0.28	76,76,76,76	0
54	MG	CA	1622	1/1	0.94	0.25	68,68,68,68	0
54	MG	BA	3133	1/1	0.94	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3031	1/1	0.94	0.08	82,82,82,82	0
54	MG	DA	3051	1/1	0.94	0.11	29,29,29,29	0
54	MG	BA	3059	1/1	0.94	0.26	59,59,59,59	0
54	MG	DA	3663	1/1	0.94	0.16	76,76,76,76	0
54	MG	DA	3436	1/1	0.94	0.11	72,72,72,72	0
54	MG	AA	1705	1/1	0.94	0.12	77,77,77,77	0
54	MG	DA	3575	1/1	0.94	0.14	80,80,80,80	0
54	MG	AA	1642	1/1	0.94	0.20	64,64,64,64	0
54	MG	DA	3371	1/1	0.94	0.23	79,79,79,79	0
54	MG	DA	3108	1/1	0.94	0.29	58,58,58,58	0
54	MG	DA	3592	1/1	0.94	0.32	78,78,78,78	0
54	MG	BA	3508	1/1	0.94	0.07	90,90,90,90	0
54	MG	CA	1643	1/1	0.94	0.28	66,66,66,66	0
54	MG	DA	3643	1/1	0.94	0.15	82,82,82,82	0
54	MG	DA	3077	1/1	0.94	0.26	48,48,48,48	0
54	MG	BA	3332	1/1	0.94	0.11	60,60,60,60	0
54	MG	BA	3513	1/1	0.94	0.13	77,77,77,77	0
54	MG	CA	1901	1/1	0.94	0.19	103,103,103,103	0
54	MG	CA	1665	1/1	0.94	0.13	84,84,84,84	0
54	MG	DA	3140	1/1	0.94	0.06	26,26,26,26	0
54	MG	BA	3303	1/1	0.94	0.11	41,41,41,41	0
54	MG	CA	1640	1/1	0.94	0.09	53,53,53,53	0
54	MG	DA	3444	1/1	0.94	0.27	86,86,86,86	0
54	MG	DA	3088	1/1	0.94	0.33	56,56,56,56	0
54	MG	AA	1707	1/1	0.94	0.17	64,64,64,64	0
54	MG	BA	3153	1/1	0.94	0.20	71,71,71,71	0
54	MG	DA	3055	1/1	0.94	0.18	41,41,41,41	0
54	MG	DA	3245	1/1	0.94	0.13	47,47,47,47	0
54	MG	DA	2935	1/1	0.94	0.18	33,33,33,33	0
54	MG	BA	3374	1/1	0.94	0.12	39,39,39,39	0
54	MG	DA	3277	1/1	0.94	0.27	59,59,59,59	0
54	MG	BA	3170	1/1	0.94	0.26	72,72,72,72	0
54	MG	CA	1611	1/1	0.94	0.23	42,42,42,42	0
54	MG	BA	2939	1/1	0.94	0.33	47,47,47,47	0
54	MG	AA	1794	1/1	0.94	0.27	93,93,93,93	0
54	MG	DA	3463	1/1	0.94	0.65	155,155,155,155	0
54	MG	DA	3360	1/1	0.94	0.06	67,67,67,67	0
54	MG	DA	3655	1/1	0.94	0.16	94,94,94,94	0
54	MG	CA	1682	1/1	0.94	0.18	67,67,67,67	0
54	MG	DA	3041	1/1	0.94	0.27	49,49,49,49	0
54	MG	AA	1612	1/1	0.94	0.42	68,68,68,68	0
54	MG	BA	3135	1/1	0.94	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1771	1/1	0.94	0.25	70,70,70,70	0
54	MG	DA	3386	1/1	0.94	0.40	75,75,75,75	0
54	MG	AA	1952	1/1	0.94	0.07	76,76,76,76	0
54	MG	AA	1906	1/1	0.94	0.32	86,86,86,86	0
54	MG	CA	1924	1/1	0.94	0.08	98,98,98,98	0
54	MG	BA	3580	1/1	0.94	0.11	89,89,89,89	0
54	MG	DA	3646	1/1	0.94	0.22	87,87,87,87	0
54	MG	CA	1853	1/1	0.94	0.15	101,101,101,101	0
54	MG	DA	3121	1/1	0.94	0.09	56,56,56,56	0
54	MG	BA	2995	1/1	0.94	0.32	52,52,52,52	0
54	MG	AA	1676	1/1	0.94	0.18	96,96,96,96	0
54	MG	BA	3001	1/1	0.94	0.15	40,40,40,40	0
54	MG	DU	204	1/1	0.94	0.25	99,99,99,99	0
54	MG	BA	3432	1/1	0.94	0.19	115,115,115,115	0
54	MG	DA	3551	1/1	0.94	0.09	68,68,68,68	0
54	MG	AA	1748	1/1	0.94	0.14	85,85,85,85	0
54	MG	DB	210	1/1	0.94	0.10	114,114,114,114	0
54	MG	CA	1932	1/1	0.94	0.16	94,94,94,94	0
54	MG	BA	3546	1/1	0.94	0.20	102,102,102,102	0
54	MG	DA	3269	1/1	0.94	0.46	99,99,99,99	0
54	MG	DA	3133	1/1	0.94	0.23	64,64,64,64	0
54	MG	BA	3169	1/1	0.94	0.24	60,60,60,60	0
54	MG	BA	3371	1/1	0.94	0.11	55,55,55,55	0
54	MG	DA	3325	1/1	0.94	0.13	64,64,64,64	0
54	MG	DB	219	1/1	0.94	0.21	77,77,77,77	0
54	MG	AA	1643	1/1	0.94	0.10	124,124,124,124	0
54	MG	CA	1699	1/1	0.94	0.21	66,66,66,66	0
54	MG	BA	3165	1/1	0.94	0.10	46,46,46,46	0
54	MG	BA	3565	1/1	0.94	0.08	99,99,99,99	0
54	MG	CA	1909	1/1	0.94	0.11	74,74,74,74	0
54	MG	AA	1653	1/1	0.94	0.07	107,107,107,107	0
54	MG	BA	3344	1/1	0.94	0.07	69,69,69,69	0
54	MG	AA	1990	1/1	0.94	0.12	97,97,97,97	0
54	MG	DA	3732	1/1	0.94	0.28	94,94,94,94	0
54	MG	BA	3138	1/1	0.94	0.20	85,85,85,85	0
54	MG	BA	3457	1/1	0.94	0.17	80,80,80,80	0
54	MG	CD	126	1/1	0.94	0.10	82,82,82,82	0
54	MG	BA	3322	1/1	0.94	0.20	72,72,72,72	0
54	MG	BA	3398	1/1	0.94	0.12	131,131,131,131	0
54	MG	BA	2936	1/1	0.94	0.23	50,50,50,50	0
54	MG	BA	3036	1/1	0.94	0.18	41,41,41,41	0
54	MG	DA	3408	1/1	0.94	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1744	1/1	0.94	0.20	77,77,77,77	0
54	MG	DA	3705	1/1	0.94	0.25	97,97,97,97	0
54	MG	CA	1737	1/1	0.94	0.05	132,132,132,132	0
54	MG	AA	1662	1/1	0.94	0.27	100,100,100,100	0
54	MG	BA	3160	1/1	0.94	0.26	65,65,65,65	0
54	MG	CA	1637	1/1	0.94	0.25	70,70,70,70	0
54	MG	BA	3329	1/1	0.95	0.14	69,69,69,69	0
54	MG	DA	3395	1/1	0.95	0.20	71,71,71,71	0
54	MG	DA	3344	1/1	0.95	0.11	44,44,44,44	0
54	MG	AA	1623	1/1	0.95	0.34	53,53,53,53	0
54	MG	BA	3084	1/1	0.95	0.33	83,83,83,83	0
54	MG	AA	1954	1/1	0.95	0.35	108,108,108,108	0
54	MG	AA	1628	1/1	0.95	0.45	69,69,69,69	0
54	MG	AA	1683	1/1	0.95	0.28	60,60,60,60	0
54	MG	BA	2980	1/1	0.95	0.28	53,53,53,53	0
54	MG	AA	1729	1/1	0.95	0.16	87,87,87,87	0
54	MG	DA	3461	1/1	0.95	0.18	66,66,66,66	0
54	MG	DA	3482	1/1	0.95	0.06	43,43,43,43	0
54	MG	AA	1650	1/1	0.95	0.14	74,74,74,74	0
54	MG	CA	1846	1/1	0.95	0.28	129,129,129,129	0
54	MG	BA	3502	1/1	0.95	0.12	91,91,91,91	0
54	MG	CA	1652	1/1	0.95	0.21	49,49,49,49	0
54	MG	BA	2949	1/1	0.95	0.35	62,62,62,62	0
54	MG	BA	3219	1/1	0.95	0.04	48,48,48,48	0
54	MG	DA	3427	1/1	0.95	0.07	65,65,65,65	0
54	MG	DE	303	1/1	0.95	0.13	20,20,20,20	0
54	MG	AA	1745	1/1	0.95	0.17	67,67,67,67	0
54	MG	DA	3104	1/1	0.95	0.35	79,79,79,79	0
54	MG	BA	2935	1/1	0.95	0.22	46,46,46,46	0
54	MG	DA	3530	1/1	0.95	0.27	59,59,59,59	0
54	MG	BA	3037	1/1	0.95	0.19	61,61,61,61	0
54	MG	DA	3353	1/1	0.95	0.22	70,70,70,70	0
54	MG	DA	2936	1/1	0.95	0.38	48,48,48,48	0
54	MG	CA	1770	1/1	0.95	0.13	85,85,85,85	0
54	MG	DA	3352	1/1	0.95	0.10	66,66,66,66	0
54	MG	DA	3676	1/1	0.95	0.28	131,131,131,131	0
54	MG	BA	3317	1/1	0.95	0.14	63,63,63,63	0
54	MG	BA	3079	1/1	0.95	0.13	59,59,59,59	0
54	MG	BA	3465	1/1	0.95	0.10	92,92,92,92	0
54	MG	BA	3446	1/1	0.95	0.15	74,74,74,74	0
54	MG	AA	2022	1/1	0.95	0.09	117,117,117,117	0
54	MG	DA	3587	1/1	0.95	0.41	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1808	1/1	0.95	0.12	92,92,92,92	0
54	MG	DA	2914	1/1	0.95	0.19	19,19,19,19	0
54	MG	DA	2909	1/1	0.95	0.33	25,25,25,25	0
54	MG	DA	3105	1/1	0.95	0.39	56,56,56,56	0
54	MG	DA	3249	1/1	0.95	0.32	65,65,65,65	0
54	MG	BA	3555	1/1	0.95	0.38	119,119,119,119	0
54	MG	DA	2966	1/1	0.95	0.25	37,37,37,37	0
54	MG	CW	201	1/1	0.95	0.26	67,67,67,67	0
54	MG	AA	2021	1/1	0.95	0.08	108,108,108,108	0
54	MG	DA	3233	1/1	0.95	0.19	51,51,51,51	0
54	MG	AA	1976	1/1	0.95	0.30	86,86,86,86	0
54	MG	AW	201	1/1	0.95	0.20	108,108,108,108	0
54	MG	DA	3390	1/1	0.95	0.33	72,72,72,72	0
54	MG	D5	101	1/1	0.95	0.16	54,54,54,54	0
54	MG	DA	3047	1/1	0.95	0.21	50,50,50,50	0
54	MG	DA	3333	1/1	0.95	0.16	50,50,50,50	0
54	MG	DA	3343	1/1	0.95	0.18	86,86,86,86	0
54	MG	CA	1830	1/1	0.95	0.18	135,135,135,135	0
54	MG	DA	3678	1/1	0.95	0.19	69,69,69,69	0
54	MG	D1	203	1/1	0.95	0.10	84,84,84,84	0
54	MG	DA	3149	1/1	0.95	0.32	56,56,56,56	0
54	MG	DA	3273	1/1	0.95	0.05	39,39,39,39	0
54	MG	BA	3166	1/1	0.95	0.09	57,57,57,57	0
54	MG	BB	220	1/1	0.95	0.26	80,80,80,80	0
54	MG	DA	3514	1/1	0.95	0.15	66,66,66,66	0
54	MG	CA	1778	1/1	0.95	0.08	55,55,55,55	0
54	MG	CA	1613	1/1	0.95	0.35	60,60,60,60	0
54	MG	DA	3524	1/1	0.95	0.16	54,54,54,54	0
54	MG	CA	1655	1/1	0.95	0.24	68,68,68,68	0
54	MG	BA	3269	1/1	0.95	0.10	90,90,90,90	0
54	MG	DA	3431	1/1	0.95	0.07	51,51,51,51	0
54	MG	D3	103	1/1	0.95	0.31	76,76,76,76	0
54	MG	BA	3324	1/1	0.95	0.24	87,87,87,87	0
54	MG	AA	1815	1/1	0.95	0.15	62,62,62,62	0
54	MG	BA	3327	1/1	0.95	0.10	65,65,65,65	0
54	MG	AA	1900	1/1	0.95	0.13	102,102,102,102	0
54	MG	DA	3721	1/1	0.95	0.09	50,50,50,50	0
54	MG	BA	3046	1/1	0.95	0.16	29,29,29,29	0
54	MG	DB	224	1/1	0.95	0.20	109,109,109,109	0
54	MG	BA	3577	1/1	0.95	0.09	80,80,80,80	0
54	MG	DA	3136	1/1	0.95	0.27	53,53,53,53	0
54	MG	CA	1915	1/1	0.95	0.19	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1712	1/1	0.95	0.08	50,50,50,50	0
54	MG	DA	3767	1/1	0.95	0.11	61,61,61,61	0
54	MG	AA	2002	1/1	0.95	0.10	81,81,81,81	0
54	MG	CA	1602	1/1	0.95	0.20	29,29,29,29	0
54	MG	DA	3039	1/1	0.95	0.16	48,48,48,48	0
54	MG	AA	1770	1/1	0.95	0.20	71,71,71,71	0
54	MG	BA	3422	1/1	0.95	0.17	83,83,83,83	0
54	MG	DA	3675	1/1	0.95	0.35	104,104,104,104	0
54	MG	BA	3195	1/1	0.95	0.08	124,124,124,124	0
54	MG	DA	3711	1/1	0.95	0.27	102,102,102,102	0
54	MG	DA	3002	1/1	0.95	0.45	62,62,62,62	0
54	MG	DA	2918	1/1	0.95	0.32	28,28,28,28	0
54	MG	BA	3308	1/1	0.95	0.32	78,78,78,78	0
54	MG	DA	3031	1/1	0.95	0.18	53,53,53,53	0
54	MG	AA	1838	1/1	0.95	0.20	77,77,77,77	0
54	MG	BA	3053	1/1	0.95	0.22	43,43,43,43	0
54	MG	DA	3635	1/1	0.95	0.20	101,101,101,101	0
54	MG	AA	1692	1/1	0.95	0.20	75,75,75,75	0
54	MG	DA	3152	1/1	0.95	0.20	52,52,52,52	0
54	MG	CA	1727	1/1	0.95	0.11	131,131,131,131	0
54	MG	BA	3441	1/1	0.95	0.09	144,144,144,144	0
54	MG	DA	3301	1/1	0.95	0.17	86,86,86,86	0
54	MG	DA	3187	1/1	0.95	0.26	64,64,64,64	0
54	MG	BA	3285	1/1	0.95	0.14	79,79,79,79	0
54	MG	DA	3607	1/1	0.95	0.19	62,62,62,62	0
54	MG	AA	2039	1/1	0.95	0.07	64,64,64,64	0
54	MG	AA	1925	1/1	0.95	0.13	87,87,87,87	0
54	MG	BA	2937	1/1	0.95	0.22	53,53,53,53	0
54	MG	BA	3007	1/1	0.95	0.21	51,51,51,51	0
54	MG	BA	2979	1/1	0.95	0.25	60,60,60,60	0
54	MG	AA	1727	1/1	0.95	0.27	104,104,104,104	0
54	MG	BA	3061	1/1	0.95	0.14	70,70,70,70	0
54	MG	DA	3618	1/1	0.95	0.48	113,113,113,113	0
54	MG	BA	3528	1/1	0.95	0.09	88,88,88,88	0
54	MG	BA	3085	1/1	0.95	0.08	40,40,40,40	0
54	MG	CA	1672	1/1	0.95	0.15	70,70,70,70	0
54	MG	DA	2982	1/1	0.95	0.28	47,47,47,47	0
54	MG	DA	3475	1/1	0.95	0.09	56,56,56,56	0
54	MG	BA	3487	1/1	0.95	0.07	74,74,74,74	0
54	MG	AA	1607	1/1	0.95	0.20	68,68,68,68	0
54	MG	CA	1902	1/1	0.95	0.10	46,46,46,46	0
54	MG	BA	3557	1/1	0.95	0.12	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1717	1/1	0.95	0.24	77,77,77,77	0
54	MG	DB	211	1/1	0.95	0.20	78,78,78,78	0
54	MG	DA	3508	1/1	0.95	0.34	73,73,73,73	0
54	MG	CX	102	1/1	0.95	0.06	104,104,104,104	0
54	MG	DA	3679	1/1	0.95	0.10	68,68,68,68	0
54	MG	CA	1943	1/1	0.95	0.10	110,110,110,110	0
54	MG	DA	3154	1/1	0.95	0.27	56,56,56,56	0
54	MG	AA	1939	1/1	0.95	0.09	118,118,118,118	0
54	MG	CA	1629	1/1	0.95	0.31	85,85,85,85	0
54	MG	BA	3257	1/1	0.95	0.07	63,63,63,63	0
54	MG	DA	3141	1/1	0.95	0.23	78,78,78,78	0
54	MG	AA	1791	1/1	0.95	0.09	68,68,68,68	0
54	MG	DA	3267	1/1	0.95	0.34	76,76,76,76	0
54	MG	BA	3142	1/1	0.95	0.18	90,90,90,90	0
54	MG	CA	1832	1/1	0.95	0.12	79,79,79,79	0
54	MG	BA	2993	1/1	0.95	0.38	52,52,52,52	0
54	MG	DA	3713	1/1	0.95	0.20	144,144,144,144	0
54	MG	AA	1633	1/1	0.95	0.30	79,79,79,79	0
54	MG	DA	3421	1/1	0.95	0.46	85,85,85,85	0
54	MG	DA	3590	1/1	0.95	0.24	93,93,93,93	0
54	MG	AA	2005	1/1	0.95	0.08	96,96,96,96	0
54	MG	DA	3057	1/1	0.95	0.30	68,68,68,68	0
54	MG	AA	1775	1/1	0.95	0.35	88,88,88,88	0
54	MG	BA	3050	1/1	0.95	0.29	67,67,67,67	0
54	MG	CA	1666	1/1	0.95	0.12	67,67,67,67	0
54	MG	AA	1920	1/1	0.95	0.07	115,115,115,115	0
54	MG	CA	1705	1/1	0.95	0.20	84,84,84,84	0
54	MG	BD	301	1/1	0.95	0.27	65,65,65,65	0
54	MG	DA	3615	1/1	0.95	0.19	78,78,78,78	0
54	MG	DA	3564	1/1	0.95	0.14	49,49,49,49	0
54	MG	DA	3103	1/1	0.95	0.17	76,76,76,76	0
54	MG	BA	3578	1/1	0.95	0.11	98,98,98,98	0
54	MG	BA	3158	1/1	0.95	0.10	39,39,39,39	0
54	MG	DA	3135	1/1	0.95	0.28	48,48,48,48	0
54	MG	BA	2989	1/1	0.95	0.39	60,60,60,60	0
54	MG	CA	1913	1/1	0.95	0.15	101,101,101,101	0
54	MG	CA	1688	1/1	0.95	0.38	76,76,76,76	0
54	MG	BA	3072	1/1	0.95	0.08	48,48,48,48	0
54	MG	AA	1974	1/1	0.95	0.20	96,96,96,96	0
54	MG	BA	3458	1/1	0.95	0.12	76,76,76,76	0
54	MG	BA	3014	1/1	0.95	0.28	49,49,49,49	0
54	MG	DA	3361	1/1	0.95	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1603	1/1	0.95	0.39	54,54,54,54	0
54	MG	DA	3510	1/1	0.95	0.13	43,43,43,43	0
54	MG	BA	3048	1/1	0.95	0.05	41,41,41,41	0
54	MG	DA	3586	1/1	0.95	0.28	72,72,72,72	0
54	MG	DA	3567	1/1	0.95	0.38	91,91,91,91	0
54	MG	CA	1787	1/1	0.95	0.27	147,147,147,147	0
54	MG	BA	2968	1/1	0.95	0.12	29,29,29,29	0
54	MG	BA	3043	1/1	0.95	0.07	51,51,51,51	0
54	MG	CA	1917	1/1	0.95	0.10	95,95,95,95	0
54	MG	CA	1940	1/1	0.95	0.14	112,112,112,112	0
54	MG	BA	3461	1/1	0.95	0.09	66,66,66,66	0
54	MG	AA	1915	1/1	0.95	0.20	172,172,172,172	0
54	MG	BE	302	1/1	0.95	0.12	85,85,85,85	0
54	MG	AA	1681	1/1	0.95	0.09	43,43,43,43	0
54	MG	CA	1686	1/1	0.95	0.16	62,62,62,62	0
54	MG	BE	303	1/1	0.95	0.06	45,45,45,45	0
54	MG	BA	2981	1/1	0.95	0.21	58,58,58,58	0
54	MG	DA	3577	1/1	0.95	0.09	80,80,80,80	0
54	MG	DA	3113	1/1	0.95	0.18	43,43,43,43	0
54	MG	BA	3088	1/1	0.95	0.15	49,49,49,49	0
54	MG	BA	3128	1/1	0.96	0.31	72,72,72,72	0
54	MG	DA	3412	1/1	0.96	0.27	105,105,105,105	0
54	MG	DA	3155	1/1	0.96	0.22	40,40,40,40	0
54	MG	DA	3307	1/1	0.96	0.36	74,74,74,74	0
54	MG	AA	1983	1/1	0.96	0.23	104,104,104,104	0
54	MG	DA	3042	1/1	0.96	0.20	48,48,48,48	0
54	MG	DA	3179	1/1	0.96	0.35	74,74,74,74	0
54	MG	AA	1739	1/1	0.96	0.15	66,66,66,66	0
54	MG	DA	2919	1/1	0.96	0.25	46,46,46,46	0
54	MG	BA	3494	1/1	0.96	0.10	65,65,65,65	0
54	MG	BA	3109	1/1	0.96	0.22	73,73,73,73	0
54	MG	DR	201	1/1	0.96	0.07	77,77,77,77	0
54	MG	AW	202	1/1	0.96	0.12	59,59,59,59	0
54	MG	BA	3542	1/1	0.96	0.08	78,78,78,78	0
54	MG	BA	2984	1/1	0.96	0.16	48,48,48,48	0
54	MG	CA	1615	1/1	0.96	0.14	40,40,40,40	0
54	MG	AA	1678	1/1	0.96	0.22	57,57,57,57	0
54	MG	BA	3287	1/1	0.96	0.31	79,79,79,79	0
54	MG	DA	2939	1/1	0.96	0.29	45,45,45,45	0
54	MG	BA	3239	1/1	0.96	0.14	49,49,49,49	0
54	MG	DA	2921	1/1	0.96	0.13	32,32,32,32	0
54	MG	CA	1829	1/1	0.96	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1605	1/1	0.96	0.33	61,61,61,61	0
54	MG	AA	1821	1/1	0.96	0.14	141,141,141,141	0
54	MG	D1	204	1/1	0.96	0.21	71,71,71,71	0
54	MG	BA	3008	1/1	0.96	0.17	95,95,95,95	0
54	MG	CA	1947	1/1	0.96	0.27	205,205,205,205	0
54	MG	DA	3796	1/1	0.96	0.09	82,82,82,82	0
54	MG	DA	3708	1/1	0.96	0.22	152,152,152,152	0
54	MG	DA	2962	1/1	0.96	0.24	33,33,33,33	0
54	MG	AA	1763	1/1	0.96	0.35	74,74,74,74	0
54	MG	AA	1836	1/1	0.96	0.12	58,58,58,58	0
54	MG	BA	2978	1/1	0.96	0.21	47,47,47,47	0
54	MG	DO	201	1/1	0.96	0.08	55,55,55,55	0
54	MG	AA	1665	1/1	0.96	0.25	59,59,59,59	0
54	MG	AA	1832	1/1	0.96	0.23	91,91,91,91	0
54	MG	AA	2035	1/1	0.96	0.34	86,86,86,86	0
54	MG	DA	3070	1/1	0.96	0.28	40,40,40,40	0
54	MG	CD	104	1/1	0.96	0.04	83,83,83,83	0
54	MG	BA	3566	1/1	0.96	0.11	56,56,56,56	0
54	MG	CD	102	1/1	0.96	0.07	99,99,99,99	0
54	MG	DA	3729	1/1	0.96	0.11	73,73,73,73	0
54	MG	BA	2965	1/1	0.96	0.07	30,30,30,30	0
54	MG	DA	2923	1/1	0.96	0.19	18,18,18,18	0
54	MG	DA	2922	1/1	0.96	0.16	17,17,17,17	0
54	MG	DA	3073	1/1	0.96	0.42	73,73,73,73	0
54	MG	DH	203	1/1	0.96	0.07	65,65,65,65	0
54	MG	CA	1874	1/1	0.96	0.07	144,144,144,144	0
54	MG	DA	2933	1/1	0.96	0.29	31,31,31,31	0
54	MG	BA	3425	1/1	0.96	0.05	98,98,98,98	0
54	MG	BA	3077	1/1	0.96	0.11	46,46,46,46	0
54	MG	DA	3576	1/1	0.96	0.10	109,109,109,109	0
54	MG	DA	3086	1/1	0.96	0.19	61,61,61,61	0
54	MG	DA	3340	1/1	0.96	0.17	76,76,76,76	0
54	MG	DA	3032	1/1	0.96	0.21	40,40,40,40	0
54	MG	DA	3123	1/1	0.96	0.23	66,66,66,66	0
54	MG	BA	3496	1/1	0.96	0.11	73,73,73,73	0
54	MG	DA	3532	1/1	0.96	0.33	87,87,87,87	0
54	MG	BA	3481	1/1	0.96	0.10	80,80,80,80	0
54	MG	BA	3243	1/1	0.96	0.06	49,49,49,49	0
54	MG	CA	1807	1/1	0.96	0.08	71,71,71,71	0
54	MG	BA	3024	1/1	0.96	0.22	40,40,40,40	0
54	MG	AA	1967	1/1	0.96	0.13	84,84,84,84	0
54	MG	BA	3346	1/1	0.96	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1902	1/1	0.96	0.11	107,107,107,107	0
54	MG	DA	2945	1/1	0.96	0.36	40,40,40,40	0
55	ZN	AQ	102	1/1	0.96	0.14	142,142,142,142	0
54	MG	DA	3210	1/1	0.96	0.32	75,75,75,75	0
54	MG	DA	3038	1/1	0.96	0.23	50,50,50,50	0
54	MG	BA	2960	1/1	0.96	0.21	49,49,49,49	0
54	MG	DA	2995	1/1	0.96	0.35	40,40,40,40	0
54	MG	DA	3394	1/1	0.96	0.26	73,73,73,73	0
54	MG	AA	1627	1/1	0.96	0.32	70,70,70,70	0
54	MG	DA	2950	1/1	0.96	0.34	52,52,52,52	0
54	MG	DA	3638	1/1	0.96	0.14	37,37,37,37	0
54	MG	BA	3115	1/1	0.96	0.23	89,89,89,89	0
54	MG	AA	1811	1/1	0.96	0.04	81,81,81,81	0
54	MG	DA	2926	1/1	0.96	0.12	23,23,23,23	0
54	MG	DA	3365	1/1	0.96	0.16	107,107,107,107	0
54	MG	BB	224	1/1	0.96	0.08	81,81,81,81	0
54	MG	BA	3041	1/1	0.96	0.09	39,39,39,39	0
54	MG	BA	3304	1/1	0.96	0.09	63,63,63,63	0
54	MG	BA	3583	1/1	0.96	0.06	79,79,79,79	0
54	MG	DA	3175	1/1	0.96	0.15	34,34,34,34	0
54	MG	DA	2999	1/1	0.96	0.24	44,44,44,44	0
54	MG	DA	3782	1/1	0.96	0.15	83,83,83,83	0
54	MG	BA	3431	1/1	0.96	0.09	96,96,96,96	0
54	MG	DA	3254	1/1	0.96	0.18	38,38,38,38	0
54	MG	DA	2915	1/1	0.96	0.28	29,29,29,29	0
54	MG	BA	3246	1/1	0.96	0.10	54,54,54,54	0
54	MG	DA	3780	1/1	0.96	0.14	72,72,72,72	0
54	MG	CA	1709	1/1	0.96	0.14	58,58,58,58	0
54	MG	BA	2918	1/1	0.96	0.29	46,46,46,46	0
54	MG	BA	3576	1/1	0.96	0.09	40,40,40,40	0
54	MG	AA	2032	1/1	0.96	0.19	84,84,84,84	0
54	MG	BA	3401	1/1	0.96	0.13	36,36,36,36	0
54	MG	DA	3119	1/1	0.96	0.34	59,59,59,59	0
54	MG	CA	1893	1/1	0.96	0.22	81,81,81,81	0
54	MG	DA	3143	1/1	0.96	0.29	68,68,68,68	0
54	MG	CA	1823	1/1	0.96	0.19	66,66,66,66	0
54	MG	DA	3201	1/1	0.96	0.15	61,61,61,61	0
54	MG	BA	3157	1/1	0.96	0.10	45,45,45,45	0
54	MG	CA	1966	1/1	0.96	0.12	82,82,82,82	0
54	MG	AA	1610	1/1	0.96	0.30	68,68,68,68	0
54	MG	BB	206	1/1	0.96	0.24	85,85,85,85	0
54	MG	CA	1701	1/1	0.96	0.17	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3382	1/1	0.96	0.22	123,123,123,123	0
54	MG	BA	3187	1/1	0.96	0.05	40,40,40,40	0
54	MG	DA	3572	1/1	0.96	0.11	60,60,60,60	0
54	MG	AA	2036	1/1	0.96	0.15	90,90,90,90	0
54	MG	DA	3221	1/1	0.96	0.29	75,75,75,75	0
54	MG	AA	1615	1/1	0.96	0.20	38,38,38,38	0
54	MG	DA	3058	1/1	0.96	0.26	54,54,54,54	0
54	MG	DO	202	1/1	0.96	0.06	42,42,42,42	0
54	MG	DA	2911	1/1	0.96	0.30	34,34,34,34	0
54	MG	D6	102	1/1	0.96	0.41	94,94,94,94	0
54	MG	BA	3188	1/1	0.96	0.19	68,68,68,68	0
54	MG	AA	1757	1/1	0.96	0.14	45,45,45,45	0
54	MG	BA	3421	1/1	0.96	0.28	88,88,88,88	0
54	MG	BE	306	1/1	0.96	0.12	72,72,72,72	0
54	MG	DA	2928	1/1	0.96	0.32	32,32,32,32	0
54	MG	AA	1755	1/1	0.96	0.29	62,62,62,62	0
54	MG	AA	1753	1/1	0.96	0.28	71,71,71,71	0
54	MG	BA	3025	1/1	0.96	0.13	47,47,47,47	0
54	MG	BA	2901	1/1	0.96	0.04	61,61,61,61	0
54	MG	CA	1849	1/1	0.96	0.20	91,91,91,91	0
54	MG	AA	1887	1/1	0.96	0.28	161,161,161,161	0
54	MG	AA	1667	1/1	0.96	0.21	61,61,61,61	0
54	MG	DA	3207	1/1	0.96	0.30	66,66,66,66	0
54	MG	CA	1624	1/1	0.96	0.25	40,40,40,40	0
54	MG	DA	3069	1/1	0.96	0.25	52,52,52,52	0
54	MG	DA	3329	1/1	0.96	0.19	62,62,62,62	0
54	MG	DA	2905	1/1	0.96	0.27	23,23,23,23	0
54	MG	AA	1989	1/1	0.96	0.20	91,91,91,91	0
54	MG	BA	3444	1/1	0.96	0.23	66,66,66,66	0
54	MG	DA	2948	1/1	0.96	0.20	40,40,40,40	0
54	MG	BA	3280	1/1	0.96	0.07	61,61,61,61	0
54	MG	CA	1843	1/1	0.96	0.06	76,76,76,76	0
54	MG	DA	2975	1/1	0.96	0.14	35,35,35,35	0
54	MG	BA	3326	1/1	0.96	0.12	54,54,54,54	0
54	MG	BA	2961	1/1	0.96	0.31	46,46,46,46	0
54	MG	CA	1703	1/1	0.96	0.17	62,62,62,62	0
55	ZN	CG	302	1/1	0.96	0.26	94,94,94,94	0
54	MG	AA	2037	1/1	0.96	0.18	97,97,97,97	0
54	MG	DA	2953	1/1	0.96	0.28	63,63,63,63	0
54	MG	DA	3521	1/1	0.96	0.08	75,75,75,75	0
54	MG	CA	1867	1/1	0.96	0.22	76,76,76,76	0
54	MG	BA	3525	1/1	0.96	0.08	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	2927	1/1	0.96	0.27	32,32,32,32	0
54	MG	CD	105	1/1	0.96	0.06	124,124,124,124	0
54	MG	BA	3471	1/1	0.96	0.21	156,156,156,156	0
54	MG	BA	2964	1/1	0.96	0.23	45,45,45,45	0
54	MG	DA	3062	1/1	0.96	0.27	50,50,50,50	0
54	MG	BT	101	1/1	0.96	0.08	65,65,65,65	0
54	MG	AA	1864	1/1	0.96	0.22	87,87,87,87	0
54	MG	AA	1714	1/1	0.96	0.10	89,89,89,89	0
54	MG	DA	3515	1/1	0.96	0.19	100,100,100,100	0
54	MG	BA	3075	1/1	0.96	0.09	37,37,37,37	0
54	MG	DA	3054	1/1	0.96	0.20	54,54,54,54	0
54	MG	BA	3119	1/1	0.96	0.14	51,51,51,51	0
54	MG	DA	3066	1/1	0.96	0.42	59,59,59,59	0
54	MG	BA	2932	1/1	0.96	0.18	37,37,37,37	0
54	MG	BA	3338	1/1	0.96	0.16	100,100,100,100	0
54	MG	BA	3214	1/1	0.96	0.20	67,67,67,67	0
54	MG	BA	3579	1/1	0.96	0.10	83,83,83,83	0
54	MG	DA	2974	1/1	0.96	0.39	51,51,51,51	0
54	MG	AA	1614	1/1	0.96	0.41	73,73,73,73	0
54	MG	BA	3141	1/1	0.96	0.12	52,52,52,52	0
54	MG	CA	1744	1/1	0.96	0.17	89,89,89,89	0
54	MG	CA	1806	1/1	0.96	0.23	106,106,106,106	0
54	MG	AA	1778	1/1	0.96	0.09	61,61,61,61	0
54	MG	AA	1810	1/1	0.96	0.14	75,75,75,75	0
54	MG	DH	202	1/1	0.96	0.62	98,98,98,98	0
54	MG	BA	2921	1/1	0.96	0.29	41,41,41,41	0
54	MG	AA	1946	1/1	0.96	0.06	82,82,82,82	0
54	MG	DA	3750	1/1	0.96	0.15	57,57,57,57	0
54	MG	CA	1710	1/1	0.96	0.17	53,53,53,53	0
54	MG	DA	3603	1/1	0.96	0.28	86,86,86,86	0
54	MG	DA	3029	1/1	0.96	0.27	34,34,34,34	0
54	MG	AA	1752	1/1	0.96	0.27	75,75,75,75	0
54	MG	DA	2904	1/1	0.96	0.22	22,22,22,22	0
54	MG	BA	3182	1/1	0.96	0.07	41,41,41,41	0
54	MG	CA	1616	1/1	0.96	0.18	68,68,68,68	0
54	MG	B3	102	1/1	0.96	0.14	58,58,58,58	0
54	MG	CA	1731	1/1	0.96	0.07	86,86,86,86	0
54	MG	BA	3004	1/1	0.96	0.17	30,30,30,30	0
54	MG	AC	106	1/1	0.96	0.12	79,79,79,79	0
54	MG	DA	3151	1/1	0.96	0.43	89,89,89,89	0
54	MG	DA	3372	1/1	0.96	0.20	57,57,57,57	0
54	MG	BA	3562	1/1	0.96	0.19	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3260	1/1	0.96	0.12	53,53,53,53	0
54	MG	CA	1936	1/1	0.96	0.08	90,90,90,90	0
54	MG	DA	3391	1/1	0.97	0.19	40,40,40,40	0
54	MG	BA	2962	1/1	0.97	0.12	20,20,20,20	0
54	MG	AA	1943	1/1	0.97	0.09	83,83,83,83	0
54	MG	D2	201	1/1	0.97	0.17	110,110,110,110	0
54	MG	DA	3068	1/1	0.97	0.34	50,50,50,50	0
54	MG	D3	101	1/1	0.97	0.18	48,48,48,48	0
54	MG	DA	3633	1/1	0.97	0.11	62,62,62,62	0
54	MG	DA	2970	1/1	0.97	0.20	49,49,49,49	0
54	MG	DA	3629	1/1	0.97	0.26	72,72,72,72	0
54	MG	DA	3737	1/1	0.97	0.18	88,88,88,88	0
54	MG	AA	1613	1/1	0.97	0.25	53,53,53,53	0
54	MG	DA	3102	1/1	0.97	0.25	49,49,49,49	0
54	MG	DA	3623	1/1	0.97	0.11	81,81,81,81	0
54	MG	CD	101	1/1	0.97	0.16	53,53,53,53	0
54	MG	DA	3426	1/1	0.97	0.18	39,39,39,39	0
54	MG	DD	303	1/1	0.97	0.12	43,43,43,43	0
54	MG	BA	3493	1/1	0.97	0.23	85,85,85,85	0
54	MG	DA	3741	1/1	0.97	0.21	97,97,97,97	0
54	MG	BA	3175	1/1	0.97	0.11	54,54,54,54	0
54	MG	BA	2929	1/1	0.97	0.23	32,32,32,32	0
54	MG	DA	3346	1/1	0.97	0.14	66,66,66,66	0
54	MG	DA	3257	1/1	0.97	0.33	64,64,64,64	0
54	MG	DA	3203	1/1	0.97	0.25	74,74,74,74	0
54	MG	BA	3294	1/1	0.97	0.23	65,65,65,65	0
54	MG	AA	1758	1/1	0.97	0.18	108,108,108,108	0
54	MG	BA	3140	1/1	0.97	0.10	51,51,51,51	0
54	MG	BA	2972	1/1	0.97	0.31	65,65,65,65	0
54	MG	CA	1693	1/1	0.97	0.10	64,64,64,64	0
54	MG	DA	3684	1/1	0.97	0.14	83,83,83,83	0
54	MG	DA	2997	1/1	0.97	0.24	41,41,41,41	0
54	MG	CA	1675	1/1	0.97	0.29	59,59,59,59	0
54	MG	AA	1686	1/1	0.97	0.19	60,60,60,60	0
54	MG	AA	1961	1/1	0.97	0.06	46,46,46,46	0
54	MG	BA	2974	1/1	0.97	0.28	39,39,39,39	0
54	MG	DA	3356	1/1	0.97	0.37	73,73,73,73	0
54	MG	AA	1777	1/1	0.97	0.27	69,69,69,69	0
54	MG	DA	3117	1/1	0.97	0.18	48,48,48,48	0
54	MG	B5	101	1/1	0.97	0.09	46,46,46,46	0
54	MG	BA	3172	1/1	0.97	0.23	72,72,72,72	0
54	MG	BU	203	1/1	0.97	0.06	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3468	1/1	0.97	0.07	73,73,73,73	0
54	MG	BA	3516	1/1	0.97	0.19	56,56,56,56	0
54	MG	DA	3255	1/1	0.97	0.24	53,53,53,53	0
54	MG	DA	2969	1/1	0.97	0.35	36,36,36,36	0
54	MG	BA	2951	1/1	0.97	0.19	38,38,38,38	0
54	MG	AA	1862	1/1	0.97	0.18	77,77,77,77	0
54	MG	BA	2977	1/1	0.97	0.16	33,33,33,33	0
54	MG	DA	3009	1/1	0.97	0.24	41,41,41,41	0
54	MG	DA	2983	1/1	0.97	0.36	34,34,34,34	0
54	MG	BA	2928	1/1	0.97	0.15	46,46,46,46	0
54	MG	BA	3256	1/1	0.97	0.17	64,64,64,64	0
54	MG	DA	3760	1/1	0.97	0.15	206,206,206,206	0
54	MG	AA	1606	1/1	0.97	0.24	55,55,55,55	0
54	MG	DA	2985	1/1	0.97	0.23	27,27,27,27	0
54	MG	DA	3341	1/1	0.97	0.23	64,64,64,64	0
54	MG	DA	3418	1/1	0.97	0.14	59,59,59,59	0
54	MG	DA	3459	1/1	0.97	0.15	64,64,64,64	0
54	MG	AA	1785	1/1	0.97	0.06	78,78,78,78	0
54	MG	DD	301	1/1	0.97	0.28	43,43,43,43	0
54	MG	BB	218	1/1	0.97	0.07	65,65,65,65	0
54	MG	CA	1935	1/1	0.97	0.08	136,136,136,136	0
54	MG	BA	3356	1/1	0.97	0.06	75,75,75,75	0
54	MG	DB	223	1/1	0.97	0.06	104,104,104,104	0
54	MG	CA	1857	1/1	0.97	0.10	80,80,80,80	0
54	MG	BA	3190	1/1	0.97	0.19	78,78,78,78	0
54	MG	CA	1642	1/1	0.97	0.23	48,48,48,48	0
54	MG	BA	2944	1/1	0.97	0.18	29,29,29,29	0
54	MG	DA	3016	1/1	0.97	0.24	23,23,23,23	0
54	MG	CA	1798	1/1	0.97	0.17	112,112,112,112	0
54	MG	AA	1942	1/1	0.97	0.12	128,128,128,128	0
54	MG	DA	3129	1/1	0.97	0.12	57,57,57,57	0
54	MG	BA	2970	1/1	0.97	0.26	32,32,32,32	0
54	MG	CA	1610	1/1	0.97	0.26	51,51,51,51	0
54	MG	DA	3651	1/1	0.97	0.20	98,98,98,98	0
54	MG	CA	1914	1/1	0.97	0.09	36,36,36,36	0
54	MG	BA	3224	1/1	0.97	0.18	54,54,54,54	0
54	MG	BA	3093	1/1	0.97	0.11	65,65,65,65	0
54	MG	CA	1619	1/1	0.97	0.24	73,73,73,73	0
54	MG	CA	1905	1/1	0.97	0.07	92,92,92,92	0
54	MG	BA	3413	1/1	0.97	0.09	92,92,92,92	0
54	MG	BA	3482	1/1	0.97	0.13	101,101,101,101	0
54	MG	CA	1733	1/1	0.97	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	2947	1/1	0.97	0.24	26,26,26,26	0
54	MG	DA	2946	1/1	0.97	0.35	40,40,40,40	0
54	MG	DA	2927	1/1	0.97	0.28	53,53,53,53	0
54	MG	AA	1750	1/1	0.97	0.21	79,79,79,79	0
54	MG	CD	109	1/1	0.97	0.02	89,89,89,89	0
54	MG	DA	2998	1/1	0.97	0.18	44,44,44,44	0
54	MG	AA	1944	1/1	0.97	0.11	111,111,111,111	0
54	MG	CA	1802	1/1	0.97	0.17	62,62,62,62	0
54	MG	DA	3696	1/1	0.97	0.08	85,85,85,85	0
54	MG	DA	3574	1/1	0.97	0.07	74,74,74,74	0
54	MG	AA	1859	1/1	0.97	0.05	77,77,77,77	0
54	MG	DA	3216	1/1	0.97	0.12	88,88,88,88	0
54	MG	DA	3452	1/1	0.97	0.15	104,104,104,104	0
54	MG	BA	3420	1/1	0.97	0.28	82,82,82,82	0
54	MG	AA	1658	1/1	0.97	0.16	57,57,57,57	0
54	MG	DA	3777	1/1	0.97	0.13	53,53,53,53	0
54	MG	CW	204	1/1	0.97	0.10	68,68,68,68	0
54	MG	BA	3288	1/1	0.97	0.08	66,66,66,66	0
54	MG	BA	2952	1/1	0.97	0.17	41,41,41,41	0
54	MG	DA	3425	1/1	0.97	0.11	68,68,68,68	0
54	MG	CA	1789	1/1	0.97	0.17	100,100,100,100	0
54	MG	BB	203	1/1	0.97	0.10	85,85,85,85	0
54	MG	BA	3162	1/1	0.97	0.23	69,69,69,69	0
54	MG	DG	202	1/1	0.97	0.05	84,84,84,84	0
54	MG	DZ	101	1/1	0.97	0.12	79,79,79,79	0
54	MG	BA	3381	1/1	0.97	0.08	45,45,45,45	0
54	MG	DA	2931	1/1	0.97	0.30	24,24,24,24	0
54	MG	DB	201	1/1	0.97	0.41	86,86,86,86	0
54	MG	BA	3171	1/1	0.97	0.06	50,50,50,50	0
54	MG	CA	1890	1/1	0.97	0.11	115,115,115,115	0
54	MG	BA	2917	1/1	0.97	0.26	37,37,37,37	0
54	MG	DA	3460	1/1	0.97	0.19	72,72,72,72	0
54	MG	D1	206	1/1	0.97	0.19	66,66,66,66	0
54	MG	BA	3466	1/1	0.97	0.06	84,84,84,84	0
54	MG	BA	3134	1/1	0.97	0.26	61,61,61,61	0
54	MG	DA	3434	1/1	0.97	0.21	63,63,63,63	0
54	MG	BA	3296	1/1	0.97	0.07	57,57,57,57	0
54	MG	BA	2997	1/1	0.97	0.30	60,60,60,60	0
54	MG	DA	2908	1/1	0.97	0.21	23,23,23,23	0
54	MG	BA	2986	1/1	0.97	0.18	41,41,41,41	0
54	MG	BA	3553	1/1	0.97	0.15	96,96,96,96	0
54	MG	DA	3063	1/1	0.97	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3540	1/1	0.97	0.19	54,54,54,54	0
54	MG	AA	2001	1/1	0.97	0.21	76,76,76,76	0
54	MG	DA	2965	1/1	0.97	0.44	49,49,49,49	0
54	MG	AA	1853	1/1	0.97	0.16	104,104,104,104	0
54	MG	BA	2933	1/1	0.97	0.12	50,50,50,50	0
54	MG	BA	2955	1/1	0.97	0.28	29,29,29,29	0
54	MG	DA	3010	1/1	0.97	0.37	86,86,86,86	0
54	MG	BA	3058	1/1	0.97	0.14	49,49,49,49	0
54	MG	BA	3418	1/1	0.97	0.08	65,65,65,65	0
54	MG	BA	3040	1/1	0.97	0.12	40,40,40,40	0
54	MG	DA	3342	1/1	0.97	0.42	77,77,77,77	0
54	MG	AA	1624	1/1	0.97	0.29	56,56,56,56	0
54	MG	CA	1679	1/1	0.97	0.18	72,72,72,72	0
54	MG	DA	3330	1/1	0.97	0.18	49,49,49,49	0
54	MG	AA	1697	1/1	0.97	0.17	77,77,77,77	0
54	MG	BA	3362	1/1	0.97	0.10	68,68,68,68	0
54	MG	CA	1713	1/1	0.97	0.14	53,53,53,53	0
54	MG	BA	3042	1/1	0.97	0.05	28,28,28,28	0
54	MG	AA	1979	1/1	0.97	0.26	75,75,75,75	0
54	MG	CA	1900	1/1	0.97	0.08	50,50,50,50	0
54	MG	CA	1681	1/1	0.97	0.20	67,67,67,67	0
54	MG	DA	3442	1/1	0.97	0.19	86,86,86,86	0
54	MG	CA	1677	1/1	0.97	0.22	57,57,57,57	0
54	MG	BA	3312	1/1	0.97	0.09	75,75,75,75	0
54	MG	BA	3453	1/1	0.97	0.27	73,73,73,73	0
54	MG	BA	3258	1/1	0.97	0.17	100,100,100,100	0
54	MG	AA	1798	1/1	0.97	0.27	79,79,79,79	0
54	MG	DA	3036	1/1	0.97	0.34	50,50,50,50	0
54	MG	DA	3582	1/1	0.97	0.09	116,116,116,116	0
54	MG	CA	1671	1/1	0.97	0.14	77,77,77,77	0
54	MG	CA	1939	1/1	0.97	0.07	87,87,87,87	0
54	MG	BA	3359	1/1	0.97	0.15	73,73,73,73	0
54	MG	DA	3786	1/1	0.97	0.16	70,70,70,70	0
54	MG	BA	3097	1/1	0.97	0.21	59,59,59,59	0
54	MG	DA	3128	1/1	0.97	0.10	40,40,40,40	0
54	MG	DA	2954	1/1	0.97	0.06	16,16,16,16	0
54	MG	DA	3585	1/1	0.97	0.09	114,114,114,114	0
54	MG	DA	3158	1/1	0.97	0.17	62,62,62,62	0
54	MG	AA	1688	1/1	0.97	0.21	39,39,39,39	0
54	MG	DA	2986	1/1	0.97	0.06	42,42,42,42	0
54	MG	DD	302	1/1	0.97	0.24	40,40,40,40	0
54	MG	DA	3664	1/1	0.97	0.14	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3176	1/1	0.97	0.17	65,65,65,65	0
54	MG	AA	1874	1/1	0.97	0.22	63,63,63,63	0
54	MG	DA	2956	1/1	0.97	0.34	47,47,47,47	0
54	MG	CA	1796	1/1	0.97	0.05	35,35,35,35	0
54	MG	AA	1912	1/1	0.97	0.15	79,79,79,79	0
54	MG	CA	1884	1/1	0.97	0.08	59,59,59,59	0
54	MG	BA	2969	1/1	0.97	0.28	33,33,33,33	0
54	MG	DA	2987	1/1	0.97	0.29	36,36,36,36	0
54	MG	AA	1980	1/1	0.97	0.06	136,136,136,136	0
54	MG	BA	2926	1/1	0.97	0.20	43,43,43,43	0
54	MG	BA	3090	1/1	0.97	0.15	61,61,61,61	0
54	MG	BA	3022	1/1	0.97	0.15	46,46,46,46	0
54	MG	DA	3278	1/1	0.97	0.28	78,78,78,78	0
54	MG	AA	1807	1/1	0.97	0.04	65,65,65,65	0
54	MG	DA	3013	1/1	0.97	0.28	58,58,58,58	0
54	MG	DA	3242	1/1	0.97	0.22	46,46,46,46	0
54	MG	DA	3001	1/1	0.97	0.20	46,46,46,46	0
54	MG	BA	3122	1/1	0.97	0.29	63,63,63,63	0
54	MG	DA	3428	1/1	0.97	0.19	55,55,55,55	0
54	MG	CA	1636	1/1	0.97	0.20	52,52,52,52	0
54	MG	DA	3160	1/1	0.98	0.13	48,48,48,48	0
54	MG	DA	2978	1/1	0.98	0.21	24,24,24,24	0
54	MG	DA	3779	1/1	0.98	0.11	72,72,72,72	0
54	MG	DA	2920	1/1	0.98	0.26	21,21,21,21	0
54	MG	CA	1856	1/1	0.98	0.04	74,74,74,74	0
54	MG	CA	1711	1/1	0.98	0.38	75,75,75,75	0
54	MG	CC	106	1/1	0.98	0.09	79,79,79,79	0
54	MG	DA	2959	1/1	0.98	0.24	26,26,26,26	0
54	MG	BA	3556	1/1	0.98	0.10	82,82,82,82	0
54	MG	DA	2929	1/1	0.98	0.28	24,24,24,24	0
54	MG	BA	2985	1/1	0.98	0.07	46,46,46,46	0
54	MG	AA	1715	1/1	0.98	0.11	76,76,76,76	0
54	MG	DA	3012	1/1	0.98	0.27	35,35,35,35	0
54	MG	BA	3044	1/1	0.98	0.10	114,114,114,114	0
54	MG	BA	3197	1/1	0.98	0.15	103,103,103,103	0
54	MG	DA	2944	1/1	0.98	0.17	35,35,35,35	0
54	MG	BA	2954	1/1	0.98	0.24	54,54,54,54	0
54	MG	DA	3040	1/1	0.98	0.16	44,44,44,44	0
54	MG	DA	3701	1/1	0.98	0.20	92,92,92,92	0
54	MG	BA	2940	1/1	0.98	0.21	27,27,27,27	0
54	MG	BA	3252	1/1	0.98	0.11	38,38,38,38	0
54	MG	BA	2966	1/1	0.98	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3027	1/1	0.98	0.15	22,22,22,22	0
54	MG	BA	3259	1/1	0.98	0.09	90,90,90,90	0
54	MG	DA	2994	1/1	0.98	0.24	37,37,37,37	0
54	MG	DA	3046	1/1	0.98	0.19	19,19,19,19	0
54	MG	DA	3266	1/1	0.98	0.12	109,109,109,109	0
54	MG	DA	2941	1/1	0.98	0.19	39,39,39,39	0
54	MG	DA	3053	1/1	0.98	0.05	28,28,28,28	0
54	MG	DA	3324	1/1	0.98	0.18	34,34,34,34	0
54	MG	DA	3485	1/1	0.98	0.10	56,56,56,56	0
54	MG	BA	3251	1/1	0.98	0.18	78,78,78,78	0
54	MG	AA	1940	1/1	0.98	0.30	91,91,91,91	0
54	MG	AA	1625	1/1	0.98	0.26	62,62,62,62	0
54	MG	CP	202	1/1	0.98	0.18	122,122,122,122	0
54	MG	CA	1625	1/1	0.98	0.34	51,51,51,51	0
54	MG	BA	2950	1/1	0.98	0.18	29,29,29,29	0
54	MG	DA	2906	1/1	0.98	0.29	27,27,27,27	0
54	MG	BA	2902	1/1	0.98	0.14	57,57,57,57	0
54	MG	BA	3067	1/1	0.98	0.23	43,43,43,43	0
54	MG	DA	3011	1/1	0.98	0.22	78,78,78,78	0
54	MG	BA	3530	1/1	0.98	0.10	110,110,110,110	0
54	MG	BA	3149	1/1	0.98	0.19	61,61,61,61	0
54	MG	BA	2924	1/1	0.98	0.18	55,55,55,55	0
54	MG	BA	3113	1/1	0.98	0.11	41,41,41,41	0
54	MG	CA	1639	1/1	0.98	0.17	42,42,42,42	0
54	MG	DA	3321	1/1	0.98	0.20	70,70,70,70	0
54	MG	DA	3604	1/1	0.98	0.15	43,43,43,43	0
54	MG	BA	2923	1/1	0.98	0.20	44,44,44,44	0
54	MG	BA	3211	1/1	0.98	0.04	43,43,43,43	0
54	MG	AA	1732	1/1	0.98	0.18	89,89,89,89	0
54	MG	AA	1817	1/1	0.98	0.09	89,89,89,89	0
54	MG	AA	1962	1/1	0.98	0.15	55,55,55,55	0
54	MG	BA	2942	1/1	0.98	0.28	36,36,36,36	0
54	MG	BA	2946	1/1	0.98	0.28	50,50,50,50	0
54	MG	DA	2968	1/1	0.98	0.12	20,20,20,20	0
54	MG	CA	1768	1/1	0.98	0.14	52,52,52,52	0
54	MG	DA	3497	1/1	0.98	0.15	68,68,68,68	0
54	MG	AC	108	1/1	0.98	0.12	61,61,61,61	0
54	MG	CA	1685	1/1	0.98	0.11	59,59,59,59	0
54	MG	DA	2917	1/1	0.98	0.29	27,27,27,27	0
54	MG	DA	3157	1/1	0.98	0.10	51,51,51,51	0
54	MG	D0	203	1/1	0.98	0.09	63,63,63,63	0
55	ZN	CQ	104	1/1	0.98	0.10	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3011	1/1	0.98	0.18	57,57,57,57	0
54	MG	CA	1607	1/1	0.98	0.30	73,73,73,73	0
54	MG	DA	2901	1/1	0.98	0.26	28,28,28,28	0
54	MG	DA	3139	1/1	0.98	0.20	33,33,33,33	0
54	MG	DA	3192	1/1	0.98	0.19	61,61,61,61	0
54	MG	DA	2961	1/1	0.98	0.17	37,37,37,37	0
54	MG	CA	1841	1/1	0.98	0.21	119,119,119,119	0
54	MG	DA	3726	1/1	0.98	0.18	75,75,75,75	0
54	MG	DA	3507	1/1	0.98	0.29	86,86,86,86	0
54	MG	AA	1788	1/1	0.98	0.13	91,91,91,91	0
54	MG	DA	3695	1/1	0.98	0.12	60,60,60,60	0
54	MG	DA	3566	1/1	0.98	0.26	78,78,78,78	0
54	MG	AA	1792	1/1	0.98	0.31	74,74,74,74	0
54	MG	DA	2938	1/1	0.98	0.13	57,57,57,57	0
54	MG	DA	2967	1/1	0.98	0.22	39,39,39,39	0
54	MG	BA	3202	1/1	0.98	0.08	65,65,65,65	0
54	MG	BA	2938	1/1	0.98	0.23	39,39,39,39	0
54	MG	DA	2930	1/1	0.98	0.31	31,31,31,31	0
54	MG	BA	3405	1/1	0.98	0.16	82,82,82,82	0
54	MG	DA	3177	1/1	0.98	0.20	38,38,38,38	0
54	MG	DA	2937	1/1	0.98	0.22	25,25,25,25	0
54	MG	BA	3026	1/1	0.98	0.23	60,60,60,60	0
54	MG	BA	3292	1/1	0.98	0.12	54,54,54,54	0
54	MG	BA	2915	1/1	0.98	0.21	34,34,34,34	0
54	MG	BA	3107	1/1	0.98	0.06	61,61,61,61	0
54	MG	BB	223	1/1	0.98	0.15	122,122,122,122	0
54	MG	DA	3026	1/1	0.98	0.33	34,34,34,34	0
54	MG	CA	1891	1/1	0.98	0.10	113,113,113,113	0
54	MG	DA	3033	1/1	0.98	0.22	42,42,42,42	0
54	MG	CA	1783	1/1	0.98	0.26	47,47,47,47	0
54	MG	DB	208	1/1	0.98	0.21	135,135,135,135	0
54	MG	AA	1679	1/1	0.98	0.22	74,74,74,74	0
54	MG	DA	3280	1/1	0.98	0.15	33,33,33,33	0
54	MG	BA	3330	1/1	0.98	0.13	62,62,62,62	0
54	MG	DZ	102	1/1	0.98	0.07	79,79,79,79	0
54	MG	DA	3017	1/1	0.98	0.31	43,43,43,43	0
54	MG	CA	1956	1/1	0.98	0.12	217,217,217,217	0
54	MG	AA	1630	1/1	0.98	0.38	55,55,55,55	0
54	MG	DA	3378	1/1	0.98	0.08	76,76,76,76	0
54	MG	BA	3110	1/1	0.98	0.17	34,34,34,34	0
54	MG	CA	1766	1/1	0.98	0.30	51,51,51,51	0
54	MG	DA	3270	1/1	0.98	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3333	1/1	0.98	0.12	62,62,62,62	0
54	MG	DA	3166	1/1	0.98	0.06	25,25,25,25	0
54	MG	BA	2920	1/1	0.98	0.21	36,36,36,36	0
54	MG	BA	2925	1/1	0.98	0.24	46,46,46,46	0
54	MG	AA	1672	1/1	0.98	0.28	68,68,68,68	0
54	MG	DA	3621	1/1	0.98	0.12	75,75,75,75	0
54	MG	BA	2990	1/1	0.98	0.22	48,48,48,48	0
54	MG	DA	3702	1/1	0.98	0.09	22,22,22,22	0
54	MG	AA	1764	1/1	0.98	0.09	96,96,96,96	0
54	MG	CA	1659	1/1	0.98	0.25	101,101,101,101	0
54	MG	BA	2916	1/1	0.98	0.25	42,42,42,42	0
54	MG	BA	3155	1/1	0.98	0.12	64,64,64,64	0
54	MG	BA	3082	1/1	0.98	0.34	59,59,59,59	0
54	MG	DA	3661	1/1	0.98	0.18	79,79,79,79	0
54	MG	DA	3423	1/1	0.98	0.14	62,62,62,62	0
54	MG	BB	219	1/1	0.98	0.05	124,124,124,124	0
54	MG	CA	1670	1/1	0.98	0.24	56,56,56,56	0
54	MG	BA	2953	1/1	0.98	0.19	32,32,32,32	0
54	MG	DA	2940	1/1	0.98	0.26	25,25,25,25	0
54	MG	BA	3311	1/1	0.98	0.14	48,48,48,48	0
54	MG	BA	3045	1/1	0.98	0.15	26,26,26,26	0
54	MG	CA	1859	1/1	0.98	0.13	121,121,121,121	0
54	MG	BA	2919	1/1	0.98	0.14	29,29,29,29	0
54	MG	DA	3196	1/1	0.98	0.26	106,106,106,106	0
54	MG	DE	301	1/1	0.98	0.21	27,27,27,27	0
54	MG	AA	1992	1/1	0.98	0.06	106,106,106,106	0
54	MG	BA	3000	1/1	0.98	0.15	25,25,25,25	0
54	MG	BA	3062	1/1	0.98	0.18	61,61,61,61	0
54	MG	DA	3677	1/1	0.98	0.14	85,85,85,85	0
54	MG	BA	3102	1/1	0.98	0.05	113,113,113,113	0
54	MG	AA	1892	1/1	0.98	0.16	99,99,99,99	0
54	MG	DA	3008	1/1	0.98	0.21	34,34,34,34	0
54	MG	DA	3458	1/1	0.98	0.10	71,71,71,71	0
54	MG	BA	3148	1/1	0.98	0.11	42,42,42,42	0
54	MG	DA	3300	1/1	0.98	0.04	28,28,28,28	0
54	MG	BA	2934	1/1	0.98	0.33	42,42,42,42	0
54	MG	AA	1703	1/1	0.98	0.23	49,49,49,49	0
54	MG	AA	1621	1/1	0.98	0.30	50,50,50,50	0
54	MG	AA	1787	1/1	0.98	0.08	65,65,65,65	0
54	MG	BA	2999	1/1	0.98	0.12	27,27,27,27	0
54	MG	DA	2916	1/1	0.98	0.24	35,35,35,35	0
54	MG	BA	2976	1/1	0.98	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	2943	1/1	0.98	0.27	29,29,29,29	0
54	MG	BA	3035	1/1	0.98	0.18	48,48,48,48	0
54	MG	DA	3147	1/1	0.98	0.17	42,42,42,42	0
54	MG	CA	1651	1/1	0.98	0.28	76,76,76,76	0
54	MG	BA	3522	1/1	0.98	0.06	54,54,54,54	0
54	MG	BA	3098	1/1	0.98	0.20	60,60,60,60	0
54	MG	DA	3118	1/1	0.98	0.13	40,40,40,40	0
54	MG	CA	1618	1/1	0.98	0.13	51,51,51,51	0
54	MG	DA	2957	1/1	0.98	0.25	20,20,20,20	0
54	MG	AA	2000	1/1	0.98	0.12	38,38,38,38	0
54	MG	DA	2971	1/1	0.98	0.30	40,40,40,40	0
54	MG	AA	1803	1/1	0.98	0.12	61,61,61,61	0
54	MG	DA	3025	1/1	0.98	0.19	25,25,25,25	0
54	MG	DA	3234	1/1	0.98	0.20	32,32,32,32	0
54	MG	DA	3722	1/1	0.98	0.26	166,166,166,166	0
54	MG	BA	3030	1/1	0.98	0.17	47,47,47,47	0
54	MG	BA	3038	1/1	0.98	0.21	39,39,39,39	0
54	MG	DA	3285	1/1	0.98	0.30	56,56,56,56	0
54	MG	DA	3282	1/1	0.98	0.13	63,63,63,63	0
54	MG	AA	1659	1/1	0.98	0.23	81,81,81,81	0
54	MG	BA	3234	1/1	0.98	0.08	42,42,42,42	0
54	MG	BA	3163	1/1	0.98	0.07	63,63,63,63	0
54	MG	BA	3192	1/1	0.98	0.06	54,54,54,54	0
54	MG	DA	3106	1/1	0.99	0.30	44,44,44,44	0
54	MG	DA	3787	1/1	0.99	0.18	59,59,59,59	0
54	MG	DA	3023	1/1	0.99	0.24	28,28,28,28	0
54	MG	CA	1958	1/1	0.99	0.13	106,106,106,106	0
54	MG	BA	3274	1/1	0.99	0.22	116,116,116,116	0
54	MG	DA	2979	1/1	0.99	0.27	31,31,31,31	0
54	MG	DA	3757	1/1	0.99	0.08	54,54,54,54	0
54	MG	BA	2973	1/1	0.99	0.23	47,47,47,47	0
54	MG	BA	2956	1/1	0.99	0.17	38,38,38,38	0
54	MG	DA	3469	1/1	0.99	0.21	51,51,51,51	0
54	MG	BA	2914	1/1	0.99	0.15	17,17,17,17	0
54	MG	DA	3021	1/1	0.99	0.30	47,47,47,47	0
54	MG	DA	2942	1/1	0.99	0.21	38,38,38,38	0
54	MG	CA	1617	1/1	0.99	0.23	44,44,44,44	0
54	MG	CA	1743	1/1	0.99	0.15	64,64,64,64	0
54	MG	AA	1670	1/1	0.99	0.16	75,75,75,75	0
54	MG	CA	1873	1/1	0.99	0.04	117,117,117,117	0
54	MG	AA	1741	1/1	0.99	0.18	93,93,93,93	0
54	MG	BA	3108	1/1	0.99	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3229	1/1	0.99	0.17	33,33,33,33	0
54	MG	DA	3165	1/1	0.99	0.15	33,33,33,33	0
54	MG	BA	3003	1/1	0.99	0.11	40,40,40,40	0
54	MG	AA	1701	1/1	0.99	0.26	72,72,72,72	0
54	MG	DA	2912	1/1	0.99	0.28	27,27,27,27	0
54	MG	DA	2977	1/1	0.99	0.05	32,32,32,32	0
54	MG	BA	2983	1/1	0.99	0.21	27,27,27,27	0
54	MG	DA	3000	1/1	0.99	0.24	31,31,31,31	0
54	MG	D0	201	1/1	0.99	0.15	38,38,38,38	0
54	MG	AA	1921	1/1	0.99	0.16	76,76,76,76	0
54	MG	BA	2930	1/1	0.99	0.15	33,33,33,33	0
54	MG	BA	3104	1/1	0.99	0.26	47,47,47,47	0
54	MG	DA	2924	1/1	0.99	0.18	17,17,17,17	0
54	MG	DA	3407	1/1	0.99	0.04	41,41,41,41	0
54	MG	DA	3309	1/1	0.99	0.14	20,20,20,20	0
54	MG	BA	3028	1/1	0.99	0.12	41,41,41,41	0
54	MG	AA	1718	1/1	0.99	0.07	63,63,63,63	0
54	MG	BA	3519	1/1	0.99	0.06	90,90,90,90	0
54	MG	DA	2903	1/1	0.99	0.35	24,24,24,24	0
54	MG	DA	2913	1/1	0.99	0.33	30,30,30,30	0
54	MG	AA	1669	1/1	0.99	0.32	54,54,54,54	0
54	MG	DA	3122	1/1	0.99	0.33	60,60,60,60	0
54	MG	BA	3047	1/1	0.99	0.17	41,41,41,41	0
54	MG	CA	1714	1/1	0.99	0.10	64,64,64,64	0
54	MG	BA	3236	1/1	0.99	0.11	33,33,33,33	0
54	MG	BA	3111	1/1	0.99	0.21	53,53,53,53	0
54	MG	DA	2932	1/1	0.99	0.21	23,23,23,23	0
54	MG	BA	2963	1/1	0.99	0.16	32,32,32,32	0
54	MG	BA	2948	1/1	0.99	0.20	29,29,29,29	0
54	MG	DA	3170	1/1	0.99	0.27	31,31,31,31	0
54	MG	BA	3096	1/1	0.99	0.20	37,37,37,37	0
54	MG	CA	1837	1/1	0.99	0.20	44,44,44,44	0
54	MG	DA	3286	1/1	0.99	0.30	58,58,58,58	0
54	MG	BA	2941	1/1	0.99	0.20	27,27,27,27	0
54	MG	CA	1948	1/1	0.99	0.17	89,89,89,89	0
54	MG	DA	3111	1/1	0.99	0.26	48,48,48,48	0
54	MG	BA	3265	1/1	0.99	0.04	40,40,40,40	0
54	MG	BA	2957	1/1	0.99	0.17	33,33,33,33	0
54	MG	DA	3030	1/1	0.99	0.26	49,49,49,49	0
55	ZN	AG	301	1/1	0.99	0.28	82,82,82,82	0
54	MG	BA	3029	1/1	0.99	0.21	40,40,40,40	0
54	MG	AA	1994	1/1	0.99	0.10	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3731	1/1	0.99	0.09	67,67,67,67	0
54	MG	DA	3388	1/1	0.99	0.10	37,37,37,37	0
54	MG	DA	2976	1/1	0.99	0.31	31,31,31,31	0
54	MG	BA	3027	1/1	0.99	0.15	46,46,46,46	0
54	MG	CQ	103	1/1	0.99	0.06	122,122,122,122	0
54	MG	DA	2973	1/1	0.99	0.29	24,24,24,24	0
54	MG	BA	3083	1/1	0.99	0.17	37,37,37,37	0
54	MG	BA	2931	1/1	0.99	0.18	29,29,29,29	0
54	MG	DA	2960	1/1	0.99	0.29	34,34,34,34	0
54	MG	DA	2907	1/1	0.99	0.27	23,23,23,23	0
54	MG	CA	1734	1/1	0.99	0.21	73,73,73,73	0
54	MG	DA	2990	1/1	0.99	0.24	27,27,27,27	0
54	MG	BA	2943	1/1	0.99	0.28	44,44,44,44	0
54	MG	DA	3334	1/1	0.99	0.29	45,45,45,45	0
54	MG	DA	3312	1/1	0.99	0.13	51,51,51,51	0
54	MG	BA	3480	1/1	0.99	0.10	87,87,87,87	0
54	MG	BA	2947	1/1	0.99	0.17	30,30,30,30	0
54	MG	DA	3479	1/1	0.99	0.11	73,73,73,73	0
54	MG	AA	1822	1/1	0.99	0.13	107,107,107,107	0
54	MG	CA	1896	1/1	0.99	0.20	67,67,67,67	0
54	MG	DA	3096	1/1	0.99	0.24	57,57,57,57	0
54	MG	DA	2934	1/1	0.99	0.13	22,22,22,22	0
54	MG	AA	1786	1/1	0.99	0.18	93,93,93,93	0
54	MG	DA	2902	1/1	0.99	0.27	44,44,44,44	0
54	MG	CA	1654	1/1	0.99	0.10	80,80,80,80	0
54	MG	DW	102	1/1	1.00	0.15	91,91,91,91	0
54	MG	AA	1880	1/1	1.00	0.09	80,80,80,80	0
54	MG	DA	3659	1/1	1.00	0.07	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.