



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 06:06 PM EST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

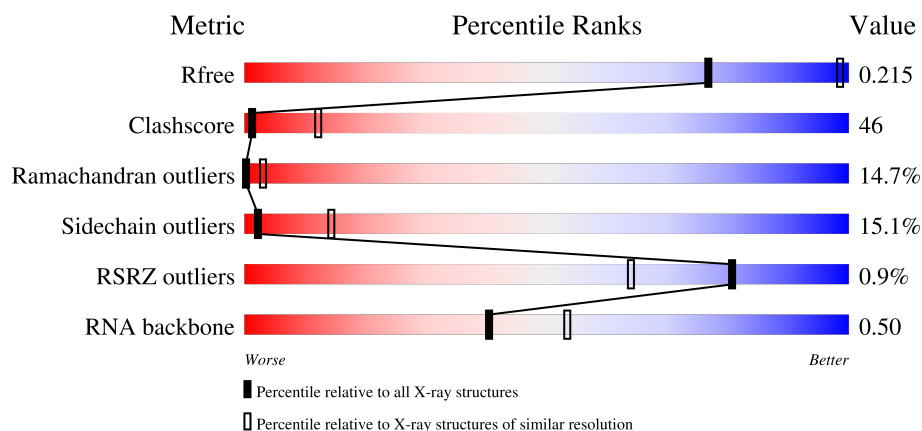
1 Overall quality at a glance

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.




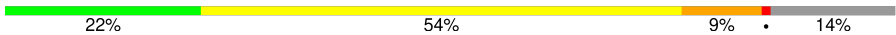
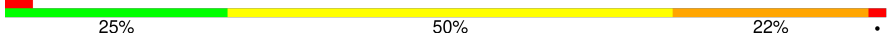

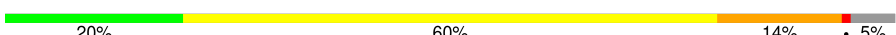

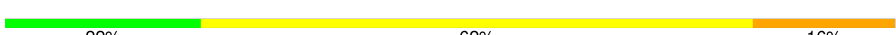




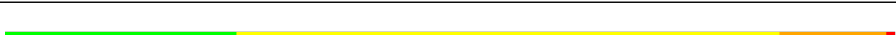

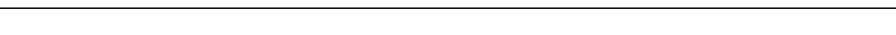
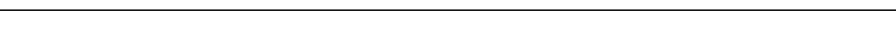
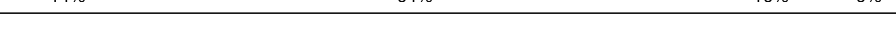
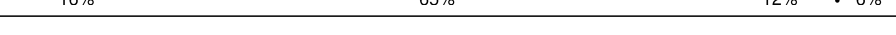
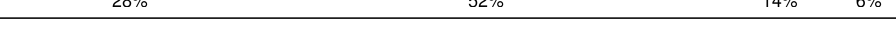

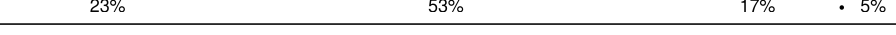


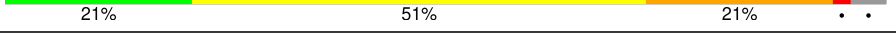

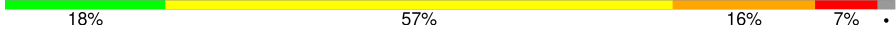
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)
RNA backbone	3690	1089 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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></div> <div>25% 50% 22% •</div> </div>
1	CA	1517	<div> <div></div> <div>25% 52% 20% •</div> </div>
2	AE	256	<div> <div></div> <div>9% 57% 23% • 8%</div> </div>
2	CE	256	<div> <div></div> <div>17% 59% 16% • 7%</div> </div>


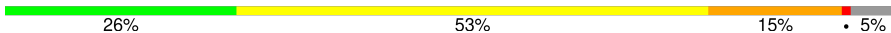
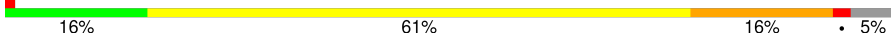


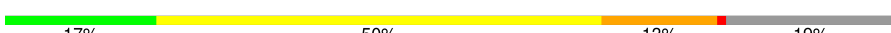
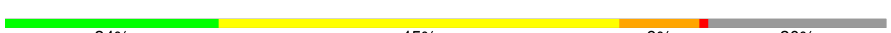




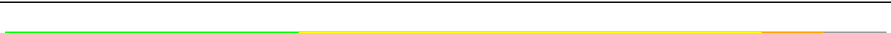









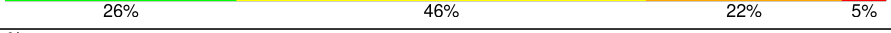
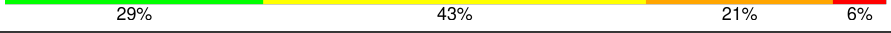
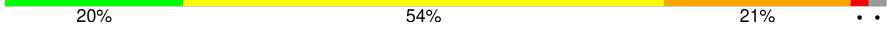

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	209	
4	CG	209	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126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

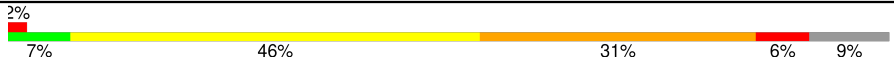


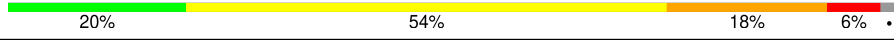
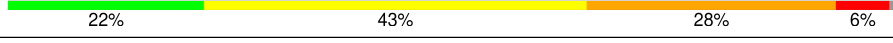
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Mol	Chain	Length	Quality of chain
39	B1	118	
39	D1	118	
40	B2	101	
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	
48	DX	60	
49	B4	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	1661	-	-	-	X
54	MG	AA	1840	-	-	-	X
54	MG	AA	1909	-	-	-	X
54	MG	AA	1911	-	-	-	X
54	MG	DA	3091	-	-	-	X
54	MG	DA	3269	-	-	-	X
54	MG	DA	3326	-	-	-	X
54	MG	DA	3440	-	-	-	X
54	MG	DA	3441	-	-	-	X
54	MG	DA	3512	-	-	-	X
54	MG	DA	3573	-	-	-	X
54	MG	DA	3668	-	-	-	X
54	MG	DA	3682	-	-	-	X

2 Entry composition

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
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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	AA	440	Total	Mg	0	0
			440	440		
54	AH	2	Total	Mg	0	0
			2	2		
54	AI	1	Total	Mg	0	0
			1	1		
54	AJ	1	Total	Mg	0	0
			1	1		
54	AK	1	Total	Mg	0	0
			1	1		
54	AL	2	Total	Mg	0	0
			2	2		
54	AO	1	Total	Mg	0	0
			1	1		
54	AP	1	Total	Mg	0	0
			1	1		
54	AQ	1	Total	Mg	0	0
			1	1		
54	AS	2	Total	Mg	0	0
			2	2		
54	AT	2	Total	Mg	0	0
			2	2		
54	AW	4	Total	Mg	0	0
			4	4		
54	AX	1	Total	Mg	0	0
			1	1		
54	AC	8	Total	Mg	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AD	3	Total 3	Mg 3	0	0
54	A1	1	Total 1	Mg 1	0	0
54	BA	683	Total 683	Mg 683	0	0
54	BB	26	Total 26	Mg 26	0	0
54	BD	2	Total 2	Mg 2	0	0
54	BE	7	Total 7	Mg 7	0	0
54	BF	2	Total 2	Mg 2	0	0
54	BG	1	Total 1	Mg 1	0	0
54	BH	1	Total 1	Mg 1	0	0
54	BK	1	Total 1	Mg 1	0	0
54	BO	1	Total 1	Mg 1	0	0
54	B0	2	Total 2	Mg 2	0	0
54	BQ	1	Total 1	Mg 1	0	0
54	BR	2	Total 2	Mg 2	0	0
54	B1	1	Total 1	Mg 1	0	0
54	BT	2	Total 2	Mg 2	0	0
54	BU	5	Total 5	Mg 5	0	0
54	B3	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	BW	1	Total 1	Mg 1	0	0
54	B4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	B5	1	Total 1	Mg 1	0	0
54	B6	1	Total 1	Mg 1	0	0
54	B8	1	Total 1	Mg 1	0	0
54	CA	384	Total 384	Mg 384	0	0
54	CG	1	Total 1	Mg 1	0	0
54	CH	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	CM	1	Total 1	Mg 1	0	0
54	CP	4	Total 4	Mg 4	0	0
54	CQ	3	Total 3	Mg 3	0	0
54	CR	1	Total 1	Mg 1	0	0
54	CS	2	Total 2	Mg 2	0	0
54	CT	1	Total 1	Mg 1	0	0
54	CW	5	Total 5	Mg 5	0	0
54	CX	2	Total 2	Mg 2	0	0
54	CC	13	Total 13	Mg 13	0	0
54	CD	26	Total 26	Mg 26	0	0
54	C1	1	Total 1	Mg 1	0	0
54	DA	905	Total 905	Mg 905	0	0
54	DB	29	Total 29	Mg 29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DD	3	Total 3	Mg 3	0	0
54	DE	3	Total 3	Mg 3	0	0
54	DF	1	Total 1	Mg 1	0	0
54	DG	3	Total 3	Mg 3	0	0
54	DH	4	Total 4	Mg 4	0	0
54	DO	5	Total 5	Mg 5	0	0
54	D0	5	Total 5	Mg 5	0	0
54	DR	2	Total 2	Mg 2	0	0
54	D1	6	Total 6	Mg 6	0	0
54	D2	1	Total 1	Mg 1	0	0
54	DS	1	Total 1	Mg 1	0	0
54	DT	2	Total 2	Mg 2	0	0
54	DU	6	Total 6	Mg 6	0	0
54	D3	4	Total 4	Mg 4	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	DW	2	Total 2	Mg 2	0	0
54	D5	1	Total 1	Mg 1	0	0
54	D6	2	Total 2	Mg 2	0	0
54	D7	1	Total 1	Mg 1	0	0

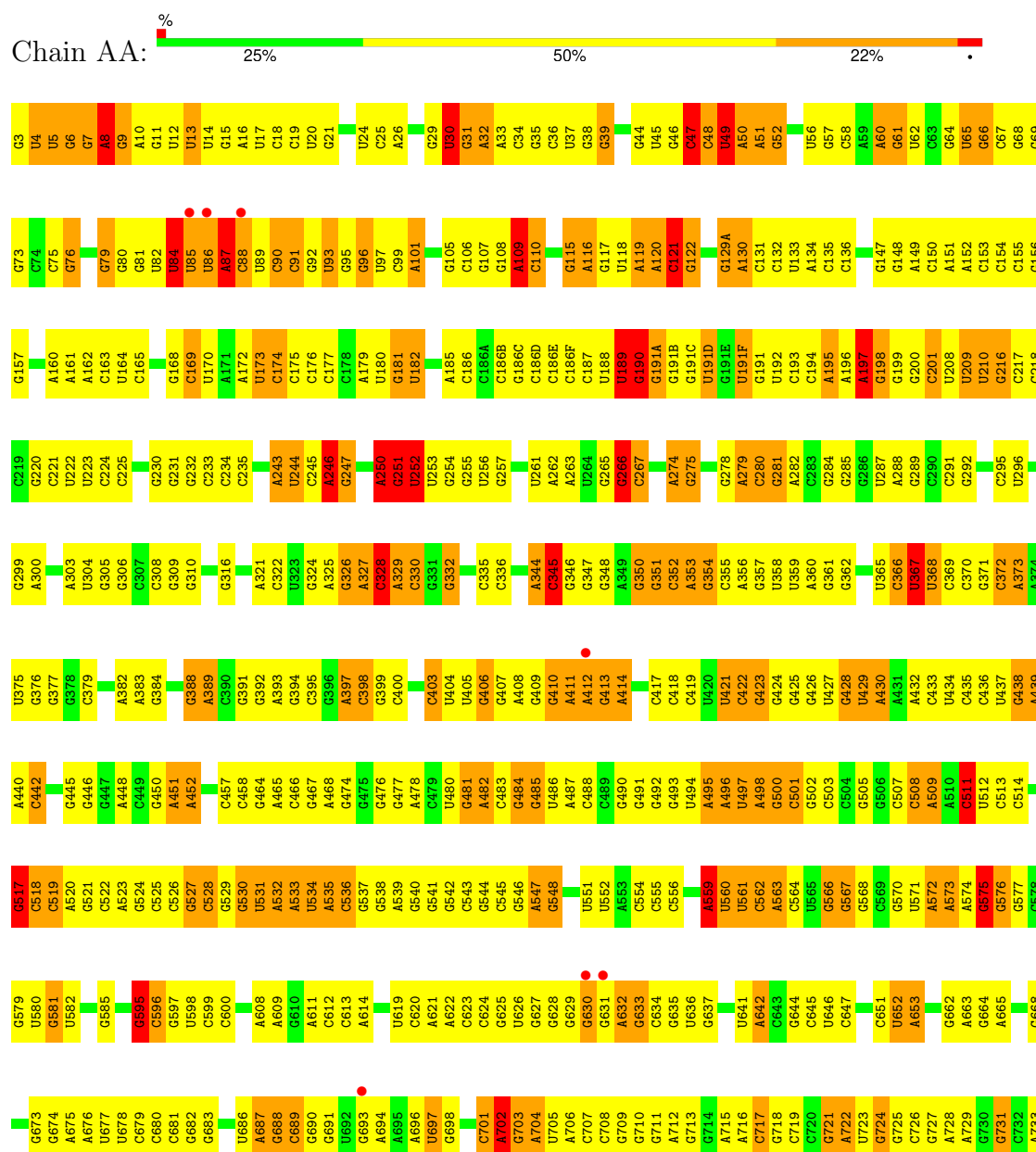
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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)



U1540	C1466	C1325	C1264	U1135	C1071	A1015	G954	G878	U804	G734
U1541	G1467	C1326	G1265	U1136	G1072	A1016	U955	C879	C805	C735
G1542	U1391	C1327	C1266	C1137	U1073	G1017	U956	C880	C806	C736
	U1392	C1328	G1267	G1138	G1207	A1018	U957	C881	A807	A737
	U1393	A1329	A1268	C1139	C1075	G1019	A958	C882	C808	C738
	U1394	C1330	C1269	C1140	G1076	U1020	A959	C883		
	C1395	G1331	C1270		G1077	G1021	U960	U884	C811	G741
	A1396	A1332	G1271	G1143	U1078	G1022	U961	C885	C812	G742
	C1397	C1333	G1272	G1144	U1079	G1023	C962		U813	U743
	A1398	C1334	G1273	C1145	A1080	G1024		A889	A814	A744
	C1399	C1335	A1213	A1146	G1081	U1025	A965	C890	A815	A745
	C1400	G1336	G1214	C1147	G1084	G1026	C967	U891	A816	A746
	G1401	G1337	G1275	U1148	U1085	C1027	C967	A892	C817	C747
	C1402	C1338	G1276	C1149	U1086	C1028	A968	C893	C818	C748
	C1403	A1339	U1277	U1150		C1028B	A969	G894	A819	C749
			U1278	U1151	G1089	C1029	C970		U820	G750
			A1280	A1152	U1090	G1030	C971	C899	U751	U751
			U1281	C1153	C1091	G1031	C972	C822	G752	G752
			C1282	G1154	U1091	A1032	C973	G823	A753	A753
			G1283	G1155	A1092	G1032A	A974	C824	C754	C754
			C1284	G1156	U1093	A1032A			G755	G755
			A1285	A1157	G1094	G1032B	A975		C756	C756
			A1286	C1158	U1095	G1033	A976		U757	U757
			A1287	U1159	C1096	G1034	A977		G758	G758
			A1288	G1160	C1097	A1035	A978		A759	A759
			A1289	C1161	G1098	G1036	C980		G760	G760
				C1162	U1099	C1037	U981		G761	G761
			U1292	C1163	C1100	C1038	U982		C762	C762
			G1293		A1169	C1039	A983		C834	C834
			G1294	A1170	A1102	U1040	C984		U835	U835
			G1295	C1171	C1103	G1041	C985		G836	G836
			C1296	G1172	G1104	G1042	A986		C837	C837
			C1297	C1173	A1105	C1043	C987		G838	G838
			A1298	G1174	G1106	A1044	G988		U841	U841
			G1300	C1175	C1107	C1045	C989		C842	C842
			U1301	G1176	G1108	A1046	C990		U843	U843
			U1302	A1177	A1111	G1047	U991		C848	C848
			C1303	G1178	C1112	G1048	U992		G778	G778
			G1304	A1179	C1113	U1049	A993		C779	C779
			C1305	C1242	C1114	G1050	A994		U880	U880
			C1306	C1243	C1115	C1051	C995		A781	A781
			C1307	C1244	C1116	G1052	A996		U782	U782
			U1308	C1245	C1117	C1053	U997		C783	C783
			C1309	C1246	G1118	A1055	C998		C784	C784
			G1310	U1247	C1118	U1056	C998A			
			G1311	A1248	C1119	G1057	U999		U788	U788
			C1312	C1249	U1120	G1058	A1000		A791	A791
			U1313	A1250	U1121	C1059	G1001		U793	U793
			C1314	A1251	U1122	G1060	A937		C794	C794
			U1315	G1253	A1123	C1061	G1002		A895	A895
			G1316	G1254	G1124	G1062	G1003		C868	C868
			C1317	C1255	U1125	C1063	A1004		C795	C795
			U1318	G1256	C1126	C1064	A1005		U796	U796
			A1319	A1257	G1127	U1065	C1006		C797	C797
			C1320	U1257	U1128	C1066	C1007		U870	U870
			C1321	G1258	C1129	C1067	C1008		U871	U871
			C1322	C1259	U1130	A1067	G1009		A872	A872
			G1323	C1262	C1132	C1068	G1010		G800	G800
			A1324	C1263	G1133	U1070	G1011		U801	U801
							A1014		A802	A802
									C877	C877

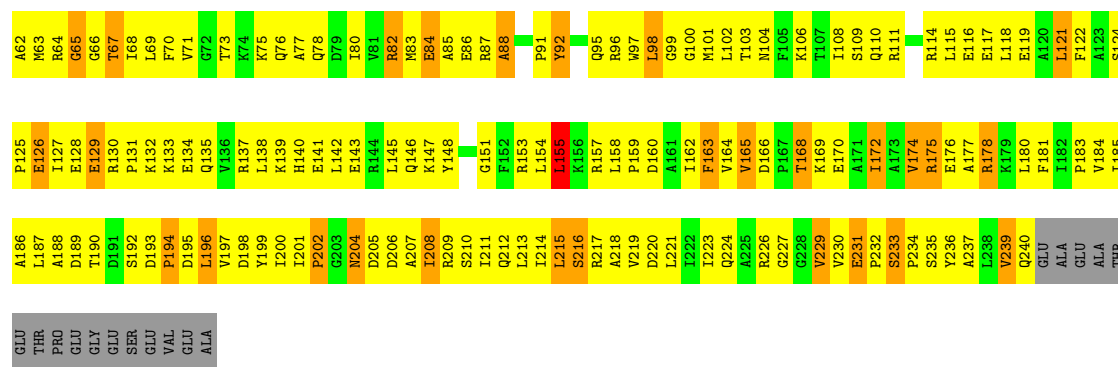
• Molecule 1: 16S rRNA (E.COLI NUMBERING)



G	U	U5	G6	G7	A8	G9	A10	G11	U12	U13	U14	G15	A16	U17	C18	C19	U20	G21	G22	C23	U30	G31	A32	A33	C34	G35	C36	U37	G38	G39	C40	G41	C43	G44	U45	G46	C47	C48	U49	A50	A51	G52	U56	G57	C58	A59	A60	G61	C63	G64	U65	C66	C67	G68	C69
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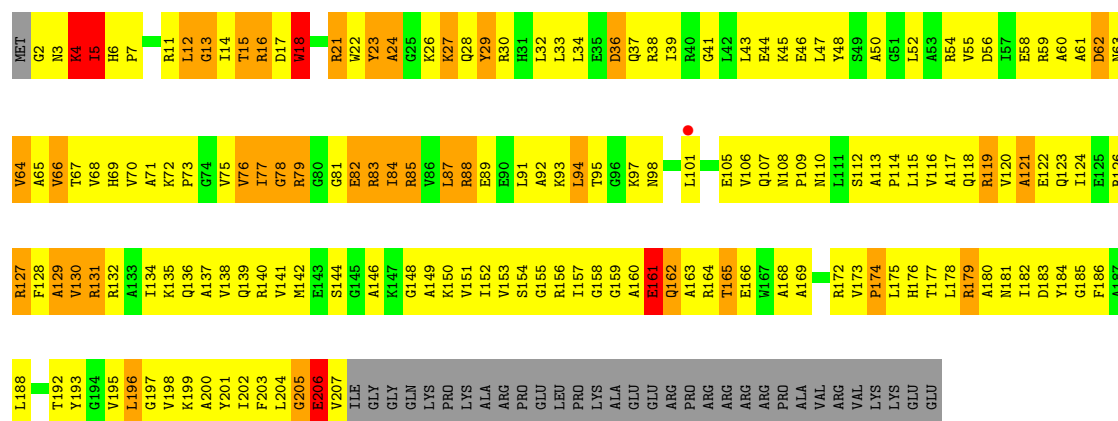
U1062	U1063	U999	A935	U863	A777	G707	G633	G558	G490	A414	A349	A279	G198	G147	G73
C1063	C1064	A1000	C936	U864	G778	C708	A640	A559	G491	A415	G350	C280	G199	G148	C74
U1065	U1066	G1001	A937	A865	A780	G709	U641	U560	G492	G416	C351	C281	G200	A149	C75
G1003	G1003	G1002	A938	G866	G709	G713	U642	U561	G493	C417	A352	G289	G201	C150	C76
A1067	A1067	A1004	C939	G867	U768	G714	C643	C562	U494	C418	A353	G290	U208	A151	C77
G1068	G1068	A1005	C941	G867	U769	G715	C644	C564	A495	C419	G354	C291	G78	G78	G78
C1071	C1071	C1006	G942	U870	A790	A716	C645	U565	A496	C422	C355	G292	G80	G80	G80
U1072	U1072	C1008	A946	U871	G791	G717	G649	G566	U497	G423	A356	C295	C217	G156	G81
U1073	U1073	G1009	G947	A872	A792	G718	G650	G567	A498	G423	G357	C295	C218	G157	G81
G1074	G1074	G1010	C948	A873	U793	G719	G651	G568	C501	G428	U358	U296	C219	U82	U82
C1075	C1075	U1020	A949	G874	A794	C720	G652	G569	G502	U429	U359	G297	G220	G159	U84
G1076	G1076	A1014	U950	C877	C796	A722	U653	A572	G503	A430	G361	A298	U222	A161	U85
U1077	U1077	A1015	G951	C878	C797	U723	A853	A573	C508	A431	G362	G299	U223	A162	U86
U1078	U1078	A1016	U952	C879	A807	U723	A854	A574	C509	A432	G363	A300	C224	C183	A87
U1079	U1079	G1017	G953	C880	G808	A728	C856	G575	A509	A433	U365	A301	C224	C183	C88
A1080	A1080	C1018	G954	G881	C808	G730	C857	G576	A510	U434	G366	G302	U229	C163	C89
U1081	U1081	C1019	U955	G882	A808	G731	U658	C578	C511	U435	U367	G303	G230	C165	C90
G1082	G1082	U1020	U956	C883	C812	G730	U659	C579	U512	C436	U368	G305	G233	G167	C91
U1083	U1083	G1021	U957	C884	U813	G731	G660	U580	G517	U437	C372	G306	C233	U170	U93
U1084	U1084	G1022	U958	C885	A814	A732	G661	U581	G518	U438	A373	G310	C234	U171	G95
U1085	U1085	G1023	A958	G885	A815	A733	A663	U582	C519	A439	A374	G311	C235	A172	G96
U1086	U1086	U1024	U960	G886	A816	G734	A664	U583	A520	A440	U375	C312	G236	U173	U97
G1089	G1089	U1025	U961	G887	C817	G735	A665	G584	G521	C442	G376	A313	G240	G174	C99
U1090	U1090	G1026	C962	U881	C818	C736	G666	G585	C522	C444	G377	C314	G240	C175	A101
U1091	U1091	C1027	G963	A892	A819	A737	G667	C586	A523	G447	G378	A315	A243	C176	G102
U1092	U1092	C1028	A964	C893	U820	A738	G668	G587	G524	A448	C379	A316	U244	C177	C103
A1093	A1093	C1028A	G965	G894	G821	C739	G671	G588	C525	A449	G380	G317	U245	C178	G105
G1094	G1094	C1028B	A966	G895	C822	U740	U672	C589	C526	C449	G381	G318	A246	A179	C106
U1095	U1095	U1029	C967	C896	G823	G741	U673	C590	G527	U450	A382	G319	G247	U180	G107
C1096	C1096	A1032	A968	G897	C824	G742	G673	C591	C528	A451	A383	G320	G247	G181	G108
U1097	U1097	G1032A	A969	G898	G825	U743	G674	G592	G529	A452	G384	A321	A250	U182	A109
C1098	C1098	C970	G971	G902	C826	C744	A675	G593	G530	A453	C385	A322	G251	G183	G110
G1099	G1099	G1033	C972	G903	U827	C745	A676	C596	U531	C454	C385	U323	U252	G184	G111
C1100	C1100	A1035	G973	G906	A828	A746	U677	C597	A532	C455	G386	G324	U253	A185	G112
A1101	A1101	G1036	A974	G906	G829	C747	U678	G597	A533	C456	A389	G325	G254	C186	G113
C1103	C1103	C1037	G976	A909	U831	C748	A684	U598	U534	C457	C390	G326	G255	C186A	U114
G1104	G1104	C1038	G977	C910	G832	C749	G885	C599	A535	C458	G391	A327	U256	C186B	G115
A1105	A1105	C1039	A978	G913	U833	G752	U886	C600	G537	C459	G392	A328	G257	C186C	U116
G1106	G1106	U1040	C979	A913	C834	G753	A887	C601	G538	C460	A393	A329	G257	C186D	U117
C1107	C1107	A1041	C980	A914	U835	G754	G888	U603	G539	C461	G394	C330	G250	C186E	A119
G1108	G1108	G1042	U981	A915	G837	C755	G889	G604	A540	C462	G394	C331	G261	C186F	A120
C1109	C1109	C1043	U982	A918	C837	C756	G890	U605	G541	C463	A397	G332	U262	C187	C121
A1110	A1110	U1043	A983	A918	U841	C757	G891	G606	G542	G475	C396	G333	A262	U188	G122
C1112	C1112	G1048	C985	U920	C842	A759	U892	G606	C543	G476	G399	C334	A263	G189	U129
G1113	G1113	U1049	A986	U921	U843	G760	A694	G607	G544	C477	C401	C335	G265	G191A	G128
C1115	C1115	G1050	G987	G922	C848	G763	A695	A622	C545	C479	C403	C337	G267	G191B	G129
G1116	G1116	C1051	U991	A923	U850	C764	A696	C623	A547	U480	U404	C338	C268	G191C	A130
C1117	C1117	U1052	U992	G924	G851	C765	G698	C624	G548	G481	U405	C339	C269	U191D	C131
G1118	G1118	G1053	U993	G925	G852	A766	G699	G625	C549	A482	C406	C341	A270	U191E	C132
C1119	C1119	A1055	A994	G926	G853	A767	C701	U626	U552	C483	G407	C342	C271	U191F	U133
G1120	G1120	U1056	G995	G927	G854	A768	A702	G627	A553	G484	A408	U343	C272	G191	A134
U1121	U1121	C1059	G996	C932	G858	G769	G703	G629	C554	G485	G409	A344	A273	U192	C135
C1122	C1122	G1060	G998	G933	A859	G775	A705	G630	C555	U486	G410	C345	A274	C193	C136
A1123	A1123	U1061	C998A	C934	A860	G776	U706	A632	C557	A487	A411	G346	G276	C194	A143
												G347	G277	A196	G144
												G348	G278	A197	





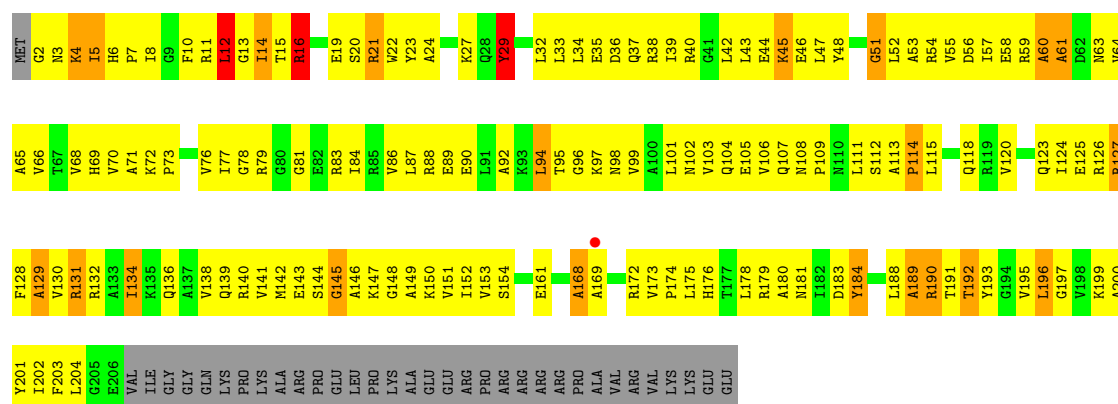
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF: 16% 53% 15% 14%



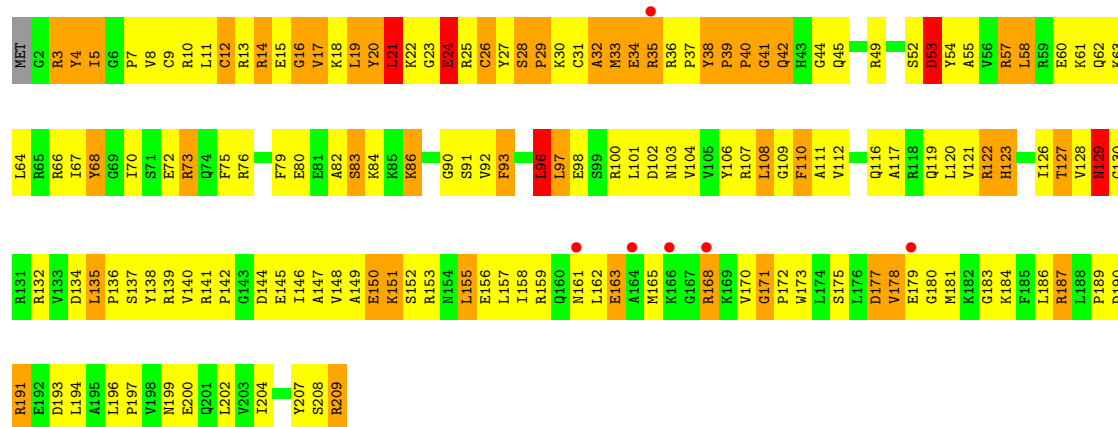
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF: 22% 54% 9% 14%

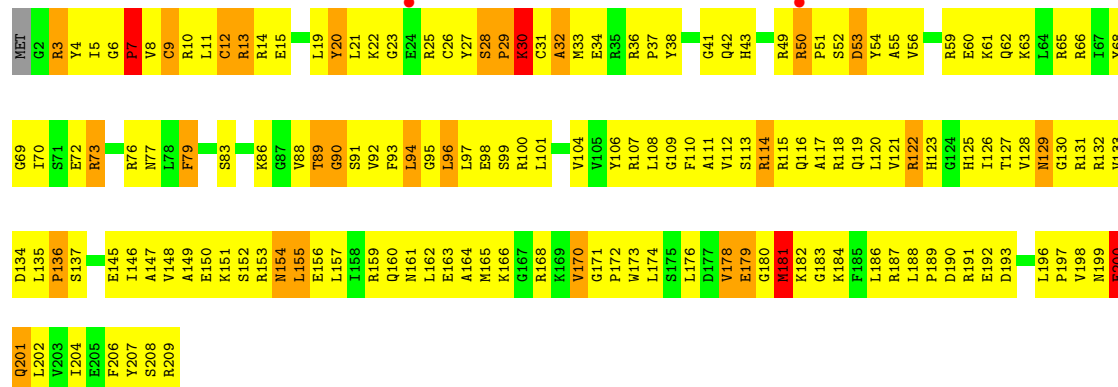


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

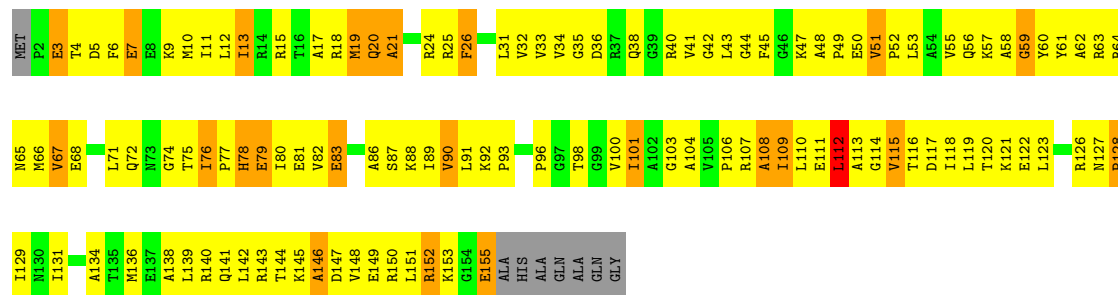
Chain AG: 3% 25% 50% 22%



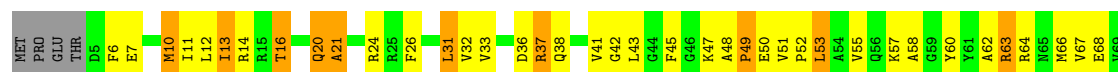
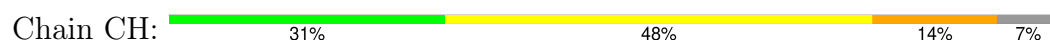
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

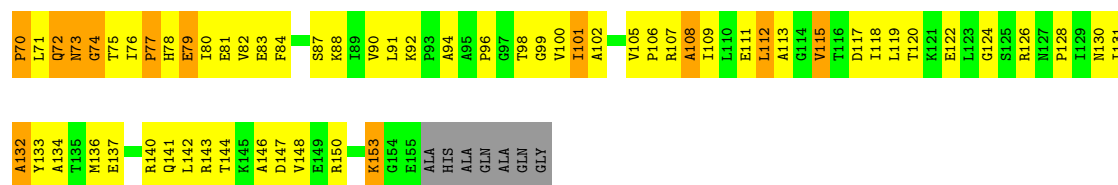


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

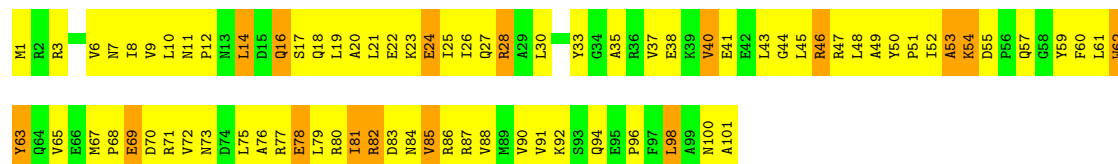


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

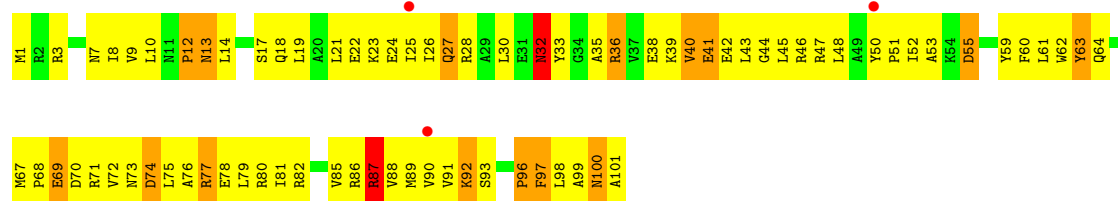




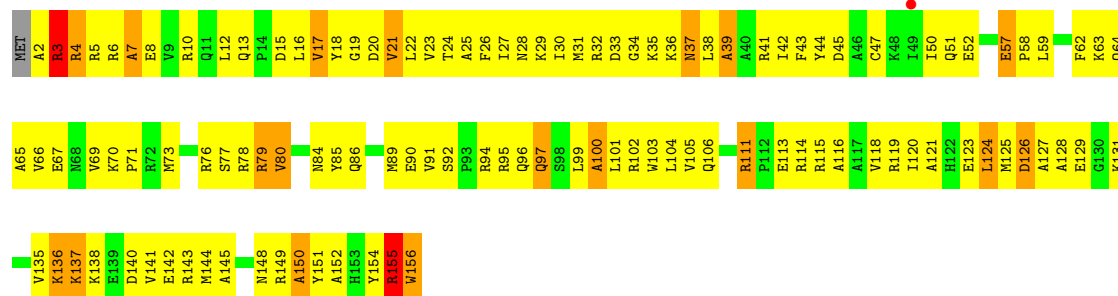
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



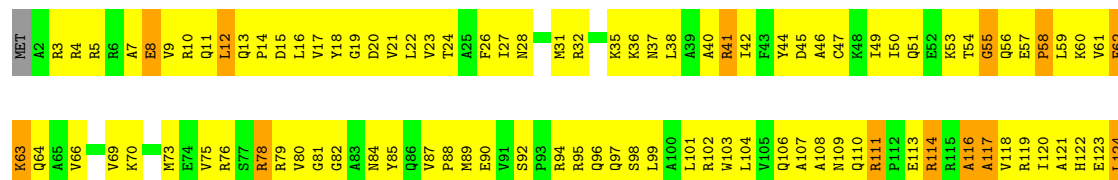
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



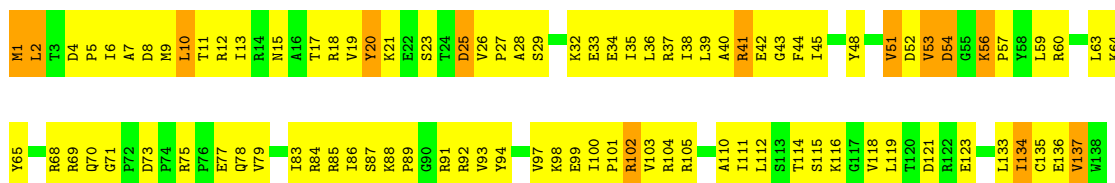
• Molecule 7: 30S RIBOSOMAL PROTEIN S7





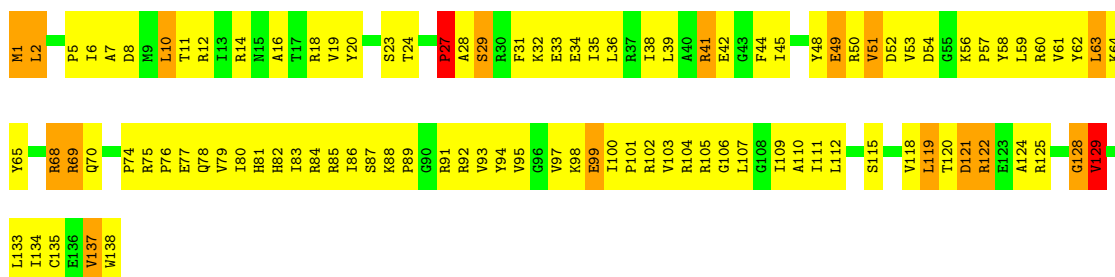
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK: 32% 59% 9%



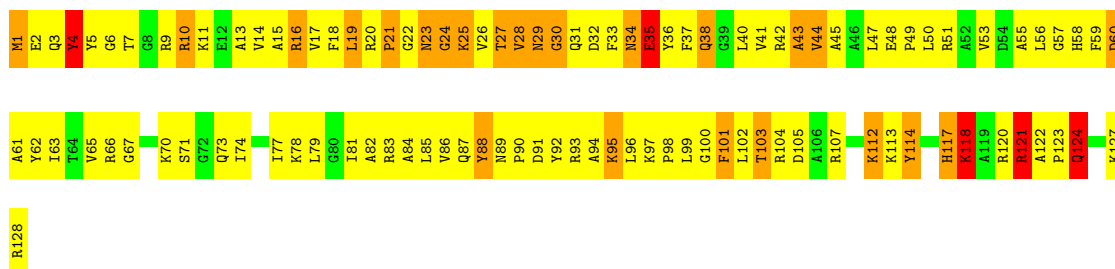
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK: 26% 61% 12%



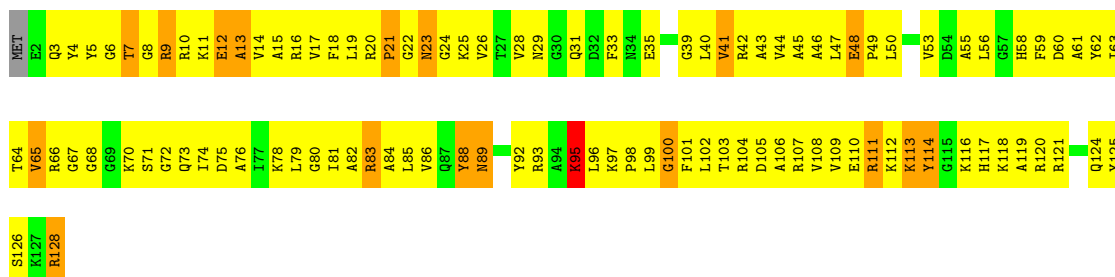
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL: 18% 59% 19%

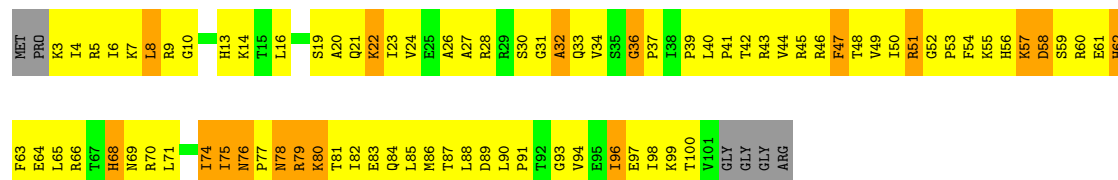


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

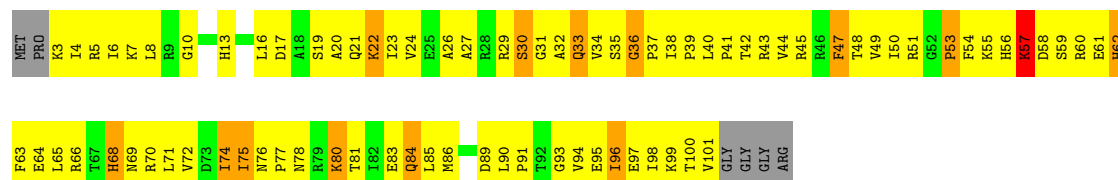
Chain CL: 17% 68% 13%



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM: 

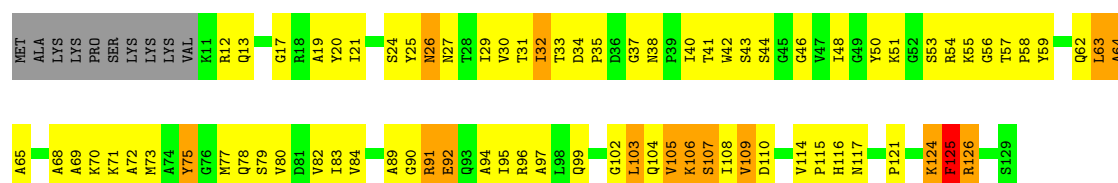
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM: 

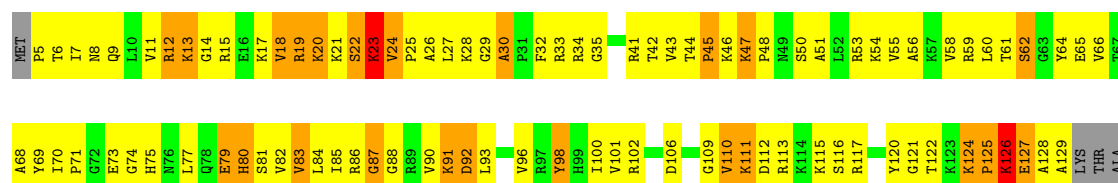
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AN: 

• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN: 

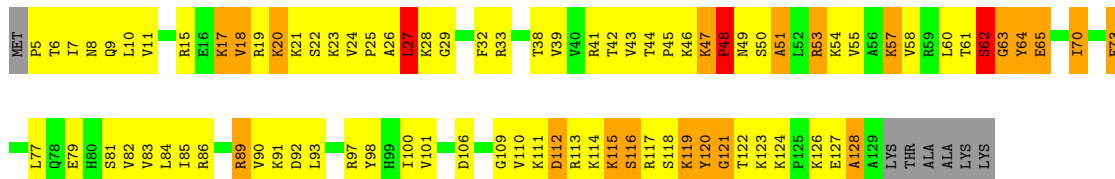
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO: 

ALA
LYS
LYS

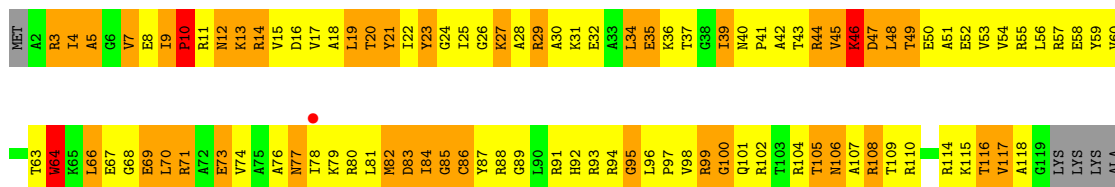
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO: 30% 48% 15% 5%



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

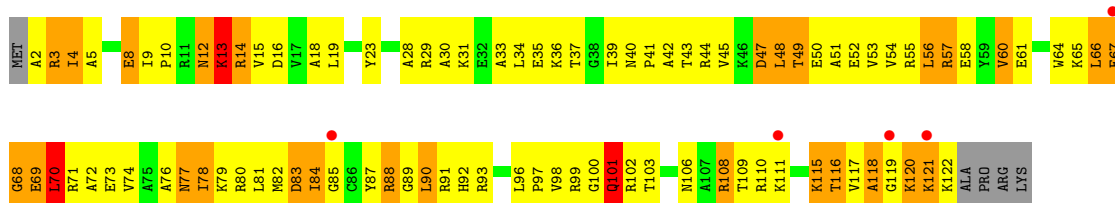
Chain AP: 12% 47% 33% 6%



PRO
ARG
LYS

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP: 4% 21% 51% 21% . .



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ: 28% 59% 8% . .

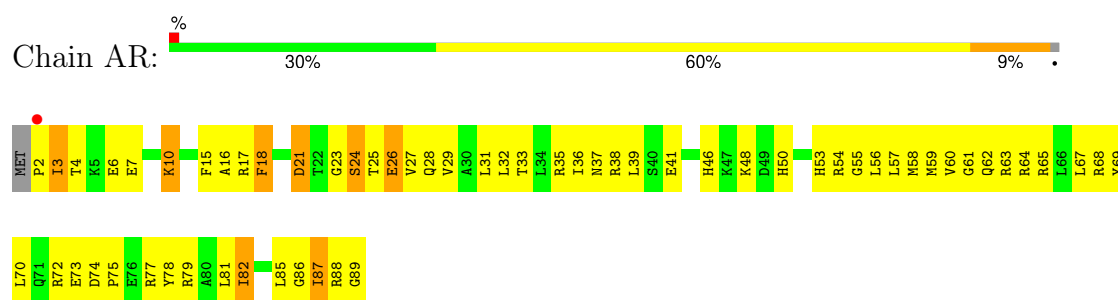


• Molecule 14: 30S RIBOSOMAL PROTEIN S14

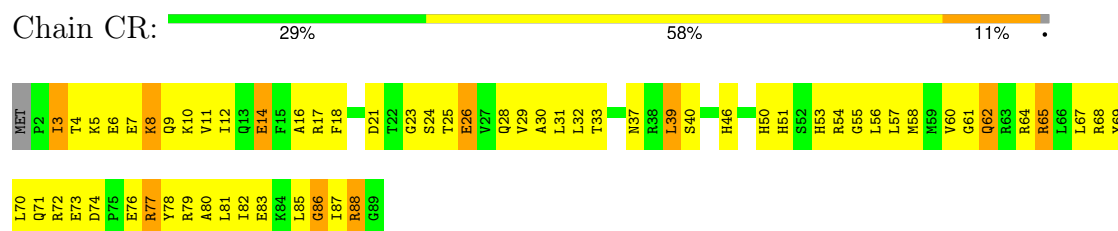
Chain CQ: 18% 57% 16% 7% .



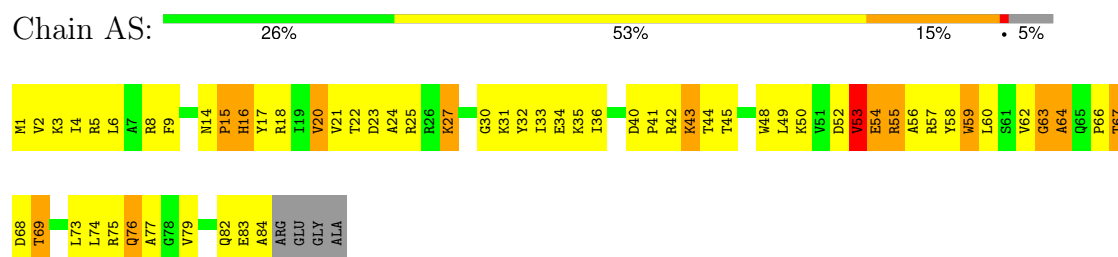
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



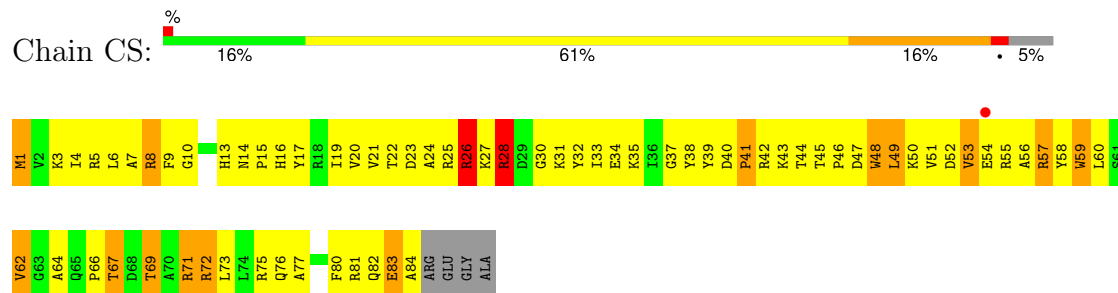
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



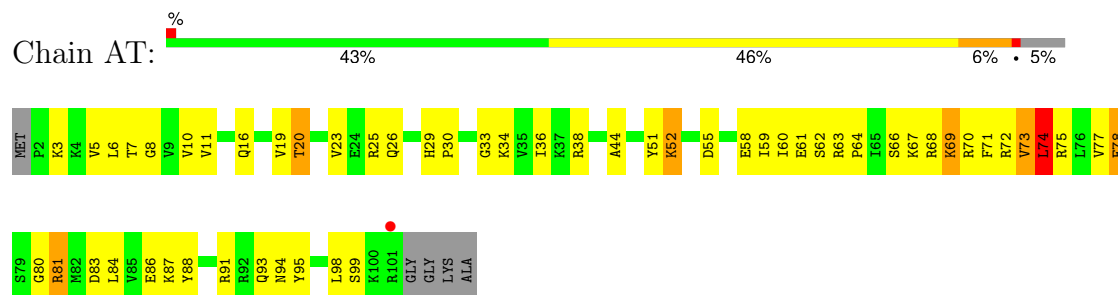
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



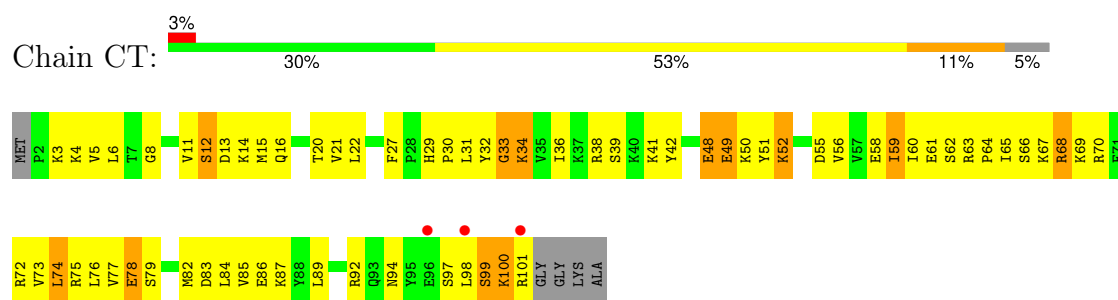
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



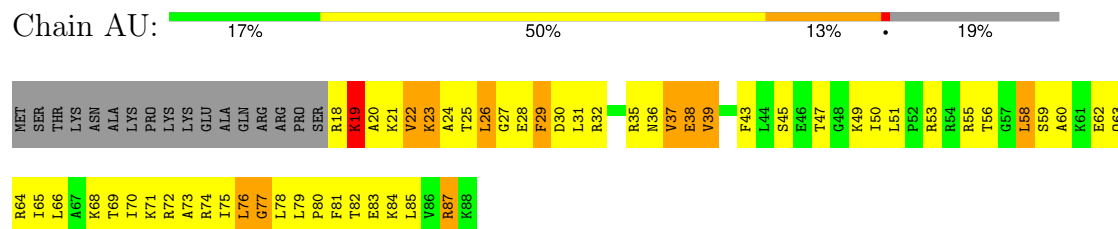
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



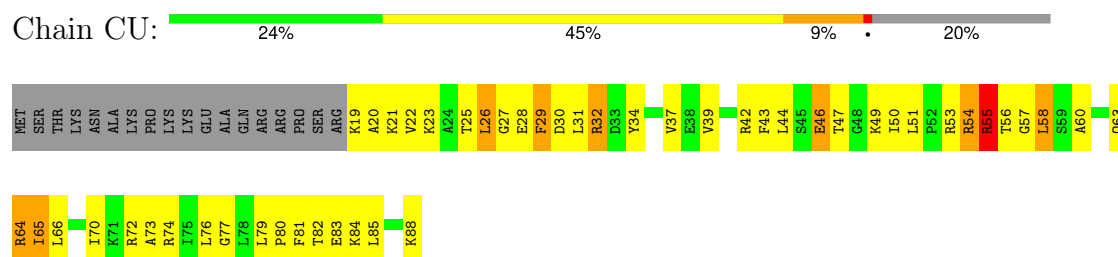
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



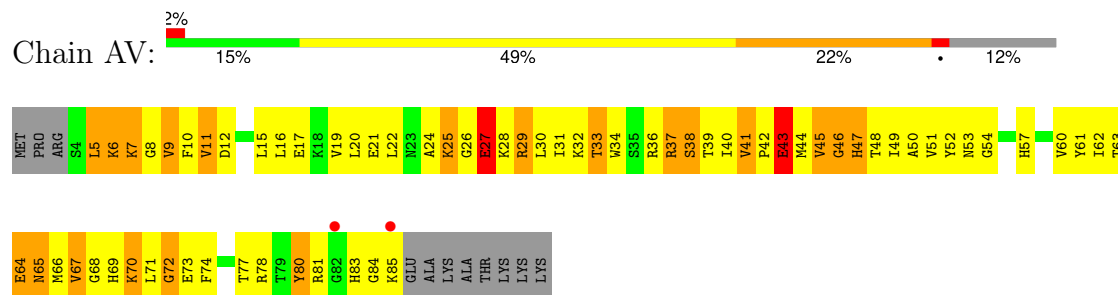
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



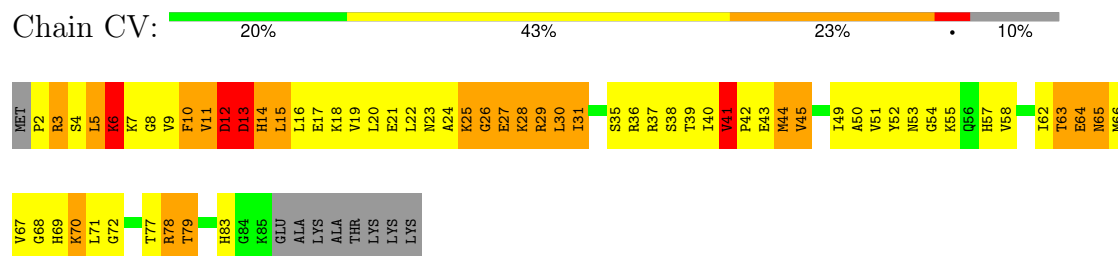
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

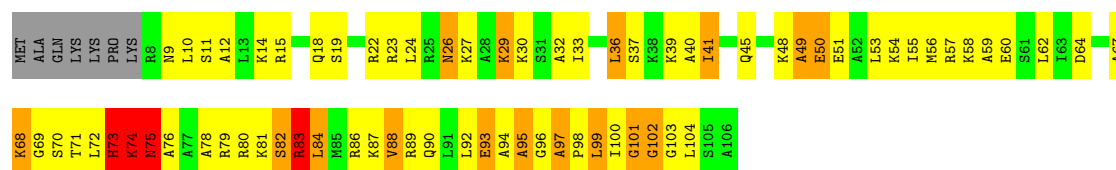


• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW: 



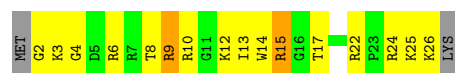
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW: 



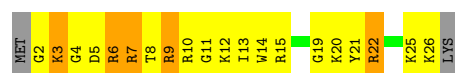
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX: 



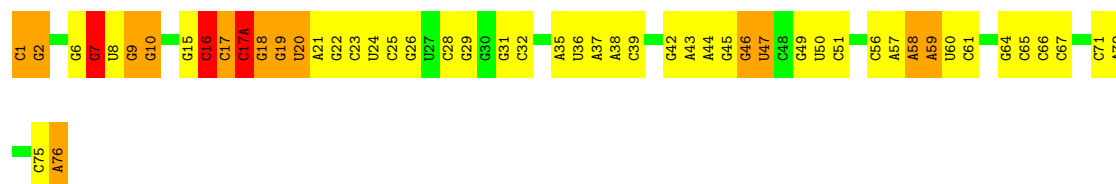
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX: 

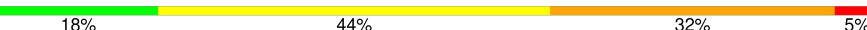


• Molecule 22: TRNA FMET (UNMODIFIED BASES)

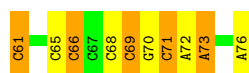
Chain AC: 



• Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain AD: 

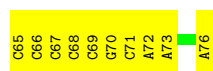
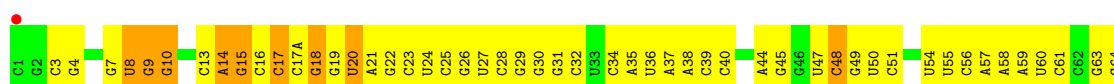




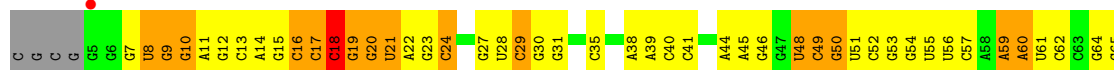
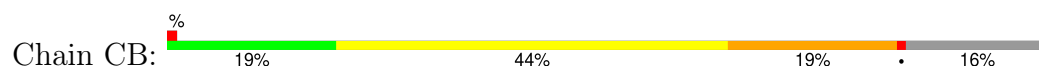
• Molecule 22: TRNA FMET (UNMODIFIED BASES)



• Molecule 22: TRNA FMET (UNMODIFIED BASES)



• Molecule 22: TRNA FMET (UNMODIFIED BASES)



• Molecule 23: MRNA



• Molecule 23: MRNA



• Molecule 24: 23S ribosomal RNA

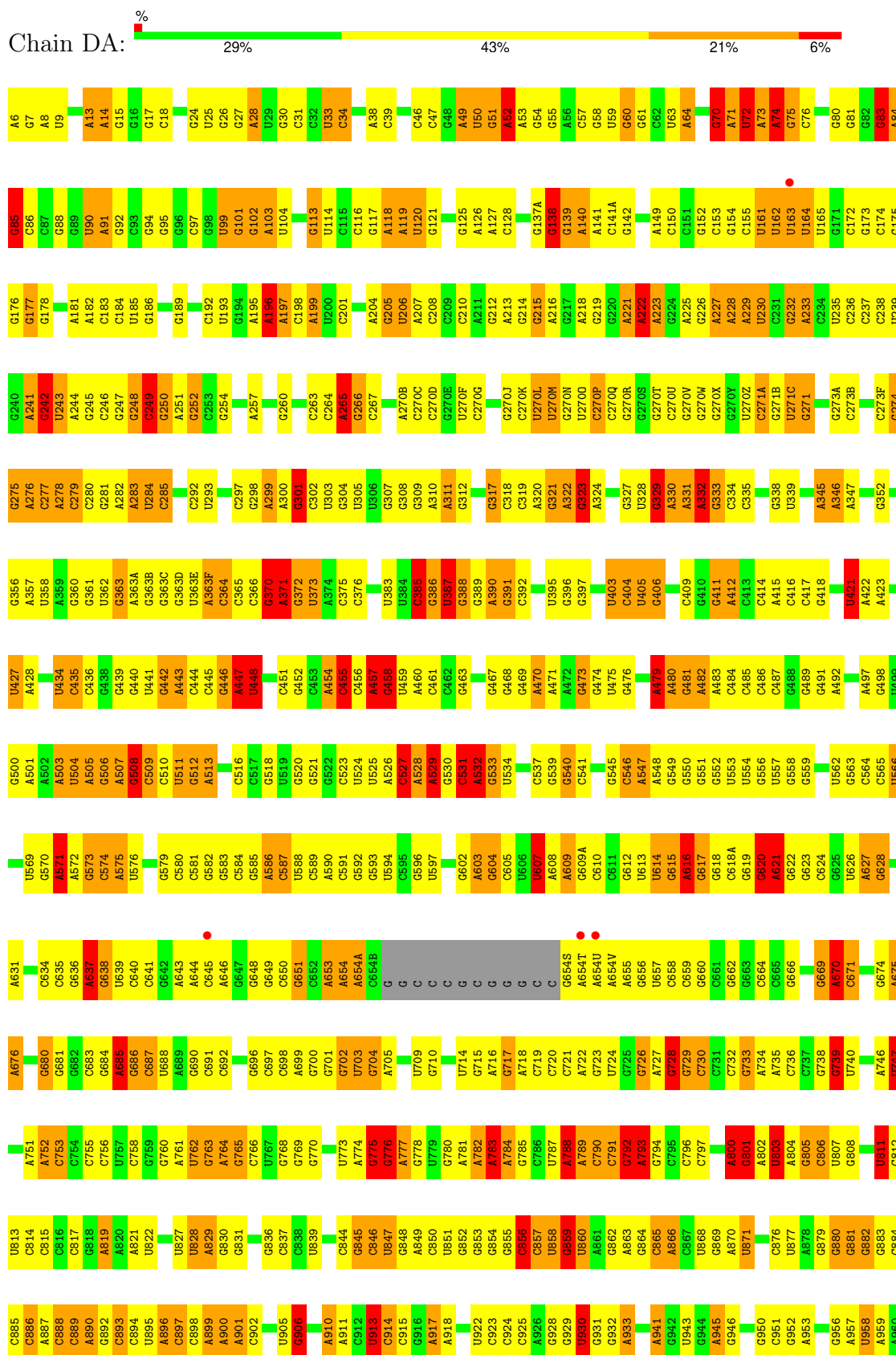




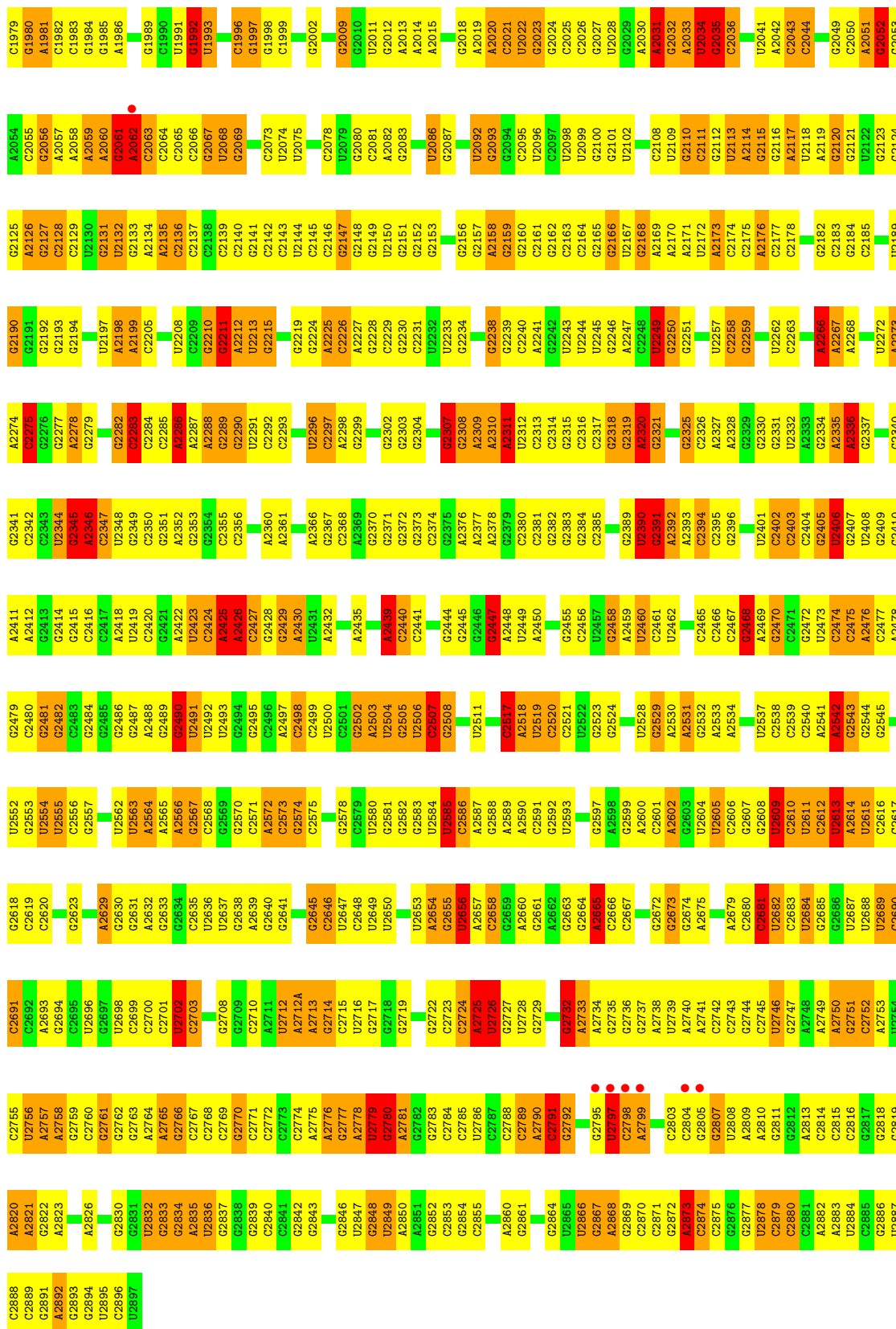
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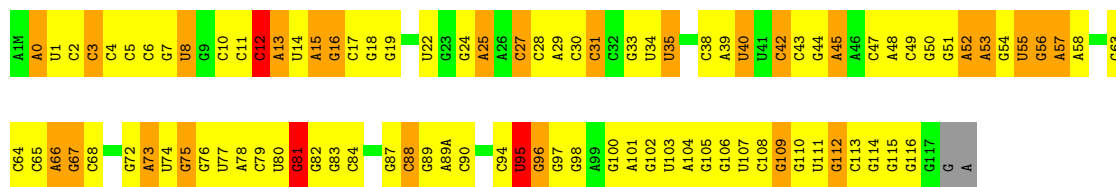


WORLDWIDE
PDB
PROTEIN DATA BANK



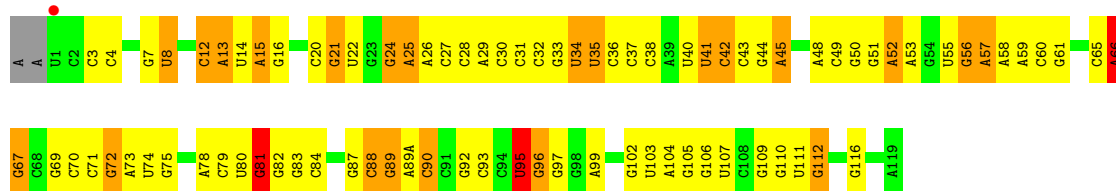
- Molecule 25: 5S ribosomal RNA

Chain BB: 20% 54% 21% ..



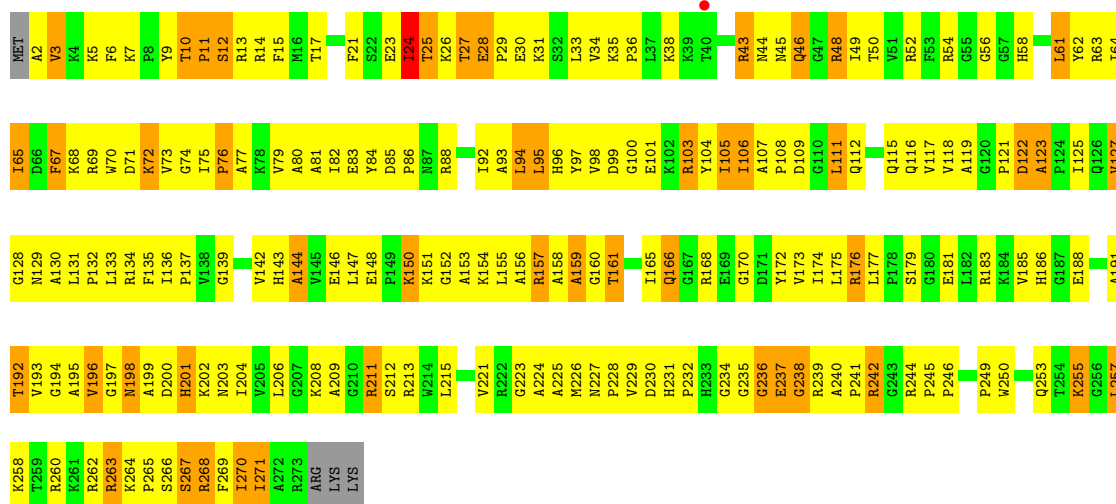
• Molecule 25: 5S ribosomal RNA

Chain DB: 29% 49% 18% ..



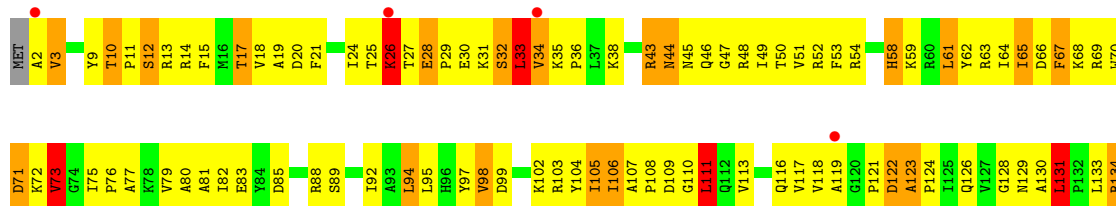
• Molecule 26: 50S ribosomal protein L2

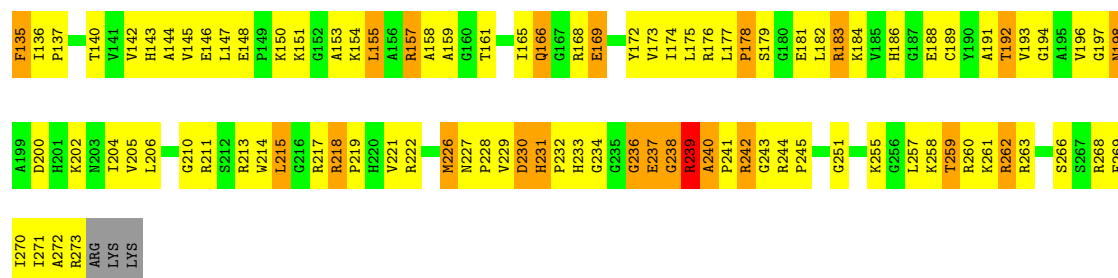
Chain BD: 26% 55% 17% ..



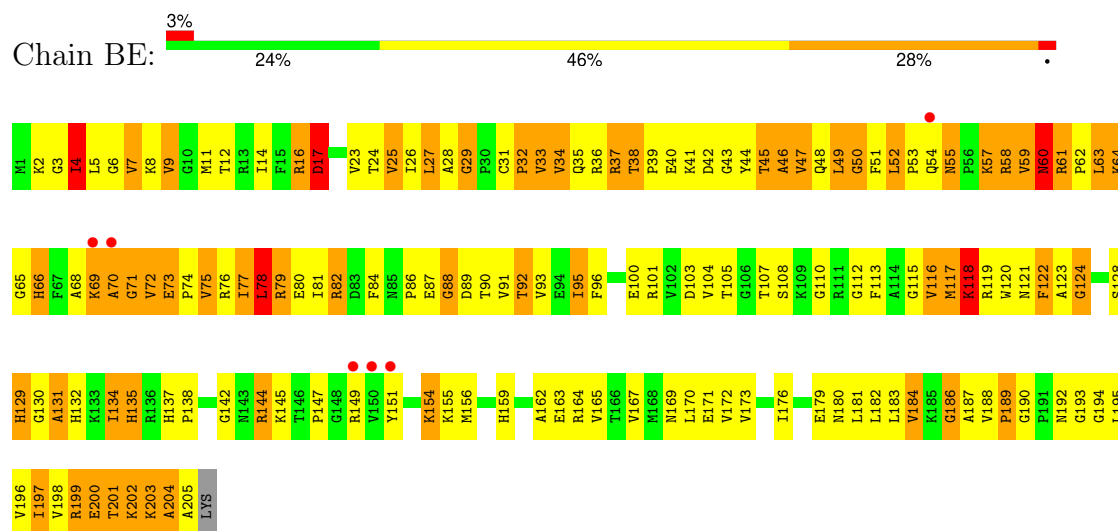
• Molecule 26: 50S ribosomal protein L2

Chain DD: 28% 53% 15% ..

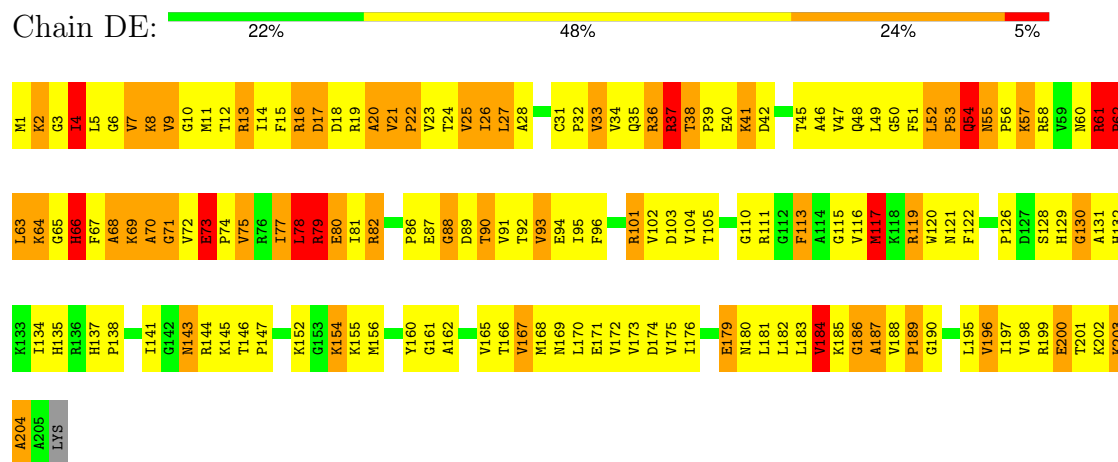




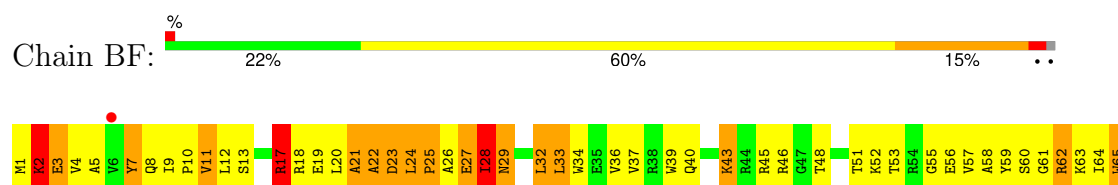
• Molecule 27: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L3



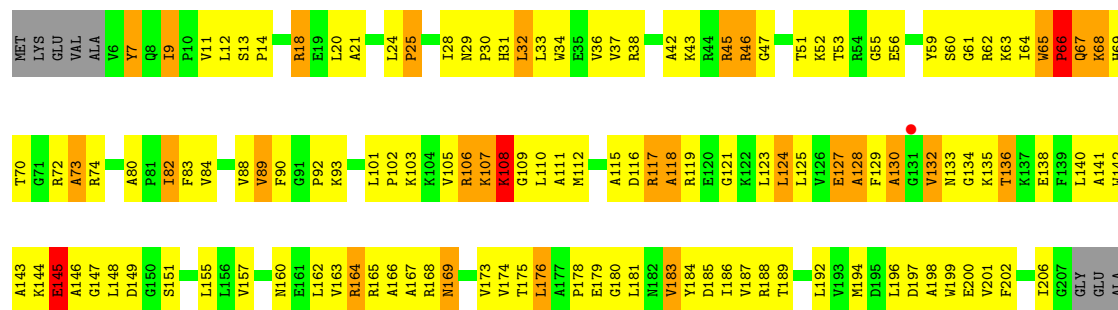
• Molecule 28: 50S ribosomal protein L4





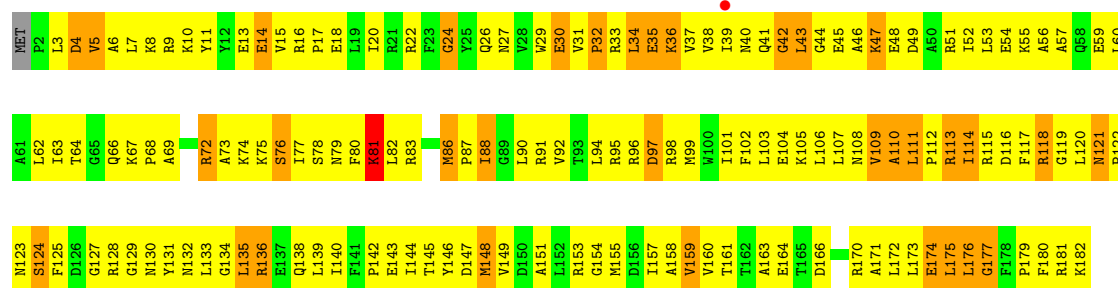
• Molecule 28: 50S ribosomal protein L4

Chain DF: 33% 49% 13% . .



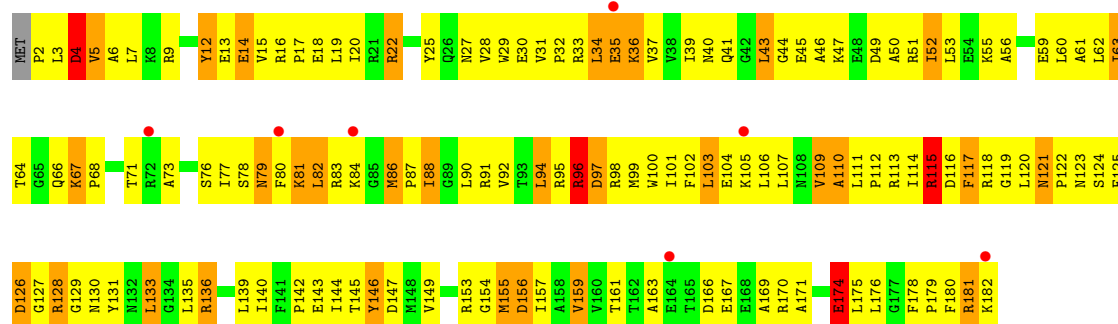
• Molecule 29: 50S ribosomal protein L5

Chain BG: 16% 64% 18% . .

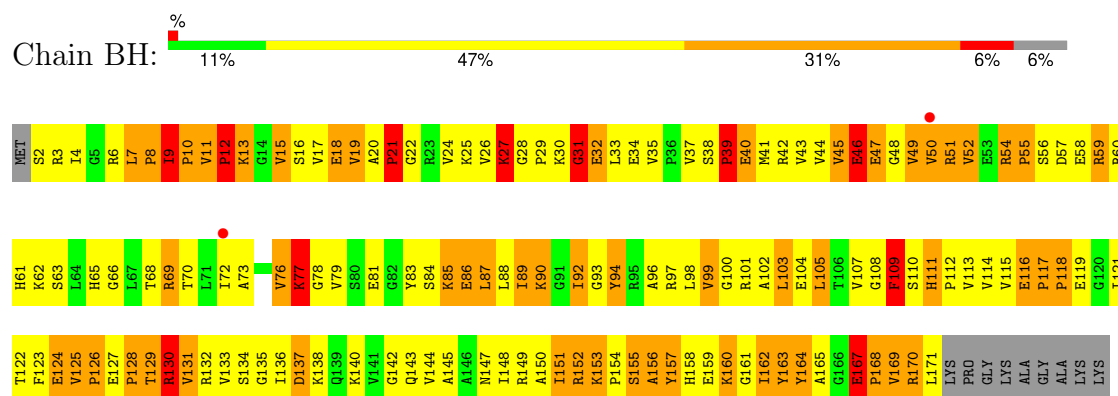


• Molecule 29: 50S ribosomal protein L5

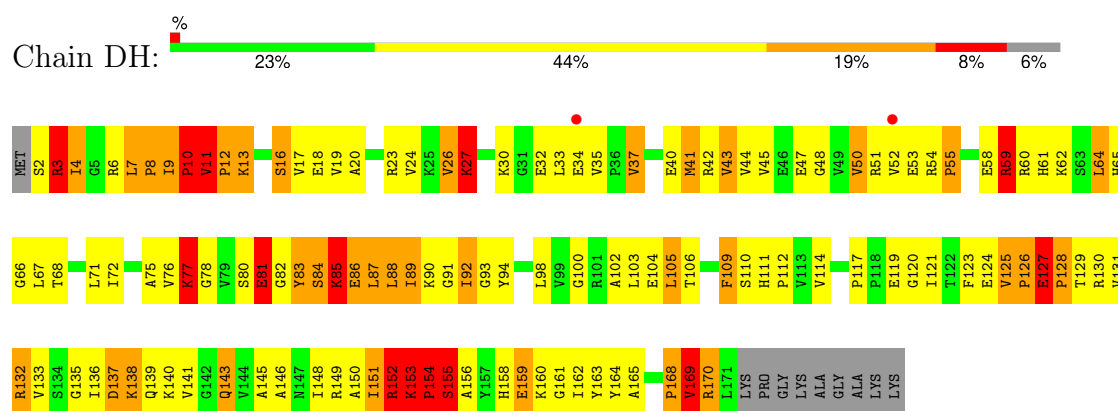
Chain DG: 4% 23% 57% 18% . .



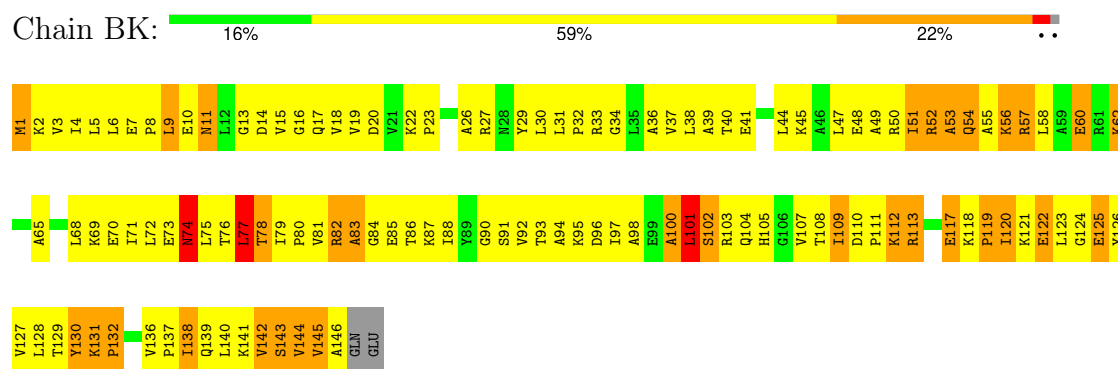
- Molecule 30: 50S ribosomal protein L6



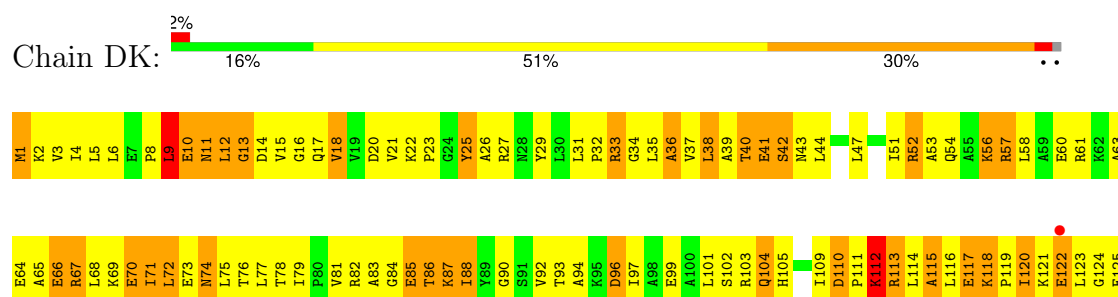
- Molecule 30: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L9

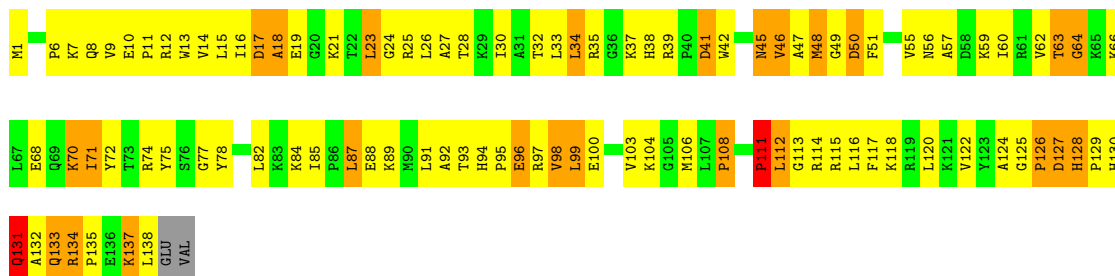


- Molecule 31: 50S ribosomal protein L9

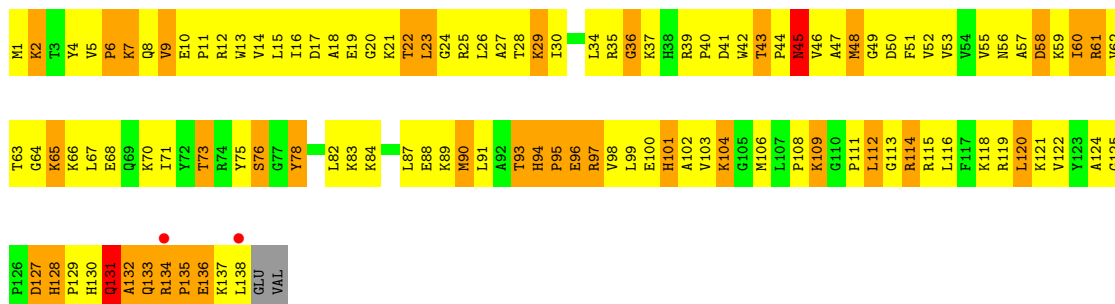
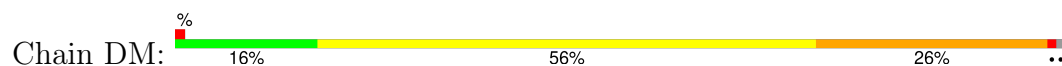




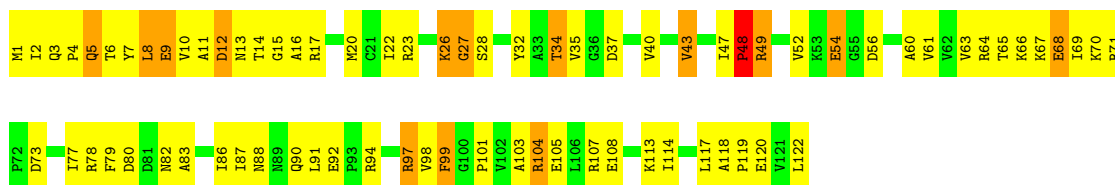
• Molecule 32: 50S ribosomal protein L13



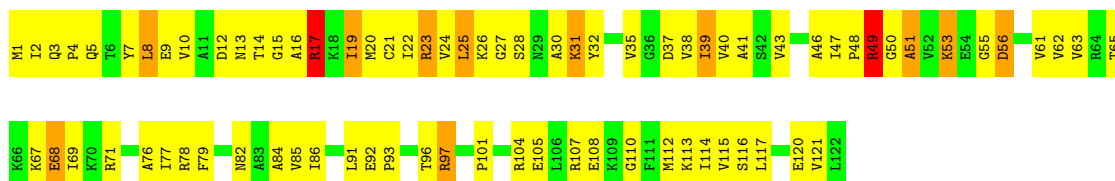
• Molecule 32: 50S ribosomal protein L13



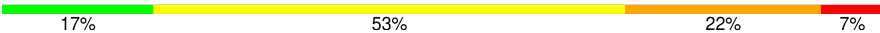
• Molecule 33: 50S ribosomal protein L14

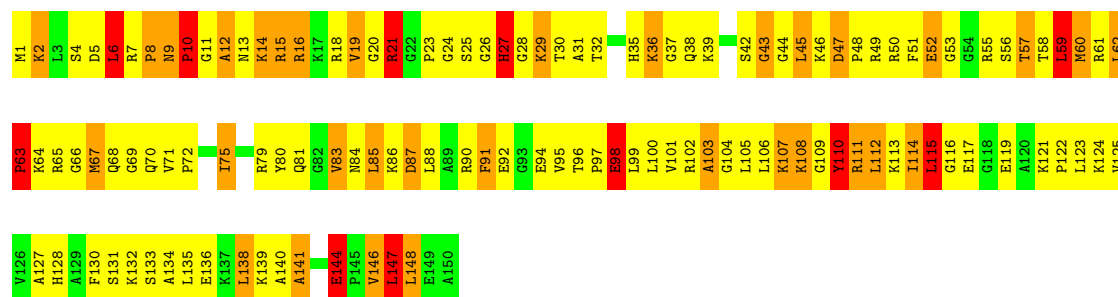


• Molecule 33: 50S ribosomal protein L14




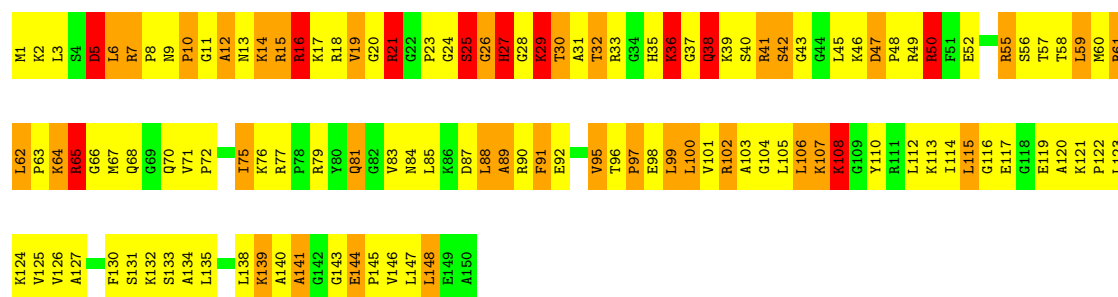
- Molecule 34: 50S ribosomal protein L15

Chain BO: 



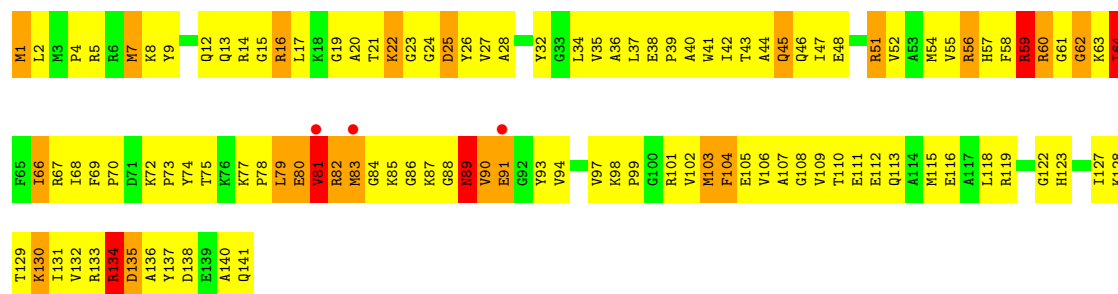
- Molecule 34: 50S ribosomal protein L15

Chain DO: 



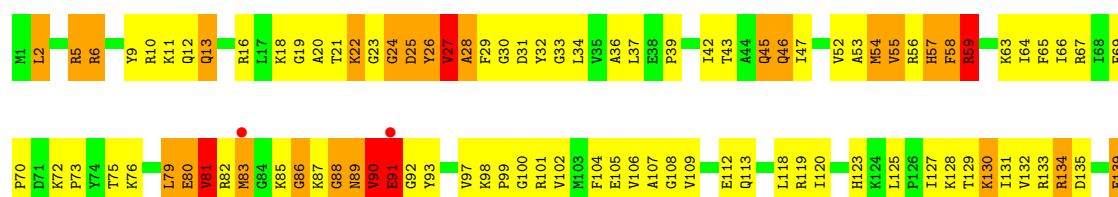
- Molecule 35: 50S ribosomal protein L16

Chain BP: 



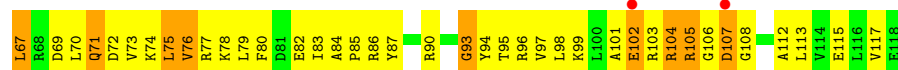
- Molecule 35: 50S ribosomal protein L16

Chain DP: 

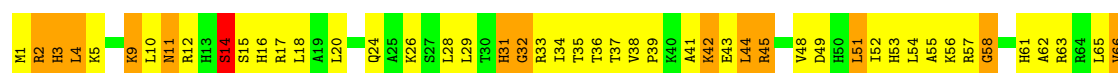




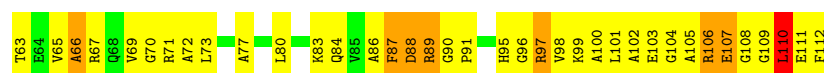
• Molecule 36: 50S ribosomal protein L17



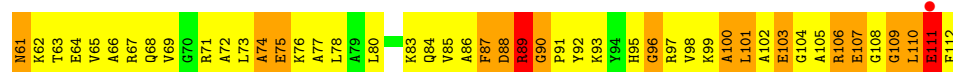
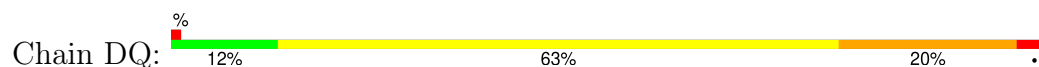
• Molecule 36: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L18

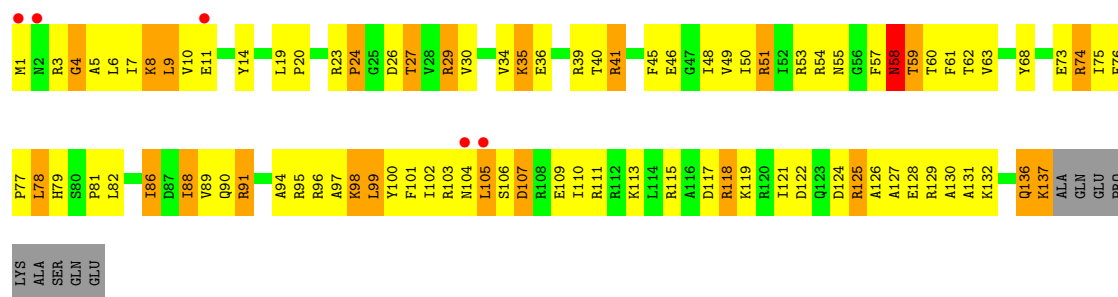


• Molecule 37: 50S ribosomal protein L18

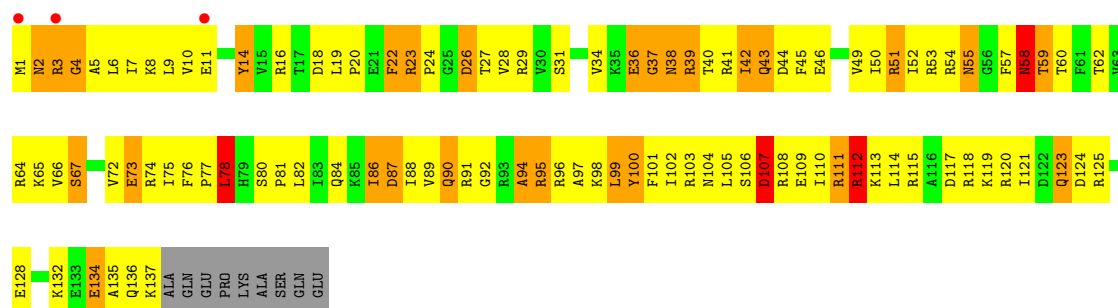


• Molecule 38: 50S ribosomal protein L19

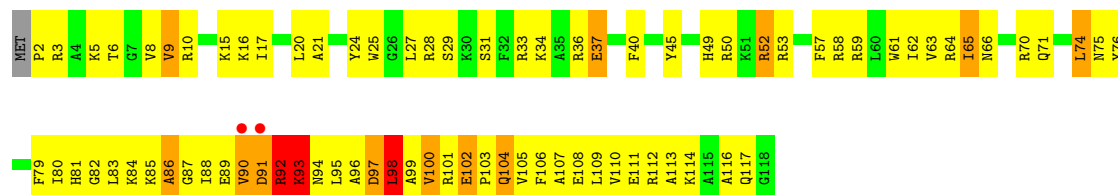




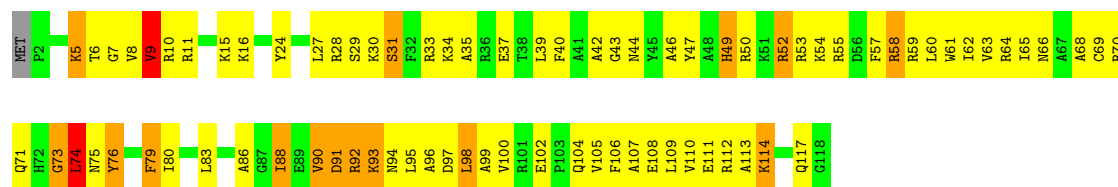
• Molecule 38: 50S ribosomal protein L19



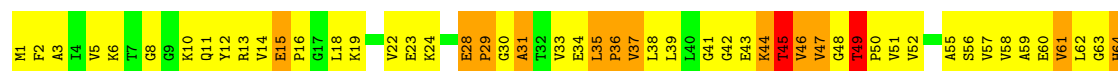
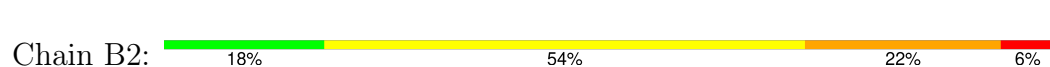
• Molecule 39: 50S ribosomal protein L20



• Molecule 39: 50S ribosomal protein L20

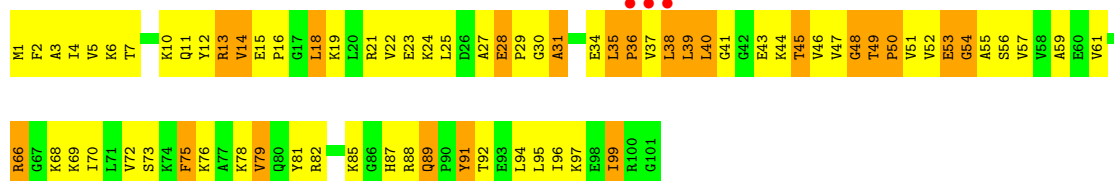


• Molecule 40: 50S ribosomal protein L21

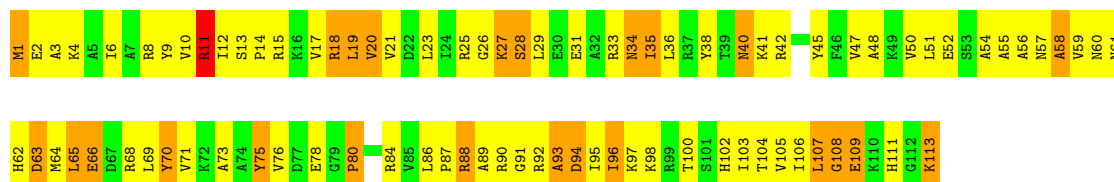




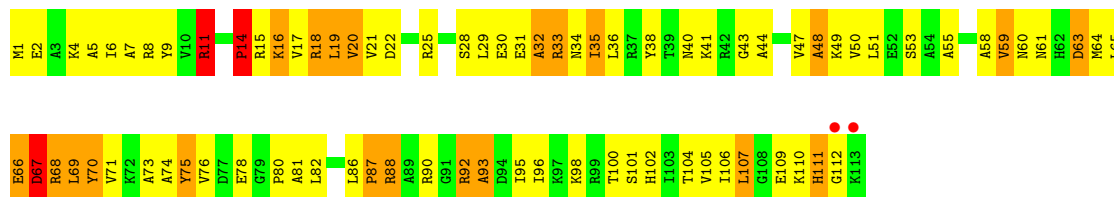
- Molecule 40: 50S ribosomal protein L21



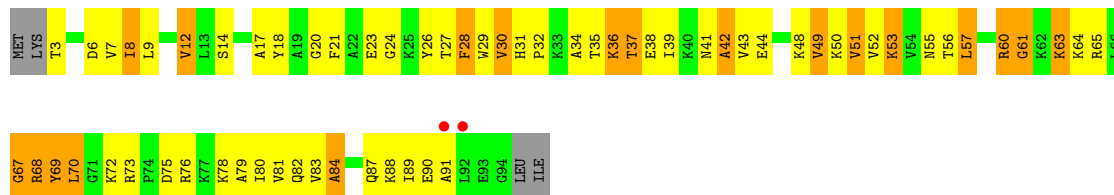
- Molecule 41: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L22

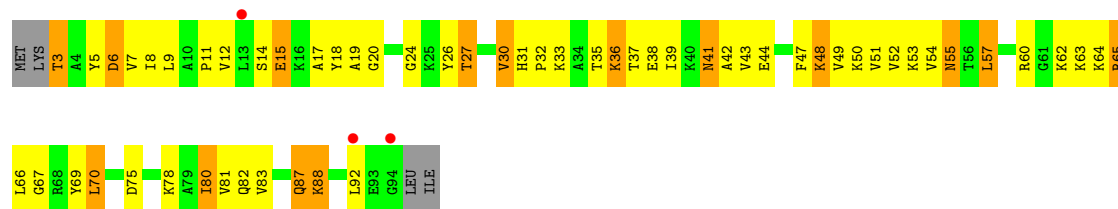


- Molecule 42: 50S ribosomal protein L23

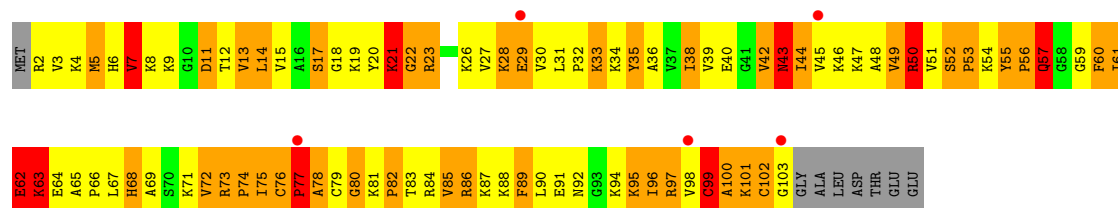


- Molecule 42: 50S ribosomal protein L23

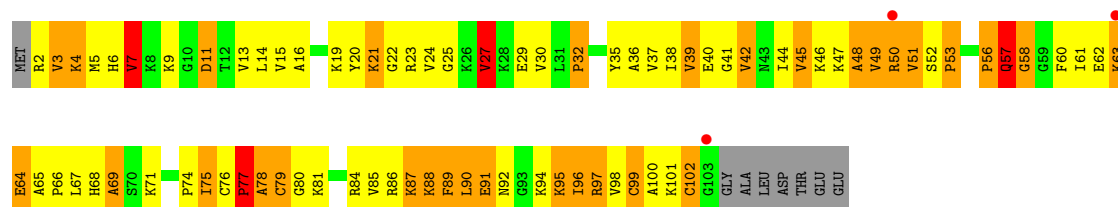
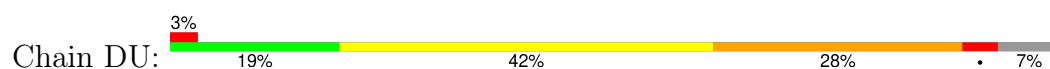




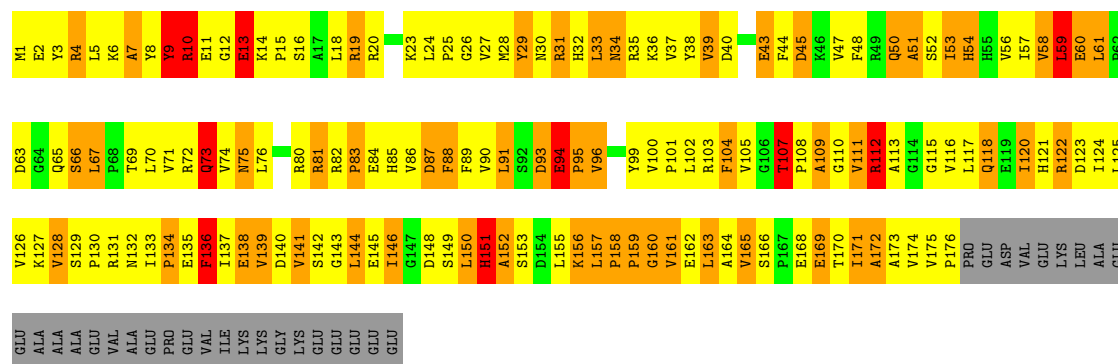
• Molecule 43: 50S ribosomal protein L24



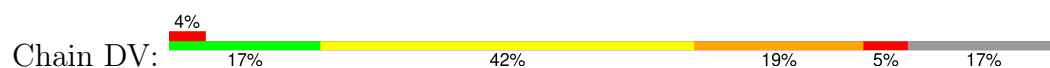
• Molecule 43: 50S ribosomal protein L24

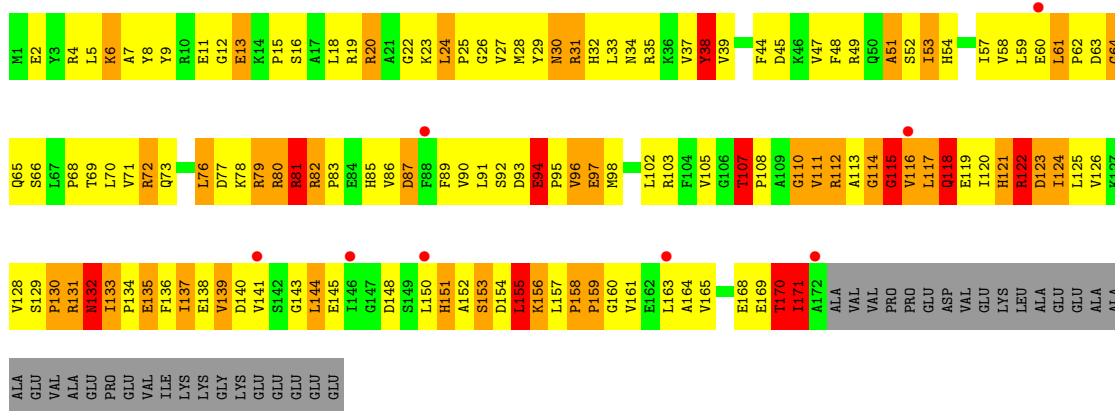


• Molecule 44: 50S ribosomal protein L25



• Molecule 44: 50S ribosomal protein L25

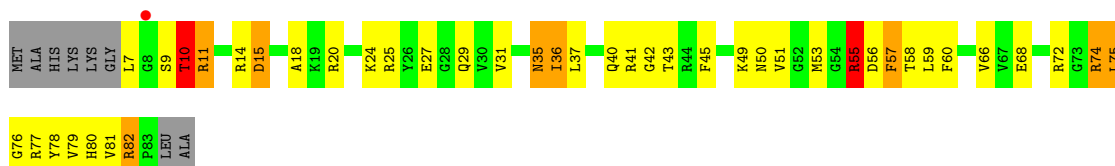




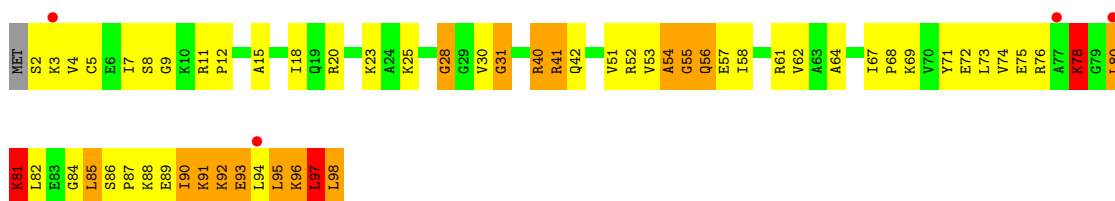
- Molecule 45: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L27

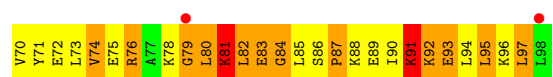


- Molecule 46: 50S ribosomal protein L28

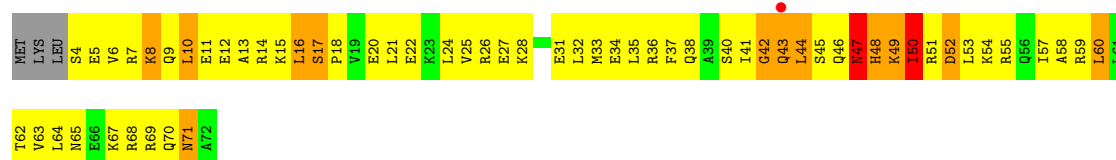
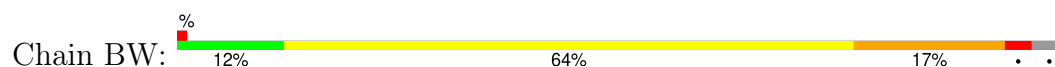


- Molecule 46: 50S ribosomal protein L28

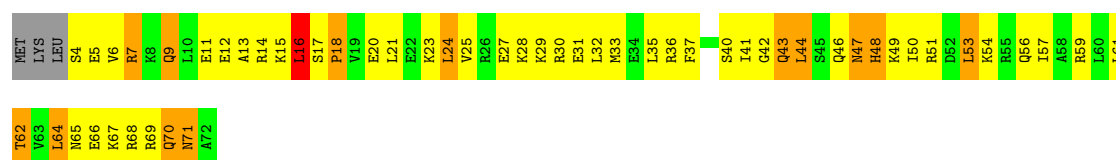




- Molecule 47: 50S ribosomal protein L29



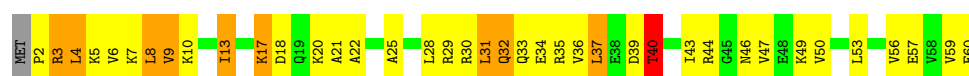
- Molecule 47: 50S ribosomal protein L29



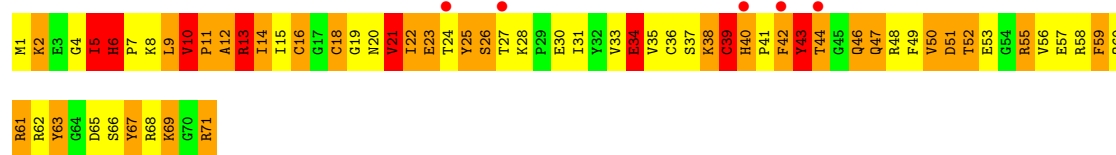
- Molecule 48: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L30

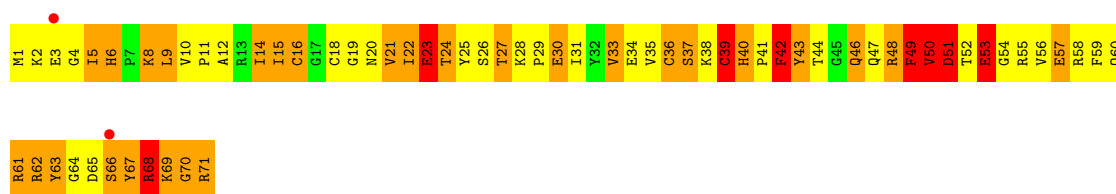


- Molecule 49: 50S ribosomal protein L31

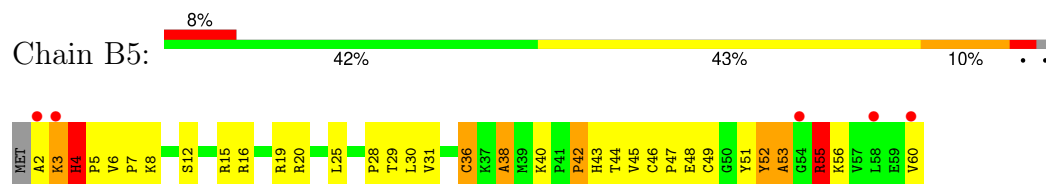


- Molecule 49: 50S ribosomal protein L31

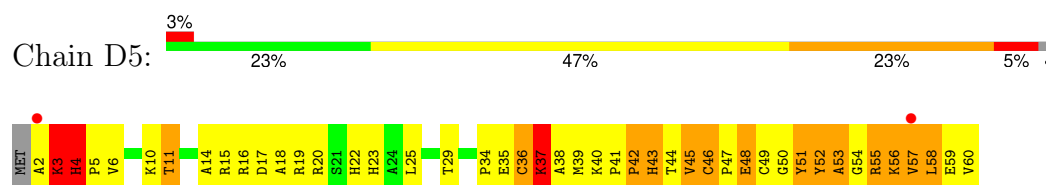




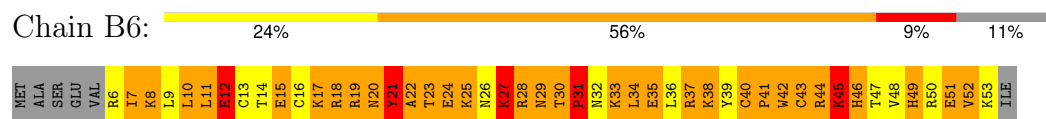
• Molecule 50: 50S ribosomal protein L32



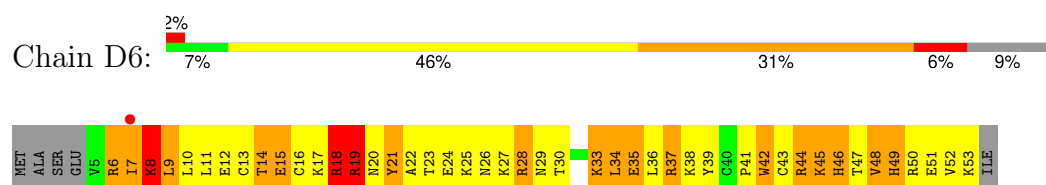
• Molecule 50: 50S ribosomal protein L32



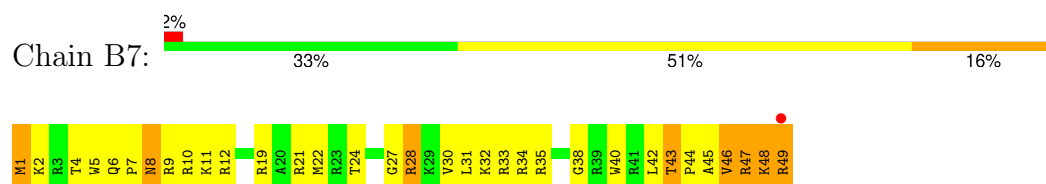
• Molecule 51: 50S ribosomal protein L33



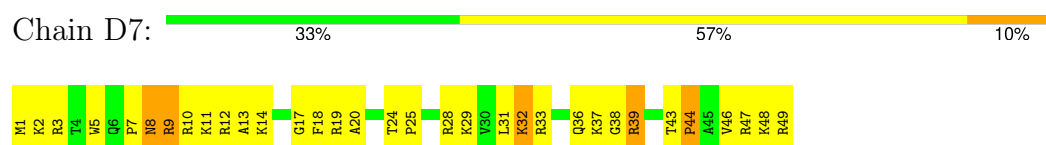
• Molecule 51: 50S ribosomal protein L33



• Molecule 52: 50S ribosomal protein L34



• Molecule 52: 50S ribosomal protein L34



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| E65 | ME1 | P2 | K3 | M4 | K5 | T6 | G9 | A10 | K11 | K12 | R13 | V14 | K15 | I16 | T17 | G20 | K21 | V22 | M25 | K26 | T27 | G28 | K29 | R30 | H31 | L32 | K33 | W34 | Q35 | K36 | K39 | E40 | T41 | R42 | Q43 | K44 | G45 | R46 | K47 | F48 | V49 | L50 | A51 | K52 | P53 | E54 | A55 | E56 | B57 | I58 | K59 | L60 | L61 | L62 | P63 | Y64 |
|-----|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 452.18Å 626.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 3.50 300.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-3.50) 100.0 (300.00-3.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.252 0.212 , 0.215	Depositor DCC
R_{free} test set	22133 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298428	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1808	2
1	CA	32554	0	16428	1772	16
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	120	0
22	CB	1385	0	704	63	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	3010	2
24	DA	62151	0	31309	2757	0
25	BB	2572	0	1305	184	0
25	DB	2573	0	1305	138	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	16
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	18

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:C2	24:BA:654(R):C:C5'	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 18 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:125:VAL:CG2	1:CA:84:U:C6[3_545]	1.17	1.03
30:BH:126:PRO:CD	1:CA:82:U:O3'[3_545]	1.41	0.79
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

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	6
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	5
5	AH	152/162 (94%)	103 (68%)	34 (22%)	15 (10%)	0	6
5	CH	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	6
6	AI	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	10
6	CI	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	7
7	AJ	153/156 (98%)	95 (62%)	42 (28%)	16 (10%)	0	5
7	CJ	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	6
8	AK	136/138 (99%)	98 (72%)	29 (21%)	9 (7%)	1	11
8	CK	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
9	AL	126/128 (98%)	71 (56%)	36 (29%)	19 (15%)	0	2
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	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CM	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	6
11	AN	119/129 (92%)	76 (64%)	29 (24%)	14 (12%)	0	4
11	CN	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
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	5
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	6
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	17
15	CR	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	10
16	AS	82/88 (93%)	57 (70%)	16 (20%)	9 (11%)	0	5
16	CS	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
17	AT	98/105 (93%)	75 (76%)	17 (17%)	6 (6%)	1	13
17	CT	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	8
18	AU	69/88 (78%)	42 (61%)	21 (30%)	6 (9%)	0	7
18	CU	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	4
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	1
21	AX	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	2	19
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	5
26	DD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	9
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	6
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	2
31	DK	144/148 (97%)	80 (56%)	36 (25%)	28 (19%)	0	1
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	13
33	DN	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	9
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	3
35	DP	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	5
36	B0	115/118 (98%)	73 (64%)	31 (27%)	11 (10%)	0	6
36	D0	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
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	9
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	6
39	D1	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	8
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	6
41	BS	111/113 (98%)	79 (71%)	20 (18%)	12 (11%)	0	5
41	DS	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	BT	90/96 (94%)	63 (70%)	18 (20%)	9 (10%)	0	6
42	DT	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	14
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	8
46	BZ	95/98 (97%)	66 (70%)	17 (18%)	12 (13%)	0	4
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	3
48	BX	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	3	24
48	DX	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	14
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	5
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	19
52	D7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	12
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%)	1	9
2	CE	205/220 (93%)	181 (88%)	24 (12%)	4	21
3	AF	160/188 (85%)	141 (88%)	19 (12%)	4	21
3	CF	159/188 (85%)	145 (91%)	14 (9%)	8	31
4	AG	180/181 (99%)	152 (84%)	28 (16%)	2	13
4	CG	180/181 (99%)	163 (91%)	17 (9%)	7	29
5	AH	119/123 (97%)	102 (86%)	17 (14%)	2	16
5	CH	116/123 (94%)	106 (91%)	10 (9%)	8	32
6	AI	90/90 (100%)	80 (89%)	10 (11%)	5	23
6	CI	90/90 (100%)	76 (84%)	14 (16%)	2	13
7	AJ	126/127 (99%)	114 (90%)	12 (10%)	7	28
7	CJ	126/127 (99%)	115 (91%)	11 (9%)	8	31
8	AK	119/119 (100%)	112 (94%)	7 (6%)	16	44
8	CK	119/119 (100%)	106 (89%)	13 (11%)	5	24
9	AL	99/99 (100%)	80 (81%)	19 (19%)	1	6
9	CL	98/99 (99%)	87 (89%)	11 (11%)	5	22
10	AM	89/92 (97%)	80 (90%)	9 (10%)	6	26
10	CM	89/92 (97%)	81 (91%)	8 (9%)	8	30
11	AN	92/99 (93%)	83 (90%)	9 (10%)	6	27
11	CN	90/99 (91%)	81 (90%)	9 (10%)	6	26
12	AO	104/109 (95%)	92 (88%)	12 (12%)	4	22
12	CO	104/109 (95%)	90 (86%)	14 (14%)	3	18
13	AP	94/101 (93%)	75 (80%)	19 (20%)	1	5
13	CP	97/101 (96%)	81 (84%)	16 (16%)	2	11
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	6	26
14	CQ	49/50 (98%)	42 (86%)	7 (14%)	2	16
15	AR	79/80 (99%)	74 (94%)	5 (6%)	15	42
15	CR	79/80 (99%)	73 (92%)	6 (8%)	11	35
16	AS	72/74 (97%)	63 (88%)	9 (12%)	3	19
16	CS	72/74 (97%)	63 (88%)	9 (12%)	3	19
17	AT	95/97 (98%)	87 (92%)	8 (8%)	9	32
17	CT	95/97 (98%)	89 (94%)	6 (6%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	62/77 (80%)	53 (86%)	9 (14%)	2	15
18	CU	61/77 (79%)	55 (90%)	6 (10%)	6	27
19	AV	71/80 (89%)	63 (89%)	8 (11%)	4	22
19	CV	73/80 (91%)	61 (84%)	12 (16%)	2	11
20	AW	76/82 (93%)	65 (86%)	11 (14%)	2	15
20	CW	76/82 (93%)	67 (88%)	9 (12%)	4	21
21	AX	20/22 (91%)	18 (90%)	2 (10%)	6	26
21	CX	20/22 (91%)	19 (95%)	1 (5%)	20	49
26	BD	214/218 (98%)	183 (86%)	31 (14%)	2	15
26	DD	214/218 (98%)	176 (82%)	38 (18%)	1	8
27	BE	165/166 (99%)	137 (83%)	28 (17%)	1	10
27	DE	165/166 (99%)	127 (77%)	38 (23%)	0	3
28	BF	165/166 (99%)	142 (86%)	23 (14%)	3	17
28	DF	161/166 (97%)	139 (86%)	22 (14%)	3	17
29	BG	155/156 (99%)	139 (90%)	16 (10%)	6	26
29	DG	155/156 (99%)	130 (84%)	25 (16%)	2	12
30	BH	142/148 (96%)	111 (78%)	31 (22%)	1	4
30	DH	142/148 (96%)	115 (81%)	27 (19%)	1	6
31	BK	122/124 (98%)	105 (86%)	17 (14%)	3	17
31	DK	122/124 (98%)	95 (78%)	27 (22%)	1	4
32	BM	117/119 (98%)	101 (86%)	16 (14%)	3	17
32	DM	117/119 (98%)	97 (83%)	20 (17%)	1	10
33	BN	100/100 (100%)	88 (88%)	12 (12%)	4	20
33	DN	100/100 (100%)	90 (90%)	10 (10%)	6	26
34	BO	116/116 (100%)	86 (74%)	30 (26%)	0	3
34	DO	116/116 (100%)	89 (77%)	27 (23%)	0	3
35	BP	111/111 (100%)	92 (83%)	19 (17%)	1	10
35	DP	111/111 (100%)	92 (83%)	19 (17%)	1	10
36	B0	100/101 (99%)	87 (87%)	13 (13%)	3	18
36	D0	101/101 (100%)	83 (82%)	18 (18%)	1	8
37	BQ	87/88 (99%)	74 (85%)	13 (15%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DQ	87/88 (99%)	74 (85%)	13 (15%)	2	15
38	BR	120/127 (94%)	99 (82%)	21 (18%)	1	8
38	DR	120/127 (94%)	96 (80%)	24 (20%)	1	6
39	B1	93/94 (99%)	82 (88%)	11 (12%)	4	21
39	D1	93/94 (99%)	79 (85%)	14 (15%)	2	14
40	B2	82/82 (100%)	67 (82%)	15 (18%)	1	7
40	D2	82/82 (100%)	70 (85%)	12 (15%)	2	15
41	BS	92/92 (100%)	76 (83%)	16 (17%)	1	9
41	DS	92/92 (100%)	77 (84%)	15 (16%)	2	11
42	BT	74/78 (95%)	61 (82%)	13 (18%)	1	8
42	DT	74/78 (95%)	62 (84%)	12 (16%)	2	11
43	BU	85/91 (93%)	61 (72%)	24 (28%)	0	2
43	DU	85/91 (93%)	70 (82%)	15 (18%)	1	8
44	BV	155/179 (87%)	120 (77%)	35 (23%)	1	4
44	DV	152/179 (85%)	124 (82%)	28 (18%)	1	7
45	B3	63/67 (94%)	55 (87%)	8 (13%)	3	18
45	D3	62/67 (92%)	54 (87%)	8 (13%)	3	18
46	BZ	82/83 (99%)	69 (84%)	13 (16%)	2	12
46	DZ	82/83 (99%)	67 (82%)	15 (18%)	1	7
47	BW	64/67 (96%)	57 (89%)	7 (11%)	5	24
47	DW	64/67 (96%)	57 (89%)	7 (11%)	5	24
48	BX	51/52 (98%)	43 (84%)	8 (16%)	2	13
48	DX	51/52 (98%)	40 (78%)	11 (22%)	1	4
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%)	6	27
50	D5	51/52 (98%)	40 (78%)	11 (22%)	1	4
51	B6	47/52 (90%)	30 (64%)	17 (36%)	0	1
51	D6	48/52 (92%)	38 (79%)	10 (21%)	1	5
52	B7	42/42 (100%)	33 (79%)	9 (21%)	1	4
52	D7	42/42 (100%)	38 (90%)	4 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	B8	54/55 (98%)	43 (80%)	11 (20%)	1	5
53	D8	54/55 (98%)	39 (72%)	15 (28%)	0	2
All	All	9616/9998 (96%)	8160 (85%)	1456 (15%)	2	14

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

Mol	Chain	Res	Type
18	CU	32	ARG
32	DM	127	ASP
26	DD	17	THR
18	CU	29	PHE
28	DF	108	LYS

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

Mol	Chain	Res	Type
31	DK	11	ASN
47	DW	9	GLN
32	DM	69	GLN
38	DR	58	ASN
35	BP	13	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	2713	A
24	DA	1962	C
1	CA	975	A
24	DA	1936	A
24	DA	2497	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1517/1517 (100%)	-0.48	10 (0%) 84 69	66, 113, 195, 251	0
1	CA	1515/1517 (99%)	-0.44	14 (0%) 81 64	47, 111, 193, 247	0
2	AE	236/256 (92%)	-0.28	2 (0%) 82 67	111, 152, 183, 188	0
2	CE	237/256 (92%)	-0.27	0 100 100	108, 138, 175, 185	0
3	AF	206/239 (86%)	0.07	1 (0%) 87 75	116, 134, 171, 178	0
3	CF	205/239 (85%)	-0.35	1 (0%) 87 75	98, 128, 150, 160	0
4	AG	208/209 (99%)	0.18	6 (2%) 54 36	72, 106, 128, 137	0
4	CG	208/209 (99%)	-0.02	2 (0%) 79 61	95, 116, 136, 143	0
5	AH	154/162 (95%)	-0.14	0 100 100	89, 109, 139, 163	0
5	CH	151/162 (93%)	-0.25	0 100 100	84, 105, 132, 157	0
6	AI	101/101 (100%)	-0.32	0 100 100	85, 106, 121, 138	0
6	CI	101/101 (100%)	0.16	3 (2%) 52 35	80, 109, 119, 139	0
7	AJ	155/156 (99%)	-0.34	1 (0%) 85 72	105, 129, 150, 160	0
7	CJ	155/156 (99%)	-0.22	0 100 100	98, 121, 141, 157	0
8	AK	138/138 (100%)	-0.40	0 100 100	91, 114, 126, 131	0
8	CK	138/138 (100%)	-0.37	0 100 100	83, 109, 121, 123	0
9	AL	128/128 (100%)	-0.39	0 100 100	109, 150, 168, 173	0
9	CL	127/128 (99%)	-0.33	0 100 100	98, 138, 160, 169	0
10	AM	99/105 (94%)	-0.24	0 100 100	118, 152, 168, 172	0
10	CM	99/105 (94%)	-0.38	0 100 100	111, 147, 168, 175	0
11	AN	121/129 (93%)	-0.27	0 100 100	88, 110, 140, 155	0
11	CN	119/129 (92%)	-0.12	0 100 100	79, 102, 128, 146	0
12	AO	125/132 (94%)	-0.11	0 100 100	77, 96, 115, 148	0
12	CO	125/132 (94%)	-0.21	0 100 100	72, 90, 115, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	118/126 (93%)	-0.02	1 (0%) 82 67	114, 146, 169, 172	0
13	CP	121/126 (96%)	0.16	5 (4%) 42 28	95, 132, 150, 153	0
14	AQ	60/61 (98%)	-0.20	0 100 100	119, 134, 148, 152	0
14	CQ	60/61 (98%)	-0.42	0 100 100	97, 116, 127, 129	0
15	AR	88/89 (98%)	-0.37	1 (1%) 77 59	80, 102, 125, 136	0
15	CR	88/89 (98%)	-0.21	0 100 100	77, 103, 122, 127	0
16	AS	84/88 (95%)	-0.28	0 100 100	86, 97, 118, 150	0
16	CS	84/88 (95%)	-0.32	1 (1%) 76 57	95, 112, 140, 156	0
17	AT	100/105 (95%)	-0.10	1 (1%) 79 61	81, 104, 130, 155	0
17	CT	100/105 (95%)	0.19	3 (3%) 52 35	82, 109, 125, 144	0
18	AU	71/88 (80%)	-0.49	0 100 100	87, 107, 135, 141	0
18	CU	70/88 (79%)	-0.07	0 100 100	84, 107, 125, 125	0
19	AV	82/93 (88%)	0.14	2 (2%) 59 41	130, 159, 169, 170	0
19	CV	84/93 (90%)	0.07	0 100 100	118, 134, 149, 152	0
20	AW	99/106 (93%)	-0.22	0 100 100	88, 106, 149, 157	0
20	CW	99/106 (93%)	-0.27	0 100 100	96, 119, 148, 155	0
21	AX	25/27 (92%)	-0.23	0 100 100	143, 151, 161, 165	0
21	CX	25/27 (92%)	-0.48	0 100 100	101, 131, 147, 158	0
22	AC	77/77 (100%)	-0.57	0 100 100	76, 119, 153, 162	0
22	AD	77/77 (100%)	-0.37	0 100 100	111, 217, 236, 246	0
22	CB	65/77 (84%)	0.05	1 (1%) 71 53	133, 199, 226, 234	0
22	CC	77/77 (100%)	-0.48	1 (1%) 74 56	68, 99, 133, 139	0
22	CD	77/77 (100%)	-0.07	1 (1%) 74 56	105, 210, 222, 228	0
23	A1	23/25 (92%)	0.16	1 (4%) 40 27	101, 193, 235, 240	0
23	C1	23/25 (92%)	-0.07	0 100 100	87, 180, 239, 241	0
24	BA	2885/2898 (99%)	-0.52	5 (0%) 92 86	53, 90, 211, 243	0
24	DA	2886/2898 (99%)	-0.58	15 (0%) 87 75	35, 74, 192, 231	0
25	BB	120/122 (98%)	-0.57	0 100 100	103, 144, 169, 214	0
25	DB	120/122 (98%)	-0.56	1 (0%) 82 67	77, 106, 126, 157	0
26	BD	272/276 (98%)	-0.00	1 (0%) 89 79	50, 78, 97, 112	0
26	DD	272/276 (98%)	0.00	4 (1%) 71 53	44, 63, 84, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	BE	205/206 (99%)	0.04	6 (2%) 54 36	60, 93, 138, 151	0
27	DE	205/206 (99%)	-0.23	0 100 100	48, 84, 123, 139	0
28	BF	208/210 (99%)	-0.08	2 (0%) 79 61	62, 98, 158, 176	0
28	DF	202/210 (96%)	-0.44	1 (0%) 87 75	40, 74, 112, 125	0
29	BG	181/182 (99%)	-0.06	1 (0%) 85 72	120, 144, 163, 175	0
29	DG	181/182 (99%)	0.19	7 (3%) 44 30	86, 109, 136, 146	0
30	BH	170/180 (94%)	0.10	2 (1%) 76 57	121, 169, 203, 209	0
30	DH	170/180 (94%)	-0.11	2 (1%) 76 57	75, 101, 123, 131	0
31	BK	146/148 (98%)	-0.08	0 100 100	82, 122, 143, 151	0
31	DK	146/148 (98%)	-0.04	3 (2%) 63 44	68, 112, 127, 142	0
32	BM	138/140 (98%)	-0.18	0 100 100	80, 105, 124, 129	0
32	DM	138/140 (98%)	-0.30	2 (1%) 73 53	66, 84, 116, 123	0
33	BN	122/122 (100%)	-0.06	0 100 100	69, 86, 99, 105	0
33	DN	122/122 (100%)	-0.35	0 100 100	50, 77, 90, 95	0
34	BO	150/150 (100%)	-0.45	0 100 100	67, 106, 135, 158	0
34	DO	150/150 (100%)	-0.29	0 100 100	45, 88, 114, 138	0
35	BP	141/141 (100%)	-0.11	3 (2%) 63 44	82, 105, 134, 178	0
35	DP	141/141 (100%)	-0.09	2 (1%) 73 53	62, 86, 107, 131	0
36	B0	117/118 (99%)	-0.25	2 (1%) 69 49	54, 80, 102, 119	0
36	D0	118/118 (100%)	-0.24	0 100 100	54, 80, 98, 107	0
37	BQ	111/112 (99%)	-0.60	0 100 100	113, 132, 155, 167	0
37	DQ	111/112 (99%)	-0.25	1 (0%) 81 64	82, 97, 130, 139	0
38	BR	137/146 (93%)	0.03	5 (3%) 46 31	77, 93, 148, 177	0
38	DR	137/146 (93%)	-0.13	3 (2%) 62 43	71, 89, 136, 157	0
39	B1	117/118 (99%)	-0.36	2 (1%) 69 49	68, 94, 135, 155	0
39	D1	117/118 (99%)	-0.47	0 100 100	53, 69, 104, 130	0
40	B2	101/101 (100%)	-0.04	0 100 100	64, 118, 132, 136	0
40	D2	101/101 (100%)	-0.05	3 (2%) 52 35	52, 97, 117, 126	0
41	BS	113/113 (100%)	-0.23	0 100 100	67, 80, 101, 141	0
41	DS	113/113 (100%)	-0.38	2 (1%) 67 48	53, 70, 100, 142	0
42	BT	92/96 (95%)	-0.07	2 (2%) 62 43	73, 89, 111, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
42	DT	92/96 (95%)	-0.23	3 (3%)	49	33	54, 70, 91, 103	0
43	BU	102/110 (92%)	0.40	5 (4%)	36	25	79, 106, 161, 172	0
43	DU	102/110 (92%)	-0.10	3 (2%)	54	36	67, 93, 134, 144	0
44	BV	176/206 (85%)	-0.18	0	100	100	113, 142, 185, 190	0
44	DV	172/206 (83%)	0.27	8 (4%)	37	26	90, 126, 184, 190	0
45	B3	80/85 (94%)	-0.73	0	100	100	84, 99, 113, 119	0
45	D3	77/85 (90%)	-0.48	1 (1%)	74	56	67, 81, 100, 115	0
46	BZ	97/98 (98%)	0.13	4 (4%)	42	28	67, 91, 149, 174	0
46	DZ	97/98 (98%)	-0.08	3 (3%)	51	35	48, 78, 141, 158	0
47	BW	69/72 (95%)	-0.11	1 (1%)	73	53	80, 105, 125, 140	0
47	DW	69/72 (95%)	-0.23	0	100	100	60, 83, 105, 122	0
48	BX	59/60 (98%)	-0.48	0	100	100	83, 107, 129, 134	0
48	DX	59/60 (98%)	-0.23	0	100	100	64, 84, 110, 124	0
49	B4	71/71 (100%)	0.44	5 (7%)	24	19	164, 193, 208, 211	0
49	D4	71/71 (100%)	0.54	2 (2%)	55	37	128, 160, 185, 188	0
50	B5	59/60 (98%)	0.23	5 (8%)	18	14	56, 91, 168, 177	0
50	D5	59/60 (98%)	-0.17	2 (3%)	48	32	46, 86, 186, 190	0
51	B6	48/54 (88%)	-0.39	0	100	100	138, 153, 169, 175	0
51	D6	49/54 (90%)	0.31	1 (2%)	64	45	132, 146, 156, 162	0
52	B7	49/49 (100%)	-0.34	1 (2%)	64	45	51, 68, 116, 148	0
52	D7	49/49 (100%)	-0.40	0	100	100	40, 49, 109, 135	0
53	B8	64/65 (98%)	-0.42	0	100	100	77, 93, 114, 152	0
53	D8	64/65 (98%)	-0.28	0	100	100	53, 72, 100, 127	0
All	All	21035/21563 (97%)	-0.31	179 (0%)	81	64	35, 102, 179, 251	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	B5	2	ALA	6.4
40	D2	36	PRO	5.5
13	CP	119	GLY	5.3
2	AE	214	ILE	4.5
1	CA	345	C	4.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1847	1/1	-0.27	0.30	133,133,133,133	0
54	MG	DA	3794	1/1	-0.18	0.27	142,142,142,142	0
54	MG	AA	1909	1/1	-0.16	0.42	128,128,128,128	0
54	MG	DA	3791	1/1	-0.09	0.30	114,114,114,114	0
54	MG	DA	3802	1/1	-0.04	0.26	138,138,138,138	0
54	MG	AA	2004	1/1	0.01	0.24	124,124,124,124	0
54	MG	AA	1911	1/1	0.04	0.42	104,104,104,104	0
54	MG	DA	3792	1/1	0.07	0.20	157,157,157,157	0
54	MG	CA	1848	1/1	0.09	0.20	130,130,130,130	0
54	MG	AA	1834	1/1	0.10	0.27	183,183,183,183	0
54	MG	DA	3049	1/1	0.12	0.38	114,114,114,114	0
54	MG	BA	3297	1/1	0.15	0.17	131,131,131,131	0
54	MG	AA	1882	1/1	0.16	0.20	134,134,134,134	0
54	MG	CA	1947	1/1	0.17	0.32	205,205,205,205	0
54	MG	AA	1915	1/1	0.17	0.19	172,172,172,172	0
54	MG	DA	3463	1/1	0.18	0.34	155,155,155,155	0
54	MG	AA	2014	1/1	0.19	0.19	175,175,175,175	0
54	MG	BA	3283	1/1	0.21	0.24	126,126,126,126	0
54	MG	AD	102	1/1	0.22	0.08	120,120,120,120	0
54	MG	AA	1932	1/1	0.22	0.29	122,122,122,122	0
54	MG	AA	1949	1/1	0.24	0.22	122,122,122,122	0
54	MG	AA	1887	1/1	0.24	0.18	161,161,161,161	0
54	MG	CA	1824	1/1	0.24	0.18	156,156,156,156	0
54	MG	DA	3570	1/1	0.25	0.35	152,152,152,152	0
54	MG	AA	2030	1/1	0.25	0.36	188,188,188,188	0
54	MG	BB	226	1/1	0.25	0.21	146,146,146,146	0
54	MG	AA	1709	1/1	0.25	0.20	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1789	1/1	0.25	0.29	128,128,128,128	0
54	MG	BA	3468	1/1	0.26	0.20	110,110,110,110	0
54	MG	AA	1865	1/1	0.26	0.29	140,140,140,140	0
54	MG	AA	1800	1/1	0.26	0.36	117,117,117,117	0
54	MG	DA	3790	1/1	0.26	0.27	109,109,109,109	0
54	MG	BA	3471	1/1	0.28	0.23	156,156,156,156	0
54	MG	CA	1956	1/1	0.28	0.11	217,217,217,217	0
54	MG	DA	3656	1/1	0.29	0.29	136,136,136,136	0
54	MG	BA	3571	1/1	0.29	0.17	94,94,94,94	0
54	MG	DU	202	1/1	0.29	0.23	139,139,139,139	0
54	MG	BH	201	1/1	0.30	0.28	193,193,193,193	0
54	MG	AA	1805	1/1	0.30	0.33	109,109,109,109	0
54	MG	BA	3554	1/1	0.30	0.15	122,122,122,122	0
54	MG	DA	3512	1/1	0.30	0.41	96,96,96,96	0
54	MG	AA	2038	1/1	0.30	0.24	116,116,116,116	0
54	MG	AA	1840	1/1	0.30	0.45	132,132,132,132	0
54	MG	AA	1622	1/1	0.32	0.20	78,78,78,78	0
54	MG	AA	1761	1/1	0.33	0.23	136,136,136,136	0
54	MG	DA	3303	1/1	0.33	0.34	113,113,113,113	0
54	MG	CA	1878	1/1	0.34	0.16	133,133,133,133	0
54	MG	BA	3417	1/1	0.34	0.13	97,97,97,97	0
54	MG	BA	2912	1/1	0.34	0.13	138,138,138,138	0
54	MG	DA	3430	1/1	0.35	0.33	95,95,95,95	0
54	MG	AA	1861	1/1	0.35	0.15	120,120,120,120	0
54	MG	DA	3491	1/1	0.35	0.35	102,102,102,102	0
54	MG	AA	1835	1/1	0.35	0.33	109,109,109,109	0
54	MG	DB	227	1/1	0.36	0.29	105,105,105,105	0
54	MG	DA	3188	1/1	0.37	0.37	96,96,96,96	0
54	MG	AA	1910	1/1	0.38	0.29	103,103,103,103	0
54	MG	DA	3293	1/1	0.38	0.28	134,134,134,134	0
54	MG	DA	3520	1/1	0.38	0.21	90,90,90,90	0
54	MG	AA	1806	1/1	0.38	0.21	118,118,118,118	0
54	MG	CA	1741	1/1	0.38	0.29	123,123,123,123	0
54	MG	CA	1860	1/1	0.38	0.31	127,127,127,127	0
54	MG	DA	3440	1/1	0.39	0.41	118,118,118,118	0
54	MG	AA	1706	1/1	0.39	0.31	143,143,143,143	0
54	MG	DA	3631	1/1	0.39	0.22	118,118,118,118	0
54	MG	BA	3232	1/1	0.39	0.13	99,99,99,99	0
54	MG	DA	3712	1/1	0.39	0.25	138,138,138,138	0
54	MG	CA	1808	1/1	0.39	0.25	98,98,98,98	0
54	MG	AA	2007	1/1	0.40	0.20	119,119,119,119	0
54	MG	AA	1878	1/1	0.40	0.20	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3266	1/1	0.41	0.29	97,97,97,97	0
54	MG	CA	1912	1/1	0.41	0.23	127,127,127,127	0
54	MG	AA	1903	1/1	0.41	0.34	95,95,95,95	0
54	MG	DA	3597	1/1	0.41	0.31	168,168,168,168	0
54	MG	BA	3464	1/1	0.41	0.22	102,102,102,102	0
54	MG	BA	3561	1/1	0.41	0.34	117,117,117,117	0
54	MG	CA	1782	1/1	0.41	0.22	123,123,123,123	0
54	MG	BA	2913	1/1	0.43	0.12	115,115,115,115	0
54	MG	CA	1813	1/1	0.43	0.16	127,127,127,127	0
54	MG	AA	1719	1/1	0.44	0.34	90,90,90,90	0
54	MG	CA	1963	1/1	0.44	0.19	145,145,145,145	0
54	MG	BA	3499	1/1	0.44	0.19	114,114,114,114	0
54	MG	CA	1680	1/1	0.45	0.18	99,99,99,99	0
54	MG	AA	1913	1/1	0.45	0.23	114,114,114,114	0
54	MG	BA	3414	1/1	0.45	0.28	105,105,105,105	0
54	MG	DA	3246	1/1	0.46	0.30	101,101,101,101	0
54	MG	AT	201	1/1	0.46	0.29	101,101,101,101	0
54	MG	CA	1910	1/1	0.46	0.14	130,130,130,130	0
54	MG	DA	3675	1/1	0.46	0.29	104,104,104,104	0
54	MG	BA	3555	1/1	0.46	0.16	119,119,119,119	0
54	MG	AA	1653	1/1	0.46	0.16	107,107,107,107	0
54	MG	AA	1812	1/1	0.47	0.22	110,110,110,110	0
54	MG	AA	1958	1/1	0.47	0.18	93,93,93,93	0
54	MG	AA	1899	1/1	0.47	0.16	112,112,112,112	0
54	MG	BA	3376	1/1	0.47	0.25	121,121,121,121	0
54	MG	BA	3136	1/1	0.47	0.28	111,111,111,111	0
54	MG	DA	3704	1/1	0.47	0.20	134,134,134,134	0
54	MG	AA	1655	1/1	0.47	0.21	91,91,91,91	0
54	MG	AA	1666	1/1	0.48	0.26	95,95,95,95	0
54	MG	CA	1818	1/1	0.48	0.17	92,92,92,92	0
54	MG	BA	3569	1/1	0.48	0.15	137,137,137,137	0
54	MG	DA	3528	1/1	0.48	0.23	80,80,80,80	0
54	MG	DA	3688	1/1	0.48	0.24	111,111,111,111	0
54	MG	BA	3018	1/1	0.48	0.33	109,109,109,109	0
54	MG	DA	3587	1/1	0.48	0.31	134,134,134,134	0
54	MG	CS	102	1/1	0.49	0.23	119,119,119,119	0
54	MG	DA	3788	1/1	0.49	0.20	111,111,111,111	0
54	MG	AA	1735	1/1	0.49	0.22	108,108,108,108	0
54	MG	BA	3080	1/1	0.49	0.19	69,69,69,69	0
54	MG	DA	3671	1/1	0.49	0.23	102,102,102,102	0
54	MG	CA	1846	1/1	0.49	0.25	129,129,129,129	0
54	MG	DA	3575	1/1	0.49	0.19	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3694	1/1	0.49	0.30	110,110,110,110	0
54	MG	CA	1975	1/1	0.49	0.17	110,110,110,110	0
54	MG	AA	1780	1/1	0.50	0.28	95,95,95,95	0
54	MG	DA	3573	1/1	0.50	0.43	124,124,124,124	0
54	MG	BA	3378	1/1	0.50	0.12	129,129,129,129	0
54	MG	BA	3479	1/1	0.50	0.21	119,119,119,119	0
54	MG	AA	2024	1/1	0.50	0.27	75,75,75,75	0
54	MG	DB	221	1/1	0.50	0.14	94,94,94,94	0
54	MG	AA	1816	1/1	0.50	0.29	107,107,107,107	0
54	MG	BA	3320	1/1	0.50	0.31	101,101,101,101	0
54	MG	AJ	201	1/1	0.51	0.13	116,116,116,116	0
54	MG	CA	1707	1/1	0.51	0.14	106,106,106,106	0
54	MG	BA	3433	1/1	0.51	0.24	109,109,109,109	0
54	MG	DA	3470	1/1	0.51	0.30	79,79,79,79	0
54	MG	DA	3091	1/1	0.51	0.41	92,92,92,92	0
54	MG	DA	3336	1/1	0.51	0.34	127,127,127,127	0
54	MG	CA	1866	1/1	0.52	0.28	118,118,118,118	0
54	MG	BF	302	1/1	0.52	0.29	117,117,117,117	0
54	MG	DA	3472	1/1	0.52	0.30	111,111,111,111	0
54	MG	DA	3134	1/1	0.52	0.34	111,111,111,111	0
54	MG	DA	3368	1/1	0.52	0.27	87,87,87,87	0
54	MG	AA	1954	1/1	0.52	0.28	108,108,108,108	0
54	MG	DA	3743	1/1	0.52	0.29	111,111,111,111	0
54	MG	CC	110	1/1	0.52	0.10	110,110,110,110	0
54	MG	BA	3245	1/1	0.53	0.12	128,128,128,128	0
54	MG	DA	3265	1/1	0.53	0.24	84,84,84,84	0
54	MG	DA	3527	1/1	0.53	0.29	127,127,127,127	0
54	MG	CA	1830	1/1	0.54	0.18	135,135,135,135	0
54	MG	AA	1696	1/1	0.54	0.23	134,134,134,134	0
54	MG	DA	3465	1/1	0.54	0.32	104,104,104,104	0
54	MG	CA	1788	1/1	0.54	0.28	86,86,86,86	0
54	MG	AA	1775	1/1	0.54	0.35	88,88,88,88	0
54	MG	BA	3572	1/1	0.54	0.27	106,106,106,106	0
54	MG	CA	1862	1/1	0.54	0.12	112,112,112,112	0
54	MG	CR	101	1/1	0.54	0.26	117,117,117,117	0
54	MG	BA	3574	1/1	0.54	0.13	86,86,86,86	0
54	MG	AA	1993	1/1	0.54	0.20	134,134,134,134	0
54	MG	CA	1888	1/1	0.54	0.14	112,112,112,112	0
54	MG	AA	1964	1/1	0.55	0.30	103,103,103,103	0
54	MG	AA	1937	1/1	0.55	0.30	95,95,95,95	0
54	MG	DA	3594	1/1	0.55	0.17	123,123,123,123	0
54	MG	DA	3477	1/1	0.55	0.15	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3611	1/1	0.55	0.31	112,112,112,112	0
54	MG	DB	213	1/1	0.55	0.25	133,133,133,133	0
54	MG	DA	3618	1/1	0.55	0.33	113,113,113,113	0
54	MG	DB	222	1/1	0.55	0.19	92,92,92,92	0
54	MG	CA	1840	1/1	0.55	0.22	113,113,113,113	0
54	MG	CA	1858	1/1	0.55	0.27	109,109,109,109	0
54	MG	BA	3335	1/1	0.56	0.36	86,86,86,86	0
54	MG	BA	2911	1/1	0.56	0.08	120,120,120,120	0
54	MG	CA	1742	1/1	0.56	0.14	124,124,124,124	0
54	MG	BA	3267	1/1	0.56	0.40	102,102,102,102	0
54	MG	BA	3394	1/1	0.56	0.19	121,121,121,121	0
54	MG	BA	3400	1/1	0.56	0.19	117,117,117,117	0
54	MG	AA	1971	1/1	0.56	0.14	123,123,123,123	0
54	MG	CA	1815	1/1	0.56	0.35	105,105,105,105	0
54	MG	AA	1919	1/1	0.56	0.35	117,117,117,117	0
54	MG	DG	203	1/1	0.56	0.31	112,112,112,112	0
54	MG	AA	2003	1/1	0.56	0.17	128,128,128,128	0
54	MG	AA	1689	1/1	0.57	0.22	93,93,93,93	0
54	MG	AA	1904	1/1	0.57	0.20	121,121,121,121	0
54	MG	DA	3451	1/1	0.57	0.22	80,80,80,80	0
54	MG	CA	1759	1/1	0.57	0.23	113,113,113,113	0
54	MG	AA	1727	1/1	0.57	0.22	104,104,104,104	0
54	MG	AW	203	1/1	0.57	0.27	114,114,114,114	0
54	MG	AA	1687	1/1	0.57	0.26	138,138,138,138	0
54	MG	DA	3269	1/1	0.57	0.45	99,99,99,99	0
54	MG	BQ	201	1/1	0.57	0.11	105,105,105,105	0
54	MG	BA	3570	1/1	0.57	0.20	104,104,104,104	0
54	MG	DA	3311	1/1	0.57	0.22	100,100,100,100	0
54	MG	AA	1956	1/1	0.57	0.22	118,118,118,118	0
54	MG	CA	1727	1/1	0.57	0.12	131,131,131,131	0
54	MG	DA	3422	1/1	0.57	0.31	82,82,82,82	0
54	MG	AA	2029	1/1	0.58	0.36	127,127,127,127	0
54	MG	CA	1722	1/1	0.58	0.23	99,99,99,99	0
54	MG	BA	3432	1/1	0.58	0.17	115,115,115,115	0
54	MG	DB	208	1/1	0.58	0.13	135,135,135,135	0
54	MG	CA	1942	1/1	0.58	0.13	101,101,101,101	0
54	MG	DA	3532	1/1	0.58	0.18	87,87,87,87	0
54	MG	CW	205	1/1	0.58	0.20	143,143,143,143	0
54	MG	DA	3644	1/1	0.58	0.36	106,106,106,106	0
54	MG	DB	228	1/1	0.58	0.32	116,116,116,116	0
54	MG	AA	1747	1/1	0.58	0.27	89,89,89,89	0
54	MG	CA	1794	1/1	0.58	0.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3205	1/1	0.59	0.22	92,92,92,92	0
54	MG	BA	3301	1/1	0.59	0.25	92,92,92,92	0
54	MG	DA	3569	1/1	0.59	0.25	92,92,92,92	0
54	MG	AA	1886	1/1	0.59	0.21	102,102,102,102	0
54	MG	AA	1826	1/1	0.59	0.34	108,108,108,108	0
54	MG	DA	3746	1/1	0.59	0.13	64,64,64,64	0
54	MG	AA	1928	1/1	0.59	0.23	117,117,117,117	0
54	MG	AA	2034	1/1	0.59	0.23	94,94,94,94	0
54	MG	AA	1720	1/1	0.59	0.16	76,76,76,76	0
54	MG	DA	3682	1/1	0.59	0.48	141,141,141,141	0
54	MG	AL	202	1/1	0.60	0.10	129,129,129,129	0
54	MG	DB	201	1/1	0.60	0.26	86,86,86,86	0
54	MG	DA	3716	1/1	0.60	0.20	86,86,86,86	0
54	MG	DA	3441	1/1	0.60	0.42	116,116,116,116	0
54	MG	BA	3181	1/1	0.60	0.39	97,97,97,97	0
54	MG	BA	3278	1/1	0.60	0.23	119,119,119,119	0
54	MG	CA	1748	1/1	0.60	0.11	71,71,71,71	0
54	MG	AH	201	1/1	0.60	0.20	103,103,103,103	0
54	MG	BA	3076	1/1	0.60	0.19	88,88,88,88	0
54	MG	AA	1957	1/1	0.60	0.16	82,82,82,82	0
54	MG	CA	1657	1/1	0.61	0.23	96,96,96,96	0
54	MG	AA	1850	1/1	0.61	0.31	112,112,112,112	0
54	MG	DA	3515	1/1	0.61	0.19	100,100,100,100	0
54	MG	DA	3281	1/1	0.61	0.18	123,123,123,123	0
54	MG	CA	1841	1/1	0.62	0.18	119,119,119,119	0
54	MG	CA	1944	1/1	0.62	0.14	99,99,99,99	0
54	MG	DA	3781	1/1	0.62	0.26	97,97,97,97	0
54	MG	BA	3450	1/1	0.62	0.20	90,90,90,90	0
54	MG	AA	1955	1/1	0.62	0.25	103,103,103,103	0
54	MG	CA	1653	1/1	0.62	0.32	86,86,86,86	0
54	MG	CA	1852	1/1	0.62	0.28	111,111,111,111	0
54	MG	AA	1662	1/1	0.62	0.19	100,100,100,100	0
54	MG	AT	202	1/1	0.62	0.21	111,111,111,111	0
54	MG	AA	1966	1/1	0.62	0.19	85,85,85,85	0
54	MG	BA	3360	1/1	0.62	0.24	117,117,117,117	0
54	MG	BB	213	1/1	0.62	0.10	122,122,122,122	0
54	MG	BB	225	1/1	0.62	0.10	90,90,90,90	0
54	MG	DA	3699	1/1	0.62	0.28	102,102,102,102	0
54	MG	CA	1904	1/1	0.62	0.33	117,117,117,117	0
54	MG	BA	3375	1/1	0.62	0.12	112,112,112,112	0
54	MG	DF	301	1/1	0.62	0.20	82,82,82,82	0
54	MG	AA	1829	1/1	0.62	0.14	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DA	3725	1/1	0.62	0.27	132,132,132,132	0
54	MG	DA	3785	1/1	0.63	0.26	117,117,117,117	0
54	MG	BA	3573	1/1	0.63	0.18	86,86,86,86	0
54	MG	AA	1664	1/1	0.63	0.20	69,69,69,69	0
54	MG	AA	1704	1/1	0.63	0.20	88,88,88,88	0
54	MG	AA	1872	1/1	0.63	0.13	108,108,108,108	0
54	MG	DA	3018	1/1	0.63	0.32	83,83,83,83	0
54	MG	DA	3299	1/1	0.63	0.24	84,84,84,84	0
54	MG	BA	3105	1/1	0.63	0.17	87,87,87,87	0
54	MG	BA	3242	1/1	0.63	0.18	82,82,82,82	0
54	MG	BA	3368	1/1	0.63	0.25	113,113,113,113	0
54	MG	DA	3719	1/1	0.63	0.20	116,116,116,116	0
54	MG	BA	3293	1/1	0.63	0.13	111,111,111,111	0
54	MG	DA	3738	1/1	0.63	0.15	114,114,114,114	0
54	MG	DA	3193	1/1	0.63	0.32	81,81,81,81	0
54	MG	DB	229	1/1	0.63	0.25	78,78,78,78	0
54	MG	DA	3235	1/1	0.63	0.20	71,71,71,71	0
54	MG	DA	3751	1/1	0.63	0.23	101,101,101,101	0
54	MG	DA	3238	1/1	0.63	0.33	100,100,100,100	0
54	MG	AA	1857	1/1	0.64	0.31	88,88,88,88	0
54	MG	DA	3410	1/1	0.64	0.28	95,95,95,95	0
54	MG	CA	1641	1/1	0.64	0.20	72,72,72,72	0
54	MG	AA	1733	1/1	0.64	0.27	102,102,102,102	0
54	MG	AA	1804	1/1	0.64	0.28	88,88,88,88	0
54	MG	BA	3201	1/1	0.64	0.17	97,97,97,97	0
54	MG	AA	1868	1/1	0.64	0.12	103,103,103,103	0
54	MG	AA	1945	1/1	0.64	0.20	67,67,67,67	0
54	MG	BA	3490	1/1	0.64	0.20	107,107,107,107	0
54	MG	AA	2023	1/1	0.64	0.10	112,112,112,112	0
54	MG	CC	102	1/1	0.64	0.09	87,87,87,87	0
54	MG	CA	1897	1/1	0.64	0.15	105,105,105,105	0
54	MG	AA	1799	1/1	0.64	0.12	91,91,91,91	0
54	MG	DA	3495	1/1	0.64	0.27	92,92,92,92	0
54	MG	BA	3422	1/1	0.64	0.28	83,83,83,83	0
54	MG	DA	3770	1/1	0.64	0.25	87,87,87,87	0
54	MG	DA	3771	1/1	0.64	0.24	97,97,97,97	0
54	MG	AA	1876	1/1	0.64	0.12	78,78,78,78	0
55	ZN	AA	2041	1/1	0.64	0.12	262,262,262,262	0
54	MG	AA	1939	1/1	0.65	0.18	118,118,118,118	0
54	MG	AA	1881	1/1	0.65	0.23	77,77,77,77	0
54	MG	AA	1742	1/1	0.65	0.19	83,83,83,83	0
54	MG	AA	1617	1/1	0.65	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3592	1/1	0.65	0.24	78,78,78,78	0
54	MG	AA	1965	1/1	0.65	0.20	117,117,117,117	0
54	MG	CA	1810	1/1	0.65	0.17	92,92,92,92	0
54	MG	DA	3728	1/1	0.65	0.15	123,123,123,123	0
54	MG	DA	3357	1/1	0.65	0.19	77,77,77,77	0
54	MG	AA	1750	1/1	0.65	0.21	79,79,79,79	0
54	MG	BA	3328	1/1	0.65	0.22	105,105,105,105	0
54	MG	DA	3517	1/1	0.65	0.27	81,81,81,81	0
54	MG	BA	3517	1/1	0.65	0.18	93,93,93,93	0
54	MG	CP	204	1/1	0.65	0.19	137,137,137,137	0
54	MG	AA	2017	1/1	0.65	0.14	92,92,92,92	0
54	MG	BA	3151	1/1	0.65	0.30	114,114,114,114	0
54	MG	BA	3270	1/1	0.65	0.34	98,98,98,98	0
54	MG	BA	2907	1/1	0.66	0.15	106,106,106,106	0
54	MG	AA	1762	1/1	0.66	0.27	104,104,104,104	0
54	MG	BA	3382	1/1	0.66	0.19	123,123,123,123	0
54	MG	AA	1870	1/1	0.66	0.12	92,92,92,92	0
54	MG	BA	3321	1/1	0.66	0.12	64,64,64,64	0
54	MG	CA	1704	1/1	0.66	0.18	88,88,88,88	0
54	MG	DA	3668	1/1	0.66	0.46	117,117,117,117	0
54	MG	AA	1917	1/1	0.66	0.35	132,132,132,132	0
54	MG	AA	1986	1/1	0.66	0.11	96,96,96,96	0
54	MG	BA	3503	1/1	0.66	0.16	66,66,66,66	0
54	MG	CD	107	1/1	0.66	0.18	122,122,122,122	0
54	MG	DA	3010	1/1	0.66	0.26	86,86,86,86	0
54	MG	CA	1828	1/1	0.66	0.18	89,89,89,89	0
54	MG	CA	1739	1/1	0.66	0.12	80,80,80,80	0
54	MG	DA	3374	1/1	0.66	0.20	75,75,75,75	0
54	MG	DA	3713	1/1	0.66	0.25	144,144,144,144	0
54	MG	DA	3085	1/1	0.66	0.30	67,67,67,67	0
54	MG	DA	3413	1/1	0.66	0.33	99,99,99,99	0
54	MG	AA	1992	1/1	0.66	0.12	106,106,106,106	0
54	MG	BA	3520	1/1	0.66	0.19	55,55,55,55	0
54	MG	BA	3223	1/1	0.66	0.24	88,88,88,88	0
54	MG	AA	1737	1/1	0.66	0.14	97,97,97,97	0
54	MG	DA	3205	1/1	0.66	0.27	115,115,115,115	0
54	MG	AA	1924	1/1	0.67	0.17	114,114,114,114	0
54	MG	AA	1926	1/1	0.67	0.17	102,102,102,102	0
54	MG	BA	3071	1/1	0.67	0.18	74,74,74,74	0
54	MG	AA	1633	1/1	0.67	0.22	79,79,79,79	0
54	MG	AA	1997	1/1	0.67	0.17	108,108,108,108	0
54	MG	CA	1762	1/1	0.67	0.19	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3628	1/1	0.67	0.22	70,70,70,70	0
54	MG	AA	1929	1/1	0.67	0.19	124,124,124,124	0
54	MG	BR	201	1/1	0.67	0.23	103,103,103,103	0
54	MG	BA	3441	1/1	0.67	0.12	144,144,144,144	0
54	MG	DA	3660	1/1	0.67	0.29	87,87,87,87	0
54	MG	AA	1866	1/1	0.67	0.23	117,117,117,117	0
54	MG	CC	103	1/1	0.67	0.10	86,86,86,86	0
54	MG	AA	1768	1/1	0.67	0.18	67,67,67,67	0
54	MG	CA	1661	1/1	0.67	0.20	64,64,64,64	0
54	MG	CD	108	1/1	0.67	0.10	174,174,174,174	0
54	MG	DA	3318	1/1	0.67	0.26	87,87,87,87	0
54	MG	BA	3161	1/1	0.67	0.26	96,96,96,96	0
54	MG	AA	1982	1/1	0.67	0.06	126,126,126,126	0
54	MG	BA	3186	1/1	0.67	0.13	83,83,83,83	0
54	MG	DA	3369	1/1	0.67	0.27	90,90,90,90	0
54	MG	AI	201	1/1	0.67	0.24	72,72,72,72	0
54	MG	DA	3401	1/1	0.67	0.13	182,182,182,182	0
54	MG	DA	3724	1/1	0.67	0.20	106,106,106,106	0
54	MG	BB	204	1/1	0.67	0.17	97,97,97,97	0
54	MG	DA	3127	1/1	0.67	0.30	78,78,78,78	0
54	MG	CA	1697	1/1	0.68	0.34	98,98,98,98	0
54	MG	AA	1724	1/1	0.68	0.35	82,82,82,82	0
54	MG	BA	2905	1/1	0.68	0.09	136,136,136,136	0
54	MG	BA	3129	1/1	0.68	0.26	72,72,72,72	0
54	MG	AA	1867	1/1	0.68	0.28	85,85,85,85	0
54	MG	CW	202	1/1	0.68	0.22	108,108,108,108	0
54	MG	DA	3563	1/1	0.68	0.18	76,76,76,76	0
54	MG	BA	3142	1/1	0.68	0.22	90,90,90,90	0
54	MG	AA	1933	1/1	0.68	0.22	98,98,98,98	0
54	MG	BB	208	1/1	0.68	0.11	91,91,91,91	0
54	MG	AA	1934	1/1	0.68	0.14	88,88,88,88	0
54	MG	BA	3380	1/1	0.68	0.28	71,71,71,71	0
54	MG	BA	3281	1/1	0.68	0.23	113,113,113,113	0
54	MG	CD	110	1/1	0.68	0.13	102,102,102,102	0
54	MG	AA	1602	1/1	0.68	0.28	53,53,53,53	0
54	MG	CA	1786	1/1	0.68	0.19	86,86,86,86	0
54	MG	DA	3419	1/1	0.68	0.31	92,92,92,92	0
54	MG	AA	1821	1/1	0.68	0.13	141,141,141,141	0
54	MG	BA	3049	1/1	0.68	0.34	71,71,71,71	0
54	MG	BA	3537	1/1	0.68	0.31	108,108,108,108	0
54	MG	DA	3652	1/1	0.68	0.21	83,83,83,83	0
54	MG	DA	3107	1/1	0.68	0.27	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1906	1/1	0.68	0.21	107,107,107,107	0
54	MG	AA	1863	1/1	0.68	0.37	92,92,92,92	0
54	MG	CA	1811	1/1	0.68	0.20	108,108,108,108	0
54	MG	CA	1922	1/1	0.68	0.28	116,116,116,116	0
54	MG	CA	1928	1/1	0.68	0.09	122,122,122,122	0
54	MG	AA	1802	1/1	0.68	0.18	98,98,98,98	0
54	MG	DA	3487	1/1	0.68	0.25	96,96,96,96	0
54	MG	BA	3423	1/1	0.68	0.19	85,85,85,85	0
54	MG	BA	3562	1/1	0.68	0.20	94,94,94,94	0
54	MG	BA	3226	1/1	0.68	0.25	88,88,88,88	0
54	MG	DA	3588	1/1	0.69	0.14	91,91,91,91	0
54	MG	CA	1908	1/1	0.69	0.23	128,128,128,128	0
54	MG	AW	201	1/1	0.69	0.24	108,108,108,108	0
54	MG	CA	1765	1/1	0.69	0.23	118,118,118,118	0
54	MG	CA	1771	1/1	0.69	0.22	101,101,101,101	0
54	MG	DA	3612	1/1	0.69	0.14	99,99,99,99	0
54	MG	CA	1924	1/1	0.69	0.09	98,98,98,98	0
54	MG	DA	3624	1/1	0.69	0.17	82,82,82,82	0
54	MG	DA	3625	1/1	0.69	0.19	99,99,99,99	0
54	MG	BA	3264	1/1	0.69	0.18	64,64,64,64	0
54	MG	AA	1999	1/1	0.69	0.20	100,100,100,100	0
54	MG	CA	1787	1/1	0.69	0.21	147,147,147,147	0
54	MG	DA	3326	1/1	0.69	0.41	105,105,105,105	0
54	MG	AD	101	1/1	0.69	0.12	85,85,85,85	0
54	MG	DA	3501	1/1	0.69	0.15	84,84,84,84	0
54	MG	DA	3351	1/1	0.69	0.07	88,88,88,88	0
54	MG	AA	1849	1/1	0.69	0.24	92,92,92,92	0
54	MG	DB	204	1/1	0.69	0.14	94,94,94,94	0
54	MG	CA	1957	1/1	0.69	0.10	90,90,90,90	0
54	MG	CA	1716	1/1	0.69	0.11	110,110,110,110	0
54	MG	AA	2018	1/1	0.69	0.14	117,117,117,117	0
54	MG	DA	3379	1/1	0.69	0.28	100,100,100,100	0
54	MG	BA	3434	1/1	0.69	0.18	88,88,88,88	0
54	MG	BA	3390	1/1	0.69	0.21	77,77,77,77	0
54	MG	CA	1629	1/1	0.69	0.25	85,85,85,85	0
54	MG	DA	3217	1/1	0.69	0.26	79,79,79,79	0
54	MG	AA	1894	1/1	0.69	0.24	103,103,103,103	0
54	MG	BA	3582	1/1	0.69	0.09	133,133,133,133	0
54	MG	AA	1931	1/1	0.69	0.22	98,98,98,98	0
54	MG	AA	2036	1/1	0.70	0.14	90,90,90,90	0
54	MG	AA	1959	1/1	0.70	0.20	104,104,104,104	0
54	MG	DA	3376	1/1	0.70	0.20	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3196	1/1	0.70	0.25	106,106,106,106	0
54	MG	AA	2027	1/1	0.70	0.24	81,81,81,81	0
54	MG	DA	3789	1/1	0.70	0.23	118,118,118,118	0
54	MG	CW	203	1/1	0.70	0.10	111,111,111,111	0
54	MG	AA	1682	1/1	0.70	0.31	87,87,87,87	0
54	MG	BA	3512	1/1	0.70	0.24	113,113,113,113	0
54	MG	DA	3243	1/1	0.70	0.23	65,65,65,65	0
54	MG	DA	3799	1/1	0.70	0.10	92,92,92,92	0
54	MG	BA	3008	1/1	0.70	0.20	95,95,95,95	0
54	MG	BA	3437	1/1	0.70	0.15	88,88,88,88	0
54	MG	CA	1930	1/1	0.70	0.15	96,96,96,96	0
54	MG	CA	1747	1/1	0.70	0.23	93,93,93,93	0
54	MG	AA	1644	1/1	0.70	0.27	90,90,90,90	0
54	MG	AK	201	1/1	0.70	0.29	90,90,90,90	0
54	MG	CA	1761	1/1	0.70	0.14	129,129,129,129	0
54	MG	BA	3358	1/1	0.70	0.21	101,101,101,101	0
54	MG	AA	1985	1/1	0.70	0.09	131,131,131,131	0
54	MG	CA	1964	1/1	0.70	0.07	94,94,94,94	0
54	MG	CA	1903	1/1	0.70	0.20	134,134,134,134	0
54	MG	DA	3116	1/1	0.70	0.34	93,93,93,93	0
54	MG	CG	301	1/1	0.70	0.38	113,113,113,113	0
54	MG	BA	3285	1/1	0.70	0.07	79,79,79,79	0
54	MG	DA	3535	1/1	0.71	0.16	79,79,79,79	0
54	MG	AA	1740	1/1	0.71	0.11	69,69,69,69	0
54	MG	DA	3377	1/1	0.71	0.17	111,111,111,111	0
54	MG	AA	1844	1/1	0.71	0.13	108,108,108,108	0
54	MG	AA	1699	1/1	0.71	0.18	95,95,95,95	0
54	MG	AA	1734	1/1	0.71	0.20	60,60,60,60	0
54	MG	DA	3580	1/1	0.71	0.18	96,96,96,96	0
54	MG	DA	3223	1/1	0.71	0.12	64,64,64,64	0
54	MG	BA	3546	1/1	0.71	0.24	102,102,102,102	0
54	MG	BB	216	1/1	0.71	0.11	83,83,83,83	0
54	MG	BA	3456	1/1	0.71	0.19	86,86,86,86	0
54	MG	DA	3437	1/1	0.71	0.29	107,107,107,107	0
54	MG	AA	1668	1/1	0.71	0.39	107,107,107,107	0
54	MG	AA	1935	1/1	0.71	0.19	94,94,94,94	0
54	MG	CA	1804	1/1	0.71	0.14	79,79,79,79	0
54	MG	AA	1902	1/1	0.71	0.11	107,107,107,107	0
54	MG	BA	3478	1/1	0.71	0.26	127,127,127,127	0
54	MG	DA	3466	1/1	0.71	0.16	85,85,85,85	0
54	MG	DA	3034	1/1	0.71	0.27	75,75,75,75	0
54	MG	AA	1832	1/1	0.71	0.23	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1754	1/1	0.71	0.21	96,96,96,96	0
54	MG	CA	1971	1/1	0.71	0.20	116,116,116,116	0
54	MG	AA	1927	1/1	0.71	0.28	98,98,98,98	0
54	MG	DA	3327	1/1	0.71	0.28	100,100,100,100	0
54	MG	DA	3669	1/1	0.71	0.13	70,70,70,70	0
54	MG	DB	209	1/1	0.71	0.34	81,81,81,81	0
54	MG	CA	1750	1/1	0.71	0.12	80,80,80,80	0
54	MG	DA	3673	1/1	0.71	0.09	94,94,94,94	0
54	MG	CK	202	1/1	0.71	0.18	87,87,87,87	0
54	MG	CA	1821	1/1	0.71	0.17	104,104,104,104	0
54	MG	DA	3363	1/1	0.71	0.27	113,113,113,113	0
54	MG	DA	3691	1/1	0.71	0.20	82,82,82,82	0
54	MG	DA	3365	1/1	0.71	0.14	107,107,107,107	0
54	MG	DA	3168	1/1	0.71	0.32	96,96,96,96	0
54	MG	D1	201	1/1	0.71	0.30	83,83,83,83	0
54	MG	DA	3169	1/1	0.71	0.21	59,59,59,59	0
54	MG	AA	1728	1/1	0.71	0.21	77,77,77,77	0
54	MG	AA	1842	1/1	0.72	0.17	72,72,72,72	0
54	MG	AA	1853	1/1	0.72	0.13	104,104,104,104	0
54	MG	CA	1776	1/1	0.72	0.12	92,92,92,92	0
54	MG	AA	1888	1/1	0.72	0.16	114,114,114,114	0
54	MG	CA	1925	1/1	0.72	0.20	90,90,90,90	0
54	MG	BA	3177	1/1	0.72	0.23	89,89,89,89	0
54	MG	AA	2033	1/1	0.72	0.22	106,106,106,106	0
54	MG	DA	3202	1/1	0.72	0.30	49,49,49,49	0
54	MG	BA	3515	1/1	0.72	0.29	80,80,80,80	0
54	MG	AC	101	1/1	0.72	0.08	88,88,88,88	0
54	MG	BA	3117	1/1	0.72	0.16	93,93,93,93	0
54	MG	BU	204	1/1	0.72	0.20	94,94,94,94	0
54	MG	DA	3496	1/1	0.72	0.21	69,69,69,69	0
54	MG	CA	1606	1/1	0.72	0.19	70,70,70,70	0
54	MG	BA	3525	1/1	0.72	0.10	95,95,95,95	0
54	MG	AA	1893	1/1	0.72	0.27	95,95,95,95	0
54	MG	BA	3474	1/1	0.72	0.15	78,78,78,78	0
54	MG	CA	1753	1/1	0.72	0.14	114,114,114,114	0
54	MG	DA	3088	1/1	0.72	0.26	56,56,56,56	0
54	MG	DA	3284	1/1	0.72	0.23	75,75,75,75	0
54	MG	DA	3765	1/1	0.72	0.20	110,110,110,110	0
54	MG	CA	1656	1/1	0.72	0.17	98,98,98,98	0
54	MG	BB	207	1/1	0.72	0.12	69,69,69,69	0
54	MG	AA	1843	1/1	0.72	0.32	93,93,93,93	0
54	MG	DA	3749	1/1	0.73	0.12	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1886	1/1	0.73	0.12	120,120,120,120	0
54	MG	AO	201	1/1	0.73	0.21	70,70,70,70	0
54	MG	AA	1674	1/1	0.73	0.20	74,74,74,74	0
54	MG	AA	1940	1/1	0.73	0.19	91,91,91,91	0
54	MG	AA	1819	1/1	0.73	0.11	98,98,98,98	0
54	MG	AA	2020	1/1	0.73	0.15	103,103,103,103	0
54	MG	BA	3454	1/1	0.73	0.13	100,100,100,100	0
54	MG	BA	3154	1/1	0.73	0.24	117,117,117,117	0
54	MG	AA	1611	1/1	0.73	0.26	63,63,63,63	0
54	MG	DA	3212	1/1	0.73	0.22	113,113,113,113	0
54	MG	CA	1918	1/1	0.73	0.10	93,93,93,93	0
54	MG	CA	1660	1/1	0.73	0.15	74,74,74,74	0
54	MG	AA	1730	1/1	0.73	0.26	85,85,85,85	0
54	MG	DA	3800	1/1	0.73	0.11	86,86,86,86	0
54	MG	CA	1664	1/1	0.73	0.16	87,87,87,87	0
54	MG	AA	1828	1/1	0.73	0.07	98,98,98,98	0
54	MG	BA	3473	1/1	0.73	0.16	93,93,93,93	0
54	MG	CD	124	1/1	0.73	0.13	109,109,109,109	0
54	MG	DA	3433	1/1	0.73	0.24	87,87,87,87	0
54	MG	DA	3710	1/1	0.73	0.12	106,106,106,106	0
54	MG	DB	220	1/1	0.73	0.13	122,122,122,122	0
54	MG	CA	1775	1/1	0.73	0.17	99,99,99,99	0
54	MG	AA	1634	1/1	0.73	0.33	97,97,97,97	0
54	MG	CA	1705	1/1	0.73	0.14	84,84,84,84	0
54	MG	CA	1950	1/1	0.73	0.20	121,121,121,121	0
54	MG	DA	3059	1/1	0.73	0.30	58,58,58,58	0
54	MG	BA	3081	1/1	0.73	0.28	72,72,72,72	0
54	MG	CA	1712	1/1	0.73	0.14	65,65,65,65	0
54	MG	BA	3424	1/1	0.73	0.30	107,107,107,107	0
54	MG	D2	201	1/1	0.73	0.12	110,110,110,110	0
54	MG	CA	1718	1/1	0.73	0.22	96,96,96,96	0
54	MG	AA	1612	1/1	0.73	0.27	68,68,68,68	0
54	MG	CA	1850	1/1	0.74	0.10	96,96,96,96	0
54	MG	DA	3568	1/1	0.74	0.14	93,93,93,93	0
54	MG	AA	1713	1/1	0.74	0.24	94,94,94,94	0
54	MG	DA	3185	1/1	0.74	0.31	75,75,75,75	0
54	MG	DA	3444	1/1	0.74	0.26	86,86,86,86	0
54	MG	AA	1640	1/1	0.74	0.19	75,75,75,75	0
54	MG	DA	3793	1/1	0.74	0.15	108,108,108,108	0
54	MG	AX	101	1/1	0.74	0.14	107,107,107,107	0
54	MG	BA	3146	1/1	0.74	0.08	78,78,78,78	0
54	MG	AA	1947	1/1	0.74	0.26	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AC	102	1/1	0.74	0.24	85,85,85,85	0
54	MG	CA	1814	1/1	0.74	0.29	84,84,84,84	0
54	MG	CA	1604	1/1	0.74	0.26	66,66,66,66	0
54	MG	DB	205	1/1	0.74	0.17	69,69,69,69	0
54	MG	AA	2015	1/1	0.74	0.18	106,106,106,106	0
54	MG	CA	1898	1/1	0.74	0.18	122,122,122,122	0
54	MG	DA	3720	1/1	0.74	0.30	82,82,82,82	0
54	MG	DB	217	1/1	0.74	0.12	122,122,122,122	0
54	MG	AA	1995	1/1	0.74	0.15	142,142,142,142	0
54	MG	CA	1772	1/1	0.74	0.22	82,82,82,82	0
54	MG	AA	1938	1/1	0.74	0.35	89,89,89,89	0
54	MG	DB	224	1/1	0.74	0.12	109,109,109,109	0
54	MG	DA	3385	1/1	0.74	0.31	99,99,99,99	0
54	MG	CA	1651	1/1	0.74	0.26	76,76,76,76	0
54	MG	CA	1781	1/1	0.74	0.29	118,118,118,118	0
54	MG	AA	1851	1/1	0.74	0.19	97,97,97,97	0
54	MG	BA	3195	1/1	0.74	0.11	124,124,124,124	0
54	MG	BA	2910	1/1	0.74	0.06	149,149,149,149	0
54	MG	AA	1960	1/1	0.74	0.19	98,98,98,98	0
54	MG	DA	3159	1/1	0.74	0.20	77,77,77,77	0
54	MG	DA	3670	1/1	0.74	0.21	98,98,98,98	0
54	MG	DA	3542	1/1	0.75	0.19	92,92,92,92	0
54	MG	CA	1960	1/1	0.75	0.21	108,108,108,108	0
54	MG	DA	3133	1/1	0.75	0.23	64,64,64,64	0
54	MG	BA	3015	1/1	0.75	0.15	70,70,70,70	0
54	MG	CA	1698	1/1	0.75	0.18	101,101,101,101	0
54	MG	CA	1699	1/1	0.75	0.22	66,66,66,66	0
54	MG	BA	3137	1/1	0.75	0.36	88,88,88,88	0
54	MG	AA	1801	1/1	0.75	0.28	94,94,94,94	0
54	MG	BE	307	1/1	0.75	0.35	84,84,84,84	0
54	MG	DA	3764	1/1	0.75	0.10	108,108,108,108	0
54	MG	CA	1711	1/1	0.75	0.34	75,75,75,75	0
54	MG	DA	3195	1/1	0.75	0.28	77,77,77,77	0
54	MG	AA	1629	1/1	0.75	0.25	74,74,74,74	0
54	MG	CA	1800	1/1	0.75	0.14	97,97,97,97	0
54	MG	DA	3784	1/1	0.75	0.29	106,106,106,106	0
54	MG	AA	1979	1/1	0.75	0.15	75,75,75,75	0
54	MG	DA	3211	1/1	0.75	0.08	71,71,71,71	0
54	MG	DA	3613	1/1	0.75	0.09	70,70,70,70	0
54	MG	AA	1980	1/1	0.75	0.08	136,136,136,136	0
54	MG	AA	2022	1/1	0.75	0.10	117,117,117,117	0
54	MG	AA	1685	1/1	0.75	0.21	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3227	1/1	0.75	0.26	66,66,66,66	0
54	MG	CA	1735	1/1	0.75	0.24	108,108,108,108	0
54	MG	BA	3084	1/1	0.75	0.33	83,83,83,83	0
54	MG	AA	1654	1/1	0.75	0.21	54,54,54,54	0
54	MG	DA	3464	1/1	0.75	0.28	93,93,93,93	0
54	MG	CA	1915	1/1	0.75	0.18	133,133,133,133	0
54	MG	DA	3665	1/1	0.75	0.26	88,88,88,88	0
54	MG	BA	3286	1/1	0.75	0.22	80,80,80,80	0
54	MG	CD	112	1/1	0.75	0.07	85,85,85,85	0
54	MG	BA	3115	1/1	0.75	0.15	89,89,89,89	0
54	MG	AA	1896	1/1	0.75	0.18	93,93,93,93	0
54	MG	BA	3118	1/1	0.75	0.17	82,82,82,82	0
54	MG	BA	3493	1/1	0.75	0.26	85,85,85,85	0
54	MG	BA	3125	1/1	0.75	0.12	94,94,94,94	0
54	MG	AA	1830	1/1	0.75	0.19	88,88,88,88	0
54	MG	DA	3072	1/1	0.75	0.21	66,66,66,66	0
54	MG	BA	3505	1/1	0.75	0.35	114,114,114,114	0
54	MG	BA	3132	1/1	0.75	0.28	90,90,90,90	0
54	MG	DA	3328	1/1	0.75	0.18	93,93,93,93	0
54	MG	CA	1676	1/1	0.75	0.24	83,83,83,83	0
54	MG	CA	1849	1/1	0.75	0.18	91,91,91,91	0
54	MG	DA	3355	1/1	0.75	0.12	60,60,60,60	0
54	MG	DA	3715	1/1	0.75	0.17	91,91,91,91	0
54	MG	BA	3237	1/1	0.75	0.12	82,82,82,82	0
54	MG	DA	3126	1/1	0.75	0.26	65,65,65,65	0
54	MG	AA	1725	1/1	0.76	0.30	92,92,92,92	0
54	MG	DA	3579	1/1	0.76	0.24	94,94,94,94	0
54	MG	CA	1797	1/1	0.76	0.16	77,77,77,77	0
54	MG	DA	3219	1/1	0.76	0.26	80,80,80,80	0
54	MG	CD	120	1/1	0.76	0.11	110,110,110,110	0
54	MG	CA	1667	1/1	0.76	0.07	93,93,93,93	0
54	MG	DA	2991	1/1	0.76	0.31	75,75,75,75	0
54	MG	AA	1771	1/1	0.76	0.21	70,70,70,70	0
54	MG	AA	1841	1/1	0.76	0.16	100,100,100,100	0
54	MG	BA	3491	1/1	0.76	0.22	104,104,104,104	0
54	MG	DA	3773	1/1	0.76	0.19	89,89,89,89	0
54	MG	DA	3261	1/1	0.76	0.26	102,102,102,102	0
54	MG	DA	3783	1/1	0.76	0.16	84,84,84,84	0
54	MG	CA	1876	1/1	0.76	0.12	83,83,83,83	0
54	MG	AA	1758	1/1	0.76	0.15	108,108,108,108	0
54	MG	DA	3457	1/1	0.76	0.11	74,74,74,74	0
54	MG	DA	3275	1/1	0.76	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3630	1/1	0.76	0.12	67,67,67,67	0
54	MG	CA	1880	1/1	0.76	0.15	130,130,130,130	0
54	MG	AA	1759	1/1	0.76	0.24	77,77,77,77	0
54	MG	AA	1760	1/1	0.76	0.21	91,91,91,91	0
54	MG	CA	1968	1/1	0.76	0.12	90,90,90,90	0
54	MG	BA	3445	1/1	0.76	0.26	96,96,96,96	0
54	MG	DA	3109	1/1	0.76	0.34	103,103,103,103	0
54	MG	CA	1817	1/1	0.76	0.27	105,105,105,105	0
54	MG	DA	3803	1/1	0.76	0.08	99,99,99,99	0
54	MG	CA	1976	1/1	0.76	0.10	103,103,103,103	0
54	MG	CA	1763	1/1	0.76	0.23	72,72,72,72	0
54	MG	AA	1809	1/1	0.76	0.17	85,85,85,85	0
54	MG	DA	3499	1/1	0.76	0.18	87,87,87,87	0
54	MG	CP	201	1/1	0.76	0.31	118,118,118,118	0
54	MG	DA	3349	1/1	0.76	0.26	56,56,56,56	0
54	MG	DA	3156	1/1	0.76	0.33	95,95,95,95	0
54	MG	AA	1621	1/1	0.76	0.19	50,50,50,50	0
54	MG	AC	106	1/1	0.76	0.17	79,79,79,79	0
54	MG	CA	1715	1/1	0.76	0.25	101,101,101,101	0
54	MG	BA	3036	1/1	0.76	0.22	41,41,41,41	0
54	MG	CA	1913	1/1	0.76	0.11	101,101,101,101	0
54	MG	DA	3534	1/1	0.76	0.24	86,86,86,86	0
54	MG	BA	3415	1/1	0.76	0.37	89,89,89,89	0
54	MG	CA	1917	1/1	0.76	0.12	95,95,95,95	0
54	MG	BB	212	1/1	0.76	0.15	81,81,81,81	0
54	MG	BA	3348	1/1	0.76	0.21	99,99,99,99	0
54	MG	D1	205	1/1	0.76	0.15	110,110,110,110	0
54	MG	AA	1661	1/1	0.76	0.45	93,93,93,93	0
54	MG	DU	201	1/1	0.76	0.14	60,60,60,60	0
54	MG	AA	2011	1/1	0.76	0.23	120,120,120,120	0
54	MG	DA	3400	1/1	0.76	0.20	73,73,73,73	0
54	MG	BA	3240	1/1	0.77	0.25	71,71,71,71	0
54	MG	DA	3536	1/1	0.77	0.17	94,94,94,94	0
54	MG	DA	3722	1/1	0.77	0.14	166,166,166,166	0
54	MG	DA	3370	1/1	0.77	0.20	79,79,79,79	0
54	MG	DA	3557	1/1	0.77	0.19	97,97,97,97	0
54	MG	AA	1781	1/1	0.77	0.25	98,98,98,98	0
54	MG	AA	1839	1/1	0.77	0.12	91,91,91,91	0
54	MG	BA	3430	1/1	0.77	0.15	90,90,90,90	0
54	MG	CA	1916	1/1	0.77	0.13	114,114,114,114	0
54	MG	CA	1831	1/1	0.77	0.17	95,95,95,95	0
54	MG	BA	3342	1/1	0.77	0.32	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CC	113	1/1	0.77	0.11	67,67,67,67	0
54	MG	CA	1689	1/1	0.77	0.13	62,62,62,62	0
54	MG	DA	3412	1/1	0.77	0.21	105,105,105,105	0
54	MG	BA	3254	1/1	0.77	0.27	101,101,101,101	0
54	MG	DA	3591	1/1	0.77	0.11	81,81,81,81	0
54	MG	AA	1746	1/1	0.77	0.18	81,81,81,81	0
54	MG	AA	1918	1/1	0.77	0.11	84,84,84,84	0
54	MG	BA	2992	1/1	0.77	0.20	63,63,63,63	0
54	MG	DA	3609	1/1	0.77	0.19	86,86,86,86	0
54	MG	DA	3228	1/1	0.77	0.25	77,77,77,77	0
54	MG	CD	121	1/1	0.77	0.13	112,112,112,112	0
54	MG	CD	122	1/1	0.77	0.07	97,97,97,97	0
54	MG	DA	3617	1/1	0.77	0.27	91,91,91,91	0
54	MG	CA	1932	1/1	0.77	0.12	94,94,94,94	0
54	MG	DA	3442	1/1	0.77	0.16	86,86,86,86	0
54	MG	CA	1938	1/1	0.77	0.22	85,85,85,85	0
54	MG	BA	3535	1/1	0.77	0.08	94,94,94,94	0
54	MG	AA	1694	1/1	0.77	0.15	66,66,66,66	0
54	MG	AA	1953	1/1	0.77	0.14	94,94,94,94	0
54	MG	BA	3279	1/1	0.77	0.21	85,85,85,85	0
54	MG	DA	3805	1/1	0.77	0.22	90,90,90,90	0
54	MG	AA	1923	1/1	0.77	0.21	85,85,85,85	0
54	MG	AA	1972	1/1	0.77	0.17	78,78,78,78	0
54	MG	DA	3467	1/1	0.77	0.24	61,61,61,61	0
54	MG	DA	3078	1/1	0.77	0.16	77,77,77,77	0
54	MG	CA	1875	1/1	0.77	0.15	110,110,110,110	0
54	MG	DA	3301	1/1	0.77	0.17	86,86,86,86	0
54	MG	BA	3386	1/1	0.77	0.15	85,85,85,85	0
54	MG	CA	1720	1/1	0.77	0.11	94,94,94,94	0
54	MG	BA	3130	1/1	0.77	0.21	75,75,75,75	0
54	MG	CA	1633	1/1	0.77	0.26	70,70,70,70	0
54	MG	DA	3498	1/1	0.77	0.20	107,107,107,107	0
54	MG	DB	225	1/1	0.77	0.16	84,84,84,84	0
54	MG	BA	3037	1/1	0.77	0.19	61,61,61,61	0
54	MG	CA	1649	1/1	0.77	0.29	86,86,86,86	0
54	MG	CA	1983	1/1	0.77	0.09	92,92,92,92	0
54	MG	DA	3130	1/1	0.77	0.36	89,89,89,89	0
54	MG	CA	1984	1/1	0.77	0.18	106,106,106,106	0
54	MG	BA	3398	1/1	0.77	0.11	131,131,131,131	0
54	MG	AA	1643	1/1	0.77	0.12	124,124,124,124	0
54	MG	AA	1765	1/1	0.77	0.22	83,83,83,83	0
54	MG	BA	3233	1/1	0.77	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1898	1/1	0.77	0.07	102,102,102,102	0
54	MG	DA	3718	1/1	0.77	0.25	88,88,88,88	0
54	MG	BA	3409	1/1	0.78	0.15	100,100,100,100	0
54	MG	AA	1970	1/1	0.78	0.19	98,98,98,98	0
54	MG	CA	1937	1/1	0.78	0.17	81,81,81,81	0
54	MG	AA	2005	1/1	0.78	0.10	96,96,96,96	0
54	MG	AA	1920	1/1	0.78	0.13	115,115,115,115	0
54	MG	BZ	101	1/1	0.78	0.12	92,92,92,92	0
54	MG	DA	3581	1/1	0.78	0.13	139,139,139,139	0
54	MG	DA	3583	1/1	0.78	0.25	99,99,99,99	0
54	MG	DA	3435	1/1	0.78	0.10	90,90,90,90	0
54	MG	AA	1871	1/1	0.78	0.09	117,117,117,117	0
54	MG	DA	3439	1/1	0.78	0.32	104,104,104,104	0
54	MG	AA	1732	1/1	0.78	0.16	89,89,89,89	0
54	MG	AA	1833	1/1	0.78	0.18	88,88,88,88	0
54	MG	BA	2991	1/1	0.78	0.20	76,76,76,76	0
54	MG	AA	2016	1/1	0.78	0.29	102,102,102,102	0
54	MG	DA	3780	1/1	0.78	0.12	72,72,72,72	0
54	MG	DA	3449	1/1	0.78	0.15	95,95,95,95	0
54	MG	DA	3283	1/1	0.78	0.14	81,81,81,81	0
54	MG	BA	3082	1/1	0.78	0.18	59,59,59,59	0
54	MG	BA	3388	1/1	0.78	0.18	95,95,95,95	0
54	MG	CA	1967	1/1	0.78	0.08	113,113,113,113	0
54	MG	CA	1730	1/1	0.78	0.17	66,66,66,66	0
54	MG	AA	1864	1/1	0.78	0.24	87,87,87,87	0
54	MG	DA	3626	1/1	0.78	0.29	109,109,109,109	0
54	MG	CA	1889	1/1	0.78	0.13	89,89,89,89	0
54	MG	CA	1655	1/1	0.78	0.17	68,68,68,68	0
54	MG	DA	3323	1/1	0.78	0.17	105,105,105,105	0
54	MG	CA	1740	1/1	0.78	0.09	104,104,104,104	0
54	MG	DA	3647	1/1	0.78	0.19	98,98,98,98	0
54	MG	BB	201	1/1	0.78	0.14	69,69,69,69	0
54	MG	BA	3511	1/1	0.78	0.08	140,140,140,140	0
54	MG	DA	3493	1/1	0.78	0.19	78,78,78,78	0
54	MG	BA	3393	1/1	0.78	0.11	82,82,82,82	0
54	MG	DA	3666	1/1	0.78	0.16	78,78,78,78	0
54	MG	AA	1744	1/1	0.78	0.18	77,77,77,77	0
54	MG	CA	1820	1/1	0.78	0.19	102,102,102,102	0
54	MG	CA	1911	1/1	0.78	0.08	123,123,123,123	0
54	MG	BA	3446	1/1	0.78	0.14	74,74,74,74	0
54	MG	DB	215	1/1	0.78	0.22	99,99,99,99	0
54	MG	DA	3509	1/1	0.78	0.12	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	218	1/1	0.78	0.16	84,84,84,84	0
54	MG	BA	3106	1/1	0.78	0.33	80,80,80,80	0
54	MG	CA	1754	1/1	0.78	0.21	82,82,82,82	0
54	MG	BA	3352	1/1	0.78	0.11	112,112,112,112	0
54	MG	DA	3690	1/1	0.78	0.20	83,83,83,83	0
54	MG	BA	3526	1/1	0.78	0.08	100,100,100,100	0
54	MG	BA	3402	1/1	0.78	0.22	96,96,96,96	0
54	MG	CA	1919	1/1	0.78	0.13	112,112,112,112	0
54	MG	CC	112	1/1	0.78	0.11	88,88,88,88	0
54	MG	DA	3705	1/1	0.78	0.19	97,97,97,97	0
54	MG	CA	1695	1/1	0.78	0.16	62,62,62,62	0
54	MG	CD	106	1/1	0.78	0.10	94,94,94,94	0
54	MG	CA	1923	1/1	0.78	0.16	104,104,104,104	0
54	MG	DA	3397	1/1	0.78	0.23	77,77,77,77	0
54	MG	CA	1845	1/1	0.78	0.21	82,82,82,82	0
54	MG	BA	3403	1/1	0.78	0.25	89,89,89,89	0
54	MG	BA	3544	1/1	0.78	0.22	71,71,71,71	0
54	MG	BA	3370	1/1	0.79	0.09	70,70,70,70	0
54	MG	AA	1914	1/1	0.79	0.16	109,109,109,109	0
54	MG	DA	3727	1/1	0.79	0.33	106,106,106,106	0
54	MG	BA	3273	1/1	0.79	0.10	72,72,72,72	0
54	MG	DA	3198	1/1	0.79	0.13	82,82,82,82	0
54	MG	CA	1757	1/1	0.79	0.08	79,79,79,79	0
54	MG	CC	105	1/1	0.79	0.23	88,88,88,88	0
54	MG	CC	109	1/1	0.79	0.21	99,99,99,99	0
54	MG	AA	1608	1/1	0.79	0.30	67,67,67,67	0
54	MG	DA	3761	1/1	0.79	0.11	112,112,112,112	0
54	MG	AA	1741	1/1	0.79	0.18	93,93,93,93	0
54	MG	AA	2028	1/1	0.79	0.19	102,102,102,102	0
54	MG	BB	222	1/1	0.79	0.08	93,93,93,93	0
54	MG	BA	2967	1/1	0.79	0.23	60,60,60,60	0
54	MG	BA	2987	1/1	0.79	0.27	57,57,57,57	0
54	MG	BE	306	1/1	0.79	0.12	72,72,72,72	0
54	MG	BA	3447	1/1	0.79	0.10	109,109,109,109	0
54	MG	BA	3217	1/1	0.79	0.23	86,86,86,86	0
54	MG	AA	1838	1/1	0.79	0.33	77,77,77,77	0
54	MG	DA	3450	1/1	0.79	0.19	98,98,98,98	0
54	MG	AA	2012	1/1	0.79	0.11	117,117,117,117	0
54	MG	BA	3545	1/1	0.79	0.14	82,82,82,82	0
54	MG	DA	2981	1/1	0.79	0.26	60,60,60,60	0
54	MG	CA	1874	1/1	0.79	0.08	144,144,144,144	0
54	MG	CA	1955	1/1	0.79	0.34	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3459	1/1	0.79	0.14	110,110,110,110	0
54	MG	DA	3024	1/1	0.79	0.08	39,39,39,39	0
54	MG	DA	3797	1/1	0.79	0.32	85,85,85,85	0
54	MG	AW	204	1/1	0.79	0.18	105,105,105,105	0
54	MG	DA	3295	1/1	0.79	0.22	104,104,104,104	0
54	MG	CA	1790	1/1	0.79	0.20	76,76,76,76	0
54	MG	AA	1907	1/1	0.79	0.12	106,106,106,106	0
54	MG	CA	1882	1/1	0.79	0.16	106,106,106,106	0
54	MG	DA	3310	1/1	0.79	0.28	66,66,66,66	0
54	MG	CA	1965	1/1	0.79	0.19	92,92,92,92	0
54	MG	AA	1895	1/1	0.79	0.12	133,133,133,133	0
54	MG	AA	1922	1/1	0.79	0.35	94,94,94,94	0
54	MG	DA	3089	1/1	0.79	0.29	66,66,66,66	0
54	MG	CA	1969	1/1	0.79	0.12	86,86,86,86	0
54	MG	DA	3094	1/1	0.79	0.16	49,49,49,49	0
54	MG	DA	3104	1/1	0.79	0.25	79,79,79,79	0
54	MG	DA	3686	1/1	0.79	0.15	93,93,93,93	0
54	MG	AC	103	1/1	0.79	0.10	86,86,86,86	0
54	MG	AA	1885	1/1	0.79	0.08	113,113,113,113	0
54	MG	CA	1733	1/1	0.79	0.14	67,67,67,67	0
54	MG	DA	3124	1/1	0.79	0.16	66,66,66,66	0
54	MG	CA	1977	1/1	0.79	0.10	100,100,100,100	0
54	MG	AA	1998	1/1	0.79	0.18	98,98,98,98	0
54	MG	CA	1736	1/1	0.79	0.17	89,89,89,89	0
54	MG	BA	3255	1/1	0.79	0.13	93,93,93,93	0
54	MG	AA	1814	1/1	0.79	0.19	63,63,63,63	0
54	MG	DG	201	1/1	0.79	0.26	76,76,76,76	0
54	MG	CM	201	1/1	0.79	0.09	91,91,91,91	0
54	MG	DO	203	1/1	0.79	0.22	100,100,100,100	0
54	MG	AA	2021	1/1	0.79	0.11	108,108,108,108	0
54	MG	BA	3580	1/1	0.79	0.13	89,89,89,89	0
54	MG	DA	3565	1/1	0.79	0.14	100,100,100,100	0
54	MG	AA	1729	1/1	0.79	0.14	87,87,87,87	0
54	MG	BA	3500	1/1	0.79	0.16	64,64,64,64	0
54	MG	DU	205	1/1	0.79	0.10	75,75,75,75	0
54	MG	CA	1749	1/1	0.79	0.18	69,69,69,69	0
54	MG	BA	3032	1/1	0.80	0.34	66,66,66,66	0
54	MG	BA	3558	1/1	0.80	0.11	108,108,108,108	0
54	MG	CA	1616	1/1	0.80	0.14	68,68,68,68	0
54	MG	CC	107	1/1	0.80	0.15	102,102,102,102	0
54	MG	DA	3396	1/1	0.80	0.11	85,85,85,85	0
54	MG	CA	1622	1/1	0.80	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3732	1/1	0.80	0.27	94,94,94,94	0
54	MG	BA	3559	1/1	0.80	0.20	104,104,104,104	0
54	MG	CA	1631	1/1	0.80	0.25	68,68,68,68	0
54	MG	DA	3404	1/1	0.80	0.26	94,94,94,94	0
54	MG	DA	3747	1/1	0.80	0.17	90,90,90,90	0
54	MG	BA	3476	1/1	0.80	0.15	97,97,97,97	0
54	MG	CA	1637	1/1	0.80	0.19	70,70,70,70	0
54	MG	AA	1676	1/1	0.80	0.16	96,96,96,96	0
54	MG	CA	1644	1/1	0.80	0.20	52,52,52,52	0
54	MG	BA	3362	1/1	0.80	0.11	68,68,68,68	0
54	MG	DA	3766	1/1	0.80	0.16	81,81,81,81	0
54	MG	DA	3226	1/1	0.80	0.16	74,74,74,74	0
54	MG	CA	1751	1/1	0.80	0.11	96,96,96,96	0
54	MG	BA	3483	1/1	0.80	0.13	103,103,103,103	0
54	MG	DA	3232	1/1	0.80	0.18	67,67,67,67	0
54	MG	BA	3488	1/1	0.80	0.15	96,96,96,96	0
54	MG	DA	3610	1/1	0.80	0.20	99,99,99,99	0
54	MG	AA	1855	1/1	0.80	0.18	101,101,101,101	0
54	MG	AS	101	1/1	0.80	0.33	84,84,84,84	0
54	MG	CA	1952	1/1	0.80	0.18	134,134,134,134	0
54	MG	DA	3247	1/1	0.80	0.10	45,45,45,45	0
54	MG	DA	3445	1/1	0.80	0.20	95,95,95,95	0
54	MG	CA	1855	1/1	0.80	0.11	99,99,99,99	0
54	MG	BA	3373	1/1	0.80	0.30	105,105,105,105	0
54	MG	AA	1963	1/1	0.80	0.26	103,103,103,103	0
54	MG	DA	3627	1/1	0.80	0.08	87,87,87,87	0
54	MG	BA	3581	1/1	0.80	0.23	125,125,125,125	0
54	MG	DA	3629	1/1	0.80	0.26	72,72,72,72	0
54	MG	AA	1808	1/1	0.80	0.11	92,92,92,92	0
54	MG	AA	2031	1/1	0.80	0.23	86,86,86,86	0
54	MG	AA	1930	1/1	0.80	0.23	82,82,82,82	0
54	MG	DA	3645	1/1	0.80	0.35	88,88,88,88	0
54	MG	BA	3510	1/1	0.80	0.14	91,91,91,91	0
54	MG	DA	3294	1/1	0.80	0.20	78,78,78,78	0
54	MG	AA	1680	1/1	0.80	0.16	70,70,70,70	0
54	MG	BB	209	1/1	0.80	0.17	59,59,59,59	0
54	MG	DA	3473	1/1	0.80	0.20	87,87,87,87	0
54	MG	AA	1671	1/1	0.80	0.13	66,66,66,66	0
54	MG	DA	3478	1/1	0.80	0.24	71,71,71,71	0
54	MG	BA	3319	1/1	0.80	0.30	108,108,108,108	0
54	MG	DA	3490	1/1	0.80	0.24	90,90,90,90	0
54	MG	AA	1845	1/1	0.80	0.13	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3448	1/1	0.80	0.07	95,95,95,95	0
54	MG	CA	1978	1/1	0.80	0.09	73,73,73,73	0
54	MG	CA	1981	1/1	0.80	0.08	65,65,65,65	0
54	MG	AA	1710	1/1	0.80	0.12	78,78,78,78	0
54	MG	BA	3256	1/1	0.80	0.09	64,64,64,64	0
54	MG	BA	3534	1/1	0.80	0.14	93,93,93,93	0
54	MG	BA	3334	1/1	0.80	0.19	75,75,75,75	0
54	MG	BA	3109	1/1	0.80	0.19	73,73,73,73	0
54	MG	BA	3541	1/1	0.80	0.15	79,79,79,79	0
54	MG	DA	3132	1/1	0.80	0.16	76,76,76,76	0
54	MG	AA	1748	1/1	0.80	0.11	85,85,85,85	0
54	MG	DR	202	1/1	0.80	0.24	102,102,102,102	0
54	MG	BA	3343	1/1	0.80	0.18	73,73,73,73	0
54	MG	DA	3364	1/1	0.80	0.28	79,79,79,79	0
54	MG	CS	101	1/1	0.80	0.22	82,82,82,82	0
54	MG	BT	102	1/1	0.80	0.14	100,100,100,100	0
54	MG	CA	1723	1/1	0.80	0.11	111,111,111,111	0
54	MG	AA	1925	1/1	0.80	0.12	87,87,87,87	0
54	MG	AA	1831	1/1	0.80	0.12	76,76,76,76	0
54	MG	DA	3741	1/1	0.81	0.18	97,97,97,97	0
54	MG	BA	3502	1/1	0.81	0.12	91,91,91,91	0
54	MG	BA	3345	1/1	0.81	0.10	80,80,80,80	0
54	MG	DA	3316	1/1	0.81	0.18	88,88,88,88	0
54	MG	DA	3317	1/1	0.81	0.11	91,91,91,91	0
54	MG	AA	1798	1/1	0.81	0.17	79,79,79,79	0
54	MG	DA	3136	1/1	0.81	0.20	53,53,53,53	0
54	MG	CA	1854	1/1	0.81	0.28	79,79,79,79	0
54	MG	BA	3138	1/1	0.81	0.22	85,85,85,85	0
54	MG	BA	3086	1/1	0.81	0.15	50,50,50,50	0
54	MG	AA	1695	1/1	0.81	0.25	73,73,73,73	0
54	MG	BA	3575	1/1	0.81	0.12	82,82,82,82	0
54	MG	AA	1631	1/1	0.81	0.25	60,60,60,60	0
54	MG	BA	3465	1/1	0.81	0.08	92,92,92,92	0
54	MG	DA	3356	1/1	0.81	0.25	73,73,73,73	0
54	MG	DA	3642	1/1	0.81	0.18	81,81,81,81	0
54	MG	BA	3365	1/1	0.81	0.16	77,77,77,77	0
54	MG	AA	1632	1/1	0.81	0.19	72,72,72,72	0
54	MG	AA	1607	1/1	0.81	0.25	68,68,68,68	0
54	MG	CA	1634	1/1	0.81	0.19	54,54,54,54	0
54	MG	BA	3298	1/1	0.81	0.14	95,95,95,95	0
54	MG	CA	1798	1/1	0.81	0.15	112,112,112,112	0
54	MG	CA	1638	1/1	0.81	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1728	1/1	0.81	0.29	85,85,85,85	0
54	MG	BA	3050	1/1	0.81	0.21	67,67,67,67	0
54	MG	BA	3051	1/1	0.81	0.26	74,74,74,74	0
54	MG	DA	3017	1/1	0.81	0.20	43,43,43,43	0
54	MG	CA	1973	1/1	0.81	0.11	116,116,116,116	0
54	MG	CA	1974	1/1	0.81	0.12	88,88,88,88	0
54	MG	CA	1648	1/1	0.81	0.29	79,79,79,79	0
54	MG	BA	3184	1/1	0.81	0.28	116,116,116,116	0
54	MG	DA	3683	1/1	0.81	0.16	100,100,100,100	0
54	MG	BA	3121	1/1	0.81	0.18	76,76,76,76	0
54	MG	BB	215	1/1	0.81	0.09	65,65,65,65	0
54	MG	DA	3538	1/1	0.81	0.19	91,91,91,91	0
54	MG	DA	3073	1/1	0.81	0.26	73,73,73,73	0
54	MG	BA	3325	1/1	0.81	0.27	98,98,98,98	0
54	MG	BB	217	1/1	0.81	0.22	102,102,102,102	0
54	MG	AA	1603	1/1	0.81	0.31	54,54,54,54	0
54	MG	DA	3268	1/1	0.81	0.37	73,73,73,73	0
54	MG	DA	3706	1/1	0.81	0.14	78,78,78,78	0
54	MG	DA	3708	1/1	0.81	0.18	152,152,152,152	0
54	MG	CA	1659	1/1	0.81	0.15	101,101,101,101	0
54	MG	DA	3711	1/1	0.81	0.12	102,102,102,102	0
54	MG	DA	3271	1/1	0.81	0.40	87,87,87,87	0
54	MG	AA	1627	1/1	0.81	0.25	70,70,70,70	0
54	MG	BA	3492	1/1	0.81	0.08	86,86,86,86	0
54	MG	CA	1663	1/1	0.81	0.25	81,81,81,81	0
54	MG	DD	301	1/1	0.81	0.32	43,43,43,43	0
54	MG	DA	3717	1/1	0.81	0.15	88,88,88,88	0
54	MG	CA	1752	1/1	0.81	0.15	90,90,90,90	0
54	MG	BE	301	1/1	0.81	0.12	60,60,60,60	0
54	MG	BA	2904	1/1	0.81	0.07	101,101,101,101	0
54	MG	D0	204	1/1	0.81	0.09	95,95,95,95	0
54	MG	BA	3495	1/1	0.81	0.49	97,97,97,97	0
54	MG	AA	1824	1/1	0.81	0.23	85,85,85,85	0
54	MG	DA	3447	1/1	0.81	0.11	84,84,84,84	0
54	MG	BG	201	1/1	0.81	0.10	117,117,117,117	0
54	MG	AA	1610	1/1	0.81	0.26	68,68,68,68	0
54	MG	DA	3304	1/1	0.81	0.08	41,41,41,41	0
54	MG	DA	3456	1/1	0.81	0.38	92,92,92,92	0
54	MG	DA	3740	1/1	0.81	0.18	88,88,88,88	0
54	MG	B0	202	1/1	0.82	0.28	111,111,111,111	0
54	MG	AA	1679	1/1	0.82	0.13	74,74,74,74	0
54	MG	AA	1906	1/1	0.82	0.19	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BR	202	1/1	0.82	0.13	105,105,105,105	0
54	MG	AA	1638	1/1	0.82	0.23	61,61,61,61	0
54	MG	DA	3567	1/1	0.82	0.23	91,91,91,91	0
54	MG	DA	3389	1/1	0.82	0.27	70,70,70,70	0
54	MG	BA	3116	1/1	0.82	0.31	64,64,64,64	0
54	MG	AA	1637	1/1	0.82	0.33	82,82,82,82	0
54	MG	BA	3509	1/1	0.82	0.15	107,107,107,107	0
54	MG	AA	1648	1/1	0.82	0.18	68,68,68,68	0
54	MG	CA	1609	1/1	0.82	0.28	54,54,54,54	0
54	MG	DA	3745	1/1	0.82	0.19	95,95,95,95	0
54	MG	DA	3405	1/1	0.82	0.16	91,91,91,91	0
54	MG	DA	2951	1/1	0.82	0.22	54,54,54,54	0
54	MG	DA	3411	1/1	0.82	0.21	86,86,86,86	0
54	MG	BA	3577	1/1	0.82	0.10	80,80,80,80	0
54	MG	DA	3237	1/1	0.82	0.22	68,68,68,68	0
54	MG	DA	3762	1/1	0.82	0.11	119,119,119,119	0
54	MG	CA	1962	1/1	0.82	0.10	90,90,90,90	0
54	MG	AA	2037	1/1	0.82	0.15	97,97,97,97	0
54	MG	BA	3462	1/1	0.82	0.23	77,77,77,77	0
54	MG	BA	3357	1/1	0.82	0.15	66,66,66,66	0
54	MG	BA	3407	1/1	0.82	0.24	106,106,106,106	0
54	MG	BA	3063	1/1	0.82	0.28	63,63,63,63	0
54	MG	DA	3038	1/1	0.82	0.17	50,50,50,50	0
54	MG	DA	3048	1/1	0.82	0.21	67,67,67,67	0
54	MG	CA	1883	1/1	0.82	0.07	80,80,80,80	0
54	MG	CA	1635	1/1	0.82	0.32	86,86,86,86	0
54	MG	DA	3278	1/1	0.82	0.17	78,78,78,78	0
54	MG	BA	3069	1/1	0.82	0.10	48,48,48,48	0
54	MG	BA	3472	1/1	0.82	0.09	125,125,125,125	0
54	MG	CA	1892	1/1	0.82	0.09	99,99,99,99	0
54	MG	CA	1895	1/1	0.82	0.11	87,87,87,87	0
54	MG	CA	1805	1/1	0.82	0.13	89,89,89,89	0
54	MG	CA	1806	1/1	0.82	0.14	106,106,106,106	0
54	MG	AA	1879	1/1	0.82	0.10	85,85,85,85	0
54	MG	DA	3461	1/1	0.82	0.13	66,66,66,66	0
54	MG	DA	3641	1/1	0.82	0.20	76,76,76,76	0
54	MG	AA	1756	1/1	0.82	0.11	68,68,68,68	0
54	MG	AA	1650	1/1	0.82	0.10	74,74,74,74	0
54	MG	BA	3539	1/1	0.82	0.22	100,100,100,100	0
54	MG	DA	3804	1/1	0.82	0.14	94,94,94,94	0
54	MG	AA	1883	1/1	0.82	0.12	64,64,64,64	0
54	MG	AA	1642	1/1	0.82	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AC	107	1/1	0.82	0.13	114,114,114,114	0
54	MG	AA	1990	1/1	0.82	0.13	97,97,97,97	0
54	MG	CQ	102	1/1	0.82	0.17	111,111,111,111	0
54	MG	DA	3474	1/1	0.82	0.33	89,89,89,89	0
54	MG	DB	211	1/1	0.82	0.18	78,78,78,78	0
54	MG	DA	3322	1/1	0.82	0.15	79,79,79,79	0
54	MG	CQ	103	1/1	0.82	0.12	122,122,122,122	0
54	MG	CA	1746	1/1	0.82	0.28	86,86,86,86	0
54	MG	BA	3377	1/1	0.82	0.07	67,67,67,67	0
54	MG	CA	1658	1/1	0.82	0.23	76,76,76,76	0
54	MG	DA	3335	1/1	0.82	0.33	93,93,93,93	0
54	MG	CA	1826	1/1	0.82	0.21	107,107,107,107	0
54	MG	DA	3343	1/1	0.82	0.18	86,86,86,86	0
54	MG	BD	302	1/1	0.82	0.13	69,69,69,69	0
54	MG	DA	3350	1/1	0.82	0.18	109,109,109,109	0
54	MG	BA	3089	1/1	0.82	0.32	74,74,74,74	0
54	MG	DA	3508	1/1	0.82	0.28	73,73,73,73	0
54	MG	CX	101	1/1	0.82	0.13	90,90,90,90	0
54	MG	BA	3557	1/1	0.82	0.22	131,131,131,131	0
54	MG	BA	3152	1/1	0.82	0.18	72,72,72,72	0
54	MG	DA	3516	1/1	0.82	0.14	99,99,99,99	0
54	MG	DA	3359	1/1	0.82	0.18	70,70,70,70	0
54	MG	DA	3518	1/1	0.82	0.14	78,78,78,78	0
54	MG	DA	3187	1/1	0.82	0.22	64,64,64,64	0
54	MG	AA	1708	1/1	0.82	0.16	70,70,70,70	0
54	MG	BA	3158	1/1	0.82	0.08	39,39,39,39	0
54	MG	DA	3529	1/1	0.82	0.32	94,94,94,94	0
54	MG	CA	1929	1/1	0.82	0.21	92,92,92,92	0
54	MG	CA	1674	1/1	0.82	0.16	73,73,73,73	0
54	MG	BA	3497	1/1	0.82	0.21	72,72,72,72	0
54	MG	DA	3371	1/1	0.82	0.21	79,79,79,79	0
54	MG	BA	3276	1/1	0.83	0.10	79,79,79,79	0
54	MG	AA	1875	1/1	0.83	0.10	113,113,113,113	0
54	MG	AA	1890	1/1	0.83	0.10	72,72,72,72	0
54	MG	AA	1779	1/1	0.83	0.06	114,114,114,114	0
54	MG	BA	2943	1/1	0.83	0.23	44,44,44,44	0
54	MG	BA	3284	1/1	0.83	0.10	74,74,74,74	0
54	MG	BA	3167	1/1	0.83	0.36	91,91,91,91	0
54	MG	DA	3723	1/1	0.83	0.23	106,106,106,106	0
54	MG	AA	2032	1/1	0.83	0.11	84,84,84,84	0
54	MG	BA	2981	1/1	0.83	0.19	58,58,58,58	0
54	MG	DA	3544	1/1	0.83	0.18	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3548	1/1	0.83	0.17	86,86,86,86	0
54	MG	DA	3555	1/1	0.83	0.24	81,81,81,81	0
54	MG	BA	3087	1/1	0.83	0.18	72,72,72,72	0
54	MG	DA	3559	1/1	0.83	0.23	103,103,103,103	0
54	MG	AA	1614	1/1	0.83	0.27	73,73,73,73	0
54	MG	DA	3381	1/1	0.83	0.11	73,73,73,73	0
54	MG	BA	3094	1/1	0.83	0.13	84,84,84,84	0
54	MG	BA	3302	1/1	0.83	0.10	61,61,61,61	0
54	MG	BA	3314	1/1	0.83	0.15	76,76,76,76	0
54	MG	DA	3218	1/1	0.83	0.24	61,61,61,61	0
54	MG	DA	3398	1/1	0.83	0.35	100,100,100,100	0
54	MG	DA	3754	1/1	0.83	0.24	99,99,99,99	0
54	MG	BA	3317	1/1	0.83	0.17	63,63,63,63	0
54	MG	DA	3577	1/1	0.83	0.09	80,80,80,80	0
54	MG	CA	1946	1/1	0.83	0.09	91,91,91,91	0
54	MG	CD	115	1/1	0.83	0.17	106,106,106,106	0
54	MG	CA	1647	1/1	0.83	0.21	81,81,81,81	0
54	MG	BA	2988	1/1	0.83	0.16	46,46,46,46	0
54	MG	AA	1989	1/1	0.83	0.11	91,91,91,91	0
54	MG	BA	3206	1/1	0.83	0.20	67,67,67,67	0
54	MG	BA	3416	1/1	0.83	0.14	74,74,74,74	0
54	MG	DA	3415	1/1	0.83	0.26	77,77,77,77	0
54	MG	DA	2965	1/1	0.83	0.28	49,49,49,49	0
54	MG	BB	202	1/1	0.83	0.15	59,59,59,59	0
54	MG	CA	1958	1/1	0.83	0.11	106,106,106,106	0
54	MG	DA	3008	1/1	0.83	0.15	34,34,34,34	0
54	MG	CA	1959	1/1	0.83	0.10	84,84,84,84	0
54	MG	DA	3263	1/1	0.83	0.29	78,78,78,78	0
54	MG	DA	3438	1/1	0.83	0.13	83,83,83,83	0
54	MG	AA	2035	1/1	0.83	0.22	86,86,86,86	0
54	MG	BA	3501	1/1	0.83	0.07	80,80,80,80	0
54	MG	BA	3421	1/1	0.83	0.20	88,88,88,88	0
54	MG	BA	2996	1/1	0.83	0.20	68,68,68,68	0
54	MG	AA	1649	1/1	0.83	0.15	84,84,84,84	0
54	MG	DA	3043	1/1	0.83	0.16	59,59,59,59	0
54	MG	AA	1852	1/1	0.83	0.24	66,66,66,66	0
54	MG	CA	1662	1/1	0.83	0.15	61,61,61,61	0
54	MG	BA	3428	1/1	0.83	0.07	93,93,93,93	0
54	MG	CA	1879	1/1	0.83	0.24	90,90,90,90	0
54	MG	AC	105	1/1	0.83	0.14	88,88,88,88	0
54	MG	AA	1825	1/1	0.83	0.10	95,95,95,95	0
54	MG	BA	3514	1/1	0.83	0.10	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	224	1/1	0.83	0.07	81,81,81,81	0
54	MG	DA	3302	1/1	0.83	0.23	76,76,76,76	0
54	MG	AA	1711	1/1	0.83	0.36	86,86,86,86	0
54	MG	DB	212	1/1	0.83	0.22	75,75,75,75	0
54	MG	CA	1684	1/1	0.83	0.15	60,60,60,60	0
54	MG	DB	214	1/1	0.83	0.08	85,85,85,85	0
54	MG	DA	3306	1/1	0.83	0.16	65,65,65,65	0
54	MG	DA	3092	1/1	0.83	0.11	39,39,39,39	0
54	MG	AA	1901	1/1	0.83	0.14	89,89,89,89	0
54	MG	DA	3313	1/1	0.83	0.09	71,71,71,71	0
54	MG	DA	3314	1/1	0.83	0.12	107,107,107,107	0
54	MG	DA	3315	1/1	0.83	0.25	81,81,81,81	0
54	MG	BA	3518	1/1	0.83	0.34	134,134,134,134	0
54	MG	DA	3106	1/1	0.83	0.20	44,44,44,44	0
54	MG	BA	3244	1/1	0.83	0.07	67,67,67,67	0
54	MG	AA	1950	1/1	0.83	0.11	90,90,90,90	0
54	MG	AD	103	1/1	0.83	0.11	101,101,101,101	0
54	MG	DA	3120	1/1	0.83	0.36	74,74,74,74	0
54	MG	CL	201	1/1	0.83	0.09	81,81,81,81	0
54	MG	DA	3125	1/1	0.83	0.14	48,48,48,48	0
54	MG	AA	1792	1/1	0.83	0.28	74,74,74,74	0
54	MG	DH	201	1/1	0.83	0.22	77,77,77,77	0
54	MG	BA	3056	1/1	0.83	0.19	71,71,71,71	0
54	MG	DA	3502	1/1	0.83	0.18	112,112,112,112	0
54	MG	AA	1860	1/1	0.83	0.12	93,93,93,93	0
54	MG	BA	3367	1/1	0.83	0.27	111,111,111,111	0
54	MG	BA	3064	1/1	0.83	0.17	76,76,76,76	0
54	MG	BA	3145	1/1	0.83	0.26	74,74,74,74	0
54	MG	AA	1978	1/1	0.83	0.07	99,99,99,99	0
54	MG	DA	3142	1/1	0.83	0.17	61,61,61,61	0
54	MG	AA	1645	1/1	0.83	0.22	55,55,55,55	0
54	MG	BA	3553	1/1	0.83	0.23	96,96,96,96	0
54	MG	BA	3533	1/1	0.84	0.13	81,81,81,81	0
54	MG	CA	1690	1/1	0.84	0.15	74,74,74,74	0
54	MG	CA	1694	1/1	0.84	0.19	55,55,55,55	0
54	MG	DA	3488	1/1	0.84	0.19	66,66,66,66	0
54	MG	AS	102	1/1	0.84	0.22	90,90,90,90	0
54	MG	DA	3622	1/1	0.84	0.27	84,84,84,84	0
54	MG	DA	3081	1/1	0.84	0.23	84,84,84,84	0
54	MG	CA	1696	1/1	0.84	0.12	84,84,84,84	0
54	MG	AA	2001	1/1	0.84	0.14	76,76,76,76	0
54	MG	DA	3256	1/1	0.84	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3536	1/1	0.84	0.23	89,89,89,89	0
54	MG	AA	1770	1/1	0.84	0.17	71,71,71,71	0
54	MG	BA	3068	1/1	0.84	0.17	72,72,72,72	0
54	MG	BB	210	1/1	0.84	0.11	62,62,62,62	0
54	MG	CA	1706	1/1	0.84	0.16	61,61,61,61	0
54	MG	BA	3228	1/1	0.84	0.06	83,83,83,83	0
54	MG	AA	1678	1/1	0.84	0.20	57,57,57,57	0
54	MG	DA	3514	1/1	0.84	0.12	66,66,66,66	0
54	MG	CA	1784	1/1	0.84	0.23	85,85,85,85	0
54	MG	BA	3135	1/1	0.84	0.18	62,62,62,62	0
54	MG	DA	3655	1/1	0.84	0.17	94,94,94,94	0
54	MG	CA	1864	1/1	0.84	0.23	90,90,90,90	0
54	MG	BA	3347	1/1	0.84	0.25	99,99,99,99	0
54	MG	BA	3550	1/1	0.84	0.13	102,102,102,102	0
54	MG	DA	3526	1/1	0.84	0.18	74,74,74,74	0
54	MG	CA	1789	1/1	0.84	0.13	100,100,100,100	0
54	MG	BB	220	1/1	0.84	0.20	80,80,80,80	0
54	MG	DA	3798	1/1	0.84	0.20	78,78,78,78	0
54	MG	BA	3235	1/1	0.84	0.10	59,59,59,59	0
54	MG	BA	3169	1/1	0.84	0.28	60,60,60,60	0
54	MG	AA	1827	1/1	0.84	0.18	88,88,88,88	0
54	MG	BA	3455	1/1	0.84	0.16	78,78,78,78	0
54	MG	CA	1803	1/1	0.84	0.20	100,100,100,100	0
54	MG	DA	3429	1/1	0.84	0.17	83,83,83,83	0
54	MG	DA	3539	1/1	0.84	0.14	76,76,76,76	0
54	MG	DA	3141	1/1	0.84	0.12	78,78,78,78	0
54	MG	CA	1961	1/1	0.84	0.19	78,78,78,78	0
54	MG	BA	3290	1/1	0.84	0.06	91,91,91,91	0
54	MG	CD	116	1/1	0.84	0.11	90,90,90,90	0
54	MG	DA	3698	1/1	0.84	0.23	89,89,89,89	0
54	MG	DA	3556	1/1	0.84	0.14	183,183,183,183	0
54	MG	AA	1701	1/1	0.84	0.26	72,72,72,72	0
54	MG	AA	1996	1/1	0.84	0.16	106,106,106,106	0
54	MG	BA	3506	1/1	0.84	0.15	77,77,77,77	0
54	MG	AA	1905	1/1	0.84	0.21	96,96,96,96	0
54	MG	DA	3709	1/1	0.84	0.15	84,84,84,84	0
54	MG	BA	3189	1/1	0.84	0.26	76,76,76,76	0
54	MG	DA	3319	1/1	0.84	0.15	71,71,71,71	0
54	MG	DA	2956	1/1	0.84	0.22	47,47,47,47	0
54	MG	BA	3143	1/1	0.84	0.25	74,74,74,74	0
54	MG	CA	1899	1/1	0.84	0.25	66,66,66,66	0
54	MG	CA	1901	1/1	0.84	0.11	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3007	1/1	0.84	0.19	48,48,48,48	0
54	MG	BK	201	1/1	0.84	0.10	68,68,68,68	0
54	MG	BA	3469	1/1	0.84	0.18	70,70,70,70	0
54	MG	BA	3199	1/1	0.84	0.30	84,84,84,84	0
54	MG	DA	3216	1/1	0.84	0.17	88,88,88,88	0
54	MG	BA	3315	1/1	0.84	0.20	84,84,84,84	0
54	MG	CA	1666	1/1	0.84	0.10	67,67,67,67	0
54	MG	BA	3200	1/1	0.84	0.19	90,90,90,90	0
54	MG	AA	1663	1/1	0.84	0.20	71,71,71,71	0
54	MG	AA	1976	1/1	0.84	0.12	86,86,86,86	0
54	MG	DA	3730	1/1	0.84	0.10	79,79,79,79	0
54	MG	D1	202	1/1	0.84	0.22	75,75,75,75	0
54	MG	BA	3477	1/1	0.84	0.14	60,60,60,60	0
54	MG	DA	3733	1/1	0.84	0.16	75,75,75,75	0
54	MG	DA	3601	1/1	0.84	0.19	95,95,95,95	0
54	MG	DA	3605	1/1	0.84	0.17	80,80,80,80	0
54	MG	DA	3361	1/1	0.84	0.26	75,75,75,75	0
54	MG	BA	3268	1/1	0.84	0.25	87,87,87,87	0
54	MG	CA	1861	1/1	0.85	0.07	109,109,109,109	0
54	MG	BA	3222	1/1	0.85	0.29	88,88,88,88	0
54	MG	DA	3752	1/1	0.85	0.09	74,74,74,74	0
54	MG	BA	3070	1/1	0.85	0.17	53,53,53,53	0
54	MG	DA	3387	1/1	0.85	0.26	83,83,83,83	0
54	MG	AA	1983	1/1	0.85	0.12	104,104,104,104	0
54	MG	BA	3521	1/1	0.85	0.32	109,109,109,109	0
54	MG	BA	3074	1/1	0.85	0.16	41,41,41,41	0
54	MG	CA	1953	1/1	0.85	0.26	103,103,103,103	0
54	MG	DA	3768	1/1	0.85	0.28	92,92,92,92	0
54	MG	DA	3769	1/1	0.85	0.17	73,73,73,73	0
54	MG	AA	1616	1/1	0.85	0.12	76,76,76,76	0
54	MG	CD	104	1/1	0.85	0.07	83,83,83,83	0
54	MG	AA	1897	1/1	0.85	0.09	56,56,56,56	0
54	MG	DA	3774	1/1	0.85	0.23	76,76,76,76	0
54	MG	BA	3144	1/1	0.85	0.12	68,68,68,68	0
54	MG	BA	2995	1/1	0.85	0.25	52,52,52,52	0
54	MG	DA	3298	1/1	0.85	0.15	70,70,70,70	0
54	MG	BA	3238	1/1	0.85	0.24	85,85,85,85	0
54	MG	DA	3661	1/1	0.85	0.17	79,79,79,79	0
54	MG	A1	101	1/1	0.85	0.10	102,102,102,102	0
54	MG	CA	1731	1/1	0.85	0.07	86,86,86,86	0
54	MG	BA	3324	1/1	0.85	0.25	87,87,87,87	0
54	MG	BA	3241	1/1	0.85	0.24	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3002	1/1	0.85	0.15	62,62,62,62	0
54	MG	AA	1641	1/1	0.85	0.15	76,76,76,76	0
54	MG	AA	1604	1/1	0.85	0.18	53,53,53,53	0
54	MG	AA	1975	1/1	0.85	0.09	86,86,86,86	0
54	MG	DA	3677	1/1	0.85	0.10	85,85,85,85	0
54	MG	DA	3681	1/1	0.85	0.23	92,92,92,92	0
54	MG	DA	3179	1/1	0.85	0.19	74,74,74,74	0
54	MG	BA	3020	1/1	0.85	0.12	72,72,72,72	0
54	MG	BA	3027	1/1	0.85	0.16	46,46,46,46	0
54	MG	AA	1675	1/1	0.85	0.16	62,62,62,62	0
54	MG	DA	3689	1/1	0.85	0.08	63,63,63,63	0
54	MG	AA	2026	1/1	0.85	0.29	90,90,90,90	0
54	MG	DA	3003	1/1	0.85	0.22	62,62,62,62	0
54	MG	DA	3443	1/1	0.85	0.35	86,86,86,86	0
54	MG	DA	3562	1/1	0.85	0.33	75,75,75,75	0
54	MG	DA	3321	1/1	0.85	0.12	70,70,70,70	0
54	MG	AA	1749	1/1	0.85	0.19	72,72,72,72	0
54	MG	CA	1822	1/1	0.85	0.12	92,92,92,92	0
54	MG	AA	2013	1/1	0.85	0.12	94,94,94,94	0
54	MG	DA	3014	1/1	0.85	0.41	68,68,68,68	0
54	MG	BA	2918	1/1	0.85	0.25	46,46,46,46	0
54	MG	DA	3455	1/1	0.85	0.08	80,80,80,80	0
54	MG	AA	1794	1/1	0.85	0.19	93,93,93,93	0
54	MG	BA	3191	1/1	0.85	0.29	79,79,79,79	0
54	MG	CA	1683	1/1	0.85	0.15	70,70,70,70	0
54	MG	CA	1832	1/1	0.85	0.09	79,79,79,79	0
54	MG	BA	2954	1/1	0.85	0.23	54,54,54,54	0
54	MG	BA	3061	1/1	0.85	0.18	70,70,70,70	0
54	MG	BA	3440	1/1	0.85	0.22	100,100,100,100	0
54	MG	BA	3127	1/1	0.85	0.33	64,64,64,64	0
54	MG	BA	2961	1/1	0.85	0.30	46,46,46,46	0
54	MG	DA	3471	1/1	0.85	0.25	94,94,94,94	0
54	MG	DA	3230	1/1	0.85	0.11	63,63,63,63	0
54	MG	BA	3507	1/1	0.85	0.11	80,80,80,80	0
54	MG	DA	3598	1/1	0.85	0.08	79,79,79,79	0
54	MG	AL	201	1/1	0.85	0.13	79,79,79,79	0
54	MG	CA	1612	1/1	0.85	0.11	37,37,37,37	0
54	MG	AA	1847	1/1	0.85	0.18	91,91,91,91	0
54	MG	DA	3480	1/1	0.85	0.12	76,76,76,76	0
54	MG	DA	3481	1/1	0.85	0.24	91,91,91,91	0
54	MG	BA	3207	1/1	0.85	0.12	67,67,67,67	0
54	MG	BA	3216	1/1	0.85	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1933	1/1	0.85	0.06	69,69,69,69	0
54	MG	AA	1651	1/1	0.85	0.24	60,60,60,60	0
54	MG	BA	3379	1/1	0.85	0.18	98,98,98,98	0
54	MG	DA	3262	1/1	0.85	0.17	84,84,84,84	0
54	MG	DA	3103	1/1	0.85	0.13	76,76,76,76	0
54	MG	CA	1834	1/1	0.86	0.15	103,103,103,103	0
54	MG	DA	3063	1/1	0.86	0.14	34,34,34,34	0
54	MG	AA	1941	1/1	0.86	0.11	93,93,93,93	0
54	MG	BB	211	1/1	0.86	0.11	80,80,80,80	0
54	MG	AA	1702	1/1	0.86	0.21	71,71,71,71	0
54	MG	CA	1769	1/1	0.86	0.12	81,81,81,81	0
54	MG	DA	3240	1/1	0.86	0.17	58,58,58,58	0
54	MG	DA	3489	1/1	0.86	0.37	79,79,79,79	0
54	MG	CA	1701	1/1	0.86	0.12	106,106,106,106	0
54	MG	AA	1639	1/1	0.86	0.35	73,73,73,73	0
54	MG	BA	3549	1/1	0.86	0.27	110,110,110,110	0
54	MG	BA	3405	1/1	0.86	0.17	82,82,82,82	0
54	MG	BA	2978	1/1	0.86	0.24	47,47,47,47	0
54	MG	BA	3150	1/1	0.86	0.28	72,72,72,72	0
54	MG	DA	3098	1/1	0.86	0.21	65,65,65,65	0
54	MG	BB	221	1/1	0.86	0.07	106,106,106,106	0
54	MG	AA	1731	1/1	0.86	0.28	63,63,63,63	0
54	MG	DA	3504	1/1	0.86	0.12	81,81,81,81	0
54	MG	DA	3506	1/1	0.86	0.27	63,63,63,63	0
54	MG	BA	3248	1/1	0.86	0.07	81,81,81,81	0
54	MG	BA	3123	1/1	0.86	0.30	71,71,71,71	0
54	MG	AA	1722	1/1	0.86	0.24	68,68,68,68	0
54	MG	DA	3110	1/1	0.86	0.16	54,54,54,54	0
54	MG	DA	3279	1/1	0.86	0.28	98,98,98,98	0
54	MG	DA	3402	1/1	0.86	0.18	70,70,70,70	0
54	MG	CA	1863	1/1	0.86	0.05	121,121,121,121	0
54	MG	CA	1949	1/1	0.86	0.18	91,91,91,91	0
54	MG	DA	3409	1/1	0.86	0.32	70,70,70,70	0
54	MG	AA	1951	1/1	0.86	0.14	79,79,79,79	0
54	MG	CA	1792	1/1	0.86	0.22	84,84,84,84	0
54	MG	DA	3795	1/1	0.86	0.10	112,112,112,112	0
54	MG	CA	1871	1/1	0.86	0.07	73,73,73,73	0
54	MG	AA	1773	1/1	0.86	0.13	81,81,81,81	0
54	MG	CA	1795	1/1	0.86	0.09	78,78,78,78	0
54	MG	DA	3417	1/1	0.86	0.08	120,120,120,120	0
54	MG	CD	109	1/1	0.86	0.07	89,89,89,89	0
54	MG	BA	3568	1/1	0.86	0.05	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1624	1/1	0.86	0.23	56,56,56,56	0
54	MG	DA	3135	1/1	0.86	0.24	48,48,48,48	0
54	MG	DA	3540	1/1	0.86	0.25	54,54,54,54	0
54	MG	CA	1729	1/1	0.86	0.12	61,61,61,61	0
54	MG	CA	1801	1/1	0.86	0.13	88,88,88,88	0
54	MG	DA	3436	1/1	0.86	0.09	72,72,72,72	0
54	MG	AA	1635	1/1	0.86	0.17	54,54,54,54	0
54	MG	AA	1817	1/1	0.86	0.09	89,89,89,89	0
54	MG	DA	3703	1/1	0.86	0.11	99,99,99,99	0
54	MG	BA	3227	1/1	0.86	0.27	82,82,82,82	0
54	MG	BA	3272	1/1	0.86	0.17	66,66,66,66	0
54	MG	B0	201	1/1	0.86	0.23	74,74,74,74	0
54	MG	AA	1900	1/1	0.86	0.07	102,102,102,102	0
54	MG	DA	3184	1/1	0.86	0.26	66,66,66,66	0
54	MG	BA	3523	1/1	0.86	0.11	104,104,104,104	0
54	MG	BA	3274	1/1	0.86	0.23	116,116,116,116	0
54	MG	DA	2989	1/1	0.86	0.19	42,42,42,42	0
54	MG	DA	3448	1/1	0.86	0.21	103,103,103,103	0
54	MG	BA	3383	1/1	0.86	0.15	63,63,63,63	0
54	MG	CA	1672	1/1	0.86	0.14	70,70,70,70	0
54	MG	BA	3229	1/1	0.86	0.15	77,77,77,77	0
54	MG	AA	1714	1/1	0.86	0.13	89,89,89,89	0
54	MG	CA	1678	1/1	0.86	0.12	66,66,66,66	0
54	MG	DA	3332	1/1	0.86	0.14	67,67,67,67	0
54	MG	BA	3583	1/1	0.86	0.05	79,79,79,79	0
54	MG	DA	3462	1/1	0.86	0.15	80,80,80,80	0
54	MG	BA	3185	1/1	0.86	0.13	84,84,84,84	0
54	MG	DA	3589	1/1	0.86	0.30	136,136,136,136	0
54	MG	BA	3280	1/1	0.86	0.08	61,61,61,61	0
54	MG	CA	1825	1/1	0.86	0.06	106,106,106,106	0
54	MG	CA	1607	1/1	0.86	0.21	73,73,73,73	0
54	MG	BA	3494	1/1	0.86	0.15	65,65,65,65	0
54	MG	DA	3468	1/1	0.86	0.09	73,73,73,73	0
54	MG	DA	3735	1/1	0.86	0.07	82,82,82,82	0
54	MG	DS	201	1/1	0.86	0.17	104,104,104,104	0
54	MG	AA	1715	1/1	0.86	0.13	76,76,76,76	0
54	MG	BA	3016	1/1	0.86	0.25	63,63,63,63	0
54	MG	BA	3543	1/1	0.86	0.10	72,72,72,72	0
54	MG	DA	3054	1/1	0.86	0.14	54,54,54,54	0
54	MG	DA	3041	1/1	0.87	0.19	49,49,49,49	0
54	MG	CA	1896	1/1	0.87	0.09	67,67,67,67	0
54	MG	AA	1783	1/1	0.87	0.35	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3406	1/1	0.87	0.12	82,82,82,82	0
54	MG	AA	2019	1/1	0.87	0.06	104,104,104,104	0
54	MG	AA	1705	1/1	0.87	0.12	77,77,77,77	0
54	MG	DA	3249	1/1	0.87	0.27	65,65,65,65	0
54	MG	DA	3056	1/1	0.87	0.26	71,71,71,71	0
54	MG	AA	1698	1/1	0.87	0.34	79,79,79,79	0
54	MG	DA	3560	1/1	0.87	0.15	79,79,79,79	0
54	MG	AA	1636	1/1	0.87	0.23	71,71,71,71	0
54	MG	DA	3066	1/1	0.87	0.31	59,59,59,59	0
54	MG	BA	3263	1/1	0.87	0.17	65,65,65,65	0
54	MG	DA	3421	1/1	0.87	0.25	85,85,85,85	0
54	MG	CK	201	1/1	0.87	0.23	90,90,90,90	0
54	MG	DA	3736	1/1	0.87	0.10	76,76,76,76	0
54	MG	DA	3424	1/1	0.87	0.16	77,77,77,77	0
54	MG	DA	3739	1/1	0.87	0.11	127,127,127,127	0
54	MG	AA	1967	1/1	0.87	0.07	84,84,84,84	0
54	MG	DA	3270	1/1	0.87	0.17	70,70,70,70	0
54	MG	BA	3336	1/1	0.87	0.13	88,88,88,88	0
54	MG	DA	3576	1/1	0.87	0.07	109,109,109,109	0
54	MG	AA	1942	1/1	0.87	0.14	128,128,128,128	0
54	MG	DA	3276	1/1	0.87	0.20	70,70,70,70	0
54	MG	DA	3748	1/1	0.87	0.18	71,71,71,71	0
54	MG	CA	1744	1/1	0.87	0.08	89,89,89,89	0
54	MG	AP	201	1/1	0.87	0.15	82,82,82,82	0
54	MG	AA	1795	1/1	0.87	0.20	70,70,70,70	0
54	MG	AA	1813	1/1	0.87	0.23	93,93,93,93	0
54	MG	AA	1774	1/1	0.87	0.21	75,75,75,75	0
54	MG	DA	3285	1/1	0.87	0.22	56,56,56,56	0
54	MG	DA	3288	1/1	0.87	0.31	91,91,91,91	0
54	MG	DA	3097	1/1	0.87	0.16	63,63,63,63	0
54	MG	CA	1665	1/1	0.87	0.12	84,84,84,84	0
54	MG	DA	3596	1/1	0.87	0.21	110,110,110,110	0
54	MG	DA	3446	1/1	0.87	0.19	86,86,86,86	0
54	MG	BA	3213	1/1	0.87	0.15	61,61,61,61	0
54	MG	DA	3297	1/1	0.87	0.13	54,54,54,54	0
54	MG	DA	3603	1/1	0.87	0.21	86,86,86,86	0
54	MG	BA	3214	1/1	0.87	0.12	67,67,67,67	0
54	MG	DA	3778	1/1	0.87	0.10	97,97,97,97	0
54	MG	AA	1869	1/1	0.87	0.07	83,83,83,83	0
54	MG	AA	1891	1/1	0.87	0.17	93,93,93,93	0
54	MG	DA	3454	1/1	0.87	0.22	69,69,69,69	0
54	MG	BA	3218	1/1	0.87	0.06	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3221	1/1	0.87	0.24	82,82,82,82	0
54	MG	DA	3114	1/1	0.87	0.16	72,72,72,72	0
54	MG	CA	1760	1/1	0.87	0.09	118,118,118,118	0
54	MG	AA	1646	1/1	0.87	0.24	66,66,66,66	0
54	MG	DA	3122	1/1	0.87	0.25	60,60,60,60	0
54	MG	AA	1652	1/1	0.87	0.17	82,82,82,82	0
54	MG	B1	201	1/1	0.87	0.11	80,80,80,80	0
54	MG	BT	101	1/1	0.87	0.16	65,65,65,65	0
54	MG	CC	111	1/1	0.87	0.08	99,99,99,99	0
54	MG	CA	1936	1/1	0.87	0.09	90,90,90,90	0
54	MG	BA	3438	1/1	0.87	0.17	54,54,54,54	0
54	MG	CD	103	1/1	0.87	0.08	113,113,113,113	0
54	MG	AA	1912	1/1	0.87	0.14	79,79,79,79	0
54	MG	CA	1941	1/1	0.87	0.07	88,88,88,88	0
54	MG	B3	102	1/1	0.87	0.07	58,58,58,58	0
54	MG	DA	3137	1/1	0.87	0.10	51,51,51,51	0
54	MG	AA	1818	1/1	0.87	0.13	64,64,64,64	0
54	MG	B4	101	1/1	0.87	0.17	85,85,85,85	0
54	MG	DA	3149	1/1	0.87	0.21	56,56,56,56	0
54	MG	BA	3156	1/1	0.87	0.18	68,68,68,68	0
54	MG	DB	207	1/1	0.87	0.12	99,99,99,99	0
54	MG	BA	3287	1/1	0.87	0.25	79,79,79,79	0
54	MG	DA	3167	1/1	0.87	0.22	68,68,68,68	0
54	MG	AA	1657	1/1	0.87	0.27	83,83,83,83	0
54	MG	BA	3160	1/1	0.87	0.20	65,65,65,65	0
54	MG	DA	3492	1/1	0.87	0.18	95,95,95,95	0
54	MG	AA	1769	1/1	0.87	0.22	80,80,80,80	0
54	MG	CA	1954	1/1	0.87	0.08	95,95,95,95	0
54	MG	BA	3451	1/1	0.87	0.23	64,64,64,64	0
54	MG	CD	123	1/1	0.87	0.06	81,81,81,81	0
54	MG	CA	1868	1/1	0.87	0.21	72,72,72,72	0
54	MG	DA	2915	1/1	0.87	0.22	29,29,29,29	0
54	MG	CA	1870	1/1	0.87	0.17	69,69,69,69	0
54	MG	BA	3453	1/1	0.87	0.29	73,73,73,73	0
54	MG	BA	2982	1/1	0.87	0.28	61,61,61,61	0
54	MG	CA	1791	1/1	0.87	0.08	85,85,85,85	0
54	MG	DA	3204	1/1	0.87	0.38	62,62,62,62	0
54	MG	AA	1822	1/1	0.87	0.13	107,107,107,107	0
54	MG	BB	205	1/1	0.87	0.13	74,74,74,74	0
54	MG	BA	3173	1/1	0.87	0.12	68,68,68,68	0
54	MG	DA	3004	1/1	0.87	0.24	52,52,52,52	0
54	MG	DA	3697	1/1	0.87	0.17	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3006	1/1	0.87	0.26	51,51,51,51	0
54	MG	BA	3307	1/1	0.87	0.29	79,79,79,79	0
54	MG	DA	3519	1/1	0.87	0.18	87,87,87,87	0
54	MG	BA	3387	1/1	0.87	0.14	67,67,67,67	0
54	MG	DA	3382	1/1	0.87	0.22	91,91,91,91	0
54	MG	BA	3176	1/1	0.87	0.18	65,65,65,65	0
54	MG	CA	1885	1/1	0.87	0.17	74,74,74,74	0
54	MG	BA	3066	1/1	0.87	0.29	99,99,99,99	0
54	MG	CA	1724	1/1	0.87	0.13	66,66,66,66	0
54	MG	BA	3391	1/1	0.87	0.19	86,86,86,86	0
54	MG	DA	3032	1/1	0.87	0.17	40,40,40,40	0
54	MG	BA	3124	1/1	0.87	0.23	75,75,75,75	0
54	MG	DU	206	1/1	0.87	0.12	83,83,83,83	0
54	MG	DZ	101	1/1	0.87	0.17	79,79,79,79	0
55	ZN	AA	2040	1/1	0.87	0.10	300,300,300,300	0
54	MG	AA	1782	1/1	0.87	0.18	106,106,106,106	0
54	MG	BA	3251	1/1	0.88	0.12	78,78,78,78	0
54	MG	BA	3540	1/1	0.88	0.15	69,69,69,69	0
54	MG	DA	3057	1/1	0.88	0.17	68,68,68,68	0
54	MG	CA	1732	1/1	0.88	0.27	82,82,82,82	0
54	MG	DA	3061	1/1	0.88	0.26	52,52,52,52	0
54	MG	DA	3550	1/1	0.88	0.26	76,76,76,76	0
54	MG	BA	3253	1/1	0.88	0.22	70,70,70,70	0
54	MG	DA	3251	1/1	0.88	0.26	83,83,83,83	0
54	MG	DA	3064	1/1	0.88	0.17	72,72,72,72	0
54	MG	BA	2903	1/1	0.88	0.08	82,82,82,82	0
54	MG	BB	223	1/1	0.88	0.10	122,122,122,122	0
54	MG	DA	3414	1/1	0.88	0.19	70,70,70,70	0
54	MG	BA	3131	1/1	0.88	0.25	76,76,76,76	0
54	MG	DA	3416	1/1	0.88	0.24	94,94,94,94	0
54	MG	CA	1907	1/1	0.88	0.11	83,83,83,83	0
54	MG	AA	1693	1/1	0.88	0.06	95,95,95,95	0
54	MG	BA	3332	1/1	0.88	0.18	60,60,60,60	0
54	MG	BA	3548	1/1	0.88	0.12	81,81,81,81	0
54	MG	BA	3257	1/1	0.88	0.09	63,63,63,63	0
54	MG	DA	3425	1/1	0.88	0.16	68,68,68,68	0
54	MG	AA	1755	1/1	0.88	0.23	62,62,62,62	0
54	MG	BA	3489	1/1	0.88	0.10	93,93,93,93	0
54	MG	AA	1856	1/1	0.88	0.20	71,71,71,71	0
54	MG	AA	1764	1/1	0.88	0.08	96,96,96,96	0
54	MG	AA	1628	1/1	0.88	0.38	69,69,69,69	0
54	MG	BA	2998	1/1	0.88	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1920	1/1	0.88	0.18	81,81,81,81	0
54	MG	CA	1921	1/1	0.88	0.22	70,70,70,70	0
54	MG	CA	1833	1/1	0.88	0.14	70,70,70,70	0
54	MG	CA	1669	1/1	0.88	0.28	71,71,71,71	0
54	MG	AA	2006	1/1	0.88	0.07	86,86,86,86	0
54	MG	DA	3593	1/1	0.88	0.11	97,97,97,97	0
54	MG	AA	1987	1/1	0.88	0.10	86,86,86,86	0
54	MG	DA	3595	1/1	0.88	0.11	80,80,80,80	0
54	MG	CA	1842	1/1	0.88	0.08	112,112,112,112	0
54	MG	CA	1844	1/1	0.88	0.12	76,76,76,76	0
54	MG	BA	3215	1/1	0.88	0.20	58,58,58,58	0
54	MG	BA	3014	1/1	0.88	0.29	49,49,49,49	0
54	MG	BA	2916	1/1	0.88	0.20	42,42,42,42	0
54	MG	CA	1934	1/1	0.88	0.19	94,94,94,94	0
54	MG	CA	1935	1/1	0.88	0.06	136,136,136,136	0
54	MG	BA	3359	1/1	0.88	0.11	73,73,73,73	0
54	MG	DA	3453	1/1	0.88	0.28	81,81,81,81	0
54	MG	DA	3307	1/1	0.88	0.24	74,74,74,74	0
54	MG	AA	1776	1/1	0.88	0.23	110,110,110,110	0
54	MG	BA	3220	1/1	0.88	0.17	59,59,59,59	0
54	MG	BA	2921	1/1	0.88	0.19	41,41,41,41	0
54	MG	BA	2923	1/1	0.88	0.16	44,44,44,44	0
54	MG	CD	113	1/1	0.88	0.07	80,80,80,80	0
54	MG	BA	3026	1/1	0.88	0.20	60,60,60,60	0
54	MG	CA	1857	1/1	0.88	0.10	80,80,80,80	0
54	MG	BW	101	1/1	0.88	0.12	65,65,65,65	0
54	MG	CA	1948	1/1	0.88	0.10	89,89,89,89	0
54	MG	CA	1774	1/1	0.88	0.11	66,66,66,66	0
54	MG	BA	2935	1/1	0.88	0.21	46,46,46,46	0
54	MG	DA	3161	1/1	0.88	0.22	60,60,60,60	0
54	MG	DA	3635	1/1	0.88	0.10	101,101,101,101	0
54	MG	DA	3163	1/1	0.88	0.26	60,60,60,60	0
54	MG	CA	1951	1/1	0.88	0.08	74,74,74,74	0
54	MG	AA	1777	1/1	0.88	0.19	69,69,69,69	0
54	MG	DA	2947	1/1	0.88	0.23	26,26,26,26	0
54	MG	DA	3176	1/1	0.88	0.23	57,57,57,57	0
54	MG	DA	3650	1/1	0.88	0.13	76,76,76,76	0
54	MG	DB	203	1/1	0.88	0.33	67,67,67,67	0
54	MG	DA	3178	1/1	0.88	0.20	72,72,72,72	0
54	MG	DA	3654	1/1	0.88	0.05	105,105,105,105	0
54	MG	DA	3337	1/1	0.88	0.23	59,59,59,59	0
54	MG	BA	3159	1/1	0.88	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3347	1/1	0.88	0.33	98,98,98,98	0
54	MG	DA	2952	1/1	0.88	0.25	39,39,39,39	0
54	MG	BA	3034	1/1	0.88	0.17	61,61,61,61	0
54	MG	AA	1620	1/1	0.88	0.15	67,67,67,67	0
54	MG	AA	1908	1/1	0.88	0.23	95,95,95,95	0
54	MG	DA	2987	1/1	0.88	0.23	36,36,36,36	0
54	MG	DB	216	1/1	0.88	0.11	94,94,94,94	0
54	MG	CA	1869	1/1	0.88	0.06	98,98,98,98	0
54	MG	CA	1613	1/1	0.88	0.24	60,60,60,60	0
54	MG	BA	3039	1/1	0.88	0.18	58,58,58,58	0
54	MG	CA	1708	1/1	0.88	0.13	77,77,77,77	0
54	MG	BA	3044	1/1	0.88	0.07	114,114,114,114	0
54	MG	BA	3299	1/1	0.88	0.10	94,94,94,94	0
54	MG	AA	1823	1/1	0.88	0.29	104,104,104,104	0
54	MG	BA	2972	1/1	0.88	0.26	65,65,65,65	0
54	MG	DA	3684	1/1	0.88	0.13	83,83,83,83	0
54	MG	DA	3214	1/1	0.88	0.23	72,72,72,72	0
54	MG	AA	1810	1/1	0.88	0.11	75,75,75,75	0
54	MG	DA	3373	1/1	0.88	0.13	75,75,75,75	0
54	MG	CA	1719	1/1	0.88	0.15	56,56,56,56	0
54	MG	BA	3310	1/1	0.88	0.09	80,80,80,80	0
54	MG	CA	1721	1/1	0.88	0.19	60,60,60,60	0
54	MG	DA	3696	1/1	0.88	0.08	85,85,85,85	0
54	MG	D0	203	1/1	0.88	0.11	63,63,63,63	0
54	MG	DA	3378	1/1	0.88	0.08	76,76,76,76	0
54	MG	DA	3220	1/1	0.88	0.15	59,59,59,59	0
54	MG	DA	3028	1/1	0.88	0.20	59,59,59,59	0
54	MG	DA	3224	1/1	0.88	0.12	55,55,55,55	0
54	MG	BA	2979	1/1	0.88	0.17	60,60,60,60	0
54	MG	DA	3386	1/1	0.88	0.28	75,75,75,75	0
54	MG	CA	1887	1/1	0.88	0.10	82,82,82,82	0
54	MG	BA	3057	1/1	0.88	0.09	65,65,65,65	0
54	MG	DA	3394	1/1	0.88	0.13	73,73,73,73	0
54	MG	DU	203	1/1	0.88	0.15	94,94,94,94	0
54	MG	AA	1717	1/1	0.88	0.16	77,77,77,77	0
54	MG	BB	214	1/1	0.88	0.14	91,91,91,91	0
54	MG	D3	104	1/1	0.88	0.09	75,75,75,75	0
54	MG	BA	3318	1/1	0.88	0.13	76,76,76,76	0
54	MG	DZ	102	1/1	0.88	0.16	79,79,79,79	0
54	MG	D6	101	1/1	0.88	0.36	98,98,98,98	0
54	MG	DA	3399	1/1	0.88	0.24	86,86,86,86	0
54	MG	AA	1753	1/1	0.88	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3120	1/1	0.89	0.21	75,75,75,75	0
54	MG	BA	3384	1/1	0.89	0.17	76,76,76,76	0
54	MG	AA	1738	1/1	0.89	0.27	84,84,84,84	0
54	MG	CA	1785	1/1	0.89	0.14	69,69,69,69	0
54	MG	CA	1688	1/1	0.89	0.22	76,76,76,76	0
54	MG	DA	3553	1/1	0.89	0.08	74,74,74,74	0
54	MG	BA	3179	1/1	0.89	0.13	51,51,51,51	0
54	MG	BA	3122	1/1	0.89	0.29	63,63,63,63	0
54	MG	AA	1793	1/1	0.89	0.09	73,73,73,73	0
54	MG	AA	1973	1/1	0.89	0.13	84,84,84,84	0
54	MG	BA	3551	1/1	0.89	0.06	98,98,98,98	0
54	MG	AA	1916	1/1	0.89	0.11	93,93,93,93	0
54	MG	BA	3249	1/1	0.89	0.28	59,59,59,59	0
54	MG	CH	201	1/1	0.89	0.12	82,82,82,82	0
54	MG	DA	3734	1/1	0.89	0.14	69,69,69,69	0
54	MG	DA	3566	1/1	0.89	0.15	78,78,78,78	0
54	MG	AA	2042	1/1	0.89	0.07	66,66,66,66	0
54	MG	DA	3737	1/1	0.89	0.18	88,88,88,88	0
54	MG	BA	3556	1/1	0.89	0.11	82,82,82,82	0
54	MG	BA	3399	1/1	0.89	0.06	82,82,82,82	0
54	MG	BU	202	1/1	0.89	0.07	73,73,73,73	0
54	MG	BA	3484	1/1	0.89	0.17	106,106,106,106	0
54	MG	DA	3267	1/1	0.89	0.31	76,76,76,76	0
54	MG	CP	202	1/1	0.89	0.07	122,122,122,122	0
54	MG	B3	101	1/1	0.89	0.08	72,72,72,72	0
54	MG	AA	1647	1/1	0.89	0.34	71,71,71,71	0
54	MG	AA	1673	1/1	0.89	0.07	91,91,91,91	0
54	MG	BA	3196	1/1	0.89	0.36	89,89,89,89	0
54	MG	BA	3565	1/1	0.89	0.18	99,99,99,99	0
54	MG	DA	3090	1/1	0.89	0.10	43,43,43,43	0
54	MG	BA	3567	1/1	0.89	0.09	69,69,69,69	0
54	MG	DA	3755	1/1	0.89	0.07	67,67,67,67	0
54	MG	DA	3758	1/1	0.89	0.13	65,65,65,65	0
54	MG	BA	3198	1/1	0.89	0.07	58,58,58,58	0
54	MG	AA	1858	1/1	0.89	0.06	83,83,83,83	0
54	MG	BA	3258	1/1	0.89	0.13	100,100,100,100	0
54	MG	BA	3261	1/1	0.89	0.14	99,99,99,99	0
54	MG	DA	3101	1/1	0.89	0.20	52,52,52,52	0
54	MG	DA	3292	1/1	0.89	0.12	83,83,83,83	0
54	MG	BA	2946	1/1	0.89	0.22	50,50,50,50	0
54	MG	BA	2948	1/1	0.89	0.16	29,29,29,29	0
54	MG	DA	3105	1/1	0.89	0.29	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1619	1/1	0.89	0.18	73,73,73,73	0
54	MG	CA	1726	1/1	0.89	0.10	54,54,54,54	0
54	MG	DA	3775	1/1	0.89	0.17	90,90,90,90	0
54	MG	CC	108	1/1	0.89	0.09	75,75,75,75	0
54	MG	CA	1621	1/1	0.89	0.19	49,49,49,49	0
54	MG	BA	3019	1/1	0.89	0.09	67,67,67,67	0
54	MG	CA	1628	1/1	0.89	0.27	87,87,87,87	0
54	MG	DA	3118	1/1	0.89	0.21	40,40,40,40	0
54	MG	AA	1874	1/1	0.89	0.13	63,63,63,63	0
54	MG	DA	3614	1/1	0.89	0.14	67,67,67,67	0
54	MG	DA	3616	1/1	0.89	0.11	59,59,59,59	0
54	MG	AA	1892	1/1	0.89	0.11	99,99,99,99	0
54	MG	BA	3579	1/1	0.89	0.12	83,83,83,83	0
54	MG	BA	2966	1/1	0.89	0.14	46,46,46,46	0
54	MG	CA	1734	1/1	0.89	0.09	73,73,73,73	0
54	MG	AA	1606	1/1	0.89	0.14	55,55,55,55	0
54	MG	BA	2971	1/1	0.89	0.19	57,57,57,57	0
54	MG	CA	1738	1/1	0.89	0.09	88,88,88,88	0
54	MG	BA	3349	1/1	0.89	0.12	82,82,82,82	0
54	MG	BA	3351	1/1	0.89	0.04	69,69,69,69	0
54	MG	CA	1642	1/1	0.89	0.16	48,48,48,48	0
54	MG	AA	1846	1/1	0.89	0.25	97,97,97,97	0
54	MG	AA	1625	1/1	0.89	0.19	62,62,62,62	0
54	MG	DA	3640	1/1	0.89	0.13	82,82,82,82	0
54	MG	BA	3435	1/1	0.89	0.16	59,59,59,59	0
54	MG	BA	3277	1/1	0.89	0.11	73,73,73,73	0
54	MG	AQ	101	1/1	0.89	0.09	83,83,83,83	0
54	MG	BA	3095	1/1	0.89	0.10	52,52,52,52	0
54	MG	DA	3329	1/1	0.89	0.18	62,62,62,62	0
54	MG	BA	3100	1/1	0.89	0.10	70,70,70,70	0
54	MG	CD	125	1/1	0.89	0.09	83,83,83,83	0
54	MG	DA	3653	1/1	0.89	0.14	88,88,88,88	0
54	MG	CD	126	1/1	0.89	0.13	82,82,82,82	0
54	MG	DA	3164	1/1	0.89	0.30	72,72,72,72	0
54	MG	DA	3339	1/1	0.89	0.20	67,67,67,67	0
54	MG	DA	2902	1/1	0.89	0.17	44,44,44,44	0
54	MG	DA	3345	1/1	0.89	0.18	80,80,80,80	0
54	MG	DA	3664	1/1	0.89	0.08	104,104,104,104	0
54	MG	DA	2909	1/1	0.89	0.25	25,25,25,25	0
54	MG	BA	3363	1/1	0.89	0.12	79,79,79,79	0
54	MG	DA	2919	1/1	0.89	0.18	46,46,46,46	0
54	MG	DA	2930	1/1	0.89	0.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3353	1/1	0.89	0.07	70,70,70,70	0
54	MG	DA	2941	1/1	0.89	0.15	39,39,39,39	0
54	MG	DA	3182	1/1	0.89	0.20	71,71,71,71	0
54	MG	BA	3043	1/1	0.89	0.10	51,51,51,51	0
54	MG	BA	3366	1/1	0.89	0.11	69,69,69,69	0
54	MG	AA	1684	1/1	0.89	0.16	74,74,74,74	0
54	MG	DA	3503	1/1	0.89	0.10	74,74,74,74	0
54	MG	BA	3524	1/1	0.89	0.09	52,52,52,52	0
54	MG	DA	3189	1/1	0.89	0.20	68,68,68,68	0
54	MG	AA	1601	1/1	0.89	0.19	42,42,42,42	0
54	MG	DA	2974	1/1	0.89	0.28	51,51,51,51	0
54	MG	BA	3112	1/1	0.89	0.13	64,64,64,64	0
54	MG	D0	202	1/1	0.89	0.18	51,51,51,51	0
54	MG	BA	3529	1/1	0.89	0.15	88,88,88,88	0
54	MG	BA	3532	1/1	0.89	0.19	83,83,83,83	0
54	MG	DA	3372	1/1	0.89	0.14	57,57,57,57	0
54	MG	BA	3114	1/1	0.89	0.15	67,67,67,67	0
54	MG	AA	1736	1/1	0.89	0.18	53,53,53,53	0
54	MG	DA	3207	1/1	0.89	0.27	66,66,66,66	0
54	MG	CA	1766	1/1	0.89	0.17	51,51,51,51	0
54	MG	AA	1948	1/1	0.89	0.10	82,82,82,82	0
54	MG	BA	3291	1/1	0.89	0.10	86,86,86,86	0
54	MG	BA	3292	1/1	0.89	0.12	54,54,54,54	0
54	MG	BA	3054	1/1	0.89	0.22	66,66,66,66	0
54	MG	DA	3531	1/1	0.89	0.23	90,90,90,90	0
54	MG	DA	3012	1/1	0.89	0.19	35,35,35,35	0
54	MG	BA	3170	1/1	0.89	0.21	72,72,72,72	0
54	MG	CA	1877	1/1	0.89	0.10	62,62,62,62	0
54	MG	AA	1677	1/1	0.89	0.24	63,63,63,63	0
54	MG	DA	3019	1/1	0.89	0.23	68,68,68,68	0
54	MG	DA	3714	1/1	0.89	0.17	92,92,92,92	0
54	MG	DA	3020	1/1	0.89	0.20	58,58,58,58	0
54	MG	BA	3419	1/1	0.90	0.07	101,101,101,101	0
54	MG	BA	3031	1/1	0.90	0.08	82,82,82,82	0
54	MG	BA	3475	1/1	0.90	0.14	73,73,73,73	0
54	MG	BA	2994	1/1	0.90	0.33	60,60,60,60	0
54	MG	BA	3530	1/1	0.90	0.13	110,110,110,110	0
54	MG	BA	3275	1/1	0.90	0.19	77,77,77,77	0
54	MG	BA	2964	1/1	0.90	0.21	45,45,45,45	0
54	MG	DA	3483	1/1	0.90	0.13	66,66,66,66	0
54	MG	AA	1884	1/1	0.90	0.08	86,86,86,86	0
54	MG	DA	3241	1/1	0.90	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3756	1/1	0.90	0.14	57,57,57,57	0
54	MG	BA	2997	1/1	0.90	0.26	60,60,60,60	0
54	MG	AA	1716	1/1	0.90	0.12	66,66,66,66	0
54	MG	AA	1788	1/1	0.90	0.08	91,91,91,91	0
54	MG	BA	3204	1/1	0.90	0.23	76,76,76,76	0
54	MG	BA	3006	1/1	0.90	0.13	54,54,54,54	0
54	MG	AA	1609	1/1	0.90	0.30	71,71,71,71	0
54	MG	B8	101	1/1	0.90	0.14	76,76,76,76	0
54	MG	CA	1745	1/1	0.90	0.09	74,74,74,74	0
54	MG	BA	3013	1/1	0.90	0.24	60,60,60,60	0
54	MG	DA	3384	1/1	0.90	0.13	62,62,62,62	0
54	MG	DA	3772	1/1	0.90	0.20	76,76,76,76	0
54	MG	DA	3264	1/1	0.90	0.24	73,73,73,73	0
54	MG	CA	1605	1/1	0.90	0.11	39,39,39,39	0
54	MG	DA	3643	1/1	0.90	0.08	82,82,82,82	0
54	MG	AA	1859	1/1	0.90	0.09	77,77,77,77	0
54	MG	DA	3505	1/1	0.90	0.22	88,88,88,88	0
54	MG	DA	2949	1/1	0.90	0.18	35,35,35,35	0
54	MG	DA	3392	1/1	0.90	0.07	66,66,66,66	0
54	MG	DA	3651	1/1	0.90	0.19	98,98,98,98	0
54	MG	BA	3052	1/1	0.90	0.10	63,63,63,63	0
54	MG	DA	3511	1/1	0.90	0.15	82,82,82,82	0
54	MG	BA	3443	1/1	0.90	0.05	79,79,79,79	0
54	MG	DA	2953	1/1	0.90	0.34	63,63,63,63	0
54	MG	BA	3547	1/1	0.90	0.09	74,74,74,74	0
54	MG	DA	2962	1/1	0.90	0.15	33,33,33,33	0
54	MG	BA	3344	1/1	0.90	0.06	69,69,69,69	0
54	MG	DA	2966	1/1	0.90	0.18	37,37,37,37	0
54	MG	CA	1829	1/1	0.90	0.09	98,98,98,98	0
54	MG	DA	2979	1/1	0.90	0.14	31,31,31,31	0
54	MG	CA	1615	1/1	0.90	0.12	40,40,40,40	0
54	MG	BA	3092	1/1	0.90	0.12	58,58,58,58	0
54	MG	DA	3287	1/1	0.90	0.15	63,63,63,63	0
54	MG	CA	1756	1/1	0.90	0.06	57,57,57,57	0
54	MG	DA	3289	1/1	0.90	0.20	63,63,63,63	0
54	MG	DA	3290	1/1	0.90	0.37	81,81,81,81	0
54	MG	BA	2929	1/1	0.90	0.26	32,32,32,32	0
54	MG	DA	2999	1/1	0.90	0.19	44,44,44,44	0
54	MG	AA	1619	1/1	0.90	0.34	55,55,55,55	0
54	MG	DA	3151	1/1	0.90	0.26	89,89,89,89	0
54	MG	CA	1835	1/1	0.90	0.19	74,74,74,74	0
54	MG	CA	1839	1/1	0.90	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2906	1/1	0.90	0.08	101,101,101,101	0
54	MG	DA	3162	1/1	0.90	0.22	55,55,55,55	0
54	MG	CA	1624	1/1	0.90	0.18	40,40,40,40	0
54	MG	CA	1625	1/1	0.90	0.25	51,51,51,51	0
54	MG	CP	203	1/1	0.90	0.09	93,93,93,93	0
54	MG	DA	3554	1/1	0.90	0.18	72,72,72,72	0
54	MG	DA	3305	1/1	0.90	0.13	63,63,63,63	0
54	MG	CA	1626	1/1	0.90	0.22	68,68,68,68	0
54	MG	CA	1700	1/1	0.90	0.18	107,107,107,107	0
54	MG	CA	1627	1/1	0.90	0.20	50,50,50,50	0
54	MG	DB	219	1/1	0.90	0.12	77,77,77,77	0
54	MG	AA	1667	1/1	0.90	0.15	61,61,61,61	0
54	MG	BA	3180	1/1	0.90	0.23	72,72,72,72	0
54	MG	AA	1767	1/1	0.90	0.20	110,110,110,110	0
54	MG	DB	223	1/1	0.90	0.06	104,104,104,104	0
54	MG	CW	201	1/1	0.90	0.30	67,67,67,67	0
54	MG	BA	3300	1/1	0.90	0.09	87,87,87,87	0
54	MG	BA	3183	1/1	0.90	0.09	80,80,80,80	0
54	MG	DA	3037	1/1	0.90	0.24	58,58,58,58	0
54	MG	BA	3457	1/1	0.90	0.21	80,80,80,80	0
54	MG	CA	1779	1/1	0.90	0.11	104,104,104,104	0
54	MG	AA	1605	1/1	0.90	0.24	61,61,61,61	0
54	MG	BA	3361	1/1	0.90	0.06	72,72,72,72	0
54	MG	BA	3563	1/1	0.90	0.21	74,74,74,74	0
54	MG	CA	1717	1/1	0.90	0.19	76,76,76,76	0
54	MG	DH	202	1/1	0.90	0.14	98,98,98,98	0
54	MG	DA	3203	1/1	0.90	0.12	74,74,74,74	0
54	MG	BA	3463	1/1	0.90	0.15	69,69,69,69	0
54	MG	DA	3452	1/1	0.90	0.07	104,104,104,104	0
54	MG	DA	3582	1/1	0.90	0.09	116,116,116,116	0
54	MG	DR	201	1/1	0.90	0.09	77,77,77,77	0
54	MG	BA	3306	1/1	0.90	0.30	105,105,105,105	0
54	MG	CA	1645	1/1	0.90	0.28	79,79,79,79	0
54	MG	CA	1646	1/1	0.90	0.06	53,53,53,53	0
54	MG	DA	3726	1/1	0.90	0.13	75,75,75,75	0
54	MG	CA	1945	1/1	0.90	0.10	77,77,77,77	0
54	MG	DA	3213	1/1	0.90	0.10	40,40,40,40	0
54	MG	CA	1867	1/1	0.90	0.21	76,76,76,76	0
54	MG	BA	3412	1/1	0.90	0.11	94,94,94,94	0
54	MG	DA	3067	1/1	0.90	0.24	47,47,47,47	0
54	MG	BA	3065	1/1	0.90	0.20	51,51,51,51	0
54	MG	AA	1921	1/1	0.90	0.11	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3075	1/1	0.90	0.12	43,43,43,43	0
54	MG	DA	3222	1/1	0.90	0.31	83,83,83,83	0
54	MG	CA	1793	1/1	0.90	0.17	66,66,66,66	0
54	MG	BA	3029	1/1	0.90	0.20	40,40,40,40	0
54	MG	D6	102	1/1	0.90	0.21	94,94,94,94	0
54	MG	BA	3190	1/1	0.90	0.22	78,78,78,78	0
54	MG	DA	3606	1/1	0.90	0.16	72,72,72,72	0
54	MG	DA	2917	1/1	0.91	0.23	27,27,27,27	0
54	MG	BA	2936	1/1	0.91	0.19	50,50,50,50	0
54	MG	DA	2920	1/1	0.91	0.19	21,21,21,21	0
54	MG	DA	2924	1/1	0.91	0.13	17,17,17,17	0
54	MG	BA	2937	1/1	0.91	0.20	53,53,53,53	0
54	MG	DA	2936	1/1	0.91	0.24	48,48,48,48	0
54	MG	BA	2942	1/1	0.91	0.27	36,36,36,36	0
54	MG	DA	3578	1/1	0.91	0.13	89,89,89,89	0
54	MG	BA	2989	1/1	0.91	0.27	60,60,60,60	0
54	MG	BA	3030	1/1	0.91	0.12	47,47,47,47	0
54	MG	DA	3291	1/1	0.91	0.28	76,76,76,76	0
54	MG	BA	3420	1/1	0.91	0.12	82,82,82,82	0
54	MG	AA	1763	1/1	0.91	0.30	74,74,74,74	0
54	MG	DA	3586	1/1	0.91	0.26	72,72,72,72	0
54	MG	BA	3485	1/1	0.91	0.25	69,69,69,69	0
54	MG	CA	1890	1/1	0.91	0.07	115,115,115,115	0
54	MG	AA	1969	1/1	0.91	0.06	89,89,89,89	0
54	MG	DA	3590	1/1	0.91	0.09	93,93,93,93	0
54	MG	CA	1807	1/1	0.91	0.10	71,71,71,71	0
54	MG	BE	304	1/1	0.91	0.34	86,86,86,86	0
54	MG	DA	3750	1/1	0.91	0.17	57,57,57,57	0
54	MG	BA	3209	1/1	0.91	0.20	58,58,58,58	0
54	MG	AA	1615	1/1	0.91	0.14	38,38,38,38	0
54	MG	DA	3145	1/1	0.91	0.27	64,64,64,64	0
54	MG	DA	3146	1/1	0.91	0.12	54,54,54,54	0
54	MG	DA	3148	1/1	0.91	0.31	76,76,76,76	0
54	MG	CA	1652	1/1	0.91	0.09	49,49,49,49	0
54	MG	DA	2982	1/1	0.91	0.21	47,47,47,47	0
54	MG	DA	3152	1/1	0.91	0.16	52,52,52,52	0
54	MG	BA	3308	1/1	0.91	0.23	78,78,78,78	0
54	MG	DA	3157	1/1	0.91	0.12	51,51,51,51	0
54	MG	DA	2988	1/1	0.91	0.17	42,42,42,42	0
54	MG	BA	2950	1/1	0.91	0.14	29,29,29,29	0
54	MG	BA	3162	1/1	0.91	0.10	69,69,69,69	0
54	MG	DA	2993	1/1	0.91	0.28	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	2997	1/1	0.91	0.14	41,41,41,41	0
54	MG	BA	2951	1/1	0.91	0.15	38,38,38,38	0
54	MG	AA	1726	1/1	0.91	0.16	68,68,68,68	0
54	MG	BA	3496	1/1	0.91	0.12	73,73,73,73	0
54	MG	BA	3560	1/1	0.91	0.11	48,48,48,48	0
54	MG	DA	3620	1/1	0.91	0.12	98,98,98,98	0
54	MG	BA	3041	1/1	0.91	0.08	39,39,39,39	0
54	MG	BA	3436	1/1	0.91	0.24	66,66,66,66	0
54	MG	BA	3172	1/1	0.91	0.23	72,72,72,72	0
54	MG	DA	3011	1/1	0.91	0.14	78,78,78,78	0
54	MG	BA	3128	1/1	0.91	0.25	72,72,72,72	0
54	MG	DA	3186	1/1	0.91	0.08	23,23,23,23	0
54	MG	BA	2958	1/1	0.91	0.14	44,44,44,44	0
54	MG	BA	3322	1/1	0.91	0.18	72,72,72,72	0
54	MG	BA	3442	1/1	0.91	0.06	89,89,89,89	0
54	MG	DA	3341	1/1	0.91	0.15	64,64,64,64	0
54	MG	DA	3636	1/1	0.91	0.15	66,66,66,66	0
54	MG	DA	3638	1/1	0.91	0.10	37,37,37,37	0
54	MG	DA	3639	1/1	0.91	0.21	71,71,71,71	0
54	MG	DA	3796	1/1	0.91	0.13	82,82,82,82	0
54	MG	DA	3191	1/1	0.91	0.27	89,89,89,89	0
54	MG	CA	1668	1/1	0.91	0.27	62,62,62,62	0
54	MG	DA	3194	1/1	0.91	0.19	65,65,65,65	0
54	MG	AA	1944	1/1	0.91	0.10	111,111,111,111	0
54	MG	DA	3801	1/1	0.91	0.11	101,101,101,101	0
54	MG	CA	1670	1/1	0.91	0.15	56,56,56,56	0
54	MG	CT	201	1/1	0.91	0.06	76,76,76,76	0
54	MG	CA	1671	1/1	0.91	0.11	77,77,77,77	0
54	MG	DA	3354	1/1	0.91	0.16	55,55,55,55	0
54	MG	DA	3033	1/1	0.91	0.10	42,42,42,42	0
54	MG	BA	3224	1/1	0.91	0.09	54,54,54,54	0
54	MG	BA	3004	1/1	0.91	0.10	30,30,30,30	0
54	MG	CA	1675	1/1	0.91	0.24	59,59,59,59	0
54	MG	DB	206	1/1	0.91	0.12	57,57,57,57	0
54	MG	CA	1926	1/1	0.91	0.22	81,81,81,81	0
54	MG	DA	3042	1/1	0.91	0.13	48,48,48,48	0
54	MG	CX	102	1/1	0.91	0.07	104,104,104,104	0
54	MG	AA	1623	1/1	0.91	0.23	53,53,53,53	0
54	MG	AA	1670	1/1	0.91	0.11	75,75,75,75	0
54	MG	B6	101	1/1	0.91	0.08	84,84,84,84	0
54	MG	CA	1682	1/1	0.91	0.09	67,67,67,67	0
54	MG	BA	3449	1/1	0.91	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	2008	1/1	0.91	0.12	69,69,69,69	0
54	MG	CA	1686	1/1	0.91	0.11	62,62,62,62	0
54	MG	CA	1764	1/1	0.91	0.05	83,83,83,83	0
54	MG	DA	3375	1/1	0.91	0.13	57,57,57,57	0
54	MG	BA	3230	1/1	0.91	0.06	67,67,67,67	0
54	MG	DA	3676	1/1	0.91	0.22	131,131,131,131	0
54	MG	BA	3340	1/1	0.91	0.14	77,77,77,77	0
54	MG	CA	1939	1/1	0.91	0.06	87,87,87,87	0
54	MG	DA	3069	1/1	0.91	0.19	52,52,52,52	0
54	MG	AA	1848	1/1	0.91	0.09	70,70,70,70	0
54	MG	DA	3231	1/1	0.91	0.34	78,78,78,78	0
54	MG	BA	3519	1/1	0.91	0.09	90,90,90,90	0
54	MG	DA	3074	1/1	0.91	0.10	52,52,52,52	0
54	MG	BA	3396	1/1	0.91	0.20	63,63,63,63	0
54	MG	BA	3097	1/1	0.91	0.10	59,59,59,59	0
54	MG	BA	3139	1/1	0.91	0.07	40,40,40,40	0
54	MG	DA	3083	1/1	0.91	0.14	56,56,56,56	0
54	MG	BA	3188	1/1	0.91	0.16	68,68,68,68	0
54	MG	BA	3461	1/1	0.91	0.12	66,66,66,66	0
54	MG	CA	1620	1/1	0.91	0.17	69,69,69,69	0
54	MG	DA	3537	1/1	0.91	0.18	73,73,73,73	0
54	MG	BA	3055	1/1	0.91	0.15	58,58,58,58	0
54	MG	CA	1703	1/1	0.91	0.18	62,62,62,62	0
54	MG	DA	3255	1/1	0.91	0.19	53,53,53,53	0
54	MG	AA	1723	1/1	0.91	0.13	89,89,89,89	0
54	MG	AA	1743	1/1	0.91	0.13	75,75,75,75	0
54	MG	DA	3403	1/1	0.91	0.14	69,69,69,69	0
54	MG	DA	3096	1/1	0.91	0.11	57,57,57,57	0
54	MG	DA	3551	1/1	0.91	0.08	68,68,68,68	0
54	MG	BA	3406	1/1	0.91	0.13	68,68,68,68	0
54	MG	AA	1697	1/1	0.91	0.08	77,77,77,77	0
54	MG	BA	3408	1/1	0.91	0.09	75,75,75,75	0
54	MG	BA	3470	1/1	0.91	0.11	79,79,79,79	0
54	MG	AA	1772	1/1	0.91	0.15	71,71,71,71	0
54	MG	DA	3558	1/1	0.91	0.20	65,65,65,65	0
54	MG	D3	102	1/1	0.91	0.10	72,72,72,72	0
54	MG	BA	3411	1/1	0.91	0.10	71,71,71,71	0
54	MG	DA	2907	1/1	0.91	0.18	23,23,23,23	0
54	MG	BA	3147	1/1	0.91	0.28	83,83,83,83	0
54	MG	DW	101	1/1	0.91	0.15	75,75,75,75	0
54	MG	DA	3274	1/1	0.91	0.19	82,82,82,82	0
54	MG	DA	2911	1/1	0.91	0.27	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3413	1/1	0.91	0.07	92,92,92,92	0
54	MG	DA	3113	1/1	0.91	0.17	43,43,43,43	0
54	MG	BA	3166	1/1	0.92	0.12	57,57,57,57	0
54	MG	DA	3545	1/1	0.92	0.26	74,74,74,74	0
54	MG	DA	3547	1/1	0.92	0.13	91,91,91,91	0
54	MG	BA	3012	1/1	0.92	0.20	56,56,56,56	0
54	MG	CA	1927	1/1	0.92	0.20	86,86,86,86	0
54	MG	DA	3076	1/1	0.92	0.13	38,38,38,38	0
54	MG	BA	3058	1/1	0.92	0.11	49,49,49,49	0
54	MG	DA	3079	1/1	0.92	0.22	59,59,59,59	0
54	MG	DA	3239	1/1	0.92	0.12	67,67,67,67	0
54	MG	BA	3356	1/1	0.92	0.07	75,75,75,75	0
54	MG	AA	1618	1/1	0.92	0.22	39,39,39,39	0
54	MG	CA	1931	1/1	0.92	0.08	84,84,84,84	0
54	MG	DA	3087	1/1	0.92	0.18	41,41,41,41	0
54	MG	BA	3062	1/1	0.92	0.12	61,61,61,61	0
54	MG	CA	1743	1/1	0.92	0.10	64,64,64,64	0
54	MG	AA	1672	1/1	0.92	0.24	68,68,68,68	0
54	MG	BO	201	1/1	0.92	0.09	50,50,50,50	0
54	MG	CD	117	1/1	0.92	0.06	85,85,85,85	0
54	MG	CA	1838	1/1	0.92	0.22	83,83,83,83	0
54	MG	DA	3095	1/1	0.92	0.10	46,46,46,46	0
54	MG	BA	3174	1/1	0.92	0.27	90,90,90,90	0
54	MG	BA	3175	1/1	0.92	0.07	54,54,54,54	0
54	MG	AA	1807	1/1	0.92	0.06	65,65,65,65	0
54	MG	BA	3431	1/1	0.92	0.09	96,96,96,96	0
54	MG	BA	2924	1/1	0.92	0.18	55,55,55,55	0
54	MG	DA	3742	1/1	0.92	0.10	58,58,58,58	0
54	MG	CA	1943	1/1	0.92	0.07	110,110,110,110	0
54	MG	BA	2970	1/1	0.92	0.21	32,32,32,32	0
54	MG	DA	3420	1/1	0.92	0.07	91,91,91,91	0
54	MG	AA	1785	1/1	0.92	0.08	78,78,78,78	0
54	MG	BA	3564	1/1	0.92	0.09	77,77,77,77	0
54	MG	DA	3423	1/1	0.92	0.07	62,62,62,62	0
54	MG	DA	3108	1/1	0.92	0.24	58,58,58,58	0
54	MG	DA	3584	1/1	0.92	0.09	86,86,86,86	0
54	MG	BA	2930	1/1	0.92	0.14	33,33,33,33	0
54	MG	DA	3753	1/1	0.92	0.23	92,92,92,92	0
54	MG	DA	3428	1/1	0.92	0.18	55,55,55,55	0
54	MG	BU	203	1/1	0.92	0.08	74,74,74,74	0
54	MG	DA	3111	1/1	0.92	0.14	48,48,48,48	0
54	MG	BA	3182	1/1	0.92	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3759	1/1	0.92	0.10	84,84,84,84	0
54	MG	CA	1851	1/1	0.92	0.19	87,87,87,87	0
54	MG	DA	3115	1/1	0.92	0.22	55,55,55,55	0
54	MG	CA	1758	1/1	0.92	0.09	90,90,90,90	0
54	MG	CA	1673	1/1	0.92	0.18	63,63,63,63	0
54	MG	DA	3119	1/1	0.92	0.31	59,59,59,59	0
54	MG	BU	205	1/1	0.92	0.12	55,55,55,55	0
54	MG	DA	2935	1/1	0.92	0.15	33,33,33,33	0
54	MG	BA	3024	1/1	0.92	0.25	40,40,40,40	0
54	MG	BA	2973	1/1	0.92	0.15	47,47,47,47	0
54	MG	CA	1859	1/1	0.92	0.08	121,121,121,121	0
54	MG	BA	3073	1/1	0.92	0.23	71,71,71,71	0
54	MG	BA	2932	1/1	0.92	0.12	37,37,37,37	0
54	MG	DA	3607	1/1	0.92	0.10	62,62,62,62	0
54	MG	DA	3296	1/1	0.92	0.30	82,82,82,82	0
54	MG	AA	1786	1/1	0.92	0.13	93,93,93,93	0
54	MG	BA	3077	1/1	0.92	0.12	46,46,46,46	0
54	MG	BA	3309	1/1	0.92	0.06	61,61,61,61	0
54	MG	CA	1770	1/1	0.92	0.11	85,85,85,85	0
54	MG	CA	1603	1/1	0.92	0.31	56,56,56,56	0
54	MG	BA	3250	1/1	0.92	0.27	93,93,93,93	0
54	MG	AA	1700	1/1	0.92	0.18	62,62,62,62	0
54	MG	BA	3578	1/1	0.92	0.17	98,98,98,98	0
54	MG	CA	1691	1/1	0.92	0.17	56,56,56,56	0
54	MG	DA	3621	1/1	0.92	0.06	75,75,75,75	0
54	MG	CA	1873	1/1	0.92	0.05	117,117,117,117	0
54	MG	DA	3460	1/1	0.92	0.16	72,72,72,72	0
54	MG	DA	3308	1/1	0.92	0.23	49,49,49,49	0
54	MG	BA	3513	1/1	0.92	0.17	77,77,77,77	0
54	MG	CA	1780	1/1	0.92	0.12	78,78,78,78	0
54	MG	CA	1608	1/1	0.92	0.11	53,53,53,53	0
54	MG	AA	1862	1/1	0.92	0.13	77,77,77,77	0
54	MG	DA	3153	1/1	0.92	0.16	51,51,51,51	0
54	MG	BA	3316	1/1	0.92	0.25	110,110,110,110	0
54	MG	DA	3632	1/1	0.92	0.07	73,73,73,73	0
54	MG	DA	3633	1/1	0.92	0.12	62,62,62,62	0
54	MG	BA	3385	1/1	0.92	0.25	64,64,64,64	0
54	MG	CA	1614	1/1	0.92	0.12	67,67,67,67	0
54	MG	DA	3002	1/1	0.92	0.31	62,62,62,62	0
54	MG	CA	1881	1/1	0.92	0.06	105,105,105,105	0
54	MG	AA	1873	1/1	0.92	0.06	80,80,80,80	0
54	MG	DA	3005	1/1	0.92	0.32	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1766	1/1	0.92	0.12	69,69,69,69	0
54	MG	CA	1702	1/1	0.92	0.12	71,71,71,71	0
54	MG	BA	2944	1/1	0.92	0.14	29,29,29,29	0
54	MG	DA	3172	1/1	0.92	0.14	53,53,53,53	0
54	MG	BB	203	1/1	0.92	0.07	85,85,85,85	0
54	MG	DA	3648	1/1	0.92	0.12	63,63,63,63	0
54	MG	BA	3389	1/1	0.92	0.08	89,89,89,89	0
54	MG	AA	2010	1/1	0.92	0.16	83,83,83,83	0
54	MG	CA	1623	1/1	0.92	0.31	71,71,71,71	0
54	MG	DA	3338	1/1	0.92	0.17	52,52,52,52	0
54	MG	DA	3183	1/1	0.92	0.23	56,56,56,56	0
54	MG	BB	206	1/1	0.92	0.15	85,85,85,85	0
54	MG	DA	3342	1/1	0.92	0.24	77,77,77,77	0
54	MG	DA	3494	1/1	0.92	0.06	110,110,110,110	0
54	MG	AA	1669	1/1	0.92	0.23	54,54,54,54	0
54	MG	DA	3662	1/1	0.92	0.11	78,78,78,78	0
54	MG	BA	2949	1/1	0.92	0.29	62,62,62,62	0
54	MG	BA	3460	1/1	0.92	0.06	90,90,90,90	0
54	MG	BA	3323	1/1	0.92	0.05	58,58,58,58	0
54	MG	DB	226	1/1	0.92	0.12	84,84,84,84	0
54	MG	CA	1802	1/1	0.92	0.14	62,62,62,62	0
54	MG	DA	3029	1/1	0.92	0.16	34,34,34,34	0
54	MG	DA	3031	1/1	0.92	0.12	53,53,53,53	0
54	MG	BA	3202	1/1	0.92	0.07	65,65,65,65	0
54	MG	CA	1630	1/1	0.92	0.22	59,59,59,59	0
54	MG	DA	3674	1/1	0.92	0.10	83,83,83,83	0
54	MG	AA	1889	1/1	0.92	0.11	68,68,68,68	0
54	MG	AA	1665	1/1	0.92	0.24	59,59,59,59	0
54	MG	DA	3201	1/1	0.92	0.09	61,61,61,61	0
54	MG	BA	3331	1/1	0.92	0.28	80,80,80,80	0
54	MG	DO	204	1/1	0.92	0.15	65,65,65,65	0
54	MG	DO	205	1/1	0.92	0.17	90,90,90,90	0
54	MG	BA	2952	1/1	0.92	0.17	41,41,41,41	0
54	MG	BA	2953	1/1	0.92	0.22	32,32,32,32	0
54	MG	CW	204	1/1	0.92	0.13	68,68,68,68	0
54	MG	DA	3685	1/1	0.92	0.05	66,66,66,66	0
54	MG	DA	3367	1/1	0.92	0.07	60,60,60,60	0
54	MG	BA	3101	1/1	0.92	0.25	56,56,56,56	0
54	MG	CA	1812	1/1	0.92	0.14	86,86,86,86	0
54	MG	D1	203	1/1	0.92	0.12	84,84,84,84	0
54	MG	BB	219	1/1	0.92	0.06	124,124,124,124	0
54	MG	DA	3055	1/1	0.92	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3522	1/1	0.92	0.07	66,66,66,66	0
54	MG	BA	3102	1/1	0.92	0.06	113,113,113,113	0
54	MG	BA	3339	1/1	0.92	0.09	74,74,74,74	0
54	MG	CA	1816	1/1	0.92	0.20	65,65,65,65	0
54	MG	DA	3060	1/1	0.92	0.13	57,57,57,57	0
54	MG	AA	1977	1/1	0.92	0.20	86,86,86,86	0
54	MG	BA	3157	1/1	0.92	0.08	45,45,45,45	0
54	MG	DA	3221	1/1	0.92	0.17	75,75,75,75	0
54	MG	BA	2957	1/1	0.92	0.12	33,33,33,33	0
54	MG	DA	3380	1/1	0.92	0.15	78,78,78,78	0
54	MG	BA	3053	1/1	0.92	0.19	43,43,43,43	0
54	MG	DW	102	1/1	0.92	0.17	91,91,91,91	0
54	MG	BA	3005	1/1	0.92	0.27	70,70,70,70	0
54	MG	AA	1877	1/1	0.92	0.19	80,80,80,80	0
54	MG	DA	3071	1/1	0.92	0.15	60,60,60,60	0
54	MG	BA	2960	1/1	0.92	0.11	49,49,49,49	0
54	MG	DA	3045	1/1	0.93	0.28	57,57,57,57	0
54	MG	DA	3507	1/1	0.93	0.12	86,86,86,86	0
54	MG	DA	3395	1/1	0.93	0.12	71,71,71,71	0
54	MG	BA	3354	1/1	0.93	0.06	57,57,57,57	0
54	MG	CA	1865	1/1	0.93	0.08	85,85,85,85	0
54	MG	DA	3050	1/1	0.93	0.28	56,56,56,56	0
54	MG	DA	3513	1/1	0.93	0.15	82,82,82,82	0
54	MG	BA	3444	1/1	0.93	0.14	66,66,66,66	0
54	MG	AA	1692	1/1	0.93	0.12	75,75,75,75	0
54	MG	DA	2918	1/1	0.93	0.26	28,28,28,28	0
54	MG	BA	3311	1/1	0.93	0.11	48,48,48,48	0
54	MG	DA	3165	1/1	0.93	0.20	33,33,33,33	0
54	MG	DA	3058	1/1	0.93	0.26	54,54,54,54	0
54	MG	CA	1650	1/1	0.93	0.09	52,52,52,52	0
54	MG	DA	2922	1/1	0.93	0.16	17,17,17,17	0
54	MG	DA	3524	1/1	0.93	0.18	54,54,54,54	0
54	MG	BA	3003	1/1	0.93	0.10	40,40,40,40	0
54	MG	DA	2926	1/1	0.93	0.09	23,23,23,23	0
54	MG	AH	202	1/1	0.93	0.08	80,80,80,80	0
54	MG	DA	3065	1/1	0.93	0.06	46,46,46,46	0
54	MG	BA	3404	1/1	0.93	0.06	82,82,82,82	0
54	MG	BA	2945	1/1	0.93	0.18	39,39,39,39	0
54	MG	DA	3782	1/1	0.93	0.12	83,83,83,83	0
54	MG	DA	3533	1/1	0.93	0.07	91,91,91,91	0
54	MG	DA	2939	1/1	0.93	0.26	45,45,45,45	0
54	MG	DA	3070	1/1	0.93	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1658	1/1	0.93	0.14	57,57,57,57	0
54	MG	DA	3658	1/1	0.93	0.33	88,88,88,88	0
54	MG	DA	2945	1/1	0.93	0.27	40,40,40,40	0
54	MG	BA	2974	1/1	0.93	0.25	39,39,39,39	0
54	MG	DA	2948	1/1	0.93	0.12	40,40,40,40	0
54	MG	DA	3190	1/1	0.93	0.09	50,50,50,50	0
54	MG	AA	1790	1/1	0.93	0.14	53,53,53,53	0
54	MG	BA	3243	1/1	0.93	0.05	49,49,49,49	0
54	MG	DA	3667	1/1	0.93	0.21	112,112,112,112	0
54	MG	CA	1823	1/1	0.93	0.07	66,66,66,66	0
54	MG	AA	1994	1/1	0.93	0.06	86,86,86,86	0
54	MG	BA	3282	1/1	0.93	0.10	103,103,103,103	0
54	MG	DA	3549	1/1	0.93	0.38	70,70,70,70	0
54	MG	DA	2957	1/1	0.93	0.19	20,20,20,20	0
54	MG	DA	3199	1/1	0.93	0.09	39,39,39,39	0
54	MG	DA	2959	1/1	0.93	0.14	26,26,26,26	0
54	MG	BA	3111	1/1	0.93	0.15	53,53,53,53	0
54	MG	AC	104	1/1	0.93	0.06	85,85,85,85	0
54	MG	DA	3680	1/1	0.93	0.07	75,75,75,75	0
54	MG	BA	3178	1/1	0.93	0.17	60,60,60,60	0
54	MG	DA	2970	1/1	0.93	0.14	49,49,49,49	0
54	MG	DA	3206	1/1	0.93	0.20	59,59,59,59	0
54	MG	BA	3374	1/1	0.93	0.12	39,39,39,39	0
54	MG	AA	1962	1/1	0.93	0.07	55,55,55,55	0
54	MG	AA	1837	1/1	0.93	0.06	59,59,59,59	0
54	MG	CA	1725	1/1	0.93	0.24	54,54,54,54	0
54	MG	DA	2984	1/1	0.93	0.26	46,46,46,46	0
54	MG	DA	3330	1/1	0.93	0.14	49,49,49,49	0
54	MG	DA	3331	1/1	0.93	0.11	70,70,70,70	0
54	MG	DA	3215	1/1	0.93	0.24	58,58,58,58	0
54	MG	DA	3695	1/1	0.93	0.06	60,60,60,60	0
54	MG	AA	1659	1/1	0.93	0.11	81,81,81,81	0
54	MG	CA	1891	1/1	0.93	0.05	113,113,113,113	0
54	MG	DA	3571	1/1	0.93	0.16	81,81,81,81	0
54	MG	DA	3100	1/1	0.93	0.06	62,62,62,62	0
54	MG	CC	104	1/1	0.93	0.11	65,65,65,65	0
54	MG	DA	3102	1/1	0.93	0.18	49,49,49,49	0
54	MG	BA	3078	1/1	0.93	0.22	57,57,57,57	0
54	MG	DA	2992	1/1	0.93	0.18	43,43,43,43	0
54	MG	CA	1894	1/1	0.93	0.08	61,61,61,61	0
54	MG	DA	2994	1/1	0.93	0.18	37,37,37,37	0
54	MG	CA	1618	1/1	0.93	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1751	1/1	0.93	0.17	73,73,73,73	0
54	MG	BD	301	1/1	0.93	0.28	65,65,65,65	0
54	MG	BA	3119	1/1	0.93	0.13	51,51,51,51	0
54	MG	AA	1981	1/1	0.93	0.05	115,115,115,115	0
54	MG	DE	301	1/1	0.93	0.20	27,27,27,27	0
54	MG	DE	302	1/1	0.93	0.12	51,51,51,51	0
54	MG	AA	1688	1/1	0.93	0.14	39,39,39,39	0
54	MG	AA	1613	1/1	0.93	0.17	53,53,53,53	0
54	MG	AA	1796	1/1	0.93	0.16	75,75,75,75	0
54	MG	CA	1905	1/1	0.93	0.04	92,92,92,92	0
54	MG	DA	3009	1/1	0.93	0.17	41,41,41,41	0
54	MG	DH	204	1/1	0.93	0.20	77,77,77,77	0
54	MG	BF	301	1/1	0.93	0.15	80,80,80,80	0
54	MG	AA	1854	1/1	0.93	0.11	97,97,97,97	0
54	MG	BA	3088	1/1	0.93	0.12	49,49,49,49	0
54	MG	DA	3244	1/1	0.93	0.27	64,64,64,64	0
54	MG	BA	3346	1/1	0.93	0.08	52,52,52,52	0
54	MG	CA	1966	1/1	0.93	0.10	82,82,82,82	0
54	MG	BA	3304	1/1	0.93	0.06	63,63,63,63	0
54	MG	DA	3600	1/1	0.93	0.23	107,107,107,107	0
54	MG	BA	3528	1/1	0.93	0.07	88,88,88,88	0
54	MG	CA	1853	1/1	0.93	0.09	101,101,101,101	0
54	MG	DA	3484	1/1	0.93	0.19	72,72,72,72	0
54	MG	CA	1970	1/1	0.93	0.17	87,87,87,87	0
54	MG	DA	3257	1/1	0.93	0.23	64,64,64,64	0
54	MG	DA	3608	1/1	0.93	0.26	74,74,74,74	0
54	MG	DA	3258	1/1	0.93	0.06	76,76,76,76	0
54	MG	BA	3059	1/1	0.93	0.20	59,59,59,59	0
54	MG	BA	3481	1/1	0.93	0.07	80,80,80,80	0
54	MG	DA	3030	1/1	0.93	0.19	49,49,49,49	0
54	MG	BA	3482	1/1	0.93	0.06	101,101,101,101	0
54	MG	AA	1797	1/1	0.93	0.13	75,75,75,75	0
54	MG	DA	3266	1/1	0.93	0.09	109,109,109,109	0
54	MG	BA	3231	1/1	0.93	0.08	68,68,68,68	0
54	MG	AA	1721	1/1	0.93	0.29	72,72,72,72	0
54	MG	BA	3487	1/1	0.93	0.08	74,74,74,74	0
54	MG	BA	3395	1/1	0.93	0.07	60,60,60,60	0
54	MG	DA	3040	1/1	0.93	0.13	44,44,44,44	0
54	MG	DA	2904	1/1	0.93	0.15	22,22,22,22	0
54	MG	DA	2906	1/1	0.93	0.17	27,27,27,27	0
54	MG	BA	3353	1/1	0.93	0.16	75,75,75,75	0
54	MG	BA	3338	1/1	0.94	0.07	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3192	1/1	0.94	0.10	61,61,61,61	0
54	MG	BA	3090	1/1	0.94	0.13	61,61,61,61	0
54	MG	DA	3325	1/1	0.94	0.07	64,64,64,64	0
54	MG	CA	1972	1/1	0.94	0.06	61,61,61,61	0
54	MG	CA	1893	1/1	0.94	0.10	81,81,81,81	0
54	MG	DA	3599	1/1	0.94	0.29	80,80,80,80	0
54	MG	DA	2927	1/1	0.94	0.16	53,53,53,53	0
54	MG	DA	3744	1/1	0.94	0.13	68,68,68,68	0
54	MG	DA	3197	1/1	0.94	0.20	64,64,64,64	0
54	MG	BA	3011	1/1	0.94	0.14	57,57,57,57	0
54	MG	AA	1936	1/1	0.94	0.09	74,74,74,74	0
54	MG	DA	3200	1/1	0.94	0.23	52,52,52,52	0
54	MG	DA	3333	1/1	0.94	0.09	50,50,50,50	0
54	MG	DA	3334	1/1	0.94	0.17	45,45,45,45	0
54	MG	BA	3397	1/1	0.94	0.23	47,47,47,47	0
54	MG	BA	2939	1/1	0.94	0.34	47,47,47,47	0
54	MG	BA	3141	1/1	0.94	0.18	52,52,52,52	0
54	MG	DA	2943	1/1	0.94	0.22	29,29,29,29	0
54	MG	AA	1991	1/1	0.94	0.08	70,70,70,70	0
54	MG	CA	1601	1/1	0.94	0.14	50,50,50,50	0
54	MG	DA	3476	1/1	0.94	0.11	68,68,68,68	0
54	MG	BA	3239	1/1	0.94	0.10	49,49,49,49	0
54	MG	DA	3210	1/1	0.94	0.20	75,75,75,75	0
54	MG	DA	3619	1/1	0.94	0.10	52,52,52,52	0
54	MG	DA	3763	1/1	0.94	0.09	71,71,71,71	0
54	MG	DA	3479	1/1	0.94	0.06	73,73,73,73	0
54	MG	DA	3344	1/1	0.94	0.09	44,44,44,44	0
54	MG	DA	3080	1/1	0.94	0.06	23,23,23,23	0
54	MG	BA	3522	1/1	0.94	0.10	54,54,54,54	0
54	MG	AA	1703	1/1	0.94	0.15	49,49,49,49	0
54	MG	CH	202	1/1	0.94	0.13	72,72,72,72	0
54	MG	AA	1946	1/1	0.94	0.13	82,82,82,82	0
54	MG	AA	1752	1/1	0.94	0.16	75,75,75,75	0
54	MG	BA	3350	1/1	0.94	0.08	63,63,63,63	0
54	MG	BA	3294	1/1	0.94	0.19	65,65,65,65	0
54	MG	CA	1679	1/1	0.94	0.10	72,72,72,72	0
54	MG	CA	1611	1/1	0.94	0.22	42,42,42,42	0
54	MG	DA	3358	1/1	0.94	0.23	78,78,78,78	0
54	MG	CA	1755	1/1	0.94	0.20	70,70,70,70	0
54	MG	DA	2968	1/1	0.94	0.13	20,20,20,20	0
54	MG	DA	3637	1/1	0.94	0.12	74,74,74,74	0
54	MG	CA	1681	1/1	0.94	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3296	1/1	0.94	0.05	57,57,57,57	0
54	MG	DA	3225	1/1	0.94	0.13	45,45,45,45	0
54	MG	BA	3103	1/1	0.94	0.18	53,53,53,53	0
54	MG	DA	3099	1/1	0.94	0.29	60,60,60,60	0
54	MG	DA	2980	1/1	0.94	0.27	44,44,44,44	0
54	MG	CA	1836	1/1	0.94	0.22	58,58,58,58	0
54	MG	BA	3531	1/1	0.94	0.14	75,75,75,75	0
54	MG	BA	3410	1/1	0.94	0.13	82,82,82,82	0
54	MG	BA	2980	1/1	0.94	0.20	53,53,53,53	0
54	MG	CA	1617	1/1	0.94	0.12	44,44,44,44	0
54	MG	AA	1984	1/1	0.94	0.06	80,80,80,80	0
54	MG	CA	1843	1/1	0.94	0.07	76,76,76,76	0
54	MG	BA	3022	1/1	0.94	0.09	46,46,46,46	0
54	MG	BA	3023	1/1	0.94	0.25	52,52,52,52	0
54	MG	DA	3242	1/1	0.94	0.09	46,46,46,46	0
54	MG	BA	2915	1/1	0.94	0.14	34,34,34,34	0
54	MG	DA	3657	1/1	0.94	0.20	88,88,88,88	0
54	MG	DA	2996	1/1	0.94	0.26	40,40,40,40	0
54	MG	DA	3112	1/1	0.94	0.14	55,55,55,55	0
54	MG	CA	1768	1/1	0.94	0.14	52,52,52,52	0
54	MG	DA	2998	1/1	0.94	0.09	44,44,44,44	0
54	MG	BA	3538	1/1	0.94	0.06	65,65,65,65	0
54	MG	DA	3000	1/1	0.94	0.17	31,31,31,31	0
54	MG	BA	3155	1/1	0.94	0.07	64,64,64,64	0
54	MG	DA	3390	1/1	0.94	0.24	72,72,72,72	0
54	MG	BA	3305	1/1	0.94	0.13	62,62,62,62	0
54	MG	BA	3113	1/1	0.94	0.17	41,41,41,41	0
54	MG	BA	2984	1/1	0.94	0.12	48,48,48,48	0
54	MG	AA	2009	1/1	0.94	0.09	71,71,71,71	0
54	MG	DA	3672	1/1	0.94	0.28	87,87,87,87	0
54	MG	BA	2917	1/1	0.94	0.21	37,37,37,37	0
54	MG	CA	1777	1/1	0.94	0.24	71,71,71,71	0
54	MG	AA	1656	1/1	0.94	0.07	71,71,71,71	0
54	MG	AA	1739	1/1	0.94	0.11	66,66,66,66	0
54	MG	BA	3427	1/1	0.94	0.11	80,80,80,80	0
54	MG	DA	3678	1/1	0.94	0.09	69,69,69,69	0
54	MG	CD	102	1/1	0.94	0.07	99,99,99,99	0
54	MG	DA	3013	1/1	0.94	0.21	58,58,58,58	0
54	MG	BA	3259	1/1	0.94	0.07	90,90,90,90	0
54	MG	CA	1783	1/1	0.94	0.15	47,47,47,47	0
54	MG	CD	105	1/1	0.94	0.05	124,124,124,124	0
54	MG	DA	3138	1/1	0.94	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3371	1/1	0.94	0.08	55,55,55,55	0
54	MG	AA	2039	1/1	0.94	0.10	64,64,64,64	0
54	MG	DA	3144	1/1	0.94	0.15	43,43,43,43	0
54	MG	CA	1636	1/1	0.94	0.14	52,52,52,52	0
54	MG	DA	3026	1/1	0.94	0.21	34,34,34,34	0
54	MG	BA	3163	1/1	0.94	0.06	63,63,63,63	0
54	MG	BA	3033	1/1	0.94	0.16	45,45,45,45	0
54	MG	CA	1639	1/1	0.94	0.12	42,42,42,42	0
54	MG	DA	3418	1/1	0.94	0.07	59,59,59,59	0
54	MG	AA	1707	1/1	0.94	0.13	64,64,64,64	0
54	MG	BA	3168	1/1	0.94	0.21	65,65,65,65	0
54	MG	DA	3700	1/1	0.94	0.10	75,75,75,75	0
54	MG	DH	203	1/1	0.94	0.06	65,65,65,65	0
54	MG	DA	3154	1/1	0.94	0.25	56,56,56,56	0
54	MG	DO	202	1/1	0.94	0.06	42,42,42,42	0
54	MG	DA	3155	1/1	0.94	0.17	40,40,40,40	0
54	MG	BA	2927	1/1	0.94	0.23	32,32,32,32	0
54	MG	BA	2928	1/1	0.94	0.18	46,46,46,46	0
54	MG	DA	3035	1/1	0.94	0.22	55,55,55,55	0
54	MG	DA	3036	1/1	0.94	0.22	50,50,50,50	0
54	MG	CD	118	1/1	0.94	0.06	60,60,60,60	0
54	MG	AA	1988	1/1	0.94	0.07	93,93,93,93	0
54	MG	DA	3432	1/1	0.94	0.19	66,66,66,66	0
54	MG	BA	3498	1/1	0.94	0.10	59,59,59,59	0
54	MG	DA	3434	1/1	0.94	0.13	63,63,63,63	0
54	MG	BA	2901	1/1	0.94	0.08	61,61,61,61	0
54	MG	D1	204	1/1	0.94	0.20	71,71,71,71	0
54	MG	BA	2931	1/1	0.94	0.09	29,29,29,29	0
54	MG	CA	1799	1/1	0.94	0.16	86,86,86,86	0
54	MG	BA	3083	1/1	0.94	0.10	37,37,37,37	0
54	MG	DT	101	1/1	0.94	0.17	51,51,51,51	0
54	MG	BA	3225	1/1	0.94	0.06	49,49,49,49	0
54	MG	BA	2965	1/1	0.94	0.05	30,30,30,30	0
54	MG	DA	3177	1/1	0.94	0.20	38,38,38,38	0
54	MG	AW	202	1/1	0.94	0.12	59,59,59,59	0
54	MG	DA	3051	1/1	0.94	0.06	29,29,29,29	0
54	MG	BA	3333	1/1	0.94	0.13	62,62,62,62	0
54	MG	AA	1745	1/1	0.94	0.15	67,67,67,67	0
54	MG	BA	3508	1/1	0.94	0.04	90,90,90,90	0
54	MG	DA	2910	1/1	0.94	0.20	25,25,25,25	0
54	MG	DA	3729	1/1	0.94	0.12	73,73,73,73	0
54	MG	BU	201	1/1	0.94	0.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2969	1/1	0.94	0.24	33,33,33,33	0
54	MG	CA	1809	1/1	0.94	0.14	78,78,78,78	0
54	MG	D7	101	1/1	0.94	0.24	55,55,55,55	0
54	MG	AA	2002	1/1	0.94	0.07	81,81,81,81	0
54	MG	BA	3392	1/1	0.94	0.04	70,70,70,70	0
54	MG	DA	3044	1/1	0.95	0.12	61,61,61,61	0
54	MG	DA	2944	1/1	0.95	0.12	35,35,35,35	0
54	MG	DA	3260	1/1	0.95	0.05	53,53,53,53	0
54	MG	DA	3047	1/1	0.95	0.20	50,50,50,50	0
54	MG	BA	3165	1/1	0.95	0.06	46,46,46,46	0
54	MG	BA	2926	1/1	0.95	0.15	43,43,43,43	0
54	MG	CA	1610	1/1	0.95	0.21	51,51,51,51	0
54	MG	BA	2938	1/1	0.95	0.15	39,39,39,39	0
54	MG	BA	2908	1/1	0.95	0.05	102,102,102,102	0
54	MG	BA	2941	1/1	0.95	0.13	27,27,27,27	0
54	MG	DA	3760	1/1	0.95	0.06	206,206,206,206	0
54	MG	DA	3383	1/1	0.95	0.07	32,32,32,32	0
54	MG	BA	3203	1/1	0.95	0.27	64,64,64,64	0
54	MG	CA	1837	1/1	0.95	0.08	44,44,44,44	0
54	MG	DA	3634	1/1	0.95	0.10	63,63,63,63	0
54	MG	BA	2955	1/1	0.95	0.23	29,29,29,29	0
54	MG	CC	106	1/1	0.95	0.04	79,79,79,79	0
54	MG	DA	3272	1/1	0.95	0.22	66,66,66,66	0
54	MG	DA	2960	1/1	0.95	0.19	34,34,34,34	0
54	MG	AA	1691	1/1	0.95	0.20	62,62,62,62	0
54	MG	DA	2963	1/1	0.95	0.22	45,45,45,45	0
54	MG	DA	2964	1/1	0.95	0.09	21,21,21,21	0
54	MG	BA	2976	1/1	0.95	0.13	38,38,38,38	0
54	MG	AA	1630	1/1	0.95	0.31	55,55,55,55	0
54	MG	BA	3466	1/1	0.95	0.04	84,84,84,84	0
54	MG	DA	3777	1/1	0.95	0.06	53,53,53,53	0
54	MG	DA	3170	1/1	0.95	0.17	31,31,31,31	0
54	MG	DA	2969	1/1	0.95	0.28	36,36,36,36	0
54	MG	DA	3173	1/1	0.95	0.06	57,57,57,57	0
54	MG	DA	3649	1/1	0.95	0.12	62,62,62,62	0
54	MG	DA	3174	1/1	0.95	0.11	66,66,66,66	0
54	MG	DA	3525	1/1	0.95	0.16	78,78,78,78	0
54	MG	DA	3175	1/1	0.95	0.18	34,34,34,34	0
54	MG	DA	3786	1/1	0.95	0.07	70,70,70,70	0
54	MG	BA	3467	1/1	0.95	0.10	81,81,81,81	0
54	MG	DA	2973	1/1	0.95	0.18	24,24,24,24	0
54	MG	BA	3067	1/1	0.95	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3530	1/1	0.95	0.21	59,59,59,59	0
54	MG	DA	3408	1/1	0.95	0.06	38,38,38,38	0
54	MG	DA	2978	1/1	0.95	0.13	24,24,24,24	0
54	MG	DA	3181	1/1	0.95	0.09	48,48,48,48	0
54	MG	BA	3327	1/1	0.95	0.10	65,65,65,65	0
54	MG	BA	3246	1/1	0.95	0.06	54,54,54,54	0
54	MG	DA	3663	1/1	0.95	0.09	76,76,76,76	0
54	MG	BA	3247	1/1	0.95	0.14	63,63,63,63	0
54	MG	BA	3211	1/1	0.95	0.04	43,43,43,43	0
54	MG	BA	3288	1/1	0.95	0.06	66,66,66,66	0
54	MG	DA	2985	1/1	0.95	0.14	27,27,27,27	0
54	MG	BA	3048	1/1	0.95	0.04	41,41,41,41	0
54	MG	DA	3541	1/1	0.95	0.21	54,54,54,54	0
54	MG	CA	1909	1/1	0.95	0.06	74,74,74,74	0
54	MG	CA	1796	1/1	0.95	0.05	35,35,35,35	0
54	MG	DA	3086	1/1	0.95	0.12	61,61,61,61	0
54	MG	DA	3546	1/1	0.95	0.24	68,68,68,68	0
54	MG	DA	2990	1/1	0.95	0.12	27,27,27,27	0
54	MG	BA	2920	1/1	0.95	0.19	36,36,36,36	0
54	MG	AA	1778	1/1	0.95	0.05	61,61,61,61	0
54	MG	BA	3429	1/1	0.95	0.09	56,56,56,56	0
54	MG	BA	3337	1/1	0.95	0.10	73,73,73,73	0
54	MG	DA	3679	1/1	0.95	0.07	68,68,68,68	0
54	MG	DA	2995	1/1	0.95	0.21	40,40,40,40	0
54	MG	DA	3093	1/1	0.95	0.23	53,53,53,53	0
54	MG	CD	114	1/1	0.95	0.04	109,109,109,109	0
54	MG	CA	1632	1/1	0.95	0.22	62,62,62,62	0
54	MG	BA	2963	1/1	0.95	0.13	32,32,32,32	0
54	MG	BA	2922	1/1	0.95	0.20	46,46,46,46	0
54	MG	BA	3295	1/1	0.95	0.07	55,55,55,55	0
54	MG	BA	3341	1/1	0.95	0.05	119,119,119,119	0
54	MG	BA	3153	1/1	0.95	0.31	71,71,71,71	0
54	MG	BA	3028	1/1	0.95	0.13	41,41,41,41	0
54	MG	DA	3324	1/1	0.95	0.14	34,34,34,34	0
54	MG	DA	3692	1/1	0.95	0.09	60,60,60,60	0
54	MG	CA	1979	1/1	0.95	0.06	104,104,104,104	0
54	MG	CA	1980	1/1	0.95	0.13	50,50,50,50	0
54	MG	BA	3126	1/1	0.95	0.05	42,42,42,42	0
54	MG	CA	1982	1/1	0.95	0.04	80,80,80,80	0
54	MG	BA	3075	1/1	0.95	0.13	37,37,37,37	0
54	MG	BA	2983	1/1	0.95	0.17	27,27,27,27	0
54	MG	DA	2905	1/1	0.95	0.21	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1643	1/1	0.95	0.18	66,66,66,66	0
54	MG	DD	302	1/1	0.95	0.11	40,40,40,40	0
54	MG	BA	3104	1/1	0.95	0.19	47,47,47,47	0
54	MG	DA	2908	1/1	0.95	0.16	23,23,23,23	0
54	MG	DA	3015	1/1	0.95	0.11	41,41,41,41	0
54	MG	BA	3187	1/1	0.95	0.03	40,40,40,40	0
54	MG	BA	2933	1/1	0.95	0.12	50,50,50,50	0
54	MG	AA	1757	1/1	0.95	0.07	45,45,45,45	0
54	MG	DA	2912	1/1	0.95	0.23	27,27,27,27	0
54	MG	DA	3023	1/1	0.95	0.13	28,28,28,28	0
54	MG	CA	1872	1/1	0.95	0.22	84,84,84,84	0
54	MG	DO	201	1/1	0.95	0.09	55,55,55,55	0
54	MG	DA	3585	1/1	0.95	0.06	114,114,114,114	0
54	MG	BA	3107	1/1	0.95	0.06	61,61,61,61	0
54	MG	DA	3459	1/1	0.95	0.05	64,64,64,64	0
54	MG	DA	3121	1/1	0.95	0.04	56,56,56,56	0
54	MG	BA	3134	1/1	0.95	0.25	61,61,61,61	0
54	MG	DA	3346	1/1	0.95	0.07	66,66,66,66	0
54	MG	DA	3123	1/1	0.95	0.16	66,66,66,66	0
54	MG	B5	101	1/1	0.95	0.16	46,46,46,46	0
54	MG	BA	3269	1/1	0.95	0.06	90,90,90,90	0
54	MG	DA	3234	1/1	0.95	0.10	32,32,32,32	0
54	MG	DA	3352	1/1	0.95	0.07	66,66,66,66	0
54	MG	BA	3193	1/1	0.95	0.21	80,80,80,80	0
54	MG	DA	3236	1/1	0.95	0.25	60,60,60,60	0
54	MG	CQ	101	1/1	0.95	0.07	71,71,71,71	0
54	MG	BA	3355	1/1	0.95	0.14	64,64,64,64	0
54	MG	DA	3131	1/1	0.95	0.21	63,63,63,63	0
54	MG	CA	1602	1/1	0.95	0.15	29,29,29,29	0
54	MG	DT	102	1/1	0.95	0.21	64,64,64,64	0
54	MG	BA	3271	1/1	0.95	0.07	59,59,59,59	0
54	MG	DA	3360	1/1	0.95	0.07	67,67,67,67	0
54	MG	CA	1940	1/1	0.95	0.06	112,112,112,112	0
54	MG	DA	3362	1/1	0.95	0.15	58,58,58,58	0
54	MG	AA	1968	1/1	0.95	0.04	80,80,80,80	0
54	MG	D3	101	1/1	0.95	0.19	48,48,48,48	0
54	MG	BA	3313	1/1	0.95	0.08	102,102,102,102	0
54	MG	D3	103	1/1	0.95	0.05	76,76,76,76	0
54	MG	DA	3482	1/1	0.95	0.06	43,43,43,43	0
54	MG	DA	3039	1/1	0.95	0.10	48,48,48,48	0
54	MG	DA	3366	1/1	0.95	0.08	50,50,50,50	0
54	MG	DA	2940	1/1	0.95	0.19	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3164	1/1	0.95	0.10	70,70,70,70	0
54	MG	DA	3615	1/1	0.95	0.06	78,78,78,78	0
54	MG	DA	2942	1/1	0.95	0.15	38,38,38,38	0
54	MG	DA	3253	1/1	0.95	0.19	67,67,67,67	0
54	MG	DA	3143	1/1	0.95	0.21	68,68,68,68	0
54	MG	BA	3552	1/1	0.95	0.18	76,76,76,76	0
54	MG	DA	3693	1/1	0.96	0.06	56,56,56,56	0
54	MG	DA	3602	1/1	0.96	0.06	116,116,116,116	0
54	MG	BA	2986	1/1	0.96	0.17	41,41,41,41	0
54	MG	AC	108	1/1	0.96	0.08	61,61,61,61	0
54	MG	BA	3542	1/1	0.96	0.06	78,78,78,78	0
54	MG	BA	3426	1/1	0.96	0.07	43,43,43,43	0
54	MG	DA	3427	1/1	0.96	0.11	65,65,65,65	0
54	MG	BA	3194	1/1	0.96	0.15	87,87,87,87	0
54	MG	DA	3701	1/1	0.96	0.13	92,92,92,92	0
54	MG	BA	3009	1/1	0.96	0.19	57,57,57,57	0
54	MG	DA	3348	1/1	0.96	0.16	58,58,58,58	0
54	MG	DA	2967	1/1	0.96	0.13	39,39,39,39	0
54	MG	BA	3260	1/1	0.96	0.30	77,77,77,77	0
54	MG	DA	3707	1/1	0.96	0.12	64,64,64,64	0
54	MG	DA	3523	1/1	0.96	0.04	64,64,64,64	0
54	MG	BA	3140	1/1	0.96	0.07	51,51,51,51	0
54	MG	BA	3197	1/1	0.96	0.09	103,103,103,103	0
54	MG	DB	202	1/1	0.96	0.06	87,87,87,87	0
54	MG	DA	2901	1/1	0.96	0.18	28,28,28,28	0
54	MG	BA	3010	1/1	0.96	0.18	55,55,55,55	0
54	MG	DA	2903	1/1	0.96	0.25	24,24,24,24	0
54	MG	AA	1836	1/1	0.96	0.07	58,58,58,58	0
54	MG	CA	1767	1/1	0.96	0.13	68,68,68,68	0
54	MG	AA	1803	1/1	0.96	0.06	61,61,61,61	0
54	MG	DA	3277	1/1	0.96	0.20	59,59,59,59	0
54	MG	BA	3364	1/1	0.96	0.07	77,77,77,77	0
54	MG	BA	2956	1/1	0.96	0.12	38,38,38,38	0
54	MG	BA	3035	1/1	0.96	0.10	48,48,48,48	0
54	MG	DA	3721	1/1	0.96	0.06	50,50,50,50	0
54	MG	DA	3282	1/1	0.96	0.17	63,63,63,63	0
54	MG	BA	3401	1/1	0.96	0.08	36,36,36,36	0
54	MG	CA	1819	1/1	0.96	0.11	61,61,61,61	0
54	MG	BA	3516	1/1	0.96	0.13	56,56,56,56	0
54	MG	DA	3128	1/1	0.96	0.07	40,40,40,40	0
54	MG	DA	2913	1/1	0.96	0.21	30,30,30,30	0
54	MG	DA	2914	1/1	0.96	0.13	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3543	1/1	0.96	0.04	96,96,96,96	0
54	MG	DA	3208	1/1	0.96	0.16	57,57,57,57	0
54	MG	AA	1683	1/1	0.96	0.20	60,60,60,60	0
54	MG	CC	101	1/1	0.96	0.05	70,70,70,70	0
54	MG	BA	2993	1/1	0.96	0.22	52,52,52,52	0
54	MG	BA	3369	1/1	0.96	0.04	73,73,73,73	0
54	MG	BB	218	1/1	0.96	0.03	65,65,65,65	0
54	MG	BA	3149	1/1	0.96	0.28	61,61,61,61	0
54	MG	DA	3068	1/1	0.96	0.21	50,50,50,50	0
54	MG	BA	3038	1/1	0.96	0.12	39,39,39,39	0
54	MG	BA	3372	1/1	0.96	0.19	53,53,53,53	0
54	MG	CA	1737	1/1	0.96	0.04	132,132,132,132	0
54	MG	DA	2929	1/1	0.96	0.15	24,24,24,24	0
54	MG	BA	2909	1/1	0.96	0.06	66,66,66,66	0
54	MG	DG	202	1/1	0.96	0.10	84,84,84,84	0
54	MG	DA	2932	1/1	0.96	0.15	23,23,23,23	0
54	MG	DA	2933	1/1	0.96	0.28	31,31,31,31	0
54	MG	DA	3469	1/1	0.96	0.14	51,51,51,51	0
54	MG	BA	3208	1/1	0.96	0.12	68,68,68,68	0
54	MG	BA	3486	1/1	0.96	0.11	90,90,90,90	0
54	MG	DA	2938	1/1	0.96	0.07	57,57,57,57	0
54	MG	DA	3388	1/1	0.96	0.05	37,37,37,37	0
54	MG	BA	2959	1/1	0.96	0.07	36,36,36,36	0
54	MG	DA	3475	1/1	0.96	0.08	56,56,56,56	0
54	MG	AA	1686	1/1	0.96	0.17	60,60,60,60	0
54	MG	DA	3391	1/1	0.96	0.09	40,40,40,40	0
54	MG	DA	3229	1/1	0.96	0.08	33,33,33,33	0
54	MG	DA	3393	1/1	0.96	0.19	60,60,60,60	0
54	MG	D0	205	1/1	0.96	0.15	95,95,95,95	0
54	MG	DA	3574	1/1	0.96	0.08	74,74,74,74	0
54	MG	DA	3082	1/1	0.96	0.37	67,67,67,67	0
54	MG	BA	2947	1/1	0.96	0.15	30,30,30,30	0
54	MG	DA	3084	1/1	0.96	0.18	47,47,47,47	0
54	MG	BA	3045	1/1	0.96	0.12	26,26,26,26	0
54	MG	BA	3046	1/1	0.96	0.14	29,29,29,29	0
54	MG	CA	1884	1/1	0.96	0.06	59,59,59,59	0
54	MG	DA	3320	1/1	0.96	0.09	131,131,131,131	0
54	MG	BE	302	1/1	0.96	0.09	85,85,85,85	0
54	MG	DA	3016	1/1	0.96	0.14	23,23,23,23	0
54	MG	DA	2946	1/1	0.96	0.25	40,40,40,40	0
54	MG	AA	1690	1/1	0.96	0.05	91,91,91,91	0
54	MG	BA	2902	1/1	0.96	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	2925	1/1	0.96	0.13	46,46,46,46	0
54	MG	DU	204	1/1	0.96	0.06	99,99,99,99	0
54	MG	DA	3021	1/1	0.96	0.17	47,47,47,47	0
54	MG	DA	3022	1/1	0.96	0.20	36,36,36,36	0
54	MG	DA	3245	1/1	0.96	0.12	47,47,47,47	0
54	MG	DA	2950	1/1	0.96	0.18	52,52,52,52	0
54	MG	BA	3025	1/1	0.96	0.10	47,47,47,47	0
54	MG	BA	3458	1/1	0.96	0.07	76,76,76,76	0
54	MG	DA	3250	1/1	0.96	0.16	44,44,44,44	0
54	MG	AA	1791	1/1	0.96	0.04	68,68,68,68	0
54	MG	DA	3252	1/1	0.96	0.22	65,65,65,65	0
54	MG	DA	2955	1/1	0.96	0.19	39,39,39,39	0
54	MG	D5	101	1/1	0.96	0.11	54,54,54,54	0
54	MG	AA	1681	1/1	0.96	0.05	43,43,43,43	0
54	MG	BA	3079	1/1	0.96	0.14	59,59,59,59	0
54	MG	DA	3787	1/1	0.96	0.07	59,59,59,59	0
54	MG	DA	2958	1/1	0.96	0.08	46,46,46,46	0
54	MG	CA	1710	1/1	0.96	0.15	53,53,53,53	0
54	MG	DA	3171	1/1	0.97	0.09	45,45,45,45	0
54	MG	DA	3510	1/1	0.97	0.05	43,43,43,43	0
54	MG	AA	1811	1/1	0.97	0.04	81,81,81,81	0
54	MG	BA	3212	1/1	0.97	0.12	87,87,87,87	0
54	MG	DA	3340	1/1	0.97	0.09	76,76,76,76	0
54	MG	CD	111	1/1	0.97	0.04	87,87,87,87	0
54	MG	BA	3060	1/1	0.97	0.07	35,35,35,35	0
54	MG	CA	1709	1/1	0.97	0.09	58,58,58,58	0
54	MG	DA	3025	1/1	0.97	0.12	25,25,25,25	0
54	MG	DA	3259	1/1	0.97	0.27	71,71,71,71	0
54	MG	BE	305	1/1	0.97	0.09	68,68,68,68	0
54	MG	DA	3431	1/1	0.97	0.08	51,51,51,51	0
54	MG	DA	3027	1/1	0.97	0.09	22,22,22,22	0
54	MG	BA	3021	1/1	0.97	0.06	35,35,35,35	0
54	MG	BA	3381	1/1	0.97	0.07	45,45,45,45	0
54	MG	CA	1714	1/1	0.97	0.05	64,64,64,64	0
54	MG	BA	3110	1/1	0.97	0.11	34,34,34,34	0
54	MG	CD	119	1/1	0.97	0.05	95,95,95,95	0
54	MG	BA	3576	1/1	0.97	0.04	40,40,40,40	0
54	MG	BA	3418	1/1	0.97	0.06	65,65,65,65	0
54	MG	AA	1712	1/1	0.97	0.06	50,50,50,50	0
54	MG	AA	2025	1/1	0.97	0.33	71,71,71,71	0
54	MG	DB	210	1/1	0.97	0.06	114,114,114,114	0
54	MG	BA	3085	1/1	0.97	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1773	1/1	0.97	0.04	87,87,87,87	0
54	MG	DA	3273	1/1	0.97	0.03	39,39,39,39	0
54	MG	AA	1820	1/1	0.97	0.04	98,98,98,98	0
54	MG	C1	101	1/1	0.97	0.05	65,65,65,65	0
54	MG	BA	3007	1/1	0.97	0.18	51,51,51,51	0
54	MG	BA	3252	1/1	0.97	0.07	38,38,38,38	0
54	MG	BA	2977	1/1	0.97	0.09	33,33,33,33	0
54	MG	DA	2971	1/1	0.97	0.23	40,40,40,40	0
54	MG	BA	3047	1/1	0.97	0.08	41,41,41,41	0
54	MG	DA	3046	1/1	0.97	0.09	19,19,19,19	0
54	MG	DA	3731	1/1	0.97	0.07	67,67,67,67	0
54	MG	BA	3504	1/1	0.97	0.04	115,115,115,115	0
54	MG	DA	2975	1/1	0.97	0.09	35,35,35,35	0
54	MG	AA	1787	1/1	0.97	0.05	65,65,65,65	0
54	MG	AA	1626	1/1	0.97	0.09	55,55,55,55	0
54	MG	BA	3289	1/1	0.97	0.27	71,71,71,71	0
54	MG	DA	3458	1/1	0.97	0.05	71,71,71,71	0
54	MG	DA	3052	1/1	0.97	0.04	42,42,42,42	0
54	MG	CA	1677	1/1	0.97	0.16	57,57,57,57	0
54	MG	BA	2919	1/1	0.97	0.13	29,29,29,29	0
54	MG	BA	3171	1/1	0.97	0.04	50,50,50,50	0
54	MG	DA	3129	1/1	0.97	0.12	57,57,57,57	0
54	MG	DE	303	1/1	0.97	0.07	20,20,20,20	0
54	MG	AA	1815	1/1	0.97	0.09	62,62,62,62	0
54	MG	BA	3096	1/1	0.97	0.08	37,37,37,37	0
54	MG	BA	3329	1/1	0.97	0.06	69,69,69,69	0
54	MG	BA	3330	1/1	0.97	0.04	62,62,62,62	0
54	MG	DA	2916	1/1	0.97	0.17	35,35,35,35	0
54	MG	DA	3062	1/1	0.97	0.18	50,50,50,50	0
54	MG	DA	3561	1/1	0.97	0.23	59,59,59,59	0
54	MG	DA	3300	1/1	0.97	0.06	28,28,28,28	0
54	MG	BA	3148	1/1	0.97	0.06	42,42,42,42	0
54	MG	DA	3564	1/1	0.97	0.09	49,49,49,49	0
54	MG	CA	1685	1/1	0.97	0.04	59,59,59,59	0
54	MG	BA	3262	1/1	0.97	0.04	58,58,58,58	0
54	MG	DA	3140	1/1	0.97	0.05	26,26,26,26	0
54	MG	CA	1687	1/1	0.97	0.06	76,76,76,76	0
54	MG	CA	1640	1/1	0.97	0.05	53,53,53,53	0
54	MG	BA	3439	1/1	0.97	0.16	73,73,73,73	0
54	MG	DA	2925	1/1	0.97	0.25	38,38,38,38	0
54	MG	AA	1880	1/1	0.97	0.04	80,80,80,80	0
54	MG	BA	3098	1/1	0.97	0.21	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3147	1/1	0.97	0.08	42,42,42,42	0
54	MG	DA	2928	1/1	0.97	0.20	32,32,32,32	0
54	MG	CA	1692	1/1	0.97	0.08	79,79,79,79	0
54	MG	DA	3150	1/1	0.97	0.22	54,54,54,54	0
54	MG	DA	3486	1/1	0.97	0.06	90,90,90,90	0
54	MG	CA	1693	1/1	0.97	0.04	64,64,64,64	0
54	MG	DA	2931	1/1	0.97	0.20	24,24,24,24	0
54	MG	DA	3233	1/1	0.97	0.18	51,51,51,51	0
54	MG	BA	3480	1/1	0.97	0.05	87,87,87,87	0
54	MG	AA	1784	1/1	0.97	0.05	76,76,76,76	0
54	MG	DA	2934	1/1	0.97	0.10	22,22,22,22	0
54	MG	BA	3234	1/1	0.97	0.05	42,42,42,42	0
54	MG	DA	3776	1/1	0.97	0.06	71,71,71,71	0
54	MG	AA	1718	1/1	0.97	0.05	63,63,63,63	0
54	MG	DA	3158	1/1	0.97	0.10	62,62,62,62	0
54	MG	DA	3779	1/1	0.97	0.07	72,72,72,72	0
54	MG	DA	2937	1/1	0.97	0.15	25,25,25,25	0
54	MG	DA	3497	1/1	0.97	0.04	68,68,68,68	0
54	MG	BA	2999	1/1	0.97	0.10	27,27,27,27	0
54	MG	CD	101	1/1	0.97	0.08	53,53,53,53	0
54	MG	DA	3500	1/1	0.97	0.04	60,60,60,60	0
54	MG	BA	3017	1/1	0.97	0.21	48,48,48,48	0
54	MG	BA	3001	1/1	0.97	0.14	40,40,40,40	0
54	MG	BA	3566	1/1	0.97	0.06	56,56,56,56	0
54	MG	BA	2985	1/1	0.97	0.04	46,46,46,46	0
54	MG	BA	3527	1/1	0.97	0.07	63,63,63,63	0
54	MG	DA	3248	1/1	0.97	0.15	56,56,56,56	0
54	MG	CA	1654	1/1	0.97	0.07	80,80,80,80	0
54	MG	BA	3210	1/1	0.97	0.05	54,54,54,54	0
54	MG	DA	3572	1/1	0.98	0.05	60,60,60,60	0
54	MG	CA	1856	1/1	0.98	0.03	74,74,74,74	0
54	MG	AA	1660	1/1	0.98	0.06	60,60,60,60	0
54	MG	DA	2983	1/1	0.98	0.29	34,34,34,34	0
54	MG	DA	3254	1/1	0.98	0.08	38,38,38,38	0
54	MG	CA	1914	1/1	0.98	0.07	36,36,36,36	0
54	MG	BE	303	1/1	0.98	0.11	45,45,45,45	0
54	MG	BA	3133	1/1	0.98	0.18	49,49,49,49	0
54	MG	BA	3042	1/1	0.98	0.04	28,28,28,28	0
54	MG	BA	3312	1/1	0.98	0.05	75,75,75,75	0
54	MG	BA	2990	1/1	0.98	0.11	48,48,48,48	0
54	MG	DA	3485	1/1	0.98	0.04	56,56,56,56	0
54	MG	DA	3687	1/1	0.98	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3139	1/1	0.98	0.10	33,33,33,33	0
54	MG	DA	2921	1/1	0.98	0.04	32,32,32,32	0
54	MG	BA	2934	1/1	0.98	0.28	42,42,42,42	0
54	MG	CA	1713	1/1	0.98	0.13	53,53,53,53	0
54	MG	BA	3219	1/1	0.98	0.04	48,48,48,48	0
54	MG	D0	201	1/1	0.98	0.10	38,38,38,38	0
54	MG	BA	3091	1/1	0.98	0.10	59,59,59,59	0
54	MG	BA	2940	1/1	0.98	0.19	27,27,27,27	0
54	MG	DA	3312	1/1	0.98	0.07	51,51,51,51	0
54	MG	BA	3108	1/1	0.98	0.06	41,41,41,41	0
54	MG	DA	2961	1/1	0.98	0.07	37,37,37,37	0
54	MG	BA	3093	1/1	0.98	0.07	65,65,65,65	0
54	MG	DA	3646	1/1	0.98	0.07	87,87,87,87	0
54	MG	BA	2914	1/1	0.98	0.12	17,17,17,17	0
54	MG	DA	3001	1/1	0.98	0.19	46,46,46,46	0
54	MG	BA	2975	1/1	0.98	0.17	40,40,40,40	0
54	MG	DA	3407	1/1	0.98	0.04	41,41,41,41	0
54	MG	D1	206	1/1	0.98	0.07	66,66,66,66	0
54	MG	DA	3757	1/1	0.98	0.06	54,54,54,54	0
54	MG	AA	1952	1/1	0.98	0.03	76,76,76,76	0
54	MG	DA	3077	1/1	0.98	0.20	48,48,48,48	0
54	MG	CA	1900	1/1	0.98	0.04	50,50,50,50	0
54	MG	BA	3192	1/1	0.98	0.04	54,54,54,54	0
54	MG	CA	1902	1/1	0.98	0.06	46,46,46,46	0
54	MG	DA	3604	1/1	0.98	0.05	43,43,43,43	0
54	MG	BA	3452	1/1	0.98	0.03	57,57,57,57	0
54	MG	DA	3280	1/1	0.98	0.06	33,33,33,33	0
54	MG	BA	3303	1/1	0.98	0.09	41,41,41,41	0
54	MG	BA	3265	1/1	0.98	0.06	40,40,40,40	0
54	MG	DA	3160	1/1	0.98	0.03	48,48,48,48	0
54	MG	DA	2972	1/1	0.98	0.27	41,41,41,41	0
54	MG	BA	2968	1/1	0.98	0.05	29,29,29,29	0
54	MG	DA	3286	1/1	0.98	0.26	58,58,58,58	0
54	MG	BA	3072	1/1	0.98	0.03	48,48,48,48	0
54	MG	AA	1974	1/1	0.98	0.12	96,96,96,96	0
54	MG	DA	2976	1/1	0.98	0.19	31,31,31,31	0
54	MG	CA	1827	1/1	0.98	0.04	100,100,100,100	0
54	MG	BA	2962	1/1	0.98	0.09	20,20,20,20	0
54	MG	DA	3426	1/1	0.98	0.09	39,39,39,39	0
54	MG	DA	3209	1/1	0.98	0.06	57,57,57,57	0
54	MG	DA	3521	1/1	0.98	0.04	75,75,75,75	0
54	MG	CA	1778	1/1	0.98	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	ZN	AG	301	1/1	0.98	0.16	82,82,82,82	0
55	ZN	CQ	104	1/1	0.98	0.03	142,142,142,142	0
54	MG	AA	1961	1/1	0.99	0.04	46,46,46,46	0
54	MG	DA	3180	1/1	0.99	0.03	102,102,102,102	0
54	MG	DA	3309	1/1	0.99	0.03	20,20,20,20	0
54	MG	BA	3040	1/1	0.99	0.07	40,40,40,40	0
54	MG	DA	3659	1/1	0.99	0.04	52,52,52,52	0
54	MG	BA	3000	1/1	0.99	0.07	25,25,25,25	0
54	MG	BA	3326	1/1	0.99	0.04	54,54,54,54	0
54	MG	DA	3702	1/1	0.99	0.04	22,22,22,22	0
54	MG	DA	3623	1/1	0.99	0.02	81,81,81,81	0
54	MG	DA	3767	1/1	0.99	0.04	61,61,61,61	0
54	MG	DA	2986	1/1	0.99	0.04	42,42,42,42	0
54	MG	DA	3552	1/1	0.99	0.04	130,130,130,130	0
54	MG	AA	2000	1/1	0.99	0.03	38,38,38,38	0
54	MG	DD	303	1/1	0.99	0.13	43,43,43,43	0
54	MG	DA	3053	1/1	0.99	0.04	28,28,28,28	0
54	MG	DA	2923	1/1	0.99	0.08	18,18,18,18	0
54	MG	DA	2954	1/1	0.99	0.03	16,16,16,16	0
54	MG	DA	2977	1/1	0.99	0.02	32,32,32,32	0
54	MG	BA	3236	1/1	0.99	0.09	33,33,33,33	0
54	MG	BA	3425	1/1	0.99	0.02	98,98,98,98	0
54	MG	AA	1943	1/1	0.99	0.06	83,83,83,83	0
54	MG	BA	3099	1/1	0.99	0.03	42,42,42,42	0
55	ZN	AQ	102	1/1	0.99	0.04	142,142,142,142	0
55	ZN	CG	302	1/1	0.99	0.15	94,94,94,94	0
54	MG	DA	3117	1/1	0.99	0.07	48,48,48,48	0
54	MG	DA	3166	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.