



# wwPDB X-ray Structure Validation Summary Report i

Jun 17, 2014 – 02:32 AM BST

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

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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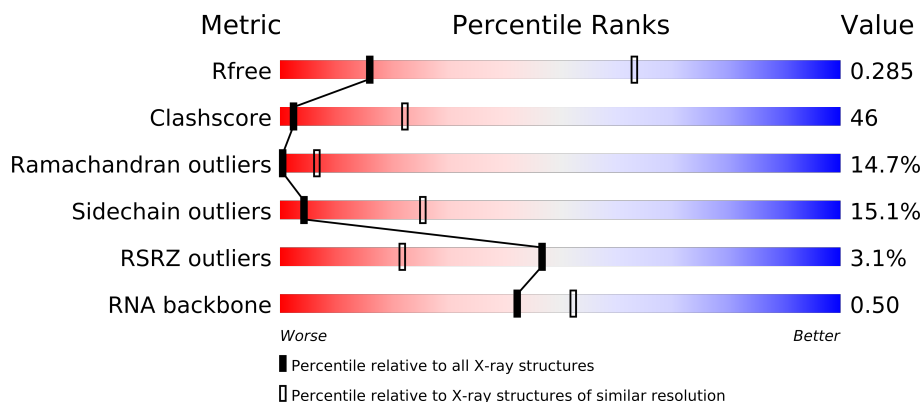
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1517	
1	CA	1517	
2	AE	256	
2	CE	256	
3	AF	239	
3	CF	239	
4	AG	209	
4	CG	209	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	

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Mol	Chain	Length	Quality of chain
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	
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	CC	77	
22	CD	77	
23	A1	25	
23	C1	25	
24	BA	2885	
25	BB	122	
26	BD	276	
26	DD	276	
27	BE	206	
27	DE	206	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
49	B4	71	<div><div></div></div>
49	D4	71	<div><div></div></div>
50	B5	60	<div><div></div></div>
50	D5	60	<div><div></div></div>
51	B6	54	<div><div></div></div>
51	D6	54	<div><div></div></div>
52	B7	49	<div><div></div></div>
52	D7	49	<div><div></div></div>
53	B8	65	<div><div></div></div>
53	D8	65	<div><div></div></div>
54	DA	2898	<div><div></div></div>
55	DB	120	<div><div></div></div>

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298428 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

- 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			

There are 19 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

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	G	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	?	-	C	DELETION	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1

- 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			

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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				
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	0	0	0
			469	298	90	81			
48	DX	59	Total	C	N	O	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			
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 a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DA	2886	Total	C	N	O	P	0	0	0
			62151	27664	11620	19982	2885			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 55 is a RNA chain called 5S ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AP	1	Total	Mg	0	0
			1	1		
56	CR	1	Total	Mg	0	0
			1	1		
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	683	Total	Mg	0	0
			683	683		
56	AK	1	Total	Mg	0	0
			1	1		
56	CH	2	Total	Mg	0	0
			2	2		
56	DF	1	Total	Mg	0	0
			1	1		
56	B8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	7	Total 7	Mg 7	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	6	Total 6	Mg 6	0	0
56	B1	1	Total 1	Mg 1	0	0
56	C1	1	Total 1	Mg 1	0	0
56	CD	26	Total 26	Mg 26	0	0
56	DZ	2	Total 2	Mg 2	0	0
56	AX	1	Total 1	Mg 1	0	0
56	D6	2	Total 2	Mg 2	0	0
56	AS	2	Total 2	Mg 2	0	0
56	CA	383	Total 383	Mg 383	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	26	Total 26	Mg 26	0	0
56	AJ	1	Total 1	Mg 1	0	0
56	BT	2	Total 2	Mg 2	0	0
56	CC	13	Total 13	Mg 13	0	0
56	DB	29	Total 29	Mg 29	0	0
56	D3	4	Total 4	Mg 4	0	0
56	BF	2	Total 2	Mg 2	0	0
56	DR	2	Total 2	Mg 2	0	0
56	DA	905	Total 905	Mg 905	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	439	Total 439	Mg 439	0	0
56	BQ	1	Total 1	Mg 1	0	0
56	CQ	3	Total 3	Mg 3	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	B6	1	Total 1	Mg 1	0	0
56	CG	1	Total 1	Mg 1	0	0
56	BU	5	Total 5	Mg 5	0	0
56	A1	2	Total 2	Mg 2	0	0
56	AD	3	Total 3	Mg 3	0	0
56	DD	3	Total 3	Mg 3	0	0
56	CT	1	Total 1	Mg 1	0	0
56	DH	4	Total 4	Mg 4	0	0
56	D0	5	Total 5	Mg 5	0	0
56	BG	1	Total 1	Mg 1	0	0
56	AI	1	Total 1	Mg 1	0	0
56	DS	1	Total 1	Mg 1	0	0
56	DE	3	Total 3	Mg 3	0	0
56	B3	2	Total 2	Mg 2	0	0
56	BR	2	Total 2	Mg 2	0	0
56	CP	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BK	1	Total 1	Mg 1	0	0
56	DW	2	Total 2	Mg 2	0	0
56	D2	1	Total 1	Mg 1	0	0
56	AL	2	Total 2	Mg 2	0	0
56	CM	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	D1	6	Total 6	Mg 6	0	0
56	AH	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DO	5	Total 5	Mg 5	0	0
56	AC	8	Total 8	Mg 8	0	0
56	CW	5	Total 5	Mg 5	0	0
56	DG	3	Total 3	Mg 3	0	0
56	D5	1	Total 1	Mg 1	0	0
56	BD	2	Total 2	Mg 2	0	0
56	AT	2	Total 2	Mg 2	0	0
56	DT	2	Total 2	Mg 2	0	0
56	B0	2	Total 2	Mg 2	0	0
56	AO	1	Total 1	Mg 1	0	0
56	BW	1	Total 1	Mg 1	0	0

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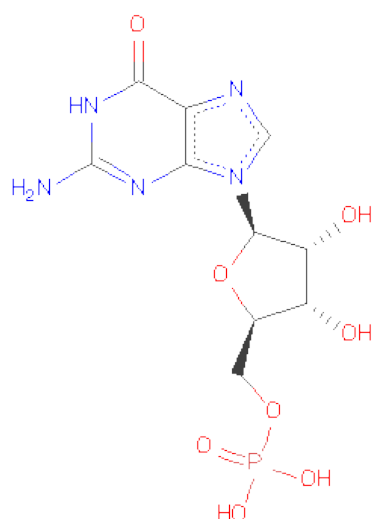
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CS	2	Total	Mg	0	0
			2	2		
56	CK	2	Total	Mg	0	0
			2	2		
56	CL	1	Total	Mg	0	0
			1	1		
56	BH	1	Total	Mg	0	0
			1	1		

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

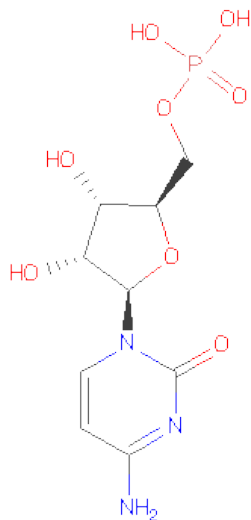
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CQ	1	Total	Zn	0	0
			1	1		
57	AG	1	Total	Zn	0	0
			1	1		
57	AA	2	Total	Zn	0	0
			2	2		
57	AQ	1	Total	Zn	0	0
			1	1		
57	CG	1	Total	Zn	0	0
			1	1		

- Molecule 58 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	CA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	CA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	CA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	CP	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	CC	1	Total 20	C 10	N 5	O 5		0	0
58	CC	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	CC	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DA	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DP	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DP	1	Total 23	C 10	N 5	O 7	P 1	0	0
58	DP	1	Total 23	C 10	N 5	O 7	P 1	0	0

- Molecule 59 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula:  $C_9H_{14}N_3O_8P$ ).



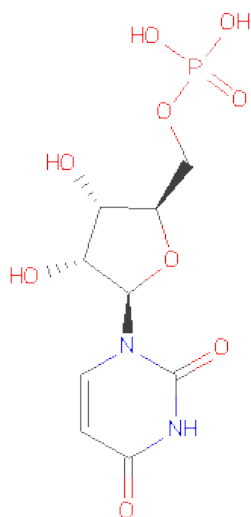
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	CA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CO	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CP	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CP	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CP	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CC	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CC	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	CC	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DA	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DP	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
59	DP	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 60 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula:  $C_9H_{13}N_2O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	CA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	C1	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

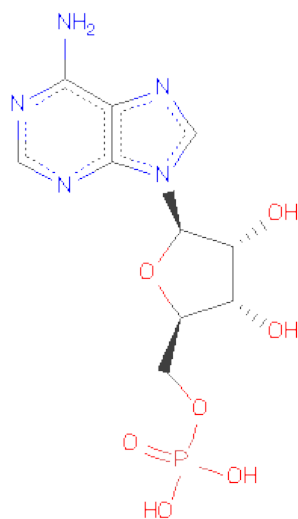
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DA	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
60	DP	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 61 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	CA	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
61	CC	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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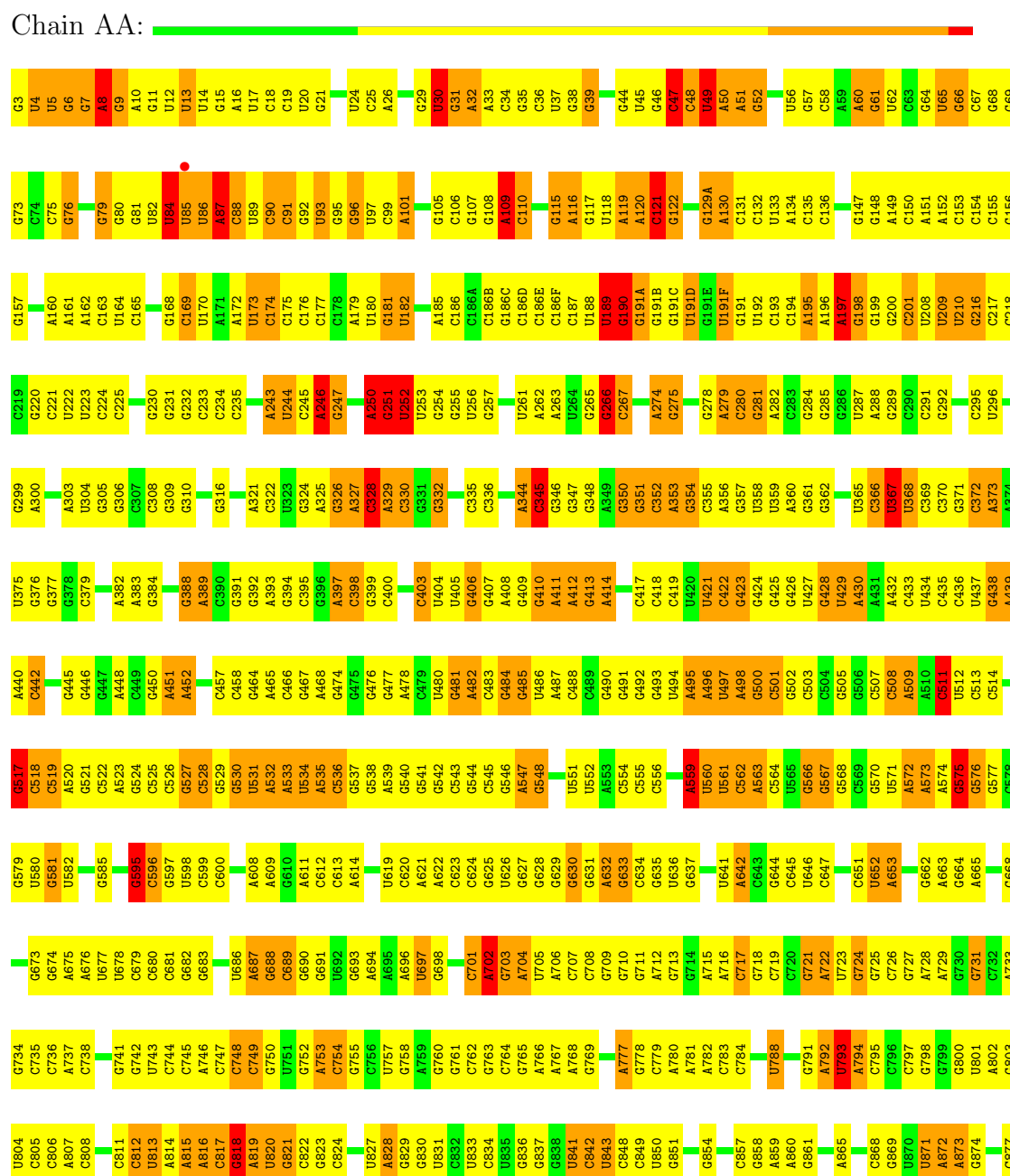
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	C1	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	C1	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0
61	DA	1	Total 22	C 10	N 5	O 6	P 1	0	0

### 3 Residue-property plots

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

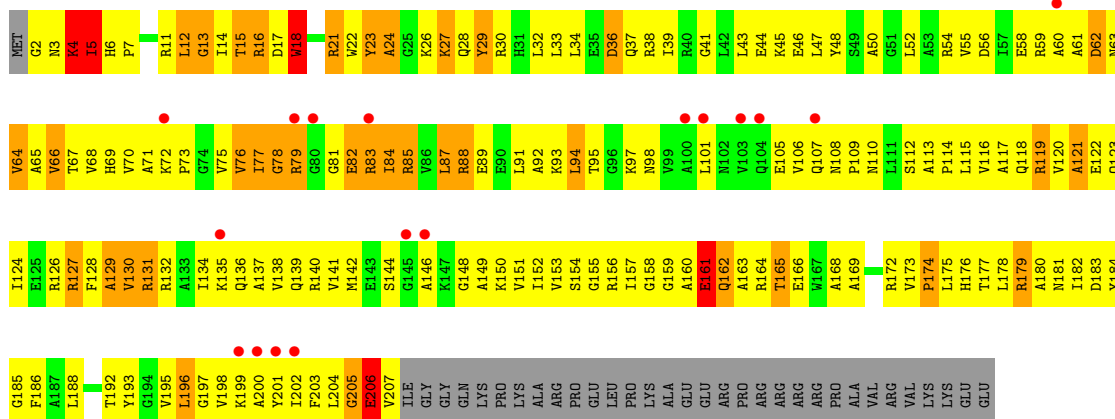
#### • Molecule 1: 16S RRNA (E.COLI NUMBERING)





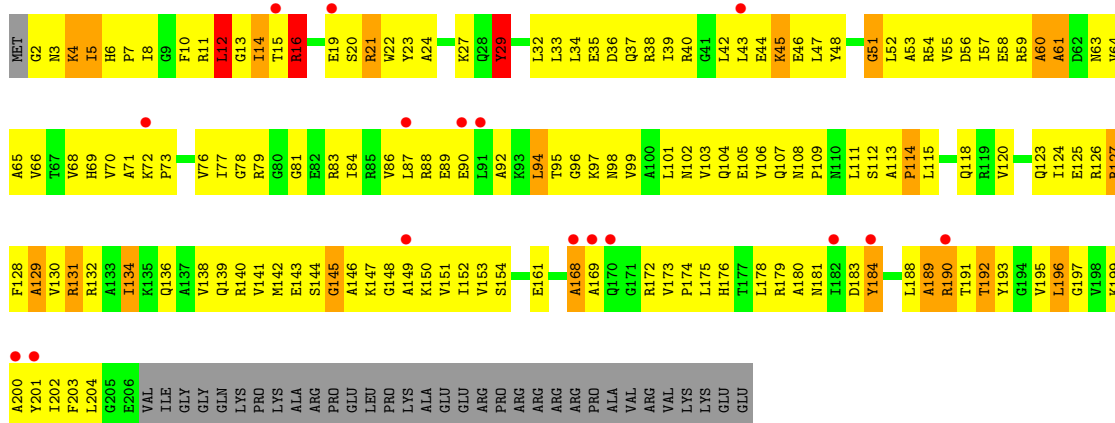






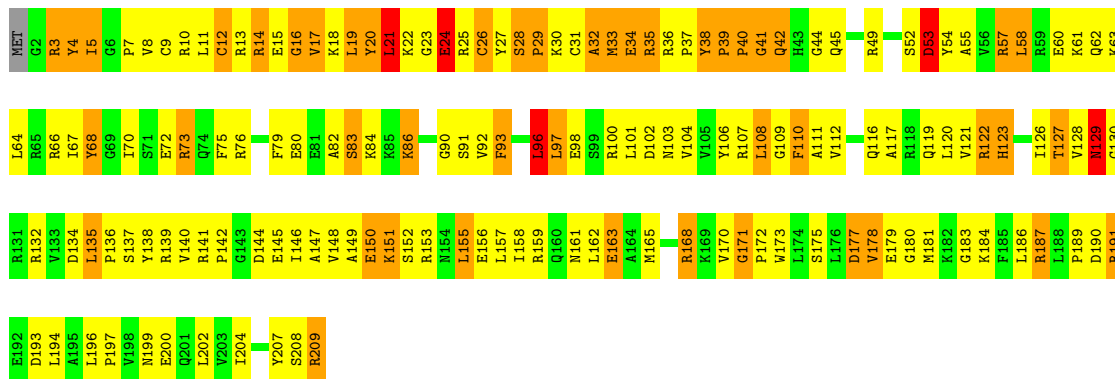
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



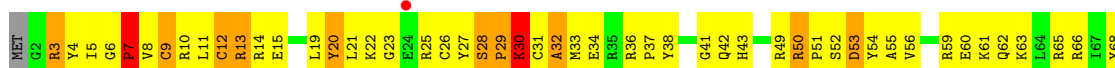
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

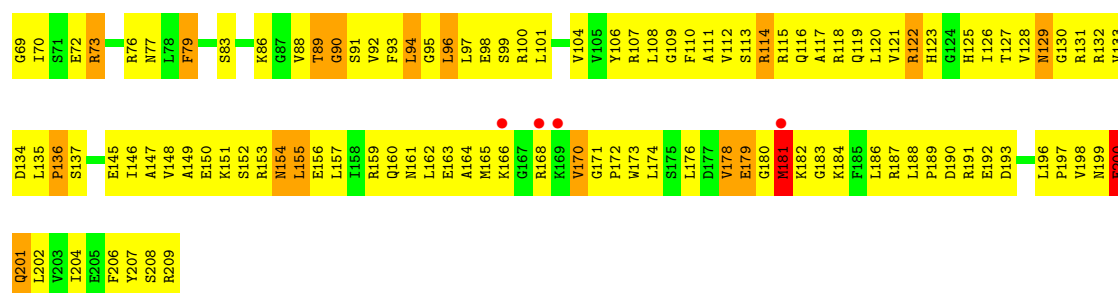
Chain AG:



### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

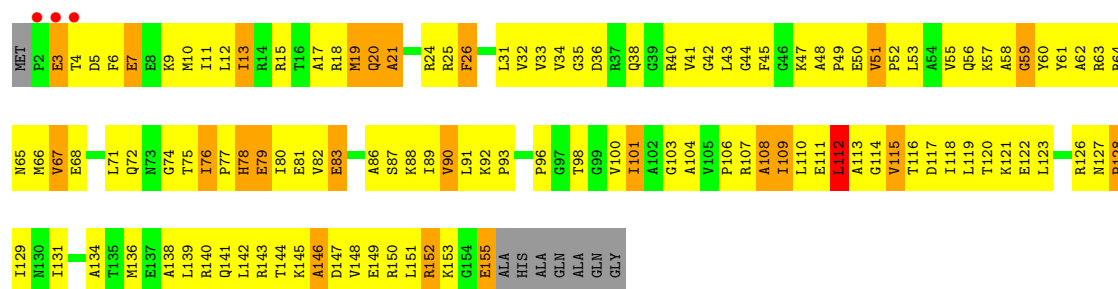
Chain CG:





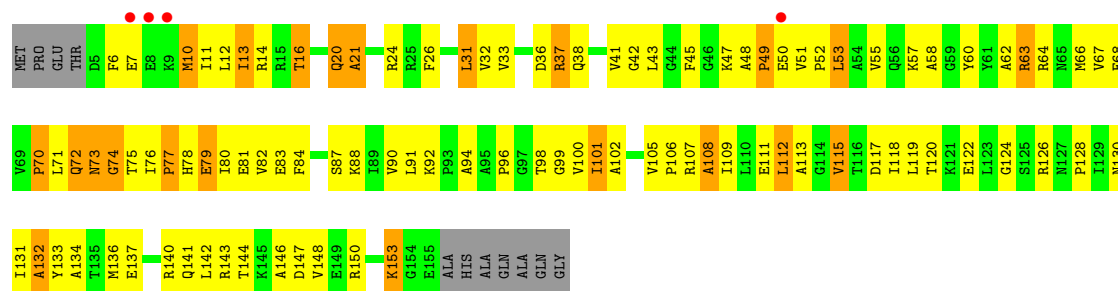
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



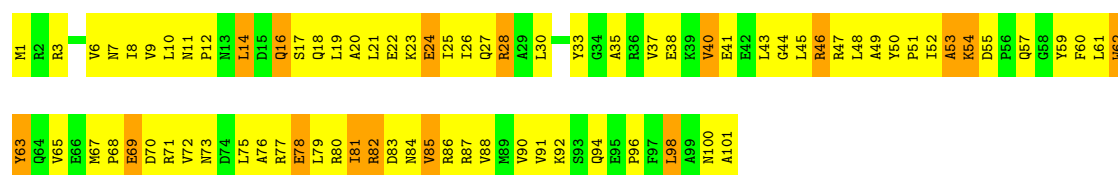
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:

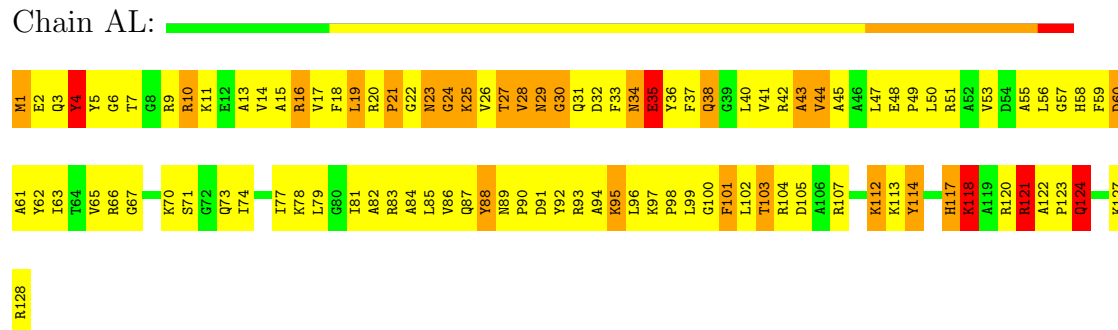






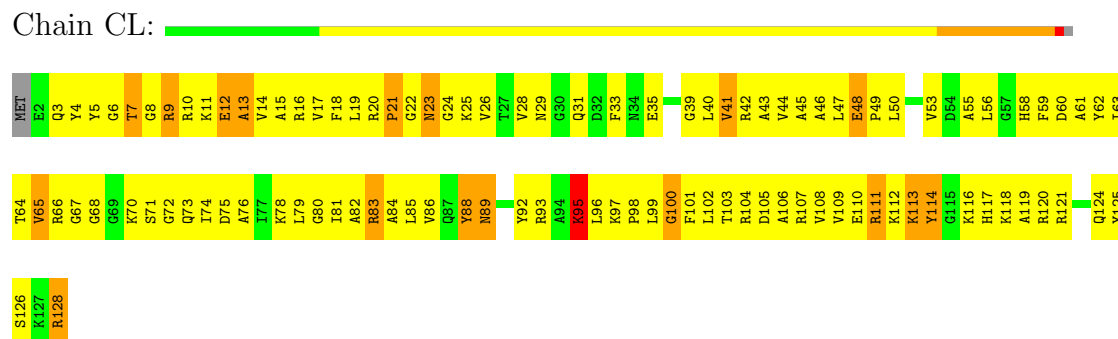
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



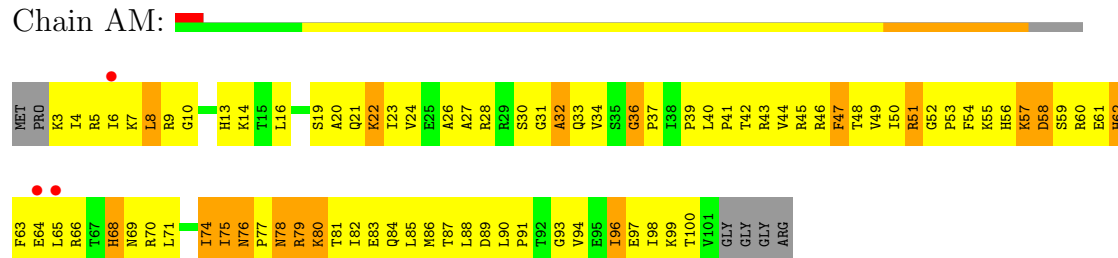
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



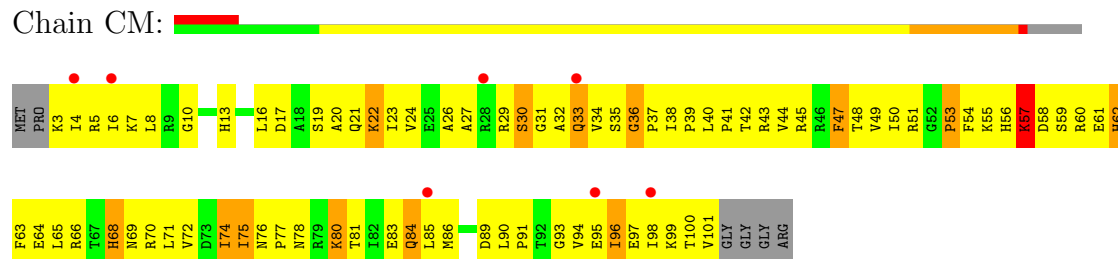
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



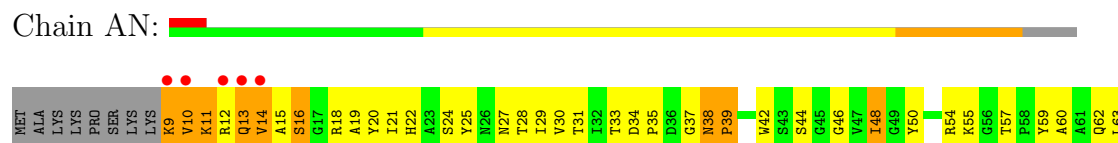
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

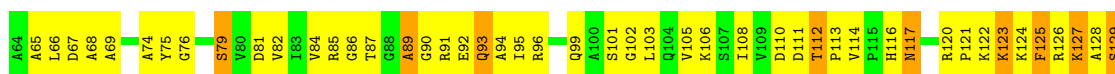
Chain CM:



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AN:





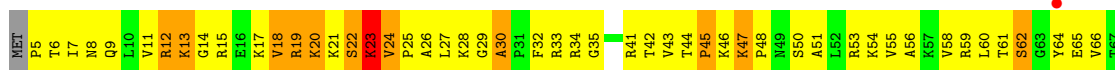
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN:



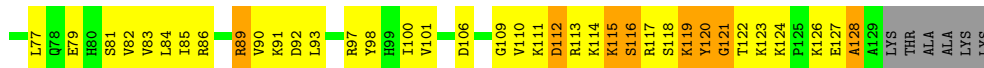
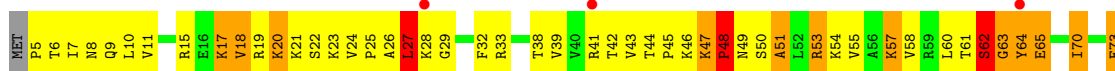
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO:



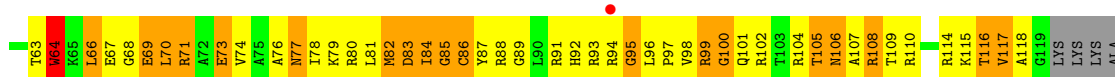
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



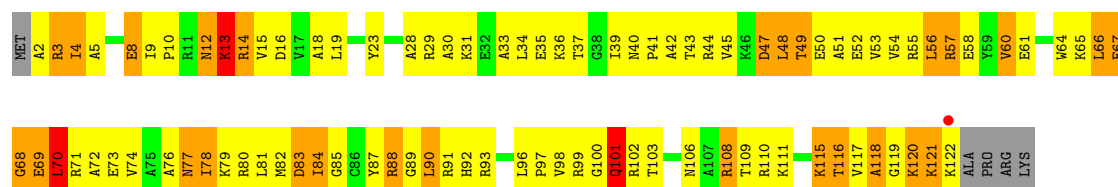
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AP:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



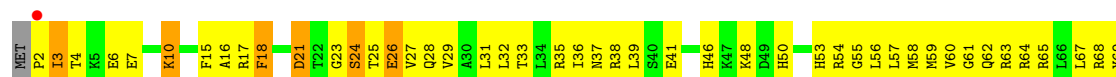
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



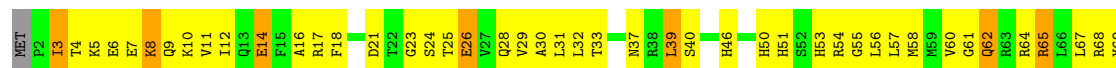
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



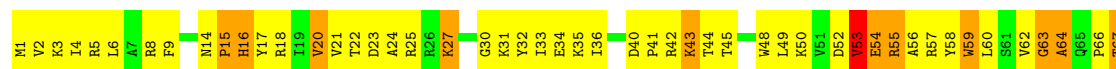
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:



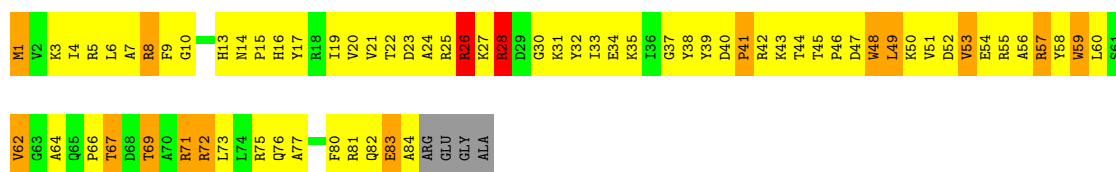
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:



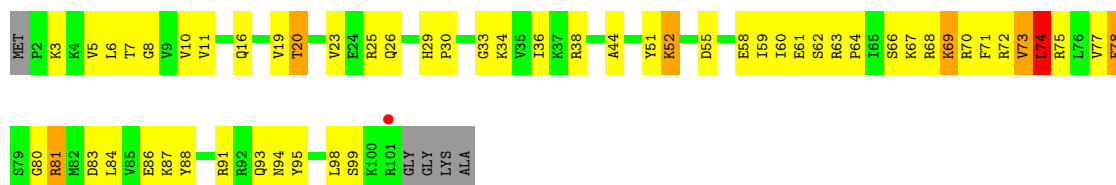
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:



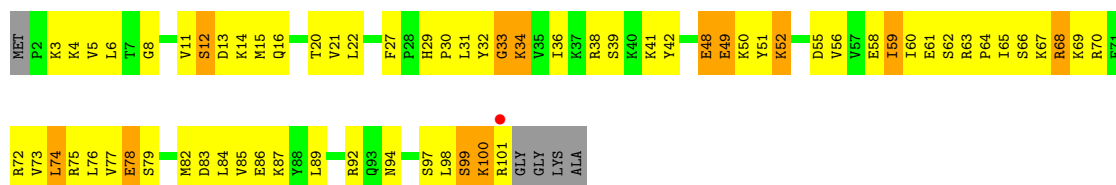
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



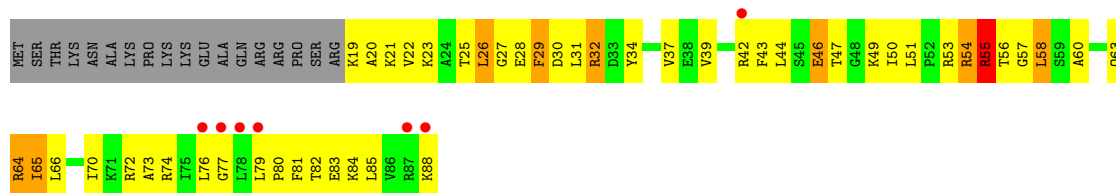
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

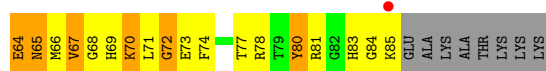
Chain CU:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

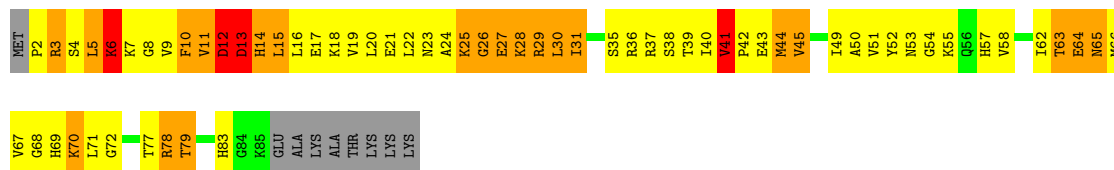
Chain AV:





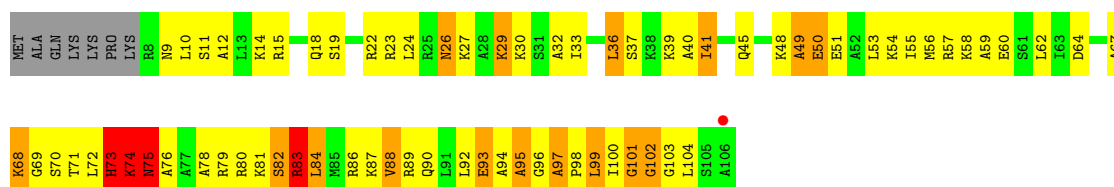
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



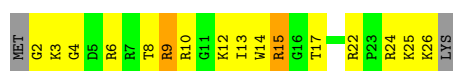
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



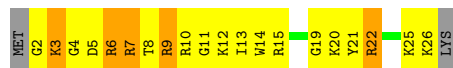
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



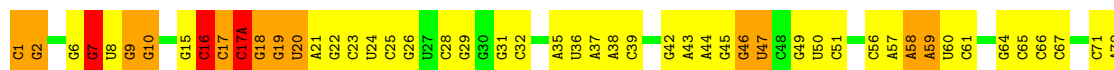
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



• Molecule 22: TRNA FMET (UNMODIFIED BASES)

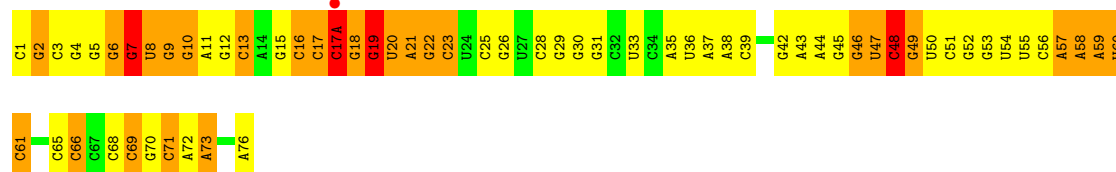
Chain AC:





- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain AD:



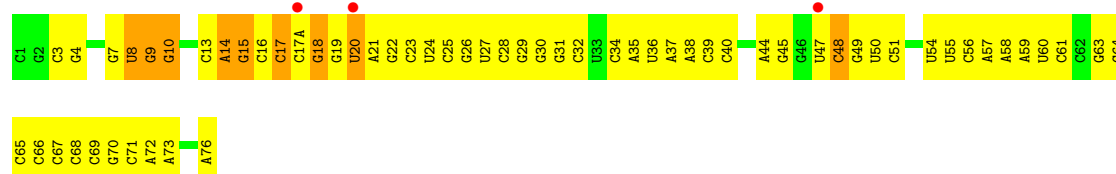
- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain CC:



- Molecule 22: TRNA FMET (UNMODIFIED BASES)

Chain CD:



- Molecule 23: MRNA

Chain A1:



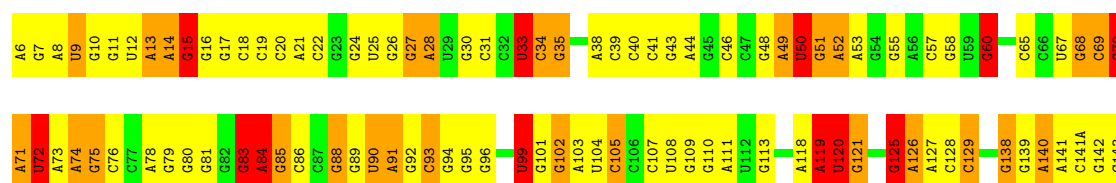
- Molecule 23: MRNA

Chain C1:



- Molecule 24: 23S ribosomal RNA

Chain BA:

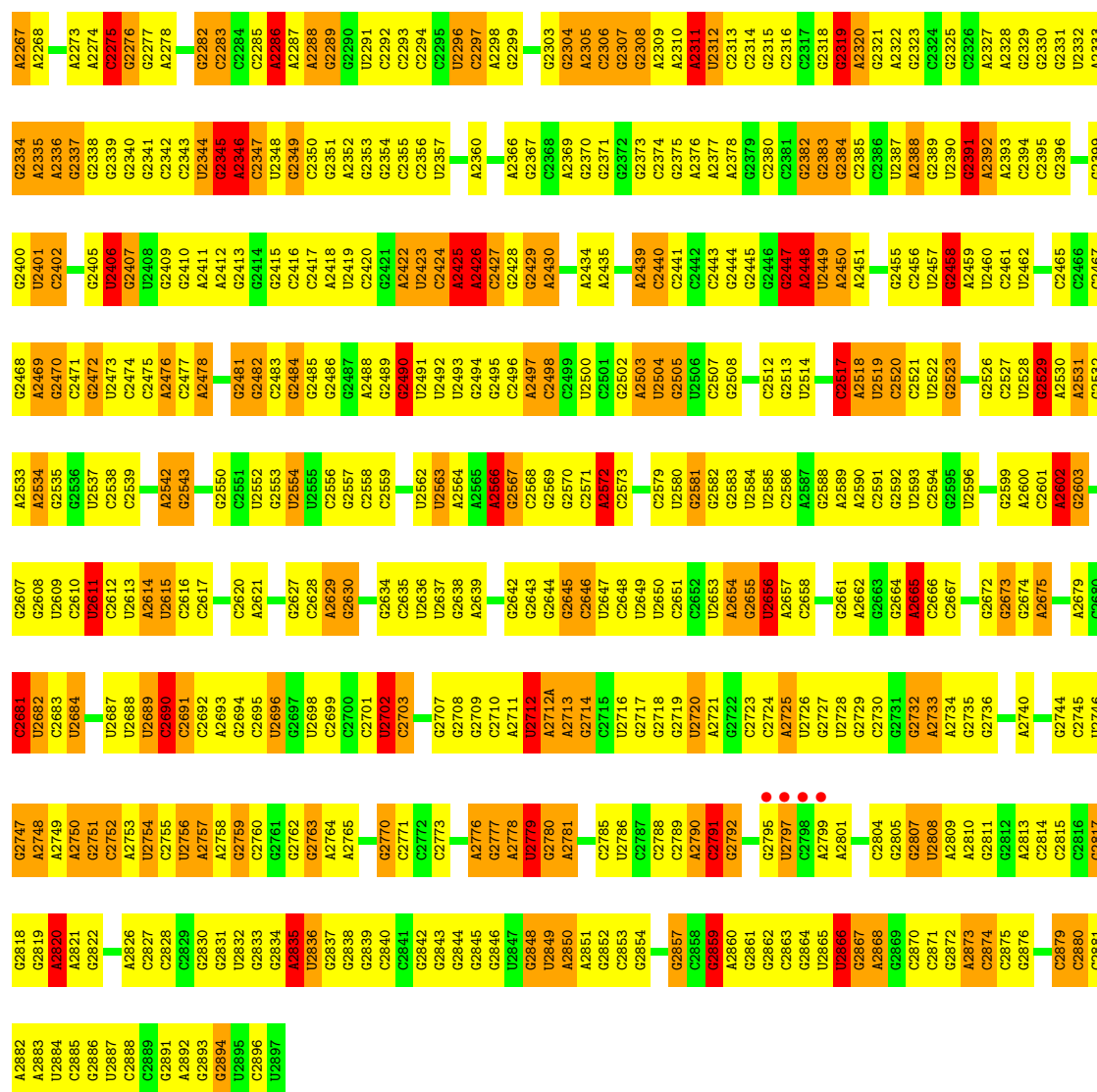


U1141	C1075	G1011	G739	C816	C672	G549	G474	A402	C328	U230	A149
U1142	C1076	U1012	G746	C817	C673	G550	U475	U403	A330	C231	C150
A1142A	A1077	U1013	A747	A818	A674	G551	G476	U404	A331	G232	C151
G1144	A1080	G1014	U747	A819	A675	U564	A477	U405	A332	A233	G152
G1145	U1081	G1015	A751	A820	A676	U565	A478	G406	G333	C234	G153
C1146	U1082	G1016	A752	U822	A677	U567	A479	G407	C334	U235	G154
C1147	U1083	G1017	A753	U823	C678	U568	A480	G408	C335	C236	C155
A1148	U1084	U1019	C754	C823	C679	G558	G481	G409	U339	U239	C156
G1149	A1085	A960	C755	A824	C680	G559	A482	G410	U339	U239	C156
C1150	U1086	C825	C756	C825	C681	C560	A483	G411	C273B	U239	C156
G1151	G1087	U826	C757	U826	G682	C561	A484	G412	C273C	G240	U162
C1152	U1088	U827	U757	U827	G683	U562	A485	C413	C273D	A241	G171
C1153	G1089	U828	U757	U828	G684	C563	C486	C414	U273E	G242	C172
G1154	U1090	A829	U762	A829	A685	C564	C487	A415	C273F	U243	G173
A1155	G1091	G830	G763	G830	G686	C565	G488	A416	G273A	G247	C174
C1156	C1092	G831	A764	G831	C687	U566	U489	C417	C273B	G248	G177
G1157	G1093	G832	G765	C832	C688	U567	U490	A422	C273C	C249	G178
U1158	U1094	U833	G766	U833	G689	U568	G493	A423	C273D	G250	G179
A1095	A1096	C834	G770	C834	C690	U569	G500	G424	C273E	A251	G180
A1096	U1097	A835	A774	A835	C691	G570	G501	G425	A283	G252	U185
U1097	G1098	U836	G775	U836	C692	A571	A501	G426	C292	G259	G189
A1098	C1099	G837	G776	C837	C693	C580	A502	U427	C292	G260	G194
G1099	C974A	U838	G777	A838	U694	C581	A503	A363A	C301	A261	A195
C1100	G975	G839	A778	G839	U695	C582	U504	A428	C302	G262	A196
U1101	C976	G840	G779	G840	C696	C583	U505	A429	C303	C263	A197
C1102	G977	G841	G780	G841	C697	C584	G506	G430	C304	C264	C198
C1103	G978	G842	A781	G842	C698	C585	A507	U431	C305	A265	A199
G1104	G979	G843	A782	A843	C699	C586	A508	U432	C306	G266	U200
U1105	C974A	A844	A783	U844	C700	C587	A509	U433	C307	C267	C208
C1106	G975	G845	A784	G845	C701	C588	U510	C435	C308	C270C	C209
U1107	C976	G846	G785	G846	C702	C589	U511	U436	C309	G270D	C210
C1108	G977	G847	G786	G847	C703	C590	U512	G440	A310	G270E	A211
G1109	A1064	U848	A787	U848	U703	C591	A513	U441	A311	U270F	G212
A1111	U1046	G849	A788	G849	U704	C592	A514	G442	A312	C270G	A213
C1112	G1047	A849	A789	U850	G705	C593	A515	G443	A313	C270H	G214
G1113	A1048	G852	C790	U851	A706	C594	U516	C444	A314	G270I	G215
C1114	C1049	G853	C791	U852	A707	C595	U517	G445	A315	G270J	A216
G1115	A1050	G854	C792	U853	A708	C596	U518	G446	A316	C270K	G217
C1116	C1053	A861	G793	U854	U709	C597	A519	U447	C316	U270L	A218
G1117	A1054	G862	A794	G862	U710	C598	U520	U448	C317	G270M	A221
U1188	G1055	C863	C795	A863	A711	C599	U521	U449	A318	U270N	A222
C1121	G1056	C864	C796	C864	A712	C601	A522	A454	A319	G270O	A223
G1124	G1059	C865	C797	A865	A713	C602	A523	C455	A320	C270P	G224
G1125	U1060	C866	U797	A866	C719	C603	A524	C456	A321	G270Q	A225
A1126	U1061	U868	A800	G868	C720	C604	A525	C457	A322	C270R	G226
A1127	G1062	C869	A801	C869	A721	C605	A526	G458	A323	G270S	A227
A1128	U1063	A870	A802	U870	G722	C606	A527	U459	A324	C270T	A228
A1129	G1064	U871	A803	U871	G723	C607	A528	G463	A325	G270U	G229
U1130	U1065	A872	A804	C872	U724	C608	A529	U464	A326	C270V	A229
G1131	U1066	G873	G805	G873	G725	C609	A530	U465	A327	U270W	
A1132	A1067	G874	C806	G874	A726	C610	A531	G466	A328	G270X	
U1133	G1068	G875	U807	C875	G727	C611	A532	A467	A329	C270Y	
C1135	A1069	C876	G808	C876	G728	C612	A533	G468	A330	G270Z	
G1136	U1070	U877	U813	U877	G729	C613	A534	U469	A331	C270A	
G1137	G1071	A878	C812	G878	C730	C614	U535	A470	A332	G270B	
G1138	C1072	G879	C813	C879	U735	C615	U536	A471	A333	C270C	
U1205	A1073	G880	U814	G880	A736	C616	A537	A472	A334	G270D	
G1206	G1074	G881	C814	G881	C737	C617	A538	A473	A335	C270E	
		G882	C815	G882	G738						



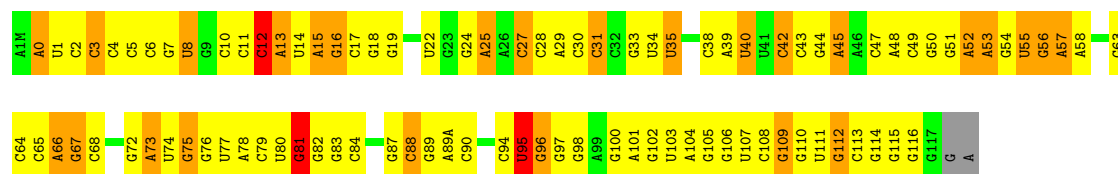


WORLD WIDE  
PDB  
PROTEIN DATA BANK



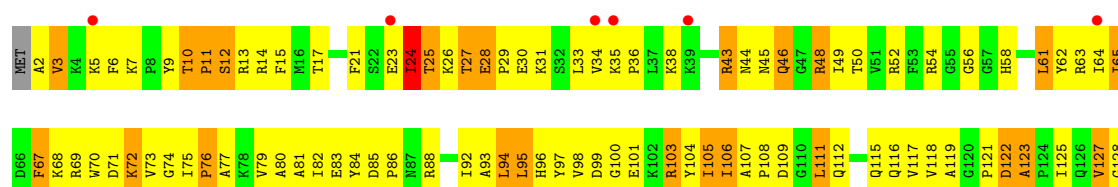
### • Molecule 25: 5S ribosomal RNA

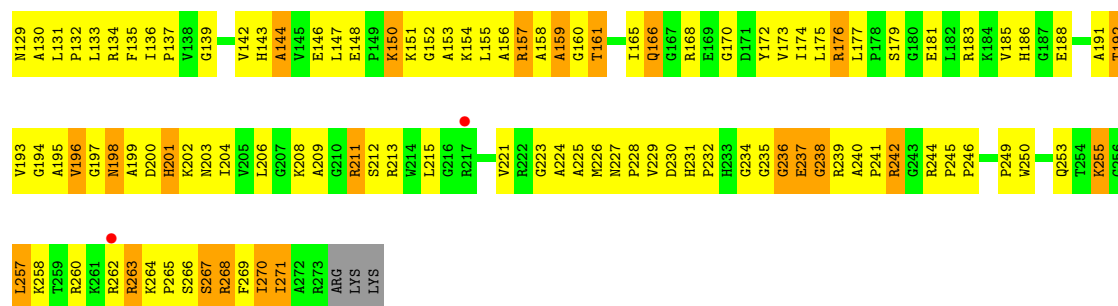
Chain BB:



### • Molecule 26: 50S ribosomal protein L2

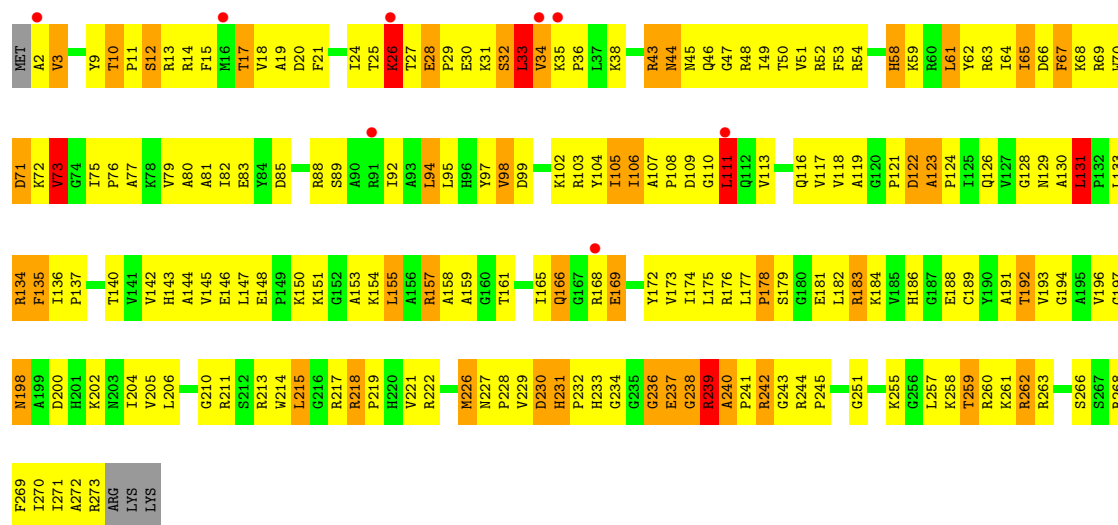
Chain BD:





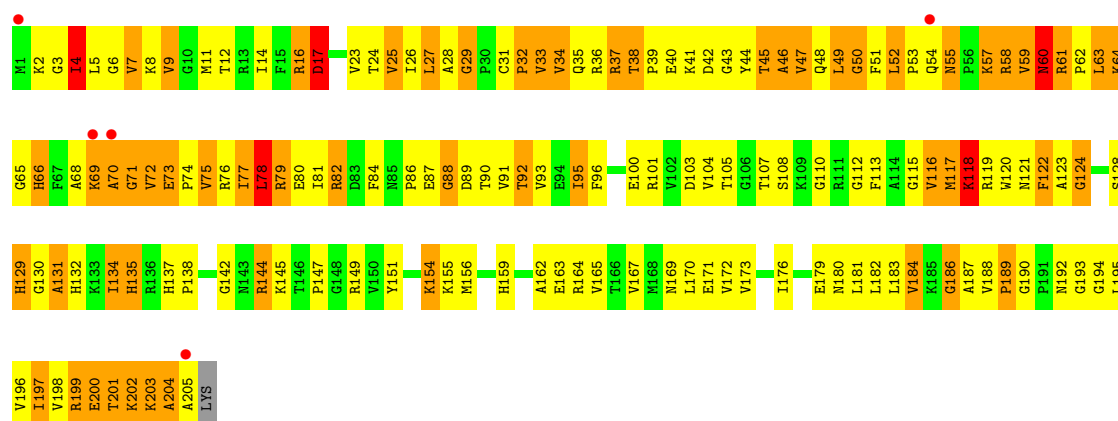
• Molecule 26: 50S ribosomal protein L2

Chain DD:



• Molecule 27: 50S ribosomal protein L3

Chain BE:



• Molecule 27: 50S ribosomal protein L3

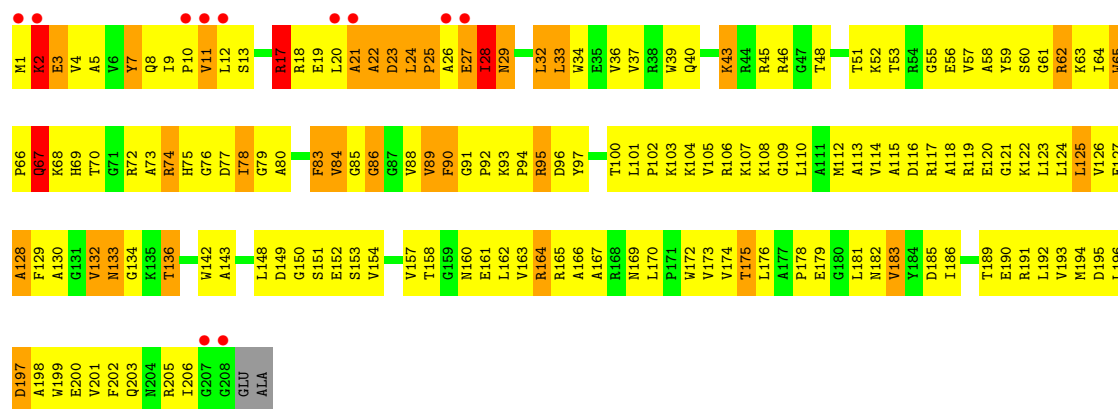
Chain DE:





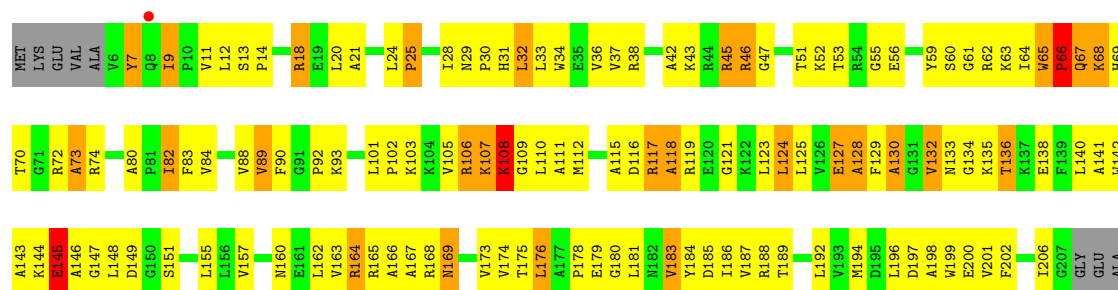
• Molecule 28: 50S ribosomal protein L4

Chain BF:



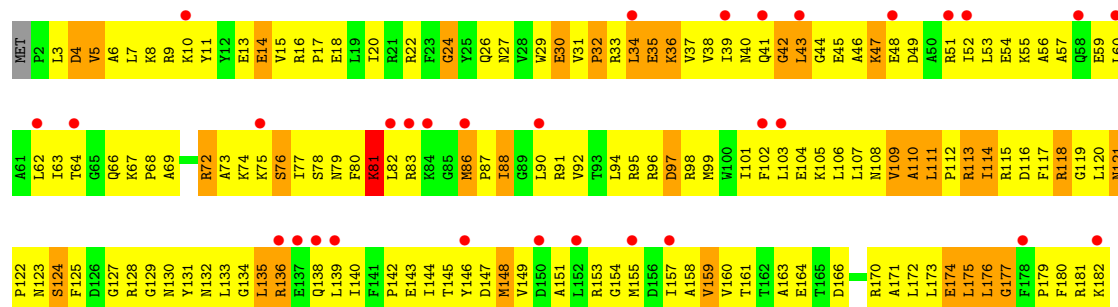
• Molecule 28: 50S ribosomal protein L4

Chain DF:



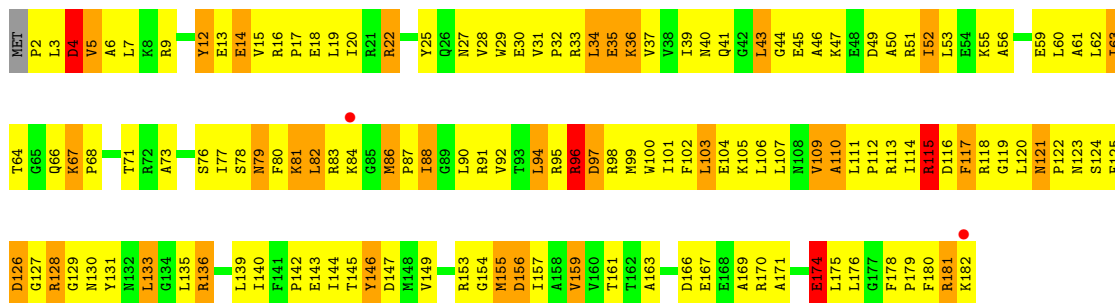
• Molecule 29: 50S ribosomal protein L5

Chain BG:



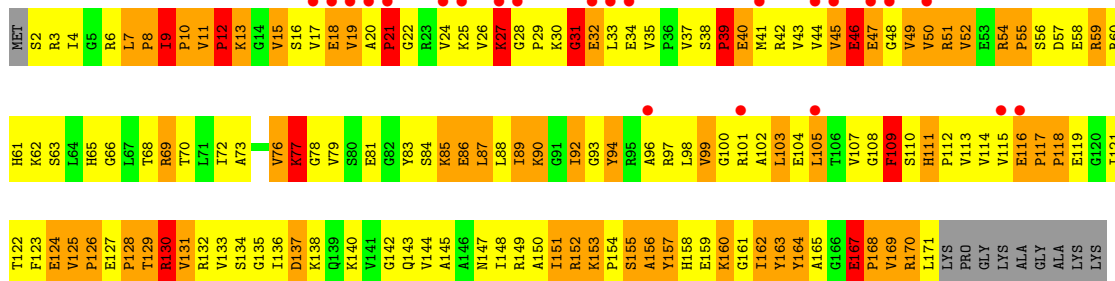
● Molecule 29: 50S ribosomal protein L5

Chain DG: 



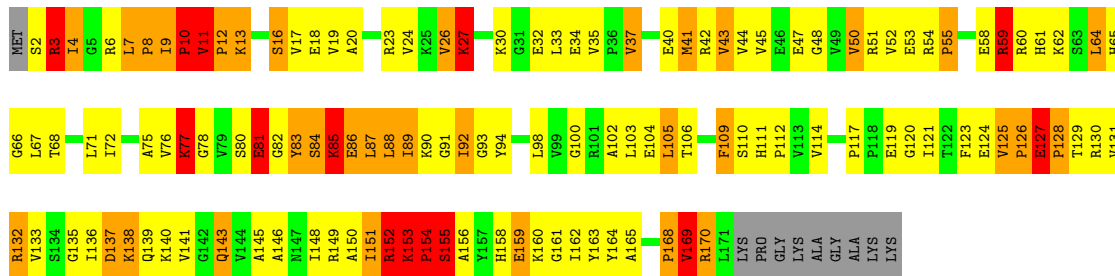
● Molecule 30: 50S ribosomal protein L6

Chain BH: 



● Molecule 30: 50S ribosomal protein L6

Chain DH: 

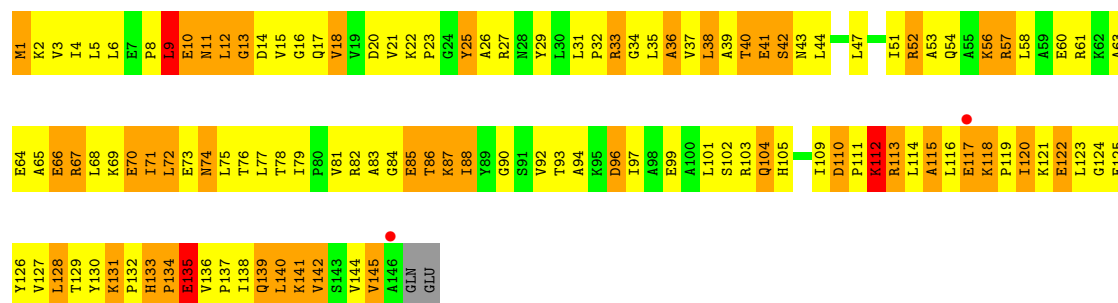


● Molecule 31: 50S ribosomal protein L9

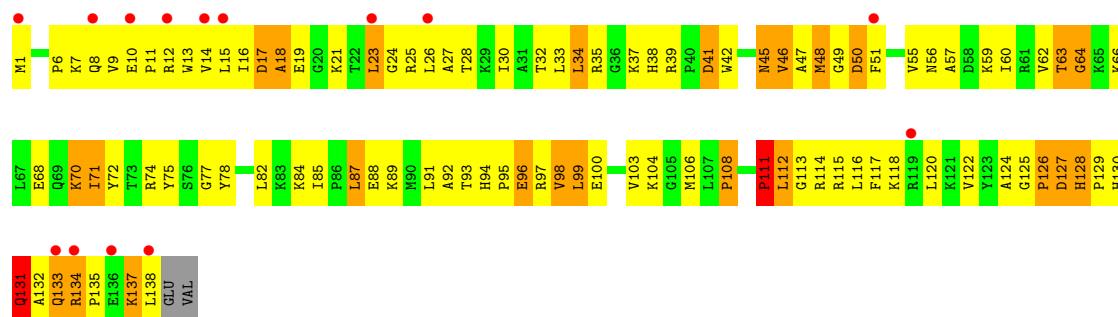
Chain BK: 



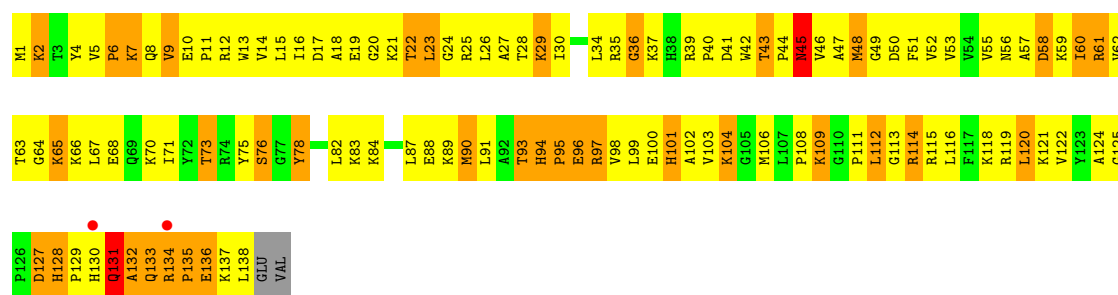
- Molecule 31: 50S ribosomal protein L9

Chain DK: 

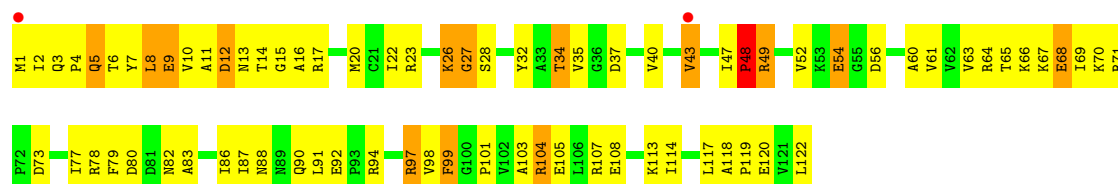
- Molecule 32: 50S ribosomal protein L13

Chain BM: 

- Molecule 32: 50S ribosomal protein L13

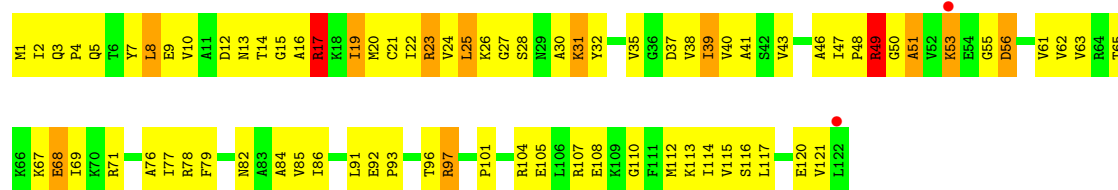
Chain DM: 

- Molecule 33: 50S ribosomal protein L14

Chain BN: 

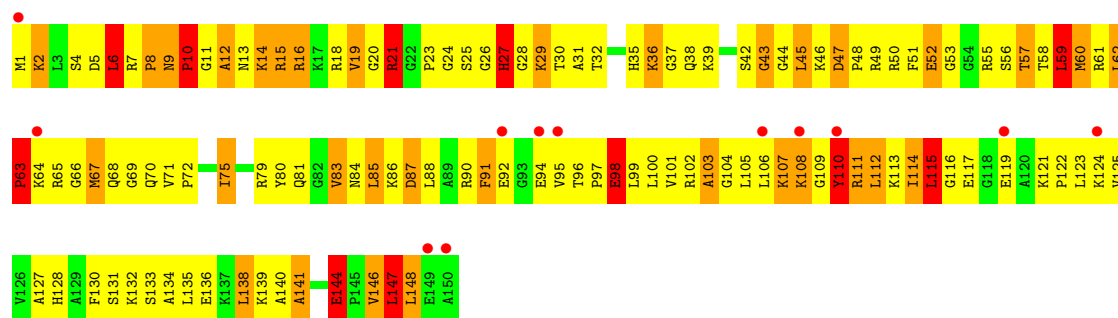
- Molecule 33: 50S ribosomal protein L14

Chain DN: 



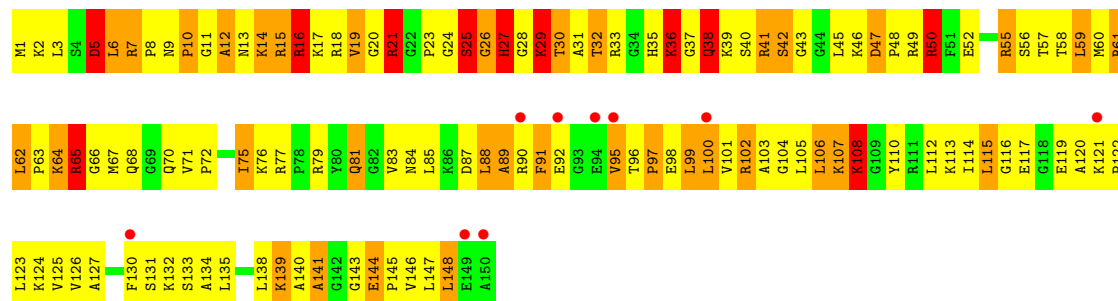
• Molecule 34: 50S ribosomal protein L15

Chain BO:



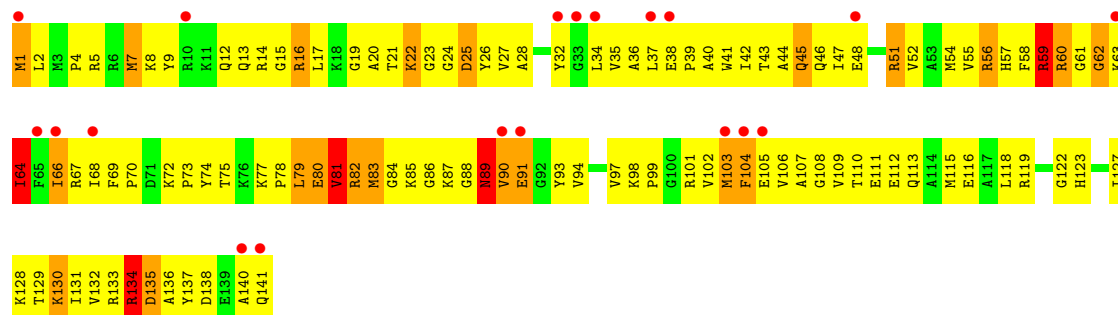
• Molecule 34: 50S ribosomal protein L15

Chain DO:



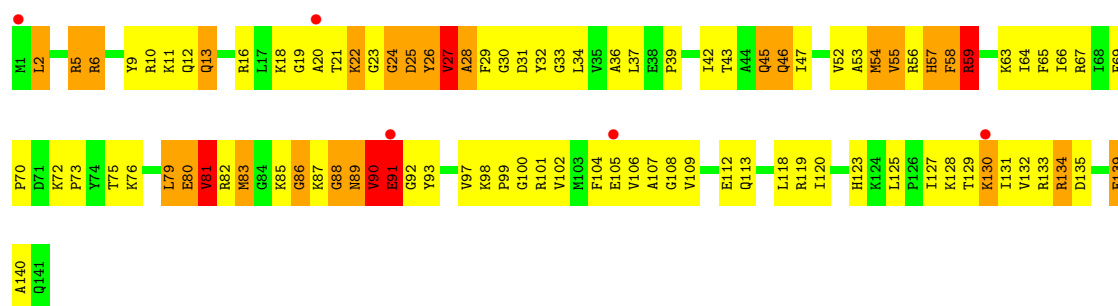
• Molecule 35: 50S ribosomal protein L16

Chain BP:



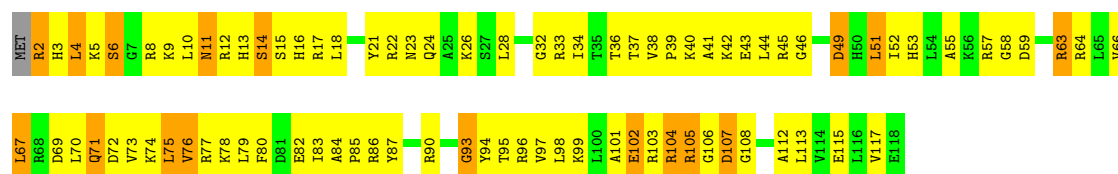
• Molecule 35: 50S ribosomal protein L16

Chain DP:



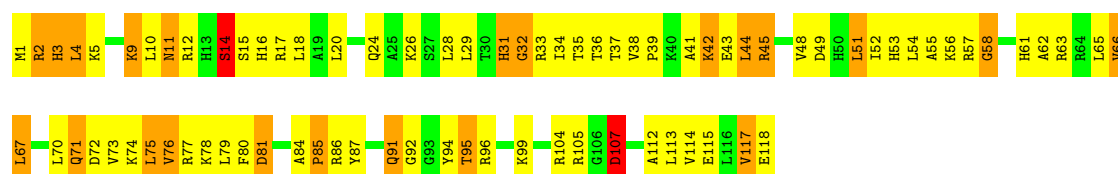
- Molecule 36: 50S ribosomal protein L17

Chain B0:



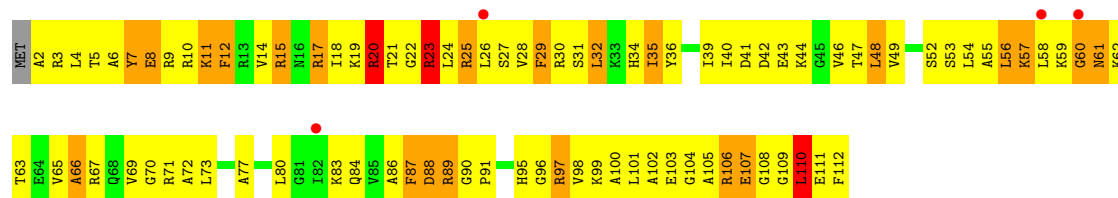
- Molecule 36: 50S ribosomal protein L17

Chain D0:



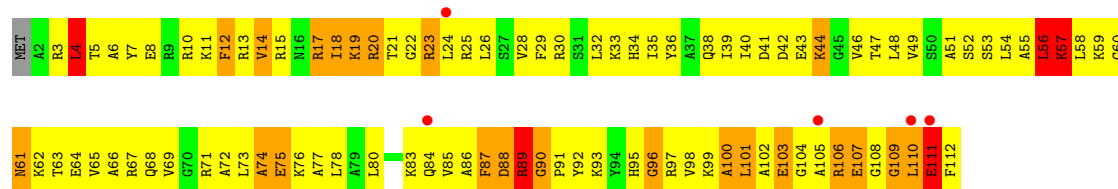
- Molecule 37: 50S ribosomal protein L18

Chain BQ:



- Molecule 37: 50S ribosomal protein L18

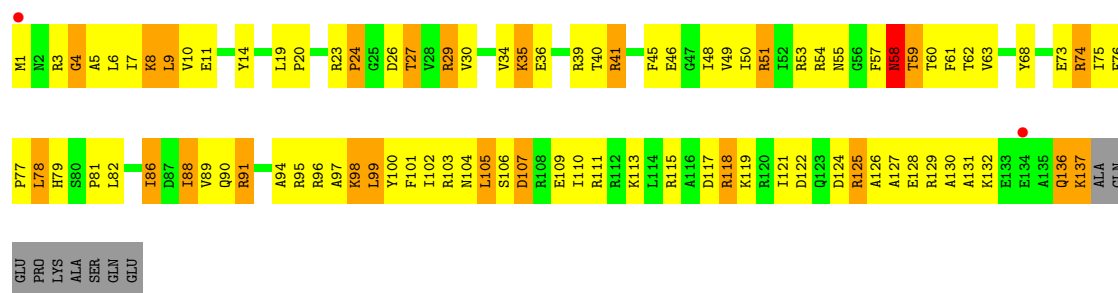
Chain DQ:



- Molecule 38: 50S ribosomal protein L19

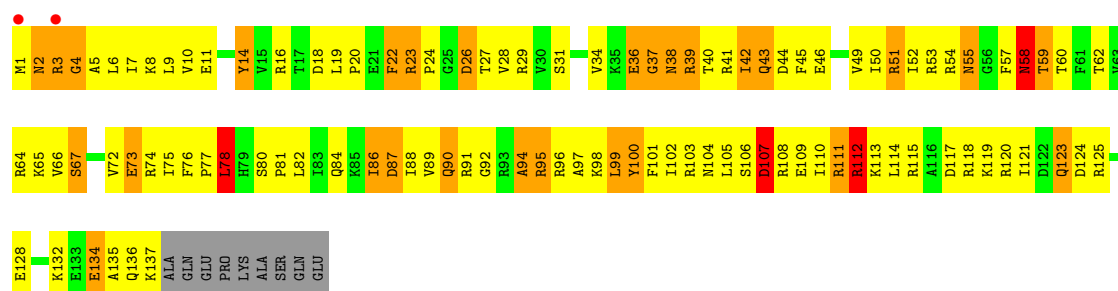
Chain BR:





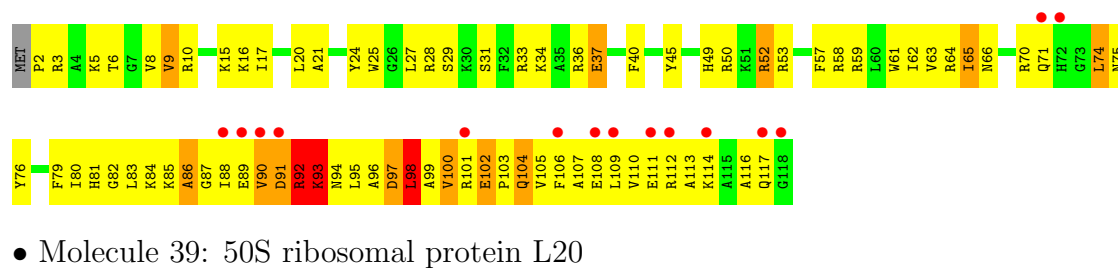
- Molecule 38: 50S ribosomal protein L19

Chain DR:



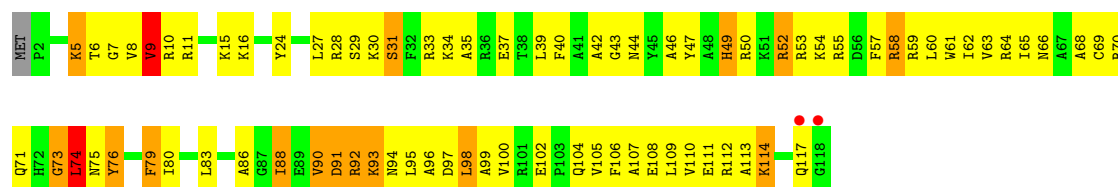
- Molecule 39: 50S ribosomal protein L20

Chain B1:



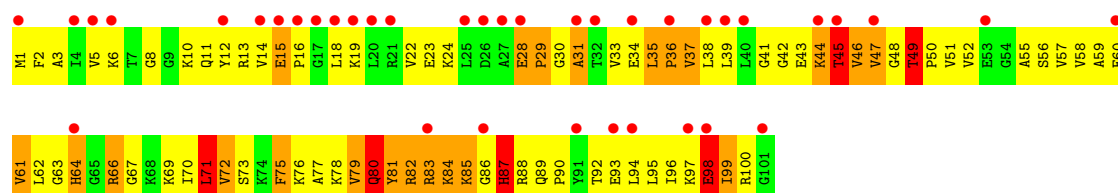
- Molecule 39: 50S ribosomal protein L20

Chain D1:



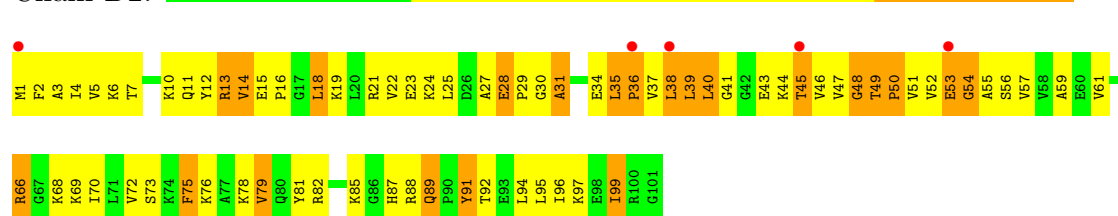
- Molecule 40: 50S ribosomal protein L21

Chain B2:



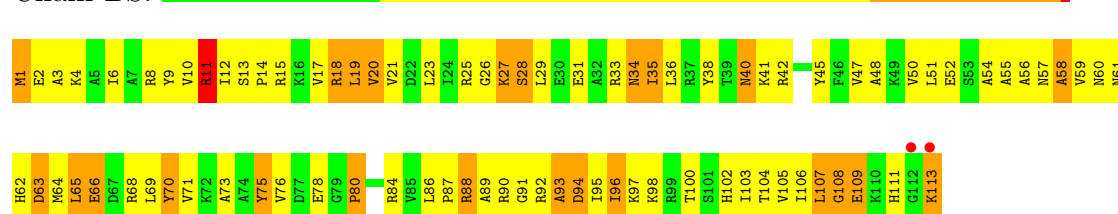
- Molecule 40: 50S ribosomal protein L21

Chain D2:



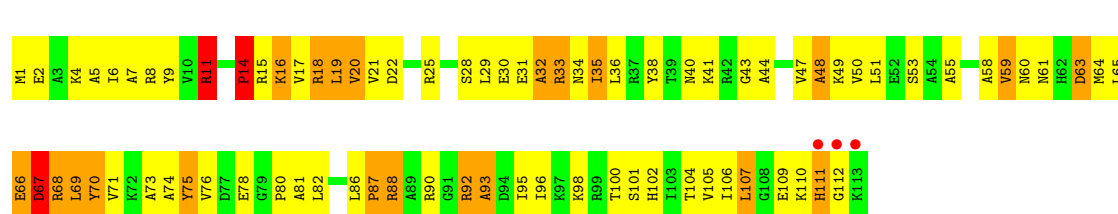
- Molecule 41: 50S ribosomal protein L22

Chain BS:



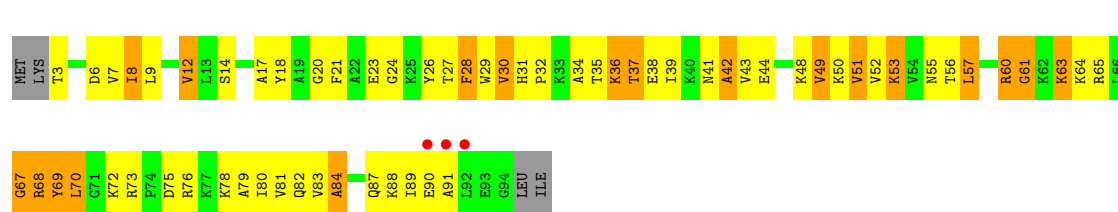
- Molecule 41: 50S ribosomal protein L22

Chain DS:



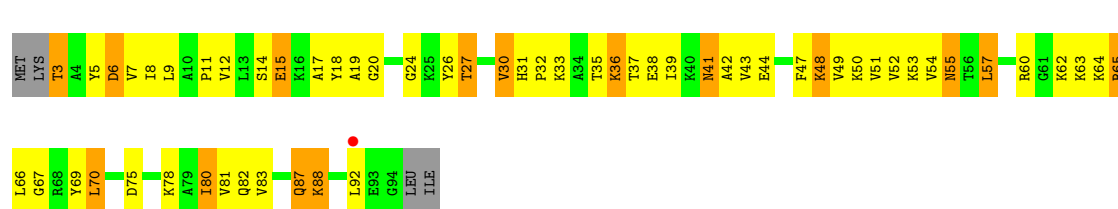
- Molecule 42: 50S ribosomal protein L23

Chain BT:



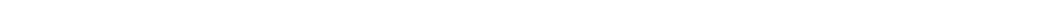
- Molecule 42: 50S ribosomal protein L23

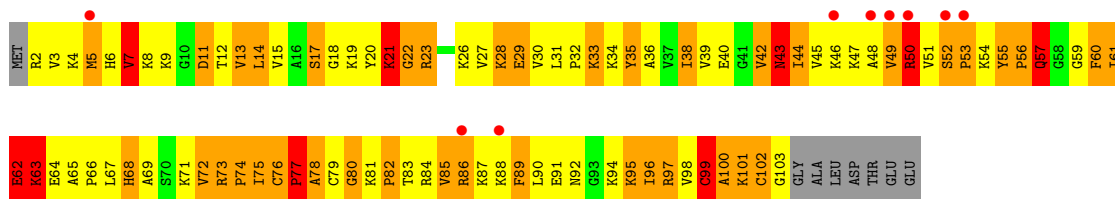
Chain DT:



- Molecule 43: 50S ribosomal protein L24

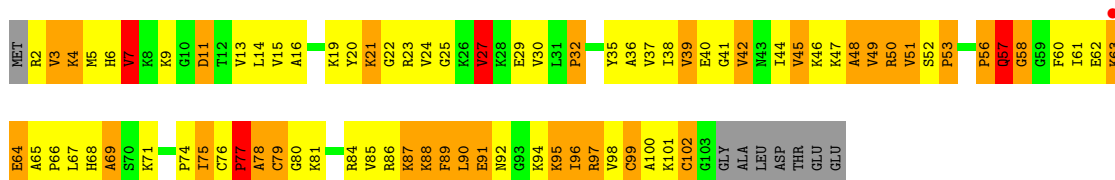
Chain BU:





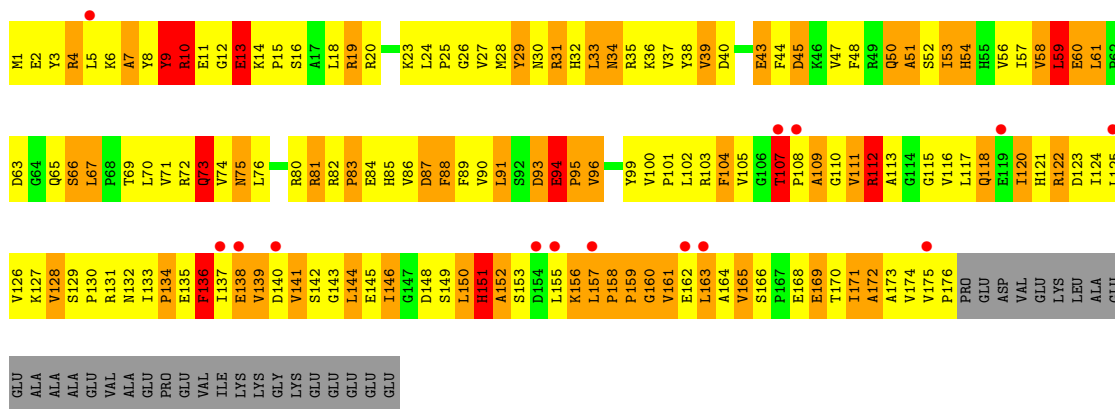
• Molecule 43: 50S ribosomal protein L24

Chain DU:



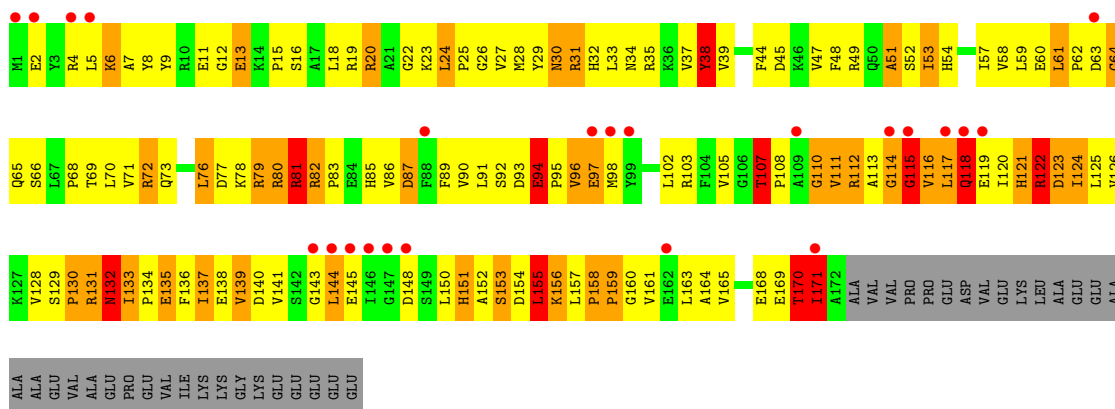
• Molecule 44: 50S ribosomal protein L25

Chain BV:



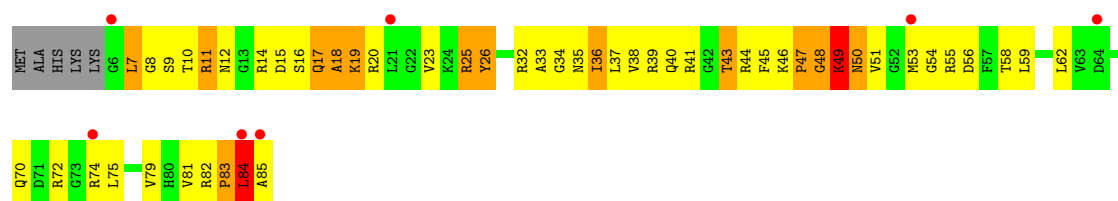
• Molecule 44: 50S ribosomal protein L25

Chain DV:



• Molecule 45: 50S ribosomal protein L27

Chain B3:



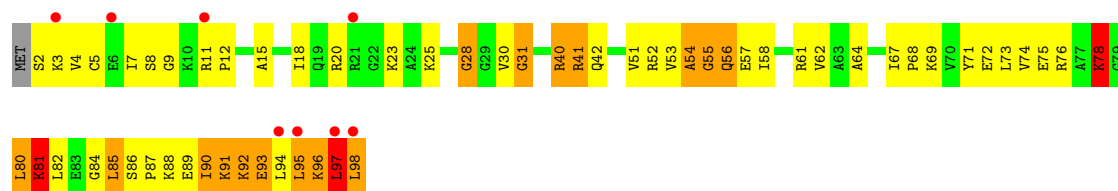
• Molecule 45: 50S ribosomal protein L27

Chain D3:



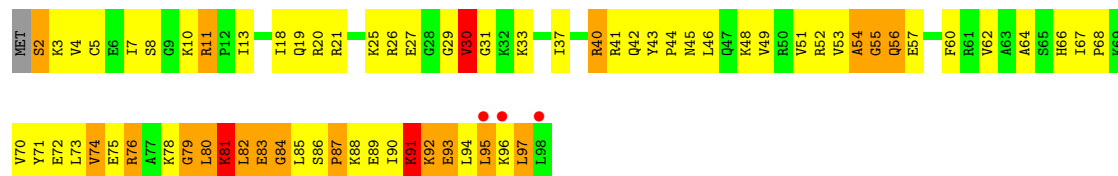
• Molecule 46: 50S ribosomal protein L28

Chain BZ:



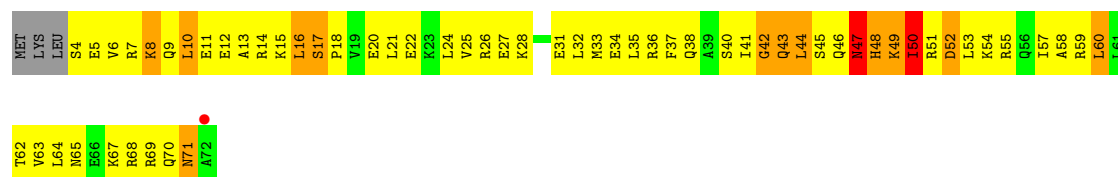
• Molecule 46: 50S ribosomal protein L28

Chain DZ:



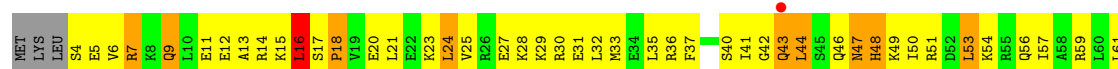
• Molecule 47: 50S ribosomal protein L29

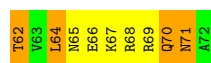
Chain BW:



• Molecule 47: 50S ribosomal protein L29

Chain DW:





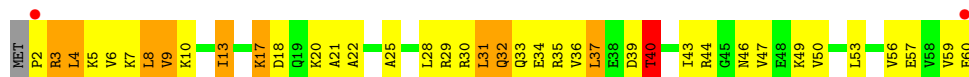
- Molecule 48: 50S ribosomal protein L30

Chain BX:



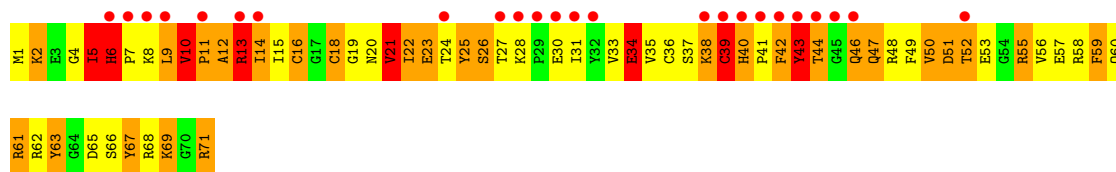
- Molecule 48: 50S ribosomal protein L30

Chain DX:



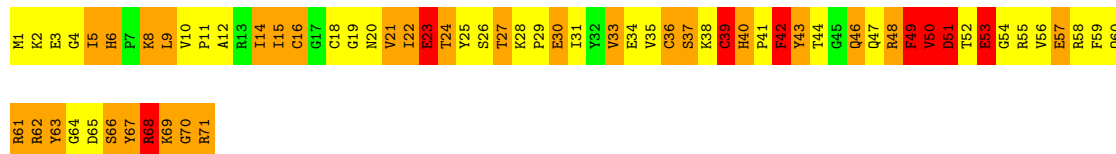
- Molecule 49: 50S ribosomal protein L31

Chain B4:



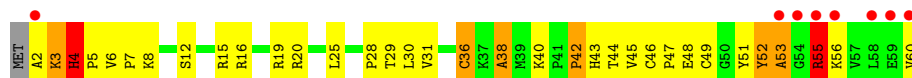
- Molecule 49: 50S ribosomal protein L31

Chain D4:



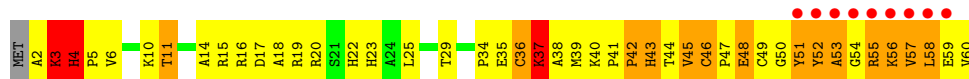
- Molecule 50: 50S ribosomal protein L32

Chain B5:



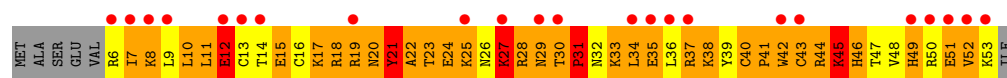
- Molecule 50: 50S ribosomal protein L32

Chain D5:



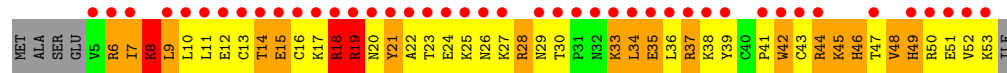
- Molecule 51: 50S ribosomal protein L33

Chain B6:



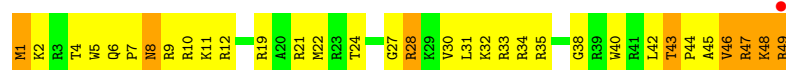
- Molecule 51: 50S ribosomal protein L33

Chain D6:



- Molecule 52: 50S ribosomal protein L34

Chain B7:



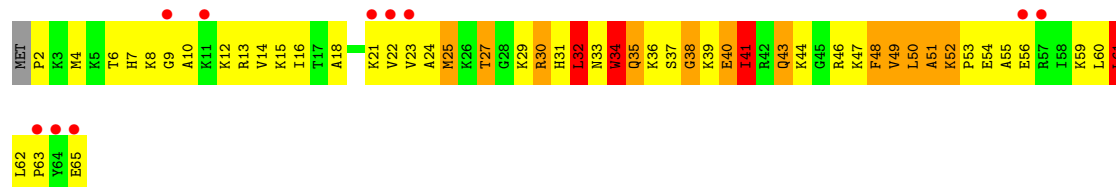
- Molecule 52: 50S ribosomal protein L34

Chain D7:



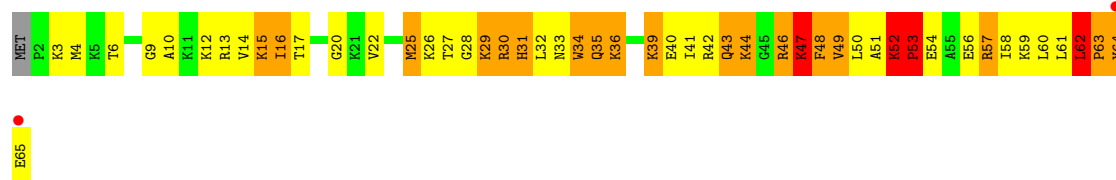
- Molecule 53: 50S ribosomal protein L35

Chain B8:



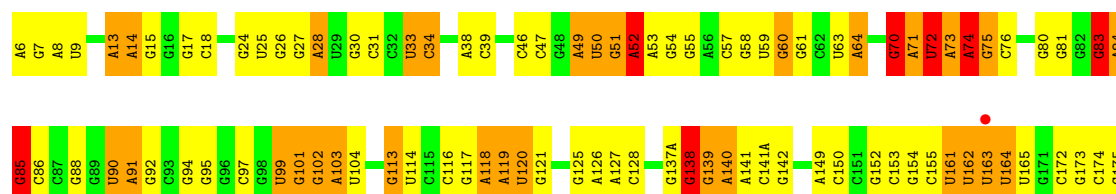
- Molecule 53: 50S ribosomal protein L35

Chain D8:



- Molecule 54: 23S ribosomal RNA

Chain DA:



U1167	G1092	A1027	C961	C985	U813	A751	A676	A631	G500	U427	G356	G275	G240	G176
G1168	G1093	A1028	G962	C986	C814	A752	G680	C634	A501	A428	A357	A276	A241	G177
G1169	A1094	A1029	U963	A987	C815	A753	G681	C635	A502		U358	C277	G242	G178
G1170	A1095	G1030		C988	C816	C754	G682	C636	A503	U434	A359	A278	U243	
G1171	A1096	U1033	G968	C989	C817	C755	G683	A637	A504	C435	G360	C279	A244	A181
G1172	A1097	G1034	U969	C890	G818	C756	G684	G638	A505	C436	G361	C280	G245	A182
A1174	A1098	A1034	C970	C992	A819	C756	G685	U639	A506	G438	U362	C281	C246	C183
U1175	G1099	U1035	C971	C993	A820	U757	A686	C640	A507	G439	G363	A282	G247	C184
G1176	C1100	G972	A821	C994	A821	C758	G686	C641	A508	G440	A363A	A283	C249	U185
A1177	U1101	A973	U895	U896	U822	G759	C687	G641	A509	U441	G363B	U284	C250	G186
C1178	C1102	G1037	C974	A896	U827	G760	U688	G642	C510	G442	G363C		G251	
C1180	A1103	C897	C974A	C998	U828	U762	A689	A643	U511	A443	G363D	C292	G252	G189
C1181	U1105	G1039	G975	A899	A829	G763	C691	C645	C581	C444	U363E	U293	G253	C192
A1182	G1106	G1042	C976	A900	G830	A764	C692	A646	C582	C445	A363F	U293	G254	C193
		G1043	G977	A901	G831	G765		G647	C583	A447	C365	C297		U193
G1187	C1109	G1044	G978	C902	G836	G766	G696	G648	C584	U448	C366	A298	A257	G194
U1188	G1110	A1045	G979	C902	U837	U767	G697	G649	C585		G370	A299		A198
A1189	A1111	A1046		U905	G837	G768	C698	C650	C518	A300	A371	A300	G260	A197
G1190	C1112	G1047	C982	G908	C838	G769	A699	G651	C519	G451	G372	G302	C263	C198
G1191	U1113	A1048	A983		U839	G770	G700	C652	G520	G452	U373	C302	C264	U200
G1192	G1114	C1049	A994	A910	C844	U773	G701	A653	G521	C453	A374	U303	C265	C201
G1193	C1115	A1050	C985	A911	G845	G774	G702	A654	C523	C454	G375	G304	A266	
A1194	C1116	G1051	C986	A912	C846	G775	U703	A654A	C524	C455	C376	U305	G266	
G1195		G1052	G987	U913	U847	G776	G704	C654B	U525	A457	U306	G307	C267	A204
C1196	A1126	C1053	A988	C914	U847		A705	G	A526	G458	U383	G308	A270B	G205
G1197	A1127	A1054	G988	C915	G848	A777		G	C527		U384	G309	C270C	U206
	C1203	G1055	A990	C916	A849	G778	U709	C	A528	A460	U385	G310	C270D	A207
G1204	A1129	A1056	C991	G916	A849	G778	G710	C	A529	A461	G386	C319	G270E	G208
A1204	U1130	G1057	C992	A917	C850	U779		C	C530	C462	U387	A311	U270F	C209
U1205	G1131	A1058	G993	A918	U851	G780		C	C531		G388	G312	U270G	C210
G1206	A1132	G1059	C994	U922	G852	A781	U714	C	C532		G389	G317		A211
C1207	U1133	U1060	C995	C923	C853	A782	G715	C	A533	G467	A390	C318	G270J	G212
G1208	G1135	A996	A996	C924	G854	A783	A716	G	U534	G468	G391	C319	C270K	G214
G1209	G1136	C997	C997	C925	C855	G785	G717	G		G469	C392	A320	G270L	G215
U1205	G1137	U999	U999	A926	C857	C786	C719	C	C537	A470	U396	G321	U270M	G216
G1210	A1211	G1065	A1000	G928	U858	U787	C720	C	C539	A471	G396	A322	U270N	A216
G1211	G1138	U1066	A1001	G929	C859	A788	C721	G654S	C541	A472	G397	G323	G270O	G217
G1212	G1139	A1067	G1002	U930	U860	A789	A722	A654T	C541	G473	U403	A324	G270P	A218
A1213	C1140	A1068	G1003	G931	A861	C790	G723	A654U	C541	G474	C404	G327	C270Q	G220
G1215	U1141	G1069	C1004	G932	G862	C791	U724	A655	C546	U475	U405	U328	G270R	A221
G1216	U1142	A1070	C1005	A933	A863	G792	G725	A655	C547	G476	G406	G329	G270S	A222
A1217	A1143	G1071	C1006	G946	G864	A793	G726	G656	C548		U406	A330	G270T	G223
	G1144		C1007	A941	C865	G794	A727	U657	A548	A479	G409	A331	C270U	G224
A1220		C1076	C1008	G942	A866	C795	G728	C658	C549	A480	G410	A332	G270V	A225
C1221	C1152	A1077	A1009	U943	C867	C796	G729	A616	C550	G481	G411	A333	G270W	G226
C1222	C1153	U1078	G944	U944	U868	C797	C730	G660	C551	A482	G412	A334	G270X	A227
	G1154	C1079	G945	A945	G869		C731	C661	C552	A483	G413	C334	G270Y	A228
G1228	A1155	A1080	U1012	G946	A870	A800	G732	G662	U554	C484	A414	C335	U270Z	A229
	A1156	U1081	C1013		U871	G801	G733	G663	C556	C485	C415		G271A	U230
C1230	G1157	U1082		G950	C876	A802	A734	C664	C557	C486	A416	G338	C271B	C231
G1231	C1158	U1083	C1018	C951	C876	U803	A735	C665	A621	G487	C417	U339	G271C	G232
G1232	U1159	A1084	U1019	G952	U877	A804	C736	G666	C622	G488	C418	C417	G271D	A233
C1233	G1160	A1085	A1020	A953	A878	G805	C737	G666	C623	G489	G419		G271E	
U1234	C1161	A1086	A1021	G879	G890	C806	C738	G669	C624	A491	G418	A345	G271F	C234
G1235	G1162	G1087	G879	G956	G880	U807	G739	A670	G695	A492		A346	G271G	U235
G1236	G1163	A1088	U1023	A957	C881	G808	U740	C671	U626	A497		A347	G271H	C236
A1237	U1164	G1089	G1024	U958	G882	U811		C672	A627	G498			G271I	C237
G1238	U1165	G1090	G1025	A959	G883	U812	A746	G674	C628	A499			G271J	C238
G1239	C1166	G1091	U1026	A960	C884	C812	U747	A675	U566	U499			G271K	U239







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.46Å 452.18Å 626.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 3.50 226.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-3.50) 100.0 (226.09-3.00)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.252 0.282 , 0.285	Depositor DCC
$R_{free}$ test set	12034 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 1177589 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	298428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

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

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

## 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	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%)
25	BB	0.46	3/2877 (0.1%)	0.79	3/4488 (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%)
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
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%)
54	DA	0.64	12/69611 (0.0%)	0.93	232/108670 (0.2%)
55	DB	0.56	3/2878 (0.1%)	0.84	6/4490 (0.1%)
All	All	0.53	54/320128 (0.0%)	0.84	638/479051 (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

*Continued on next page...*

*Continued from previous page...*

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
25	BB	0	4
54	DA	0	153
55	DB	0	5
All	All	0	416

The worst 5 of 54 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 638 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
54	DA	1379	A	C1'-O4'-C4'	-24.15	90.58	109.90
54	DA	945	A	C1'-O4'-C4'	-23.55	91.06	109.90
54	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32600	0	16446	1806	2
1	CA	32554	0	16428	1768	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CU	574	0	644	73	0
19	AV	656	0	678	168	0
19	CV	674	0	699	141	0
20	AW	763	0	861	84	0
20	CW	763	0	861	117	0
21	AX	217	0	234	35	0
21	CX	217	0	234	33	0
22	AC	1640	0	836	72	0
22	AD	1640	0	836	121	0
22	CC	1640	0	836	41	0
22	CD	1640	0	834	93	0
23	A1	502	0	253	40	0
23	C1	502	0	253	38	0
24	BA	62134	0	31302	3009	2
25	BB	2572	0	1305	184	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
39	B1	964	0	1022	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	DA	62151	0	31309	2761	0
55	DB	2573	0	1305	138	0
56	A1	2	0	0	0	0
56	AA	439	0	0	0	0
56	AC	8	0	0	0	0
56	AD	3	0	0	0	0
56	AH	2	0	0	0	0
56	AI	1	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AQ	1	0	0	0	0
56	AS	2	0	0	0	0
56	AT	2	0	0	0	0
56	AW	4	0	0	0	0
56	AX	1	0	0	0	0
56	B0	2	0	0	0	0
56	B1	1	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	1	0	0	0	0
56	B6	1	0	0	0	0
56	B8	1	0	0	0	0
56	BA	683	0	0	0	0
56	BB	26	0	0	0	0
56	BD	2	0	0	0	0
56	BE	7	0	0	0	0
56	BF	2	0	0	0	0
56	BG	1	0	0	0	0
56	BH	1	0	0	0	0
56	BK	1	0	0	0	0
56	BO	1	0	0	0	0
56	BQ	1	0	0	0	0
56	BR	2	0	0	0	0
56	BT	2	0	0	0	0
56	BU	5	0	0	0	0
56	BW	1	0	0	0	0
56	BZ	1	0	0	0	0
56	C1	1	0	0	0	0
56	CA	383	0	0	0	0
56	CC	13	0	0	0	0
56	CD	26	0	0	0	0
56	CG	1	0	0	0	0
56	CH	2	0	0	0	0
56	CK	2	0	0	0	0
56	CL	1	0	0	0	0
56	CM	1	0	0	0	0
56	CP	4	0	0	0	0
56	CQ	3	0	0	0	0
56	CR	1	0	0	0	0
56	CS	2	0	0	0	0
56	CT	1	0	0	0	0
56	CW	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CX	3	0	0	0	0
56	D0	5	0	0	0	0
56	D1	6	0	0	0	0
56	D2	1	0	0	0	0
56	D3	4	0	0	0	0
56	D5	1	0	0	0	0
56	D6	2	0	0	0	0
56	D7	1	0	0	0	0
56	DA	905	0	0	0	0
56	DB	29	0	0	0	0
56	DD	3	0	0	0	0
56	DE	3	0	0	0	0
56	DF	1	0	0	0	0
56	DG	3	0	0	0	0
56	DH	4	0	0	0	0
56	DO	5	0	0	0	0
56	DR	2	0	0	0	0
56	DS	1	0	0	0	0
56	DT	2	0	0	0	0
56	DU	6	0	0	0	0
56	DW	2	0	0	0	0
56	DZ	2	0	0	0	0
57	AA	2	0	0	0	0
57	AG	1	0	0	0	0
57	AQ	1	0	0	0	0
57	CG	1	0	0	0	0
57	CQ	1	0	0	0	0
58	CA	69	0	33	1	0
58	CC	66	0	34	2	0
58	CP	23	0	11	1	0
58	DA	276	0	132	26	0
58	DP	69	0	33	4	0
59	CA	40	0	22	4	0
59	CC	60	0	31	4	0
59	CO	20	0	11	2	0
59	CP	60	0	33	4	0
59	DA	200	0	111	21	0
59	DP	40	0	22	2	0
60	C1	20	0	10	0	0
60	CA	20	0	10	0	0
60	DA	160	0	80	15	0
60	DP	20	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	C1	44	0	22	3	0
61	CA	22	0	11	1	0
61	CC	22	0	11	3	0
61	DA	154	0	77	9	0
All	All	298428	0	200046	22779	18

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

The worst 5 of 22779 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:DH:127:GLU:CG	30:DH:128:PRO:HD3	1.36	1.52
24:BA:654(R):C:C5'	24:BA:654(R):C:C2	1.96	1.45
54:DA:1378:A:O2'	54: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	Distance(Å)	Clash(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 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AF	204/239 (85%)	119 (58%)	49 (24%)	36 (18%)	0	4
3	CF	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	17
4	AG	206/209 (99%)	117 (57%)	56 (27%)	33 (16%)	0	5
4	CG	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	1	13
5	AH	152/162 (94%)	103 (68%)	34 (22%)	15 (10%)	1	15
5	CH	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	15
6	AI	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	2	25
6	CI	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	18
7	AJ	153/156 (98%)	95 (62%)	42 (28%)	16 (10%)	1	14
7	CJ	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	16
8	AK	136/138 (99%)	98 (72%)	29 (21%)	9 (7%)	2	28
8	CK	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	13
9	AL	126/128 (98%)	71 (56%)	36 (29%)	19 (15%)	0	6
9	CL	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	10
10	AM	97/105 (92%)	67 (69%)	20 (21%)	10 (10%)	1	14
10	CM	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	14
11	AN	119/129 (92%)	76 (64%)	29 (24%)	14 (12%)	1	12
11	CN	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	22
12	AO	123/132 (93%)	80 (65%)	22 (18%)	21 (17%)	0	4
12	CO	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	12
13	AP	116/126 (92%)	62 (53%)	23 (20%)	31 (27%)	0	1
13	CP	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	4
14	AQ	58/61 (95%)	37 (64%)	15 (26%)	6 (10%)	1	14
14	CQ	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	4
15	AR	86/89 (97%)	55 (64%)	27 (31%)	4 (5%)	4	39
15	CR	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	26
16	AS	82/88 (93%)	57 (70%)	16 (20%)	9 (11%)	1	13
16	CS	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	9
17	AT	98/105 (93%)	75 (76%)	17 (17%)	6 (6%)	2	30
17	CT	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	21
18	AU	69/88 (78%)	42 (61%)	21 (30%)	6 (9%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CU	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	12
19	AV	80/93 (86%)	43 (54%)	20 (25%)	17 (21%)	0	2
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	4
20	CW	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	3
21	AX	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	4	42
21	CX	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	4
26	BD	270/276 (98%)	193 (72%)	46 (17%)	31 (12%)	1	12
26	DD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	2	24
27	BE	203/206 (98%)	114 (56%)	46 (23%)	43 (21%)	0	2
27	DE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	BF	206/210 (98%)	137 (66%)	45 (22%)	24 (12%)	1	12
28	DF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	15
29	BG	179/182 (98%)	114 (64%)	39 (22%)	26 (14%)	0	7
29	DG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	1	12
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	6
31	DK	144/148 (97%)	80 (56%)	36 (25%)	28 (19%)	0	3
32	BM	136/140 (97%)	88 (65%)	29 (21%)	19 (14%)	0	8
32	DM	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
33	BN	120/122 (98%)	96 (80%)	17 (14%)	7 (6%)	3	32
33	DN	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	24
34	BO	148/150 (99%)	80 (54%)	32 (22%)	36 (24%)	0	1
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	8
35	DP	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	1	13
36	B0	115/118 (98%)	73 (64%)	31 (27%)	11 (10%)	1	17
36	D0	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	11
37	BQ	109/112 (97%)	58 (53%)	32 (29%)	19 (17%)	0	4
37	DQ	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	135/146 (92%)	94 (70%)	31 (23%)	10 (7%)	2	24
38	DR	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	6
39	B1	115/118 (98%)	81 (70%)	22 (19%)	12 (10%)	1	14
39	D1	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	22
40	B2	99/101 (98%)	67 (68%)	12 (12%)	20 (20%)	0	2
40	D2	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	15
41	BS	111/113 (98%)	79 (71%)	20 (18%)	12 (11%)	1	13
41	DS	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	10
42	BT	90/96 (94%)	63 (70%)	18 (20%)	9 (10%)	1	15
42	DT	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	34
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	1
44	BV	174/206 (84%)	85 (49%)	43 (25%)	46 (26%)	0	1
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	8
45	D3	75/85 (88%)	56 (75%)	13 (17%)	6 (8%)	1	21
46	BZ	95/98 (97%)	66 (70%)	17 (18%)	12 (13%)	0	10
46	DZ	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	12
47	BW	67/72 (93%)	43 (64%)	12 (18%)	12 (18%)	0	4
47	DW	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	9
48	BX	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	6	50
48	DX	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	35
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%)	1	14
50	D5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
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%)	4	42
52	D7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	29
53	B8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	D8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	4
All	All	11381/12054 (94%)	7244 (64%)	2468 (22%)	1669 (15%)	0	6

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%)	3	18
2	CE	205/220 (93%)	181 (88%)	24 (12%)	8	38
3	AF	160/188 (85%)	141 (88%)	19 (12%)	8	37
3	CF	159/188 (85%)	145 (91%)	14 (9%)	14	57
4	AG	180/181 (99%)	152 (84%)	28 (16%)	4	23
4	CG	180/181 (99%)	163 (91%)	17 (9%)	13	52
5	AH	119/123 (97%)	102 (86%)	17 (14%)	5	28
5	CH	116/123 (94%)	106 (91%)	10 (9%)	15	58
6	AI	90/90 (100%)	80 (89%)	10 (11%)	9	42
6	CI	90/90 (100%)	76 (84%)	14 (16%)	4	23
7	AJ	126/127 (99%)	114 (90%)	12 (10%)	12	51
7	CJ	126/127 (99%)	115 (91%)	11 (9%)	15	57
8	AK	119/119 (100%)	112 (94%)	7 (6%)	28	75
8	CK	119/119 (100%)	106 (89%)	13 (11%)	9	43
9	AL	99/99 (100%)	80 (81%)	19 (19%)	2	12
9	CL	98/99 (99%)	87 (89%)	11 (11%)	9	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AM	89/92 (97%)	80 (90%)	9 (10%)	11	48
10	CM	89/92 (97%)	81 (91%)	8 (9%)	14	55
11	AN	92/99 (93%)	83 (90%)	9 (10%)	12	50
11	CN	90/99 (91%)	81 (90%)	9 (10%)	11	49
12	AO	104/109 (95%)	92 (88%)	12 (12%)	8	39
12	CO	104/109 (95%)	90 (86%)	14 (14%)	6	30
13	AP	94/101 (93%)	75 (80%)	19 (20%)	2	11
13	CP	97/101 (96%)	81 (84%)	16 (16%)	3	20
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	11	48
14	CQ	49/50 (98%)	42 (86%)	7 (14%)	5	28
15	AR	79/80 (99%)	74 (94%)	5 (6%)	25	73
15	CR	79/80 (99%)	73 (92%)	6 (8%)	19	65
16	AS	72/74 (97%)	63 (88%)	9 (12%)	7	35
16	CS	72/74 (97%)	63 (88%)	9 (12%)	7	35
17	AT	95/97 (98%)	87 (92%)	8 (8%)	16	59
17	CT	95/97 (98%)	89 (94%)	6 (6%)	25	73
18	AU	62/77 (80%)	53 (86%)	9 (14%)	5	27
18	CU	61/77 (79%)	55 (90%)	6 (10%)	12	50
19	AV	71/80 (89%)	63 (89%)	8 (11%)	9	40
19	CV	73/80 (91%)	61 (84%)	12 (16%)	3	20
20	AW	76/82 (93%)	65 (86%)	11 (14%)	5	27
20	CW	76/82 (93%)	67 (88%)	9 (12%)	8	38
21	AX	20/22 (91%)	18 (90%)	2 (10%)	11	49
21	CX	20/22 (91%)	19 (95%)	1 (5%)	34	79
26	BD	214/218 (98%)	183 (86%)	31 (14%)	5	27
26	DD	214/218 (98%)	176 (82%)	38 (18%)	2	16
27	BE	165/166 (99%)	137 (83%)	28 (17%)	3	18
27	DE	165/166 (99%)	127 (77%)	38 (23%)	1	7
28	BF	165/166 (99%)	142 (86%)	23 (14%)	5	29
28	DF	161/166 (97%)	139 (86%)	22 (14%)	5	29
29	BG	155/156 (99%)	139 (90%)	16 (10%)	10	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DG	155/156 (99%)	130 (84%)	25 (16%)	3	22
30	BH	142/148 (96%)	111 (78%)	31 (22%)	1	8
30	DH	142/148 (96%)	115 (81%)	27 (19%)	2	13
31	BK	122/124 (98%)	105 (86%)	17 (14%)	5	29
31	DK	122/124 (98%)	95 (78%)	27 (22%)	1	8
32	BM	117/119 (98%)	101 (86%)	16 (14%)	5	29
32	DM	117/119 (98%)	97 (83%)	20 (17%)	3	18
33	BN	100/100 (100%)	88 (88%)	12 (12%)	7	37
33	DN	100/100 (100%)	90 (90%)	10 (10%)	11	49
34	BO	116/116 (100%)	86 (74%)	30 (26%)	1	5
34	DO	116/116 (100%)	89 (77%)	27 (23%)	1	7
35	BP	111/111 (100%)	92 (83%)	19 (17%)	3	18
35	DP	111/111 (100%)	92 (83%)	19 (17%)	3	18
36	B0	100/101 (99%)	87 (87%)	13 (13%)	6	33
36	D0	101/101 (100%)	83 (82%)	18 (18%)	2	16
37	BQ	87/88 (99%)	74 (85%)	13 (15%)	4	26
37	DQ	87/88 (99%)	74 (85%)	13 (15%)	4	26
38	BR	120/127 (94%)	99 (82%)	21 (18%)	3	17
38	DR	120/127 (94%)	96 (80%)	24 (20%)	2	11
39	B1	93/94 (99%)	82 (88%)	11 (12%)	8	38
39	D1	93/94 (99%)	79 (85%)	14 (15%)	4	25
40	B2	82/82 (100%)	67 (82%)	15 (18%)	2	14
40	D2	82/82 (100%)	70 (85%)	12 (15%)	5	27
41	BS	92/92 (100%)	76 (83%)	16 (17%)	3	17
41	DS	92/92 (100%)	77 (84%)	15 (16%)	3	21
42	BT	74/78 (95%)	61 (82%)	13 (18%)	3	16
42	DT	74/78 (95%)	62 (84%)	12 (16%)	3	21
43	BU	85/91 (93%)	61 (72%)	24 (28%)	0	4
43	DU	85/91 (93%)	70 (82%)	15 (18%)	3	16
44	BV	155/179 (87%)	120 (77%)	35 (23%)	1	8
44	DV	152/179 (85%)	124 (82%)	28 (18%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	B3	63/67 (94%)	55 (87%)	8 (13%)	6	33
45	D3	62/67 (92%)	54 (87%)	8 (13%)	6	33
46	BZ	82/83 (99%)	69 (84%)	13 (16%)	4	22
46	DZ	82/83 (99%)	67 (82%)	15 (18%)	2	14
47	BW	64/67 (96%)	57 (89%)	7 (11%)	9	43
47	DW	64/67 (96%)	57 (89%)	7 (11%)	9	43
48	BX	51/52 (98%)	43 (84%)	8 (16%)	4	23
48	DX	51/52 (98%)	40 (78%)	11 (22%)	1	9
49	B4	63/63 (100%)	43 (68%)	20 (32%)	0	3
49	D4	63/63 (100%)	44 (70%)	19 (30%)	0	4
50	B5	51/52 (98%)	46 (90%)	5 (10%)	12	50
50	D5	51/52 (98%)	40 (78%)	11 (22%)	1	9
51	B6	47/52 (90%)	30 (64%)	17 (36%)	0	2
51	D6	48/52 (92%)	38 (79%)	10 (21%)	2	10
52	B7	42/42 (100%)	33 (79%)	9 (21%)	1	9
52	D7	42/42 (100%)	38 (90%)	4 (10%)	12	51
53	B8	54/55 (98%)	43 (80%)	11 (20%)	2	10
53	D8	54/55 (98%)	39 (72%)	15 (28%)	0	4
All	All	9616/9998 (96%)	8160 (85%)	1456 (15%)	4	25

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

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

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

Mol	Chain	Res	Type
48	BX	46	ASN
6	CI	7	ASN
42	DT	55	ASN

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Mol	Chain	Res	Type
50	B5	43	HIS
3	CF	37	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1516/1517 (99%)	341 (22%)	139 (9%)
1	CA	1514/1517 (99%)	316 (20%)	133 (8%)
22	AC	77/77 (100%)	15 (19%)	5 (6%)
22	AD	76/77 (98%)	28 (36%)	6 (7%)
22	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	2884/2885 (99%)	762 (26%)	325 (11%)
25	BB	119/122 (97%)	25 (21%)	3 (2%)
54	DA	2884/2898 (99%)	776 (26%)	354 (12%)
55	DB	119/120 (99%)	21 (17%)	6 (5%)
All	All	9385/9417 (99%)	2329 (24%)	988 (10%)

5 of 2329 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 988 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2497	A
1	CA	753	A
54	DA	2250	G
24	BA	2681	C
1	CA	243	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2724 ligands modelled in this entry, 2659 are monoatomic - leaving 65 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
61	A	C1	101	-	22,24,25	0.75	0	32,35,38	0.68	0
60	U	C1	102	-	19,21,22	1.61	3 (15%)	23,30,33	0.66	0
61	A	C1	103	-	22,24,25	0.73	0	32,35,38	0.69	0
58	G	CA	1601	-	23,25,26	1.01	1 (4%)	32,37,40	5.23	4 (12%)
58	G	CA	1602	-	23,25,26	0.99	2 (8%)	32,37,40	5.71	3 (9%)
59	C	CA	1603	-	19,21,22	1.10	3 (15%)	24,30,33	0.72	1 (4%)
60	U	CA	1604	-	19,21,22	1.55	2 (10%)	23,30,33	0.82	0
59	C	CA	1605	-	19,21,22	1.11	2 (10%)	24,30,33	0.79	1 (4%)
58	G	CA	1606	-	23,25,26	0.99	1 (4%)	32,37,40	5.25	4 (12%)
61	A	CA	1607	-	22,24,25	0.71	1 (4%)	32,35,38	0.69	0
58	G	CC	101	-	22,22,26	0.86	1 (4%)	31,33,40	5.15	4 (12%)
58	G	CC	102	-	23,25,26	0.97	2 (8%)	32,37,40	5.25	4 (12%)
61	A	CC	103	-	22,24,25	0.73	1 (4%)	32,35,38	0.73	0
58	G	CC	104	-	23,25,26	0.95	1 (4%)	32,37,40	5.36	4 (12%)
59	C	CC	105	-	19,21,22	1.13	3 (15%)	24,30,33	1.14	2 (8%)
59	C	CC	106	-	19,21,22	1.00	1 (5%)	24,30,33	0.72	1 (4%)
59	C	CC	107	-	19,21,22	1.29	1 (5%)	24,30,33	2.31	4 (16%)
59	C	CO	201	-	19,21,22	1.00	2 (10%)	24,30,33	0.78	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	G	CP	201	-	23,25,26	0.97	2 (8%)	32,37,40	5.17	4 (12%)
59	C	CP	202	-	19,21,22	1.07	2 (10%)	24,30,33	0.73	1 (4%)
59	C	CP	203	-	19,21,22	1.07	2 (10%)	24,30,33	0.81	1 (4%)
59	C	CP	204	-	19,21,22	1.11	2 (10%)	24,30,33	0.77	1 (4%)
58	G	DA	2901	-	23,25,26	0.96	2 (8%)	32,37,40	5.11	4 (12%)
60	U	DA	2902	-	19,21,22	1.48	1 (5%)	23,30,33	0.70	0
58	G	DA	2903	-	23,25,26	0.96	1 (4%)	32,37,40	5.13	5 (15%)
58	G	DA	2904	-	23,25,26	0.93	1 (4%)	32,37,40	5.26	4 (12%)
61	A	DA	2905	-	22,24,25	0.76	0	32,35,38	0.68	0
58	G	DA	2906	-	23,25,26	0.95	1 (4%)	32,37,40	5.50	4 (12%)
59	C	DA	2907	-	19,21,22	0.97	1 (5%)	24,30,33	0.75	1 (4%)
58	G	DA	2908	-	23,25,26	0.96	1 (4%)	32,37,40	4.98	4 (12%)
58	G	DA	2909	-	23,25,26	1.01	2 (8%)	32,37,40	4.92	4 (12%)
60	U	DA	2910	-	19,21,22	1.60	2 (10%)	23,30,33	0.70	0
61	A	DA	2911	-	22,24,25	0.70	1 (4%)	32,35,38	0.67	0
58	G	DA	2912	-	23,25,26	0.92	1 (4%)	32,37,40	4.92	4 (12%)
59	C	DA	2913	-	19,21,22	1.08	3 (15%)	24,30,33	0.79	1 (4%)
60	U	DA	2914	-	19,21,22	1.52	2 (10%)	23,30,33	0.68	0
59	C	DA	2915	-	19,21,22	1.06	3 (15%)	24,30,33	0.74	1 (4%)
58	G	DA	2916	-	23,25,26	0.93	1 (4%)	32,37,40	5.38	4 (12%)
60	U	DA	2917	-	19,21,22	1.59	1 (5%)	23,30,33	0.79	0
61	A	DA	2918	-	22,24,25	0.72	0	32,35,38	0.65	0
61	A	DA	2919	-	22,24,25	0.72	0	32,35,38	0.66	0
58	G	DA	2920	-	23,25,26	0.96	1 (4%)	32,37,40	5.22	4 (12%)
58	G	DA	2921	-	23,25,26	0.93	2 (8%)	32,37,40	5.27	4 (12%)
60	U	DA	2922	-	19,21,22	1.56	1 (5%)	23,30,33	0.78	0
59	C	DA	2923	-	19,21,22	1.02	1 (5%)	24,30,33	1.11	1 (4%)
58	G	DA	2924	-	23,25,26	0.94	1 (4%)	32,37,40	5.31	4 (12%)
60	U	DA	2925	-	19,21,22	1.56	2 (10%)	23,30,33	0.80	0
59	C	DA	2926	-	19,21,22	0.98	2 (10%)	24,30,33	0.77	1 (4%)
60	U	DA	2927	-	19,21,22	1.60	2 (10%)	23,30,33	0.89	0
59	C	DA	2928	-	19,21,22	0.96	0	24,30,33	0.75	1 (4%)
61	A	DA	2929	-	22,24,25	0.73	1 (4%)	32,35,38	0.80	0
61	A	DA	2930	-	22,24,25	0.68	1 (4%)	32,35,38	1.12	4 (12%)
61	A	DA	2931	-	22,24,25	0.77	1 (4%)	32,35,38	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	U	DA	2932	-	19,21,22	1.54	2 (10%)	23,30,33	1.12	0
58	G	DA	2933	-	23,25,26	1.00	1 (4%)	32,37,40	5.26	4 (12%)
59	C	DA	2934	-	19,21,22	1.04	1 (5%)	24,30,33	0.74	1 (4%)
59	C	DA	2935	-	19,21,22	1.02	1 (5%)	24,30,33	0.72	1 (4%)
59	C	DA	2936	-	19,21,22	0.95	2 (10%)	24,30,33	0.73	1 (4%)
59	C	DA	2937	-	19,21,22	1.06	2 (10%)	24,30,33	0.84	1 (4%)
58	G	DP	201	-	23,25,26	0.97	2 (8%)	32,37,40	4.73	4 (12%)
58	G	DP	202	-	23,25,26	1.01	2 (8%)	32,37,40	4.72	4 (12%)
60	U	DP	203	-	19,21,22	1.62	1 (5%)	23,30,33	0.70	0
59	C	DP	204	-	19,21,22	1.13	3 (15%)	24,30,33	0.76	1 (4%)
59	C	DP	205	-	19,21,22	0.97	1 (5%)	24,30,33	0.84	1 (4%)
58	G	DP	206	-	23,25,26	0.94	0	32,37,40	4.95	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	A	C1	101	-	-	0/8/25/26	0/3/3/3
60	U	C1	102	-	-	0/6/25/26	0/2/2/2
61	A	C1	103	-	-	0/8/25/26	0/3/3/3
58	G	CA	1601	-	-	0/8/25/26	0/3/3/3
58	G	CA	1602	-	-	0/8/25/26	0/3/3/3
59	C	CA	1603	-	-	0/6/25/26	0/2/2/2
60	U	CA	1604	-	-	0/6/25/26	0/2/2/2
59	C	CA	1605	-	-	0/6/25/26	0/2/2/2
58	G	CA	1606	-	-	0/8/25/26	0/3/3/3
61	A	CA	1607	-	-	0/8/25/26	0/3/3/3
58	G	CC	101	-	-	0/6/22/26	0/3/3/3
58	G	CC	102	-	-	0/8/25/26	0/3/3/3
61	A	CC	103	-	-	0/8/25/26	0/3/3/3
58	G	CC	104	-	-	0/8/25/26	0/3/3/3
59	C	CC	105	-	-	0/6/25/26	0/2/2/2
59	C	CC	106	-	-	0/6/25/26	0/2/2/2
59	C	CC	107	-	-	0/6/25/26	0/2/2/2
59	C	CO	201	-	-	0/6/25/26	0/2/2/2
58	G	CP	201	-	-	0/8/25/26	0/3/3/3
59	C	CP	202	-	-	0/6/25/26	0/2/2/2
59	C	CP	203	-	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	C	CP	204	-	-	0/6/25/26	0/2/2/2
58	G	DA	2901	-	-	0/8/25/26	0/3/3/3
60	U	DA	2902	-	-	0/6/25/26	0/2/2/2
58	G	DA	2903	-	-	1/8/25/26	0/3/3/3
58	G	DA	2904	-	-	1/8/25/26	0/3/3/3
61	A	DA	2905	-	-	0/8/25/26	0/3/3/3
58	G	DA	2906	-	-	0/8/25/26	0/3/3/3
59	C	DA	2907	-	-	0/6/25/26	0/2/2/2
58	G	DA	2908	-	-	1/8/25/26	0/3/3/3
58	G	DA	2909	-	-	0/8/25/26	0/3/3/3
60	U	DA	2910	-	-	0/6/25/26	0/2/2/2
61	A	DA	2911	-	-	1/8/25/26	0/3/3/3
58	G	DA	2912	-	-	0/8/25/26	0/3/3/3
59	C	DA	2913	-	-	0/6/25/26	0/2/2/2
60	U	DA	2914	-	-	0/6/25/26	0/2/2/2
59	C	DA	2915	-	-	0/6/25/26	0/2/2/2
58	G	DA	2916	-	-	0/8/25/26	0/3/3/3
60	U	DA	2917	-	-	0/6/25/26	0/2/2/2
61	A	DA	2918	-	-	0/8/25/26	0/3/3/3
61	A	DA	2919	-	-	0/8/25/26	0/3/3/3
58	G	DA	2920	-	-	0/8/25/26	0/3/3/3
58	G	DA	2921	-	-	0/8/25/26	0/3/3/3
60	U	DA	2922	-	-	0/6/25/26	0/2/2/2
59	C	DA	2923	-	-	0/6/25/26	0/2/2/2
58	G	DA	2924	-	-	0/8/25/26	0/3/3/3
60	U	DA	2925	-	-	0/6/25/26	0/2/2/2
59	C	DA	2926	-	-	0/6/25/26	0/2/2/2
60	U	DA	2927	-	-	0/6/25/26	0/2/2/2
59	C	DA	2928	-	-	0/6/25/26	0/2/2/2
61	A	DA	2929	-	-	0/8/25/26	0/3/3/3
61	A	DA	2930	-	-	0/8/25/26	0/3/3/3
61	A	DA	2931	-	-	1/8/25/26	0/3/3/3
60	U	DA	2932	-	-	0/6/25/26	0/2/2/2
58	G	DA	2933	-	-	0/8/25/26	0/3/3/3
59	C	DA	2934	-	-	0/6/25/26	0/2/2/2
59	C	DA	2935	-	-	0/6/25/26	0/2/2/2
59	C	DA	2936	-	-	0/6/25/26	0/2/2/2
59	C	DA	2937	-	-	0/6/25/26	0/2/2/2
58	G	DP	201	-	-	0/8/25/26	0/3/3/3
58	G	DP	202	-	-	0/8/25/26	0/3/3/3
60	U	DP	203	-	-	0/6/25/26	0/2/2/2
59	C	DP	204	-	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	C	DP	205	-	-	0/6/25/26	0/2/2/2
58	G	DP	206	-	-	0/8/25/26	0/3/3/3

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	DA	2917	U	C5-C4	5.87	1.43	1.37
60	DP	203	U	C5-C4	5.87	1.43	1.37
60	DA	2932	U	C5-C4	5.65	1.43	1.37
60	CA	1604	U	C5-C4	5.61	1.43	1.37
60	DA	2910	U	C5-C4	5.51	1.43	1.37

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	1602	G	C6-C5-N7	-30.65	130.01	134.14
58	DA	2906	G	C6-C5-N7	-29.39	130.18	134.14
58	DA	2916	G	C6-C5-N7	-28.69	130.28	134.14
58	CC	104	G	C6-C5-N7	-28.47	130.31	134.14
58	DA	2924	G	C6-C5-N7	-28.23	130.34	134.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DA	2904	G	OP2-P-O5'-C5'
61	DA	2911	A	OP2-P-O5'-C5'
58	DA	2903	G	OP2-P-O5'-C5'
61	DA	2931	A	OP2-P-O5'-C5'
58	DA	2908	G	OP2-P-O5'-C5'

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1517/1517 (100%)	-0.76	2 (0%) 93 84	66, 113, 195, 251	0
1	CA	1515/1517 (99%)	-0.83	10 (0%) 84 56	47, 111, 193, 247	0
2	AE	236/256 (92%)	0.65	18 (7%) 14 7	111, 152, 183, 188	0
2	CE	237/256 (92%)	0.52	18 (7%) 14 7	108, 138, 175, 185	0
3	AF	206/239 (86%)	0.62	17 (8%) 11 6	116, 134, 171, 178	0
3	CF	205/239 (85%)	0.76	16 (7%) 13 7	98, 128, 150, 160	0
4	AG	208/209 (99%)	-0.04	0 100 100	72, 106, 128, 137	0
4	CG	208/209 (99%)	0.10	5 (2%) 56 26	95, 116, 136, 143	0
5	AH	154/162 (95%)	0.06	3 (1%) 64 32	89, 109, 139, 163	0
5	CH	151/162 (93%)	0.25	4 (2%) 53 24	84, 105, 132, 157	0
6	AI	101/101 (100%)	0.41	0 100 100	85, 106, 121, 138	0
6	CI	101/101 (100%)	0.52	2 (1%) 62 30	80, 109, 119, 139	0
7	AJ	155/156 (99%)	0.47	10 (6%) 18 8	105, 129, 150, 160	0
7	CJ	155/156 (99%)	0.18	4 (2%) 53 24	98, 121, 141, 157	0
8	AK	138/138 (100%)	-0.37	0 100 100	91, 114, 126, 131	0
8	CK	138/138 (100%)	-0.01	1 (0%) 84 56	83, 109, 121, 123	0
9	AL	128/128 (100%)	-0.11	0 100 100	109, 150, 168, 173	0
9	CL	127/128 (99%)	-0.16	0 100 100	98, 138, 160, 169	0
10	AM	99/105 (94%)	0.16	3 (3%) 48 22	118, 152, 168, 172	0
10	CM	99/105 (94%)	0.35	7 (7%) 16 7	111, 147, 168, 175	0
11	AN	121/129 (93%)	0.62	5 (4%) 35 15	88, 110, 140, 155	0
11	CN	119/129 (92%)	0.79	8 (6%) 17 8	79, 102, 128, 146	0
12	AO	125/132 (94%)	0.24	3 (2%) 56 26	77, 96, 115, 148	0
12	CO	125/132 (94%)	0.48	3 (2%) 56 26	72, 90, 115, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	118/126 (93%)	0.08	3 (2%) 54 25	114, 146, 169, 172	0
13	CP	121/126 (96%)	-0.22	1 (0%) 83 53	95, 132, 150, 153	0
14	AQ	60/61 (98%)	-0.07	0 100 100	119, 134, 148, 152	0
14	CQ	60/61 (98%)	-0.14	0 100 100	97, 116, 127, 129	0
15	AR	88/89 (98%)	-0.05	1 (1%) 77 44	80, 102, 125, 136	0
15	CR	88/89 (98%)	-0.18	1 (1%) 77 44	77, 103, 122, 127	0
16	AS	84/88 (95%)	-0.51	0 100 100	86, 97, 118, 150	0
16	CS	84/88 (95%)	-0.33	0 100 100	95, 112, 140, 156	0
17	AT	100/105 (95%)	-0.24	1 (1%) 79 47	81, 104, 130, 155	0
17	CT	100/105 (95%)	-0.14	1 (1%) 79 47	82, 109, 125, 144	0
18	AU	71/88 (80%)	0.27	3 (4%) 35 14	87, 107, 135, 141	0
18	CU	70/88 (79%)	0.80	7 (10%) 8 5	84, 107, 125, 125	0
19	AV	82/93 (88%)	0.10	1 (1%) 75 42	130, 159, 169, 170	0
19	CV	84/93 (90%)	-0.03	0 100 100	118, 134, 149, 152	0
20	AW	99/106 (93%)	-0.30	1 (1%) 79 47	88, 106, 149, 157	0
20	CW	99/106 (93%)	-0.40	0 100 100	96, 119, 148, 155	0
21	AX	25/27 (92%)	-0.12	0 100 100	143, 151, 161, 165	0
21	CX	25/27 (92%)	-0.58	0 100 100	101, 131, 147, 158	0
22	AC	77/77 (100%)	-0.56	0 100 100	76, 119, 153, 162	0
22	AD	77/77 (100%)	-0.11	1 (1%) 74 40	111, 217, 236, 246	0
22	CC	77/77 (100%)	-0.57	0 100 100	68, 99, 133, 139	0
22	CD	77/77 (100%)	0.01	3 (3%) 37 16	105, 210, 222, 228	0
23	A1	23/25 (92%)	0.77	4 (17%) 2 2	101, 193, 235, 240	0
23	C1	23/25 (92%)	1.21	4 (17%) 2 2	87, 180, 239, 241	0
24	BA	2885/2885 (100%)	-0.73	17 (0%) 86 59	53, 90, 211, 243	0
25	BB	120/122 (98%)	-0.75	0 100 100	103, 144, 169, 214	0
26	BD	272/276 (98%)	0.34	8 (2%) 49 23	50, 78, 97, 112	0
26	DD	272/276 (98%)	0.33	8 (2%) 49 23	44, 63, 84, 100	0
27	BE	205/206 (99%)	0.21	5 (2%) 56 26	60, 93, 138, 151	0
27	DE	205/206 (99%)	0.49	13 (6%) 19 8	48, 84, 123, 139	0
28	BF	208/210 (99%)	0.51	11 (5%) 25 10	62, 98, 158, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	202/210 (96%)	-0.16	1 (0%) 88 64	40, 74, 112, 125	0
29	BG	181/182 (99%)	1.00	31 (17%) 2 2	120, 144, 163, 175	0
29	DG	181/182 (99%)	0.03	2 (1%) 77 44	86, 109, 136, 146	0
30	BH	170/180 (94%)	0.62	23 (13%) 4 3	121, 169, 203, 209	0
30	DH	170/180 (94%)	0.06	0 100 100	75, 101, 123, 131	0
31	BK	146/148 (98%)	0.45	2 (1%) 72 38	82, 122, 143, 151	0
31	DK	146/148 (98%)	0.17	2 (1%) 72 38	68, 112, 127, 142	0
32	BM	138/140 (98%)	0.82	14 (10%) 7 5	80, 105, 124, 129	0
32	DM	138/140 (98%)	0.16	2 (1%) 72 38	66, 84, 116, 123	0
33	BN	122/122 (100%)	0.46	2 (1%) 68 35	69, 86, 99, 105	0
33	DN	122/122 (100%)	0.55	2 (1%) 68 35	50, 77, 90, 95	0
34	BO	150/150 (100%)	0.70	12 (8%) 12 7	67, 106, 135, 158	0
34	DO	150/150 (100%)	0.43	9 (6%) 21 9	45, 88, 114, 138	0
35	BP	141/141 (100%)	0.96	19 (13%) 4 3	82, 105, 134, 178	0
35	DP	141/141 (100%)	0.46	5 (3%) 42 19	62, 86, 107, 131	0
36	B0	117/118 (99%)	-0.35	0 100 100	54, 80, 102, 119	0
36	D0	118/118 (100%)	0.01	0 100 100	54, 80, 98, 107	0
37	BQ	111/112 (99%)	0.21	4 (3%) 41 18	113, 132, 155, 167	0
37	DQ	111/112 (99%)	0.54	5 (4%) 32 14	82, 97, 130, 139	0
38	BR	137/146 (93%)	-0.09	2 (1%) 70 36	77, 93, 148, 177	0
38	DR	137/146 (93%)	0.09	2 (1%) 70 36	71, 89, 136, 157	0
39	B1	117/118 (99%)	0.87	15 (12%) 4 3	68, 94, 135, 155	0
39	D1	117/118 (99%)	-0.15	2 (1%) 67 34	53, 69, 104, 130	0
40	B2	101/101 (100%)	1.69	38 (37%) 1 1	64, 118, 132, 136	0
40	D2	101/101 (100%)	0.31	5 (4%) 28 12	52, 97, 117, 126	0
41	BS	113/113 (100%)	0.06	2 (1%) 65 33	67, 80, 101, 141	0
41	DS	113/113 (100%)	0.18	3 (2%) 52 24	53, 70, 100, 142	0
42	BT	92/96 (95%)	0.12	3 (3%) 44 20	73, 89, 111, 121	0
42	DT	92/96 (95%)	-0.19	1 (1%) 77 44	54, 70, 91, 103	0
43	BU	102/110 (92%)	0.65	9 (8%) 10 6	79, 106, 161, 172	0
43	DU	102/110 (92%)	-0.12	1 (0%) 79 47	67, 93, 134, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BV	176/206 (85%)	0.79	14 (7%) 12 7	113, 142, 185, 190	0
44	DV	172/206 (83%)	1.06	23 (13%) 4 3	90, 126, 184, 190	0
45	B3	80/85 (94%)	0.94	7 (8%) 10 6	84, 99, 113, 119	0
45	D3	77/85 (90%)	0.42	1 (1%) 74 40	67, 81, 100, 115	0
46	BZ	97/98 (98%)	0.65	8 (8%) 12 6	67, 91, 149, 174	0
46	DZ	97/98 (98%)	0.17	3 (3%) 47 22	48, 78, 141, 158	0
47	BW	69/72 (95%)	0.08	1 (1%) 72 38	80, 105, 125, 140	0
47	DW	69/72 (95%)	-0.17	1 (1%) 72 38	60, 83, 105, 122	0
48	BX	59/60 (98%)	1.31	13 (22%) 1 2	83, 107, 129, 134	0
48	DX	59/60 (98%)	0.32	2 (3%) 43 19	64, 84, 110, 124	0
49	B4	71/71 (100%)	1.69	24 (33%) 1 1	164, 193, 208, 211	0
49	D4	71/71 (100%)	0.28	0 100 100	128, 160, 185, 188	0
50	B5	59/60 (98%)	0.41	8 (13%) 4 3	57, 91, 168, 177	0
50	D5	59/60 (98%)	0.73	9 (15%) 3 3	46, 86, 186, 190	0
51	B6	48/54 (88%)	2.17	23 (47%) 1 1	138, 153, 169, 175	0
51	D6	49/54 (90%)	3.54	43 (87%) 0 0	132, 146, 156, 162	0
52	B7	49/49 (100%)	0.13	1 (2%) 62 30	51, 68, 116, 148	0
52	D7	49/49 (100%)	-0.14	2 (4%) 35 15	40, 49, 109, 135	0
53	B8	64/65 (98%)	1.13	10 (15%) 3 2	77, 93, 114, 152	0
53	D8	64/65 (98%)	0.55	2 (3%) 47 22	53, 72, 100, 127	0
54	DA	2886/2898 (99%)	-0.63	14 (0%) 88 64	35, 74, 192, 231	0
55	DB	120/120 (100%)	-0.72	0 100 100	77, 106, 126, 157	0
All	All	20970/21471 (97%)	-0.13	660 (3%) 47 22	35, 102, 176, 251	0

The worst 5 of 660 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	B8	65	GLU	12.4
24	BA	1176	G	12.2
41	DS	113	LYS	10.3
28	BF	1	MET	9.1
54	DA	2798	C	8.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	1864	1/1	0.24	-	87,87,87,87	0
56	MG	DA	3377	1/1	0.09	-	76,76,76,76	0
56	MG	CA	1881	1/1	0.07	-	144,144,144,144	0
56	MG	BA	3478	1/1	0.52	-	127,127,127,127	0
56	MG	CA	1779	1/1	0.22	-	82,82,82,82	0
56	MG	AA	1628	1/1	0.40	-	69,69,69,69	0
56	MG	DA	3154	1/1	0.14	-	48,48,48,48	0
56	MG	CA	1708	1/1	0.17	-	106,106,106,106	0
56	MG	AA	1866	1/1	0.32	-	117,117,117,117	0
56	MG	DA	3349	1/1	0.14	-	51,51,51,51	0
56	MG	BA	2936	1/1	0.24	-	50,50,50,50	0
56	MG	BA	3197	1/1	0.16	-	103,103,103,103	0
56	MG	CA	1869	1/1	0.28	-	112,112,112,112	0
56	MG	AA	1642	1/1	0.18	-	64,64,64,64	0
56	MG	DA	3425	1/1	0.15	-	37,37,37,37	0
56	MG	BA	3428	1/1	0.12	-	93,93,93,93	0
56	MG	BA	3099	1/1	0.06	-	42,42,42,42	0
56	MG	DA	3670	1/1	0.16	-	62,62,62,62	0
56	MG	BA	3556	1/1	0.14	-	82,82,82,82	0
59	C	DA	2915	20/21	0.54	-	200,201,203,204	0
56	MG	DA	3384	1/1	0.48	-	98,98,98,98	0
56	MG	AA	1957	1/1	0.17	-	82,82,82,82	0
56	MG	BA	2945	1/1	0.19	-	39,39,39,39	0
56	MG	DA	3708	1/1	0.33	-	102,102,102,102	0
56	MG	AA	1839	1/1	0.14	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3010	1/1	0.33	-	55,55,55,55	0
56	MG	CD	124	1/1	0.17	-	109,109,109,109	0
56	MG	CA	1760	1/1	0.14	-	114,114,114,114	0
56	MG	DA	3549	1/1	0.56	-	96,96,96,96	0
56	MG	DA	2972	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3446	1/1	0.14	-	74,74,74,74	0
56	MG	DA	3010	1/1	0.30	-	24,24,24,24	0
56	MG	CA	1894	1/1	0.16	-	82,82,82,82	0
56	MG	BA	3350	1/1	0.15	-	63,63,63,63	0
56	MG	DA	3588	1/1	0.08	-	68,68,68,68	0
56	MG	AA	1877	1/1	0.35	-	80,80,80,80	0
56	MG	DA	3135	1/1	0.45	-	65,65,65,65	0
56	MG	DA	3652	1/1	0.25	-	78,78,78,78	0
56	MG	AI	201	1/1	0.13	-	72,72,72,72	0
56	MG	DA	3560	1/1	0.07	-	64,64,64,64	0
56	MG	AA	1750	1/1	0.20	-	79,79,79,79	0
56	MG	DA	3663	1/1	0.46	-	109,109,109,109	0
56	MG	CA	1663	1/1	0.24	-	98,98,98,98	0
56	MG	AA	1814	1/1	0.25	-	63,63,63,63	0
56	MG	BA	3285	1/1	0.17	-	79,79,79,79	0
56	MG	DA	3125	1/1	0.32	-	56,56,56,56	0
56	MG	CG	301	1/1	0.48	-	113,113,113,113	0
56	MG	BA	3473	1/1	0.19	-	93,93,93,93	0
56	MG	BA	3186	1/1	0.16	-	83,83,83,83	0
56	MG	D5	101	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3592	1/1	0.35	-	81,81,81,81	0
56	MG	AA	1602	1/1	0.24	-	53,53,53,53	0
56	MG	AA	1920	1/1	0.07	-	115,115,115,115	0
56	MG	BE	306	1/1	0.13	-	72,72,72,72	0
56	MG	BA	3203	1/1	0.23	-	64,64,64,64	0
56	MG	CA	1658	1/1	0.23	-	76,76,76,76	0
56	MG	BA	3024	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3353	1/1	0.20	-	88,88,88,88	0
56	MG	CA	1785	1/1	0.06	-	55,55,55,55	0
56	MG	BA	3485	1/1	0.15	-	69,69,69,69	0
56	MG	DA	3177	1/1	0.05	-	26,26,26,26	0
56	MG	BA	3327	1/1	0.12	-	65,65,65,65	0
56	MG	AA	1743	1/1	0.09	-	75,75,75,75	0
56	MG	CA	1800	1/1	0.17	-	66,66,66,66	0
56	MG	BK	201	1/1	0.19	-	68,68,68,68	0
56	MG	CA	1858	1/1	0.19	-	87,87,87,87	0
56	MG	BA	3157	1/1	0.12	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3410	1/1	0.14	-	75,75,75,75	0
56	MG	BA	3378	1/1	0.33	-	129,129,129,129	0
56	MG	CC	112	1/1	0.29	-	88,88,88,88	0
56	MG	CA	1722	1/1	0.32	-	101,101,101,101	0
56	MG	AA	1686	1/1	0.19	-	60,60,60,60	0
56	MG	DA	3822	1/1	0.24	-	117,117,117,117	0
56	MG	BA	3150	1/1	0.25	-	72,72,72,72	0
56	MG	CC	108	1/1	0.08	-	70,70,70,70	0
56	MG	DA	3544	1/1	0.32	-	86,86,86,86	0
56	MG	DA	3806	1/1	0.15	-	73,73,73,73	0
56	MG	AA	1824	1/1	0.17	-	85,85,85,85	0
56	MG	AA	1751	1/1	0.22	-	73,73,73,73	0
56	MG	BA	2959	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3138	1/1	0.34	-	52,52,52,52	0
56	MG	BA	3497	1/1	0.21	-	72,72,72,72	0
61	A	CA	1607	22/23	0.33	-	188,192,193,194	0
56	MG	DA	2969	1/1	0.18	-	23,23,23,23	0
56	MG	BA	3440	1/1	0.13	-	100,100,100,100	0
56	MG	AA	1930	1/1	0.35	-	82,82,82,82	0
56	MG	DA	3365	1/1	0.40	-	93,93,93,93	0
56	MG	AA	1997	1/1	0.40	-	108,108,108,108	0
56	MG	BA	3261	1/1	0.27	-	99,99,99,99	0
56	MG	CD	110	1/1	0.21	-	102,102,102,102	0
56	MG	AA	1821	1/1	0.21	-	141,141,141,141	0
56	MG	BD	301	1/1	0.25	-	65,65,65,65	0
56	MG	DA	3487	1/1	0.25	-	98,98,98,98	0
56	MG	AA	1857	1/1	0.34	-	88,88,88,88	0
56	MG	BA	3251	1/1	0.24	-	78,78,78,78	0
56	MG	BA	3434	1/1	0.32	-	88,88,88,88	0
56	MG	DA	3826	1/1	0.40	-	118,118,118,118	0
56	MG	DA	3589	1/1	0.12	-	130,130,130,130	0
56	MG	DA	3539	1/1	0.52	-	112,112,112,112	0
56	MG	AA	1829	1/1	0.21	-	109,109,109,109	0
60	U	DA	2917	20/21	0.58	-	190,192,196,196	0
56	MG	BA	3259	1/1	0.06	-	90,90,90,90	0
56	MG	BA	3389	1/1	0.28	-	89,89,89,89	0
56	MG	DA	3469	1/1	0.26	-	66,66,66,66	0
56	MG	BA	3281	1/1	0.36	-	113,113,113,113	0
56	MG	DA	3604	1/1	0.28	-	91,91,91,91	0
56	MG	DA	3829	1/1	0.17	-	157,157,157,157	0
56	MG	BA	3357	1/1	0.15	-	66,66,66,66	0
56	MG	AA	1706	1/1	0.33	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3003	1/1	0.11	-	40,40,40,40	0
56	MG	BA	3453	1/1	0.31	-	73,73,73,73	0
56	MG	BA	3394	1/1	0.14	-	121,121,121,121	0
56	MG	BA	3064	1/1	0.33	-	76,76,76,76	0
56	MG	AD	103	1/1	0.16	-	101,101,101,101	0
56	MG	D0	204	1/1	0.27	-	95,95,95,95	0
56	MG	CX	101	1/1	0.09	-	90,90,90,90	0
56	MG	AA	1863	1/1	0.41	-	92,92,92,92	0
56	MG	BA	3304	1/1	0.10	-	63,63,63,63	0
56	MG	BA	2966	1/1	0.28	-	46,46,46,46	0
56	MG	CA	1799	1/1	0.25	-	84,84,84,84	0
56	MG	AA	1746	1/1	0.26	-	81,81,81,81	0
56	MG	BA	3013	1/1	0.23	-	60,60,60,60	0
56	MG	A1	101	1/1	0.10	-	102,102,102,102	0
56	MG	BA	3136	1/1	0.48	-	111,111,111,111	0
56	MG	DA	3227	1/1	0.17	-	50,50,50,50	0
56	MG	B5	101	1/1	0.10	-	46,46,46,46	0
56	MG	AC	101	1/1	0.10	-	88,88,88,88	0
56	MG	DA	3083	1/1	0.16	-	19,19,19,19	0
56	MG	CA	1830	1/1	0.15	-	66,66,66,66	0
56	MG	AA	1904	1/1	0.23	-	121,121,121,121	0
56	MG	DA	3155	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3525	1/1	0.16	-	66,66,66,66	0
56	MG	DA	3076	1/1	0.14	-	48,48,48,48	0
56	MG	BA	3111	1/1	0.23	-	53,53,53,53	0
56	MG	DA	3205	1/1	0.47	-	96,96,96,96	0
56	MG	BA	3069	1/1	0.09	-	48,48,48,48	0
56	MG	BA	3339	1/1	0.09	-	74,74,74,74	0
56	MG	AA	1603	1/1	0.35	-	54,54,54,54	0
56	MG	DA	3203	1/1	0.05	-	25,25,25,25	0
56	MG	AA	1936	1/1	0.06	-	74,74,74,74	0
56	MG	AA	1989	1/1	0.21	-	91,91,91,91	0
56	MG	DA	3091	1/1	0.19	-	54,54,54,54	0
56	MG	BA	3218	1/1	0.11	-	70,70,70,70	0
56	MG	AA	1725	1/1	0.32	-	92,92,92,92	0
56	MG	BA	3106	1/1	0.28	-	80,80,80,80	0
56	MG	AA	1763	1/1	0.37	-	74,74,74,74	0
56	MG	DA	3480	1/1	0.32	-	86,86,86,86	0
56	MG	D3	102	1/1	0.11	-	72,72,72,72	0
56	MG	DA	3355	1/1	0.41	-	87,87,87,87	0
56	MG	DA	3294	1/1	0.32	-	64,64,64,64	0
56	MG	BA	3367	1/1	0.39	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3162	1/1	0.20	-	48,48,48,48	0
56	MG	BA	2917	1/1	0.28	-	37,37,37,37	0
56	MG	BA	3072	1/1	0.12	-	48,48,48,48	0
56	MG	AA	1932	1/1	0.28	-	122,122,122,122	0
56	MG	BA	2996	1/1	0.28	-	68,68,68,68	0
56	MG	BA	3030	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3436	1/1	0.22	-	66,66,66,66	0
56	MG	DA	3839	1/1	0.53	-	138,138,138,138	0
56	MG	CA	1861	1/1	0.21	-	79,79,79,79	0
56	MG	AA	1635	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3049	1/1	0.22	-	71,71,71,71	0
56	MG	DA	3504	1/1	0.18	-	61,61,61,61	0
56	MG	CA	1723	1/1	0.10	-	110,110,110,110	0
56	MG	DA	2996	1/1	0.25	-	26,26,26,26	0
56	MG	DA	3442	1/1	0.24	-	91,91,91,91	0
56	MG	AA	1764	1/1	0.10	-	96,96,96,96	0
56	MG	DB	225	1/1	0.34	-	84,84,84,84	0
56	MG	BA	3375	1/1	0.15	-	112,112,112,112	0
56	MG	DA	3615	1/1	0.23	-	89,89,89,89	0
56	MG	BA	3368	1/1	0.53	-	113,113,113,113	0
56	MG	AO	201	1/1	0.17	-	70,70,70,70	0
56	MG	DB	219	1/1	0.22	-	77,77,77,77	0
56	MG	BA	3539	1/1	0.14	-	100,100,100,100	0
56	MG	DA	3647	1/1	0.50	-	99,99,99,99	0
56	MG	DA	2949	1/1	0.26	-	27,27,27,27	0
56	MG	AA	1669	1/1	0.33	-	54,54,54,54	0
56	MG	DA	3720	1/1	0.27	-	100,100,100,100	0
56	MG	BA	2941	1/1	0.21	-	27,27,27,27	0
56	MG	DA	3756	1/1	0.36	-	116,116,116,116	0
56	MG	BA	3122	1/1	0.32	-	63,63,63,63	0
56	MG	DA	3801	1/1	0.23	-	108,108,108,108	0
56	MG	CX	103	1/1	0.21	-	106,106,106,106	0
56	MG	CA	1630	1/1	0.36	-	71,71,71,71	0
56	MG	BA	2973	1/1	0.21	-	47,47,47,47	0
56	MG	DB	214	1/1	0.10	-	85,85,85,85	0
56	MG	DA	3056	1/1	0.27	-	68,68,68,68	0
56	MG	BA	3512	1/1	0.23	-	113,113,113,113	0
56	MG	BA	3158	1/1	0.10	-	39,39,39,39	0
56	MG	DA	3100	1/1	0.07	-	34,34,34,34	0
56	MG	AA	2010	1/1	0.13	-	83,83,83,83	0
56	MG	AA	1869	1/1	0.11	-	83,83,83,83	0
56	MG	DA	3591	1/1	0.40	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3461	1/1	0.15	-	77,77,77,77	0
56	MG	BE	307	1/1	0.15	-	84,84,84,84	0
56	MG	DA	3676	1/1	0.34	-	71,71,71,71	0
56	MG	CA	1933	1/1	0.20	-	81,81,81,81	0
56	MG	AA	1749	1/1	0.31	-	72,72,72,72	0
56	MG	AS	102	1/1	0.15	-	90,90,90,90	0
56	MG	DA	2991	1/1	0.02	-	16,16,16,16	0
56	MG	CA	1670	1/1	0.33	-	81,81,81,81	0
56	MG	BA	3531	1/1	0.08	-	75,75,75,75	0
56	MG	DA	2978	1/1	0.20	-	39,39,39,39	0
56	MG	DA	3342	1/1	0.11	-	63,63,63,63	0
56	MG	DA	3765	1/1	0.58	-	123,123,123,123	0
56	MG	CA	1952	1/1	0.09	-	77,77,77,77	0
56	MG	DA	3327	1/1	0.42	-	81,81,81,81	0
56	MG	DA	3426	1/1	0.27	-	70,70,70,70	0
56	MG	AA	1935	1/1	0.23	-	94,94,94,94	0
56	MG	AA	1947	1/1	0.14	-	119,119,119,119	0
56	MG	DA	3515	1/1	0.24	-	71,71,71,71	0
56	MG	BA	3160	1/1	0.25	-	65,65,65,65	0
56	MG	DA	3314	1/1	0.24	-	59,59,59,59	0
56	MG	AA	1787	1/1	0.09	-	65,65,65,65	0
56	MG	AA	1786	1/1	0.17	-	93,93,93,93	0
56	MG	DU	202	1/1	0.66	-	139,139,139,139	0
56	MG	AA	1927	1/1	0.34	-	98,98,98,98	0
56	MG	BA	3237	1/1	0.18	-	82,82,82,82	0
56	MG	CA	1846	1/1	0.10	-	65,65,65,65	0
56	MG	DA	3494	1/1	0.18	-	74,74,74,74	0
56	MG	DA	3399	1/1	0.10	-	58,58,58,58	0
56	MG	AA	2036	1/1	0.14	-	90,90,90,90	0
56	MG	DA	3694	1/1	0.13	-	88,88,88,88	0
56	MG	BA	2924	1/1	0.20	-	55,55,55,55	0
56	MG	AW	201	1/1	0.17	-	108,108,108,108	0
56	MG	BA	2964	1/1	0.25	-	45,45,45,45	0
56	MG	AA	1616	1/1	0.13	-	76,76,76,76	0
56	MG	DA	3255	1/1	0.32	-	61,61,61,61	0
56	MG	DA	3654	1/1	0.28	-	91,91,91,91	0
56	MG	BA	2951	1/1	0.21	-	38,38,38,38	0
56	MG	AA	1648	1/1	0.36	-	68,68,68,68	0
56	MG	CA	1827	1/1	0.24	-	102,102,102,102	0
56	MG	DA	3685	1/1	0.21	-	63,63,63,63	0
56	MG	CA	1702	1/1	0.23	-	62,62,62,62	0
56	MG	BA	3243	1/1	0.08	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3751	1/1	0.47	-	92,92,92,92	0
56	MG	AA	1801	1/1	0.47	-	94,94,94,94	0
56	MG	BA	3022	1/1	0.13	-	46,46,46,46	0
56	MG	CA	1758	1/1	0.16	-	96,96,96,96	0
56	MG	DA	3192	1/1	0.23	-	40,40,40,40	0
56	MG	BA	3202	1/1	0.06	-	65,65,65,65	0
56	MG	BU	202	1/1	0.12	-	73,73,73,73	0
56	MG	DA	3033	1/1	0.31	-	40,40,40,40	0
56	MG	BA	3175	1/1	0.10	-	54,54,54,54	0
56	MG	DA	3659	1/1	0.35	-	84,84,84,84	0
56	MG	DA	3834	1/1	0.68	-	85,85,85,85	0
56	MG	DA	3630	1/1	0.15	-	97,97,97,97	0
56	MG	AA	1992	1/1	0.07	-	106,106,106,106	0
56	MG	DA	3309	1/1	0.28	-	66,66,66,66	0
56	MG	AA	1699	1/1	0.27	-	95,95,95,95	0
56	MG	DA	3364	1/1	0.31	-	100,100,100,100	0
56	MG	DA	3536	1/1	0.26	-	87,87,87,87	0
56	MG	AA	1799	1/1	0.20	-	91,91,91,91	0
56	MG	CA	1836	1/1	0.06	-	98,98,98,98	0
56	MG	BA	3413	1/1	0.10	-	92,92,92,92	0
56	MG	AA	1614	1/1	0.47	-	73,73,73,73	0
56	MG	AA	1810	1/1	0.19	-	75,75,75,75	0
56	MG	DA	3029	1/1	0.22	-	43,43,43,43	0
56	MG	DA	3144	1/1	0.33	-	91,91,91,91	0
56	MG	DA	3491	1/1	0.41	-	69,69,69,69	0
56	MG	DA	3481	1/1	0.26	-	86,86,86,86	0
56	MG	DA	3030	1/1	0.44	-	57,57,57,57	0
56	MG	D0	203	1/1	0.08	-	63,63,63,63	0
56	MG	CA	1794	1/1	0.21	-	147,147,147,147	0
56	MG	BA	3189	1/1	0.30	-	76,76,76,76	0
56	MG	BB	212	1/1	0.27	-	81,81,81,81	0
56	MG	BA	3196	1/1	0.45	-	89,89,89,89	0
56	MG	DA	3068	1/1	0.24	-	53,53,53,53	0
56	MG	DA	3038	1/1	0.19	-	46,46,46,46	0
56	MG	CA	1627	1/1	0.31	-	69,69,69,69	0
56	MG	DA	3101	1/1	0.28	-	72,72,72,72	0
56	MG	DA	3119	1/1	0.39	-	67,67,67,67	0
56	MG	AA	1978	1/1	0.06	-	99,99,99,99	0
56	MG	CA	1955	1/1	0.14	-	89,89,89,89	0
56	MG	BA	3180	1/1	0.16	-	72,72,72,72	0
56	MG	BA	3392	1/1	0.14	-	70,70,70,70	0
56	MG	AA	2037	1/1	0.14	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3682	1/1	0.37	-	88,88,88,88	0
56	MG	CD	121	1/1	0.12	-	112,112,112,112	0
56	MG	AA	1974	1/1	0.25	-	96,96,96,96	0
56	MG	DA	3066	1/1	0.27	-	34,34,34,34	0
56	MG	BA	3131	1/1	0.35	-	76,76,76,76	0
56	MG	A1	102	1/1	0.10	-	66,66,66,66	0
56	MG	BA	3249	1/1	0.20	-	59,59,59,59	0
56	MG	DG	201	1/1	0.11	-	76,76,76,76	0
56	MG	DA	3427	1/1	0.36	-	72,72,72,72	0
56	MG	CA	1650	1/1	0.26	-	66,66,66,66	0
56	MG	BA	2998	1/1	0.14	-	51,51,51,51	0
56	MG	BA	2953	1/1	0.18	-	32,32,32,32	0
56	MG	BA	3227	1/1	0.25	-	82,82,82,82	0
56	MG	BB	204	1/1	0.34	-	97,97,97,97	0
56	MG	BA	2906	1/1	0.25	-	101,101,101,101	0
56	MG	DA	3439	1/1	0.14	-	70,70,70,70	0
56	MG	DA	3311	1/1	0.28	-	82,82,82,82	0
56	MG	AA	1644	1/1	0.46	-	90,90,90,90	0
56	MG	DA	3788	1/1	0.35	-	101,101,101,101	0
56	MG	AA	1842	1/1	0.16	-	72,72,72,72	0
56	MG	CA	1640	1/1	0.23	-	70,70,70,70	0
56	MG	DA	3262	1/1	0.20	-	45,45,45,45	0
56	MG	CA	1797	1/1	0.15	-	76,76,76,76	0
56	MG	BA	3466	1/1	0.07	-	84,84,84,84	0
56	MG	BA	2914	1/1	0.16	-	17,17,17,17	0
56	MG	BA	3471	1/1	0.35	-	156,156,156,156	0
56	MG	BA	3216	1/1	0.26	-	86,86,86,86	0
56	MG	BA	3056	1/1	0.28	-	71,71,71,71	0
56	MG	BA	3298	1/1	0.16	-	95,95,95,95	0
56	MG	DA	3736	1/1	0.45	-	102,102,102,102	0
56	MG	DA	3449	1/1	0.32	-	105,105,105,105	0
56	MG	AA	2017	1/1	0.12	-	92,92,92,92	0
56	MG	BA	3517	1/1	0.11	-	93,93,93,93	0
56	MG	DA	3714	1/1	0.10	-	85,85,85,85	0
56	MG	CA	1745	1/1	0.14	-	88,88,88,88	0
56	MG	DA	3219	1/1	0.23	-	71,71,71,71	0
56	MG	CA	1852	1/1	0.26	-	82,82,82,82	0
56	MG	AA	2035	1/1	0.33	-	86,86,86,86	0
56	MG	CA	1621	1/1	0.09	-	67,67,67,67	0
56	MG	DA	3027	1/1	0.25	-	27,27,27,27	0
56	MG	BA	3480	1/1	0.11	-	87,87,87,87	0
56	MG	DA	3296	1/1	0.31	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1682	1/1	0.28	-	59,59,59,59	0
56	MG	AA	1944	1/1	0.10	-	111,111,111,111	0
56	MG	BA	3039	1/1	0.21	-	58,58,58,58	0
56	MG	AA	1854	1/1	0.21	-	97,97,97,97	0
56	MG	AA	1925	1/1	0.12	-	87,87,87,87	0
56	MG	DA	3080	1/1	0.16	-	59,59,59,59	0
56	MG	BA	3050	1/1	0.36	-	67,67,67,67	0
56	MG	BA	3581	1/1	0.37	-	125,125,125,125	0
56	MG	BA	3210	1/1	0.05	-	54,54,54,54	0
56	MG	AA	1795	1/1	0.25	-	70,70,70,70	0
56	MG	DA	3001	1/1	0.18	-	21,21,21,21	0
56	MG	DA	2953	1/1	0.24	-	35,35,35,35	0
56	MG	AA	1719	1/1	0.36	-	90,90,90,90	0
56	MG	BQ	201	1/1	0.24	-	105,105,105,105	0
56	MG	CA	1862	1/1	0.14	-	99,99,99,99	0
56	MG	DA	3282	1/1	0.13	-	47,47,47,47	0
56	MG	DA	3619	1/1	0.07	-	116,116,116,116	0
56	MG	CQ	102	1/1	0.15	-	111,111,111,111	0
56	MG	BA	3031	1/1	0.08	-	82,82,82,82	0
56	MG	B0	202	1/1	0.36	-	111,111,111,111	0
56	MG	DA	3674	1/1	0.15	-	74,74,74,74	0
56	MG	DA	3018	1/1	0.26	-	60,60,60,60	0
56	MG	BA	2970	1/1	0.26	-	32,32,32,32	0
56	MG	AA	1739	1/1	0.07	-	66,66,66,66	0
56	MG	DA	3523	1/1	0.26	-	90,90,90,90	0
56	MG	DR	201	1/1	0.08	-	77,77,77,77	0
56	MG	DA	3463	1/1	0.19	-	39,39,39,39	0
56	MG	DA	2984	1/1	0.24	-	26,26,26,26	0
56	MG	DA	3533	1/1	0.26	-	69,69,69,69	0
56	MG	D7	101	1/1	0.13	-	55,55,55,55	0
56	MG	DA	3445	1/1	0.13	-	38,38,38,38	0
56	MG	BA	3023	1/1	0.27	-	52,52,52,52	0
56	MG	BA	3312	1/1	0.08	-	75,75,75,75	0
56	MG	AA	1902	1/1	0.12	-	107,107,107,107	0
56	MG	DA	3306	1/1	0.39	-	99,99,99,99	0
56	MG	AA	1627	1/1	0.33	-	70,70,70,70	0
56	MG	DA	3302	1/1	0.24	-	84,84,84,84	0
56	MG	BA	3103	1/1	0.16	-	53,53,53,53	0
56	MG	CA	1801	1/1	0.26	-	80,80,80,80	0
56	MG	AA	1730	1/1	0.46	-	85,85,85,85	0
56	MG	BB	206	1/1	0.26	-	85,85,85,85	0
56	MG	DA	3049	1/1	0.23	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CC	118	1/1	0.18	-	99,99,99,99	0
56	MG	BA	3271	1/1	0.10	-	59,59,59,59	0
56	MG	AA	1761	1/1	0.51	-	136,136,136,136	0
56	MG	CA	1980	1/1	0.13	-	116,116,116,116	0
56	MG	AA	1785	1/1	0.09	-	78,78,78,78	0
56	MG	DD	301	1/1	0.23	-	43,43,43,43	0
56	MG	AA	1942	1/1	0.11	-	128,128,128,128	0
56	MG	DA	3600	1/1	0.10	-	76,76,76,76	0
56	MG	DA	3272	1/1	0.30	-	71,71,71,71	0
56	MG	CA	1948	1/1	0.10	-	88,88,88,88	0
56	MG	AA	1879	1/1	0.04	-	85,85,85,85	0
56	MG	BA	3374	1/1	0.13	-	39,39,39,39	0
56	MG	DA	3502	1/1	0.69	-	104,104,104,104	0
56	MG	BA	3119	1/1	0.17	-	51,51,51,51	0
56	MG	BA	3087	1/1	0.25	-	72,72,72,72	0
56	MG	CA	1875	1/1	0.21	-	72,72,72,72	0
56	MG	BA	3058	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3549	1/1	0.30	-	110,110,110,110	0
56	MG	CA	1908	1/1	0.16	-	103,103,103,103	0
56	MG	AA	1716	1/1	0.08	-	66,66,66,66	0
56	MG	BA	3521	1/1	0.21	-	109,109,109,109	0
56	MG	AA	1980	1/1	0.10	-	136,136,136,136	0
56	MG	AA	1870	1/1	0.16	-	92,92,92,92	0
56	MG	BA	3526	1/1	0.09	-	100,100,100,100	0
56	MG	BA	3173	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3693	1/1	0.68	-	136,136,136,136	0
56	MG	CA	1646	1/1	0.13	-	42,42,42,42	0
56	MG	DA	3257	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3481	1/1	0.09	-	80,80,80,80	0
56	MG	BA	3028	1/1	0.11	-	41,41,41,41	0
56	MG	CA	1641	1/1	0.18	-	54,54,54,54	0
56	MG	CA	1666	1/1	0.22	-	101,101,101,101	0
56	MG	BA	2915	1/1	0.20	-	34,34,34,34	0
56	MG	DA	3790	1/1	0.29	-	92,92,92,92	0
56	MG	DA	3518	1/1	0.19	-	91,91,91,91	0
56	MG	CA	1697	1/1	0.13	-	74,74,74,74	0
56	MG	DA	3371	1/1	0.33	-	45,45,45,45	0
56	MG	CA	1898	1/1	0.10	-	113,113,113,113	0
56	MG	DA	3323	1/1	0.29	-	58,58,58,58	0
56	MG	DA	3025	1/1	0.26	-	42,42,42,42	0
56	MG	BE	301	1/1	0.14	-	60,60,60,60	0
56	MG	AA	1895	1/1	0.13	-	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1905	1/1	0.27	-	122,122,122,122	0
56	MG	BA	3329	1/1	0.15	-	69,69,69,69	0
56	MG	BA	3482	1/1	0.12	-	101,101,101,101	0
56	MG	BA	3005	1/1	0.34	-	70,70,70,70	0
56	MG	DA	3325	1/1	0.32	-	91,91,91,91	0
56	MG	DA	3072	1/1	0.24	-	55,55,55,55	0
56	MG	DA	2948	1/1	0.32	-	34,34,34,34	0
56	MG	DA	3614	1/1	0.10	-	80,80,80,80	0
56	MG	BA	3036	1/1	0.19	-	41,41,41,41	0
56	MG	BA	3568	1/1	0.12	-	123,123,123,123	0
56	MG	DA	3065	1/1	0.29	-	59,59,59,59	0
56	MG	DA	3139	1/1	0.24	-	49,49,49,49	0
56	MG	BA	3468	1/1	0.39	-	110,110,110,110	0
56	MG	BB	225	1/1	0.23	-	90,90,90,90	0
56	MG	BA	3129	1/1	0.23	-	72,72,72,72	0
56	MG	CD	118	1/1	0.09	-	60,60,60,60	0
56	MG	BA	3372	1/1	0.16	-	53,53,53,53	0
56	MG	DA	3798	1/1	0.30	-	112,112,112,112	0
56	MG	DA	3731	1/1	0.35	-	110,110,110,110	0
56	MG	AA	1607	1/1	0.20	-	68,68,68,68	0
56	MG	DA	3633	1/1	0.21	-	110,110,110,110	0
56	MG	BA	3290	1/1	0.08	-	91,91,91,91	0
56	MG	BA	3380	1/1	0.19	-	71,71,71,71	0
56	MG	DA	3253	1/1	0.09	-	88,88,88,88	0
56	MG	BA	3410	1/1	0.13	-	82,82,82,82	0
56	MG	CA	1947	1/1	0.14	-	112,112,112,112	0
56	MG	CA	1620	1/1	0.31	-	60,60,60,60	0
56	MG	AJ	201	1/1	0.20	-	116,116,116,116	0
56	MG	DA	3103	1/1	0.42	-	59,59,59,59	0
56	MG	DA	3274	1/1	0.31	-	68,68,68,68	0
56	MG	DA	3495	1/1	0.10	-	71,71,71,71	0
56	MG	BA	3123	1/1	0.35	-	71,71,71,71	0
56	MG	BA	3346	1/1	0.17	-	52,52,52,52	0
56	MG	AA	1826	1/1	0.37	-	108,108,108,108	0
56	MG	AA	1977	1/1	0.30	-	86,86,86,86	0
56	MG	DA	3347	1/1	0.42	-	66,66,66,66	0
56	MG	AA	1704	1/1	0.28	-	88,88,88,88	0
56	MG	AA	1738	1/1	0.30	-	84,84,84,84	0
56	MG	DA	3093	1/1	0.36	-	71,71,71,71	0
56	MG	BA	2938	1/1	0.23	-	39,39,39,39	0
56	MG	BA	3417	1/1	0.10	-	97,97,97,97	0
56	MG	CW	204	1/1	0.06	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	2952	1/1	0.17	-	41,41,41,41	0
56	MG	DA	3732	1/1	0.10	-	60,60,60,60	0
56	MG	BB	203	1/1	0.10	-	85,85,85,85	0
56	MG	CD	126	1/1	0.21	-	82,82,82,82	0
56	MG	D6	102	1/1	0.38	-	94,94,94,94	0
56	MG	AA	1914	1/1	0.12	-	109,109,109,109	0
58	G	CA	1606	23/24	0.44	-	180,186,187,187	0
56	MG	DA	3376	1/1	0.37	-	67,67,67,67	0
56	MG	AA	1744	1/1	0.20	-	77,77,77,77	0
56	MG	BA	3379	1/1	0.18	-	98,98,98,98	0
56	MG	BB	220	1/1	0.32	-	80,80,80,80	0
56	MG	DA	3021	1/1	0.39	-	46,46,46,46	0
56	MG	DA	3424	1/1	0.23	-	83,83,83,83	0
56	MG	BA	3195	1/1	0.13	-	124,124,124,124	0
56	MG	BA	3554	1/1	0.16	-	122,122,122,122	0
56	MG	BA	3441	1/1	0.12	-	144,144,144,144	0
56	MG	BA	3484	1/1	0.18	-	106,106,106,106	0
56	MG	BA	3075	1/1	0.08	-	37,37,37,37	0
56	MG	AA	1940	1/1	0.21	-	91,91,91,91	0
56	MG	DB	202	1/1	0.13	-	87,87,87,87	0
56	MG	AA	1867	1/1	0.30	-	85,85,85,85	0
56	MG	DA	2976	1/1	0.25	-	45,45,45,45	0
56	MG	DA	3022	1/1	0.22	-	27,27,27,27	0
56	MG	DA	3337	1/1	0.03	-	28,28,28,28	0
56	MG	BA	3575	1/1	0.13	-	82,82,82,82	0
56	MG	DA	3707	1/1	0.18	-	98,98,98,98	0
56	MG	CA	1705	1/1	0.20	-	101,101,101,101	0
56	MG	BA	3017	1/1	0.15	-	48,48,48,48	0
56	MG	BA	3494	1/1	0.16	-	65,65,65,65	0
56	MG	DA	3754	1/1	0.25	-	88,88,88,88	0
56	MG	BA	3519	1/1	0.05	-	90,90,90,90	0
56	MG	BA	3408	1/1	0.09	-	75,75,75,75	0
56	MG	CA	1714	1/1	0.19	-	106,106,106,106	0
56	MG	DA	3796	1/1	0.33	-	84,84,84,84	0
56	MG	DA	3020	1/1	0.37	-	34,34,34,34	0
56	MG	DA	3697	1/1	0.26	-	87,87,87,87	0
56	MG	CA	1818	1/1	0.22	-	108,108,108,108	0
56	MG	BA	2968	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3038	1/1	0.19	-	39,39,39,39	0
56	MG	DA	3653	1/1	0.20	-	59,59,59,59	0
56	MG	DA	3516	1/1	0.10	-	73,73,73,73	0
56	MG	BA	2912	1/1	0.20	-	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3554	1/1	0.14	-	81,81,81,81	0
56	MG	DA	3290	1/1	0.43	-	67,67,67,67	0
56	MG	DA	3386	1/1	0.18	-	56,56,56,56	0
56	MG	BA	3248	1/1	0.08	-	81,81,81,81	0
56	MG	BA	3317	1/1	0.14	-	63,63,63,63	0
56	MG	CA	1893	1/1	0.29	-	120,120,120,120	0
56	MG	DA	3006	1/1	0.35	-	36,36,36,36	0
56	MG	AA	1643	1/1	0.10	-	124,124,124,124	0
56	MG	CA	1900	1/1	0.34	-	81,81,81,81	0
56	MG	BA	3344	1/1	0.12	-	69,69,69,69	0
56	MG	DA	3595	1/1	0.19	-	65,65,65,65	0
56	MG	BA	3397	1/1	0.17	-	47,47,47,47	0
56	MG	AP	201	1/1	0.13	-	82,82,82,82	0
56	MG	CA	1748	1/1	0.39	-	123,123,123,123	0
56	MG	AA	1964	1/1	0.53	-	103,103,103,103	0
56	MG	DA	3795	1/1	0.13	-	65,65,65,65	0
56	MG	CA	1944	1/1	0.17	-	81,81,81,81	0
56	MG	DA	3734	1/1	0.32	-	89,89,89,89	0
56	MG	BA	2979	1/1	0.25	-	60,60,60,60	0
56	MG	DA	3741	1/1	0.49	-	134,134,134,134	0
56	MG	DA	3248	1/1	0.18	-	71,71,71,71	0
56	MG	CA	1954	1/1	0.21	-	205,205,205,205	0
56	MG	CA	1618	1/1	0.19	-	42,42,42,42	0
56	MG	BB	222	1/1	0.14	-	93,93,93,93	0
56	MG	DA	3369	1/1	0.21	-	67,67,67,67	0
56	MG	CA	1741	1/1	0.22	-	73,73,73,73	0
56	MG	BA	3563	1/1	0.18	-	74,74,74,74	0
56	MG	CA	1895	1/1	0.10	-	112,112,112,112	0
56	MG	DA	3316	1/1	0.27	-	98,98,98,98	0
56	MG	CA	1725	1/1	0.29	-	96,96,96,96	0
56	MG	DA	2980	1/1	0.28	-	29,29,29,29	0
56	MG	BA	3272	1/1	0.17	-	66,66,66,66	0
56	MG	CA	1913	1/1	0.12	-	107,107,107,107	0
60	U	CA	1604	20/21	0.24	-	135,138,147,147	0
56	MG	BA	3213	1/1	0.12	-	61,61,61,61	0
56	MG	AA	1671	1/1	0.15	-	66,66,66,66	0
56	MG	BA	3279	1/1	0.26	-	85,85,85,85	0
56	MG	CA	1882	1/1	0.20	-	110,110,110,110	0
56	MG	BA	3229	1/1	0.21	-	77,77,77,77	0
56	MG	DA	3454	1/1	0.12	-	120,120,120,120	0
56	MG	DA	3140	1/1	0.21	-	76,76,76,76	0
56	MG	DA	3142	1/1	0.34	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1820	1/1	0.14	-	98,98,98,98	0
56	MG	CA	1979	1/1	0.11	-	61,61,61,61	0
56	MG	CA	1770	1/1	0.15	-	72,72,72,72	0
56	MG	CD	123	1/1	0.10	-	81,81,81,81	0
56	MG	CA	1644	1/1	0.25	-	70,70,70,70	0
56	MG	DA	3202	1/1	0.15	-	33,33,33,33	0
56	MG	CA	1912	1/1	0.05	-	92,92,92,92	0
56	MG	BA	3362	1/1	0.12	-	68,68,68,68	0
56	MG	CA	1732	1/1	0.24	-	54,54,54,54	0
56	MG	BB	201	1/1	0.22	-	69,69,69,69	0
56	MG	DA	3273	1/1	0.23	-	60,60,60,60	0
56	MG	AA	1848	1/1	0.13	-	70,70,70,70	0
56	MG	AA	1873	1/1	0.11	-	80,80,80,80	0
56	MG	BA	3090	1/1	0.19	-	61,61,61,61	0
56	MG	BA	3422	1/1	0.21	-	83,83,83,83	0
56	MG	CA	1755	1/1	0.12	-	71,71,71,71	0
56	MG	AA	1733	1/1	0.20	-	102,102,102,102	0
56	MG	DA	3428	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3635	1/1	0.15	-	79,79,79,79	0
56	MG	AA	1872	1/1	0.12	-	108,108,108,108	0
56	MG	DA	2970	1/1	0.24	-	31,31,31,31	0
56	MG	BA	3506	1/1	0.07	-	77,77,77,77	0
56	MG	AA	1674	1/1	0.22	-	74,74,74,74	0
56	MG	BR	202	1/1	0.22	-	105,105,105,105	0
56	MG	CA	1788	1/1	0.36	-	118,118,118,118	0
56	MG	CA	1904	1/1	0.28	-	105,105,105,105	0
56	MG	DA	3007	1/1	0.22	-	49,49,49,49	0
56	MG	DA	3500	1/1	0.48	-	155,155,155,155	0
56	MG	CP	206	1/1	0.19	-	122,122,122,122	0
56	MG	BA	3254	1/1	0.23	-	101,101,101,101	0
56	MG	DA	3054	1/1	0.31	-	43,43,43,43	0
56	MG	DA	3258	1/1	0.38	-	75,75,75,75	0
56	MG	DA	3385	1/1	0.13	-	58,58,58,58	0
56	MG	CA	1726	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3172	1/1	0.31	-	48,48,48,48	0
56	MG	CA	1989	1/1	0.07	-	80,80,80,80	0
56	MG	DA	3650	1/1	0.12	-	70,70,70,70	0
56	MG	BA	3277	1/1	0.13	-	73,73,73,73	0
56	MG	D0	201	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3314	1/1	0.20	-	76,76,76,76	0
56	MG	BA	3034	1/1	0.19	-	61,61,61,61	0
56	MG	DA	3250	1/1	0.21	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3416	1/1	0.49	-	100,100,100,100	0
56	MG	BA	2984	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3609	1/1	0.10	-	60,60,60,60	0
56	MG	DA	2963	1/1	0.12	-	23,23,23,23	0
56	MG	AA	1889	1/1	0.07	-	68,68,68,68	0
56	MG	CA	1782	1/1	0.23	-	99,99,99,99	0
56	MG	CA	1776	1/1	0.18	-	81,81,81,81	0
56	MG	DA	2973	1/1	0.39	-	48,48,48,48	0
56	MG	BA	3496	1/1	0.10	-	73,73,73,73	0
56	MG	AA	1970	1/1	0.27	-	98,98,98,98	0
56	MG	BA	3548	1/1	0.26	-	81,81,81,81	0
56	MG	DA	2994	1/1	0.23	-	20,20,20,20	0
56	MG	DA	3324	1/1	0.21	-	63,63,63,63	0
56	MG	AA	1928	1/1	0.30	-	117,117,117,117	0
56	MG	BA	3306	1/1	0.53	-	105,105,105,105	0
56	MG	DA	3688	1/1	0.20	-	98,98,98,98	0
56	MG	AA	1701	1/1	0.23	-	72,72,72,72	0
56	MG	DA	2992	1/1	0.38	-	39,39,39,39	0
56	MG	CA	1982	1/1	0.25	-	110,110,110,110	0
56	MG	BA	2969	1/1	0.28	-	33,33,33,33	0
56	MG	AA	1849	1/1	0.23	-	92,92,92,92	0
56	MG	AA	1682	1/1	0.39	-	87,87,87,87	0
56	MG	DA	3780	1/1	0.36	-	111,111,111,111	0
56	MG	BA	3266	1/1	0.35	-	97,97,97,97	0
56	MG	BA	3310	1/1	0.14	-	80,80,80,80	0
56	MG	CA	1974	1/1	0.07	-	113,113,113,113	0
58	G	DP	206	23/24	0.49	-	189,190,191,193	0
56	MG	DA	3367	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3319	1/1	0.49	-	108,108,108,108	0
56	MG	AA	1922	1/1	0.22	-	94,94,94,94	0
56	MG	DA	3031	1/1	0.26	-	37,37,37,37	0
56	MG	DA	3329	1/1	0.21	-	83,83,83,83	0
56	MG	CA	1792	1/1	0.23	-	69,69,69,69	0
56	MG	DA	3345	1/1	0.23	-	49,49,49,49	0
56	MG	DA	3059	1/1	0.26	-	36,36,36,36	0
56	MG	AA	1691	1/1	0.25	-	62,62,62,62	0
56	MG	BA	3490	1/1	0.32	-	107,107,107,107	0
56	MG	DA	3542	1/1	0.32	-	88,88,88,88	0
56	MG	DO	204	1/1	0.19	-	65,65,65,65	0
56	MG	AA	1742	1/1	0.31	-	83,83,83,83	0
56	MG	CA	1635	1/1	0.37	-	87,87,87,87	0
56	MG	CA	1608	1/1	0.21	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3255	1/1	0.25	-	93,93,93,93	0
56	MG	CA	1938	1/1	0.13	-	84,84,84,84	0
56	MG	DA	3555	1/1	0.26	-	78,78,78,78	0
56	MG	AA	1782	1/1	0.29	-	106,106,106,106	0
56	MG	BA	3201	1/1	0.30	-	97,97,97,97	0
56	MG	CA	1812	1/1	0.07	-	89,89,89,89	0
56	MG	DA	2946	1/1	0.30	-	25,25,25,25	0
56	MG	BA	2948	1/1	0.19	-	29,29,29,29	0
56	MG	CC	120	1/1	0.15	-	67,67,67,67	0
56	MG	DA	3151	1/1	0.43	-	72,72,72,72	0
56	MG	DA	3813	1/1	0.13	-	71,71,71,71	0
56	MG	AA	1732	1/1	0.18	-	89,89,89,89	0
56	MG	DA	3583	1/1	0.22	-	68,68,68,68	0
56	MG	DA	3388	1/1	0.15	-	88,88,88,88	0
56	MG	DA	3042	1/1	0.42	-	69,69,69,69	0
56	MG	CA	1717	1/1	0.21	-	53,53,53,53	0
56	MG	BA	3328	1/1	0.20	-	105,105,105,105	0
56	MG	DA	3019	1/1	0.29	-	47,47,47,47	0
56	MG	AW	203	1/1	0.23	-	114,114,114,114	0
56	MG	AA	1905	1/1	0.19	-	96,96,96,96	0
56	MG	DA	2939	1/1	0.29	-	44,44,44,44	0
56	MG	AA	1734	1/1	0.24	-	60,60,60,60	0
56	MG	D1	204	1/1	0.25	-	71,71,71,71	0
56	MG	DA	3778	1/1	0.17	-	97,97,97,97	0
56	MG	DA	3256	1/1	0.36	-	80,80,80,80	0
56	MG	DA	3783	1/1	0.09	-	64,64,64,64	0
56	MG	BA	3390	1/1	0.12	-	77,77,77,77	0
56	MG	AA	1823	1/1	0.35	-	104,104,104,104	0
56	MG	BA	3425	1/1	0.04	-	98,98,98,98	0
56	MG	DA	3032	1/1	0.32	-	40,40,40,40	0
56	MG	CA	1820	1/1	0.18	-	127,127,127,127	0
56	MG	DA	3825	1/1	0.32	-	111,111,111,111	0
56	MG	BA	3135	1/1	0.30	-	62,62,62,62	0
56	MG	AA	1847	1/1	0.26	-	91,91,91,91	0
56	MG	BA	3001	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3363	1/1	0.61	-	105,105,105,105	0
56	MG	BA	3360	1/1	0.33	-	117,117,117,117	0
56	MG	DA	3092	1/1	0.16	-	41,41,41,41	0
56	MG	CA	1803	1/1	0.05	-	35,35,35,35	0
56	MG	DA	3046	1/1	0.24	-	41,41,41,41	0
56	MG	BA	3269	1/1	0.09	-	90,90,90,90	0
56	MG	AA	1815	1/1	0.17	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3558	1/1	0.18	-	108,108,108,108	0
56	MG	CA	1969	1/1	0.16	-	90,90,90,90	0
56	MG	BA	3398	1/1	0.10	-	131,131,131,131	0
56	MG	BA	2910	1/1	0.10	-	149,149,149,149	0
56	MG	CA	1868	1/1	0.15	-	109,109,109,109	0
56	MG	DA	3581	1/1	0.29	-	87,87,87,87	0
56	MG	DA	3221	1/1	0.22	-	66,66,66,66	0
60	U	DA	2922	20/21	0.61	-	202,204,205,206	0
56	MG	AA	1844	1/1	0.30	-	108,108,108,108	0
56	MG	AA	2006	1/1	0.12	-	86,86,86,86	0
56	MG	AA	2025	1/1	0.33	-	71,71,71,71	0
56	MG	CC	109	1/1	0.15	-	87,87,87,87	0
56	MG	CA	1930	1/1	0.15	-	104,104,104,104	0
56	MG	CA	1653	1/1	0.08	-	53,53,53,53	0
56	MG	DA	3280	1/1	0.17	-	65,65,65,65	0
56	MG	AA	1630	1/1	0.35	-	55,55,55,55	0
56	MG	CA	1766	1/1	0.29	-	113,113,113,113	0
56	MG	BA	2990	1/1	0.22	-	48,48,48,48	0
56	MG	BA	2963	1/1	0.15	-	32,32,32,32	0
56	MG	DA	3833	1/1	0.09	-	82,82,82,82	0
56	MG	DA	3651	1/1	0.15	-	67,67,67,67	0
56	MG	BA	3096	1/1	0.20	-	37,37,37,37	0
56	MG	DA	3661	1/1	0.22	-	82,82,82,82	0
56	MG	DA	3211	1/1	0.10	-	66,66,66,66	0
56	MG	BA	3443	1/1	0.07	-	79,79,79,79	0
56	MG	AA	1837	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3384	1/1	0.20	-	76,76,76,76	0
56	MG	BB	216	1/1	0.15	-	83,83,83,83	0
56	MG	DA	3433	1/1	0.22	-	85,85,85,85	0
56	MG	AA	1708	1/1	0.28	-	70,70,70,70	0
56	MG	BA	3455	1/1	0.19	-	78,78,78,78	0
56	MG	AA	1611	1/1	0.37	-	63,63,63,63	0
60	U	C1	102	20/21	0.22	-	126,134,138,138	0
56	MG	CA	1789	1/1	0.37	-	123,123,123,123	0
56	MG	BA	3511	1/1	0.09	-	140,140,140,140	0
56	MG	DA	3701	1/1	0.15	-	104,104,104,104	0
56	MG	CA	1688	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3730	1/1	0.17	-	56,56,56,56	0
58	G	DA	2909	23/24	0.26	-	232,233,236,236	0
56	MG	BA	3004	1/1	0.16	-	30,30,30,30	0
56	MG	DA	3486	1/1	0.11	-	95,95,95,95	0
56	MG	DA	3183	1/1	0.18	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1934	1/1	0.14	-	88,88,88,88	0
56	MG	BA	3033	1/1	0.24	-	45,45,45,45	0
56	MG	DA	3704	1/1	0.34	-	112,112,112,112	0
56	MG	BA	3228	1/1	0.18	-	83,83,83,83	0
56	MG	BA	3359	1/1	0.10	-	73,73,73,73	0
56	MG	AL	202	1/1	0.29	-	129,129,129,129	0
56	MG	AC	108	1/1	0.10	-	61,61,61,61	0
56	MG	CA	1685	1/1	0.13	-	66,66,66,66	0
56	MG	BA	3543	1/1	0.19	-	72,72,72,72	0
56	MG	DA	3104	1/1	0.24	-	47,47,47,47	0
56	MG	AA	2003	1/1	0.10	-	128,128,128,128	0
56	MG	AA	1883	1/1	0.16	-	64,64,64,64	0
56	MG	BA	3470	1/1	0.15	-	79,79,79,79	0
56	MG	DA	3836	1/1	0.20	-	92,92,92,92	0
56	MG	DA	3004	1/1	0.17	-	39,39,39,39	0
56	MG	BA	3303	1/1	0.10	-	41,41,41,41	0
56	MG	DA	3562	1/1	0.31	-	78,78,78,78	0
56	MG	AA	1679	1/1	0.25	-	74,74,74,74	0
56	MG	DA	3466	1/1	0.15	-	83,83,83,83	0
56	MG	CD	104	1/1	0.05	-	83,83,83,83	0
56	MG	DA	3180	1/1	0.22	-	68,68,68,68	0
56	MG	BA	3077	1/1	0.12	-	46,46,46,46	0
56	MG	DA	3612	1/1	0.18	-	80,80,80,80	0
56	MG	AA	1612	1/1	0.42	-	68,68,68,68	0
56	MG	BA	3070	1/1	0.21	-	53,53,53,53	0
56	MG	BA	3324	1/1	0.27	-	87,87,87,87	0
56	MG	BA	2982	1/1	0.38	-	61,61,61,61	0
56	MG	AA	1621	1/1	0.29	-	50,50,50,50	0
56	MG	CA	1614	1/1	0.29	-	73,73,73,73	0
56	MG	BA	3098	1/1	0.23	-	60,60,60,60	0
56	MG	CK	202	1/1	0.10	-	87,87,87,87	0
56	MG	BA	2977	1/1	0.16	-	33,33,33,33	0
56	MG	AA	1606	1/1	0.23	-	55,55,55,55	0
56	MG	AA	1937	1/1	0.21	-	95,95,95,95	0
56	MG	DA	3394	1/1	0.21	-	77,77,77,77	0
56	MG	DA	3052	1/1	0.18	-	41,41,41,41	0
56	MG	AA	1737	1/1	0.17	-	97,97,97,97	0
56	MG	BA	2985	1/1	0.06	-	46,46,46,46	0
56	MG	AA	1931	1/1	0.32	-	98,98,98,98	0
56	MG	AA	1818	1/1	0.11	-	64,64,64,64	0
60	U	DA	2914	20/21	0.52	-	199,203,205,205	0
56	MG	AA	1899	1/1	0.24	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3690	1/1	0.34	-	88,88,88,88	0
56	MG	BA	2931	1/1	0.20	-	29,29,29,29	0
56	MG	DA	3171	1/1	0.54	-	111,111,111,111	0
56	MG	CD	119	1/1	0.04	-	95,95,95,95	0
56	MG	BA	3015	1/1	0.24	-	70,70,70,70	0
56	MG	BA	3400	1/1	0.09	-	117,117,117,117	0
60	U	DA	2927	20/21	0.41	-	197,201,202,203	0
56	MG	DA	3642	1/1	0.16	-	80,80,80,80	0
56	MG	CA	1802	1/1	0.06	-	78,78,78,78	0
56	MG	BA	3289	1/1	0.28	-	71,71,71,71	0
56	MG	DA	3173	1/1	0.30	-	53,53,53,53	0
56	MG	BA	3206	1/1	0.18	-	67,67,67,67	0
56	MG	D1	205	1/1	0.40	-	110,110,110,110	0
56	MG	CA	1768	1/1	0.09	-	129,129,129,129	0
56	MG	CA	1855	1/1	0.25	-	130,130,130,130	0
56	MG	BA	3162	1/1	0.28	-	69,69,69,69	0
56	MG	CA	1822	1/1	0.38	-	105,105,105,105	0
56	MG	DA	3460	1/1	0.16	-	62,62,62,62	0
56	MG	DA	3259	1/1	0.53	-	83,83,83,83	0
56	MG	DA	3540	1/1	0.21	-	74,74,74,74	0
56	MG	CA	1678	1/1	0.12	-	77,77,77,77	0
56	MG	DA	3571	1/1	0.19	-	86,86,86,86	0
56	MG	DA	3522	1/1	0.10	-	56,56,56,56	0
56	MG	AA	1629	1/1	0.33	-	74,74,74,74	0
56	MG	CA	1750	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3214	1/1	0.18	-	38,38,38,38	0
56	MG	BA	3048	1/1	0.08	-	41,41,41,41	0
56	MG	CA	1879	1/1	0.19	-	84,84,84,84	0
56	MG	DA	3270	1/1	0.22	-	51,51,51,51	0
56	MG	DA	3036	1/1	0.29	-	44,44,44,44	0
56	MG	CA	1917	1/1	0.26	-	130,130,130,130	0
56	MG	BA	3082	1/1	0.37	-	59,59,59,59	0
56	MG	CA	1884	1/1	0.29	-	62,62,62,62	0
56	MG	C1	104	1/1	0.09	-	65,65,65,65	0
56	MG	AA	1609	1/1	0.39	-	71,71,71,71	0
56	MG	AA	1946	1/1	0.07	-	82,82,82,82	0
56	MG	CA	1710	1/1	0.18	-	62,62,62,62	0
56	MG	AA	1892	1/1	0.13	-	99,99,99,99	0
56	MG	DA	3368	1/1	0.15	-	70,70,70,70	0
56	MG	AA	1731	1/1	0.30	-	63,63,63,63	0
56	MG	CA	1616	1/1	0.34	-	54,54,54,54	0
56	MG	B3	101	1/1	0.15	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	2000	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3231	1/1	0.10	-	68,68,68,68	0
56	MG	CA	1828	1/1	0.40	-	104,104,104,104	0
56	MG	DA	3313	1/1	0.25	-	70,70,70,70	0
56	MG	AT	202	1/1	0.25	-	111,111,111,111	0
56	MG	DA	3800	1/1	0.15	-	71,71,71,71	0
56	MG	CA	1856	1/1	0.16	-	91,91,91,91	0
56	MG	BW	101	1/1	0.11	-	65,65,65,65	0
56	MG	DA	3753	1/1	0.26	-	86,86,86,86	0
56	MG	CA	1667	1/1	0.23	-	74,74,74,74	0
56	MG	BA	2958	1/1	0.20	-	44,44,44,44	0
56	MG	DA	3761	1/1	0.24	-	106,106,106,106	0
61	A	C1	101	22/23	0.17	-	138,139,140,140	0
56	MG	BA	2957	1/1	0.18	-	33,33,33,33	0
56	MG	DA	3077	1/1	0.17	-	44,44,44,44	0
56	MG	BA	3161	1/1	0.47	-	96,96,96,96	0
56	MG	DA	3578	1/1	0.16	-	54,54,54,54	0
56	MG	DA	3594	1/1	0.30	-	97,97,97,97	0
56	MG	DA	3009	1/1	0.30	-	41,41,41,41	0
56	MG	AA	1707	1/1	0.23	-	64,64,64,64	0
56	MG	AA	1665	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3245	1/1	0.18	-	57,57,57,57	0
56	MG	DA	3163	1/1	0.30	-	65,65,65,65	0
56	MG	CA	1654	1/1	0.24	-	81,81,81,81	0
56	MG	BA	3146	1/1	0.18	-	78,78,78,78	0
56	MG	AA	1769	1/1	0.22	-	80,80,80,80	0
56	MG	DA	3641	1/1	0.15	-	43,43,43,43	0
56	MG	CW	203	1/1	0.11	-	111,111,111,111	0
56	MG	DA	3348	1/1	0.31	-	100,100,100,100	0
56	MG	BA	3429	1/1	0.18	-	56,56,56,56	0
56	MG	CA	1971	1/1	0.12	-	94,94,94,94	0
56	MG	DA	3819	1/1	0.12	-	83,83,83,83	0
56	MG	DA	3000	1/1	0.35	-	45,45,45,45	0
58	G	DP	201	23/24	0.31	-	190,191,192,193	0
56	MG	DA	3373	1/1	0.50	-	127,127,127,127	0
56	MG	AA	1955	1/1	0.32	-	103,103,103,103	0
56	MG	DA	3766	1/1	0.09	-	73,73,73,73	0
56	MG	BA	3487	1/1	0.10	-	74,74,74,74	0
56	MG	AD	102	1/1	0.19	-	120,120,120,120	0
56	MG	AA	1990	1/1	0.13	-	97,97,97,97	0
56	MG	DA	3057	1/1	0.26	-	58,58,58,58	0
56	MG	DA	3375	1/1	0.14	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BB	221	1/1	0.12	-	106,106,106,106	0
56	MG	AA	2032	1/1	0.17	-	84,84,84,84	0
56	MG	BA	3322	1/1	0.25	-	72,72,72,72	0
56	MG	CA	1835	1/1	0.20	-	89,89,89,89	0
56	MG	BA	3407	1/1	0.37	-	106,106,106,106	0
56	MG	D1	206	1/1	0.15	-	66,66,66,66	0
56	MG	DA	3457	1/1	0.10	-	91,91,91,91	0
56	MG	CA	1762	1/1	0.30	-	70,70,70,70	0
56	MG	CA	1754	1/1	0.34	-	93,93,93,93	0
56	MG	BA	3552	1/1	0.10	-	76,76,76,76	0
56	MG	BA	3045	1/1	0.18	-	26,26,26,26	0
56	MG	DA	3107	1/1	0.24	-	40,40,40,40	0
56	MG	BA	3144	1/1	0.15	-	68,68,68,68	0
56	MG	AA	1949	1/1	0.16	-	122,122,122,122	0
56	MG	AL	201	1/1	0.21	-	79,79,79,79	0
61	A	DA	2911	22/23	0.51	-	216,217,221,222	0
56	MG	CA	1669	1/1	0.18	-	61,61,61,61	0
56	MG	CA	1826	1/1	0.07	-	61,61,61,61	0
56	MG	BA	2927	1/1	0.28	-	32,32,32,32	0
56	MG	DA	2986	1/1	0.20	-	35,35,35,35	0
56	MG	DA	3148	1/1	0.30	-	48,48,48,48	0
56	MG	DA	3820	1/1	0.35	-	84,84,84,84	0
56	MG	DA	3577	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3097	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3500	1/1	0.07	-	64,64,64,64	0
56	MG	DA	3398	1/1	0.27	-	75,75,75,75	0
56	MG	AA	1918	1/1	0.09	-	84,84,84,84	0
56	MG	BA	3219	1/1	0.04	-	48,48,48,48	0
56	MG	CA	1910	1/1	0.24	-	134,134,134,134	0
56	MG	DA	2974	1/1	0.19	-	25,25,25,25	0
56	MG	DA	3450	1/1	0.33	-	99,99,99,99	0
56	MG	DA	3530	1/1	0.15	-	78,78,78,78	0
56	MG	DA	3420	1/1	0.18	-	32,32,32,32	0
56	MG	DA	3553	1/1	0.17	-	99,99,99,99	0
56	MG	DA	3352	1/1	0.37	-	81,81,81,81	0
56	MG	CA	1987	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3305	1/1	0.12	-	62,62,62,62	0
56	MG	BA	3182	1/1	0.09	-	41,41,41,41	0
56	MG	BA	3294	1/1	0.20	-	65,65,65,65	0
56	MG	AA	1758	1/1	0.14	-	108,108,108,108	0
56	MG	DA	3321	1/1	0.23	-	75,75,75,75	0
56	MG	CA	1773	1/1	0.28	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1626	1/1	0.21	-	73,73,73,73	0
59	C	CP	203	20/21	0.38	-	164,172,175,176	0
58	G	DA	2906	23/24	0.44	-	200,204,206,207	0
56	MG	CA	1738	1/1	0.08	-	86,86,86,86	0
56	MG	DA	3047	1/1	0.32	-	86,86,86,86	0
56	MG	DA	3343	1/1	0.24	-	65,65,65,65	0
56	MG	AA	2027	1/1	0.14	-	81,81,81,81	0
56	MG	DA	3493	1/1	0.40	-	92,92,92,92	0
56	MG	DA	2938	1/1	0.30	-	28,28,28,28	0
56	MG	AA	1651	1/1	0.31	-	60,60,60,60	0
56	MG	CA	1613	1/1	0.19	-	70,70,70,70	0
56	MG	AA	1605	1/1	0.33	-	61,61,61,61	0
56	MG	CA	1655	1/1	0.31	-	79,79,79,79	0
56	MG	CP	208	1/1	0.36	-	137,137,137,137	0
56	MG	CW	202	1/1	0.04	-	108,108,108,108	0
56	MG	BE	305	1/1	0.15	-	68,68,68,68	0
56	MG	DA	3758	1/1	0.09	-	50,50,50,50	0
56	MG	CD	112	1/1	0.09	-	85,85,85,85	0
56	MG	BA	3046	1/1	0.17	-	29,29,29,29	0
56	MG	BA	3577	1/1	0.12	-	80,80,80,80	0
56	MG	AA	1890	1/1	0.13	-	72,72,72,72	0
56	MG	BA	3449	1/1	0.16	-	76,76,76,76	0
56	MG	CD	102	1/1	0.10	-	99,99,99,99	0
56	MG	AA	1859	1/1	0.08	-	77,77,77,77	0
56	MG	AA	1658	1/1	0.20	-	57,57,57,57	0
56	MG	DA	3777	1/1	0.29	-	88,88,88,88	0
56	MG	BB	226	1/1	0.20	-	146,146,146,146	0
56	MG	DA	3168	1/1	0.24	-	63,63,63,63	0
56	MG	AA	1948	1/1	0.07	-	82,82,82,82	0
56	MG	BA	2934	1/1	0.36	-	42,42,42,42	0
56	MG	DA	3193	1/1	0.44	-	95,95,95,95	0
56	MG	DA	2989	1/1	0.36	-	39,39,39,39	0
56	MG	CA	1656	1/1	0.43	-	86,86,86,86	0
56	MG	CA	1978	1/1	0.21	-	116,116,116,116	0
56	MG	AA	1967	1/1	0.16	-	84,84,84,84	0
56	MG	CA	1831	1/1	0.34	-	156,156,156,156	0
56	MG	CA	1781	1/1	0.17	-	66,66,66,66	0
57	ZN	AQ	102	1/1	0.12	-	142,142,142,142	0
56	MG	AA	1853	1/1	0.19	-	104,104,104,104	0
56	MG	BA	2955	1/1	0.28	-	29,29,29,29	0
56	MG	CA	1638	1/1	0.26	-	68,68,68,68	0
56	MG	CA	1897	1/1	0.06	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3503	1/1	0.15	-	66,66,66,66	0
56	MG	CA	1724	1/1	0.26	-	76,76,76,76	0
56	MG	DA	3241	1/1	0.42	-	62,62,62,62	0
56	MG	DA	3782	1/1	0.17	-	95,95,95,95	0
56	MG	DA	3598	1/1	0.21	-	59,59,59,59	0
56	MG	CA	1709	1/1	0.22	-	71,71,71,71	0
56	MG	CA	1983	1/1	0.17	-	103,103,103,103	0
56	MG	AA	1898	1/1	0.14	-	102,102,102,102	0
56	MG	CA	1927	1/1	0.20	-	81,81,81,81	0
60	U	DA	2902	20/21	0.51	-	207,208,214,214	0
56	MG	DA	3552	1/1	0.14	-	100,100,100,100	0
56	MG	CA	1662	1/1	0.26	-	68,68,68,68	0
56	MG	BA	3457	1/1	0.20	-	80,80,80,80	0
56	MG	DA	3823	1/1	0.19	-	70,70,70,70	0
56	MG	DA	3832	1/1	0.50	-	112,112,112,112	0
56	MG	BA	3535	1/1	0.15	-	94,94,94,94	0
56	MG	CA	1692	1/1	0.13	-	59,59,59,59	0
56	MG	AA	1999	1/1	0.18	-	100,100,100,100	0
56	MG	AA	1755	1/1	0.33	-	62,62,62,62	0
56	MG	DA	3069	1/1	0.17	-	40,40,40,40	0
56	MG	AA	1876	1/1	0.28	-	78,78,78,78	0
56	MG	BA	3474	1/1	0.29	-	78,78,78,78	0
56	MG	BA	3120	1/1	0.22	-	75,75,75,75	0
56	MG	DA	3737	1/1	0.10	-	75,75,75,75	0
56	MG	BA	3114	1/1	0.15	-	67,67,67,67	0
57	ZN	CG	302	1/1	0.24	-	94,94,94,94	0
56	MG	DA	3733	1/1	0.10	-	85,85,85,85	0
56	MG	CA	1940	1/1	0.11	-	69,69,69,69	0
56	MG	BE	303	1/1	0.07	-	45,45,45,45	0
56	MG	BU	204	1/1	0.18	-	94,94,94,94	0
56	MG	CA	1647	1/1	0.07	-	53,53,53,53	0
56	MG	AA	1954	1/1	0.32	-	108,108,108,108	0
56	MG	AA	1961	1/1	0.06	-	46,46,46,46	0
56	MG	DA	3838	1/1	0.49	-	101,101,101,101	0
56	MG	DA	3356	1/1	0.19	-	71,71,71,71	0
56	MG	AA	1656	1/1	0.16	-	71,71,71,71	0
56	MG	BA	3560	1/1	0.10	-	48,48,48,48	0
56	MG	DA	3743	1/1	0.25	-	78,78,78,78	0
56	MG	DA	3725	1/1	0.42	-	111,111,111,111	0
56	MG	DA	3263	1/1	0.17	-	74,74,74,74	0
56	MG	DA	3189	1/1	0.25	-	52,52,52,52	0
56	MG	DA	2983	1/1	0.39	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1817	1/1	0.17	-	92,92,92,92	0
56	MG	DO	205	1/1	0.18	-	90,90,90,90	0
61	A	DA	2930	22/23	0.41	-	193,196,197,197	0
56	MG	CA	1690	1/1	0.20	-	70,70,70,70	0
56	MG	BA	3236	1/1	0.13	-	33,33,33,33	0
56	MG	DA	3750	1/1	0.16	-	144,144,144,144	0
56	MG	CA	1749	1/1	0.18	-	124,124,124,124	0
56	MG	DA	3464	1/1	0.09	-	65,65,65,65	0
56	MG	AA	2004	1/1	0.32	-	124,124,124,124	0
56	MG	DA	3706	1/1	0.29	-	70,70,70,70	0
56	MG	DA	3587	1/1	0.24	-	76,76,76,76	0
56	MG	AA	1619	1/1	0.39	-	55,55,55,55	0
56	MG	DA	3213	1/1	0.26	-	57,57,57,57	0
56	MG	BE	304	1/1	0.25	-	86,86,86,86	0
56	MG	CA	1747	1/1	0.14	-	104,104,104,104	0
56	MG	DA	3179	1/1	0.30	-	61,61,61,61	0
56	MG	AA	1740	1/1	0.17	-	69,69,69,69	0
56	MG	DA	3160	1/1	0.24	-	66,66,66,66	0
56	MG	DA	3574	1/1	0.42	-	73,73,73,73	0
56	MG	CA	1740	1/1	0.19	-	67,67,67,67	0
56	MG	BA	3080	1/1	0.20	-	69,69,69,69	0
56	MG	AA	1649	1/1	0.17	-	84,84,84,84	0
56	MG	DA	3514	1/1	0.15	-	83,83,83,83	0
56	MG	AA	1678	1/1	0.24	-	57,57,57,57	0
56	MG	DA	3791	1/1	0.46	-	99,99,99,99	0
56	MG	DB	221	1/1	0.28	-	94,94,94,94	0
56	MG	BA	3340	1/1	0.09	-	77,77,77,77	0
56	MG	BA	3006	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3419	1/1	0.28	-	91,91,91,91	0
56	MG	AA	1759	1/1	0.28	-	77,77,77,77	0
56	MG	CA	1883	1/1	0.20	-	83,83,83,83	0
56	MG	DA	3568	1/1	0.45	-	90,90,90,90	0
56	MG	BA	3530	1/1	0.12	-	110,110,110,110	0
56	MG	DA	3499	1/1	0.32	-	80,80,80,80	0
56	MG	BA	3377	1/1	0.12	-	67,67,67,67	0
56	MG	DA	3496	1/1	0.18	-	64,64,64,64	0
56	MG	DH	203	1/1	0.05	-	65,65,65,65	0
59	C	DA	2934	20/21	0.42	-	199,202,203,204	0
56	MG	BA	3308	1/1	0.34	-	78,78,78,78	0
56	MG	DA	3095	1/1	0.28	-	54,54,54,54	0
56	MG	CD	120	1/1	0.08	-	110,110,110,110	0
56	MG	AA	1660	1/1	0.12	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1718	1/1	0.35	-	75,75,75,75	0
56	MG	DA	3188	1/1	0.46	-	89,89,89,89	0
56	MG	DA	3028	1/1	0.46	-	75,75,75,75	0
56	MG	CA	1986	1/1	0.12	-	104,104,104,104	0
56	MG	AA	1792	1/1	0.31	-	74,74,74,74	0
56	MG	AA	1617	1/1	0.39	-	77,77,77,77	0
56	MG	DA	3382	1/1	0.29	-	80,80,80,80	0
56	MG	AA	1721	1/1	0.35	-	72,72,72,72	0
56	MG	BA	3242	1/1	0.19	-	82,82,82,82	0
56	MG	BA	3057	1/1	0.17	-	65,65,65,65	0
56	MG	CA	1891	1/1	0.07	-	59,59,59,59	0
56	MG	CA	1634	1/1	0.28	-	50,50,50,50	0
56	MG	DA	3667	1/1	0.18	-	67,67,67,67	0
56	MG	AA	1668	1/1	0.54	-	107,107,107,107	0
56	MG	DU	204	1/1	0.30	-	99,99,99,99	0
56	MG	DA	3175	1/1	0.33	-	56,56,56,56	0
59	C	DA	2923	20/21	0.32	-	207,209,210,210	0
56	MG	DA	3391	1/1	0.16	-	55,55,55,55	0
56	MG	BA	2962	1/1	0.13	-	20,20,20,20	0
56	MG	DA	3133	1/1	0.26	-	57,57,57,57	0
56	MG	BA	3371	1/1	0.09	-	55,55,55,55	0
56	MG	BA	3352	1/1	0.18	-	112,112,112,112	0
56	MG	AA	1926	1/1	0.15	-	102,102,102,102	0
56	MG	DA	3742	1/1	0.24	-	97,97,97,97	0
56	MG	DA	3827	1/1	0.19	-	109,109,109,109	0
56	MG	AA	1881	1/1	0.13	-	77,77,77,77	0
60	U	DA	2910	20/21	0.69	-	222,224,231,231	0
56	MG	CA	1823	1/1	0.20	-	65,65,65,65	0
56	MG	DA	3346	1/1	0.14	-	20,20,20,20	0
56	MG	BA	3438	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3366	1/1	0.14	-	69,69,69,69	0
56	MG	BA	3143	1/1	0.36	-	74,74,74,74	0
56	MG	DA	3405	1/1	0.31	-	87,87,87,87	0
56	MG	CA	1786	1/1	0.27	-	104,104,104,104	0
56	MG	BA	3188	1/1	0.22	-	68,68,68,68	0
56	MG	CA	1959	1/1	0.52	-	134,134,134,134	0
56	MG	BA	3358	1/1	0.20	-	101,101,101,101	0
56	MG	BU	203	1/1	0.08	-	74,74,74,74	0
56	MG	BA	3516	1/1	0.17	-	56,56,56,56	0
56	MG	AA	1659	1/1	0.22	-	81,81,81,81	0
56	MG	AA	1667	1/1	0.23	-	61,61,61,61	0
56	MG	CQ	103	1/1	0.09	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1624	1/1	0.21	-	44,44,44,44	0
56	MG	CA	1645	1/1	0.28	-	60,60,60,60	0
56	MG	DA	3408	1/1	0.19	-	79,79,79,79	0
56	MG	DA	3799	1/1	0.08	-	119,119,119,119	0
56	MG	BA	3118	1/1	0.20	-	82,82,82,82	0
56	MG	CA	1878	1/1	0.08	-	73,73,73,73	0
56	MG	AA	1680	1/1	0.21	-	70,70,70,70	0
56	MG	CA	1866	1/1	0.14	-	121,121,121,121	0
56	MG	DA	3016	1/1	0.26	-	31,31,31,31	0
56	MG	BA	3502	1/1	0.14	-	91,91,91,91	0
56	MG	CA	1968	1/1	0.23	-	78,78,78,78	0
56	MG	DA	3547	1/1	0.11	-	43,43,43,43	0
56	MG	DA	3315	1/1	0.24	-	78,78,78,78	0
56	MG	CA	1877	1/1	0.14	-	69,69,69,69	0
56	MG	AA	1714	1/1	0.06	-	89,89,89,89	0
56	MG	CC	114	1/1	0.13	-	102,102,102,102	0
56	MG	DB	220	1/1	0.33	-	122,122,122,122	0
56	MG	CA	1664	1/1	0.29	-	96,96,96,96	0
59	C	DA	2928	20/21	0.36	-	192,195,200,200	0
56	MG	DA	3700	1/1	0.11	-	76,76,76,76	0
56	MG	BA	3198	1/1	0.12	-	58,58,58,58	0
56	MG	BA	2923	1/1	0.20	-	44,44,44,44	0
56	MG	BF	302	1/1	0.40	-	117,117,117,117	0
56	MG	DA	2968	1/1	0.28	-	24,24,24,24	0
56	MG	BA	3079	1/1	0.14	-	59,59,59,59	0
56	MG	CA	1744	1/1	0.04	-	132,132,132,132	0
56	MG	CA	1949	1/1	0.14	-	101,101,101,101	0
56	MG	DH	202	1/1	0.55	-	98,98,98,98	0
57	ZN	CQ	104	1/1	0.09	-	142,142,142,142	0
56	MG	CP	205	1/1	0.25	-	118,118,118,118	0
56	MG	DA	3161	1/1	0.18	-	66,66,66,66	0
56	MG	DA	3328	1/1	0.20	-	76,76,76,76	0
56	MG	AA	1690	1/1	0.13	-	91,91,91,91	0
56	MG	AA	2028	1/1	0.14	-	102,102,102,102	0
56	MG	AC	105	1/1	0.10	-	88,88,88,88	0
56	MG	AA	1965	1/1	0.30	-	117,117,117,117	0
56	MG	BA	3145	1/1	0.16	-	74,74,74,74	0
56	MG	D1	203	1/1	0.12	-	84,84,84,84	0
56	MG	CA	1696	1/1	0.14	-	62,62,62,62	0
56	MG	DA	3026	1/1	0.24	-	42,42,42,42	0
56	MG	AA	1783	1/1	0.34	-	90,90,90,90	0
56	MG	DA	3656	1/1	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1830	1/1	0.25	-	88,88,88,88	0
56	MG	AA	2011	1/1	0.35	-	120,120,120,120	0
61	A	DA	2929	22/23	0.32	-	188,191,195,195	0
56	MG	BA	3393	1/1	0.12	-	82,82,82,82	0
56	MG	DA	3498	1/1	0.23	-	66,66,66,66	0
56	MG	DH	201	1/1	0.10	-	77,77,77,77	0
56	MG	BA	3542	1/1	0.08	-	78,78,78,78	0
56	MG	DA	3235	1/1	0.24	-	82,82,82,82	0
56	MG	D0	205	1/1	0.81	-	95,95,95,95	0
56	MG	DU	203	1/1	0.18	-	94,94,94,94	0
56	MG	AA	1919	1/1	0.30	-	117,117,117,117	0
56	MG	BA	2975	1/1	0.20	-	40,40,40,40	0
56	MG	BA	3051	1/1	0.26	-	74,74,74,74	0
56	MG	AA	1756	1/1	0.21	-	68,68,68,68	0
56	MG	DA	3658	1/1	0.12	-	75,75,75,75	0
56	MG	BA	3148	1/1	0.11	-	42,42,42,42	0
56	MG	CA	1928	1/1	0.20	-	70,70,70,70	0
56	MG	DA	3643	1/1	0.33	-	72,72,72,72	0
56	MG	DA	3671	1/1	0.49	-	63,63,63,63	0
56	MG	BA	3332	1/1	0.11	-	60,60,60,60	0
56	MG	AA	2039	1/1	0.09	-	64,64,64,64	0
56	MG	CA	1880	1/1	0.03	-	117,117,117,117	0
56	MG	BA	3007	1/1	0.23	-	51,51,51,51	0
56	MG	BA	3492	1/1	0.07	-	86,86,86,86	0
56	MG	BA	3076	1/1	0.20	-	88,88,88,88	0
56	MG	DA	3285	1/1	0.24	-	56,56,56,56	0
56	MG	AA	1909	1/1	0.51	-	128,128,128,128	0
56	MG	DW	102	1/1	0.16	-	91,91,91,91	0
56	MG	DA	3546	1/1	0.26	-	94,94,94,94	0
56	MG	CA	1832	1/1	0.14	-	106,106,106,106	0
59	C	CC	106	20/21	0.71	-	226,229,230,230	0
56	MG	DA	3178	1/1	0.23	-	78,78,78,78	0
56	MG	AA	1775	1/1	0.31	-	88,88,88,88	0
56	MG	DA	3130	1/1	0.29	-	53,53,53,53	0
56	MG	DA	3655	1/1	0.30	-	113,113,113,113	0
56	MG	DA	3411	1/1	0.17	-	75,75,75,75	0
56	MG	DA	3287	1/1	0.22	-	44,44,44,44	0
56	MG	AA	2033	1/1	0.24	-	106,106,106,106	0
56	MG	DA	3772	1/1	0.14	-	82,82,82,82	0
56	MG	DA	3660	1/1	0.10	-	81,81,81,81	0
56	MG	BA	3060	1/1	0.09	-	35,35,35,35	0
56	MG	BA	3092	1/1	0.10	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3698	1/1	0.15	-	79,79,79,79	0
56	MG	DA	3014	1/1	0.05	-	32,32,32,32	0
56	MG	BA	3117	1/1	0.14	-	93,93,93,93	0
56	MG	DW	101	1/1	0.23	-	75,75,75,75	0
56	MG	DA	3035	1/1	0.17	-	44,44,44,44	0
56	MG	DA	3387	1/1	0.35	-	109,109,109,109	0
56	MG	DA	3567	1/1	0.23	-	59,59,59,59	0
56	MG	CA	1657	1/1	0.11	-	52,52,52,52	0
56	MG	DA	3317	1/1	0.14	-	33,33,33,33	0
56	MG	AA	1610	1/1	0.29	-	68,68,68,68	0
56	MG	BA	3256	1/1	0.21	-	64,64,64,64	0
56	MG	BA	2946	1/1	0.31	-	50,50,50,50	0
56	MG	CA	1674	1/1	0.05	-	93,93,93,93	0
56	MG	BA	3185	1/1	0.13	-	84,84,84,84	0
56	MG	BA	3337	1/1	0.17	-	73,73,73,73	0
56	MG	BA	2944	1/1	0.18	-	29,29,29,29	0
56	MG	DA	3113	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3307	1/1	0.19	-	79,79,79,79	0
56	MG	BA	3421	1/1	0.25	-	88,88,88,88	0
56	MG	DA	3657	1/1	0.35	-	98,98,98,98	0
56	MG	CA	1816	1/1	0.18	-	78,78,78,78	0
56	MG	CA	1914	1/1	0.09	-	83,83,83,83	0
56	MG	AA	1788	1/1	0.12	-	91,91,91,91	0
56	MG	AA	1683	1/1	0.28	-	60,60,60,60	0
56	MG	DA	3207	1/1	0.25	-	31,31,31,31	0
56	MG	DA	3417	1/1	0.19	-	78,78,78,78	0
56	MG	CA	1777	1/1	0.13	-	85,85,85,85	0
56	MG	DA	3565	1/1	0.33	-	80,80,80,80	0
56	MG	DA	3145	1/1	0.35	-	58,58,58,58	0
59	C	DA	2937	20/21	0.87	-	217,217,218,218	0
56	MG	BB	223	1/1	0.11	-	122,122,122,122	0
56	MG	CA	1945	1/1	0.25	-	85,85,85,85	0
56	MG	DA	3807	1/1	0.32	-	87,87,87,87	0
56	MG	DE	303	1/1	0.10	-	20,20,20,20	0
56	MG	DA	3438	1/1	0.07	-	182,182,182,182	0
56	MG	DA	2964	1/1	0.29	-	53,53,53,53	0
56	MG	AA	1840	1/1	0.45	-	132,132,132,132	0
56	MG	DA	3521	1/1	0.13	-	72,72,72,72	0
56	MG	CA	1687	1/1	0.25	-	99,99,99,99	0
56	MG	CD	105	1/1	0.06	-	124,124,124,124	0
56	MG	DA	3166	1/1	0.12	-	57,57,57,57	0
56	MG	CA	1844	1/1	0.17	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3510	1/1	0.24	-	91,91,91,91	0
56	MG	AA	1972	1/1	0.22	-	78,78,78,78	0
56	MG	AA	1784	1/1	0.04	-	76,76,76,76	0
56	MG	DA	3291	1/1	0.18	-	38,38,38,38	0
56	MG	BA	3524	1/1	0.14	-	52,52,52,52	0
56	MG	BA	2919	1/1	0.13	-	29,29,29,29	0
56	MG	DB	217	1/1	0.33	-	122,122,122,122	0
56	MG	DA	3541	1/1	0.07	-	81,81,81,81	0
56	MG	AA	1694	1/1	0.31	-	66,66,66,66	0
56	MG	AA	1994	1/1	0.10	-	86,86,86,86	0
56	MG	CA	1609	1/1	0.19	-	29,29,29,29	0
56	MG	DA	3837	1/1	0.20	-	86,86,86,86	0
56	MG	BA	3139	1/1	0.10	-	40,40,40,40	0
56	MG	CA	1729	1/1	0.20	-	99,99,99,99	0
56	MG	DA	3299	1/1	0.12	-	84,84,84,84	0
56	MG	BA	3351	1/1	0.07	-	69,69,69,69	0
56	MG	BA	2921	1/1	0.31	-	41,41,41,41	0
56	MG	DA	3488	1/1	0.24	-	80,80,80,80	0
56	MG	BA	3544	1/1	0.13	-	71,71,71,71	0
56	MG	BA	3316	1/1	0.38	-	110,110,110,110	0
56	MG	BA	3456	1/1	0.10	-	86,86,86,86	0
56	MG	BA	3226	1/1	0.29	-	88,88,88,88	0
56	MG	BA	3163	1/1	0.07	-	63,63,63,63	0
56	MG	DA	3447	1/1	0.28	-	95,95,95,95	0
56	MG	B3	102	1/1	0.09	-	58,58,58,58	0
56	MG	BA	3451	1/1	0.18	-	64,64,64,64	0
56	MG	CA	1711	1/1	0.16	-	88,88,88,88	0
56	MG	AA	1693	1/1	0.10	-	95,95,95,95	0
56	MG	DA	3721	1/1	0.18	-	83,83,83,83	0
56	MG	AA	1924	1/1	0.26	-	114,114,114,114	0
56	MG	AA	1921	1/1	0.16	-	76,76,76,76	0
56	MG	BA	3335	1/1	0.41	-	86,86,86,86	0
56	MG	AA	1720	1/1	0.13	-	76,76,76,76	0
56	MG	DA	3543	1/1	0.30	-	63,63,63,63	0
56	MG	DA	3740	1/1	0.23	-	99,99,99,99	0
56	MG	D2	201	1/1	0.34	-	110,110,110,110	0
56	MG	DA	3683	1/1	0.23	-	87,87,87,87	0
56	MG	D3	101	1/1	0.20	-	48,48,48,48	0
56	MG	AH	201	1/1	0.30	-	103,103,103,103	0
56	MG	CA	1946	1/1	0.08	-	87,87,87,87	0
56	MG	CA	1795	1/1	0.22	-	86,86,86,86	0
56	MG	BA	2902	1/1	0.20	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1829	1/1	0.15	-	92,92,92,92	0
56	MG	DA	3570	1/1	0.10	-	91,91,91,91	0
56	MG	DA	3397	1/1	0.09	-	67,67,67,67	0
56	MG	CA	1649	1/1	0.21	-	48,48,48,48	0
56	MG	BA	3547	1/1	0.20	-	74,74,74,74	0
56	MG	CA	1805	1/1	0.07	-	112,112,112,112	0
56	MG	BA	3012	1/1	0.17	-	56,56,56,56	0
56	MG	DA	3034	1/1	0.27	-	41,41,41,41	0
56	MG	DA	3679	1/1	0.26	-	81,81,81,81	0
56	MG	BA	2907	1/1	0.31	-	106,106,106,106	0
56	MG	CA	1925	1/1	0.14	-	93,93,93,93	0
56	MG	BA	3205	1/1	0.17	-	92,92,92,92	0
56	MG	AA	1645	1/1	0.20	-	55,55,55,55	0
56	MG	DA	3665	1/1	0.11	-	70,70,70,70	0
56	MG	AA	1735	1/1	0.41	-	108,108,108,108	0
56	MG	DA	3646	1/1	0.26	-	86,86,86,86	0
56	MG	DA	3507	1/1	0.28	-	79,79,79,79	0
56	MG	CA	1873	1/1	0.16	-	118,118,118,118	0
56	MG	BG	201	1/1	0.20	-	117,117,117,117	0
58	G	DA	2933	23/24	0.44	-	193,200,205,206	0
56	MG	BA	3207	1/1	0.14	-	67,67,67,67	0
56	MG	BA	3073	1/1	0.30	-	71,71,71,71	0
56	MG	AA	1956	1/1	0.29	-	118,118,118,118	0
56	MG	BA	3318	1/1	0.18	-	76,76,76,76	0
56	MG	BA	2988	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3292	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3430	1/1	0.14	-	90,90,90,90	0
56	MG	DA	3746	1/1	0.19	-	84,84,84,84	0
56	MG	CA	1661	1/1	0.11	-	80,80,80,80	0
56	MG	AA	1702	1/1	0.26	-	71,71,71,71	0
56	MG	CA	1695	1/1	0.39	-	76,76,76,76	0
56	MG	BA	3091	1/1	0.16	-	59,59,59,59	0
56	MG	DA	3586	1/1	0.41	-	70,70,70,70	0
56	MG	BA	3212	1/1	0.20	-	87,87,87,87	0
56	MG	DA	3378	1/1	0.21	-	64,64,64,64	0
56	MG	CA	1619	1/1	0.08	-	37,37,37,37	0
56	MG	DA	3264	1/1	0.22	-	66,66,66,66	0
56	MG	CQ	101	1/1	0.04	-	71,71,71,71	0
59	C	DA	2907	20/21	0.59	-	206,207,208,208	0
56	MG	BA	2918	1/1	0.32	-	46,46,46,46	0
56	MG	DA	2947	1/1	0.23	-	25,25,25,25	0
56	MG	DA	3218	1/1	0.13	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1962	1/1	0.44	-	102,102,102,102	0
56	MG	BA	2981	1/1	0.23	-	58,58,58,58	0
56	MG	AA	1841	1/1	0.35	-	100,100,100,100	0
56	MG	CD	106	1/1	0.18	-	94,94,94,94	0
56	MG	CA	1870	1/1	0.12	-	121,121,121,121	0
56	MG	DA	3120	1/1	0.18	-	56,56,56,56	0
56	MG	CA	1887	1/1	0.21	-	130,130,130,130	0
56	MG	DA	3232	1/1	0.32	-	77,77,77,77	0
56	MG	CA	1730	1/1	0.13	-	111,111,111,111	0
56	MG	CD	107	1/1	0.20	-	122,122,122,122	0
56	MG	CA	1716	1/1	0.11	-	58,58,58,58	0
56	MG	CA	1651	1/1	0.17	-	52,52,52,52	0
56	MG	BA	2949	1/1	0.39	-	62,62,62,62	0
56	MG	BA	3479	1/1	0.23	-	119,119,119,119	0
56	MG	DA	3043	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3439	1/1	0.24	-	73,73,73,73	0
56	MG	DA	3722	1/1	0.12	-	66,66,66,66	0
56	MG	CA	1863	1/1	0.04	-	74,74,74,74	0
56	MG	DA	3476	1/1	0.51	-	104,104,104,104	0
56	MG	BA	3283	1/1	0.37	-	126,126,126,126	0
56	MG	CA	1972	1/1	0.33	-	92,92,92,92	0
56	MG	DA	3374	1/1	0.18	-	59,59,59,59	0
56	MG	AA	1850	1/1	0.41	-	112,112,112,112	0
56	MG	AA	1718	1/1	0.06	-	63,63,63,63	0
56	MG	BA	2933	1/1	0.15	-	50,50,50,50	0
56	MG	BA	3467	1/1	0.06	-	81,81,81,81	0
56	MG	DA	3305	1/1	0.45	-	73,73,73,73	0
56	MG	CA	1771	1/1	0.12	-	83,83,83,83	0
58	G	CP	201	23/24	0.40	-	175,178,181,181	0
56	MG	DT	101	1/1	0.10	-	51,51,51,51	0
56	MG	AA	2022	1/1	0.11	-	117,117,117,117	0
56	MG	CA	1680	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3044	1/1	0.11	-	114,114,114,114	0
56	MG	DA	3181	1/1	0.16	-	43,43,43,43	0
56	MG	AA	1981	1/1	0.09	-	115,115,115,115	0
56	MG	DA	3062	1/1	0.16	-	25,25,25,25	0
56	MG	DA	3520	1/1	0.18	-	66,66,66,66	0
56	MG	BA	3086	1/1	0.25	-	50,50,50,50	0
56	MG	DA	3492	1/1	0.09	-	80,80,80,80	0
56	MG	BA	2909	1/1	0.07	-	66,66,66,66	0
56	MG	DA	2941	1/1	0.20	-	22,22,22,22	0
56	MG	AA	1809	1/1	0.34	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3369	1/1	0.06	-	73,73,73,73	0
56	MG	AA	2012	1/1	0.18	-	117,117,117,117	0
56	MG	DA	3067	1/1	0.26	-	49,49,49,49	0
56	MG	CA	1778	1/1	0.14	-	101,101,101,101	0
56	MG	BA	3067	1/1	0.26	-	43,43,43,43	0
56	MG	DA	3559	1/1	0.09	-	66,66,66,66	0
56	MG	BA	3191	1/1	0.39	-	79,79,79,79	0
56	MG	BA	3386	1/1	0.16	-	85,85,85,85	0
56	MG	BA	3078	1/1	0.21	-	57,57,57,57	0
56	MG	AA	1943	1/1	0.07	-	83,83,83,83	0
56	MG	BA	3325	1/1	0.16	-	98,98,98,98	0
56	MG	DA	2942	1/1	0.27	-	23,23,23,23	0
56	MG	AA	1962	1/1	0.16	-	55,55,55,55	0
56	MG	AA	1695	1/1	0.40	-	73,73,73,73	0
56	MG	BA	3215	1/1	0.17	-	58,58,58,58	0
56	MG	DB	204	1/1	0.16	-	94,94,94,94	0
56	MG	CA	1623	1/1	0.15	-	68,68,68,68	0
56	MG	DA	3085	1/1	0.25	-	67,67,67,67	0
56	MG	AA	1779	1/1	0.09	-	114,114,114,114	0
56	MG	DA	3436	1/1	0.27	-	86,86,86,86	0
56	MG	DA	3575	1/1	0.12	-	91,91,91,91	0
56	MG	DA	3002	1/1	0.42	-	49,49,49,49	0
56	MG	BA	3562	1/1	0.20	-	94,94,94,94	0
56	MG	BA	3529	1/1	0.12	-	88,88,88,88	0
56	MG	AA	1675	1/1	0.20	-	62,62,62,62	0
56	MG	CA	1839	1/1	0.14	-	79,79,79,79	0
56	MG	CA	1675	1/1	0.27	-	62,62,62,62	0
56	MG	AA	1838	1/1	0.22	-	77,77,77,77	0
56	MG	BA	3240	1/1	0.41	-	71,71,71,71	0
56	MG	CA	1727	1/1	0.18	-	94,94,94,94	0
56	MG	BA	3156	1/1	0.32	-	68,68,68,68	0
56	MG	DA	3358	1/1	0.29	-	70,70,70,70	0
56	MG	DA	3150	1/1	0.19	-	43,43,43,43	0
56	MG	BA	3267	1/1	0.29	-	102,102,102,102	0
56	MG	DA	3292	1/1	0.30	-	53,53,53,53	0
56	MG	DA	3088	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3551	1/1	0.08	-	98,98,98,98	0
56	MG	CA	1612	1/1	0.16	-	39,39,39,39	0
56	MG	BA	3557	1/1	0.16	-	131,131,131,131	0
56	MG	BA	2928	1/1	0.16	-	46,46,46,46	0
56	MG	DA	3828	1/1	0.24	-	114,114,114,114	0
56	MG	CC	117	1/1	0.14	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	C	DA	2913	20/21	0.47	-	206,207,211,211	0
56	MG	DB	211	1/1	0.25	-	78,78,78,78	0
56	MG	CA	1943	1/1	0.05	-	90,90,90,90	0
56	MG	DA	3252	1/1	0.33	-	58,58,58,58	0
56	MG	DA	3625	1/1	0.12	-	91,91,91,91	0
56	MG	BA	3347	1/1	0.18	-	99,99,99,99	0
56	MG	DA	3164	1/1	0.28	-	78,78,78,78	0
56	MG	DA	3787	1/1	0.13	-	57,57,57,57	0
56	MG	DA	3276	1/1	0.23	-	67,67,67,67	0
56	MG	BB	219	1/1	0.04	-	124,124,124,124	0
56	MG	AA	1689	1/1	0.16	-	93,93,93,93	0
56	MG	BA	3002	1/1	0.24	-	62,62,62,62	0
56	MG	BA	3068	1/1	0.25	-	72,72,72,72	0
56	MG	CA	1853	1/1	0.21	-	129,129,129,129	0
56	MG	AA	1700	1/1	0.29	-	62,62,62,62	0
56	MG	DA	2993	1/1	0.35	-	47,47,47,47	0
56	MG	DA	3579	1/1	0.19	-	92,92,92,92	0
56	MG	DA	3268	1/1	0.34	-	78,78,78,78	0
56	MG	BO	201	1/1	0.13	-	50,50,50,50	0
56	MG	AA	1760	1/1	0.42	-	91,91,91,91	0
56	MG	BA	2991	1/1	0.29	-	76,76,76,76	0
56	MG	BA	3165	1/1	0.11	-	46,46,46,46	0
56	MG	DA	3271	1/1	0.18	-	32,32,32,32	0
56	MG	BA	2960	1/1	0.22	-	49,49,49,49	0
56	MG	DA	3810	1/1	0.22	-	89,89,89,89	0
56	MG	CA	1903	1/1	0.19	-	67,67,67,67	0
56	MG	DA	3234	1/1	0.34	-	64,64,64,64	0
56	MG	BA	3420	1/1	0.20	-	82,82,82,82	0
56	MG	AA	1897	1/1	0.10	-	56,56,56,56	0
56	MG	D3	103	1/1	0.33	-	76,76,76,76	0
56	MG	DA	3467	1/1	0.50	-	95,95,95,95	0
56	MG	BA	3178	1/1	0.23	-	60,60,60,60	0
56	MG	DA	2951	1/1	0.16	-	19,19,19,19	0
56	MG	BA	3246	1/1	0.11	-	54,54,54,54	0
56	MG	CA	1686	1/1	0.15	-	72,72,72,72	0
56	MG	DA	3794	1/1	0.09	-	54,54,54,54	0
57	ZN	AG	301	1/1	0.26	-	82,82,82,82	0
56	MG	CA	1988	1/1	0.07	-	65,65,65,65	0
56	MG	CM	201	1/1	0.19	-	91,91,91,91	0
56	MG	AA	2016	1/1	0.34	-	102,102,102,102	0
56	MG	DA	2959	1/1	0.12	-	17,17,17,17	0
56	MG	DA	3627	1/1	0.25	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3295	1/1	0.11	-	76,76,76,76	0
56	MG	DA	3395	1/1	0.23	-	78,78,78,78	0
56	MG	BA	2986	1/1	0.20	-	41,41,41,41	0
56	MG	BB	202	1/1	0.14	-	59,59,59,59	0
56	MG	DA	2944	1/1	0.31	-	23,23,23,23	0
56	MG	DA	3842	1/1	0.28	-	90,90,90,90	0
56	MG	BA	3571	1/1	0.23	-	94,94,94,94	0
56	MG	BA	3094	1/1	0.14	-	84,84,84,84	0
56	MG	DA	3572	1/1	0.21	-	79,79,79,79	0
56	MG	BA	2980	1/1	0.31	-	53,53,53,53	0
56	MG	AA	1729	1/1	0.20	-	87,87,87,87	0
56	MG	DO	202	1/1	0.05	-	42,42,42,42	0
56	MG	DA	3749	1/1	0.95	-	138,138,138,138	0
56	MG	AA	1963	1/1	0.53	-	103,103,103,103	0
56	MG	BA	3151	1/1	0.51	-	114,114,114,114	0
56	MG	CA	1677	1/1	0.20	-	56,56,56,56	0
56	MG	AA	1625	1/1	0.32	-	62,62,62,62	0
56	MG	BA	3361	1/1	0.14	-	72,72,72,72	0
56	MG	DA	3448	1/1	0.33	-	86,86,86,86	0
56	MG	AA	1753	1/1	0.29	-	71,71,71,71	0
56	MG	CA	1886	1/1	0.29	-	90,90,90,90	0
56	MG	BA	3149	1/1	0.21	-	61,61,61,61	0
56	MG	AA	2009	1/1	0.08	-	71,71,71,71	0
56	MG	DD	302	1/1	0.33	-	40,40,40,40	0
56	MG	DA	3226	1/1	0.18	-	68,68,68,68	0
56	MG	BA	3116	1/1	0.28	-	64,64,64,64	0
56	MG	BA	2994	1/1	0.30	-	60,60,60,60	0
59	C	CP	202	20/21	0.38	-	147,160,162,163	0
56	MG	D0	202	1/1	0.19	-	51,51,51,51	0
56	MG	CA	1850	1/1	0.08	-	76,76,76,76	0
56	MG	AA	2023	1/1	0.05	-	112,112,112,112	0
56	MG	BA	2911	1/1	0.11	-	120,120,120,120	0
56	MG	DA	3497	1/1	0.15	-	72,72,72,72	0
56	MG	DB	205	1/1	0.20	-	69,69,69,69	0
56	MG	DA	3220	1/1	0.27	-	56,56,56,56	0
56	MG	AA	1806	1/1	0.33	-	118,118,118,118	0
56	MG	BA	3208	1/1	0.24	-	68,68,68,68	0
56	MG	BA	3260	1/1	0.22	-	77,77,77,77	0
56	MG	CA	1763	1/1	0.11	-	57,57,57,57	0
56	MG	DA	3105	1/1	0.31	-	50,50,50,50	0
56	MG	DA	3249	1/1	0.12	-	113,113,113,113	0
56	MG	BA	3555	1/1	0.49	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	2966	1/1	0.30	-	24,24,24,24	0
56	MG	AA	1789	1/1	0.20	-	128,128,128,128	0
56	MG	DA	3200	1/1	0.29	-	60,60,60,60	0
56	MG	CA	1819	1/1	0.16	-	86,86,86,86	0
56	MG	BA	3083	1/1	0.18	-	37,37,37,37	0
56	MG	AA	1843	1/1	0.37	-	93,93,93,93	0
56	MG	DA	3517	1/1	0.24	-	76,76,76,76	0
56	MG	DA	3334	1/1	0.31	-	54,54,54,54	0
56	MG	AA	1620	1/1	0.23	-	67,67,67,67	0
56	MG	DA	3197	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3293	1/1	0.33	-	55,55,55,55	0
56	MG	BA	2972	1/1	0.39	-	65,65,65,65	0
56	MG	CA	1693	1/1	0.09	-	62,62,62,62	0
56	MG	BA	3121	1/1	0.21	-	76,76,76,76	0
56	MG	DA	3045	1/1	0.22	-	34,34,34,34	0
56	MG	DA	3622	1/1	0.07	-	114,114,114,114	0
56	MG	BA	2974	1/1	0.29	-	39,39,39,39	0
56	MG	BA	3137	1/1	0.36	-	88,88,88,88	0
56	MG	AA	1777	1/1	0.28	-	69,69,69,69	0
56	MG	AA	1670	1/1	0.14	-	75,75,75,75	0
56	MG	DA	2952	1/1	0.30	-	29,29,29,29	0
56	MG	CA	1720	1/1	0.14	-	53,53,53,53	0
56	MG	AA	1664	1/1	0.33	-	69,69,69,69	0
56	MG	BA	3164	1/1	0.09	-	70,70,70,70	0
56	MG	AA	1900	1/1	0.11	-	102,102,102,102	0
56	MG	BA	3427	1/1	0.07	-	80,80,80,80	0
56	MG	AA	2029	1/1	0.29	-	127,127,127,127	0
56	MG	BA	3241	1/1	0.30	-	92,92,92,92	0
56	MG	DA	3686	1/1	0.23	-	62,62,62,62	0
56	MG	CA	1936	1/1	0.24	-	92,92,92,92	0
56	MG	DA	3611	1/1	0.05	-	74,74,74,74	0
56	MG	DA	2985	1/1	0.19	-	40,40,40,40	0
56	MG	AA	1698	1/1	0.39	-	79,79,79,79	0
56	MG	BA	3278	1/1	0.20	-	119,119,119,119	0
56	MG	BB	218	1/1	0.10	-	65,65,65,65	0
56	MG	BA	3268	1/1	0.40	-	87,87,87,87	0
56	MG	DA	3527	1/1	0.18	-	90,90,90,90	0
56	MG	BA	3472	1/1	0.14	-	125,125,125,125	0
58	G	CC	101	20/24	0.66	-	213,214,215,215	0
56	MG	AA	1966	1/1	0.30	-	85,85,85,85	0
56	MG	CD	122	1/1	0.16	-	97,97,97,97	0
56	MG	DA	3243	1/1	0.30	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1692	1/1	0.19	-	75,75,75,75	0
56	MG	DA	3094	1/1	0.33	-	68,68,68,68	0
56	MG	CA	1735	1/1	0.28	-	85,85,85,85	0
56	MG	DA	3817	1/1	0.10	-	72,72,72,72	0
56	MG	DA	3301	1/1	0.43	-	73,73,73,73	0
56	MG	CA	1752	1/1	0.12	-	74,74,74,74	0
56	MG	DA	2988	1/1	0.40	-	54,54,54,54	0
56	MG	DA	3784	1/1	0.10	-	90,90,90,90	0
56	MG	BA	3020	1/1	0.24	-	72,72,72,72	0
56	MG	DA	3506	1/1	0.23	-	51,51,51,51	0
56	MG	BA	3528	1/1	0.14	-	88,88,88,88	0
56	MG	BA	2978	1/1	0.23	-	47,47,47,47	0
56	MG	CA	1672	1/1	0.12	-	84,84,84,84	0
56	MG	DA	3475	1/1	0.17	-	83,83,83,83	0
56	MG	BA	3168	1/1	0.25	-	65,65,65,65	0
56	MG	AA	1711	1/1	0.39	-	86,86,86,86	0
56	MG	BA	3124	1/1	0.36	-	75,75,75,75	0
56	MG	CA	1874	1/1	0.18	-	76,76,76,76	0
59	C	CO	201	20/21	0.41	-	186,186,189,189	0
56	MG	BB	205	1/1	0.20	-	74,74,74,74	0
56	MG	DA	3803	1/1	0.21	-	81,81,81,81	0
56	MG	CA	1838	1/1	0.40	-	95,95,95,95	0
56	MG	CA	1743	1/1	0.25	-	89,89,89,89	0
56	MG	AA	2020	1/1	0.15	-	103,103,103,103	0
56	MG	AD	101	1/1	0.34	-	85,85,85,85	0
56	MG	DA	3548	1/1	0.28	-	82,82,82,82	0
56	MG	BA	3052	1/1	0.19	-	63,63,63,63	0
56	MG	AA	1906	1/1	0.36	-	86,86,86,86	0
58	G	CC	104	23/24	0.81	-	211,216,216,218	0
56	MG	DA	3338	1/1	0.18	-	86,86,86,86	0
56	MG	BA	2997	1/1	0.31	-	60,60,60,60	0
56	MG	DA	3793	1/1	0.13	-	57,57,57,57	0
56	MG	DA	3818	1/1	0.21	-	97,97,97,97	0
56	MG	BA	3505	1/1	0.33	-	114,114,114,114	0
56	MG	AA	1993	1/1	0.28	-	134,134,134,134	0
56	MG	DB	213	1/1	0.70	-	133,133,133,133	0
56	MG	BA	3194	1/1	0.26	-	87,87,87,87	0
59	C	DA	2926	20/21	0.30	-	191,195,202,202	0
56	MG	DA	3198	1/1	0.29	-	60,60,60,60	0
56	MG	AA	1811	1/1	0.08	-	81,81,81,81	0
56	MG	BA	3406	1/1	0.10	-	68,68,68,68	0
56	MG	BB	224	1/1	0.09	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3759	1/1	0.29	-	166,166,166,166	0
56	MG	BA	3583	1/1	0.07	-	79,79,79,79	0
56	MG	AA	1817	1/1	0.04	-	89,89,89,89	0
56	MG	CA	1699	1/1	0.18	-	79,79,79,79	0
56	MG	AA	1736	1/1	0.17	-	53,53,53,53	0
56	MG	BA	3431	1/1	0.10	-	96,96,96,96	0
56	MG	DA	3254	1/1	0.46	-	79,79,79,79	0
56	MG	AA	1688	1/1	0.23	-	39,39,39,39	0
56	MG	DA	3769	1/1	0.30	-	94,94,94,94	0
56	MG	DA	3157	1/1	0.50	-	74,74,74,74	0
56	MG	DA	3361	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3129	1/1	0.12	-	39,39,39,39	0
56	MG	AA	1884	1/1	0.11	-	86,86,86,86	0
56	MG	BA	3138	1/1	0.21	-	85,85,85,85	0
56	MG	CA	1876	1/1	0.10	-	98,98,98,98	0
56	MG	AA	1604	1/1	0.28	-	53,53,53,53	0
56	MG	DA	3013	1/1	0.34	-	31,31,31,31	0
56	MG	DA	3096	1/1	0.30	-	58,58,58,58	0
56	MG	DB	229	1/1	0.18	-	78,78,78,78	0
56	MG	DA	3048	1/1	0.24	-	78,78,78,78	0
56	MG	BA	3461	1/1	0.10	-	66,66,66,66	0
56	MG	DA	3745	1/1	0.19	-	152,152,152,152	0
56	MG	BA	3320	1/1	0.40	-	101,101,101,101	0
56	MG	CA	1648	1/1	0.18	-	72,72,72,72	0
56	MG	DA	3137	1/1	0.10	-	62,62,62,62	0
56	MG	DA	3835	1/1	0.61	-	78,78,78,78	0
56	MG	AA	1615	1/1	0.23	-	38,38,38,38	0
56	MG	AA	1662	1/1	0.30	-	100,100,100,100	0
56	MG	DH	204	1/1	0.15	-	77,77,77,77	0
56	MG	DA	3723	1/1	0.14	-	93,93,93,93	0
56	MG	BA	3084	1/1	0.38	-	83,83,83,83	0
56	MG	CA	1783	1/1	0.11	-	92,92,92,92	0
56	MG	DA	3165	1/1	0.08	-	40,40,40,40	0
56	MG	AA	1613	1/1	0.27	-	53,53,53,53	0
56	MG	DA	3102	1/1	0.08	-	46,46,46,46	0
56	MG	CA	1956	1/1	0.17	-	91,91,91,91	0
56	MG	BA	3336	1/1	0.25	-	88,88,88,88	0
56	MG	CA	1811	1/1	0.14	-	79,79,79,79	0
56	MG	DA	3402	1/1	0.18	-	107,107,107,107	0
56	MG	DA	3407	1/1	0.35	-	79,79,79,79	0
56	MG	BA	2929	1/1	0.23	-	32,32,32,32	0
56	MG	CA	1739	1/1	0.17	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BF	301	1/1	0.12	-	80,80,80,80	0
56	MG	BA	3355	1/1	0.14	-	64,64,64,64	0
56	MG	AA	1650	1/1	0.14	-	74,74,74,74	0
56	MG	CA	1746	1/1	0.09	-	80,80,80,80	0
56	MG	BA	3232	1/1	0.12	-	99,99,99,99	0
56	MG	DA	3620	1/1	0.21	-	99,99,99,99	0
56	MG	CD	111	1/1	0.10	-	87,87,87,87	0
56	MG	DA	2940	1/1	0.32	-	24,24,24,24	0
56	MG	DA	3672	1/1	0.25	-	101,101,101,101	0
56	MG	AA	1833	1/1	0.30	-	88,88,88,88	0
56	MG	DA	3196	1/1	0.12	-	77,77,77,77	0
56	MG	DA	3111	1/1	0.11	-	52,52,52,52	0
56	MG	AA	1661	1/1	0.41	-	93,93,93,93	0
56	MG	BA	3000	1/1	0.14	-	25,25,25,25	0
56	MG	DA	3636	1/1	0.49	-	80,80,80,80	0
56	MG	DA	3304	1/1	0.37	-	76,76,76,76	0
56	MG	BA	3515	1/1	0.20	-	80,80,80,80	0
56	MG	BA	3309	1/1	0.09	-	61,61,61,61	0
56	MG	BA	2971	1/1	0.15	-	57,57,57,57	0
56	MG	DA	3775	1/1	0.16	-	114,114,114,114	0
56	MG	AA	1626	1/1	0.18	-	55,55,55,55	0
56	MG	CD	125	1/1	0.34	-	83,83,83,83	0
56	MG	DA	3812	1/1	0.27	-	90,90,90,90	0
56	MG	CW	205	1/1	0.15	-	143,143,143,143	0
56	MG	CA	1660	1/1	0.35	-	86,86,86,86	0
56	MG	DR	202	1/1	0.11	-	102,102,102,102	0
56	MG	DU	206	1/1	0.17	-	83,83,83,83	0
56	MG	DB	227	1/1	0.20	-	105,105,105,105	0
56	MG	DA	3764	1/1	0.46	-	106,106,106,106	0
56	MG	AA	1901	1/1	0.08	-	89,89,89,89	0
56	MG	BA	3442	1/1	0.08	-	89,89,89,89	0
56	MG	AA	1976	1/1	0.37	-	86,86,86,86	0
56	MG	BA	3342	1/1	0.23	-	90,90,90,90	0
56	MG	DA	2979	1/1	0.21	-	38,38,38,38	0
56	MG	CA	1642	1/1	0.29	-	86,86,86,86	0
56	MG	AA	1790	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3303	1/1	0.13	-	109,109,109,109	0
56	MG	DA	3333	1/1	0.39	-	82,82,82,82	0
56	MG	BA	3545	1/1	0.33	-	82,82,82,82	0
56	MG	AA	2015	1/1	0.18	-	106,106,106,106	0
56	MG	CA	1610	1/1	0.30	-	56,56,56,56	0
56	MG	AA	1908	1/1	0.26	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3149	1/1	0.19	-	55,55,55,55	0
56	MG	DA	3012	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3414	1/1	0.37	-	111,111,111,111	0
56	MG	DA	3771	1/1	0.14	-	69,69,69,69	0
56	MG	AA	1724	1/1	0.44	-	82,82,82,82	0
56	MG	DA	3217	1/1	0.11	-	102,102,102,102	0
56	MG	BA	3174	1/1	0.33	-	90,90,90,90	0
56	MG	AA	1723	1/1	0.17	-	89,89,89,89	0
56	MG	AA	1684	1/1	0.26	-	74,74,74,74	0
56	MG	BA	3331	1/1	0.34	-	80,80,80,80	0
56	MG	CD	109	1/1	0.03	-	89,89,89,89	0
56	MG	DA	3699	1/1	0.23	-	78,78,78,78	0
56	MG	CA	1691	1/1	0.13	-	60,60,60,60	0
56	MG	B8	101	1/1	0.14	-	76,76,76,76	0
56	MG	DA	3224	1/1	0.30	-	64,64,64,64	0
56	MG	DA	3452	1/1	0.19	-	77,77,77,77	0
56	MG	CA	1926	1/1	0.38	-	112,112,112,112	0
56	MG	BA	2950	1/1	0.17	-	29,29,29,29	0
56	MG	DA	3441	1/1	0.18	-	94,94,94,94	0
56	MG	DB	224	1/1	0.24	-	109,109,109,109	0
56	MG	DA	3446	1/1	0.29	-	70,70,70,70	0
56	MG	AW	204	1/1	0.13	-	105,105,105,105	0
56	MG	CA	1871	1/1	0.26	-	90,90,90,90	0
56	MG	BA	3391	1/1	0.16	-	86,86,86,86	0
56	MG	CA	1965	1/1	0.11	-	106,106,106,106	0
56	MG	D1	201	1/1	0.40	-	83,83,83,83	0
56	MG	AA	1959	1/1	0.44	-	104,104,104,104	0
56	MG	DA	3204	1/1	0.28	-	68,68,68,68	0
56	MG	DA	3380	1/1	0.18	-	86,86,86,86	0
56	MG	CA	1901	1/1	0.11	-	61,61,61,61	0
56	MG	DO	203	1/1	0.37	-	100,100,100,100	0
56	MG	BA	3134	1/1	0.23	-	61,61,61,61	0
56	MG	DO	201	1/1	0.14	-	55,55,55,55	0
56	MG	BA	3364	1/1	0.12	-	77,77,77,77	0
56	MG	DA	3768	1/1	0.05	-	67,67,67,67	0
56	MG	DA	3563	1/1	0.18	-	74,74,74,74	0
56	MG	AA	2001	1/1	0.23	-	76,76,76,76	0
56	MG	AA	1673	1/1	0.12	-	91,91,91,91	0
56	MG	CA	1772	1/1	0.36	-	118,118,118,118	0
56	MG	BA	3313	1/1	0.27	-	102,102,102,102	0
59	C	CA	1605	20/21	0.20	-	136,138,139,139	0
56	MG	BA	3100	1/1	0.14	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3055	1/1	0.18	-	58,58,58,58	0
56	MG	AA	2030	1/1	0.47	-	188,188,188,188	0
56	MG	DA	3618	1/1	0.24	-	139,139,139,139	0
56	MG	BA	3463	1/1	0.21	-	69,69,69,69	0
56	MG	DA	3279	1/1	0.24	-	46,46,46,46	0
56	MG	DA	2967	1/1	0.27	-	31,31,31,31	0
56	MG	DA	3238	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3019	1/1	0.13	-	67,67,67,67	0
56	MG	CA	1617	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3423	1/1	0.17	-	85,85,85,85	0
56	MG	BA	3026	1/1	0.22	-	60,60,60,60	0
56	MG	BA	3580	1/1	0.11	-	89,89,89,89	0
56	MG	CA	1906	1/1	0.24	-	66,66,66,66	0
58	G	DA	2912	23/24	0.44	-	207,210,214,215	0
56	MG	DA	3128	1/1	0.43	-	92,92,92,92	0
56	MG	DA	3666	1/1	0.24	-	72,72,72,72	0
56	MG	DA	3815	1/1	0.09	-	97,97,97,97	0
56	MG	DA	3210	1/1	0.12	-	57,57,57,57	0
56	MG	D3	104	1/1	0.24	-	75,75,75,75	0
56	MG	DA	3664	1/1	0.12	-	87,87,87,87	0
56	MG	BA	3176	1/1	0.21	-	65,65,65,65	0
56	MG	BA	2930	1/1	0.18	-	33,33,33,33	0
56	MG	CA	1721	1/1	0.06	-	64,64,64,64	0
56	MG	DA	3141	1/1	0.27	-	79,79,79,79	0
56	MG	DA	3551	1/1	0.15	-	66,66,66,66	0
56	MG	BA	2993	1/1	0.39	-	52,52,52,52	0
56	MG	DA	3421	1/1	0.24	-	62,62,62,62	0
56	MG	AA	1797	1/1	0.14	-	75,75,75,75	0
56	MG	DA	3124	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3047	1/1	0.16	-	41,41,41,41	0
56	MG	BA	2904	1/1	0.17	-	101,101,101,101	0
56	MG	DB	209	1/1	0.48	-	81,81,81,81	0
56	MG	BA	3155	1/1	0.19	-	64,64,64,64	0
56	MG	CA	1764	1/1	0.12	-	79,79,79,79	0
56	MG	DA	3109	1/1	0.22	-	66,66,66,66	0
56	MG	BA	3509	1/1	0.24	-	107,107,107,107	0
56	MG	CA	1761	1/1	0.18	-	82,82,82,82	0
56	MG	DU	201	1/1	0.19	-	60,60,60,60	0
56	MG	BA	3578	1/1	0.14	-	98,98,98,98	0
56	MG	AA	1713	1/1	0.38	-	94,94,94,94	0
56	MG	CA	1859	1/1	0.26	-	111,111,111,111	0
56	MG	CA	1804	1/1	0.22	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1917	1/1	0.41	-	132,132,132,132	0
56	MG	CD	108	1/1	0.08	-	174,174,174,174	0
56	MG	BA	3235	1/1	0.14	-	59,59,59,59	0
56	MG	B4	101	1/1	0.14	-	85,85,85,85	0
56	MG	DA	3222	1/1	0.31	-	75,75,75,75	0
56	MG	DA	3300	1/1	0.31	-	78,78,78,78	0
56	MG	CA	1966	1/1	0.20	-	84,84,84,84	0
56	MG	AA	1632	1/1	0.21	-	72,72,72,72	0
56	MG	AA	1929	1/1	0.19	-	124,124,124,124	0
56	MG	AA	1996	1/1	0.34	-	106,106,106,106	0
56	MG	BA	3167	1/1	0.40	-	91,91,91,91	0
56	MG	DA	3437	1/1	0.23	-	73,73,73,73	0
59	C	CP	204	20/21	0.40	-	171,177,179,179	0
56	MG	BU	205	1/1	0.17	-	55,55,55,55	0
56	MG	DA	3240	1/1	0.25	-	74,74,74,74	0
56	MG	CA	1633	1/1	0.28	-	68,68,68,68	0
56	MG	DA	3684	1/1	0.28	-	98,98,98,98	0
56	MG	DA	3331	1/1	0.26	-	78,78,78,78	0
56	MG	BA	3504	1/1	0.15	-	115,115,115,115	0
56	MG	DA	3087	1/1	0.31	-	56,56,56,56	0
56	MG	DA	3176	1/1	0.18	-	33,33,33,33	0
56	MG	CA	1975	1/1	0.36	-	90,90,90,90	0
56	MG	BA	3222	1/1	0.36	-	88,88,88,88	0
56	MG	AA	1772	1/1	0.32	-	71,71,71,71	0
56	MG	DA	3344	1/1	0.44	-	74,74,74,74	0
56	MG	AA	1896	1/1	0.37	-	93,93,93,93	0
56	MG	DA	3649	1/1	0.20	-	99,99,99,99	0
56	MG	AA	1812	1/1	0.35	-	110,110,110,110	0
56	MG	CA	1751	1/1	0.15	-	89,89,89,89	0
56	MG	AA	1862	1/1	0.14	-	77,77,77,77	0
56	MG	DA	3153	1/1	0.47	-	93,93,93,93	0
59	C	DP	204	20/21	0.37	-	191,193,194,195	0
56	MG	DA	3393	1/1	0.50	-	73,73,73,73	0
56	MG	BA	3476	1/1	0.22	-	97,97,97,97	0
56	MG	DA	3453	1/1	0.43	-	94,94,94,94	0
56	MG	DA	3601	1/1	0.13	-	49,49,49,49	0
56	MG	AA	1677	1/1	0.36	-	63,63,63,63	0
56	MG	AA	1986	1/1	0.17	-	96,96,96,96	0
56	MG	DA	3341	1/1	0.08	-	41,41,41,41	0
56	MG	BA	2913	1/1	0.42	-	115,115,115,115	0
56	MG	AA	1831	1/1	0.13	-	76,76,76,76	0
56	MG	AA	1825	1/1	0.08	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1935	1/1	0.06	-	122,122,122,122	0
56	MG	DA	3266	1/1	0.20	-	33,33,33,33	0
56	MG	BA	3301	1/1	0.28	-	92,92,92,92	0
56	MG	BB	213	1/1	0.16	-	122,122,122,122	0
56	MG	BA	3037	1/1	0.19	-	61,61,61,61	0
56	MG	CK	201	1/1	0.15	-	90,90,90,90	0
56	MG	AA	1639	1/1	0.39	-	73,73,73,73	0
56	MG	DA	3597	1/1	0.27	-	79,79,79,79	0
56	MG	DA	3186	1/1	0.29	-	56,56,56,56	0
56	MG	BA	2932	1/1	0.17	-	37,37,37,37	0
56	MG	BA	3021	1/1	0.14	-	35,35,35,35	0
56	MG	DA	3320	1/1	0.09	-	81,81,81,81	0
56	MG	AA	1907	1/1	0.08	-	106,106,106,106	0
56	MG	DA	3191	1/1	0.32	-	56,56,56,56	0
56	MG	BA	3564	1/1	0.08	-	77,77,77,77	0
56	MG	DA	3580	1/1	0.16	-	96,96,96,96	0
56	MG	CA	1842	1/1	0.13	-	74,74,74,74	0
56	MG	CA	1967	1/1	0.21	-	108,108,108,108	0
56	MG	CA	1970	1/1	0.13	-	145,145,145,145	0
58	G	DA	2920	23/24	0.49	-	196,198,199,200	0
56	MG	DA	3603	1/1	0.38	-	78,78,78,78	0
56	MG	DA	3451	1/1	0.40	-	70,70,70,70	0
56	MG	BA	3152	1/1	0.35	-	72,72,72,72	0
56	MG	DA	3696	1/1	0.07	-	52,52,52,52	0
56	MG	AA	2018	1/1	0.21	-	117,117,117,117	0
56	MG	DB	207	1/1	0.21	-	99,99,99,99	0
56	MG	DA	3390	1/1	0.25	-	70,70,70,70	0
56	MG	BA	3353	1/1	0.20	-	75,75,75,75	0
56	MG	BA	3220	1/1	0.18	-	59,59,59,59	0
56	MG	CD	115	1/1	0.23	-	106,106,106,106	0
56	MG	CA	1757	1/1	0.10	-	80,80,80,80	0
56	MG	BA	3288	1/1	0.08	-	66,66,66,66	0
56	MG	BA	3128	1/1	0.31	-	72,72,72,72	0
56	MG	DA	3412	1/1	0.07	-	57,57,57,57	0
56	MG	CA	1767	1/1	0.08	-	118,118,118,118	0
56	MG	BA	2956	1/1	0.17	-	38,38,38,38	0
56	MG	DA	3307	1/1	0.26	-	70,70,70,70	0
56	MG	DA	3566	1/1	0.19	-	94,94,94,94	0
56	MG	AA	1726	1/1	0.18	-	68,68,68,68	0
56	MG	BA	3381	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3574	1/1	0.15	-	86,86,86,86	0
56	MG	DA	3406	1/1	0.29	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3727	1/1	0.29	-	83,83,83,83	0
56	MG	B6	101	1/1	0.11	-	84,84,84,84	0
56	MG	AC	102	1/1	0.40	-	85,85,85,85	0
56	MG	DA	3396	1/1	0.28	-	70,70,70,70	0
56	MG	DA	3524	1/1	0.42	-	96,96,96,96	0
56	MG	AA	1938	1/1	0.26	-	89,89,89,89	0
56	MG	BA	3204	1/1	0.30	-	76,76,76,76	0
56	MG	CA	1622	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3190	1/1	0.10	-	51,51,51,51	0
56	MG	DA	3281	1/1	0.21	-	64,64,64,64	0
56	MG	DA	3422	1/1	0.46	-	99,99,99,99	0
56	MG	BA	3573	1/1	0.22	-	86,86,86,86	0
56	MG	CA	1957	1/1	0.19	-	121,121,121,121	0
56	MG	BA	3040	1/1	0.13	-	40,40,40,40	0
56	MG	DA	3703	1/1	0.15	-	78,78,78,78	0
56	MG	DA	3108	1/1	0.27	-	60,60,60,60	0
56	MG	CA	1713	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3042	1/1	0.05	-	28,28,28,28	0
56	MG	BA	2967	1/1	0.30	-	60,60,60,60	0
56	MG	DA	3318	1/1	0.25	-	123,123,123,123	0
56	MG	BA	3399	1/1	0.14	-	82,82,82,82	0
56	MG	DA	3747	1/1	0.32	-	106,106,106,106	0
56	MG	BA	3507	1/1	0.17	-	80,80,80,80	0
56	MG	AA	1709	1/1	0.44	-	130,130,130,130	0
56	MG	BA	2965	1/1	0.08	-	30,30,30,30	0
56	MG	AA	1910	1/1	0.12	-	103,103,103,103	0
56	MG	DA	3512	1/1	0.08	-	56,56,56,56	0
56	MG	AA	1652	1/1	0.21	-	82,82,82,82	0
56	MG	BA	3348	1/1	0.37	-	99,99,99,99	0
56	MG	BA	3029	1/1	0.20	-	40,40,40,40	0
56	MG	BA	3153	1/1	0.24	-	71,71,71,71	0
56	MG	DA	3576	1/1	0.33	-	76,76,76,76	0
56	MG	CD	103	1/1	0.15	-	113,113,113,113	0
56	MG	DA	3078	1/1	0.31	-	49,49,49,49	0
56	MG	DA	2987	1/1	0.36	-	52,52,52,52	0
56	MG	DA	2958	1/1	0.15	-	32,32,32,32	0
56	MG	CA	1611	1/1	0.24	-	66,66,66,66	0
56	MG	DA	3477	1/1	0.48	-	118,118,118,118	0
56	MG	AA	1987	1/1	0.21	-	86,86,86,86	0
56	MG	BA	3433	1/1	0.28	-	109,109,109,109	0
56	MG	DA	2943	1/1	0.25	-	27,27,27,27	0
56	MG	CA	1728	1/1	0.18	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3177	1/1	0.33	-	89,89,89,89	0
56	MG	BT	102	1/1	0.15	-	100,100,100,100	0
56	MG	AA	1913	1/1	0.24	-	114,114,114,114	0
56	MG	AA	1865	1/1	0.43	-	140,140,140,140	0
56	MG	DA	3735	1/1	0.28	-	89,89,89,89	0
56	MG	DA	3354	1/1	0.15	-	91,91,91,91	0
56	MG	DA	3638	1/1	0.54	-	95,95,95,95	0
56	MG	BA	3276	1/1	0.18	-	79,79,79,79	0
56	MG	DA	3534	1/1	0.12	-	68,68,68,68	0
56	MG	DA	3629	1/1	0.41	-	78,78,78,78	0
56	MG	DA	2955	1/1	0.30	-	28,28,28,28	0
56	MG	CX	102	1/1	0.05	-	104,104,104,104	0
56	MG	AA	1748	1/1	0.17	-	85,85,85,85	0
56	MG	CD	101	1/1	0.16	-	53,53,53,53	0
56	MG	DA	3269	1/1	0.23	-	67,67,67,67	0
56	MG	DD	303	1/1	0.17	-	43,43,43,43	0
56	MG	DA	3359	1/1	0.33	-	79,79,79,79	0
56	MG	CA	1629	1/1	0.21	-	68,68,68,68	0
56	MG	BA	3354	1/1	0.10	-	57,57,57,57	0
56	MG	DA	3267	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3632	1/1	0.12	-	80,80,80,80	0
56	MG	AA	2024	1/1	0.22	-	75,75,75,75	0
56	MG	DA	3689	1/1	0.25	-	83,83,83,83	0
56	MG	BA	3334	1/1	0.24	-	75,75,75,75	0
56	MG	BA	3450	1/1	0.14	-	90,90,90,90	0
56	MG	BA	3401	1/1	0.12	-	36,36,36,36	0
56	MG	CA	1815	1/1	0.20	-	98,98,98,98	0
56	MG	AC	104	1/1	0.11	-	85,85,85,85	0
56	MG	BB	209	1/1	0.16	-	59,59,59,59	0
56	MG	CA	1919	1/1	0.14	-	127,127,127,127	0
56	MG	BA	3343	1/1	0.27	-	73,73,73,73	0
58	G	DP	202	23/24	0.32	-	188,189,190,190	0
56	MG	BA	3284	1/1	0.13	-	74,74,74,74	0
56	MG	BA	3293	1/1	0.47	-	111,111,111,111	0
56	MG	DA	3265	1/1	0.32	-	77,77,77,77	0
56	MG	AA	1975	1/1	0.22	-	86,86,86,86	0
56	MG	AA	1641	1/1	0.13	-	76,76,76,76	0
56	MG	DA	3379	1/1	0.49	-	77,77,77,77	0
58	G	CA	1602	23/24	0.39	-	162,165,174,174	0
56	MG	CA	1625	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3089	1/1	0.40	-	74,74,74,74	0
56	MG	BA	3561	1/1	0.39	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3617	1/1	0.27	-	96,96,96,96	0
56	MG	AA	1728	1/1	0.28	-	77,77,77,77	0
56	MG	BA	3270	1/1	0.45	-	98,98,98,98	0
56	MG	BA	3101	1/1	0.18	-	56,56,56,56	0
56	MG	BA	3489	1/1	0.17	-	93,93,93,93	0
56	MG	DA	3501	1/1	0.51	-	93,93,93,93	0
56	MG	CA	1787	1/1	0.18	-	78,78,78,78	0
56	MG	CA	1753	1/1	0.48	-	86,86,86,86	0
56	MG	BA	3043	1/1	0.08	-	51,51,51,51	0
56	MG	DA	3459	1/1	0.33	-	82,82,82,82	0
56	MG	CD	117	1/1	0.07	-	85,85,85,85	0
59	C	DP	205	20/21	0.47	-	189,190,191,191	0
56	MG	AC	107	1/1	0.58	-	114,114,114,114	0
56	MG	DA	3182	1/1	0.32	-	64,64,64,64	0
56	MG	AA	1915	1/1	0.17	-	172,172,172,172	0
56	MG	BA	3356	1/1	0.06	-	75,75,75,75	0
56	MG	BA	2947	1/1	0.17	-	30,30,30,30	0
56	MG	DA	3561	1/1	0.15	-	54,54,54,54	0
56	MG	DA	3584	1/1	0.19	-	91,91,91,91	0
56	MG	DA	3802	1/1	0.29	-	110,110,110,110	0
56	MG	BA	3414	1/1	0.24	-	105,105,105,105	0
56	MG	CA	1867	1/1	0.41	-	127,127,127,127	0
56	MG	AA	1766	1/1	0.10	-	69,69,69,69	0
56	MG	BA	3209	1/1	0.21	-	58,58,58,58	0
56	MG	BA	2922	1/1	0.21	-	46,46,46,46	0
56	MG	BA	3054	1/1	0.22	-	66,66,66,66	0
56	MG	BA	3365	1/1	0.16	-	77,77,77,77	0
56	MG	CH	201	1/1	0.14	-	82,82,82,82	0
56	MG	DA	3841	1/1	0.17	-	94,94,94,94	0
56	MG	AA	1984	1/1	0.17	-	80,80,80,80	0
56	MG	BA	3540	1/1	0.20	-	69,69,69,69	0
56	MG	AA	1774	1/1	0.25	-	75,75,75,75	0
56	MG	DA	3774	1/1	0.20	-	88,88,88,88	0
56	MG	DA	2981	1/1	0.16	-	35,35,35,35	0
56	MG	DA	3482	1/1	0.36	-	95,95,95,95	0
56	MG	DA	3223	1/1	0.10	-	23,23,23,23	0
56	MG	CA	1769	1/1	0.23	-	110,110,110,110	0
56	MG	CA	1851	1/1	0.19	-	76,76,76,76	0
56	MG	AA	1958	1/1	0.35	-	93,93,93,93	0
56	MG	AA	1816	1/1	0.21	-	107,107,107,107	0
56	MG	AA	1856	1/1	0.20	-	71,71,71,71	0
56	MG	DA	3082	1/1	0.32	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3624	1/1	0.32	-	134,134,134,134	0
56	MG	DA	3821	1/1	0.32	-	106,106,106,106	0
56	MG	BA	2935	1/1	0.25	-	46,46,46,46	0
56	MG	CA	1834	1/1	0.05	-	100,100,100,100	0
56	MG	BA	3063	1/1	0.25	-	63,63,63,63	0
56	MG	DA	3430	1/1	0.09	-	60,60,60,60	0
56	MG	AA	1941	1/1	0.11	-	93,93,93,93	0
56	MG	DA	3596	1/1	0.26	-	103,103,103,103	0
56	MG	DB	216	1/1	0.19	-	94,94,94,94	0
56	MG	DA	3199	1/1	0.25	-	55,55,55,55	0
56	MG	CA	1984	1/1	0.19	-	100,100,100,100	0
56	MG	DA	3702	1/1	0.29	-	88,88,88,88	0
56	MG	DA	3781	1/1	0.14	-	68,68,68,68	0
56	MG	AA	1608	1/1	0.39	-	67,67,67,67	0
56	MG	CA	1890	1/1	0.08	-	80,80,80,80	0
56	MG	DB	206	1/1	0.21	-	57,57,57,57	0
56	MG	BA	3184	1/1	0.45	-	116,116,116,116	0
56	MG	BA	3370	1/1	0.11	-	70,70,70,70	0
56	MG	AA	1793	1/1	0.20	-	73,73,73,73	0
56	MG	BA	3426	1/1	0.07	-	43,43,43,43	0
56	MG	CA	1668	1/1	0.15	-	64,64,64,64	0
56	MG	DT	102	1/1	0.14	-	64,64,64,64	0
56	MG	DA	3401	1/1	0.33	-	79,79,79,79	0
56	MG	AA	1663	1/1	0.23	-	71,71,71,71	0
56	MG	BA	3469	1/1	0.24	-	70,70,70,70	0
56	MG	BA	3109	1/1	0.21	-	73,73,73,73	0
56	MG	DA	3716	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3569	1/1	0.26	-	87,87,87,87	0
56	MG	DA	3529	1/1	0.27	-	95,95,95,95	0
56	MG	DA	3435	1/1	0.39	-	100,100,100,100	0
56	MG	CA	1985	1/1	0.22	-	73,73,73,73	0
58	G	DA	2903	23/24	0.44	-	200,202,205,206	0
56	MG	DA	3792	1/1	0.23	-	67,67,67,67	0
56	MG	CA	1679	1/1	0.15	-	70,70,70,70	0
56	MG	AA	1697	1/1	0.22	-	77,77,77,77	0
56	MG	DA	3132	1/1	0.15	-	46,46,46,46	0
56	MG	AA	1657	1/1	0.38	-	83,83,83,83	0
56	MG	BA	3419	1/1	0.07	-	101,101,101,101	0
56	MG	DA	2957	1/1	0.25	-	21,21,21,21	0
56	MG	CA	1736	1/1	0.13	-	61,61,61,61	0
56	MG	AA	1803	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3081	1/1	0.29	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1765	1/1	0.08	-	90,90,90,90	0
56	MG	DS	201	1/1	0.37	-	104,104,104,104	0
56	MG	DA	2962	1/1	0.43	-	38,38,38,38	0
56	MG	AA	1798	1/1	0.32	-	79,79,79,79	0
56	MG	DA	3805	1/1	0.20	-	92,92,92,92	0
56	MG	CA	1671	1/1	0.13	-	87,87,87,87	0
56	MG	CA	1939	1/1	0.11	-	94,94,94,94	0
56	MG	AA	1960	1/1	0.17	-	98,98,98,98	0
56	MG	DA	3513	1/1	0.13	-	68,68,68,68	0
56	MG	BA	3221	1/1	0.28	-	82,82,82,82	0
56	MG	AA	1741	1/1	0.16	-	93,93,93,93	0
56	MG	DA	3776	1/1	0.20	-	127,127,127,127	0
56	MG	CA	1683	1/1	0.35	-	83,83,83,83	0
56	MG	DA	3724	1/1	0.23	-	78,78,78,78	0
56	MG	DA	3472	1/1	0.19	-	90,90,90,90	0
56	MG	CA	1796	1/1	0.15	-	100,100,100,100	0
58	G	DA	2908	23/24	0.23	-	230,232,233,233	0
56	MG	DA	3073	1/1	0.38	-	50,50,50,50	0
56	MG	AA	1715	1/1	0.12	-	76,76,76,76	0
59	C	DA	2936	20/21	0.48	-	211,214,215,216	0
56	MG	CC	113	1/1	0.06	-	79,79,79,79	0
56	MG	BA	3245	1/1	0.12	-	128,128,128,128	0
56	MG	DA	3429	1/1	0.13	-	66,66,66,66	0
58	G	CA	1601	23/24	0.44	-	179,181,186,186	0
56	MG	CA	1689	1/1	0.17	-	67,67,67,67	0
56	MG	DA	3040	1/1	0.31	-	62,62,62,62	0
56	MG	CA	1665	1/1	0.24	-	76,76,76,76	0
56	MG	BA	2940	1/1	0.20	-	27,27,27,27	0
56	MG	BA	3252	1/1	0.12	-	38,38,38,38	0
56	MG	DA	3039	1/1	0.44	-	62,62,62,62	0
56	MG	BA	3395	1/1	0.08	-	60,60,60,60	0
56	MG	DA	3675	1/1	0.13	-	37,37,37,37	0
56	MG	DA	3005	1/1	0.11	-	20,20,20,20	0
56	MG	DA	3711	1/1	0.13	-	83,83,83,83	0
56	MG	DA	3767	1/1	0.14	-	79,79,79,79	0
56	MG	DA	3444	1/1	0.06	-	41,41,41,41	0
56	MG	DA	3308	1/1	0.49	-	87,87,87,87	0
56	MG	DA	3485	1/1	0.43	-	103,103,103,103	0
56	MG	AA	1696	1/1	0.32	-	134,134,134,134	0
56	MG	DA	2945	1/1	0.23	-	23,23,23,23	0
56	MG	BA	3483	1/1	0.15	-	103,103,103,103	0
56	MG	AA	1640	1/1	0.23	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3668	1/1	0.46	-	118,118,118,118	0
56	MG	DA	3811	1/1	0.34	-	76,76,76,76	0
56	MG	CA	1941	1/1	0.30	-	94,94,94,94	0
56	MG	DA	3277	1/1	0.17	-	58,58,58,58	0
56	MG	DA	3623	1/1	0.21	-	72,72,72,72	0
56	MG	DA	3011	1/1	0.43	-	51,51,51,51	0
56	MG	AA	1804	1/1	0.36	-	88,88,88,88	0
61	A	DA	2905	22/23	0.43	-	198,198,199,199	0
56	MG	DA	3187	1/1	0.35	-	54,54,54,54	0
56	MG	DA	2960	1/1	0.15	-	18,18,18,18	0
56	MG	BA	3115	1/1	0.31	-	89,89,89,89	0
56	MG	DA	3608	1/1	0.37	-	81,81,81,81	0
56	MG	BA	3402	1/1	0.17	-	96,96,96,96	0
56	MG	DA	3535	1/1	0.14	-	107,107,107,107	0
56	MG	BA	3041	1/1	0.09	-	39,39,39,39	0
56	MG	AK	201	1/1	0.13	-	90,90,90,90	0
56	MG	DA	3392	1/1	0.21	-	60,60,60,60	0
56	MG	BA	2942	1/1	0.30	-	36,36,36,36	0
56	MG	AA	1727	1/1	0.24	-	104,104,104,104	0
56	MG	DA	3455	1/1	0.07	-	59,59,59,59	0
56	MG	CP	207	1/1	0.17	-	93,93,93,93	0
56	MG	BA	3140	1/1	0.11	-	51,51,51,51	0
56	MG	DA	3237	1/1	0.24	-	52,52,52,52	0
56	MG	CA	1924	1/1	0.08	-	95,95,95,95	0
56	MG	DA	2982	1/1	0.39	-	40,40,40,40	0
56	MG	BA	3383	1/1	0.20	-	63,63,63,63	0
56	MG	AA	1969	1/1	0.13	-	89,89,89,89	0
56	MG	DA	3206	1/1	0.37	-	59,59,59,59	0
56	MG	DA	3121	1/1	0.27	-	47,47,47,47	0
56	MG	BA	2995	1/1	0.29	-	52,52,52,52	0
56	MG	AA	1676	1/1	0.15	-	96,96,96,96	0
56	MG	DA	3117	1/1	0.07	-	23,23,23,23	0
56	MG	AA	2019	1/1	0.05	-	104,104,104,104	0
56	MG	CC	119	1/1	0.13	-	88,88,88,88	0
56	MG	CA	1977	1/1	0.24	-	87,87,87,87	0
56	MG	BA	3432	1/1	0.21	-	115,115,115,115	0
56	MG	DA	3695	1/1	0.47	-	88,88,88,88	0
56	MG	DA	3201	1/1	0.34	-	72,72,72,72	0
56	MG	CC	110	1/1	0.16	-	86,86,86,86	0
56	MG	BA	3257	1/1	0.07	-	63,63,63,63	0
56	MG	BA	3445	1/1	0.44	-	96,96,96,96	0
56	MG	DB	210	1/1	0.14	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1701	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3187	1/1	0.06	-	40,40,40,40	0
56	MG	BA	3546	1/1	0.24	-	102,102,102,102	0
61	A	C1	103	22/23	0.24	-	133,135,137,138	0
56	MG	DB	218	1/1	0.43	-	84,84,84,84	0
56	MG	DA	3403	1/1	0.14	-	50,50,50,50	0
56	MG	CA	1950	1/1	0.10	-	110,110,110,110	0
56	MG	DA	3122	1/1	0.37	-	67,67,67,67	0
56	MG	BA	3016	1/1	0.28	-	63,63,63,63	0
56	MG	DA	3687	1/1	0.23	-	76,76,76,76	0
56	MG	CA	1942	1/1	0.07	-	136,136,136,136	0
56	MG	CA	1964	1/1	0.09	-	90,90,90,90	0
56	MG	DA	3298	1/1	0.32	-	102,102,102,102	0
56	MG	AA	1894	1/1	0.40	-	103,103,103,103	0
56	MG	DB	223	1/1	0.05	-	104,104,104,104	0
56	MG	BA	3110	1/1	0.17	-	34,34,34,34	0
56	MG	AA	1998	1/1	0.29	-	98,98,98,98	0
56	MG	AA	1654	1/1	0.26	-	54,54,54,54	0
56	MG	BA	3130	1/1	0.27	-	75,75,75,75	0
61	A	CC	103	22/23	0.59	-	208,209,210,210	0
56	MG	BA	2920	1/1	0.18	-	36,36,36,36	0
56	MG	BA	2925	1/1	0.23	-	46,46,46,46	0
56	MG	DA	3261	1/1	0.21	-	55,55,55,55	0
60	U	DA	2932	20/21	0.51	-	191,194,195,195	0
56	MG	DA	3465	1/1	0.18	-	55,55,55,55	0
56	MG	BA	2989	1/1	0.39	-	60,60,60,60	0
56	MG	AA	1796	1/1	0.44	-	75,75,75,75	0
56	MG	BA	3065	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3773	1/1	0.20	-	76,76,76,76	0
56	MG	BA	3093	1/1	0.12	-	65,65,65,65	0
56	MG	CA	1703	1/1	0.23	-	84,84,84,84	0
56	MG	AA	1776	1/1	0.40	-	110,110,110,110	0
58	G	DA	2904	23/24	0.60	-	199,200,202,202	0
56	MG	BA	3458	1/1	0.10	-	76,76,76,76	0
56	MG	BA	3275	1/1	0.30	-	77,77,77,77	0
56	MG	AA	1923	1/1	0.12	-	85,85,85,85	0
56	MG	AA	1911	1/1	0.31	-	104,104,104,104	0
56	MG	BA	3409	1/1	0.16	-	100,100,100,100	0
56	MG	CA	1929	1/1	0.29	-	116,116,116,116	0
56	MG	AT	201	1/1	0.20	-	101,101,101,101	0
56	MG	DA	3677	1/1	0.30	-	82,82,82,82	0
56	MG	DA	3537	1/1	0.12	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1784	1/1	0.19	-	71,71,71,71	0
56	MG	BT	101	1/1	0.07	-	65,65,65,65	0
56	MG	BA	2987	1/1	0.29	-	57,57,57,57	0
56	MG	BA	3541	1/1	0.23	-	79,79,79,79	0
56	MG	DA	3216	1/1	0.39	-	74,74,74,74	0
56	MG	BA	3147	1/1	0.44	-	83,83,83,83	0
56	MG	BA	2976	1/1	0.24	-	38,38,38,38	0
56	MG	DA	3081	1/1	0.18	-	61,61,61,61	0
56	MG	CA	1911	1/1	0.26	-	117,117,117,117	0
56	MG	BA	3522	1/1	0.04	-	54,54,54,54	0
56	MG	BA	3181	1/1	0.34	-	97,97,97,97	0
56	MG	CA	1865	1/1	0.15	-	109,109,109,109	0
56	MG	CA	1825	1/1	0.24	-	92,92,92,92	0
56	MG	BA	3579	1/1	0.10	-	83,83,83,83	0
56	MG	DA	3631	1/1	0.45	-	123,123,123,123	0
56	MG	DB	226	1/1	0.17	-	84,84,84,84	0
56	MG	CA	1953	1/1	0.06	-	91,91,91,91	0
56	MG	BA	2983	1/1	0.24	-	27,27,27,27	0
56	MG	AA	1778	1/1	0.07	-	61,61,61,61	0
56	MG	DG	202	1/1	0.09	-	84,84,84,84	0
56	MG	CA	1976	1/1	0.24	-	86,86,86,86	0
56	MG	AA	1623	1/1	0.34	-	53,53,53,53	0
56	MG	BA	3104	1/1	0.29	-	47,47,47,47	0
56	MG	CR	101	1/1	0.35	-	117,117,117,117	0
56	MG	BA	3533	1/1	0.10	-	81,81,81,81	0
56	MG	DA	3709	1/1	0.29	-	87,87,87,87	0
56	MG	AA	1834	1/1	0.51	-	183,183,183,183	0
56	MG	BA	3112	1/1	0.26	-	64,64,64,64	0
56	MG	AA	1903	1/1	0.23	-	95,95,95,95	0
56	MG	DA	3760	1/1	0.18	-	106,106,106,106	0
56	MG	BA	3286	1/1	0.22	-	80,80,80,80	0
56	MG	CA	1628	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3454	1/1	0.09	-	100,100,100,100	0
56	MG	BA	3179	1/1	0.19	-	51,51,51,51	0
56	MG	DA	2965	1/1	0.28	-	32,32,32,32	0
56	MG	CA	1848	1/1	0.14	-	119,119,119,119	0
56	MG	AA	1710	1/1	0.18	-	78,78,78,78	0
56	MG	AA	1995	1/1	0.26	-	142,142,142,142	0
56	MG	BA	3323	1/1	0.08	-	58,58,58,58	0
56	MG	AA	1875	1/1	0.20	-	113,113,113,113	0
56	MG	AA	2031	1/1	0.29	-	86,86,86,86	0
56	MG	BA	3514	1/1	0.38	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1624	1/1	0.33	-	56,56,56,56	0
56	MG	CA	1706	1/1	0.17	-	66,66,66,66	0
56	MG	DA	3443	1/1	0.19	-	82,82,82,82	0
56	MG	BA	3273	1/1	0.09	-	72,72,72,72	0
56	MG	DA	3044	1/1	0.19	-	48,48,48,48	0
56	MG	CA	1698	1/1	0.20	-	56,56,56,56	0
56	MG	AA	1979	1/1	0.28	-	75,75,75,75	0
56	MG	CT	201	1/1	0.21	-	76,76,76,76	0
56	MG	AA	1988	1/1	0.19	-	93,93,93,93	0
56	MG	BA	3388	1/1	0.44	-	95,95,95,95	0
56	MG	BA	3465	1/1	0.20	-	92,92,92,92	0
56	MG	CA	1615	1/1	0.15	-	53,53,53,53	0
56	MG	DA	3236	1/1	0.09	-	39,39,39,39	0
56	MG	AA	1861	1/1	0.20	-	120,120,120,120	0
56	MG	AA	1808	1/1	0.12	-	92,92,92,92	0
56	MG	BA	3376	1/1	0.17	-	121,121,121,121	0
56	MG	DA	3613	1/1	0.10	-	109,109,109,109	0
56	MG	DA	2954	1/1	0.26	-	27,27,27,27	0
56	MG	AA	1968	1/1	0.09	-	80,80,80,80	0
56	MG	AA	2026	1/1	0.28	-	90,90,90,90	0
56	MG	CA	1715	1/1	0.15	-	77,77,77,77	0
56	MG	BR	201	1/1	0.15	-	103,103,103,103	0
56	MG	BA	3520	1/1	0.24	-	55,55,55,55	0
56	MG	DA	2956	1/1	0.26	-	46,46,46,46	0
56	MG	DA	3350	1/1	0.25	-	71,71,71,71	0
56	MG	AA	1860	1/1	0.28	-	93,93,93,93	0
56	MG	BA	3211	1/1	0.04	-	43,43,43,43	0
56	MG	CA	1775	1/1	0.15	-	52,52,52,52	0
56	MG	BA	3009	1/1	0.18	-	57,57,57,57	0
56	MG	AA	1832	1/1	0.21	-	91,91,91,91	0
56	MG	BA	2926	1/1	0.18	-	43,43,43,43	0
56	MG	BA	3159	1/1	0.26	-	61,61,61,61	0
56	MG	DA	3229	1/1	0.20	-	61,61,61,61	0
56	MG	CH	202	1/1	0.17	-	72,72,72,72	0
56	MG	DA	3678	1/1	0.23	-	76,76,76,76	0
56	MG	DA	3478	1/1	0.56	-	116,116,116,116	0
56	MG	CS	102	1/1	0.14	-	119,119,119,119	0
56	MG	BA	3532	1/1	0.23	-	83,83,83,83	0
56	MG	DA	3717	1/1	0.18	-	75,75,75,75	0
56	MG	BA	3095	1/1	0.15	-	52,52,52,52	0
56	MG	BA	3582	1/1	0.27	-	133,133,133,133	0
56	MG	DA	3509	1/1	0.47	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3341	1/1	0.05	-	119,119,119,119	0
56	MG	DA	3639	1/1	0.13	-	116,116,116,116	0
56	MG	DA	3340	1/1	0.62	-	113,113,113,113	0
56	MG	BA	3321	1/1	0.15	-	64,64,64,64	0
56	MG	DA	2961	1/1	0.14	-	17,17,17,17	0
56	MG	CA	1841	1/1	0.29	-	103,103,103,103	0
56	MG	BA	3225	1/1	0.08	-	49,49,49,49	0
56	MG	DA	3532	1/1	0.30	-	92,92,92,92	0
56	MG	AA	1888	1/1	0.14	-	114,114,114,114	0
56	MG	CA	1916	1/1	0.13	-	74,74,74,74	0
56	MG	AA	2034	1/1	0.35	-	94,94,94,94	0
56	MG	AA	1637	1/1	0.54	-	82,82,82,82	0
56	MG	BA	3538	1/1	0.15	-	65,65,65,65	0
56	MG	AA	1953	1/1	0.17	-	94,94,94,94	0
56	MG	B1	201	1/1	0.18	-	80,80,80,80	0
56	MG	BA	3405	1/1	0.19	-	82,82,82,82	0
56	MG	DA	3286	1/1	0.28	-	65,65,65,65	0
56	MG	AA	1638	1/1	0.24	-	61,61,61,61	0
56	MG	BA	3460	1/1	0.20	-	90,90,90,90	0
56	MG	BA	3373	1/1	0.36	-	105,105,105,105	0
56	MG	CA	1824	1/1	0.27	-	105,105,105,105	0
56	MG	DU	205	1/1	0.19	-	75,75,75,75	0
56	MG	BA	3183	1/1	0.14	-	80,80,80,80	0
56	MG	DA	3024	1/1	0.25	-	36,36,36,36	0
56	MG	BA	2905	1/1	0.23	-	136,136,136,136	0
56	MG	CA	1921	1/1	0.08	-	36,36,36,36	0
56	MG	AA	2013	1/1	0.15	-	94,94,94,94	0
56	MG	DA	3336	1/1	0.30	-	84,84,84,84	0
56	MG	BA	3027	1/1	0.17	-	46,46,46,46	0
56	MG	CA	1742	1/1	0.41	-	108,108,108,108	0
56	MG	DA	3744	1/1	0.08	-	64,64,64,64	0
56	MG	CA	1774	1/1	0.20	-	68,68,68,68	0
56	MG	CA	1780	1/1	0.05	-	87,87,87,87	0
58	G	DA	2901	23/24	0.59	-	214,217,220,220	0
56	MG	DA	2999	1/1	0.20	-	33,33,33,33	0
56	MG	DA	3152	1/1	0.34	-	55,55,55,55	0
56	MG	BA	3333	1/1	0.13	-	62,62,62,62	0
56	MG	DA	3538	1/1	0.33	-	84,84,84,84	0
57	ZN	AA	2040	1/1	0.55	-	300,300,300,300	0
56	MG	CA	1896	1/1	0.20	-	89,89,89,89	0
56	MG	BA	3172	1/1	0.24	-	72,72,72,72	0
56	MG	DA	3389	1/1	0.22	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1871	1/1	0.07	-	117,117,117,117	0
56	MG	DA	3748	1/1	0.29	-	102,102,102,102	0
56	MG	BA	2916	1/1	0.25	-	42,42,42,42	0
56	MG	DA	3366	1/1	0.26	-	62,62,62,62	0
56	MG	DA	3474	1/1	0.55	-	107,107,107,107	0
56	MG	AA	1851	1/1	0.18	-	97,97,97,97	0
56	MG	DA	3084	1/1	0.18	-	50,50,50,50	0
56	MG	BA	3534	1/1	0.15	-	93,93,93,93	0
56	MG	AA	1885	1/1	0.24	-	113,113,113,113	0
56	MG	DA	3691	1/1	0.11	-	105,105,105,105	0
56	MG	CL	201	1/1	0.48	-	81,81,81,81	0
56	MG	AA	1952	1/1	0.06	-	76,76,76,76	0
56	MG	BA	3475	1/1	0.17	-	73,73,73,73	0
56	MG	AA	1747	1/1	0.29	-	89,89,89,89	0
61	A	DA	2919	22/23	0.35	-	194,198,199,199	0
56	MG	CA	1864	1/1	0.11	-	80,80,80,80	0
56	MG	DA	3808	1/1	0.30	-	97,97,97,97	0
56	MG	DA	3610	1/1	0.64	-	124,124,124,124	0
56	MG	AA	1717	1/1	0.30	-	77,77,77,77	0
56	MG	BA	3291	1/1	0.17	-	86,86,86,86	0
56	MG	DA	3008	1/1	0.25	-	40,40,40,40	0
56	MG	BA	3499	1/1	0.37	-	114,114,114,114	0
56	MG	BB	214	1/1	0.33	-	91,91,91,91	0
56	MG	BB	211	1/1	0.23	-	80,80,80,80	0
56	MG	AA	1618	1/1	0.29	-	39,39,39,39	0
56	MG	CA	1712	1/1	0.17	-	84,84,84,84	0
56	MG	BA	2999	1/1	0.14	-	27,27,27,27	0
56	MG	AA	1845	1/1	0.14	-	88,88,88,88	0
56	MG	CA	1923	1/1	0.14	-	114,114,114,114	0
56	MG	AA	1757	1/1	0.15	-	45,45,45,45	0
56	MG	AA	1791	1/1	0.07	-	68,68,68,68	0
56	MG	DA	3134	1/1	0.38	-	63,63,63,63	0
56	MG	CA	1918	1/1	0.16	-	123,123,123,123	0
56	MG	DA	3118	1/1	0.35	-	84,84,84,84	0
56	MG	BA	3491	1/1	0.27	-	104,104,104,104	0
56	MG	BA	2901	1/1	0.12	-	61,61,61,61	0
56	MG	AA	1633	1/1	0.31	-	79,79,79,79	0
56	MG	DA	2971	1/1	0.09	-	22,22,22,22	0
56	MG	AA	1666	1/1	0.25	-	95,95,95,95	0
56	MG	CA	1704	1/1	0.25	-	98,98,98,98	0
56	MG	AA	1827	1/1	0.19	-	88,88,88,88	0
56	MG	DA	3231	1/1	0.28	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	1733	1/1	0.14	-	54,54,54,54	0
56	MG	BA	3437	1/1	0.17	-	88,88,88,88	0
56	MG	DA	3809	1/1	0.25	-	76,76,76,76	0
56	MG	CA	1837	1/1	0.17	-	135,135,135,135	0
56	MG	DA	3275	1/1	0.35	-	100,100,100,100	0
56	MG	DA	3739	1/1	0.07	-	22,22,22,22	0
56	MG	BA	3326	1/1	0.10	-	54,54,54,54	0
56	MG	DA	3519	1/1	0.07	-	43,43,43,43	0
56	MG	DA	2998	1/1	0.19	-	37,37,37,37	0
56	MG	DA	3789	1/1	0.19	-	74,74,74,74	0
56	MG	AA	1646	1/1	0.22	-	66,66,66,66	0
56	MG	DA	3015	1/1	0.22	-	24,24,24,24	0
56	MG	DA	3605	1/1	0.13	-	93,93,93,93	0
56	MG	DA	3763	1/1	0.15	-	75,75,75,75	0
56	MG	BA	3525	1/1	0.09	-	95,95,95,95	0
56	MG	CA	1808	1/1	0.30	-	88,88,88,88	0
56	MG	AA	1634	1/1	0.42	-	97,97,97,97	0
56	MG	BA	3477	1/1	0.15	-	60,60,60,60	0
56	MG	CA	1631	1/1	0.22	-	40,40,40,40	0
56	MG	BA	2903	1/1	0.14	-	82,82,82,82	0
56	MG	DA	3383	1/1	0.07	-	66,66,66,66	0
56	MG	BA	3014	1/1	0.30	-	49,49,49,49	0
56	MG	DA	3718	1/1	0.25	-	92,92,92,92	0
56	MG	BA	2943	1/1	0.30	-	44,44,44,44	0
56	MG	BA	2954	1/1	0.26	-	54,54,54,54	0
56	MG	DA	3156	1/1	0.32	-	59,59,59,59	0
56	MG	DA	3510	1/1	0.34	-	87,87,87,87	0
56	MG	BU	201	1/1	0.29	-	75,75,75,75	0
56	MG	DA	3673	1/1	0.15	-	66,66,66,66	0
56	MG	DZ	101	1/1	0.06	-	79,79,79,79	0
56	MG	DA	3194	1/1	0.08	-	51,51,51,51	0
56	MG	BA	3126	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3338	1/1	0.16	-	100,100,100,100	0
56	MG	CC	116	1/1	0.31	-	99,99,99,99	0
56	MG	BA	3214	1/1	0.22	-	67,67,67,67	0
56	MG	CA	1958	1/1	0.16	-	74,74,74,74	0
56	MG	DA	3284	1/1	0.14	-	45,45,45,45	0
56	MG	DB	212	1/1	0.38	-	75,75,75,75	0
61	A	DA	2918	22/23	0.25	-	137,139,140,145	0
56	MG	DA	3602	1/1	0.18	-	100,100,100,100	0
56	MG	BA	3141	1/1	0.16	-	52,52,52,52	0
56	MG	DA	3626	1/1	0.69	-	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3003	1/1	0.27	-	37,37,37,37	0
56	MG	BA	3537	1/1	0.31	-	108,108,108,108	0
56	MG	DA	3063	1/1	0.30	-	34,34,34,34	0
56	MG	BE	302	1/1	0.12	-	85,85,85,85	0
56	MG	AA	1828	1/1	0.15	-	98,98,98,98	0
56	MG	DA	3483	1/1	0.32	-	86,86,86,86	0
56	MG	CA	1814	1/1	0.09	-	71,71,71,71	0
56	MG	DA	3606	1/1	0.33	-	92,92,92,92	0
56	MG	AA	1878	1/1	0.20	-	99,99,99,99	0
56	MG	BA	3088	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3200	1/1	0.28	-	90,90,90,90	0
56	MG	CA	1892	1/1	0.18	-	74,74,74,74	0
56	MG	BA	3113	1/1	0.11	-	41,41,41,41	0
56	MG	DA	3247	1/1	0.40	-	75,75,75,75	0
56	MG	CA	1676	1/1	0.25	-	71,71,71,71	0
56	MG	CA	1731	1/1	0.13	-	66,66,66,66	0
56	MG	DA	3637	1/1	0.25	-	107,107,107,107	0
56	MG	CA	1756	1/1	0.22	-	69,69,69,69	0
56	MG	DA	3372	1/1	0.35	-	93,93,93,93	0
56	MG	BA	2908	1/1	0.15	-	102,102,102,102	0
56	MG	AA	1855	1/1	0.24	-	101,101,101,101	0
56	MG	BA	3193	1/1	0.26	-	80,80,80,80	0
56	MG	CA	1681	1/1	0.16	-	73,73,73,73	0
56	MG	CA	1813	1/1	0.24	-	106,106,106,106	0
56	MG	AA	1647	1/1	0.44	-	71,71,71,71	0
56	MG	BA	3032	1/1	0.40	-	66,66,66,66	0
56	MG	AA	1983	1/1	0.28	-	104,104,104,104	0
56	MG	BA	3154	1/1	0.25	-	117,117,117,117	0
56	MG	DB	222	1/1	0.26	-	92,92,92,92	0
56	MG	DA	3582	1/1	0.26	-	74,74,74,74	0
56	MG	DA	3404	1/1	0.15	-	60,60,60,60	0
56	MG	DA	3061	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3412	1/1	0.20	-	94,94,94,94	0
56	MG	DA	3786	1/1	0.21	-	102,102,102,102	0
56	MG	BA	3097	1/1	0.22	-	59,59,59,59	0
56	MG	BA	3550	1/1	0.21	-	102,102,102,102	0
56	MG	DA	3557	1/1	0.29	-	90,90,90,90	0
56	MG	DA	3585	1/1	0.24	-	86,86,86,86	0
56	MG	DA	3158	1/1	0.08	-	56,56,56,56	0
56	MG	AA	1745	1/1	0.20	-	67,67,67,67	0
56	MG	AA	1622	1/1	0.18	-	78,78,78,78	0
56	MG	DA	3728	1/1	0.28	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3558	1/1	0.06	-	75,75,75,75	0
56	MG	BA	3287	1/1	0.37	-	79,79,79,79	0
56	MG	AA	1916	1/1	0.17	-	93,93,93,93	0
56	MG	BA	3239	1/1	0.15	-	49,49,49,49	0
56	MG	AA	1912	1/1	0.17	-	79,79,79,79	0
56	MG	CA	1889	1/1	0.31	-	106,106,106,106	0
56	MG	AH	202	1/1	0.07	-	80,80,80,80	0
56	MG	DB	228	1/1	0.33	-	116,116,116,116	0
56	MG	BA	3127	1/1	0.30	-	64,64,64,64	0
56	MG	D6	101	1/1	0.74	-	98,98,98,98	0
56	MG	BD	302	1/1	0.13	-	69,69,69,69	0
56	MG	AA	1765	1/1	0.24	-	83,83,83,83	0
56	MG	AA	1807	1/1	0.06	-	65,65,65,65	0
56	MG	DA	3503	1/1	0.37	-	85,85,85,85	0
56	MG	DB	208	1/1	0.22	-	135,135,135,135	0
56	MG	AA	1822	1/1	0.10	-	107,107,107,107	0
56	MG	CA	1759	1/1	0.24	-	90,90,90,90	0
56	MG	AA	2014	1/1	0.28	-	175,175,175,175	0
56	MG	BA	3330	1/1	0.11	-	62,62,62,62	0
56	MG	DA	3017	1/1	0.26	-	44,44,44,44	0
56	MG	AA	1836	1/1	0.14	-	58,58,58,58	0
58	G	CC	102	23/24	0.57	-	211,212,213,214	0
56	MG	CA	1636	1/1	0.29	-	85,85,85,85	0
56	MG	BA	3264	1/1	0.14	-	64,64,64,64	0
56	MG	DA	3195	1/1	0.17	-	62,62,62,62	0
56	MG	BA	3274	1/1	0.15	-	116,116,116,116	0
56	MG	BA	3415	1/1	0.21	-	89,89,89,89	0
56	MG	AA	1636	1/1	0.41	-	71,71,71,71	0
56	MG	DA	3351	1/1	0.14	-	107,107,107,107	0
56	MG	DA	3070	1/1	0.22	-	42,42,42,42	0
56	MG	AA	1886	1/1	0.33	-	102,102,102,102	0
56	MG	BA	3566	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3132	1/1	0.41	-	90,90,90,90	0
56	MG	CW	201	1/1	0.24	-	67,67,67,67	0
56	MG	AA	1722	1/1	0.37	-	68,68,68,68	0
56	MG	AA	1601	1/1	0.23	-	42,42,42,42	0
56	MG	DA	3225	1/1	0.40	-	96,96,96,96	0
56	MG	BA	3105	1/1	0.25	-	87,87,87,87	0
56	MG	AC	103	1/1	0.09	-	86,86,86,86	0
56	MG	BA	3493	1/1	0.21	-	85,85,85,85	0
56	MG	DA	3831	1/1	0.19	-	142,142,142,142	0
56	MG	DA	3644	1/1	0.18	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1694	1/1	0.10	-	76,76,76,76	0
56	MG	DB	215	1/1	0.20	-	99,99,99,99	0
56	MG	DA	3840	1/1	0.06	-	99,99,99,99	0
56	MG	DA	3086	1/1	0.40	-	114,114,114,114	0
58	G	DA	2916	23/24	0.47	-	195,197,199,199	0
56	MG	BA	3125	1/1	0.16	-	94,94,94,94	0
56	MG	AA	1780	1/1	0.29	-	95,95,95,95	0
56	MG	DA	3123	1/1	0.20	-	61,61,61,61	0
56	MG	BA	3435	1/1	0.08	-	59,59,59,59	0
56	MG	CA	1793	1/1	0.19	-	86,86,86,86	0
56	MG	BA	3102	1/1	0.06	-	113,113,113,113	0
56	MG	CA	1931	1/1	0.09	-	98,98,98,98	0
56	MG	DA	3230	1/1	0.32	-	81,81,81,81	0
56	MG	CA	1807	1/1	0.16	-	97,97,97,97	0
56	MG	DA	2997	1/1	0.29	-	34,34,34,34	0
56	MG	DA	3381	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3415	1/1	0.08	-	76,76,76,76	0
56	MG	DA	3471	1/1	0.23	-	63,63,63,63	0
56	MG	AA	2008	1/1	0.10	-	69,69,69,69	0
56	MG	DA	3064	1/1	0.14	-	22,22,22,22	0
56	MG	AA	1685	1/1	0.19	-	96,96,96,96	0
56	MG	BA	3297	1/1	0.22	-	131,131,131,131	0
56	MG	DA	3147	1/1	0.15	-	54,54,54,54	0
56	MG	DA	3170	1/1	0.19	-	64,64,64,64	0
56	MG	CA	1840	1/1	0.11	-	70,70,70,70	0
56	MG	BZ	101	1/1	0.24	-	92,92,92,92	0
56	MG	DA	2995	1/1	0.10	-	46,46,46,46	0
56	MG	CA	1684	1/1	0.20	-	57,57,57,57	0
56	MG	DA	2950	1/1	0.34	-	30,30,30,30	0
56	MG	AA	1819	1/1	0.36	-	98,98,98,98	0
56	MG	BA	3527	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3217	1/1	0.26	-	86,86,86,86	0
56	MG	DA	3816	1/1	0.10	-	72,72,72,72	0
56	MG	DA	3136	1/1	0.38	-	60,60,60,60	0
60	U	DA	2925	20/21	0.60	-	203,208,208,208	0
56	MG	BA	3133	1/1	0.18	-	49,49,49,49	0
56	MG	AA	2002	1/1	0.08	-	81,81,81,81	0
56	MG	AA	1805	1/1	0.44	-	109,109,109,109	0
56	MG	DA	3051	1/1	0.43	-	68,68,68,68	0
56	MG	AA	1770	1/1	0.24	-	71,71,71,71	0
56	MG	BA	3059	1/1	0.33	-	59,59,59,59	0
56	MG	DA	3770	1/1	0.23	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3332	1/1	0.12	-	104,104,104,104	0
56	MG	CA	1791	1/1	0.31	-	85,85,85,85	0
56	MG	DA	3779	1/1	0.25	-	58,58,58,58	0
56	MG	CA	1990	1/1	0.12	-	92,92,92,92	0
56	MG	CA	1734	1/1	0.11	-	131,131,131,131	0
56	MG	DA	3505	1/1	0.11	-	73,73,73,73	0
56	MG	DA	3167	1/1	0.45	-	89,89,89,89	0
56	MG	CA	1673	1/1	0.14	-	67,67,67,67	0
56	MG	DA	3098	1/1	0.29	-	52,52,52,52	0
56	MG	CA	1857	1/1	0.12	-	96,96,96,96	0
56	MG	BA	3190	1/1	0.20	-	78,78,78,78	0
56	MG	AA	1687	1/1	0.62	-	138,138,138,138	0
56	MG	BA	3576	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3053	1/1	0.23	-	43,43,43,43	0
56	MG	CA	1798	1/1	0.06	-	85,85,85,85	0
56	MG	DA	3528	1/1	0.45	-	102,102,102,102	0
56	MG	BA	3263	1/1	0.32	-	65,65,65,65	0
56	MG	AA	1951	1/1	0.17	-	79,79,79,79	0
56	MG	AA	1802	1/1	0.21	-	98,98,98,98	0
56	MG	DA	3114	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3074	1/1	0.21	-	41,41,41,41	0
56	MG	BA	3224	1/1	0.23	-	54,54,54,54	0
56	MG	BA	3247	1/1	0.19	-	63,63,63,63	0
56	MG	CA	1845	1/1	0.23	-	83,83,83,83	0
56	MG	DA	3607	1/1	0.54	-	152,152,152,152	0
56	MG	DA	3297	1/1	0.14	-	53,53,53,53	0
56	MG	BA	3382	1/1	0.24	-	123,123,123,123	0
56	MG	DA	3112	1/1	0.15	-	43,43,43,43	0
56	MG	DA	3212	1/1	0.10	-	34,34,34,34	0
56	MG	DA	3055	1/1	0.39	-	83,83,83,83	0
56	MG	DA	3053	1/1	0.23	-	23,23,23,23	0
56	MG	DE	302	1/1	0.10	-	51,51,51,51	0
56	MG	DA	3830	1/1	0.12	-	108,108,108,108	0
56	MG	BA	3061	1/1	0.15	-	70,70,70,70	0
56	MG	DA	3058	1/1	0.36	-	47,47,47,47	0
56	MG	AA	1773	1/1	0.16	-	81,81,81,81	0
56	MG	CA	1937	1/1	0.23	-	96,96,96,96	0
56	MG	BA	3085	1/1	0.08	-	40,40,40,40	0
56	MG	AA	2038	1/1	0.35	-	116,116,116,116	0
56	MG	BA	3170	1/1	0.31	-	72,72,72,72	0
56	MG	CC	111	1/1	0.10	-	65,65,65,65	0
56	MG	AA	1945	1/1	0.32	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3360	1/1	0.13	-	105,105,105,105	0
56	MG	BB	210	1/1	0.24	-	62,62,62,62	0
56	MG	BA	3452	1/1	0.16	-	57,57,57,57	0
56	MG	AA	1887	1/1	0.33	-	161,161,161,161	0
56	MG	DA	3041	1/1	0.29	-	52,52,52,52	0
56	MG	BA	3253	1/1	0.17	-	70,70,70,70	0
56	MG	DA	3712	1/1	0.29	-	104,104,104,104	0
56	MG	DA	3797	1/1	0.14	-	206,206,206,206	0
56	MG	BA	3363	1/1	0.15	-	79,79,79,79	0
56	MG	AA	1939	1/1	0.08	-	118,118,118,118	0
56	MG	DA	3669	1/1	0.09	-	73,73,73,73	0
56	MG	BA	3444	1/1	0.24	-	66,66,66,66	0
56	MG	DA	3462	1/1	0.06	-	68,68,68,68	0
56	MG	BA	3233	1/1	0.14	-	84,84,84,84	0
56	MG	BA	2961	1/1	0.31	-	46,46,46,46	0
56	MG	BA	3448	1/1	0.27	-	95,95,95,95	0
56	MG	BA	3411	1/1	0.19	-	71,71,71,71	0
56	MG	BA	3018	1/1	0.40	-	109,109,109,109	0
56	MG	CA	1847	1/1	0.23	-	113,113,113,113	0
56	MG	DA	3713	1/1	0.29	-	131,131,131,131	0
56	MG	BA	3296	1/1	0.11	-	57,57,57,57	0
56	MG	DA	3680	1/1	0.11	-	82,82,82,82	0
56	MG	BA	3265	1/1	0.04	-	40,40,40,40	0
56	MG	DA	3738	1/1	0.22	-	92,92,92,92	0
56	MG	AA	2005	1/1	0.07	-	96,96,96,96	0
56	MG	BA	3553	1/1	0.17	-	96,96,96,96	0
56	MG	BA	3262	1/1	0.14	-	58,58,58,58	0
56	MG	DA	3640	1/1	0.23	-	86,86,86,86	0
56	MG	BA	2992	1/1	0.27	-	63,63,63,63	0
56	MG	AA	1893	1/1	0.11	-	95,95,95,95	0
56	MG	DA	3185	1/1	0.36	-	76,76,76,76	0
56	MG	CA	1932	1/1	0.14	-	90,90,90,90	0
56	MG	DA	3752	1/1	0.43	-	91,91,91,91	0
56	MG	BA	3523	1/1	0.12	-	104,104,104,104	0
56	MG	AA	1891	1/1	0.27	-	93,93,93,93	0
59	C	CC	105	20/21	0.72	-	219,224,225,225	0
56	MG	DA	3071	1/1	0.27	-	75,75,75,75	0
56	MG	DA	3804	1/1	0.04	-	61,61,61,61	0
56	MG	AA	1781	1/1	0.36	-	98,98,98,98	0
56	MG	AA	1933	1/1	0.27	-	98,98,98,98	0
56	MG	CA	1885	1/1	0.26	-	133,133,133,133	0
56	MG	DA	2990	1/1	0.25	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3330	1/1	0.72	-	134,134,134,134	0
56	MG	DA	3089	1/1	0.09	-	42,42,42,42	0
56	MG	DA	3312	1/1	0.24	-	62,62,62,62	0
59	C	CC	107	20/21	0.60	-	229,229,230,230	0
56	MG	BB	208	1/1	0.13	-	91,91,91,91	0
56	MG	CA	1790	1/1	0.22	-	47,47,47,47	0
56	MG	DA	3432	1/1	0.20	-	71,71,71,71	0
56	MG	BA	3572	1/1	0.32	-	106,106,106,106	0
56	MG	AA	1800	1/1	0.46	-	117,117,117,117	0
56	MG	DA	3050	1/1	0.30	-	58,58,58,58	0
56	MG	CA	1806	1/1	0.39	-	86,86,86,86	0
56	MG	BA	3559	1/1	0.24	-	104,104,104,104	0
56	MG	BA	3462	1/1	0.26	-	77,77,77,77	0
56	MG	BA	3536	1/1	0.27	-	89,89,89,89	0
56	MG	CA	1960	1/1	0.47	-	103,103,103,103	0
56	MG	BA	3315	1/1	0.15	-	84,84,84,84	0
56	MG	DA	3757	1/1	0.51	-	82,82,82,82	0
56	MG	DA	3573	1/1	0.38	-	94,94,94,94	0
56	MG	DA	3456	1/1	0.55	-	92,92,92,92	0
59	C	DA	2935	20/21	0.42	-	205,208,209,210	0
56	MG	BA	3396	1/1	0.20	-	63,63,63,63	0
56	MG	BA	3501	1/1	0.17	-	80,80,80,80	0
56	MG	AA	1752	1/1	0.34	-	75,75,75,75	0
56	MG	DA	3710	1/1	0.30	-	94,94,94,94	0
56	MG	CA	1872	1/1	0.13	-	85,85,85,85	0
56	MG	DA	3662	1/1	0.32	-	99,99,99,99	0
56	MG	DA	3115	1/1	0.20	-	77,77,77,77	0
56	MG	AA	1768	1/1	0.18	-	67,67,67,67	0
56	MG	AA	1813	1/1	0.32	-	93,93,93,93	0
56	MG	AA	1672	1/1	0.30	-	68,68,68,68	0
56	MG	DA	3621	1/1	0.25	-	86,86,86,86	0
56	MG	DA	3545	1/1	0.27	-	73,73,73,73	0
56	MG	CA	1833	1/1	0.10	-	107,107,107,107	0
59	C	CA	1603	20/21	0.29	-	147,151,160,160	0
56	MG	BA	3223	1/1	0.24	-	88,88,88,88	0
56	MG	DA	3260	1/1	0.16	-	64,64,64,64	0
56	MG	AA	1874	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3556	1/1	0.39	-	87,87,87,87	0
56	MG	CC	115	1/1	0.11	-	75,75,75,75	0
56	MG	DA	3322	1/1	0.33	-	56,56,56,56	0
56	MG	DA	3423	1/1	0.37	-	75,75,75,75	0
56	MG	DA	3126	1/1	0.34	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3288	1/1	0.36	-	83,83,83,83	0
56	MG	BA	3238	1/1	0.34	-	85,85,85,85	0
56	MG	DA	3357	1/1	0.20	-	131,131,131,131	0
56	MG	BA	3311	1/1	0.20	-	48,48,48,48	0
56	MG	AA	1880	1/1	0.12	-	80,80,80,80	0
56	MG	BA	3459	1/1	0.26	-	110,110,110,110	0
56	MG	DA	3511	1/1	0.43	-	89,89,89,89	0
56	MG	BA	3066	1/1	0.41	-	99,99,99,99	0
56	MG	AA	1971	1/1	0.36	-	123,123,123,123	0
56	MG	DA	3326	1/1	0.19	-	63,63,63,63	0
56	MG	DA	3228	1/1	0.40	-	89,89,89,89	0
56	MG	BA	3387	1/1	0.14	-	67,67,67,67	0
56	MG	AW	202	1/1	0.08	-	59,59,59,59	0
56	MG	DA	3484	1/1	0.24	-	84,84,84,84	0
56	MG	CA	1821	1/1	0.31	-	84,84,84,84	0
56	MG	DA	3814	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3416	1/1	0.21	-	74,74,74,74	0
56	MG	CA	1652	1/1	0.31	-	79,79,79,79	0
56	MG	DA	3310	1/1	0.05	-	39,39,39,39	0
56	MG	BA	3199	1/1	0.30	-	84,84,84,84	0
56	MG	DA	3370	1/1	0.15	-	50,50,50,50	0
56	MG	D1	202	1/1	0.14	-	75,75,75,75	0
56	MG	CA	1973	1/1	0.10	-	82,82,82,82	0
56	MG	CA	1934	1/1	0.13	-	86,86,86,86	0
56	MG	BA	3447	1/1	0.20	-	109,109,109,109	0
56	MG	BA	3498	1/1	0.22	-	59,59,59,59	0
56	MG	BA	3008	1/1	0.22	-	95,95,95,95	0
56	MG	BA	3424	1/1	0.24	-	107,107,107,107	0
56	MG	BA	3518	1/1	0.40	-	134,134,134,134	0
56	MG	BA	3404	1/1	0.08	-	82,82,82,82	0
56	MG	BA	3250	1/1	0.25	-	93,93,93,93	0
56	MG	AX	101	1/1	0.17	-	107,107,107,107	0
56	MG	CA	1810	1/1	0.26	-	100,100,100,100	0
56	MG	DA	3335	1/1	0.23	-	70,70,70,70	0
56	MG	DA	3755	1/1	0.15	-	88,88,88,88	0
56	MG	DA	3645	1/1	0.37	-	74,74,74,74	0
56	MG	DA	3319	1/1	0.11	-	63,63,63,63	0
56	MG	AS	101	1/1	0.27	-	84,84,84,84	0
56	MG	DA	3251	1/1	0.29	-	72,72,72,72	0
56	MG	DG	203	1/1	0.24	-	112,112,112,112	0
56	MG	CD	114	1/1	0.07	-	109,109,109,109	0
56	MG	DA	3729	1/1	0.13	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3239	1/1	0.15	-	49,49,49,49	0
56	MG	BA	3192	1/1	0.05	-	54,54,54,54	0
56	MG	AA	1982	1/1	0.11	-	126,126,126,126	0
56	MG	DA	3131	1/1	0.21	-	49,49,49,49	0
56	MG	DA	3479	1/1	0.24	-	86,86,86,86	0
56	MG	BA	3345	1/1	0.15	-	80,80,80,80	0
56	MG	BA	3299	1/1	0.32	-	94,94,94,94	0
56	MG	AA	2021	1/1	0.07	-	108,108,108,108	0
56	MG	DA	3233	1/1	0.25	-	106,106,106,106	0
56	MG	BA	3567	1/1	0.11	-	69,69,69,69	0
56	MG	CA	1700	1/1	0.14	-	64,64,64,64	0
56	MG	CA	1899	1/1	0.05	-	99,99,99,99	0
56	MG	DA	3550	1/1	0.40	-	82,82,82,82	0
56	MG	DA	3023	1/1	0.07	-	42,42,42,42	0
57	ZN	AA	2041	1/1	0.31	-	262,262,262,262	0
56	MG	DA	3490	1/1	0.39	-	81,81,81,81	0
56	MG	DA	3468	1/1	0.07	-	51,51,51,51	0
56	MG	CA	1951	1/1	0.13	-	99,99,99,99	0
56	MG	DA	3628	1/1	0.16	-	81,81,81,81	0
56	MG	CA	1809	1/1	0.11	-	62,62,62,62	0
56	MG	DA	3184	1/1	0.19	-	42,42,42,42	0
56	MG	BA	3488	1/1	0.28	-	96,96,96,96	0
56	MG	DA	3616	1/1	0.45	-	94,94,94,94	0
56	MG	BA	3166	1/1	0.08	-	57,57,57,57	0
56	MG	DA	3362	1/1	0.10	-	64,64,64,64	0
56	MG	BA	3385	1/1	0.21	-	64,64,64,64	0
56	MG	CA	1632	1/1	0.30	-	51,51,51,51	0
56	MG	DA	3090	1/1	0.05	-	28,28,28,28	0
56	MG	CA	1907	1/1	0.07	-	50,50,50,50	0
56	MG	DA	3074	1/1	0.32	-	58,58,58,58	0
56	MG	BB	217	1/1	0.38	-	102,102,102,102	0
56	MG	DA	3418	1/1	0.23	-	73,73,73,73	0
56	MG	DA	3431	1/1	0.27	-	73,73,73,73	0
56	MG	CA	1963	1/1	0.09	-	217,217,217,217	0
56	MG	DA	3037	1/1	0.23	-	31,31,31,31	0
56	MG	AQ	101	1/1	0.06	-	83,83,83,83	0
56	MG	DA	3715	1/1	0.10	-	69,69,69,69	0
56	MG	DA	3648	1/1	0.46	-	112,112,112,112	0
56	MG	DA	3470	1/1	0.21	-	87,87,87,87	0
56	MG	BH	201	1/1	0.48	-	193,193,193,193	0
56	MG	AA	1631	1/1	0.28	-	60,60,60,60	0
56	MG	CS	101	1/1	0.25	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3127	1/1	0.12	-	43,43,43,43	0
56	MG	CA	1915	1/1	0.28	-	128,128,128,128	0
56	MG	AA	1712	1/1	0.09	-	50,50,50,50	0
56	MG	BA	3282	1/1	0.22	-	103,103,103,103	0
56	MG	AA	1846	1/1	0.42	-	97,97,97,97	0
56	MG	CA	1920	1/1	0.12	-	101,101,101,101	0
56	MG	DA	3209	1/1	0.14	-	53,53,53,53	0
56	MG	CA	1639	1/1	0.24	-	62,62,62,62	0
56	MG	AA	2007	1/1	0.38	-	119,119,119,119	0
56	MG	BA	3403	1/1	0.33	-	89,89,89,89	0
56	MG	DA	3215	1/1	0.37	-	72,72,72,72	0
56	MG	BA	3570	1/1	0.20	-	104,104,104,104	0
56	MG	DA	3531	1/1	0.09	-	110,110,110,110	0
56	MG	DA	3099	1/1	0.23	-	50,50,50,50	0
56	MG	DA	3116	1/1	0.39	-	59,59,59,59	0
56	MG	AA	1705	1/1	0.15	-	77,77,77,77	0
56	MG	AA	1991	1/1	0.09	-	70,70,70,70	0
56	MG	DA	3489	1/1	0.11	-	104,104,104,104	0
56	MG	DA	3060	1/1	0.22	-	28,28,28,28	0
56	MG	DA	3244	1/1	0.26	-	66,66,66,66	0
56	MG	DA	3143	1/1	0.29	-	44,44,44,44	0
56	MG	BB	207	1/1	0.26	-	69,69,69,69	0
56	MG	BA	3508	1/1	0.07	-	90,90,90,90	0
56	MG	CA	1643	1/1	0.19	-	52,52,52,52	0
56	MG	DA	3440	1/1	0.26	-	69,69,69,69	0
56	MG	BA	3244	1/1	0.08	-	67,67,67,67	0
56	MG	BA	3011	1/1	0.18	-	57,57,57,57	0
56	MG	BA	3300	1/1	0.13	-	87,87,87,87	0
56	MG	BA	3513	1/1	0.11	-	77,77,77,77	0
56	MG	DA	3289	1/1	0.31	-	65,65,65,65	0
56	MG	DA	3719	1/1	0.71	-	141,141,141,141	0
56	MG	BA	2937	1/1	0.23	-	53,53,53,53	0
56	MG	DA	3726	1/1	0.17	-	63,63,63,63	0
56	MG	AA	1868	1/1	0.23	-	103,103,103,103	0
56	MG	DA	3146	1/1	0.67	-	103,103,103,103	0
56	MG	CA	1961	1/1	0.12	-	95,95,95,95	0
56	MG	BA	3230	1/1	0.10	-	67,67,67,67	0
56	MG	BA	3495	1/1	0.20	-	97,97,97,97	0
60	U	DP	203	20/21	0.23	-	190,195,196,196	0
56	MG	AA	1973	1/1	0.15	-	84,84,84,84	0
56	MG	DA	3634	1/1	1.33	-	168,168,168,168	0
56	MG	CA	1922	1/1	0.15	-	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3246	1/1	0.11	-	57,57,57,57	0
56	MG	AA	1985	1/1	0.47	-	131,131,131,131	0
56	MG	AA	1950	1/1	0.13	-	90,90,90,90	0
56	MG	DA	3409	1/1	0.30	-	57,57,57,57	0
56	MG	DB	201	1/1	0.37	-	86,86,86,86	0
56	MG	BA	3171	1/1	0.07	-	50,50,50,50	0
56	MG	CA	1902	1/1	0.16	-	87,87,87,87	0
56	MG	BA	3107	1/1	0.07	-	61,61,61,61	0
56	MG	DA	3106	1/1	0.20	-	52,52,52,52	0
56	MG	BA	3025	1/1	0.13	-	47,47,47,47	0
56	MG	BA	3464	1/1	0.30	-	102,102,102,102	0
56	MG	CA	1849	1/1	0.13	-	112,112,112,112	0
56	MG	BA	2939	1/1	0.34	-	47,47,47,47	0
56	MG	AA	1794	1/1	0.33	-	93,93,93,93	0
58	G	DA	2924	23/24	0.46	-	203,205,210,210	0
56	MG	DA	3434	1/1	0.23	-	77,77,77,77	0
56	MG	DA	3508	1/1	0.24	-	94,94,94,94	0
56	MG	CA	1854	1/1	0.28	-	133,133,133,133	0
56	MG	CA	1707	1/1	0.40	-	107,107,107,107	0
56	MG	DZ	102	1/1	0.05	-	79,79,79,79	0
56	MG	DA	3110	1/1	0.40	-	73,73,73,73	0
56	MG	DF	301	1/1	0.16	-	82,82,82,82	0
56	MG	CA	1888	1/1	0.13	-	105,105,105,105	0
58	G	DA	2921	23/24	0.51	-	199,201,202,202	0
56	MG	DA	3169	1/1	0.32	-	76,76,76,76	0
56	MG	AA	1767	1/1	0.52	-	110,110,110,110	0
56	MG	BA	3280	1/1	0.12	-	61,61,61,61	0
56	MG	CA	1843	1/1	0.25	-	58,58,58,58	0
56	MG	BA	3108	1/1	0.11	-	41,41,41,41	0
56	MG	DA	2975	1/1	0.12	-	57,57,57,57	0
61	A	DA	2931	22/23	0.42	-	181,188,194,194	0
56	MG	AA	1771	1/1	0.26	-	70,70,70,70	0
56	MG	BA	3569	1/1	0.18	-	137,137,137,137	0
56	MG	BA	3349	1/1	0.12	-	82,82,82,82	0
56	MG	BA	3418	1/1	0.08	-	65,65,65,65	0
56	MG	DA	2977	1/1	0.24	-	25,25,25,25	0
56	MG	BA	3142	1/1	0.13	-	90,90,90,90	0
56	MG	B0	201	1/1	0.17	-	74,74,74,74	0
56	MG	DA	3159	1/1	0.28	-	60,60,60,60	0
56	MG	DA	3526	1/1	0.47	-	79,79,79,79	0
56	MG	CA	1659	1/1	0.19	-	49,49,49,49	0
56	MG	DA	3413	1/1	0.39	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1655	1/1	0.21	-	91,91,91,91	0
56	MG	DA	3590	1/1	0.18	-	74,74,74,74	0
56	MG	BA	3302	1/1	0.07	-	61,61,61,61	0
56	MG	AA	1754	1/1	0.33	-	96,96,96,96	0
56	MG	AA	1858	1/1	0.09	-	83,83,83,83	0
56	MG	DA	3599	1/1	0.24	-	75,75,75,75	0
56	MG	DA	3593	1/1	0.30	-	183,183,183,183	0
56	MG	DA	3762	1/1	0.19	-	132,132,132,132	0
56	MG	DA	3079	1/1	0.26	-	48,48,48,48	0
56	MG	DA	3339	1/1	0.25	-	76,76,76,76	0
56	MG	BA	3258	1/1	0.16	-	100,100,100,100	0
56	MG	DA	3564	1/1	0.51	-	127,127,127,127	0
56	MG	DE	301	1/1	0.18	-	27,27,27,27	0
56	MG	CA	1719	1/1	0.10	-	65,65,65,65	0
56	MG	DA	3692	1/1	0.15	-	94,94,94,94	0
56	MG	BA	3062	1/1	0.21	-	61,61,61,61	0
56	MG	AA	1882	1/1	0.42	-	134,134,134,134	0
56	MG	AA	1762	1/1	0.25	-	104,104,104,104	0
56	MG	BA	3169	1/1	0.26	-	60,60,60,60	0
56	MG	BA	3295	1/1	0.11	-	55,55,55,55	0
56	MG	DA	3458	1/1	0.55	-	85,85,85,85	0
56	MG	DA	3473	1/1	0.14	-	72,72,72,72	0
56	MG	BA	3486	1/1	0.24	-	90,90,90,90	0
56	MG	DB	203	1/1	0.42	-	67,67,67,67	0
56	MG	AA	1703	1/1	0.25	-	49,49,49,49	0
56	MG	DA	3208	1/1	0.12	-	45,45,45,45	0
56	MG	BB	215	1/1	0.13	-	65,65,65,65	0
56	MG	BA	3565	1/1	0.13	-	99,99,99,99	0
56	MG	DA	3824	1/1	0.15	-	59,59,59,59	0
56	MG	CA	1909	1/1	0.09	-	46,46,46,46	0
56	MG	AA	1653	1/1	0.07	-	107,107,107,107	0
56	MG	AA	1852	1/1	0.19	-	66,66,66,66	0
56	MG	BA	3035	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3283	1/1	0.53	-	101,101,101,101	0
56	MG	DA	3681	1/1	0.25	-	106,106,106,106	0
56	MG	CA	1860	1/1	0.16	-	101,101,101,101	0
56	MG	AA	1835	1/1	0.30	-	109,109,109,109	0
56	MG	BA	3071	1/1	0.19	-	74,74,74,74	0
56	MG	DA	3174	1/1	0.17	-	51,51,51,51	0
56	MG	CD	116	1/1	0.12	-	90,90,90,90	0
56	MG	CD	113	1/1	0.12	-	80,80,80,80	0
56	MG	CA	1981	1/1	0.10	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1681	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3075	1/1	0.19	-	50,50,50,50	0
56	MG	DA	3278	1/1	0.13	-	56,56,56,56	0
56	MG	AC	106	1/1	0.17	-	79,79,79,79	0
56	MG	DA	3705	1/1	0.39	-	117,117,117,117	0
56	MG	DA	3242	1/1	0.29	-	115,115,115,115	0
56	MG	CA	1737	1/1	0.20	-	66,66,66,66	0
56	MG	DA	3400	1/1	0.28	-	113,113,113,113	0
56	MG	BA	3234	1/1	0.07	-	42,42,42,42	0
56	MG	DA	3785	1/1	0.54	-	71,71,71,71	0
56	MG	CA	1637	1/1	0.30	-	59,59,59,59	0

## 6.5 Other polymers

There are no such residues in this entry.