



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:55 PM BST

PDB ID : 4V9B  
Title : Crystal Structure of the 70S ribosome with tigecycline. This entry contains the 30S subunit of molecule A.  
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.  
Deposited on : 2012-07-18  
Resolution : 3.10 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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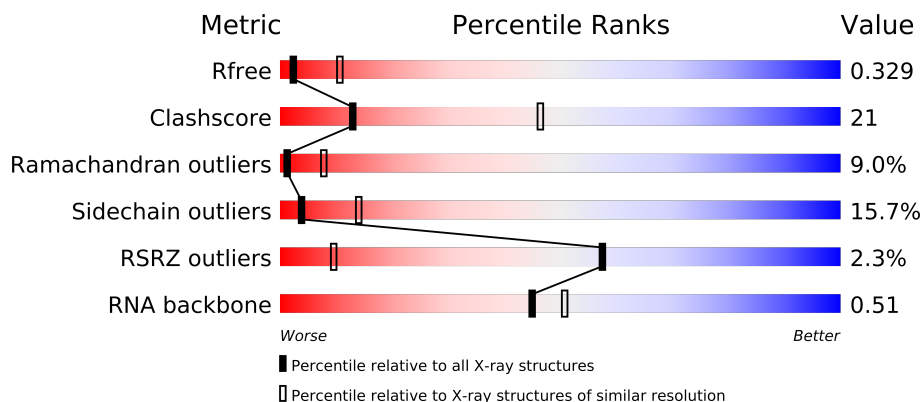
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	1506	
1	CA	1506	
2	AE	256	
2	CE	256	
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
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	128	
12	CO	128	
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	6	
23	C1	6	
24	BA	2912	
24	DA	2912	
25	BB	122	
25	DB	122	
26	BD	276	
26	DD	276	

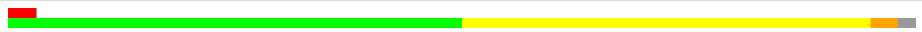



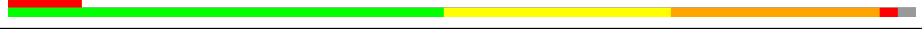




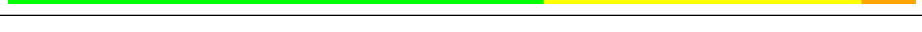

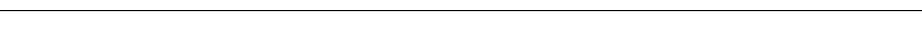
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Mol	Chain	Length	Quality of chain
27	BE	206	
27	DE	206	
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0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

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Mol	Chain	Length	Quality of chain
48	BX	60	
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
51	B6	54	
51	D6	54	
52	B7	49	
52	D7	49	
53	B8	65	
53	D8	65	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 295766 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	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	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	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			
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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	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	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	127	Total	C	N	O		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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	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	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	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			
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.

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			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	17A	C	U	CONFLICT	GB AP008226.1
AC	50	U	C	CONFLICT	GB AP008226.1
AC	51	C	G	CONFLICT	GB AP008226.1
AC	63	G	C	CONFLICT	GB AP008226.1
AD	17A	C	U	CONFLICT	GB AP008226.1
AD	50	U	C	CONFLICT	GB AP008226.1
AD	51	C	G	CONFLICT	GB AP008226.1
AD	63	G	C	CONFLICT	GB AP008226.1
CC	17A	C	U	CONFLICT	GB AP008226.1
CC	50	U	C	CONFLICT	GB AP008226.1
CC	51	C	G	CONFLICT	GB AP008226.1
CC	63	G	C	CONFLICT	GB AP008226.1
CD	17A	C	U	CONFLICT	GB AP008226.1
CD	50	U	C	CONFLICT	GB AP008226.1
CD	51	C	G	CONFLICT	GB AP008226.1
CD	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	C1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	DA	2906	Total	C	N	O	P	0	0	0
			62587	27857	11709	20116	2905			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	EXPRESSION TAG	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	166	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- 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			

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

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

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

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

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

- 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	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
36	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- 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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
44	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
45	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	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	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
49	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	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	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
51	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	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	61	Total 488	C 312	N 99	O 75	S 2	0	0	0
53	D8	61	Total 488	C 312	N 99	O 75	S 2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	632	Total 632	Mg 632	0	0
54	CA	199	Total 199	Mg 199	0	0
54	B8	2	Total 2	Mg 2	0	0
54	BE	4	Total 4	Mg 4	0	0
54	DU	2	Total 2	Mg 2	0	0
54	B1	1	Total 1	Mg 1	0	0
54	AN	2	Total 2	Mg 2	0	0
54	CN	1	Total 1	Mg 1	0	0
54	B5	1	Total 1	Mg 1	0	0
54	BB	16	Total 16	Mg 16	0	0
54	D8	1	Total 1	Mg 1	0	0
54	D3	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	1	Total 1	Mg 1	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	236	Total 236	Mg 236	0	0
54	CX	1	Total 1	Mg 1	0	0
54	CG	2	Total 2	Mg 2	0	0

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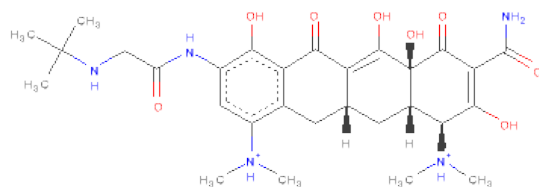
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BU	2	Total 2	Mg 2	0	0
54	A1	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	CC	9	Total 9	Mg 9	0	0
54	DE	4	Total 4	Mg 4	0	0
54	B3	2	Total 2	Mg 2	0	0
54	DA	523	Total 523	Mg 523	0	0
54	B7	3	Total 3	Mg 3	0	0
54	AG	1	Total 1	Mg 1	0	0
54	BO	2	Total 2	Mg 2	0	0
54	AQ	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	AH	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	AC	8	Total 8	Mg 8	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	1	Total 1	Mg 1	0	0
54	AT	1	Total 1	Mg 1	0	0
54	B0	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	CL	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DB	15	Total	Mg	0	0
			15	15		

- Molecule 55 is TIGECYCLINE (three-letter code: T1C) (formula:  $C_{29}H_{41}N_5O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			42	29	5	8		
55	CA	1	Total	C	N	O	0	0
			42	29	5	8		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

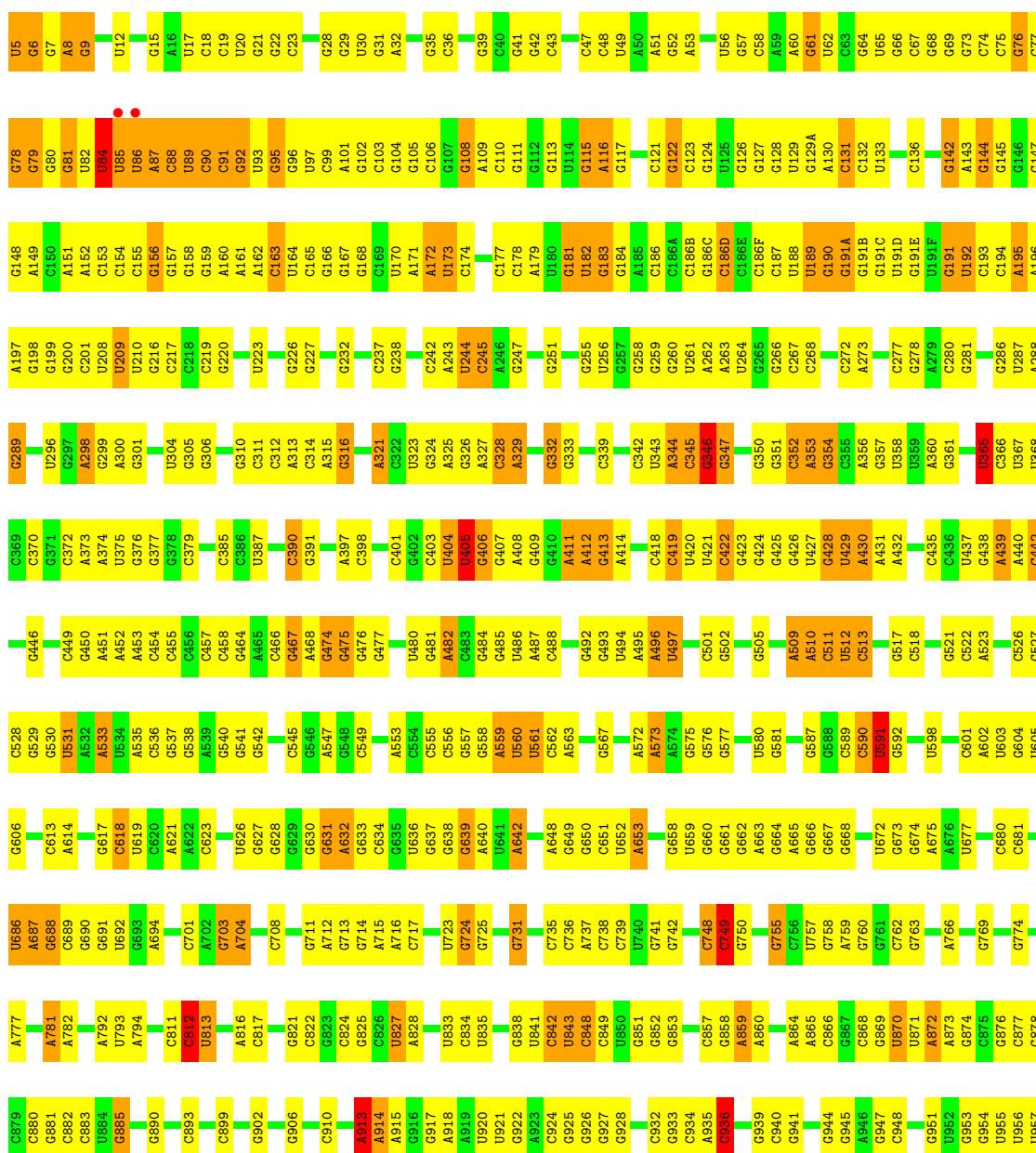
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total	Zn	0	0
			1	1		
56	AQ	1	Total	Zn	0	0
			1	1		
56	CQ	1	Total	Zn	0	0
			1	1		
56	CG	1	Total	Zn	0	0
			1	1		

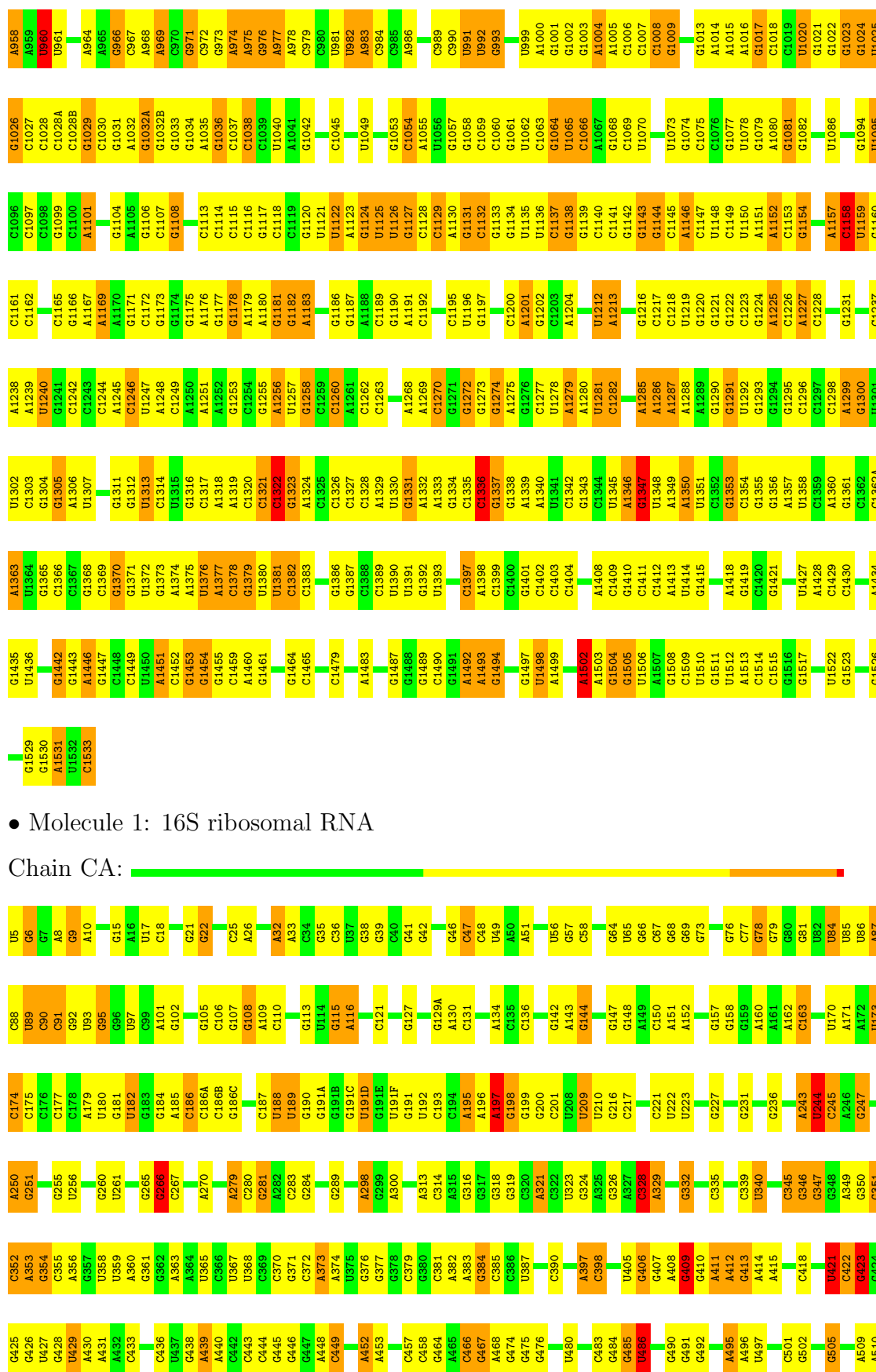
### 3 Residue-property plots

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

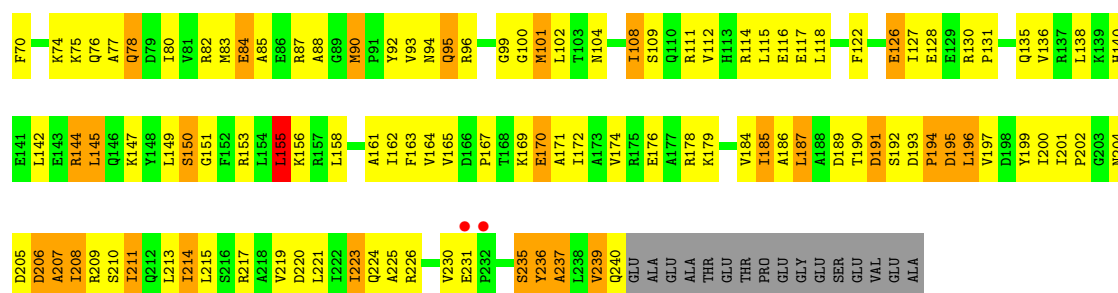
- Molecule 1: 16S ribosomal RNA

Chain AA: 



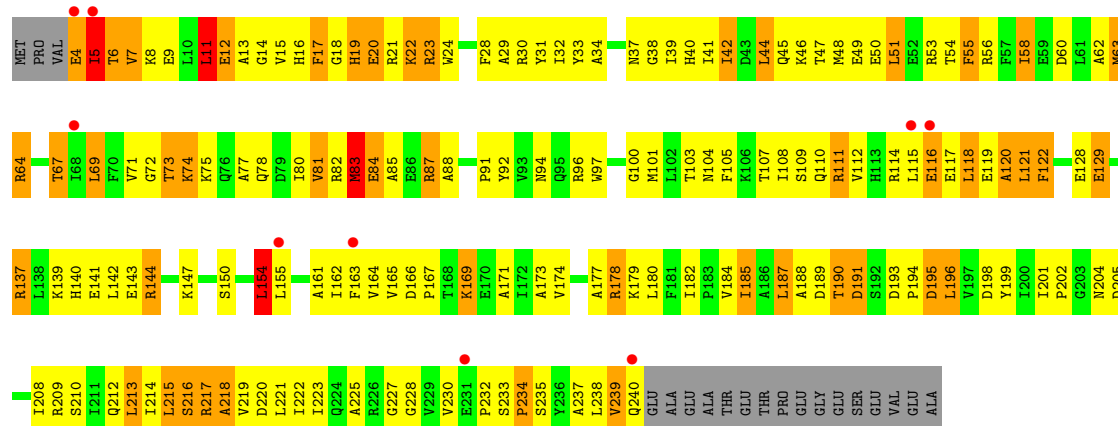






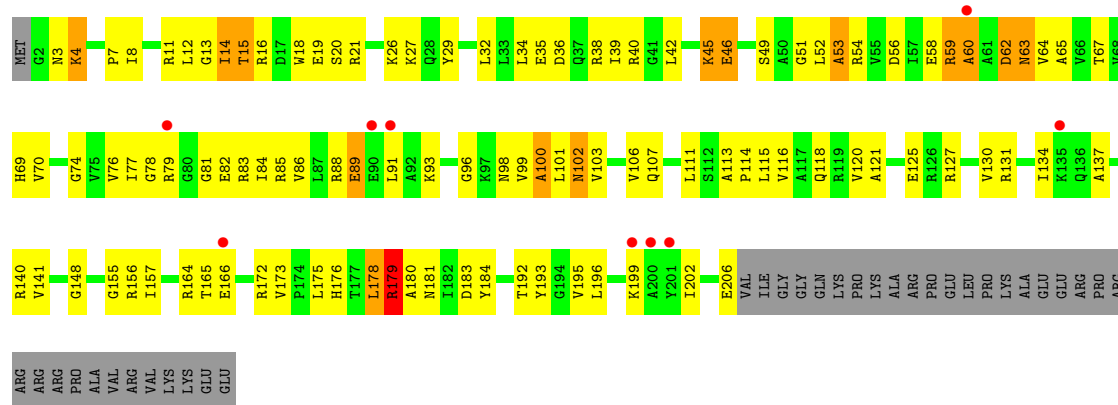
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CE:



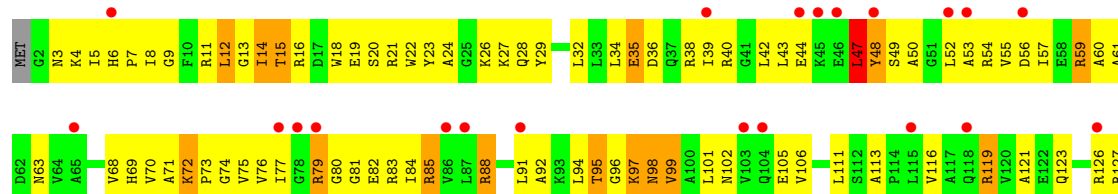
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

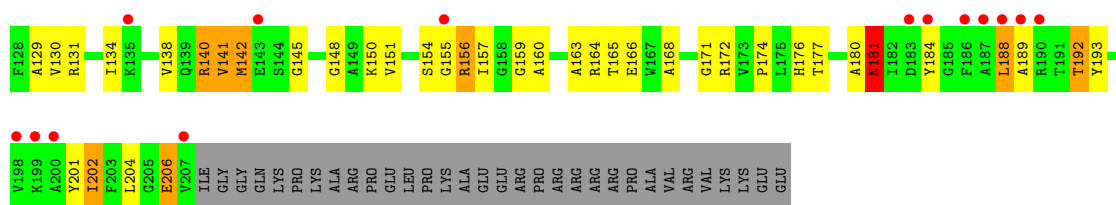
Chain AF:



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

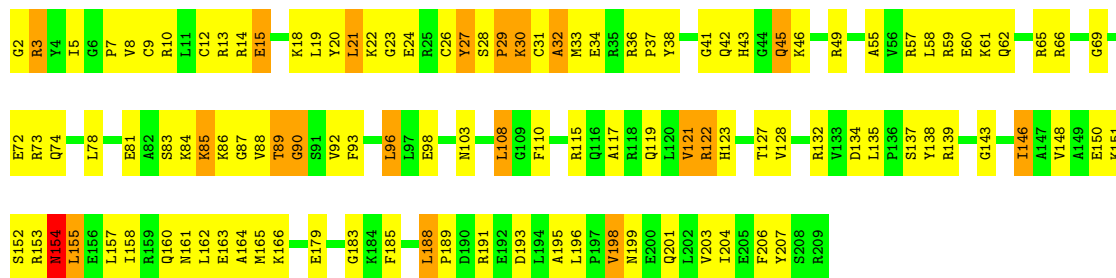
Chain CF:





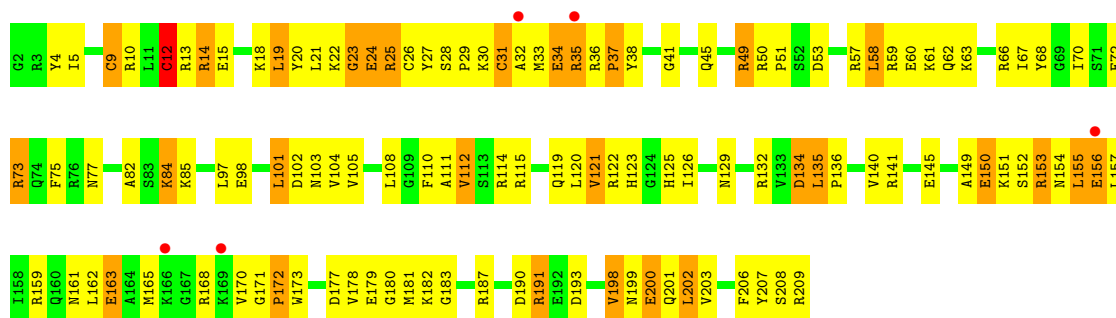
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG:



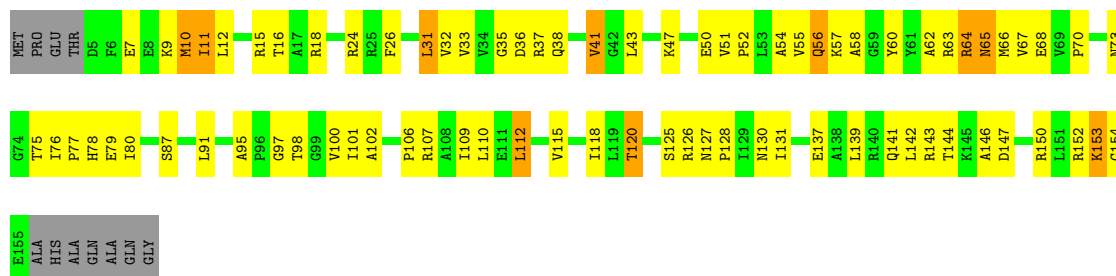
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:



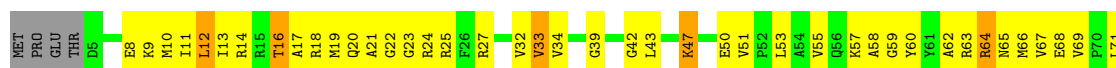
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:

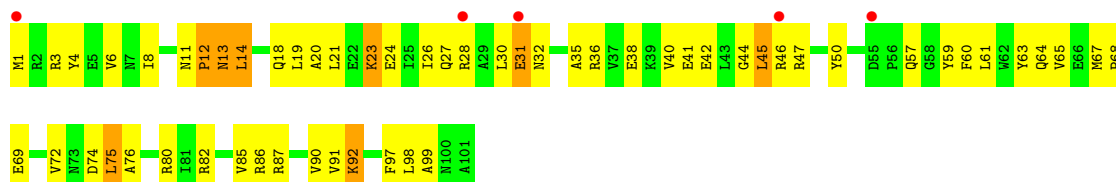






- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



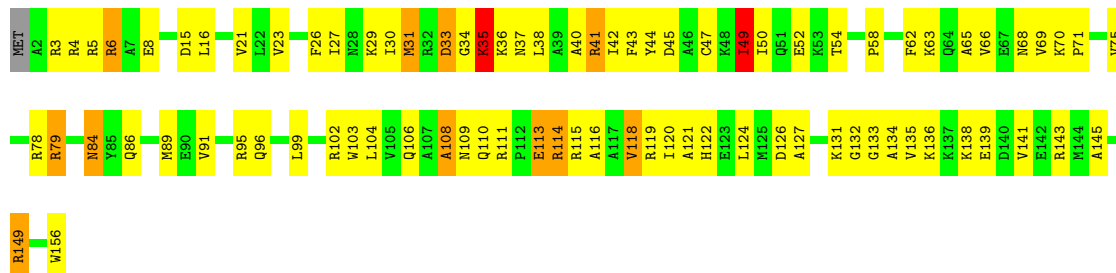
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



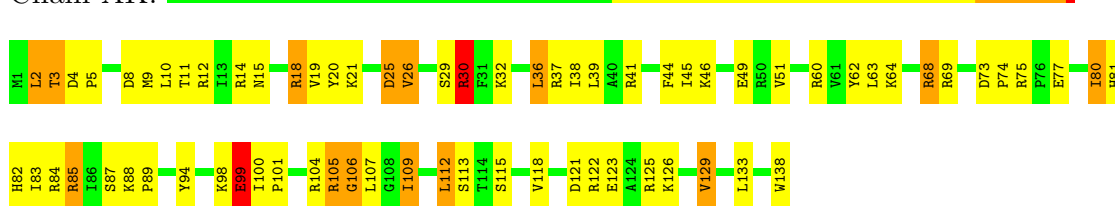
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



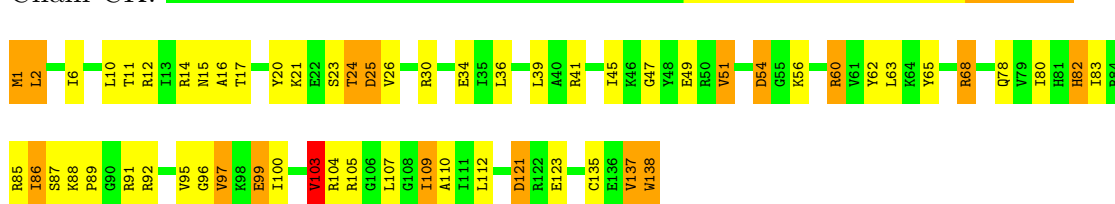
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



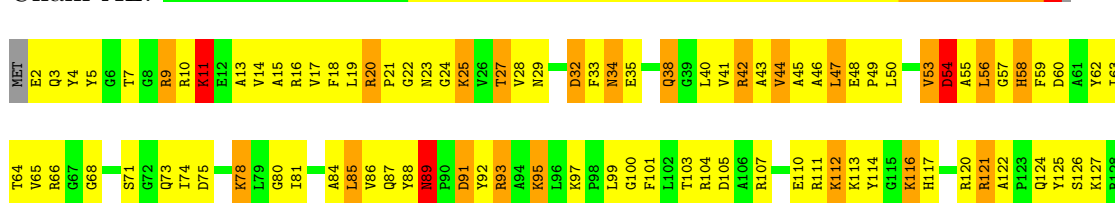
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



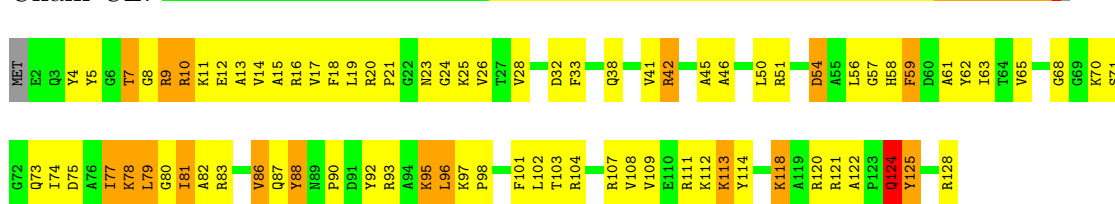
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



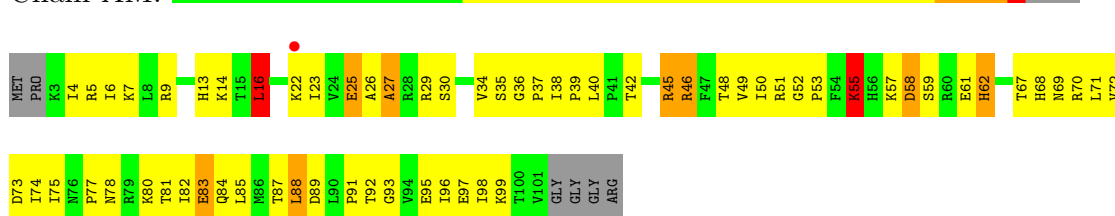
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



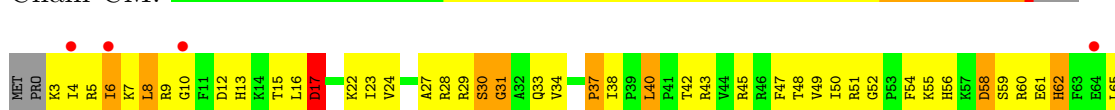
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

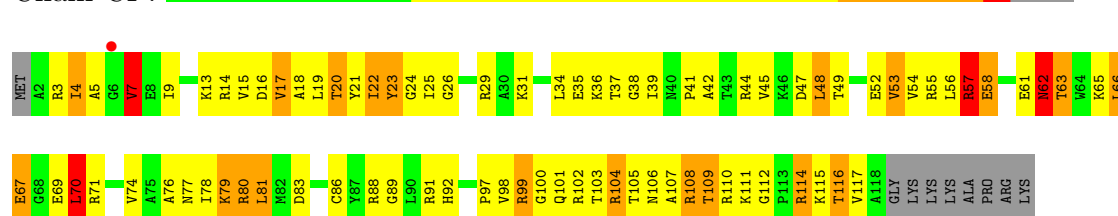
Chain CM:





- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



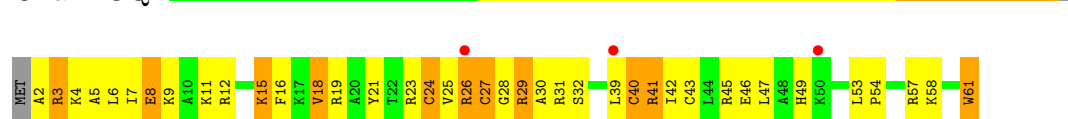
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



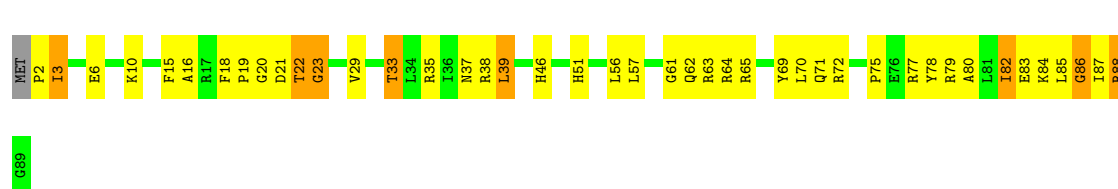
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



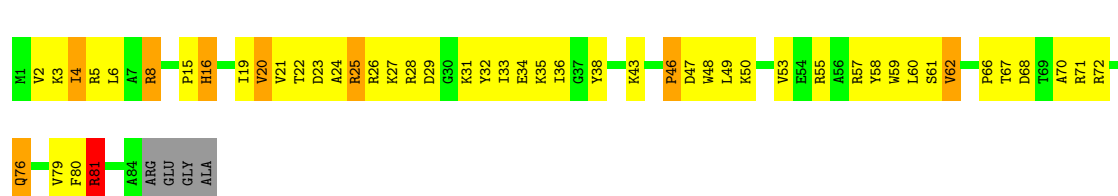
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:



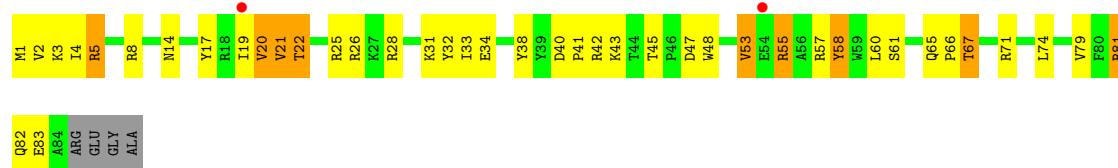
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:



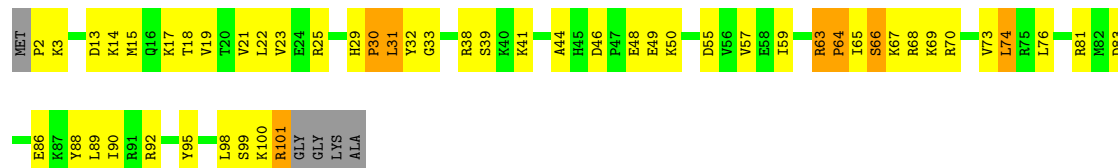
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:



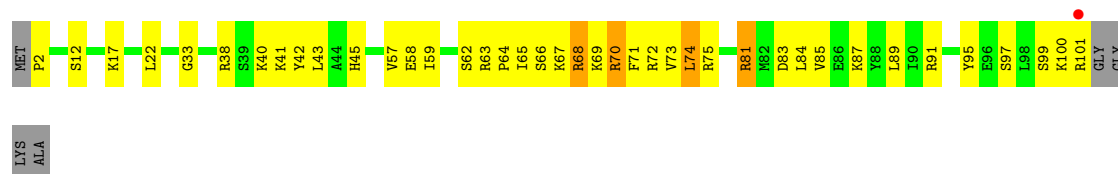
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:



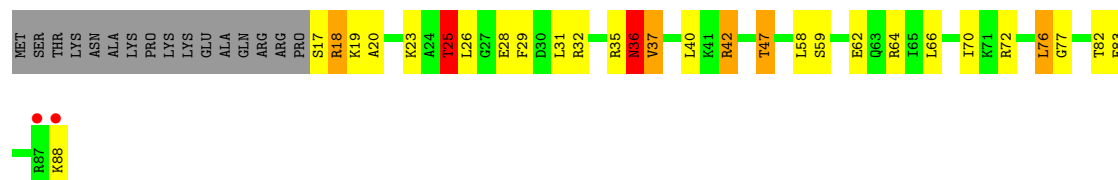
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



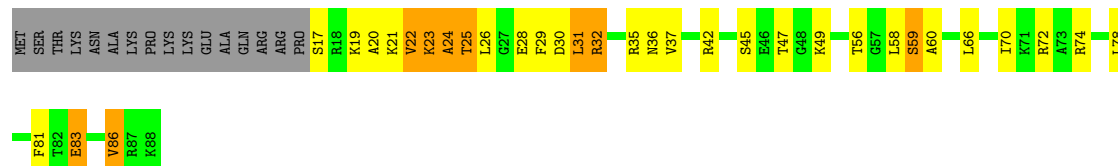
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CU:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

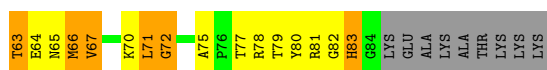
Chain AV:





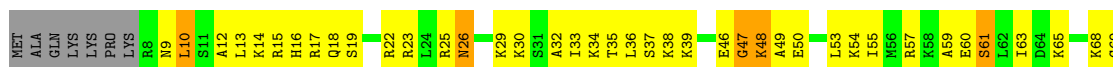
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV:



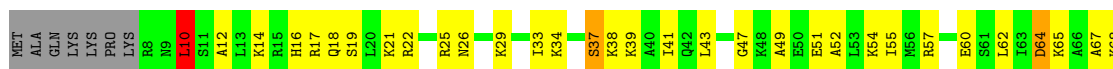
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



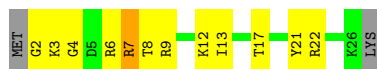
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



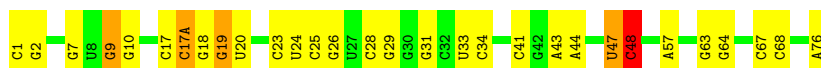
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



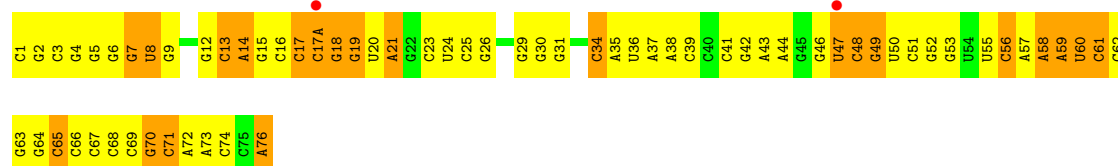
• Molecule 22: TRNA-FMET

Chain AC:



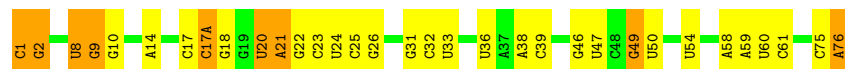
• Molecule 22: TRNA-FMET

Chain AD:



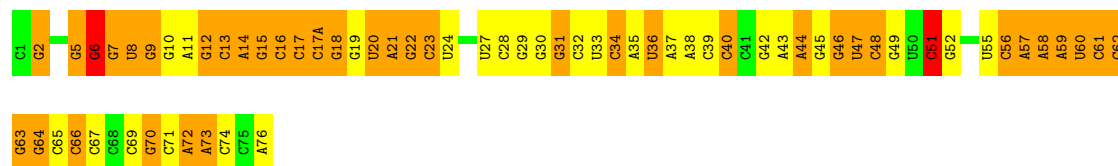
- Molecule 22: TRNA-FMET

Chain CC:



- Molecule 22: TRNA-FMET

Chain CD:



- Molecule 23: MRNA

Chain A1:



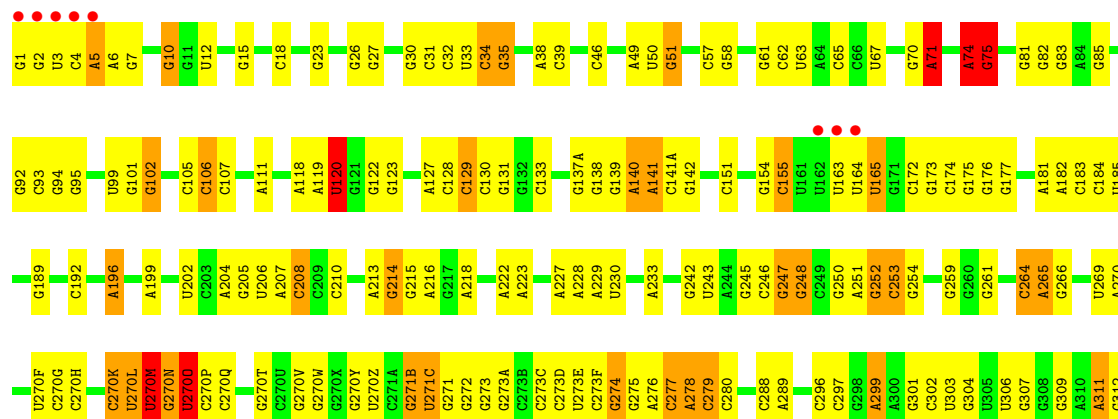
- Molecule 23: MRNA

Chain C1:



- Molecule 24: 23S ribosomal RNA

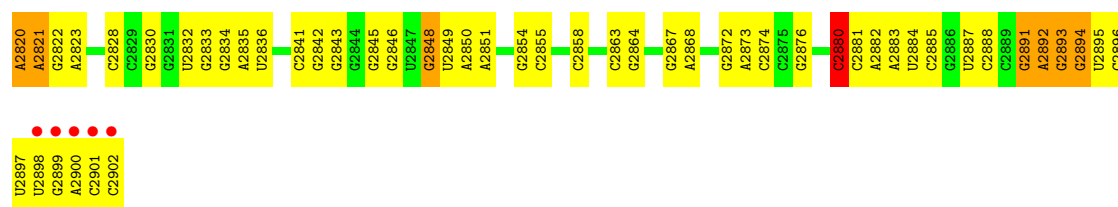
Chain BA:



C1505	C1506	C1507	A1508	C1509	A1510	A1511	G1512	A1433	A1434	G1435	U1438	A1439	A1440	G1441	G1442	A1444A	C1445	G1446	G1447	G1448	A1449	G1449A	A1453	U1454	G1455	C1458	G1459	A1460	G1461	G1466	C1467	G1470	A1471	A1472	G1473	G1479	G1480	U1482	G1483	A1486	G1487	G1488	U1489	A1490	G1491	C1492	C1493	A1566	A1567	G1568	A1569	C1577		
G1339	A1242	G1344	A1349	A1354	G1355	G1356	U1357	G1358	A1359	A1360	G1364	A1365	U1366	A1367	G1368	U1372	C1375	C1376	G1377	A1378	A1379	G1380	A1384	G1385	A1392	A1393	U1394	A1395	C1398	C1402	U1313	C1403	C1404	U1405	U1406	C1407	C1408	C1409	G1410	C1411	G1414	U1415	C1416	C1417	G1418	A1419	U1420	G1421	G1422	G1423				
G1170	G1171	G1173	A1174	U1175	G1176	A1177	G1178	C1179	G1180	C1181	A1182	G1186	U1187	U1188	A1189	G1190	G1191	G1195	U1198	U1199	C1200	C1201	U1291	A1292	G1203	U1294	C1295	G1296	C1297	C1298	G1299	U1300	A1301	G1309	U1312	U1313	C1314	U1315	U1316	A1317	A1322	U1323	G1324	G1328	U1329	C1330	A1331	C1332	G1333	G1334	U1335	G1338		
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G962	U963	C964	G968	A973	G974	C974A	C975	C976	G977	A980	A981	C982	A983	A984	C985	G986	G987	C989	U995	A996	C997	U999	A1000	G1003	C1004	C1005	U1006	C1007	C1008	A1009	U1010	G1011	U1012	C1013	U1014	G1015	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	U1089	U1090	G1091	A1028						
G882	G883	C884	C885	C886	A887	C888	C889	A890	C892	C893	C894	U895	A896	C897	C898	A899	A900	A901	C902	C903	C904	U905	U906	U907	C908	A909	A910	A911	C912	U913	C914	A917	A918	C919	C929	U930	C931	C932	U938	C939	G940	A941	C942	U943	G946	G950	C951	G956	U957	U958	A959	A960	C961	
C797	U803	A804	G805	C806	C812	U813	C814	C815	C816	C817	G818	A819	C825	U826	U827	U828	G831	G832	U833	C838	U839	C844	G845	C846	U847	G848	A849	C850	U851	C857	U858	G859	C860	A863	C864	A865	C866	A867	C868	C869	A870	G873	G874	G875	C876	U877	A878	G879	C880	G881				
C409	G410	G411	C416	C417	U421	A428	C433	U434	C439	G440	A441	A442	A443	C444	C445	U448	G450	C453	A454	C455	C456	A457	G458	U459	A460	G463	A466	G467	C468	A470	A471	U475	A480	A481	A482	A483	C484	C485	C486	U489	G491	A492	G493	C494										
A575	U576	G577	A578	C579	C580	C581	G582	C583	C584	G585	C586	C587	U588	C589	C590	G591	G592	G593	U594	C595	C596	C601	G602	A603	G604	C605	U606	U607	U614	G615	A616	G617	G620	A621	G622	A627	G628	G629	G630	A631	A632	A633	C634	C635	G636	A637	U638	A639	U640	A644	C645	G646	C647	G648
G495	G498	U499	A500	G501	A502	A503	U504	A505	G506	A507	C508	C509	C510	U511	G512	A513	A514	C517	C523	A526	C527	A528	A529	G530	C531	A532	G533	U534	C537	G539	G540	C541	G545	C546	A547	A548	G549	U553	G558	G563	U566	A567	U568	U569	G570	A571	A572	G573	C574					
G651	A654	A654A	C654B	G654C	G654D	C654E	C654F	C654G	C654H	C654I	A654J	C654K	C654L	C654M	G654N	G654O	C654P	C654Q	C654R	A654T	A655	G656	U657	C658	C661	G662	G663	C664	G674	A675	A676	A677	C678	C679	G680	G681	G684	A685	G686	C691	G696	C697	C698	G699	G700	A705	A706	G715						
C720	C721	A722	G723	U724	G725	G726	A727	G728	G729	C730	G733	U740	G741	G742	G743	A746	U747	A752	C753	C754	C755	A761	A764	G765	G768	G771	A774	G775	G776	A777	G778	U779	G780	A781	A782	A783	A784	G785	C786	U787	A788	A789	G790	G791	G792	A793	G794	C796						
G851	A854	A854A	C854B	G854C	G854D	C854E	C854F	C854G	C854H	C854I	A854J	C854K	C854L	C854M	G854N	G854O	C854P	C854Q	C854R	A854T	A855	G856	U857	C858	C861	G862	G863	C864	G874	A875	A876	A877	C878	C879	G880	G881	G884	A885	G886	C891	G896	C897	C898	G899	G900	A905	A906	G915						
C720	C721	A722	G723	U724	G725	G726	A727	G728	G729	C730	G733	U740	G741	G742	G743	A746	U747	A752	C753	C754	C755	A761	A764	G765	G768	G771	A774	G775	G776	A777	G778	U779	G780	A781	A782	A783	A784	G785	C786	U787	A788	A789	G790	G791	G792	A793	G794	C796						

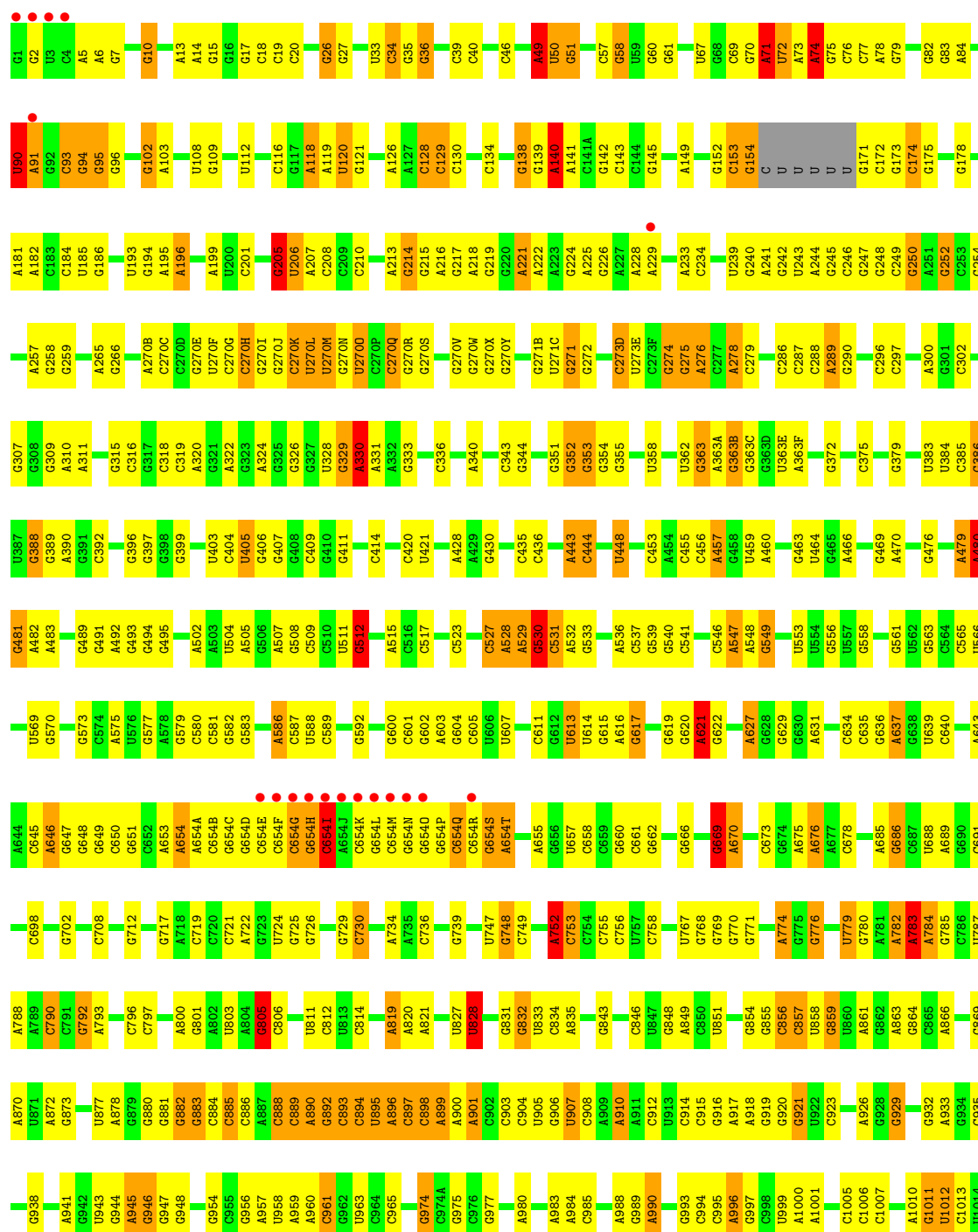


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	C2751	C2666	C2496	A2422	A2346	G2279	C2188	G2125		U1955	G1858	C1774	A1669	A1583
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C2700	U2785	C2700	G2534	G2447	C2381	C2306	U2232	U2150	C2078	G1994	G1903	A1803	C1617	A1618
C2701		C2701	A2534	U2448	G2382	G2307	G2234	G2151	U2086	C1996	C1906	C1804	U1717	
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	U2789		G2544	C2452	C2386	A2311	G2239	G2156	C2090	G2000	C1908	A1812	A1730	
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A2713	A2632	A2713	G2550	C2464	U2390	G2316	G2246	C2161	C2097	G2012	A1916	G1817	A1637	A1637
C2714		C2714	U2554	C2464	G2391	C2316	U2246	G2162	U2098	A2015	A1919	U1818	C1638	C1638
	U2795			A2392	A2392	G2317	A2247	C2162	U2098	A2015	A1919	U1818	G1741	
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U2720	U2797	U2720	G2557	G2468	C2394	G2319	C2246	C2164	G2100	A2015	A1919	U1820	G1742	C1640
A2721	U2637	A2721	C2558	A2469	C2394	A2320	G2250	G2165	G2101	C1925	C1925	A1821	C1742	
C2722	C2798	C2722	A2561	G2470	G2397	G2321	U2257	G2166	U2102	G1929	G1929	G1822	G1748	C1644
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	A2801		U2563	C2472	G2399	G2323	C2258	G2168	G2104	G2023	G1930	G1824	G1750	C1646
U2726	C2803	U2726	C2563	U2473	C2399	C2324	U2259	A2169		G2024	U1931	A1825	C1647	
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	U2812		C2571	C2480	G2407	G2331	A2267	C2176	G2116	A2031	A1937	G1836	A1762	A1654
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C2738	U2814	C2738	C2573	G2482	G2407	G2331	A2267	C2176	G2116	A2031	A1937	G1836	A1762	A1654
U2739	A2815	U2739	G2483	G2483	G2410	G2332	G2270	C2178	A2117	U1940	G1839	G1764	C1657	C1656
A2740	C2816	A2740	C2484	C2484	G2411	A2334	G2271	C2179	U2118	C2039	G1949	C1844	C1765	C1658
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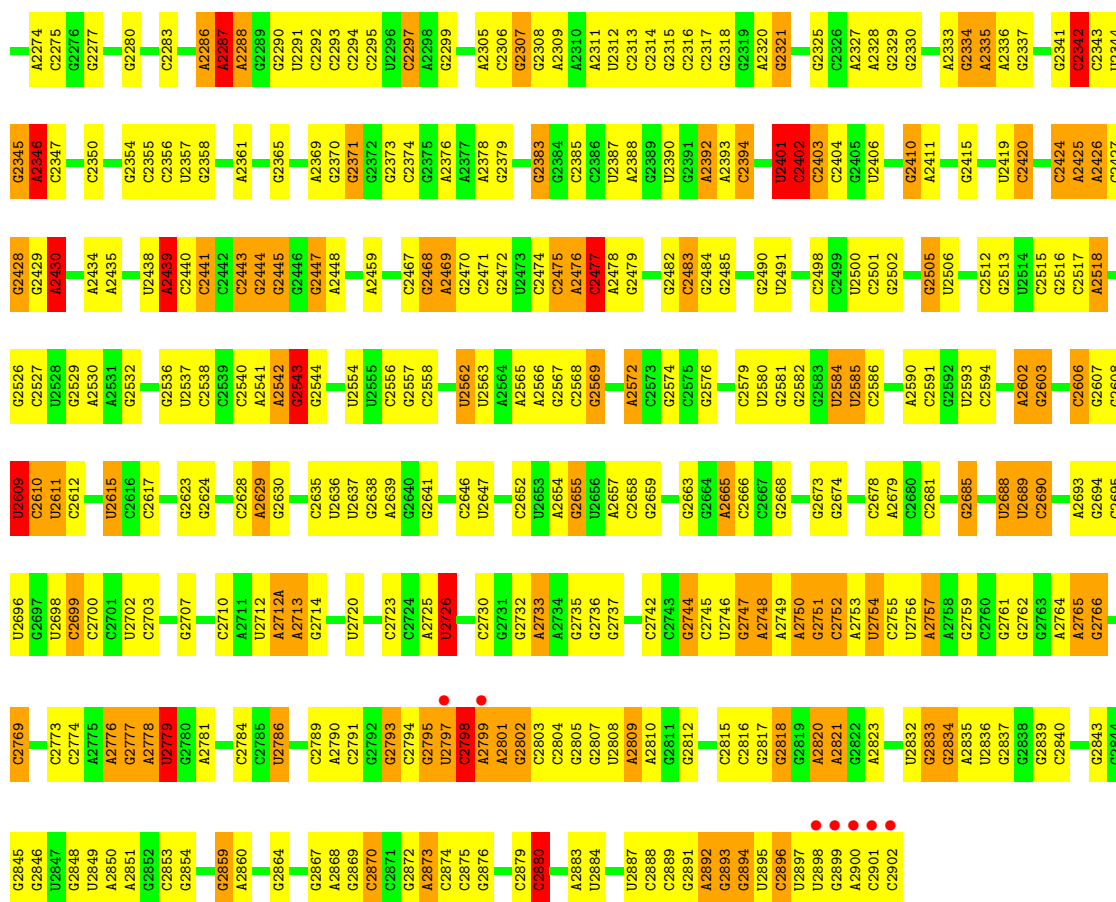


• Molecule 24: 23S ribosomal RNA

Chain DA:



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G2046	G2049	G2052	G2053	G2054	G2055	G2056	A2059	G2060	G2061	A2062	G2065	G2066	G2067	G2068	G2069	G2070	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122				
U1956	C1962	U1963	G1965	G1966	G1967	U1970	A1971	G1980	G1989	G1990	U1991	G1989	G1987	G1988	G1989	G1990	G1991	G1992	U1993	U1994	U1995	G1996	C1999	G2006	C2007	G2008	G2009	G2012	G2013	A2014	G2015	G2016	G2017	G2018	A2019	A2020	G2023	G2024	G2027	G2028	G2029	A2030	G2031	G2032	A2033	C2036	G2040	U2041	C2043								
U1757	G1758	C1761	G1762	G1763	G1764	C1771	G1772	A1773	U1779	A1780	C1781	A1782	A1783	A1784	A1785	A1786	G1787	A1788	A1789	G1790	A1791	C1797	U1798	G1799	C1800	G1801	A1802	U1805	A1809	A1810	G1811	A1812	G1813	A1814	A1815	G1816	G1817	U1818	U1819	U1820	G1823	A1829	U1834	G1835	G1839	G1842	G1846										
A1847	A1848	G1849	G1850	U1851	G1852	A1853	G1856	G1857	G1858	U1864	G1869	C1870	A1871	G1872	G1873	G1879	G1883	A1884	A1885	G1886	G1887	G1888	A1889	C1894	G1895	U1898	G1899	G1900	A1901	C1902	G1906	G1910	U1911	A1912	G1913	G1914	U1915	G1916	U1917	G1929	G1930	U1931	G1935	A1936	G1950	U1951	A1952	U1955									
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G1478	G1479	G1483	G1484	G1485	A1486	G1487	G1488	G1489	A1490	G1491	G1492	C1493	A1496	U1497	C1505	A1507	A1508	C1509	A1510	A1511	G1512	U1516	G1517	G1518	G1519	U1520	G1522	G1525	G1526	G1527	A1528	C1533	G1534	U1535	A1536	C1537	G1538	G1539	U1540	U1541	G1542	A1543	A1544	A1545A	G1546	G1547	C1550	C1556	A1558								
C1407	C1408	G1409	G1410	C1411	A1412	G1413	G1414	U1415	G1416	G1417	G1418	A1419	U1420	G1421	G1424	A1427	C1428	A1434	G1435	G1436	C1437	G1441	G1442	G1443	A1444A	G1447	G1448	A1449	G1449A	C1450	C1451	A1453	U1454	C1455	G1458	G1459	A1460	G1461	C1462	G1463	G1464	G1465	G1466	C1467	G1470	A1471	A1472	G1473	C1474	G1475	A1477						
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A1220	C1223	G1224	C1225	G1228	C1230	G1236	G1239	U1240	G1245	A1246	A1247	G1248	C1251	G1252	A1253	U1254	U1255	G1256	C1257	A1262	G1266	A1269	C1270	G1271	A1272	U1273	U1274	A1275	A1276	A1277	A1278	G1279	G1280	A1286	A1287	U1288	U1292	C1293	U1294	C1295	G1299	U1300	A1301	G1309													
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G1016	G1017	C1018	G1019	U1019	U1021	G1022	U1023	G1024	G1025	G1026	U1027	A1028	G1029	G1030	U1033	G1034	U1035	G1036	G1037	C1038	G1039	C1040	C1041	G1042	C1043	U1044	A1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	G1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075



• Molecule 25: 5S RIBOSOMAL RNA

Chain BB:



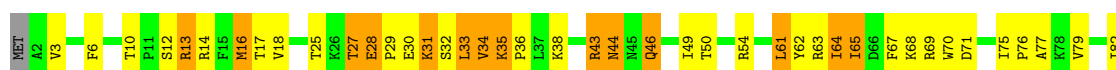
• Molecule 25: 5S RIBOSOMAL RNA

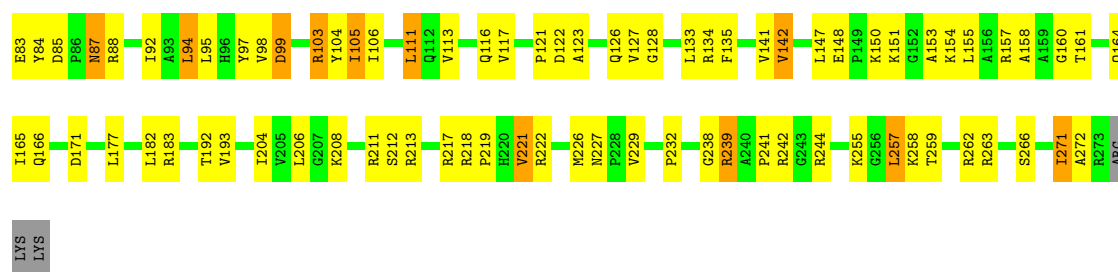
Chain DB:



• Molecule 26: 50S ribosomal protein L2

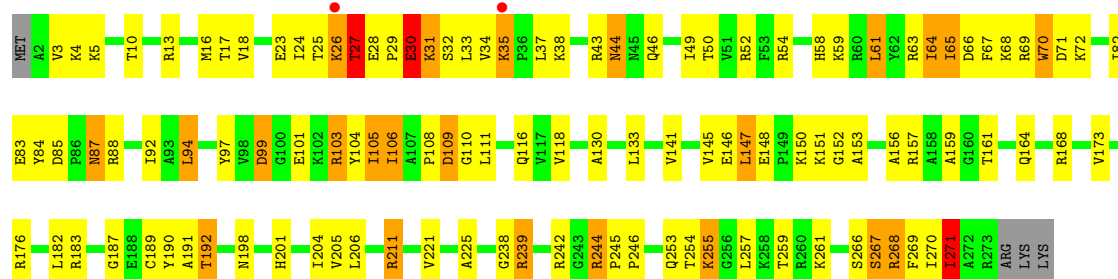
Chain BD:





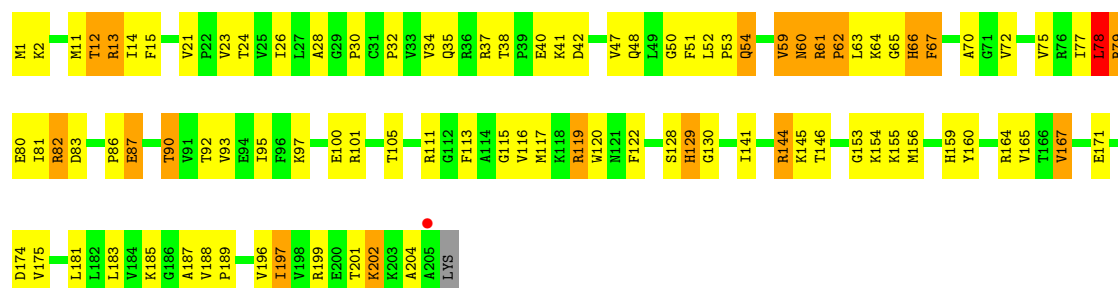
- Molecule 26: 50S ribosomal protein L2

Chain DD:



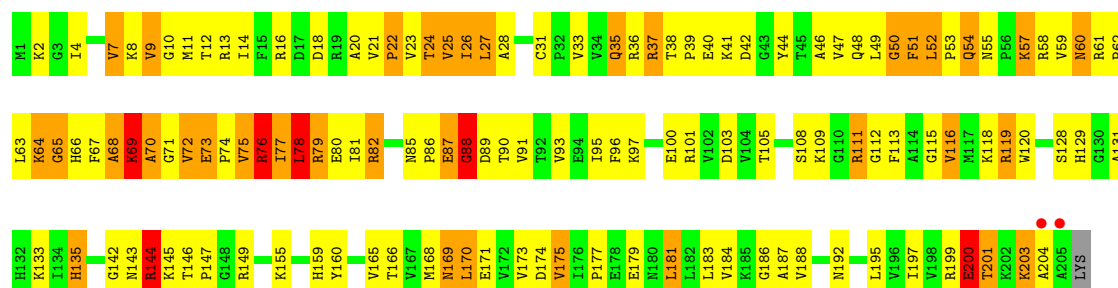
- Molecule 27: 50S ribosomal protein L3

Chain BE:



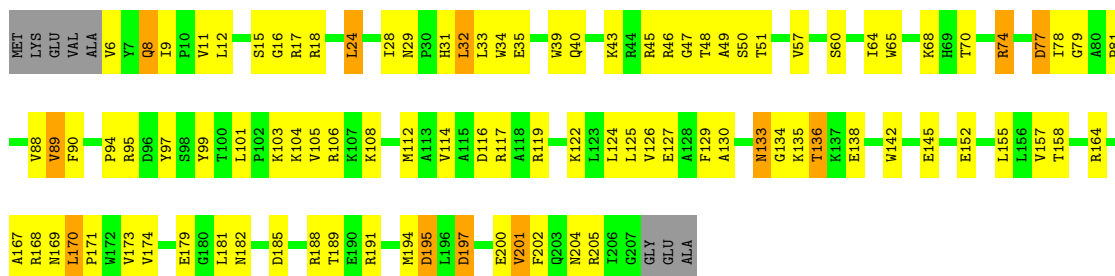
- Molecule 27: 50S ribosomal protein L3

Chain DE:



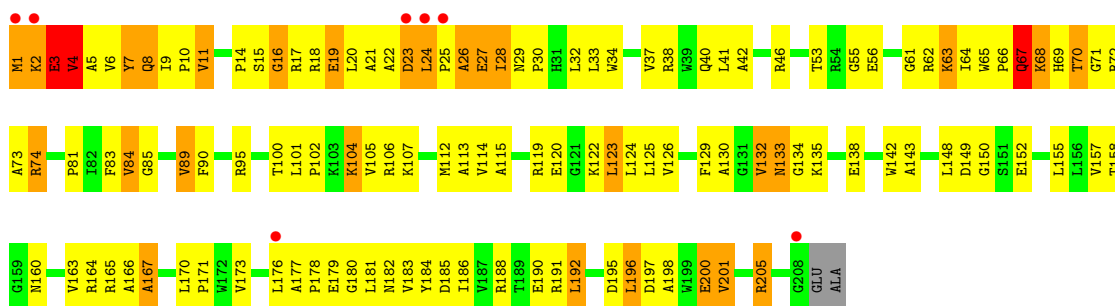
- Molecule 28: 50S ribosomal protein L4

Chain BF:



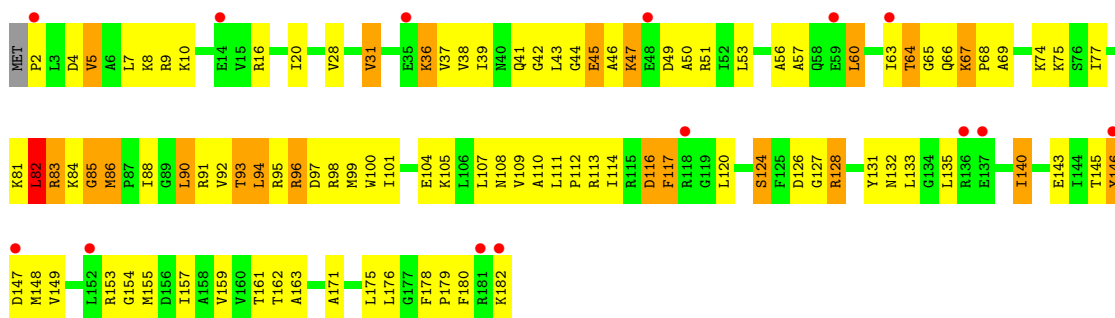
• Molecule 28: 50S ribosomal protein L4

Chain DF:



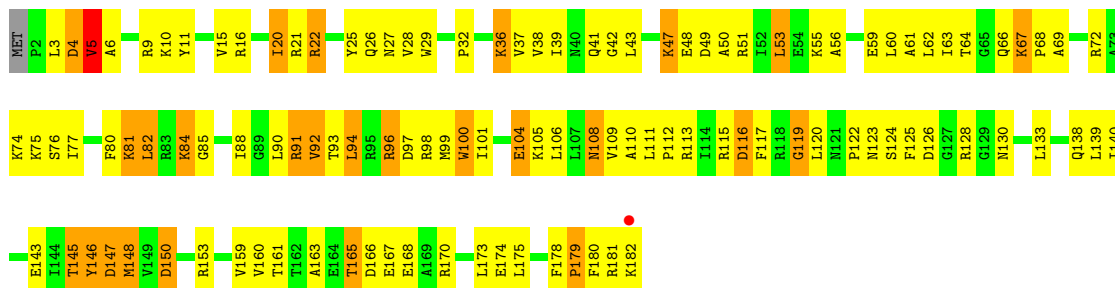
• Molecule 29: 50S ribosomal protein L5

Chain BG:



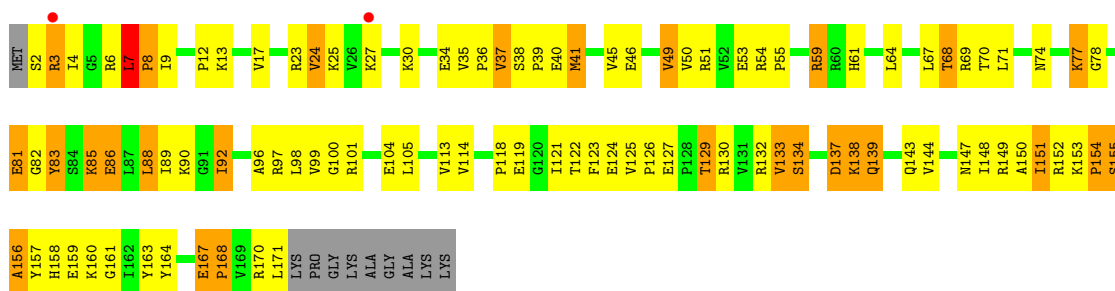
• Molecule 29: 50S ribosomal protein L5

Chain DG:



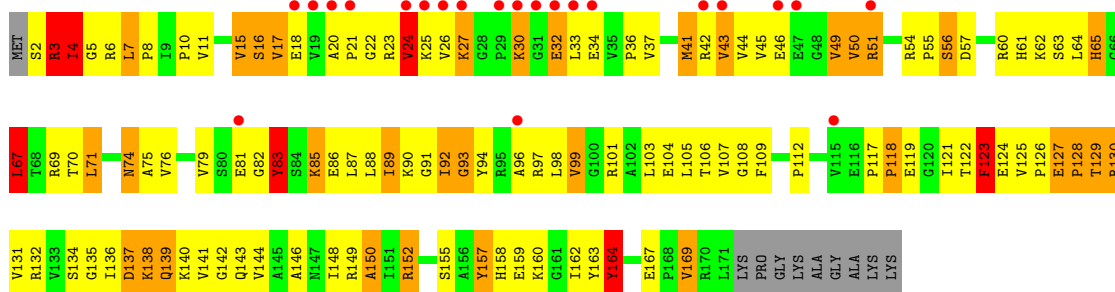
• Molecule 30: 50S ribosomal protein L6

Chain BH:



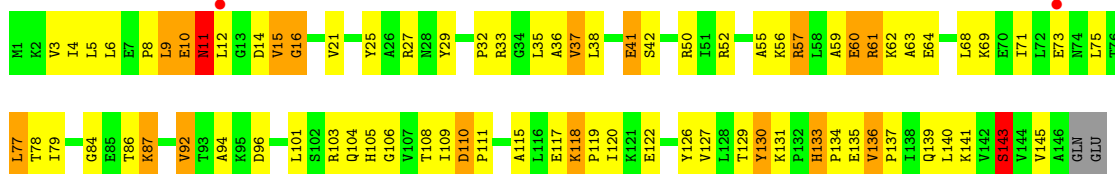
- Molecule 30: 50S ribosomal protein L6

Chain DH:



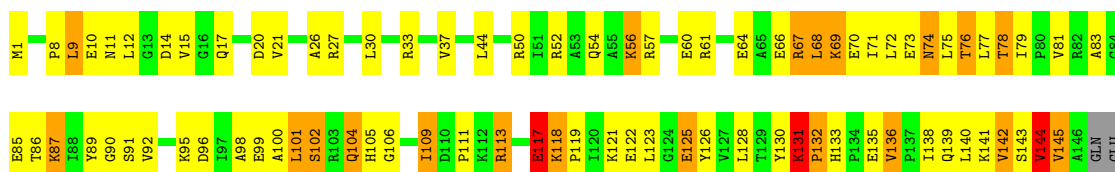
- Molecule 31: 50S ribosomal protein L9

Chain BK:



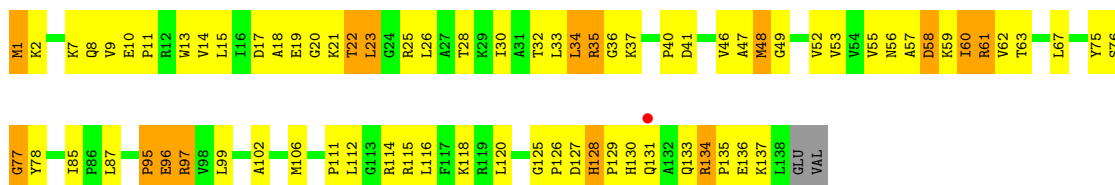
- Molecule 31: 50S ribosomal protein L9

Chain DK:



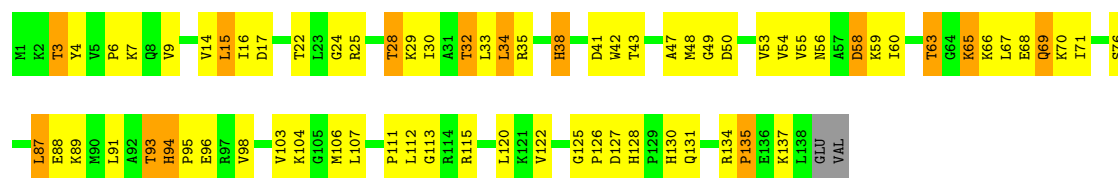
- Molecule 32: 50S ribosomal protein L13

Chain BM:



- Molecule 32: 50S ribosomal protein L13

Chain DM:



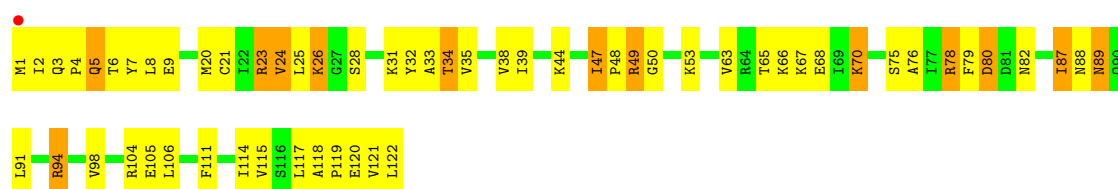
- Molecule 33: 50S ribosomal protein L14

Chain BN:



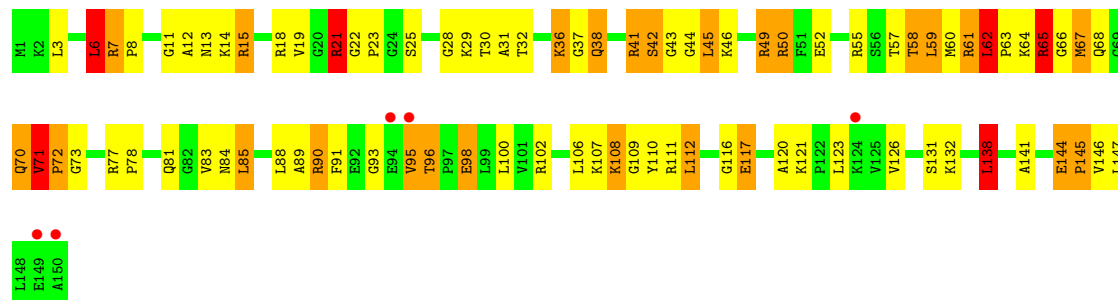
- Molecule 33: 50S ribosomal protein L14

Chain DN:



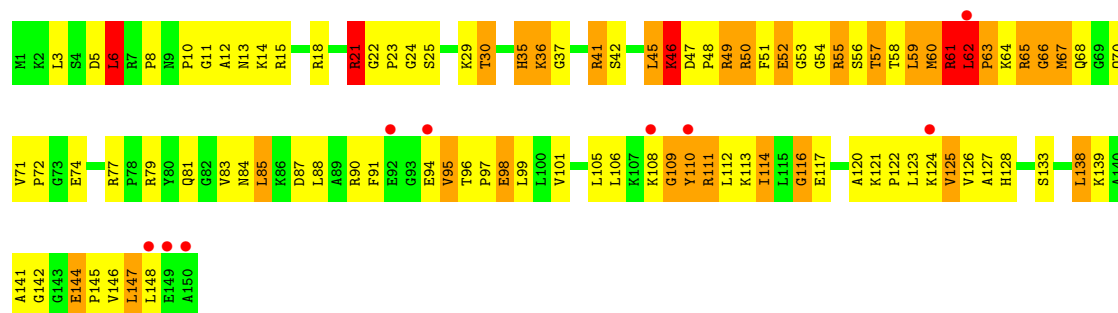
- Molecule 34: 50S ribosomal protein L15

Chain BO:



- Molecule 34: 50S ribosomal protein L15

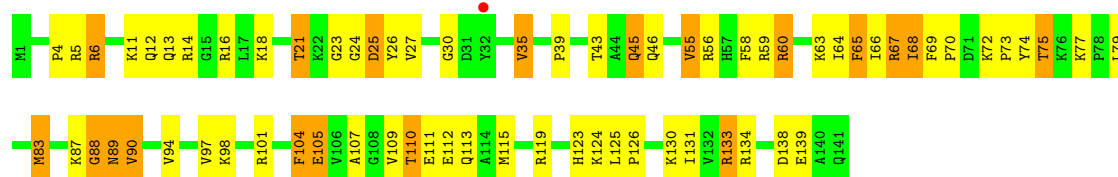
Chain DO:



- Molecule 35: 50S ribosomal protein L16

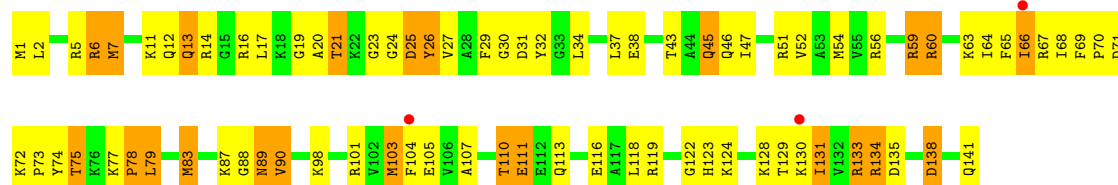


Chain BP:



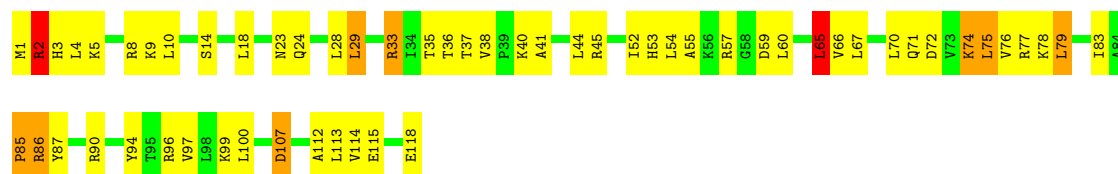
- Molecule 35: 50S ribosomal protein L16

Chain DP:



- Molecule 36: 50S ribosomal protein L17

Chain B0:



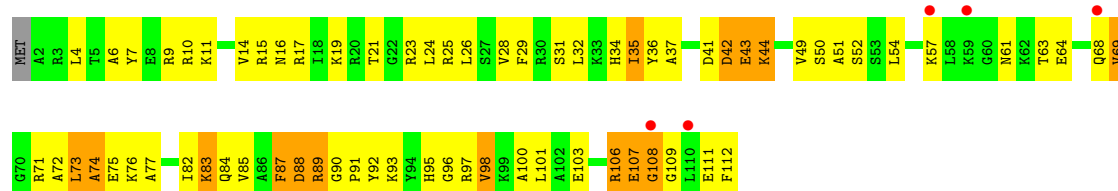
- Molecule 36: 50S ribosomal protein L17

Chain D0:



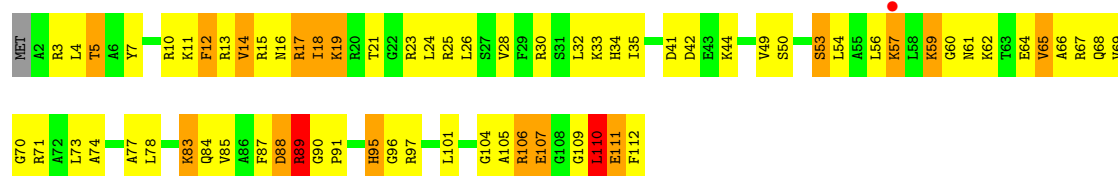
- Molecule 37: 50S ribosomal protein L18

Chain BQ:



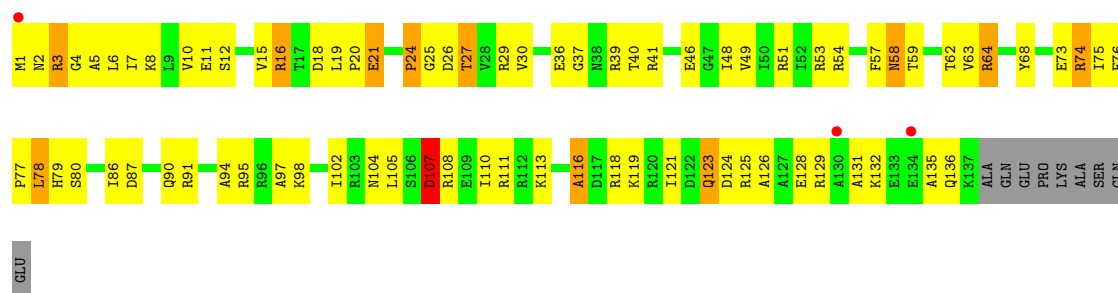
- Molecule 37: 50S ribosomal protein L18

Chain DQ:



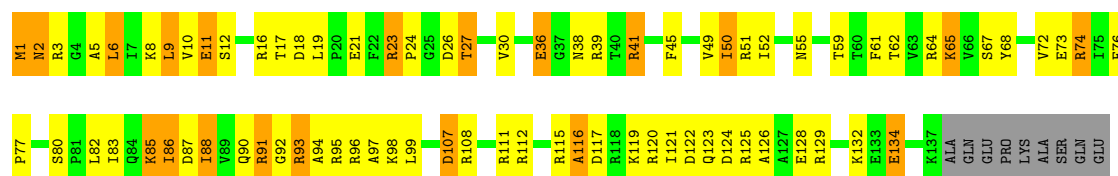
• Molecule 38: 50S ribosomal protein L19

Chain BR:



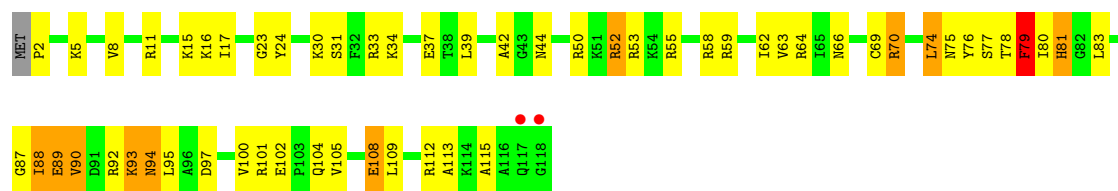
• Molecule 38: 50S ribosomal protein L19

Chain DR:



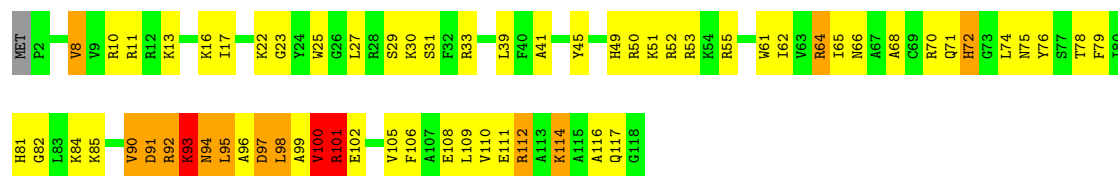
• Molecule 39: 50S ribosomal protein L20

Chain B1:



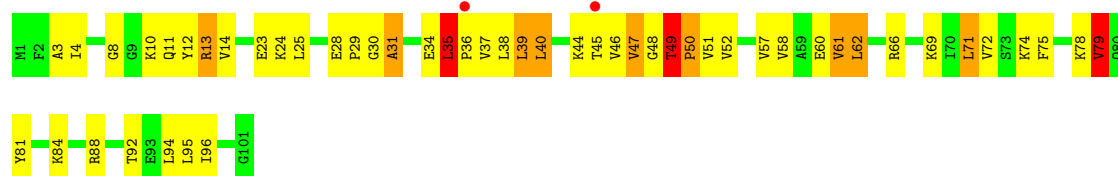
• Molecule 39: 50S ribosomal protein L20

Chain D1:



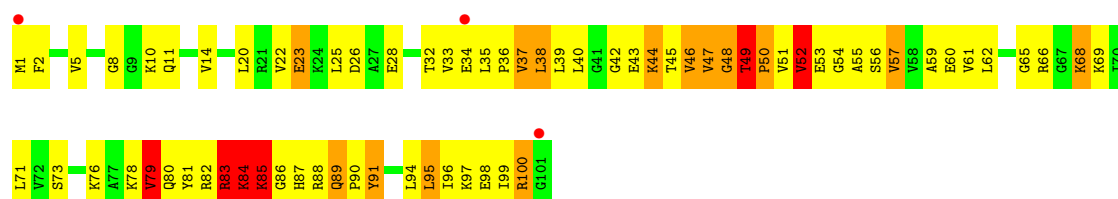
• Molecule 40: 50S ribosomal protein L21

Chain B2:



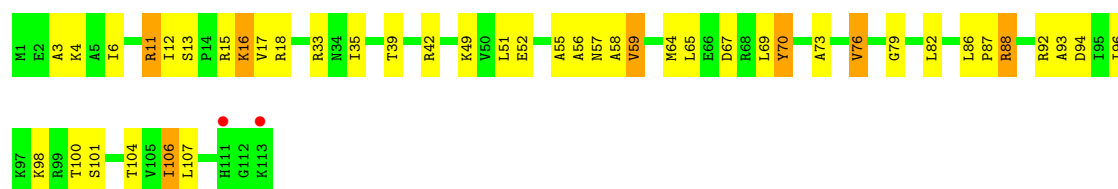
• Molecule 40: 50S ribosomal protein L21

Chain D2:



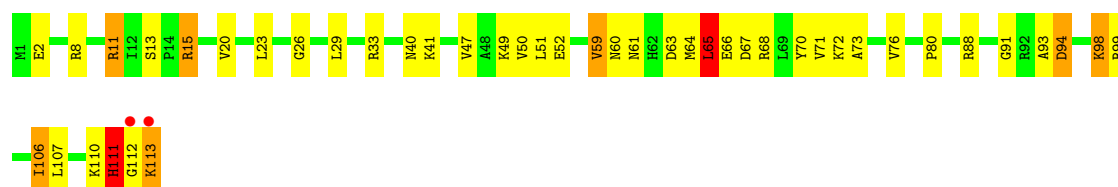
• Molecule 41: 50S ribosomal protein L22

Chain BS:



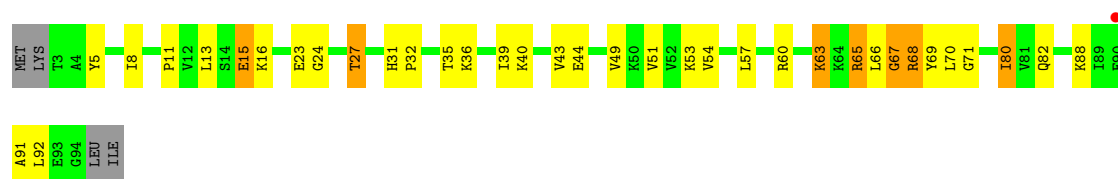
• Molecule 41: 50S ribosomal protein L22

Chain DS:



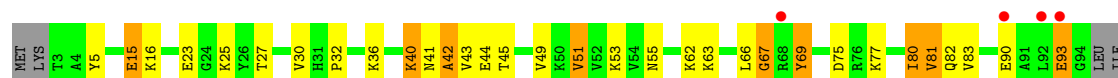
• Molecule 42: 50S ribosomal protein L23

Chain BT:



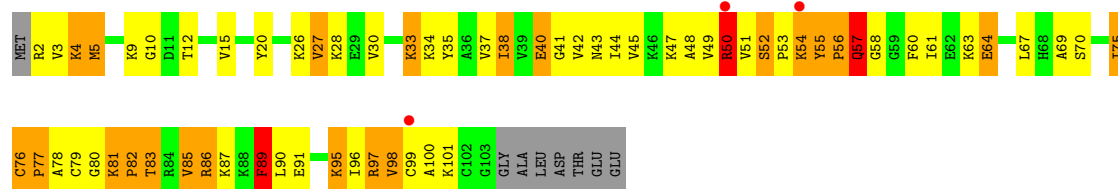
• Molecule 42: 50S ribosomal protein L23

Chain DT:



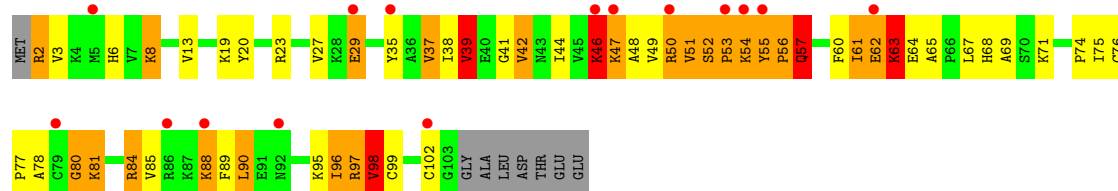
- Molecule 43: 50S ribosomal protein L24

Chain BU:



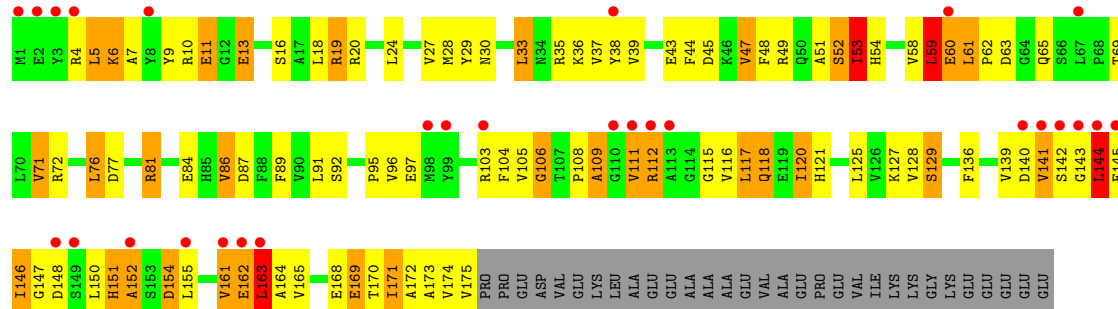
- Molecule 43: 50S ribosomal protein L24

Chain DU:



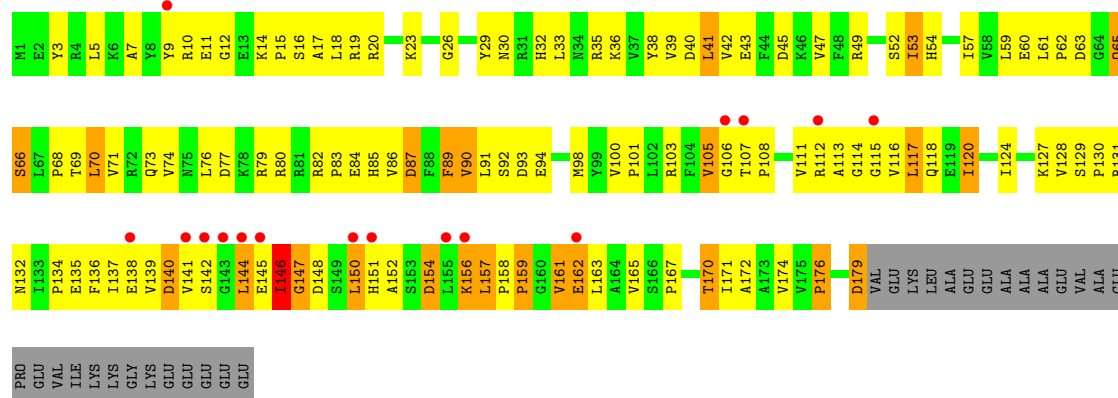
- Molecule 44: 50S ribosomal protein L25

Chain BV:



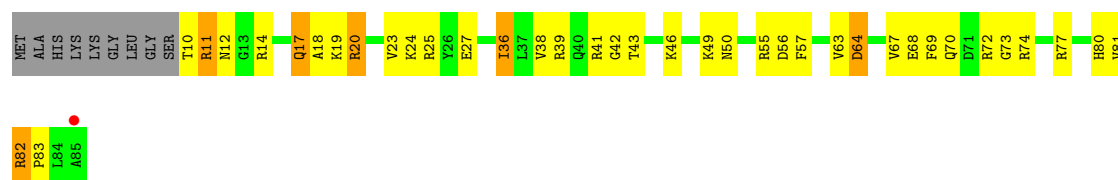
- Molecule 44: 50S ribosomal protein L25

Chain DV:



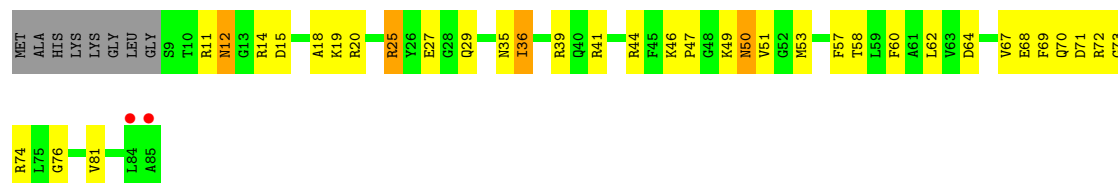
- Molecule 45: 50S ribosomal protein L27

Chain B3: 



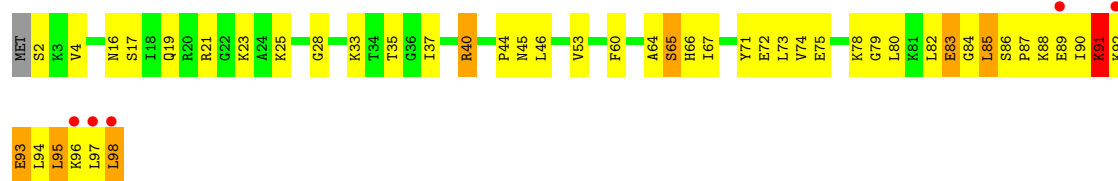
- Molecule 45: 50S ribosomal protein L27

Chain D3: 



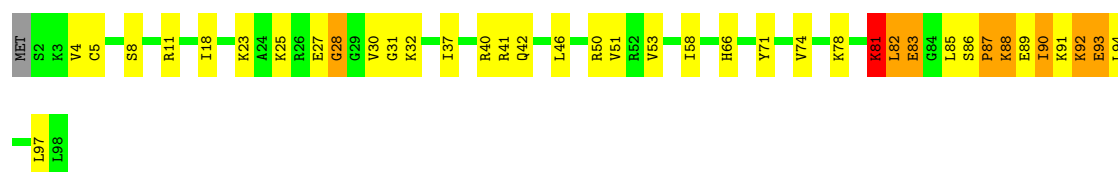
- Molecule 46: 50S ribosomal protein L28

Chain BZ: 



- Molecule 46: 50S ribosomal protein L28

Chain DZ: 



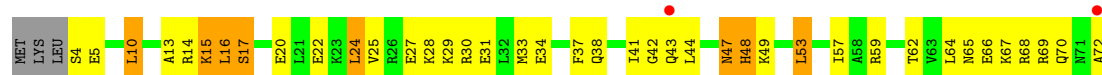
- Molecule 47: 50S ribosomal protein L29

Chain BW: 



- Molecule 47: 50S ribosomal protein L29

Chain DW: 



- Molecule 48: 50S ribosomal protein L30

Chain BX: 



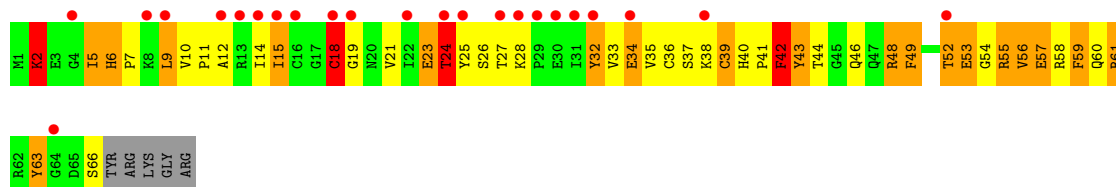
- Molecule 48: 50S ribosomal protein L30

Chain DX: 



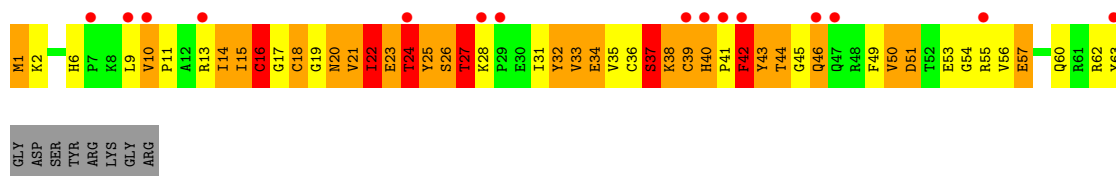
- Molecule 49: 50S ribosomal protein L31

Chain B4: 



- Molecule 49: 50S ribosomal protein L31

Chain D4: 



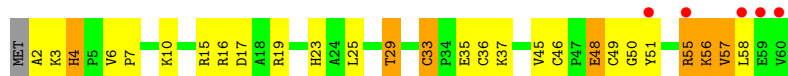
- Molecule 50: 50S ribosomal protein L32

Chain B5: 



- Molecule 50: 50S ribosomal protein L32

Chain D5: 



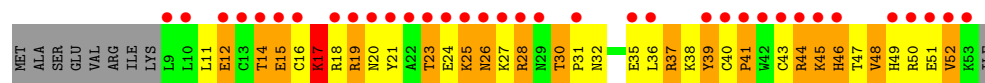
- Molecule 51: 50S ribosomal protein L33

Chain B6: 



- Molecule 51: 50S ribosomal protein L33

Chain D6:



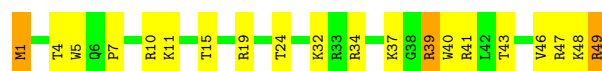
- Molecule 52: 50S ribosomal protein L34

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:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
$R_{merge}$	0.47	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, $R_{free}$	0.213 , 0.269 0.265 , 0.329	Depositor DCC
$R_{free}$ test set	921 reflections (0.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045188 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	295766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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, T1C

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	0.58	23/36234 (0.1%)	1.04	97/56554 (0.2%)
1	CA	0.50	5/36237 (0.0%)	0.95	67/56558 (0.1%)
2	AE	0.37	0/1959	0.60	1/2642 (0.0%)
2	CE	0.38	0/1959	0.68	4/2642 (0.2%)
3	AF	0.39	0/1629	0.57	0/2195
3	CF	0.37	0/1636	0.56	0/2205
4	AG	0.48	1/1733 (0.1%)	0.66	1/2318 (0.0%)
4	CG	0.45	1/1733 (0.1%)	0.63	1/2318 (0.0%)
5	AH	0.42	0/1171	0.60	0/1576
5	CH	0.38	0/1171	0.57	0/1576
6	AI	0.43	0/856	0.61	0/1154
6	CI	0.37	0/856	0.52	0/1154
7	AJ	0.45	0/1276	0.65	2/1709 (0.1%)
7	CJ	0.39	0/1276	0.59	0/1709
8	AK	0.39	0/1136	0.68	3/1527 (0.2%)
8	CK	0.35	0/1136	0.56	0/1527
9	AL	0.45	0/1029	0.65	0/1379
9	CL	0.41	0/1029	0.62	0/1379
10	AM	0.34	0/814	0.56	0/1095
10	CM	0.38	0/814	0.58	0/1095
11	AN	0.41	0/900	0.58	0/1213
11	CN	0.52	1/900 (0.1%)	0.66	1/1213 (0.1%)
12	AO	0.44	0/991	0.62	0/1327
12	CO	0.42	0/991	0.65	1/1327 (0.1%)
13	AP	0.39	0/938	0.59	0/1258
13	CP	0.35	0/943	0.63	1/1265 (0.1%)
14	AQ	0.45	0/501	0.68	0/664
14	CQ	0.45	0/501	0.64	0/664
15	AR	0.41	0/745	0.57	0/992
15	CR	0.42	0/745	0.54	0/992
16	AS	0.40	0/721	0.79	3/970 (0.3%)
16	CS	0.40	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.40	0/847	0.57	0/1131
17	CT	0.39	0/847	0.55	0/1131
18	AU	0.41	0/596	0.64	0/790
18	CU	0.41	0/596	0.60	0/790
19	AV	0.46	0/680	0.75	1/915 (0.1%)
19	CV	0.47	0/638	0.78	0/860
20	AW	0.36	0/765	0.59	0/1007
20	CW	0.37	0/765	0.58	0/1007
21	AX	0.37	0/221	0.55	0/288
21	CX	0.36	0/221	0.63	0/288
22	AC	0.66	2/1832 (0.1%)	1.08	8/2855 (0.3%)
22	AD	0.52	2/1832 (0.1%)	1.08	9/2855 (0.3%)
22	CC	0.56	2/1832 (0.1%)	1.00	9/2855 (0.3%)
22	CD	0.54	2/1832 (0.1%)	1.15	11/2855 (0.4%)
23	A1	0.63	0/144	0.84	0/222
23	C1	0.55	0/144	0.86	0/222
24	BA	0.67	14/70233 (0.0%)	1.18	443/109643 (0.4%)
24	DA	0.61	4/70100 (0.0%)	1.09	282/109435 (0.3%)
25	BB	0.63	0/2928	1.12	12/4568 (0.3%)
25	DB	0.55	0/2928	0.99	3/4568 (0.1%)
26	BD	0.54	0/2165	0.73	0/2919
26	DD	0.57	1/2165 (0.0%)	0.70	0/2919
27	BE	0.49	0/1601	0.64	0/2160
27	DE	0.50	0/1601	0.67	1/2160 (0.0%)
28	BF	0.49	0/1620	0.69	0/2194
28	DF	0.44	0/1662	0.64	0/2249
29	BG	0.42	0/1499	0.59	0/2016
29	DG	0.36	0/1499	0.59	0/2016
30	BH	0.44	0/1332	0.63	1/1802 (0.1%)
30	DH	0.34	0/1332	0.70	1/1802 (0.1%)
31	BK	0.41	0/1151	0.63	0/1558
31	DK	0.40	0/1151	0.63	1/1558 (0.1%)
32	BM	0.47	0/1131	0.62	0/1525
32	DM	0.39	0/1131	0.58	0/1525
33	BN	0.47	0/943	0.61	0/1269
33	DN	0.46	0/943	0.61	0/1269
34	BO	0.54	0/1162	0.82	2/1544 (0.1%)
34	DO	0.42	0/1162	0.71	0/1544
35	BP	0.50	0/1143	0.66	0/1527
35	DP	0.45	0/1143	0.63	0/1527
36	B0	0.51	0/982	0.74	1/1312 (0.1%)
36	D0	0.46	0/974	0.63	0/1302
37	BQ	0.51	0/892	0.69	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DQ	0.44	0/892	0.73	1/1187 (0.1%)
38	BR	0.45	0/1155	0.62	0/1542
38	DR	0.43	0/1155	0.60	0/1542
39	B1	0.52	0/982	0.67	0/1306
39	D1	0.42	0/982	0.64	0/1306
40	B2	0.50	0/790	0.68	1/1057 (0.1%)
40	D2	0.42	0/790	0.69	1/1057 (0.1%)
41	BS	0.47	0/911	0.63	0/1220
41	DS	0.47	0/911	0.59	0/1220
42	BT	0.58	0/739	0.65	0/993
42	DT	0.55	0/739	0.64	0/993
43	BU	0.54	0/798	0.74	0/1064
43	DU	0.50	0/798	0.69	1/1064 (0.1%)
44	BV	0.40	0/1427	0.63	0/1935
44	DV	0.37	0/1460	0.67	1/1982 (0.1%)
45	B3	0.65	2/615 (0.3%)	0.70	0/819
45	D3	0.46	0/621	0.61	0/827
46	BZ	0.50	0/770	0.65	0/1022
46	DZ	0.49	0/770	0.68	0/1022
47	BW	0.56	1/560 (0.2%)	0.70	0/741
47	DW	0.48	0/583	0.71	1/771 (0.1%)
48	BX	0.44	0/474	0.58	0/635
48	DX	0.40	0/474	0.56	0/635
49	B4	0.65	2/545 (0.4%)	0.77	1/733 (0.1%)
49	D4	0.44	0/527	0.69	0/709
50	B5	0.52	0/473	0.76	0/639
50	D5	0.45	0/473	0.67	0/639
51	B6	0.48	0/396	0.70	0/529
51	D6	0.52	0/396	0.68	0/529
52	B7	0.59	0/438	0.74	0/575
52	D7	0.54	0/438	0.65	0/575
53	B8	0.66	0/494	0.77	0/649
53	D8	0.61	0/494	0.93	1/649 (0.2%)
All	All	0.57	63/319716 (0.0%)	0.99	976/478502 (0.2%)

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	193	C	P-O5'	13.92	1.73	1.59
1	AA	193	C	C5'-C4'	13.77	1.67	1.51
1	AA	1381	U	C2-N3	-13.28	1.28	1.37
22	AD	17(A)	C	C4-N4	-11.47	1.23	1.33

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CC	17(A)	C	C4-N4	-11.41	1.23	1.33

The worst 5 of 976 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1381	U	N3-C4-C5	34.37	135.22	114.60
1	AA	193	C	C6-N1-C2	-33.39	106.94	120.30
1	AA	193	C	C5-C6-N1	30.48	136.24	121.00
1	AA	1381	U	C4-C5-C6	-26.85	103.59	119.70
22	CD	17(A)	C	N3-C4-C5	-19.72	114.01	121.90

There are no chirality outliers.

There are no planarity outliers.

## 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	32369	0	16338	913	10
1	CA	32372	0	16336	884	0
2	AE	1924	0	1975	117	0
2	CE	1924	0	1975	144	0
3	AF	1605	0	1668	70	0
3	CF	1612	0	1677	118	0
4	AG	1703	0	1763	112	0
4	CG	1703	0	1764	215	0
5	AH	1155	0	1213	58	0
5	CH	1155	0	1212	56	0
6	AI	843	0	857	42	0
6	CI	843	0	857	28	0
7	AJ	1257	0	1296	74	0
7	CJ	1257	0	1296	67	0
8	AK	1116	0	1177	58	0
8	CK	1116	0	1177	43	0
9	AL	1010	0	1037	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	CL	1010	0	1037	94	0
10	AM	801	0	849	57	0
10	CM	801	0	849	56	1
11	AN	885	0	904	38	0
11	CN	885	0	904	39	0
12	AO	975	0	1062	76	0
12	CO	975	0	1062	44	0
13	AP	928	0	987	62	0
13	CP	933	0	992	89	0
14	AQ	492	0	529	40	0
14	CQ	492	0	531	43	0
15	AR	734	0	771	25	0
15	CR	734	0	771	32	0
16	AS	705	0	725	37	0
16	CS	705	0	725	29	0
17	AT	834	0	904	44	0
17	CT	834	0	904	28	0
18	AU	591	0	662	23	0
18	CU	591	0	662	25	0
19	AV	665	0	686	49	0
19	CV	624	0	636	80	0
20	AW	763	0	861	57	0
20	CW	763	0	861	48	0
21	AX	217	0	234	8	0
21	CX	217	0	234	20	0
22	AC	1640	0	836	20	0
22	AD	1640	0	836	97	0
22	CC	1640	0	836	23	0
22	CD	1640	0	836	90	0
23	A1	129	0	65	0	0
23	C1	129	0	65	0	0
24	BA	62707	0	31612	1372	0
24	DA	62587	0	31554	1346	0
25	BB	2617	0	1328	59	0
25	DB	2617	0	1328	85	0
26	BD	2115	0	2195	113	0
26	DD	2115	0	2195	141	0
27	BE	1568	0	1634	101	0
27	DE	1568	0	1634	207	0
28	BF	1585	0	1632	76	0
28	DF	1627	0	1680	130	0
29	BG	1474	0	1535	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	DG	1474	0	1535	105	0
30	BH	1307	0	1382	135	0
30	DH	1307	0	1382	122	9
31	BK	1136	0	1223	49	0
31	DK	1136	0	1223	47	0
32	BM	1104	0	1180	70	0
32	DM	1104	0	1180	50	0
33	BN	933	0	996	29	0
33	DN	933	0	996	43	0
34	BO	1145	0	1227	112	0
34	DO	1145	0	1228	155	0
35	BP	1122	0	1179	86	0
35	DP	1122	0	1179	59	0
36	B0	968	0	1033	59	0
36	D0	960	0	1021	37	0
37	BQ	882	0	943	54	0
37	DQ	882	0	943	72	0
38	BR	1141	0	1202	68	0
38	DR	1141	0	1202	65	0
39	B1	964	0	1022	64	0
39	D1	964	0	1022	69	0
40	B2	779	0	852	43	1
40	D2	779	0	852	89	0
41	BS	900	0	964	27	0
41	DS	900	0	964	27	0
42	BT	725	0	778	25	0
42	DT	725	0	778	20	0
43	BU	785	0	878	79	0
43	DU	785	0	878	57	0
44	BV	1397	0	1430	79	0
44	DV	1428	0	1454	87	0
45	B3	607	0	628	40	0
45	D3	613	0	633	35	0
46	BZ	763	0	848	30	0
46	DZ	763	0	848	34	0
47	BW	558	0	610	25	0
47	DW	581	0	629	30	0
48	BX	469	0	518	17	0
48	DX	469	0	518	19	0
49	B4	533	0	522	57	0
49	D4	515	0	510	74	0
50	B5	459	0	480	35	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	D5	459	0	480	25	0
51	B6	389	0	404	42	0
51	D6	389	0	404	76	0
52	B7	430	0	480	16	0
52	D7	430	0	480	13	0
53	B8	488	0	559	51	0
53	D8	488	0	560	71	0
54	A1	1	0	0	0	0
54	AA	236	0	0	0	0
54	AC	8	0	0	0	0
54	AD	1	0	0	0	0
54	AG	1	0	0	0	0
54	AH	1	0	0	0	0
54	AN	2	0	0	0	0
54	AQ	1	0	0	0	0
54	AT	1	0	0	0	0
54	B0	1	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	2	0	0	0	0
54	B5	1	0	0	0	0
54	B7	3	0	0	0	0
54	B8	2	0	0	0	0
54	BA	632	0	0	0	0
54	BB	16	0	0	0	0
54	BD	1	0	0	0	0
54	BE	4	0	0	0	0
54	BF	2	0	0	0	0
54	BO	2	0	0	0	0
54	BU	2	0	0	0	0
54	CA	199	0	0	0	0
54	CC	9	0	0	0	0
54	CG	2	0	0	0	0
54	CL	1	0	0	0	0
54	CN	1	0	0	0	0
54	CS	1	0	0	0	0
54	CX	1	0	0	0	0
54	D1	1	0	0	0	0
54	D3	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	523	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DB	15	0	0	0	0
54	DE	4	0	0	0	0
54	DP	1	0	0	0	0
54	DR	1	0	0	0	0
54	DU	2	0	0	0	0
55	AA	42	0	39	2	0
55	CA	42	0	38	5	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	295766	0	199075	9375	11

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 21.

The worst 5 of 9375 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:BA:2751:G:C2	30:BH:3:ARG:HD3	1.42	1.55
30:DH:127:GLU:CG	30:DH:128:PRO:HD3	1.36	1.54
27:DE:11:MET:SD	27:DE:24:THR:HG22	1.47	1.52
40:D2:49:THR:HB	40:D2:50:PRO:CD	1.45	1.47
26:DD:34:VAL:HG22	26:DD:35:LYS:CE	1.44	1.46

The worst 5 of 11 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)
1:AA:85:U:O5'	30:DH:126:PRO:CA[3_555]	1.25	0.95
1:AA:85:U:C4'	30:DH:126:PRO:CB[3_555]	1.47	0.73
1:AA:84:U:O3'	30:DH:127:GLU:N[3_555]	1.76	0.44
1:AA:84:U:OP2	30:DH:127:GLU:CG[3_555]	1.98	0.22
1:AA:85:U:C5'	30:DH:126:PRO:CB[3_555]	2.00	0.20

## 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	235/256 (92%)	170 (72%)	41 (17%)	24 (10%)	1	6
2	CE	235/256 (92%)	165 (70%)	38 (16%)	32 (14%)	0	2
3	AF	203/239 (85%)	138 (68%)	44 (22%)	21 (10%)	1	6
3	CF	204/239 (85%)	135 (66%)	48 (24%)	21 (10%)	1	6
4	AG	206/208 (99%)	154 (75%)	35 (17%)	17 (8%)	1	9
4	CG	206/208 (99%)	150 (73%)	36 (18%)	20 (10%)	1	6
5	AH	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	6	32
5	CH	149/162 (92%)	130 (87%)	13 (9%)	6 (4%)	5	28
6	AI	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	5	28
6	CI	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	11	49
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	6	33
7	CJ	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	3	21
8	AK	136/138 (99%)	103 (76%)	23 (17%)	10 (7%)	2	11
8	CK	136/138 (99%)	120 (88%)	10 (7%)	6 (4%)	4	25
9	AL	125/128 (98%)	87 (70%)	26 (21%)	12 (10%)	1	7
9	CL	125/128 (98%)	90 (72%)	31 (25%)	4 (3%)	6	35
10	AM	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	1	7
10	CM	97/105 (92%)	65 (67%)	24 (25%)	8 (8%)	1	10
11	AN	117/129 (91%)	90 (77%)	19 (16%)	8 (7%)	2	14
11	CN	117/129 (91%)	96 (82%)	16 (14%)	5 (4%)	4	26
12	AO	123/128 (96%)	87 (71%)	24 (20%)	12 (10%)	1	6
12	CO	123/128 (96%)	103 (84%)	10 (8%)	10 (8%)	1	10
13	AP	114/126 (90%)	81 (71%)	20 (18%)	13 (11%)	1	4
13	CP	115/126 (91%)	75 (65%)	22 (19%)	18 (16%)	0	1
14	AQ	58/61 (95%)	40 (69%)	7 (12%)	11 (19%)	0	0
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	6
15	AR	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	2	13
15	CR	86/89 (97%)	73 (85%)	6 (7%)	7 (8%)	1	10
16	AS	82/88 (93%)	65 (79%)	16 (20%)	1 (1%)	19	62
16	CS	82/88 (93%)	66 (80%)	15 (18%)	1 (1%)	19	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AT	98/105 (93%)	78 (80%)	14 (14%)	6 (6%)	2	16
17	CT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	11	49
18	AU	70/88 (80%)	59 (84%)	7 (10%)	4 (6%)	3	18
18	CU	70/88 (80%)	56 (80%)	7 (10%)	7 (10%)	1	6
19	AV	81/93 (87%)	54 (67%)	19 (24%)	8 (10%)	1	6
19	CV	76/93 (82%)	44 (58%)	17 (22%)	15 (20%)	0	0
20	AW	97/106 (92%)	72 (74%)	12 (12%)	13 (13%)	0	2
20	CW	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	1	7
21	AX	23/27 (85%)	14 (61%)	7 (30%)	2 (9%)	1	9
21	CX	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	3
26	BD	270/276 (98%)	231 (86%)	26 (10%)	13 (5%)	4	23
26	DD	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	4	23
27	BE	203/206 (98%)	161 (79%)	28 (14%)	14 (7%)	2	13
27	DE	203/206 (98%)	133 (66%)	33 (16%)	37 (18%)	0	0
28	BF	200/210 (95%)	175 (88%)	20 (10%)	5 (2%)	9	42
28	DF	206/210 (98%)	151 (73%)	29 (14%)	26 (13%)	0	3
29	BG	179/182 (98%)	120 (67%)	42 (24%)	17 (10%)	1	7
29	DG	179/182 (98%)	121 (68%)	38 (21%)	20 (11%)	1	5
30	BH	168/180 (93%)	124 (74%)	24 (14%)	20 (12%)	1	4
30	DH	168/180 (93%)	92 (55%)	45 (27%)	31 (18%)	0	0
31	BK	144/148 (97%)	102 (71%)	25 (17%)	17 (12%)	1	4
31	DK	144/148 (97%)	104 (72%)	28 (19%)	12 (8%)	1	9
32	BM	136/140 (97%)	101 (74%)	25 (18%)	10 (7%)	2	11
32	DM	136/140 (97%)	110 (81%)	22 (16%)	4 (3%)	7	38
33	BN	120/122 (98%)	113 (94%)	5 (4%)	2 (2%)	14	54
33	DN	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	9	42
34	BO	148/150 (99%)	99 (67%)	21 (14%)	28 (19%)	0	0
34	DO	148/150 (99%)	83 (56%)	44 (30%)	21 (14%)	0	2
35	BP	139/141 (99%)	96 (69%)	26 (19%)	17 (12%)	1	4
35	DP	139/141 (99%)	105 (76%)	19 (14%)	15 (11%)	1	5
36	B0	116/118 (98%)	88 (76%)	19 (16%)	9 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D0	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	8	41
37	BQ	109/112 (97%)	78 (72%)	19 (17%)	12 (11%)	1	5
37	DQ	109/112 (97%)	78 (72%)	20 (18%)	11 (10%)	1	6
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	2	14
38	DR	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	4	25
39	B1	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	6	32
39	D1	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	11
40	B2	99/101 (98%)	78 (79%)	11 (11%)	10 (10%)	1	6
40	D2	99/101 (98%)	73 (74%)	12 (12%)	14 (14%)	0	2
41	BS	111/113 (98%)	102 (92%)	6 (5%)	3 (3%)	8	39
41	DS	111/113 (98%)	98 (88%)	8 (7%)	5 (4%)	4	24
42	BT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	10	46
42	DT	90/96 (94%)	69 (77%)	13 (14%)	8 (9%)	1	8
43	BU	100/110 (91%)	69 (69%)	14 (14%)	17 (17%)	0	0
43	DU	100/110 (91%)	53 (53%)	22 (22%)	25 (25%)	0	0
44	BV	173/206 (84%)	117 (68%)	31 (18%)	25 (14%)	0	2
44	DV	177/206 (86%)	111 (63%)	35 (20%)	31 (18%)	0	0
45	B3	74/85 (87%)	65 (88%)	7 (10%)	2 (3%)	8	39
45	D3	75/85 (88%)	66 (88%)	7 (9%)	2 (3%)	8	39
46	BZ	95/98 (97%)	78 (82%)	10 (10%)	7 (7%)	2	11
46	DZ	95/98 (97%)	71 (75%)	14 (15%)	10 (10%)	1	5
47	BW	64/72 (89%)	52 (81%)	9 (14%)	3 (5%)	4	23
47	DW	67/72 (93%)	53 (79%)	6 (9%)	8 (12%)	1	4
48	BX	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	6	32
48	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	3	21
49	B4	64/71 (90%)	34 (53%)	15 (23%)	15 (23%)	0	0
49	D4	61/71 (86%)	25 (41%)	18 (30%)	18 (30%)	0	0
50	B5	57/60 (95%)	41 (72%)	9 (16%)	7 (12%)	1	3
50	D5	57/60 (95%)	46 (81%)	7 (12%)	4 (7%)	2	13
51	B6	43/54 (80%)	24 (56%)	14 (33%)	5 (12%)	1	4
51	D6	43/54 (80%)	19 (44%)	13 (30%)	11 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
52	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
53	B8	59/65 (91%)	45 (76%)	8 (14%)	6 (10%)	1	6
53	D8	59/65 (91%)	42 (71%)	8 (14%)	9 (15%)	0	1
All	All	11341/12044 (94%)	8521 (75%)	1799 (16%)	1021 (9%)	1	8

5 of 1021 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	29	ALA
2	AE	30	ARG
2	AE	95	GLN
2	AE	101	MET
2	AE	208	ILE

### 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	205/220 (93%)	166 (81%)	39 (19%)	2	9
2	CE	205/220 (93%)	166 (81%)	39 (19%)	2	9
3	AF	159/188 (85%)	141 (89%)	18 (11%)	9	32
3	CF	160/188 (85%)	138 (86%)	22 (14%)	5	21
4	AG	180/180 (100%)	157 (87%)	23 (13%)	6	24
4	CG	180/180 (100%)	160 (89%)	20 (11%)	9	33
5	AH	116/123 (94%)	103 (89%)	13 (11%)	9	33
5	CH	116/123 (94%)	102 (88%)	14 (12%)	7	27
6	AI	90/90 (100%)	82 (91%)	8 (9%)	14	47
6	CI	90/90 (100%)	77 (86%)	13 (14%)	5	19
7	AJ	126/127 (99%)	105 (83%)	21 (17%)	3	11
7	CJ	126/127 (99%)	107 (85%)	19 (15%)	4	16
8	AK	119/119 (100%)	105 (88%)	14 (12%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CK	119/119 (100%)	102 (86%)	17 (14%)	5	19
9	AL	98/99 (99%)	74 (76%)	24 (24%)	1	4
9	CL	98/99 (99%)	80 (82%)	18 (18%)	2	9
10	AM	89/92 (97%)	78 (88%)	11 (12%)	7	25
10	CM	89/92 (97%)	72 (81%)	17 (19%)	2	9
11	AN	90/99 (91%)	80 (89%)	10 (11%)	9	33
11	CN	90/99 (91%)	73 (81%)	17 (19%)	2	9
12	AO	104/107 (97%)	89 (86%)	15 (14%)	5	19
12	CO	104/107 (97%)	93 (89%)	11 (11%)	10	35
13	AP	94/101 (93%)	85 (90%)	9 (10%)	12	42
13	CP	94/101 (93%)	75 (80%)	19 (20%)	2	8
14	AQ	49/50 (98%)	39 (80%)	10 (20%)	2	8
14	CQ	49/50 (98%)	40 (82%)	9 (18%)	2	9
15	AR	79/80 (99%)	70 (89%)	9 (11%)	8	31
15	CR	79/80 (99%)	72 (91%)	7 (9%)	14	47
16	AS	72/74 (97%)	55 (76%)	17 (24%)	1	5
16	CS	72/74 (97%)	61 (85%)	11 (15%)	4	15
17	AT	95/97 (98%)	85 (90%)	10 (10%)	10	35
17	CT	95/97 (98%)	87 (92%)	8 (8%)	16	52
18	AU	63/77 (82%)	54 (86%)	9 (14%)	5	19
18	CU	63/77 (82%)	55 (87%)	8 (13%)	6	24
19	AV	72/80 (90%)	56 (78%)	16 (22%)	1	6
19	CV	67/80 (84%)	54 (81%)	13 (19%)	2	8
20	AW	76/82 (93%)	66 (87%)	10 (13%)	6	23
20	CW	76/82 (93%)	68 (90%)	8 (10%)	10	35
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	19 (95%)	1 (5%)	34	75
26	BD	214/218 (98%)	178 (83%)	36 (17%)	3	11
26	DD	214/218 (98%)	183 (86%)	31 (14%)	5	18
27	BE	165/166 (99%)	144 (87%)	21 (13%)	6	24
27	DE	165/166 (99%)	143 (87%)	22 (13%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BF	161/166 (97%)	142 (88%)	19 (12%)	8	29
28	DF	165/166 (99%)	138 (84%)	27 (16%)	3	12
29	BG	155/156 (99%)	138 (89%)	17 (11%)	9	34
29	DG	155/156 (99%)	132 (85%)	23 (15%)	4	17
30	BH	142/148 (96%)	123 (87%)	19 (13%)	6	22
30	DH	142/148 (96%)	109 (77%)	33 (23%)	1	5
31	BK	122/124 (98%)	103 (84%)	19 (16%)	4	14
31	DK	122/124 (98%)	92 (75%)	30 (25%)	1	3
32	BM	117/119 (98%)	95 (81%)	22 (19%)	2	9
32	DM	117/119 (98%)	96 (82%)	21 (18%)	2	10
33	BN	100/100 (100%)	90 (90%)	10 (10%)	11	38
33	DN	100/100 (100%)	87 (87%)	13 (13%)	6	23
34	BO	116/116 (100%)	91 (78%)	25 (22%)	1	6
34	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
35	BP	111/111 (100%)	100 (90%)	11 (10%)	11	39
35	DP	111/111 (100%)	94 (85%)	17 (15%)	4	15
36	B0	101/101 (100%)	87 (86%)	14 (14%)	5	21
36	D0	100/101 (99%)	89 (89%)	11 (11%)	9	34
37	BQ	87/88 (99%)	74 (85%)	13 (15%)	4	17
37	DQ	87/88 (99%)	69 (79%)	18 (21%)	2	8
38	BR	120/127 (94%)	105 (88%)	15 (12%)	7	25
38	DR	120/127 (94%)	98 (82%)	22 (18%)	2	10
39	B1	93/94 (99%)	79 (85%)	14 (15%)	4	16
39	D1	93/94 (99%)	79 (85%)	14 (15%)	4	16
40	B2	82/82 (100%)	69 (84%)	13 (16%)	4	13
40	D2	82/82 (100%)	62 (76%)	20 (24%)	1	4
41	BS	92/92 (100%)	80 (87%)	12 (13%)	6	23
41	DS	92/92 (100%)	75 (82%)	17 (18%)	2	9
42	BT	74/78 (95%)	63 (85%)	11 (15%)	4	17
42	DT	74/78 (95%)	66 (89%)	8 (11%)	9	34
43	BU	85/91 (93%)	62 (73%)	23 (27%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DU	85/91 (93%)	59 (69%)	26 (31%)	0	1
44	BV	154/179 (86%)	126 (82%)	28 (18%)	2	10
44	DV	158/179 (88%)	136 (86%)	22 (14%)	5	21
45	B3	61/67 (91%)	54 (88%)	7 (12%)	8	31
45	D3	62/67 (92%)	58 (94%)	4 (6%)	24	65
46	BZ	82/83 (99%)	67 (82%)	15 (18%)	2	10
46	DZ	82/83 (99%)	76 (93%)	6 (7%)	20	59
47	BW	62/67 (92%)	54 (87%)	8 (13%)	6	24
47	DW	64/67 (96%)	61 (95%)	3 (5%)	36	78
48	BX	51/52 (98%)	44 (86%)	7 (14%)	5	21
48	DX	51/52 (98%)	43 (84%)	8 (16%)	4	14
49	B4	59/63 (94%)	41 (70%)	18 (30%)	0	1
49	D4	57/63 (90%)	36 (63%)	21 (37%)	0	0
50	B5	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	D5	51/52 (98%)	43 (84%)	8 (16%)	4	14
51	B6	44/52 (85%)	33 (75%)	11 (25%)	1	3
51	D6	44/52 (85%)	31 (70%)	13 (30%)	0	1
52	B7	42/42 (100%)	36 (86%)	6 (14%)	5	19
52	D7	42/42 (100%)	33 (79%)	9 (21%)	1	7
53	B8	51/55 (93%)	39 (76%)	12 (24%)	1	5
53	D8	51/55 (93%)	41 (80%)	10 (20%)	2	8
All	All	9584/9992 (96%)	8081 (84%)	1503 (16%)	4	14

5 of 1503 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B4	57	GLU
7	CJ	75	VAL
43	DU	62	GLU
51	B6	37	ARG
3	CF	29	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	CG	43	HIS
12	CO	49	ASN
41	DS	40	ASN
4	CG	45	GLN
7	CJ	28	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1506 (100%)	316 (20%)	26 (1%)
1	CA	1505/1506 (99%)	312 (20%)	30 (1%)
22	AC	76/77 (98%)	8 (10%)	1 (1%)
22	AD	76/77 (98%)	24 (31%)	1 (1%)
22	CC	77/77 (100%)	12 (15%)	1 (1%)
22	CD	76/77 (98%)	45 (59%)	5 (6%)
23	A1	5/6 (83%)	1 (20%)	0
23	C1	5/6 (83%)	1 (20%)	0
24	BA	2911/2912 (99%)	593 (20%)	44 (1%)
24	DA	2904/2912 (99%)	645 (22%)	39 (1%)
25	BB	121/122 (99%)	27 (22%)	0
25	DB	121/122 (99%)	32 (26%)	0
All	All	9383/9400 (99%)	2016 (21%)	147 (1%)

5 of 2016 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2481	G
1	CA	412	A
24	DA	2211	G
24	BA	2610	C
1	CA	197	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 1692 ligands modelled in this entry, 1690 are monoatomic - leaving 2 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	$\# Z  > 2$
55	T1C	AA	1837	54	45,45,45	1.54	7 (15%)	72,72,72	2.25	21 (29%)
55	T1C	CA	1800	54	45,45,45	1.58	6 (13%)	72,72,72	1.87	20 (27%)

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
55	T1C	AA	1837	54	-	1/22/80/80	0/4/4/4
55	T1C	CA	1800	54	-	1/22/80/80	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1800	T1C	C7-N7	-7.10	1.41	1.48
55	AA	1837	T1C	C7-N7	-7.08	1.41	1.48
55	CA	1800	T1C	C4-N4	-3.64	1.47	1.51
55	AA	1837	T1C	C4-N4	-2.79	1.48	1.51
55	CA	1800	T1C	C9-N9	-2.66	1.36	1.41

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
55	CA	1800	T1C	O12-C12-C1B	-6.65	117.73	123.88
55	AA	1837	T1C	C41-C1C-C1	-6.56	103.46	111.12
55	AA	1837	T1C	O12-C12-C1B	-6.40	117.95	123.88
55	AA	1837	T1C	C51-C1B-C12	-6.18	119.28	122.96
55	AA	1837	T1C	C1C-C41-C4	5.49	116.22	111.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	AA	1837	T1C	C92-C91-N9-C9
55	CA	1800	T1C	C92-C91-N9-C9

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	1506/1506 (100%)	-0.68	2 (0%) 93 70	66, 112, 190, 248	0
1	CA	1506/1506 (100%)	-0.72	3 (0%) 93 61	76, 117, 189, 249	0
2	AE	237/256 (92%)	0.13	5 (2%) 60 11	116, 147, 183, 193	0
2	CE	237/256 (92%)	0.37	9 (3%) 38 5	126, 162, 192, 208	0
3	AF	205/239 (85%)	0.52	9 (4%) 33 5	99, 124, 157, 164	0
3	CF	206/239 (86%)	1.13	35 (16%) 2 0	121, 145, 174, 184	0
4	AG	208/208 (100%)	-0.30	0 100 100	95, 118, 140, 145	0
4	CG	208/208 (100%)	0.29	5 (2%) 56 9	93, 113, 133, 142	0
5	AH	151/162 (93%)	-0.14	0 100 100	90, 110, 132, 163	0
5	CH	151/162 (93%)	0.20	0 100 100	97, 117, 139, 165	0
6	AI	101/101 (100%)	0.73	5 (4%) 28 4	91, 112, 125, 144	0
6	CI	101/101 (100%)	0.01	1 (0%) 79 23	90, 107, 128, 148	0
7	AJ	155/156 (99%)	0.58	11 (7%) 16 3	111, 129, 157, 167	0
7	CJ	155/156 (99%)	0.09	0 100 100	116, 133, 162, 173	0
8	AK	138/138 (100%)	-0.20	0 100 100	97, 117, 127, 137	0
8	CK	138/138 (100%)	0.03	0 100 100	105, 122, 135, 143	0
9	AL	127/128 (99%)	-0.07	0 100 100	100, 144, 163, 167	0
9	CL	127/128 (99%)	-0.13	0 100 100	114, 155, 170, 176	0
10	AM	99/105 (94%)	0.33	1 (1%) 79 23	100, 146, 171, 175	0
10	CM	99/105 (94%)	0.51	4 (4%) 36 5	117, 159, 174, 180	0
11	AN	119/129 (92%)	0.90	11 (9%) 9 2	83, 108, 138, 168	0
11	CN	119/129 (92%)	0.14	1 (0%) 83 28	91, 112, 138, 163	0
12	AO	125/128 (97%)	0.00	2 (1%) 68 15	78, 92, 116, 168	0
12	CO	125/128 (97%)	0.46	7 (5%) 24 3	84, 104, 129, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	116/126 (92%)	0.07	1 (0%) 81 25	100, 133, 147, 157	0
13	CP	117/126 (92%)	-0.14	1 (0%) 81 25	121, 155, 170, 177	0
14	AQ	60/61 (98%)	-0.13	0 100 100	103, 114, 127, 135	0
14	CQ	60/61 (98%)	0.57	3 (5%) 28 4	130, 139, 155, 162	0
15	AR	88/89 (98%)	-0.16	0 100 100	89, 108, 124, 127	0
15	CR	88/89 (98%)	-0.14	0 100 100	89, 113, 131, 136	0
16	AS	84/88 (95%)	-0.30	0 100 100	107, 122, 145, 171	0
16	CS	84/88 (95%)	0.21	2 (2%) 56 9	91, 107, 126, 167	0
17	AT	100/105 (95%)	-0.12	0 100 100	96, 114, 126, 133	0
17	CT	100/105 (95%)	0.11	1 (1%) 79 23	91, 111, 128, 149	0
18	AU	72/88 (81%)	0.29	2 (2%) 50 8	95, 112, 141, 169	0
18	CU	72/88 (81%)	-0.13	0 100 100	96, 117, 152, 173	0
19	AV	83/93 (89%)	-0.30	0 100 100	115, 136, 151, 157	0
19	CV	78/93 (83%)	0.10	0 100 100	135, 166, 181, 188	0
20	AW	99/106 (93%)	-0.29	0 100 100	111, 127, 157, 162	0
20	CW	99/106 (93%)	-0.11	1 (1%) 79 23	91, 116, 148, 165	0
21	AX	25/27 (92%)	-0.39	0 100 100	111, 120, 140, 160	0
21	CX	25/27 (92%)	-0.32	0 100 100	117, 138, 154, 170	0
22	AC	77/77 (100%)	-0.60	0 100 100	77, 100, 135, 151	0
22	AD	77/77 (100%)	0.13	2 (2%) 53 8	93, 214, 228, 234	0
22	CC	77/77 (100%)	-0.76	0 100 100	80, 118, 151, 171	0
22	CD	77/77 (100%)	-0.62	0 100 100	93, 220, 238, 248	0
23	A1	6/6 (100%)	-0.49	0 100 100	85, 89, 129, 143	0
23	C1	6/6 (100%)	-0.34	0 100 100	103, 111, 138, 153	0
24	BA	2912/2912 (100%)	-0.41	32 (1%) 77 22	53, 82, 212, 247	0
24	DA	2906/2912 (99%)	-0.57	27 (0%) 81 25	60, 90, 232, 251	0
25	BB	122/122 (100%)	-0.60	1 (0%) 83 28	78, 106, 126, 184	0
25	DB	122/122 (100%)	-0.81	0 100 100	91, 127, 154, 200	0
26	BD	272/276 (98%)	0.14	0 100 100	55, 75, 94, 102	0
26	DD	272/276 (98%)	-0.11	2 (0%) 84 32	58, 81, 99, 122	0
27	BE	205/206 (99%)	0.09	1 (0%) 88 39	60, 92, 135, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DE	205/206 (99%)	-0.13	2 (0%) 79 23	60, 97, 142, 165	0
28	BF	202/210 (96%)	0.01	0 100 100	54, 84, 118, 133	0
28	DF	208/210 (99%)	0.44	7 (3%) 43 6	66, 102, 156, 182	0
29	BG	181/182 (99%)	0.62	14 (7%) 13 2	95, 116, 145, 154	0
29	DG	181/182 (99%)	0.16	1 (0%) 86 36	117, 141, 165, 177	0
30	BH	170/180 (94%)	0.14	2 (1%) 75 20	88, 113, 132, 151	0
30	DH	170/180 (94%)	0.82	22 (12%) 4 1	146, 200, 223, 235	0
31	BK	146/148 (98%)	0.22	2 (1%) 72 17	87, 129, 146, 151	0
31	DK	146/148 (98%)	-0.21	0 100 100	88, 132, 151, 159	0
32	BM	138/140 (98%)	0.30	1 (0%) 84 32	78, 93, 128, 145	0
32	DM	138/140 (98%)	-0.05	0 100 100	80, 107, 137, 157	0
33	BN	122/122 (100%)	0.18	0 100 100	69, 87, 102, 112	0
33	DN	122/122 (100%)	0.06	1 (0%) 83 28	70, 91, 109, 116	0
34	BO	150/150 (100%)	0.21	5 (3%) 44 6	60, 91, 114, 167	0
34	DO	150/150 (100%)	0.56	9 (6%) 21 3	66, 105, 140, 179	0
35	BP	141/141 (100%)	0.16	1 (0%) 84 32	68, 91, 113, 135	0
35	DP	141/141 (100%)	0.27	3 (2%) 60 11	80, 106, 130, 152	0
36	B0	118/118 (100%)	0.08	0 100 100	72, 89, 104, 118	0
36	D0	117/118 (99%)	-0.06	0 100 100	71, 89, 108, 119	0
37	BQ	111/112 (99%)	0.33	5 (4%) 32 5	85, 104, 127, 137	0
37	DQ	111/112 (99%)	-0.09	1 (0%) 81 25	98, 121, 142, 151	0
38	BR	137/146 (93%)	0.12	3 (2%) 59 11	80, 102, 150, 169	0
38	DR	137/146 (93%)	-0.07	0 100 100	80, 99, 159, 185	0
39	B1	117/118 (99%)	-0.02	2 (1%) 67 15	63, 83, 112, 138	0
39	D1	117/118 (99%)	-0.16	0 100 100	72, 101, 136, 155	0
40	B2	101/101 (100%)	0.22	2 (1%) 62 12	64, 102, 126, 145	0
40	D2	101/101 (100%)	0.41	3 (2%) 48 7	71, 123, 139, 148	0
41	BS	113/113 (100%)	0.11	2 (1%) 65 14	63, 80, 110, 161	0
41	DS	113/113 (100%)	0.28	2 (1%) 65 14	68, 83, 113, 161	0
42	BT	92/96 (95%)	0.37	1 (1%) 77 22	64, 78, 101, 111	0
42	DT	92/96 (95%)	0.21	4 (4%) 34 5	77, 94, 118, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BU	102/110 (92%)	0.41	3 (2%) 49 7	75, 99, 149, 163	0
43	DU	102/110 (92%)	1.07	15 (14%) 3 1	93, 118, 160, 182	0
44	BV	175/206 (84%)	1.12	28 (16%) 3 1	97, 131, 195, 201	0
44	DV	179/206 (86%)	0.91	16 (8%) 10 2	118, 157, 213, 219	0
45	B3	76/85 (89%)	0.13	1 (1%) 74 19	69, 85, 101, 140	0
45	D3	77/85 (90%)	0.11	2 (2%) 53 8	74, 95, 111, 151	0
46	BZ	97/98 (98%)	0.65	5 (5%) 26 4	65, 85, 132, 164	0
46	DZ	97/98 (98%)	0.09	0 100 100	67, 91, 135, 157	0
47	BW	66/72 (91%)	0.26	1 (1%) 70 16	70, 87, 108, 132	0
47	DW	69/72 (95%)	0.21	2 (2%) 49 7	90, 112, 133, 164	0
48	BX	59/60 (98%)	0.17	2 (3%) 43 6	73, 86, 121, 137	0
48	DX	59/60 (98%)	0.34	1 (1%) 67 15	79, 102, 145, 162	0
49	B4	66/71 (92%)	1.66	23 (34%) 1 0	122, 158, 180, 186	0
49	D4	63/71 (88%)	1.23	15 (23%) 1 0	154, 187, 197, 205	0
50	B5	59/60 (98%)	0.35	5 (8%) 11 2	57, 90, 166, 172	0
50	D5	59/60 (98%)	0.48	5 (8%) 11 2	68, 91, 178, 192	0
51	B6	45/54 (83%)	4.34	40 (88%) 0 0	128, 153, 163, 164	0
51	D6	45/54 (83%)	3.13	35 (77%) 0 0	138, 164, 181, 183	0
52	B7	49/49 (100%)	0.14	2 (4%) 35 5	55, 61, 92, 120	0
52	D7	49/49 (100%)	0.17	0 100 100	63, 70, 107, 130	0
53	B8	61/65 (93%)	0.38	0 100 100	66, 81, 98, 124	0
53	D8	61/65 (93%)	0.34	0 100 100	73, 87, 106, 121	0
All	All	20927/21444 (97%)	-0.12	483 (2%) 57 9	53, 106, 186, 251	0

The worst 5 of 483 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	DA	654(K)	C	14.5
51	B6	16	CYS	12.3
24	DA	654(J)	A	10.8
44	DV	143	GLY	9.9
24	DA	2901	C	9.6

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
54	MG	BA	3172	1/1	0.47	-	62,62,62,62	0
54	MG	BA	3511	1/1	0.18	-	80,80,80,80	0
54	MG	CA	1661	1/1	0.25	-	88,88,88,88	0
54	MG	DA	3327	1/1	0.21	-	75,75,75,75	0
54	MG	AA	1686	1/1	0.33	-	88,88,88,88	0
54	MG	AA	1769	1/1	0.30	-	122,122,122,122	0
54	MG	BA	3239	1/1	0.28	-	71,71,71,71	0
54	MG	BA	3351	1/1	0.20	-	62,62,62,62	0
54	MG	BA	3269	1/1	0.20	-	49,49,49,49	0
54	MG	BA	3403	1/1	0.31	-	103,103,103,103	0
54	MG	BA	3084	1/1	0.18	-	109,109,109,109	0
54	MG	CA	1664	1/1	0.24	-	169,169,169,169	0
54	MG	CA	1633	1/1	0.22	-	85,85,85,85	0
54	MG	AA	1734	1/1	0.40	-	135,135,135,135	0
54	MG	DA	3207	1/1	0.30	-	72,72,72,72	0
54	MG	DA	3004	1/1	0.47	-	105,105,105,105	0
54	MG	CA	1616	1/1	0.17	-	102,102,102,102	0
54	MG	DA	3079	1/1	0.08	-	95,95,95,95	0
54	MG	BA	3603	1/1	0.27	-	93,93,93,93	0
54	MG	CA	1611	1/1	0.42	-	106,106,106,106	0
54	MG	AA	1774	1/1	0.28	-	79,79,79,79	0
54	MG	BA	3246	1/1	0.39	-	62,62,62,62	0
54	MG	CA	1717	1/1	0.23	-	86,86,86,86	0
54	MG	BA	3325	1/1	0.15	-	79,79,79,79	0
54	MG	AA	1651	1/1	0.26	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3174	1/1	0.26	-	63,63,63,63	0
54	MG	AA	1797	1/1	0.42	-	102,102,102,102	0
54	MG	DA	3274	1/1	0.39	-	100,100,100,100	0
54	MG	CC	103	1/1	0.24	-	73,73,73,73	0
54	MG	BA	3400	1/1	0.17	-	72,72,72,72	0
54	MG	DA	3344	1/1	0.32	-	82,82,82,82	0
54	MG	CA	1606	1/1	0.26	-	83,83,83,83	0
54	MG	BA	3406	1/1	0.19	-	88,88,88,88	0
54	MG	DA	3078	1/1	0.20	-	65,65,65,65	0
54	MG	BA	3453	1/1	0.19	-	78,78,78,78	0
54	MG	BA	3194	1/1	0.25	-	64,64,64,64	0
54	MG	BA	3596	1/1	0.25	-	85,85,85,85	0
54	MG	DA	3125	1/1	0.33	-	71,71,71,71	0
54	MG	AA	1829	1/1	0.20	-	81,81,81,81	0
54	MG	DA	3023	1/1	0.16	-	76,76,76,76	0
54	MG	AA	1822	1/1	0.21	-	101,101,101,101	0
54	MG	AA	1672	1/1	0.50	-	86,86,86,86	0
54	MG	CA	1770	1/1	0.16	-	65,65,65,65	0
54	MG	BA	3234	1/1	0.17	-	79,79,79,79	0
54	MG	BA	3220	1/1	0.12	-	76,76,76,76	0
54	MG	BA	3050	1/1	0.27	-	79,79,79,79	0
54	MG	DA	3407	1/1	0.18	-	94,94,94,94	0
54	MG	BA	3354	1/1	0.22	-	83,83,83,83	0
54	MG	DA	3450	1/1	0.09	-	94,94,94,94	0
54	MG	DA	3136	1/1	0.25	-	63,63,63,63	0
54	MG	DA	3036	1/1	0.47	-	114,114,114,114	0
54	MG	DA	3278	1/1	0.30	-	91,91,91,91	0
54	MG	AA	1659	1/1	0.25	-	56,56,56,56	0
54	MG	DA	3394	1/1	0.17	-	75,75,75,75	0
56	ZN	CQ	101	1/1	0.11	-	123,123,123,123	0
54	MG	DA	3163	1/1	0.33	-	66,66,66,66	0
54	MG	AA	1670	1/1	0.24	-	86,86,86,86	0
54	MG	BA	3306	1/1	0.54	-	94,94,94,94	0
54	MG	DA	3054	1/1	0.37	-	65,65,65,65	0
54	MG	BA	3275	1/1	0.40	-	90,90,90,90	0
54	MG	AA	1705	1/1	0.16	-	104,104,104,104	0
54	MG	DE	304	1/1	0.20	-	66,66,66,66	0
54	MG	AA	1738	1/1	0.43	-	120,120,120,120	0
54	MG	BA	3212	1/1	0.44	-	52,52,52,52	0
54	MG	AA	1741	1/1	0.17	-	99,99,99,99	0
54	MG	BA	3432	1/1	0.28	-	81,81,81,81	0
54	MG	BA	3032	1/1	0.37	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3222	1/1	0.53	-	82,82,82,82	0
54	MG	DA	3464	1/1	0.12	-	89,89,89,89	0
54	MG	BA	3138	1/1	0.34	-	65,65,65,65	0
54	MG	BA	3442	1/1	0.24	-	89,89,89,89	0
54	MG	DA	3232	1/1	0.31	-	54,54,54,54	0
54	MG	BA	3563	1/1	0.39	-	59,59,59,59	0
54	MG	BA	3528	1/1	0.21	-	74,74,74,74	0
54	MG	DA	3041	1/1	0.14	-	82,82,82,82	0
54	MG	DA	3212	1/1	0.32	-	48,48,48,48	0
54	MG	AA	1745	1/1	0.38	-	78,78,78,78	0
54	MG	BA	3561	1/1	0.33	-	57,57,57,57	0
54	MG	DA	3332	1/1	0.29	-	94,94,94,94	0
54	MG	BA	3618	1/1	0.24	-	87,87,87,87	0
54	MG	AA	1806	1/1	0.42	-	87,87,87,87	0
54	MG	AA	1788	1/1	0.24	-	91,91,91,91	0
54	MG	B1	201	1/1	0.32	-	68,68,68,68	0
54	MG	AA	1762	1/1	0.35	-	92,92,92,92	0
54	MG	DA	3518	1/1	0.33	-	83,83,83,83	0
54	MG	CA	1624	1/1	0.16	-	92,92,92,92	0
54	MG	BA	3259	1/1	0.36	-	56,56,56,56	0
54	MG	BB	209	1/1	0.27	-	112,112,112,112	0
54	MG	AA	1627	1/1	0.49	-	76,76,76,76	0
54	MG	DA	3003	1/1	0.10	-	77,77,77,77	0
54	MG	AA	1772	1/1	0.39	-	110,110,110,110	0
54	MG	DA	3503	1/1	0.26	-	76,76,76,76	0
54	MG	DA	3506	1/1	0.38	-	91,91,91,91	0
54	MG	BA	3451	1/1	0.47	-	93,93,93,93	0
54	MG	BA	3527	1/1	0.21	-	78,78,78,78	0
54	MG	DB	207	1/1	0.31	-	133,133,133,133	0
54	MG	AA	1721	1/1	0.34	-	95,95,95,95	0
54	MG	BA	3581	1/1	0.16	-	59,59,59,59	0
54	MG	DA	3098	1/1	0.07	-	112,112,112,112	0
54	MG	BA	3588	1/1	0.45	-	77,77,77,77	0
54	MG	DA	3139	1/1	0.17	-	63,63,63,63	0
54	MG	BA	3180	1/1	0.52	-	92,92,92,92	0
54	MG	BA	3111	1/1	0.45	-	85,85,85,85	0
54	MG	DA	3033	1/1	0.25	-	93,93,93,93	0
54	MG	CA	1680	1/1	0.04	-	104,104,104,104	0
54	MG	CA	1714	1/1	0.13	-	161,161,161,161	0
54	MG	BA	3468	1/1	0.35	-	99,99,99,99	0
54	MG	DP	201	1/1	0.11	-	76,76,76,76	0
54	MG	BA	3399	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
54	MG	DA	3091	1/1	0.32	-	73,73,73,73	0
54	MG	CA	1790	1/1	0.31	-	105,105,105,105	0
54	MG	AA	1729	1/1	0.31	-	102,102,102,102	0
54	MG	BA	3152	1/1	0.10	-	80,80,80,80	0
54	MG	DA	3362	1/1	0.42	-	79,79,79,79	0
54	MG	DA	3393	1/1	0.33	-	92,92,92,92	0
54	MG	DA	3392	1/1	0.12	-	82,82,82,82	0
54	MG	BA	3631	1/1	0.24	-	96,96,96,96	0
54	MG	BA	3343	1/1	0.43	-	73,73,73,73	0
54	MG	BA	3570	1/1	0.13	-	65,65,65,65	0
54	MG	D8	101	1/1	0.26	-	80,80,80,80	0
54	MG	BA	3093	1/1	0.15	-	72,72,72,72	0
54	MG	AA	1735	1/1	0.29	-	104,104,104,104	0
54	MG	BA	3195	1/1	0.20	-	43,43,43,43	0
54	MG	AA	1742	1/1	0.21	-	82,82,82,82	0
54	MG	AA	1792	1/1	0.24	-	108,108,108,108	0
54	MG	CA	1702	1/1	0.31	-	84,84,84,84	0
54	MG	BA	3620	1/1	0.15	-	63,63,63,63	0
54	MG	BA	3373	1/1	0.23	-	85,85,85,85	0
54	MG	DA	3446	1/1	0.24	-	99,99,99,99	0
54	MG	BA	3460	1/1	0.07	-	189,189,189,189	0
54	MG	DA	3012	1/1	0.36	-	87,87,87,87	0
54	MG	DA	3472	1/1	0.14	-	88,88,88,88	0
54	MG	BA	3420	1/1	0.13	-	65,65,65,65	0
54	MG	AC	107	1/1	0.20	-	94,94,94,94	0
54	MG	BA	3369	1/1	0.51	-	68,68,68,68	0
54	MG	BA	3271	1/1	0.14	-	98,98,98,98	0
54	MG	DA	3333	1/1	0.39	-	90,90,90,90	0
54	MG	BA	3305	1/1	0.45	-	79,79,79,79	0
54	MG	DA	3067	1/1	0.40	-	93,93,93,93	0
54	MG	CA	1722	1/1	0.34	-	104,104,104,104	0
54	MG	CA	1756	1/1	0.39	-	76,76,76,76	0
54	MG	CA	1757	1/1	0.13	-	100,100,100,100	0
54	MG	CA	1784	1/1	0.39	-	95,95,95,95	0
54	MG	AA	1749	1/1	0.12	-	130,130,130,130	0
54	MG	DA	3138	1/1	0.12	-	121,121,121,121	0
54	MG	DB	215	1/1	0.11	-	120,120,120,120	0
54	MG	B8	102	1/1	0.24	-	107,107,107,107	0
54	MG	BA	3467	1/1	0.28	-	62,62,62,62	0
54	MG	BA	3365	1/1	0.23	-	86,86,86,86	0
54	MG	AA	1644	1/1	0.36	-	68,68,68,68	0
54	MG	DA	3257	1/1	0.36	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1724	1/1	0.59	-	126,126,126,126	0
54	MG	DA	3418	1/1	0.18	-	97,97,97,97	0
54	MG	DA	3463	1/1	0.28	-	75,75,75,75	0
54	MG	BA	3051	1/1	0.38	-	74,74,74,74	0
54	MG	DA	3051	1/1	0.35	-	78,78,78,78	0
54	MG	DA	3223	1/1	0.36	-	73,73,73,73	0
54	MG	BA	3129	1/1	0.29	-	84,84,84,84	0
54	MG	BA	3487	1/1	0.18	-	72,72,72,72	0
54	MG	AA	1730	1/1	0.25	-	90,90,90,90	0
54	MG	AA	1815	1/1	0.41	-	98,98,98,98	0
54	MG	BA	3319	1/1	0.24	-	82,82,82,82	0
54	MG	BA	3066	1/1	0.18	-	60,60,60,60	0
54	MG	BA	3110	1/1	0.26	-	58,58,58,58	0
54	MG	BA	3108	1/1	0.28	-	56,56,56,56	0
54	MG	DA	3194	1/1	0.42	-	54,54,54,54	0
54	MG	AA	1832	1/1	0.28	-	87,87,87,87	0
54	MG	DA	3367	1/1	0.38	-	89,89,89,89	0
54	MG	AA	1763	1/1	0.44	-	89,89,89,89	0
54	MG	DA	3096	1/1	0.44	-	88,88,88,88	0
54	MG	BA	3562	1/1	0.39	-	53,53,53,53	0
54	MG	D3	101	1/1	0.34	-	78,78,78,78	0
54	MG	CA	1776	1/1	0.32	-	98,98,98,98	0
54	MG	BA	3026	1/1	0.29	-	59,59,59,59	0
54	MG	DA	3015	1/1	0.37	-	64,64,64,64	0
54	MG	B5	1701	1/1	0.26	-	60,60,60,60	0
54	MG	AA	1706	1/1	0.25	-	94,94,94,94	0
54	MG	BA	3572	1/1	0.43	-	45,45,45,45	0
54	MG	CA	1666	1/1	0.06	-	76,76,76,76	0
54	MG	CA	1621	1/1	0.23	-	82,82,82,82	0
54	MG	BA	3519	1/1	0.40	-	115,115,115,115	0
54	MG	BA	3143	1/1	0.42	-	63,63,63,63	0
54	MG	CA	1789	1/1	0.17	-	82,82,82,82	0
54	MG	DA	3008	1/1	0.23	-	77,77,77,77	0
54	MG	DA	3048	1/1	0.34	-	61,61,61,61	0
54	MG	BA	3094	1/1	0.43	-	103,103,103,103	0
54	MG	AA	1785	1/1	0.34	-	146,146,146,146	0
54	MG	AA	1783	1/1	0.45	-	88,88,88,88	0
54	MG	BA	3238	1/1	0.44	-	63,63,63,63	0
54	MG	BB	215	1/1	0.14	-	110,110,110,110	0
54	MG	AA	1754	1/1	0.19	-	91,91,91,91	0
54	MG	CA	1772	1/1	0.17	-	128,128,128,128	0
54	MG	DA	3034	1/1	0.13	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1810	1/1	0.27	-	89,89,89,89	0
54	MG	DA	3341	1/1	0.28	-	68,68,68,68	0
54	MG	DA	3230	1/1	0.28	-	64,64,64,64	0
54	MG	BA	3045	1/1	0.16	-	64,64,64,64	0
54	MG	BA	3462	1/1	0.33	-	94,94,94,94	0
54	MG	CA	1721	1/1	0.29	-	74,74,74,74	0
54	MG	DA	3435	1/1	0.09	-	134,134,134,134	0
54	MG	DA	3010	1/1	0.33	-	74,74,74,74	0
54	MG	DA	3351	1/1	0.14	-	85,85,85,85	0
54	MG	BA	3264	1/1	0.31	-	78,78,78,78	0
54	MG	CA	1775	1/1	0.13	-	84,84,84,84	0
54	MG	BA	3057	1/1	0.38	-	70,70,70,70	0
54	MG	BA	3289	1/1	0.34	-	94,94,94,94	0
54	MG	BA	3291	1/1	0.27	-	85,85,85,85	0
54	MG	DA	3497	1/1	0.30	-	86,86,86,86	0
54	MG	CA	1648	1/1	0.27	-	88,88,88,88	0
54	MG	BA	3217	1/1	0.34	-	98,98,98,98	0
54	MG	DA	3465	1/1	0.29	-	50,50,50,50	0
54	MG	CA	1638	1/1	0.29	-	100,100,100,100	0
54	MG	CA	1646	1/1	0.13	-	92,92,92,92	0
54	MG	DA	3112	1/1	0.29	-	58,58,58,58	0
54	MG	AA	1712	1/1	0.37	-	94,94,94,94	0
54	MG	DA	3411	1/1	0.36	-	88,88,88,88	0
54	MG	BA	3304	1/1	0.47	-	81,81,81,81	0
54	MG	BA	3425	1/1	0.14	-	87,87,87,87	0
54	MG	BA	3410	1/1	0.43	-	83,83,83,83	0
54	MG	CA	1632	1/1	0.23	-	88,88,88,88	0
54	MG	CA	1607	1/1	0.29	-	81,81,81,81	0
54	MG	AA	1630	1/1	0.22	-	88,88,88,88	0
54	MG	BA	3428	1/1	0.17	-	90,90,90,90	0
54	MG	DA	3193	1/1	0.18	-	76,76,76,76	0
54	MG	BA	3331	1/1	0.23	-	88,88,88,88	0
54	MG	CA	1708	1/1	0.26	-	98,98,98,98	0
54	MG	CA	1678	1/1	0.34	-	75,75,75,75	0
54	MG	BA	3130	1/1	0.39	-	105,105,105,105	0
54	MG	BA	3233	1/1	0.06	-	82,82,82,82	0
54	MG	BA	3300	1/1	0.24	-	95,95,95,95	0
54	MG	BA	3555	1/1	0.15	-	105,105,105,105	0
54	MG	AA	1807	1/1	0.46	-	79,79,79,79	0
54	MG	CA	1660	1/1	0.17	-	101,101,101,101	0
54	MG	CA	1684	1/1	0.24	-	91,91,91,91	0
54	MG	DA	3313	1/1	0.30	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1618	1/1	0.17	-	108,108,108,108	0
54	MG	DA	3060	1/1	0.36	-	78,78,78,78	0
54	MG	DA	3259	1/1	0.38	-	78,78,78,78	0
54	MG	DA	3340	1/1	0.28	-	83,83,83,83	0
54	MG	CA	1743	1/1	0.12	-	85,85,85,85	0
54	MG	DA	3507	1/1	0.12	-	117,117,117,117	0
54	MG	CA	1645	1/1	0.37	-	78,78,78,78	0
54	MG	BA	3186	1/1	0.40	-	69,69,69,69	0
54	MG	DA	3428	1/1	0.15	-	86,86,86,86	0
54	MG	DA	3145	1/1	0.20	-	86,86,86,86	0
54	MG	DA	3382	1/1	0.33	-	94,94,94,94	0
54	MG	BA	3517	1/1	0.41	-	90,90,90,90	0
54	MG	DA	3184	1/1	0.17	-	87,87,87,87	0
54	MG	BA	3381	1/1	0.37	-	89,89,89,89	0
54	MG	BA	3162	1/1	0.25	-	85,85,85,85	0
54	MG	DA	3343	1/1	0.40	-	72,72,72,72	0
54	MG	BA	3541	1/1	0.33	-	74,74,74,74	0
54	MG	DA	3009	1/1	0.18	-	71,71,71,71	0
54	MG	DA	3490	1/1	0.06	-	77,77,77,77	0
54	MG	DA	3265	1/1	0.26	-	91,91,91,91	0
54	MG	DA	3363	1/1	0.35	-	92,92,92,92	0
54	MG	CA	1739	1/1	0.29	-	120,120,120,120	0
54	MG	AA	1698	1/1	0.21	-	85,85,85,85	0
54	MG	BB	216	1/1	0.06	-	111,111,111,111	0
54	MG	CA	1762	1/1	0.14	-	83,83,83,83	0
54	MG	DA	3268	1/1	0.35	-	76,76,76,76	0
54	MG	CA	1617	1/1	0.27	-	109,109,109,109	0
54	MG	DA	3377	1/1	0.24	-	85,85,85,85	0
54	MG	BA	3232	1/1	0.28	-	95,95,95,95	0
54	MG	AA	1647	1/1	0.39	-	92,92,92,92	0
54	MG	B8	101	1/1	0.24	-	91,91,91,91	0
54	MG	DA	3169	1/1	0.30	-	74,74,74,74	0
54	MG	DA	3319	1/1	0.10	-	97,97,97,97	0
54	MG	DA	3487	1/1	0.15	-	95,95,95,95	0
54	MG	DA	3442	1/1	0.24	-	105,105,105,105	0
54	MG	DA	3449	1/1	0.22	-	88,88,88,88	0
54	MG	DA	3053	1/1	0.35	-	70,70,70,70	0
54	MG	BA	3478	1/1	0.43	-	64,64,64,64	0
54	MG	DA	3198	1/1	0.29	-	57,57,57,57	0
54	MG	AA	1800	1/1	0.20	-	89,89,89,89	0
54	MG	AA	1697	1/1	0.09	-	90,90,90,90	0
54	MG	BA	3510	1/1	0.53	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3083	1/1	0.37	-	90,90,90,90	0
54	MG	DA	3251	1/1	0.28	-	87,87,87,87	0
54	MG	BA	3448	1/1	0.24	-	79,79,79,79	0
54	MG	B7	103	1/1	0.28	-	79,79,79,79	0
54	MG	DA	3345	1/1	0.18	-	91,91,91,91	0
54	MG	DA	3185	1/1	0.30	-	77,77,77,77	0
54	MG	DA	3203	1/1	0.31	-	73,73,73,73	0
54	MG	BA	3589	1/1	0.29	-	66,66,66,66	0
54	MG	DA	3270	1/1	0.46	-	90,90,90,90	0
54	MG	BA	3624	1/1	0.19	-	98,98,98,98	0
54	MG	DA	3170	1/1	0.20	-	58,58,58,58	0
54	MG	DA	3089	1/1	0.34	-	81,81,81,81	0
54	MG	DA	3249	1/1	0.22	-	74,74,74,74	0
54	MG	DA	3381	1/1	0.28	-	93,93,93,93	0
54	MG	CA	1748	1/1	0.14	-	110,110,110,110	0
54	MG	AA	1650	1/1	0.35	-	87,87,87,87	0
54	MG	DA	3143	1/1	0.13	-	84,84,84,84	0
54	MG	DA	3064	1/1	0.37	-	88,88,88,88	0
54	MG	CA	1609	1/1	0.14	-	121,121,121,121	0
54	MG	CL	201	1/1	0.32	-	104,104,104,104	0
54	MG	DA	3087	1/1	0.35	-	79,79,79,79	0
54	MG	BA	3370	1/1	0.18	-	100,100,100,100	0
54	MG	DA	3305	1/1	0.35	-	78,78,78,78	0
54	MG	BA	3456	1/1	0.08	-	225,225,225,225	0
54	MG	DA	3236	1/1	0.26	-	56,56,56,56	0
54	MG	BA	3254	1/1	0.33	-	72,72,72,72	0
54	MG	CA	1655	1/1	0.36	-	93,93,93,93	0
54	MG	BA	3235	1/1	0.35	-	79,79,79,79	0
54	MG	DA	3250	1/1	0.29	-	105,105,105,105	0
54	MG	CA	1761	1/1	0.22	-	103,103,103,103	0
54	MG	DA	3400	1/1	0.26	-	95,95,95,95	0
54	MG	DA	3485	1/1	0.32	-	77,77,77,77	0
54	MG	BA	3098	1/1	0.38	-	45,45,45,45	0
54	MG	DA	3099	1/1	0.29	-	60,60,60,60	0
54	MG	CA	1710	1/1	0.20	-	102,102,102,102	0
54	MG	AA	1759	1/1	0.18	-	101,101,101,101	0
54	MG	AA	1744	1/1	0.35	-	81,81,81,81	0
54	MG	CA	1686	1/1	0.20	-	96,96,96,96	0
54	MG	DA	3140	1/1	0.31	-	80,80,80,80	0
54	MG	CC	101	1/1	0.08	-	110,110,110,110	0
54	MG	BA	3006	1/1	0.35	-	56,56,56,56	0
54	MG	DA	3521	1/1	0.41	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1786	1/1	0.11	-	145,145,145,145	0
54	MG	AA	1791	1/1	0.25	-	96,96,96,96	0
54	MG	AA	1750	1/1	0.08	-	92,92,92,92	0
54	MG	BA	3237	1/1	0.50	-	64,64,64,64	0
54	MG	BA	3224	1/1	0.45	-	76,76,76,76	0
54	MG	CA	1700	1/1	0.09	-	133,133,133,133	0
54	MG	BA	3159	1/1	0.34	-	69,69,69,69	0
54	MG	DA	3165	1/1	0.32	-	64,64,64,64	0
54	MG	BA	3579	1/1	0.50	-	51,51,51,51	0
54	MG	BA	3187	1/1	0.48	-	71,71,71,71	0
54	MG	DA	3515	1/1	0.33	-	101,101,101,101	0
54	MG	BA	3213	1/1	0.14	-	61,61,61,61	0
54	MG	BA	3121	1/1	0.23	-	98,98,98,98	0
54	MG	DA	3324	1/1	0.47	-	90,90,90,90	0
54	MG	AA	1622	1/1	0.39	-	70,70,70,70	0
54	MG	BA	3564	1/1	0.13	-	71,71,71,71	0
54	MG	DA	3370	1/1	0.42	-	87,87,87,87	0
54	MG	BE	302	1/1	0.15	-	76,76,76,76	0
54	MG	DA	3020	1/1	0.28	-	81,81,81,81	0
54	MG	CA	1612	1/1	0.09	-	94,94,94,94	0
54	MG	AA	1761	1/1	0.17	-	94,94,94,94	0
54	MG	AA	1641	1/1	0.21	-	74,74,74,74	0
54	MG	AA	1619	1/1	0.20	-	96,96,96,96	0
54	MG	DA	3205	1/1	0.32	-	80,80,80,80	0
54	MG	BA	3396	1/1	0.20	-	117,117,117,117	0
54	MG	DA	3500	1/1	0.20	-	98,98,98,98	0
54	MG	CA	1620	1/1	0.26	-	75,75,75,75	0
54	MG	BA	3112	1/1	0.45	-	71,71,71,71	0
54	MG	DA	3044	1/1	0.14	-	78,78,78,78	0
54	MG	BA	3210	1/1	0.28	-	59,59,59,59	0
54	MG	DB	202	1/1	0.20	-	116,116,116,116	0
54	MG	DA	3068	1/1	0.43	-	86,86,86,86	0
54	MG	DA	3210	1/1	0.30	-	57,57,57,57	0
54	MG	BA	3546	1/1	0.17	-	98,98,98,98	0
54	MG	CA	1759	1/1	0.33	-	100,100,100,100	0
54	MG	DA	3476	1/1	0.20	-	66,66,66,66	0
54	MG	BA	3357	1/1	0.49	-	77,77,77,77	0
54	MG	BA	3592	1/1	0.24	-	73,73,73,73	0
54	MG	AA	1635	1/1	0.18	-	111,111,111,111	0
54	MG	DA	3206	1/1	0.36	-	73,73,73,73	0
54	MG	BA	3559	1/1	0.44	-	65,65,65,65	0
54	MG	DB	212	1/1	0.24	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3310	1/1	0.22	-	70,70,70,70	0
54	MG	BA	3622	1/1	0.25	-	97,97,97,97	0
54	MG	DA	3126	1/1	0.26	-	67,67,67,67	0
54	MG	DA	3187	1/1	0.27	-	83,83,83,83	0
54	MG	AA	1718	1/1	0.24	-	87,87,87,87	0
54	MG	BA	3565	1/1	0.36	-	45,45,45,45	0
54	MG	BA	3061	1/1	0.23	-	84,84,84,84	0
54	MG	DA	3017	1/1	0.34	-	105,105,105,105	0
54	MG	DA	3391	1/1	0.30	-	107,107,107,107	0
54	MG	AA	1809	1/1	0.31	-	105,105,105,105	0
54	MG	DA	3208	1/1	0.30	-	57,57,57,57	0
54	MG	CA	1619	1/1	0.11	-	75,75,75,75	0
54	MG	DA	3299	1/1	0.29	-	99,99,99,99	0
54	MG	DA	3452	1/1	0.34	-	95,95,95,95	0
54	MG	BA	3526	1/1	0.07	-	97,97,97,97	0
54	MG	CA	1777	1/1	0.17	-	78,78,78,78	0
54	MG	DA	3133	1/1	0.09	-	76,76,76,76	0
54	MG	AA	1775	1/1	0.17	-	113,113,113,113	0
54	MG	DA	3459	1/1	0.31	-	87,87,87,87	0
54	MG	DA	3256	1/1	0.27	-	60,60,60,60	0
54	MG	CA	1747	1/1	0.42	-	96,96,96,96	0
54	MG	DA	3304	1/1	0.22	-	88,88,88,88	0
54	MG	BA	3202	1/1	0.29	-	71,71,71,71	0
54	MG	DA	3361	1/1	0.28	-	77,77,77,77	0
54	MG	DA	3330	1/1	0.42	-	95,95,95,95	0
54	MG	DA	3049	1/1	0.37	-	92,92,92,92	0
54	MG	AA	1610	1/1	0.18	-	102,102,102,102	0
54	MG	BF	301	1/1	0.08	-	76,76,76,76	0
54	MG	BA	3389	1/1	0.30	-	74,74,74,74	0
54	MG	DA	3123	1/1	0.40	-	92,92,92,92	0
54	MG	B0	201	1/1	0.24	-	67,67,67,67	0
54	MG	AA	1787	1/1	0.09	-	89,89,89,89	0
54	MG	AA	1676	1/1	0.29	-	109,109,109,109	0
54	MG	DA	3197	1/1	0.11	-	82,82,82,82	0
54	MG	AA	1661	1/1	0.29	-	81,81,81,81	0
54	MG	BA	3192	1/1	0.26	-	100,100,100,100	0
54	MG	CA	1758	1/1	0.22	-	94,94,94,94	0
54	MG	CA	1796	1/1	0.14	-	81,81,81,81	0
54	MG	CA	1605	1/1	0.29	-	87,87,87,87	0
54	MG	DA	3247	1/1	0.39	-	76,76,76,76	0
54	MG	CA	1653	1/1	0.24	-	124,124,124,124	0
54	MG	BA	3606	1/1	0.10	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3461	1/1	0.21	-	93,93,93,93	0
54	MG	DA	3164	1/1	0.26	-	84,84,84,84	0
54	MG	DA	3046	1/1	0.25	-	78,78,78,78	0
54	MG	DA	3021	1/1	0.32	-	63,63,63,63	0
54	MG	DA	3502	1/1	0.16	-	67,67,67,67	0
54	MG	BA	3568	1/1	0.23	-	55,55,55,55	0
54	MG	DA	3199	1/1	0.24	-	63,63,63,63	0
54	MG	BA	3008	1/1	0.45	-	59,59,59,59	0
54	MG	DA	3013	1/1	0.13	-	95,95,95,95	0
54	MG	BA	3540	1/1	0.24	-	78,78,78,78	0
54	MG	DA	3228	1/1	0.23	-	70,70,70,70	0
54	MG	CA	1690	1/1	0.26	-	86,86,86,86	0
54	MG	BA	3200	1/1	0.39	-	76,76,76,76	0
54	MG	DA	3220	1/1	0.25	-	60,60,60,60	0
54	MG	CG	302	1/1	0.08	-	114,114,114,114	0
54	MG	BA	3273	1/1	0.28	-	80,80,80,80	0
54	MG	BA	3197	1/1	0.28	-	89,89,89,89	0
54	MG	DA	3253	1/1	0.20	-	88,88,88,88	0
54	MG	AA	1743	1/1	0.24	-	100,100,100,100	0
54	MG	AA	1720	1/1	0.11	-	113,113,113,113	0
54	MG	DA	3043	1/1	0.32	-	88,88,88,88	0
54	MG	BA	3042	1/1	0.20	-	62,62,62,62	0
54	MG	BA	3115	1/1	0.42	-	74,74,74,74	0
54	MG	BA	3021	1/1	0.31	-	63,63,63,63	0
54	MG	BA	3286	1/1	0.41	-	73,73,73,73	0
54	MG	BA	3267	1/1	0.33	-	75,75,75,75	0
54	MG	CA	1746	1/1	0.39	-	97,97,97,97	0
54	MG	DA	3105	1/1	0.25	-	65,65,65,65	0
54	MG	BA	3575	1/1	0.33	-	52,52,52,52	0
54	MG	CA	1733	1/1	0.44	-	79,79,79,79	0
54	MG	BA	3279	1/1	0.38	-	68,68,68,68	0
54	MG	AA	1653	1/1	0.36	-	89,89,89,89	0
54	MG	DA	3408	1/1	0.15	-	76,76,76,76	0
54	MG	DB	206	1/1	0.36	-	104,104,104,104	0
54	MG	BA	3532	1/1	0.28	-	82,82,82,82	0
54	MG	AA	1693	1/1	0.25	-	106,106,106,106	0
54	MG	DA	3273	1/1	0.23	-	54,54,54,54	0
54	MG	DA	3470	1/1	0.20	-	54,54,54,54	0
54	MG	BA	3360	1/1	0.25	-	85,85,85,85	0
54	MG	CA	1738	1/1	0.44	-	74,74,74,74	0
54	MG	AA	1740	1/1	0.43	-	83,83,83,83	0
54	MG	CA	1699	1/1	0.37	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1679	1/1	0.24	-	97,97,97,97	0
54	MG	BA	3214	1/1	0.30	-	56,56,56,56	0
54	MG	AA	1746	1/1	0.30	-	110,110,110,110	0
54	MG	DA	3356	1/1	0.10	-	84,84,84,84	0
54	MG	DA	3115	1/1	0.31	-	66,66,66,66	0
54	MG	DA	3063	1/1	0.25	-	95,95,95,95	0
54	MG	CA	1779	1/1	0.21	-	97,97,97,97	0
54	MG	CA	1763	1/1	0.31	-	80,80,80,80	0
54	MG	CA	1647	1/1	0.18	-	84,84,84,84	0
54	MG	DA	3171	1/1	0.37	-	64,64,64,64	0
54	MG	CA	1604	1/1	0.16	-	91,91,91,91	0
54	MG	DA	3396	1/1	0.26	-	73,73,73,73	0
54	MG	DA	3094	1/1	0.16	-	107,107,107,107	0
54	MG	BA	3055	1/1	0.41	-	84,84,84,84	0
54	MG	DA	3052	1/1	0.35	-	60,60,60,60	0
54	MG	DA	3113	1/1	0.38	-	83,83,83,83	0
54	MG	BA	3314	1/1	0.41	-	81,81,81,81	0
54	MG	BA	3466	1/1	0.16	-	81,81,81,81	0
54	MG	DA	3025	1/1	0.18	-	91,91,91,91	0
54	MG	AA	1726	1/1	0.19	-	95,95,95,95	0
54	MG	BA	3205	1/1	0.28	-	51,51,51,51	0
54	MG	BA	3619	1/1	0.32	-	87,87,87,87	0
54	MG	CA	1724	1/1	0.31	-	94,94,94,94	0
54	MG	CA	1734	1/1	0.22	-	78,78,78,78	0
54	MG	BA	3019	1/1	0.35	-	48,48,48,48	0
54	MG	BA	3550	1/1	0.28	-	98,98,98,98	0
54	MG	AA	1660	1/1	0.17	-	68,68,68,68	0
54	MG	B7	101	1/1	0.37	-	69,69,69,69	0
54	MG	BA	3165	1/1	0.37	-	48,48,48,48	0
54	MG	AA	1790	1/1	0.28	-	97,97,97,97	0
54	MG	CA	1627	1/1	0.07	-	111,111,111,111	0
54	MG	DA	3074	1/1	0.50	-	102,102,102,102	0
54	MG	BA	3090	1/1	0.30	-	85,85,85,85	0
54	MG	CA	1751	1/1	0.20	-	95,95,95,95	0
54	MG	DA	3360	1/1	0.39	-	86,86,86,86	0
54	MG	DA	3378	1/1	0.30	-	70,70,70,70	0
54	MG	CA	1729	1/1	0.07	-	108,108,108,108	0
54	MG	DA	3520	1/1	0.29	-	99,99,99,99	0
54	MG	DA	3072	1/1	0.11	-	109,109,109,109	0
54	MG	AA	1803	1/1	0.39	-	75,75,75,75	0
54	MG	DA	3037	1/1	0.39	-	101,101,101,101	0
54	MG	BA	3272	1/1	0.20	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3423	1/1	0.18	-	83,83,83,83	0
54	MG	CA	1651	1/1	0.12	-	114,114,114,114	0
54	MG	DA	3275	1/1	0.23	-	76,76,76,76	0
54	MG	DA	3466	1/1	0.19	-	123,123,123,123	0
54	MG	BA	3299	1/1	0.36	-	79,79,79,79	0
54	MG	BA	3393	1/1	0.52	-	89,89,89,89	0
54	MG	BA	3368	1/1	0.21	-	98,98,98,98	0
54	MG	CA	1711	1/1	0.19	-	100,100,100,100	0
54	MG	BA	3445	1/1	0.48	-	64,64,64,64	0
54	MG	DA	3108	1/1	0.27	-	65,65,65,65	0
54	MG	BA	3126	1/1	0.46	-	73,73,73,73	0
54	MG	BA	3529	1/1	0.29	-	87,87,87,87	0
54	MG	D1	201	1/1	0.29	-	72,72,72,72	0
54	MG	BA	3178	1/1	0.37	-	51,51,51,51	0
54	MG	AA	1632	1/1	0.15	-	94,94,94,94	0
54	MG	AA	1770	1/1	0.11	-	110,110,110,110	0
54	MG	BA	3288	1/1	0.43	-	115,115,115,115	0
54	MG	CC	102	1/1	0.28	-	77,77,77,77	0
54	MG	BA	3193	1/1	0.38	-	56,56,56,56	0
54	MG	AA	1737	1/1	0.33	-	95,95,95,95	0
54	MG	BA	3515	1/1	0.38	-	93,93,93,93	0
54	MG	DA	3346	1/1	0.21	-	93,93,93,93	0
54	MG	DA	3231	1/1	0.16	-	74,74,74,74	0
54	MG	BA	3513	1/1	0.29	-	78,78,78,78	0
54	MG	BA	3095	1/1	0.48	-	57,57,57,57	0
54	MG	BA	3417	1/1	0.40	-	82,82,82,82	0
54	MG	BA	3412	1/1	0.48	-	78,78,78,78	0
54	MG	BA	3327	1/1	0.38	-	85,85,85,85	0
54	MG	AA	1680	1/1	0.15	-	105,105,105,105	0
54	MG	BA	3240	1/1	0.22	-	84,84,84,84	0
54	MG	BA	3080	1/1	0.22	-	82,82,82,82	0
54	MG	CA	1636	1/1	0.28	-	100,100,100,100	0
54	MG	AC	101	1/1	0.23	-	68,68,68,68	0
54	MG	CA	1799	1/1	0.09	-	115,115,115,115	0
54	MG	AA	1808	1/1	0.40	-	125,125,125,125	0
54	MG	BA	3116	1/1	0.28	-	84,84,84,84	0
54	MG	DA	3458	1/1	0.11	-	91,91,91,91	0
54	MG	CA	1771	1/1	0.35	-	96,96,96,96	0
54	MG	DA	3122	1/1	0.32	-	84,84,84,84	0
54	MG	BA	3382	1/1	0.51	-	89,89,89,89	0
54	MG	AA	1767	1/1	0.24	-	82,82,82,82	0
54	MG	DA	3167	1/1	0.33	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3311	1/1	0.21	-	73,73,73,73	0
54	MG	DA	3201	1/1	0.37	-	66,66,66,66	0
54	MG	DA	3318	1/1	0.37	-	88,88,88,88	0
54	MG	CA	1766	1/1	0.25	-	74,74,74,74	0
54	MG	DA	3302	1/1	0.23	-	64,64,64,64	0
54	MG	DA	3334	1/1	0.26	-	84,84,84,84	0
54	MG	DA	3495	1/1	0.20	-	125,125,125,125	0
54	MG	BA	3188	1/1	0.27	-	47,47,47,47	0
54	MG	DA	3254	1/1	0.24	-	79,79,79,79	0
54	MG	BA	3278	1/1	0.41	-	64,64,64,64	0
54	MG	BA	3149	1/1	0.24	-	91,91,91,91	0
54	MG	BA	3530	1/1	0.30	-	85,85,85,85	0
54	MG	DA	3376	1/1	0.27	-	62,62,62,62	0
54	MG	AA	1626	1/1	0.30	-	84,84,84,84	0
54	MG	CA	1725	1/1	0.26	-	115,115,115,115	0
54	MG	BA	3179	1/1	0.52	-	60,60,60,60	0
54	MG	CA	1768	1/1	0.29	-	97,97,97,97	0
54	MG	AC	102	1/1	0.45	-	102,102,102,102	0
54	MG	BA	3167	1/1	0.23	-	68,68,68,68	0
54	MG	DA	3196	1/1	0.19	-	72,72,72,72	0
54	MG	DA	3441	1/1	0.16	-	111,111,111,111	0
54	MG	BA	3323	1/1	0.36	-	87,87,87,87	0
54	MG	AA	1602	1/1	0.19	-	82,82,82,82	0
54	MG	AA	1666	1/1	0.40	-	88,88,88,88	0
54	MG	DA	3178	1/1	0.38	-	70,70,70,70	0
54	MG	BA	3255	1/1	0.19	-	69,69,69,69	0
54	MG	BA	3350	1/1	0.47	-	72,72,72,72	0
54	MG	DA	3129	1/1	0.26	-	79,79,79,79	0
54	MG	AA	1728	1/1	0.40	-	70,70,70,70	0
54	MG	BA	3122	1/1	0.45	-	98,98,98,98	0
54	MG	AA	1623	1/1	0.15	-	82,82,82,82	0
54	MG	DA	3114	1/1	0.28	-	70,70,70,70	0
54	MG	BA	3298	1/1	0.32	-	43,43,43,43	0
54	MG	DA	3303	1/1	0.09	-	94,94,94,94	0
54	MG	BA	3309	1/1	0.36	-	69,69,69,69	0
54	MG	BA	3359	1/1	0.26	-	83,83,83,83	0
54	MG	BA	3628	1/1	0.34	-	78,78,78,78	0
54	MG	BA	3621	1/1	0.21	-	93,93,93,93	0
54	MG	DA	3505	1/1	0.25	-	73,73,73,73	0
54	MG	CA	1628	1/1	0.05	-	110,110,110,110	0
54	MG	DA	3387	1/1	0.14	-	89,89,89,89	0
54	MG	A1	101	1/1	0.18	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3427	1/1	0.24	-	74,74,74,74	0
54	MG	DA	3430	1/1	0.22	-	110,110,110,110	0
54	MG	BA	3262	1/1	0.23	-	61,61,61,61	0
54	MG	AA	1716	1/1	0.30	-	106,106,106,106	0
54	MG	DA	3516	1/1	0.28	-	76,76,76,76	0
54	MG	CA	1705	1/1	0.12	-	135,135,135,135	0
54	MG	DA	3402	1/1	0.25	-	91,91,91,91	0
54	MG	BA	3113	1/1	0.28	-	54,54,54,54	0
54	MG	DA	3077	1/1	0.34	-	110,110,110,110	0
54	MG	DA	3416	1/1	0.36	-	86,86,86,86	0
54	MG	BA	3196	1/1	0.34	-	85,85,85,85	0
54	MG	AA	1612	1/1	0.20	-	131,131,131,131	0
54	MG	DA	3385	1/1	0.28	-	63,63,63,63	0
54	MG	DB	211	1/1	0.41	-	90,90,90,90	0
54	MG	DA	3336	1/1	0.50	-	90,90,90,90	0
54	MG	AA	1758	1/1	0.21	-	71,71,71,71	0
54	MG	BA	3342	1/1	0.28	-	85,85,85,85	0
54	MG	BA	3141	1/1	0.31	-	76,76,76,76	0
54	MG	AA	1756	1/1	0.34	-	121,121,121,121	0
54	MG	DB	201	1/1	0.37	-	90,90,90,90	0
54	MG	BA	3148	1/1	0.34	-	85,85,85,85	0
54	MG	DB	204	1/1	0.11	-	87,87,87,87	0
54	MG	DA	3492	1/1	0.26	-	96,96,96,96	0
54	MG	AA	1751	1/1	0.28	-	90,90,90,90	0
54	MG	BA	3552	1/1	0.09	-	79,79,79,79	0
54	MG	DA	3186	1/1	0.22	-	84,84,84,84	0
54	MG	CA	1670	1/1	0.37	-	73,73,73,73	0
54	MG	CC	109	1/1	0.22	-	111,111,111,111	0
54	MG	BA	3372	1/1	0.38	-	81,81,81,81	0
54	MG	DA	3144	1/1	0.25	-	79,79,79,79	0
54	MG	BA	3499	1/1	0.22	-	82,82,82,82	0
54	MG	DA	3481	1/1	0.27	-	55,55,55,55	0
54	MG	DA	3028	1/1	0.26	-	74,74,74,74	0
54	MG	AA	1708	1/1	0.11	-	96,96,96,96	0
54	MG	CA	1774	1/1	0.16	-	105,105,105,105	0
54	MG	DA	3320	1/1	0.07	-	105,105,105,105	0
54	MG	DA	3419	1/1	0.13	-	97,97,97,97	0
54	MG	DA	3195	1/1	0.25	-	82,82,82,82	0
54	MG	BA	3036	1/1	0.40	-	73,73,73,73	0
54	MG	BA	3257	1/1	0.36	-	73,73,73,73	0
54	MG	DA	3160	1/1	0.32	-	69,69,69,69	0
54	MG	BA	3427	1/1	0.10	-	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3183	1/1	0.36	-	70,70,70,70	0
54	MG	BA	3610	1/1	0.27	-	55,55,55,55	0
54	MG	BA	3422	1/1	0.35	-	52,52,52,52	0
54	MG	BA	3632	1/1	0.11	-	114,114,114,114	0
54	MG	BA	3284	1/1	0.34	-	76,76,76,76	0
54	MG	BA	3380	1/1	0.21	-	74,74,74,74	0
54	MG	BA	3505	1/1	0.22	-	51,51,51,51	0
54	MG	BA	3355	1/1	0.43	-	86,86,86,86	0
54	MG	CC	105	1/1	0.39	-	86,86,86,86	0
54	MG	DA	3084	1/1	0.12	-	67,67,67,67	0
54	MG	BA	3560	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3493	1/1	0.26	-	74,74,74,74	0
54	MG	DB	213	1/1	0.36	-	111,111,111,111	0
54	MG	BA	3455	1/1	0.17	-	74,74,74,74	0
54	MG	DA	3379	1/1	0.35	-	88,88,88,88	0
54	MG	BB	207	1/1	0.26	-	84,84,84,84	0
54	MG	DA	3069	1/1	0.28	-	85,85,85,85	0
54	MG	DA	3279	1/1	0.17	-	70,70,70,70	0
54	MG	CA	1781	1/1	0.32	-	148,148,148,148	0
54	MG	CA	1626	1/1	0.30	-	115,115,115,115	0
54	MG	CA	1795	1/1	0.10	-	87,87,87,87	0
54	MG	DA	3308	1/1	0.20	-	78,78,78,78	0
54	MG	BB	205	1/1	0.36	-	91,91,91,91	0
54	MG	BA	3170	1/1	0.18	-	57,57,57,57	0
54	MG	BA	3155	1/1	0.42	-	55,55,55,55	0
54	MG	CA	1793	1/1	0.39	-	82,82,82,82	0
54	MG	BA	3027	1/1	0.28	-	53,53,53,53	0
54	MG	DA	3311	1/1	0.45	-	74,74,74,74	0
54	MG	BA	3498	1/1	0.33	-	94,94,94,94	0
54	MG	CA	1744	1/1	0.11	-	70,70,70,70	0
54	MG	CA	1639	1/1	0.21	-	95,95,95,95	0
54	MG	BA	3139	1/1	0.45	-	48,48,48,48	0
54	MG	BA	3226	1/1	0.13	-	64,64,64,64	0
54	MG	BA	3258	1/1	0.39	-	74,74,74,74	0
54	MG	AA	1654	1/1	0.27	-	99,99,99,99	0
54	MG	AA	1755	1/1	0.21	-	88,88,88,88	0
54	MG	BA	3312	1/1	0.53	-	84,84,84,84	0
54	MG	CA	1663	1/1	0.16	-	90,90,90,90	0
54	MG	BA	3443	1/1	0.09	-	116,116,116,116	0
54	MG	BA	3413	1/1	0.18	-	87,87,87,87	0
54	MG	BA	3537	1/1	0.12	-	65,65,65,65	0
54	MG	BA	3429	1/1	0.56	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3383	1/1	0.38	-	87,87,87,87	0
54	MG	DA	3322	1/1	0.27	-	104,104,104,104	0
54	MG	DU	201	1/1	0.23	-	89,89,89,89	0
54	MG	BA	3341	1/1	0.21	-	67,67,67,67	0
54	MG	DA	3293	1/1	0.38	-	72,72,72,72	0
54	MG	DA	3479	1/1	0.17	-	68,68,68,68	0
54	MG	AH	201	1/1	0.22	-	91,91,91,91	0
54	MG	BA	3587	1/1	0.16	-	88,88,88,88	0
54	MG	BA	3268	1/1	0.36	-	86,86,86,86	0
54	MG	DA	3350	1/1	0.40	-	85,85,85,85	0
54	MG	B3	102	1/1	0.15	-	80,80,80,80	0
54	MG	AA	1677	1/1	0.43	-	109,109,109,109	0
54	MG	AA	1679	1/1	0.35	-	86,86,86,86	0
54	MG	CA	1677	1/1	0.32	-	73,73,73,73	0
54	MG	CA	1773	1/1	0.29	-	113,113,113,113	0
54	MG	BA	3471	1/1	0.43	-	78,78,78,78	0
54	MG	BA	3398	1/1	0.30	-	78,78,78,78	0
54	MG	BA	3153	1/1	0.20	-	76,76,76,76	0
54	MG	BA	3252	1/1	0.49	-	63,63,63,63	0
54	MG	AA	1607	1/1	0.17	-	89,89,89,89	0
54	MG	BA	3469	1/1	0.31	-	94,94,94,94	0
54	MG	DA	3221	1/1	0.33	-	74,74,74,74	0
54	MG	BA	3135	1/1	0.41	-	85,85,85,85	0
54	MG	CA	1674	1/1	0.24	-	87,87,87,87	0
54	MG	BA	3265	1/1	0.57	-	82,82,82,82	0
56	ZN	AQ	102	1/1	0.09	-	138,138,138,138	0
54	MG	BA	3059	1/1	0.30	-	78,78,78,78	0
54	MG	DA	3326	1/1	0.27	-	82,82,82,82	0
54	MG	BA	3379	1/1	0.23	-	101,101,101,101	0
54	MG	BA	3102	1/1	0.29	-	80,80,80,80	0
54	MG	DA	3517	1/1	0.37	-	80,80,80,80	0
54	MG	CA	1794	1/1	0.18	-	112,112,112,112	0
54	MG	DA	3056	1/1	0.24	-	97,97,97,97	0
54	MG	AA	1828	1/1	0.26	-	107,107,107,107	0
54	MG	BA	3333	1/1	0.17	-	83,83,83,83	0
54	MG	DA	3110	1/1	0.33	-	60,60,60,60	0
54	MG	BA	3040	1/1	0.36	-	58,58,58,58	0
54	MG	AA	1636	1/1	0.29	-	76,76,76,76	0
54	MG	AA	1668	1/1	0.40	-	81,81,81,81	0
54	MG	BA	3465	1/1	0.24	-	79,79,79,79	0
54	MG	DA	3081	1/1	0.28	-	91,91,91,91	0
54	MG	AA	1825	1/1	0.16	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3237	1/1	0.34	-	52,52,52,52	0
54	MG	BA	3337	1/1	0.42	-	64,64,64,64	0
54	MG	BA	3402	1/1	0.24	-	83,83,83,83	0
54	MG	B7	102	1/1	0.29	-	78,78,78,78	0
54	MG	BA	3077	1/1	0.33	-	82,82,82,82	0
54	MG	BA	3362	1/1	0.34	-	83,83,83,83	0
54	MG	DA	3523	1/1	0.13	-	90,90,90,90	0
54	MG	CA	1672	1/1	0.26	-	79,79,79,79	0
54	MG	DA	3434	1/1	0.21	-	92,92,92,92	0
54	MG	CA	1767	1/1	0.36	-	80,80,80,80	0
54	MG	BA	3480	1/1	0.36	-	75,75,75,75	0
54	MG	BA	3221	1/1	0.32	-	93,93,93,93	0
54	MG	CA	1622	1/1	0.41	-	113,113,113,113	0
54	MG	AA	1835	1/1	0.34	-	100,100,100,100	0
54	MG	BA	3321	1/1	0.49	-	100,100,100,100	0
54	MG	DA	3014	1/1	0.32	-	67,67,67,67	0
54	MG	BA	3037	1/1	0.17	-	68,68,68,68	0
54	MG	BB	210	1/1	0.43	-	76,76,76,76	0
54	MG	CA	1685	1/1	0.20	-	82,82,82,82	0
54	MG	DA	3323	1/1	0.15	-	84,84,84,84	0
54	MG	DA	3426	1/1	0.18	-	95,95,95,95	0
54	MG	DA	3439	1/1	0.15	-	95,95,95,95	0
54	MG	BA	3358	1/1	0.39	-	82,82,82,82	0
54	MG	CA	1603	1/1	0.40	-	115,115,115,115	0
54	MG	AA	1683	1/1	0.31	-	97,97,97,97	0
54	MG	BA	3260	1/1	0.37	-	62,62,62,62	0
54	MG	DA	3128	1/1	0.30	-	56,56,56,56	0
54	MG	BA	3522	1/1	0.48	-	100,100,100,100	0
54	MG	DA	3499	1/1	0.15	-	92,92,92,92	0
54	MG	DB	214	1/1	0.12	-	101,101,101,101	0
54	MG	BA	3154	1/1	0.37	-	59,59,59,59	0
54	MG	AA	1657	1/1	0.38	-	58,58,58,58	0
54	MG	DA	3131	1/1	0.22	-	77,77,77,77	0
54	MG	CA	1654	1/1	0.24	-	107,107,107,107	0
54	MG	BA	3303	1/1	0.31	-	69,69,69,69	0
54	MG	CA	1662	1/1	0.11	-	110,110,110,110	0
54	MG	CA	1745	1/1	0.37	-	102,102,102,102	0
54	MG	BA	3441	1/1	0.20	-	95,95,95,95	0
54	MG	BA	3394	1/1	0.22	-	102,102,102,102	0
54	MG	AA	1656	1/1	0.34	-	73,73,73,73	0
54	MG	BA	3414	1/1	0.88	-	102,102,102,102	0
54	MG	DA	3380	1/1	0.14	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3486	1/1	0.38	-	73,73,73,73	0
54	MG	BA	3158	1/1	0.19	-	79,79,79,79	0
54	MG	BA	3025	1/1	0.34	-	61,61,61,61	0
54	MG	CA	1740	1/1	0.19	-	103,103,103,103	0
54	MG	BA	3600	1/1	0.26	-	65,65,65,65	0
54	MG	BA	3209	1/1	0.37	-	64,64,64,64	0
54	MG	DA	3042	1/1	0.21	-	78,78,78,78	0
54	MG	BA	3397	1/1	0.34	-	84,84,84,84	0
54	MG	BA	3322	1/1	0.26	-	76,76,76,76	0
54	MG	CA	1752	1/1	0.12	-	94,94,94,94	0
54	MG	BA	3243	1/1	0.39	-	63,63,63,63	0
54	MG	DA	3294	1/1	0.25	-	77,77,77,77	0
54	MG	DA	3353	1/1	0.28	-	83,83,83,83	0
54	MG	AA	1713	1/1	0.45	-	82,82,82,82	0
54	MG	BU	201	1/1	0.12	-	95,95,95,95	0
54	MG	CA	1797	1/1	0.41	-	101,101,101,101	0
54	MG	CA	1643	1/1	0.25	-	86,86,86,86	0
54	MG	BA	3496	1/1	0.40	-	97,97,97,97	0
54	MG	CA	1696	1/1	0.12	-	121,121,121,121	0
54	MG	BA	3512	1/1	0.14	-	87,87,87,87	0
54	MG	DA	3478	1/1	0.41	-	63,63,63,63	0
54	MG	BA	3363	1/1	0.34	-	79,79,79,79	0
54	MG	BA	3047	1/1	0.35	-	77,77,77,77	0
54	MG	BA	3615	1/1	0.14	-	83,83,83,83	0
54	MG	DA	3369	1/1	0.31	-	91,91,91,91	0
54	MG	AA	1637	1/1	0.34	-	122,122,122,122	0
54	MG	DA	3226	1/1	0.28	-	75,75,75,75	0
54	MG	DA	3111	1/1	0.36	-	105,105,105,105	0
54	MG	BA	3554	1/1	0.23	-	94,94,94,94	0
54	MG	DA	3429	1/1	0.28	-	103,103,103,103	0
54	MG	BA	3163	1/1	0.31	-	94,94,94,94	0
54	MG	DA	3086	1/1	0.26	-	109,109,109,109	0
54	MG	DA	3475	1/1	0.34	-	66,66,66,66	0
54	MG	AA	1618	1/1	0.26	-	82,82,82,82	0
54	MG	BA	3222	1/1	0.28	-	62,62,62,62	0
54	MG	DA	3177	1/1	0.33	-	65,65,65,65	0
54	MG	DA	3007	1/1	0.38	-	76,76,76,76	0
54	MG	BA	3183	1/1	0.36	-	75,75,75,75	0
54	MG	AA	1794	1/1	0.51	-	93,93,93,93	0
54	MG	AA	1628	1/1	0.37	-	96,96,96,96	0
54	MG	BA	3092	1/1	0.36	-	72,72,72,72	0
54	MG	D5	101	1/1	0.12	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1791	1/1	0.15	-	95,95,95,95	0
54	MG	BA	3276	1/1	0.47	-	91,91,91,91	0
54	MG	BA	3198	1/1	0.42	-	71,71,71,71	0
54	MG	BA	3608	1/1	0.21	-	89,89,89,89	0
54	MG	DA	3218	1/1	0.40	-	56,56,56,56	0
54	MG	BA	3566	1/1	0.44	-	70,70,70,70	0
54	MG	BA	3184	1/1	0.30	-	66,66,66,66	0
54	MG	DA	3245	1/1	0.35	-	76,76,76,76	0
54	MG	BA	3349	1/1	0.14	-	64,64,64,64	0
54	MG	BA	3543	1/1	0.21	-	98,98,98,98	0
54	MG	AA	1673	1/1	0.14	-	131,131,131,131	0
54	MG	DA	3219	1/1	0.35	-	70,70,70,70	0
54	MG	DA	3234	1/1	0.11	-	94,94,94,94	0
54	MG	DA	3181	1/1	0.29	-	78,78,78,78	0
54	MG	BA	3083	1/1	0.24	-	68,68,68,68	0
54	MG	DA	3440	1/1	0.13	-	86,86,86,86	0
54	MG	DA	3453	1/1	0.45	-	92,92,92,92	0
54	MG	DA	3272	1/1	0.18	-	65,65,65,65	0
54	MG	BA	3085	1/1	0.35	-	75,75,75,75	0
54	MG	DA	3155	1/1	0.22	-	74,74,74,74	0
54	MG	CA	1652	1/1	0.30	-	106,106,106,106	0
54	MG	BA	3483	1/1	0.30	-	105,105,105,105	0
54	MG	DA	3486	1/1	0.14	-	78,78,78,78	0
54	MG	BA	3199	1/1	0.38	-	80,80,80,80	0
54	MG	DA	3522	1/1	0.23	-	81,81,81,81	0
54	MG	DA	3352	1/1	0.14	-	71,71,71,71	0
54	MG	BA	3416	1/1	0.17	-	92,92,92,92	0
54	MG	AA	1613	1/1	0.33	-	97,97,97,97	0
54	MG	BA	3125	1/1	0.29	-	75,75,75,75	0
54	MG	DA	3508	1/1	0.38	-	65,65,65,65	0
54	MG	DA	3292	1/1	0.29	-	78,78,78,78	0
54	MG	BA	3160	1/1	0.45	-	92,92,92,92	0
54	MG	AA	1638	1/1	0.19	-	109,109,109,109	0
54	MG	DA	3409	1/1	0.31	-	95,95,95,95	0
54	MG	CA	1719	1/1	0.13	-	104,104,104,104	0
54	MG	BA	3293	1/1	0.21	-	89,89,89,89	0
54	MG	CA	1687	1/1	0.21	-	84,84,84,84	0
54	MG	CA	1682	1/1	0.28	-	94,94,94,94	0
54	MG	DA	3180	1/1	0.35	-	68,68,68,68	0
54	MG	BA	3041	1/1	0.48	-	66,66,66,66	0
54	MG	DA	3141	1/1	0.33	-	88,88,88,88	0
54	MG	DA	3501	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
54	MG	DA	3233	1/1	0.14	-	75,75,75,75	0
54	MG	BA	3017	1/1	0.32	-	53,53,53,53	0
54	MG	BA	3458	1/1	0.50	-	78,78,78,78	0
54	MG	CA	1676	1/1	0.20	-	90,90,90,90	0
54	MG	AA	1820	1/1	0.07	-	112,112,112,112	0
54	MG	AA	1682	1/1	0.33	-	103,103,103,103	0
54	MG	DA	3306	1/1	0.15	-	88,88,88,88	0
54	MG	DA	3188	1/1	0.18	-	82,82,82,82	0
54	MG	BA	3318	1/1	0.39	-	71,71,71,71	0
54	MG	AA	1782	1/1	0.44	-	124,124,124,124	0
54	MG	DA	3260	1/1	0.41	-	72,72,72,72	0
54	MG	BA	3216	1/1	0.31	-	62,62,62,62	0
54	MG	DA	3405	1/1	0.12	-	153,153,153,153	0
54	MG	DA	3331	1/1	0.28	-	79,79,79,79	0
54	MG	DA	3448	1/1	0.45	-	89,89,89,89	0
54	MG	AT	201	1/1	0.10	-	87,87,87,87	0
54	MG	AA	1813	1/1	0.22	-	88,88,88,88	0
54	MG	CA	1669	1/1	0.31	-	81,81,81,81	0
54	MG	BA	3385	1/1	0.41	-	79,79,79,79	0
54	MG	DA	3016	1/1	0.19	-	74,74,74,74	0
54	MG	BA	3114	1/1	0.16	-	98,98,98,98	0
54	MG	BA	3087	1/1	0.22	-	72,72,72,72	0
54	MG	BA	3211	1/1	0.22	-	48,48,48,48	0
54	MG	DA	3246	1/1	0.30	-	89,89,89,89	0
54	MG	AA	1687	1/1	0.14	-	137,137,137,137	0
54	MG	BA	3551	1/1	0.19	-	93,93,93,93	0
54	MG	BA	3371	1/1	0.33	-	77,77,77,77	0
54	MG	DE	303	1/1	0.12	-	85,85,85,85	0
54	MG	AA	1773	1/1	0.47	-	125,125,125,125	0
54	MG	BA	3065	1/1	0.48	-	68,68,68,68	0
54	MG	DA	3235	1/1	0.31	-	74,74,74,74	0
54	MG	BA	3580	1/1	0.43	-	68,68,68,68	0
54	MG	DA	3386	1/1	0.27	-	71,71,71,71	0
54	MG	BA	3586	1/1	0.40	-	71,71,71,71	0
54	MG	DA	3471	1/1	0.31	-	51,51,51,51	0
54	MG	CA	1659	1/1	0.21	-	92,92,92,92	0
54	MG	BA	3473	1/1	0.54	-	84,84,84,84	0
54	MG	BA	3290	1/1	0.19	-	82,82,82,82	0
54	MG	BB	204	1/1	0.41	-	87,87,87,87	0
54	MG	BA	3542	1/1	0.24	-	77,77,77,77	0
54	MG	DA	3266	1/1	0.15	-	87,87,87,87	0
54	MG	DA	3157	1/1	0.29	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3602	1/1	0.28	-	71,71,71,71	0
54	MG	BB	211	1/1	0.33	-	99,99,99,99	0
54	MG	DA	3151	1/1	0.17	-	106,106,106,106	0
54	MG	DA	3410	1/1	0.15	-	67,67,67,67	0
54	MG	BA	3086	1/1	0.52	-	73,73,73,73	0
54	MG	CA	1701	1/1	0.29	-	90,90,90,90	0
54	MG	DA	3425	1/1	0.16	-	82,82,82,82	0
54	MG	DA	3454	1/1	0.33	-	90,90,90,90	0
54	MG	BA	3446	1/1	0.51	-	94,94,94,94	0
54	MG	BA	3626	1/1	0.22	-	87,87,87,87	0
54	MG	DA	3116	1/1	0.24	-	60,60,60,60	0
54	MG	BA	3383	1/1	0.22	-	86,86,86,86	0
54	MG	CA	1681	1/1	0.32	-	88,88,88,88	0
54	MG	DA	3415	1/1	0.24	-	92,92,92,92	0
54	MG	DA	3175	1/1	0.20	-	71,71,71,71	0
54	MG	BA	3549	1/1	0.11	-	74,74,74,74	0
54	MG	BA	3120	1/1	0.15	-	76,76,76,76	0
54	MG	BA	3014	1/1	0.36	-	49,49,49,49	0
54	MG	DA	3055	1/1	0.21	-	51,51,51,51	0
54	MG	AA	1614	1/1	0.19	-	132,132,132,132	0
54	MG	AA	1812	1/1	0.51	-	99,99,99,99	0
54	MG	DA	3027	1/1	0.14	-	93,93,93,93	0
54	MG	BA	3423	1/1	0.41	-	100,100,100,100	0
54	MG	AA	1771	1/1	0.20	-	94,94,94,94	0
54	MG	DA	3190	1/1	0.30	-	67,67,67,67	0
54	MG	DA	3457	1/1	0.20	-	84,84,84,84	0
54	MG	BA	3157	1/1	0.22	-	72,72,72,72	0
54	MG	DA	3519	1/1	0.12	-	81,81,81,81	0
54	MG	DA	3314	1/1	0.28	-	91,91,91,91	0
54	MG	CC	104	1/1	0.21	-	103,103,103,103	0
54	MG	AA	1818	1/1	0.58	-	121,121,121,121	0
54	MG	AA	1764	1/1	0.39	-	111,111,111,111	0
54	MG	AA	1752	1/1	0.19	-	134,134,134,134	0
54	MG	DA	3496	1/1	0.17	-	86,86,86,86	0
54	MG	BA	3593	1/1	0.28	-	78,78,78,78	0
54	MG	AA	1616	1/1	0.34	-	81,81,81,81	0
54	MG	DA	3146	1/1	0.13	-	86,86,86,86	0
54	MG	AA	1714	1/1	0.26	-	88,88,88,88	0
54	MG	BA	3627	1/1	0.34	-	69,69,69,69	0
54	MG	DA	3127	1/1	0.09	-	91,91,91,91	0
54	MG	BA	3536	1/1	0.27	-	74,74,74,74	0
54	MG	AA	1631	1/1	0.29	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3215	1/1	0.32	-	68,68,68,68	0
54	MG	DA	3359	1/1	0.44	-	91,91,91,91	0
54	MG	DA	3390	1/1	0.20	-	76,76,76,76	0
54	MG	DB	209	1/1	0.15	-	97,97,97,97	0
54	MG	CA	1755	1/1	0.26	-	104,104,104,104	0
54	MG	BA	3629	1/1	0.30	-	100,100,100,100	0
54	MG	AA	1799	1/1	0.52	-	111,111,111,111	0
54	MG	BA	3173	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3447	1/1	0.12	-	80,80,80,80	0
54	MG	BA	3281	1/1	0.38	-	72,72,72,72	0
54	MG	BA	3018	1/1	0.36	-	55,55,55,55	0
54	MG	AA	1814	1/1	0.14	-	91,91,91,91	0
54	MG	CA	1785	1/1	0.49	-	101,101,101,101	0
54	MG	DA	3388	1/1	0.28	-	78,78,78,78	0
54	MG	BA	3248	1/1	0.22	-	76,76,76,76	0
54	MG	AA	1765	1/1	0.40	-	122,122,122,122	0
54	MG	BA	3491	1/1	0.11	-	84,84,84,84	0
54	MG	BA	3330	1/1	0.51	-	91,91,91,91	0
54	MG	BA	3361	1/1	0.26	-	76,76,76,76	0
54	MG	AA	1689	1/1	0.35	-	73,73,73,73	0
54	MG	BB	202	1/1	0.22	-	101,101,101,101	0
54	MG	AA	1725	1/1	0.17	-	105,105,105,105	0
54	MG	DA	3451	1/1	0.33	-	81,81,81,81	0
54	MG	DA	3264	1/1	0.16	-	68,68,68,68	0
54	MG	BA	3556	1/1	0.38	-	49,49,49,49	0
54	MG	DA	3493	1/1	0.12	-	90,90,90,90	0
54	MG	CA	1783	1/1	0.27	-	80,80,80,80	0
54	MG	DA	3469	1/1	0.37	-	50,50,50,50	0
54	MG	BA	3518	1/1	0.56	-	87,87,87,87	0
54	MG	DA	3001	1/1	0.36	-	77,77,77,77	0
54	MG	AA	1757	1/1	0.15	-	102,102,102,102	0
54	MG	BA	3538	1/1	0.15	-	76,76,76,76	0
54	MG	BA	3507	1/1	0.33	-	79,79,79,79	0
54	MG	BA	3545	1/1	0.23	-	76,76,76,76	0
54	MG	BA	3012	1/1	0.30	-	66,66,66,66	0
54	MG	DA	3148	1/1	0.19	-	86,86,86,86	0
54	MG	AA	1634	1/1	0.24	-	97,97,97,97	0
54	MG	BA	3100	1/1	0.24	-	105,105,105,105	0
54	MG	BB	201	1/1	0.34	-	77,77,77,77	0
54	MG	AA	1642	1/1	0.30	-	88,88,88,88	0
54	MG	AA	1776	1/1	0.31	-	102,102,102,102	0
54	MG	BA	3253	1/1	0.30	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3356	1/1	0.56	-	81,81,81,81	0
54	MG	AA	1611	1/1	0.13	-	118,118,118,118	0
54	MG	BA	3485	1/1	0.20	-	79,79,79,79	0
54	MG	BA	3479	1/1	0.38	-	80,80,80,80	0
54	MG	BA	3336	1/1	0.20	-	72,72,72,72	0
54	MG	DA	3189	1/1	0.38	-	56,56,56,56	0
54	MG	BA	3449	1/1	0.35	-	70,70,70,70	0
54	MG	BE	304	1/1	0.09	-	90,90,90,90	0
54	MG	DA	3269	1/1	0.36	-	97,97,97,97	0
54	MG	DA	3483	1/1	0.29	-	79,79,79,79	0
54	MG	DA	3443	1/1	0.13	-	85,85,85,85	0
54	MG	BA	3097	1/1	0.51	-	69,69,69,69	0
54	MG	DA	3399	1/1	0.13	-	103,103,103,103	0
54	MG	AA	1621	1/1	0.27	-	101,101,101,101	0
54	MG	AA	1780	1/1	0.32	-	90,90,90,90	0
54	MG	CA	1780	1/1	0.27	-	74,74,74,74	0
54	MG	DA	3191	1/1	0.33	-	62,62,62,62	0
54	MG	CA	1649	1/1	0.33	-	88,88,88,88	0
54	MG	CA	1650	1/1	0.13	-	93,93,93,93	0
54	MG	AA	1604	1/1	0.10	-	88,88,88,88	0
54	MG	BA	3033	1/1	0.35	-	62,62,62,62	0
54	MG	BA	3206	1/1	0.32	-	89,89,89,89	0
54	MG	BA	3034	1/1	0.41	-	78,78,78,78	0
54	MG	DA	3368	1/1	0.31	-	82,82,82,82	0
54	MG	AA	1817	1/1	0.14	-	137,137,137,137	0
54	MG	DA	3384	1/1	0.35	-	81,81,81,81	0
54	MG	BA	3508	1/1	0.19	-	83,83,83,83	0
54	MG	CA	1726	1/1	0.30	-	82,82,82,82	0
54	MG	BA	3068	1/1	0.34	-	94,94,94,94	0
54	MG	BA	3447	1/1	0.29	-	83,83,83,83	0
54	MG	BF	302	1/1	0.19	-	71,71,71,71	0
54	MG	BA	3407	1/1	0.49	-	85,85,85,85	0
54	MG	BA	3215	1/1	0.45	-	74,74,74,74	0
54	MG	BA	3190	1/1	0.28	-	75,75,75,75	0
54	MG	BA	3348	1/1	0.06	-	140,140,140,140	0
54	MG	BA	3533	1/1	0.23	-	89,89,89,89	0
54	MG	DA	3124	1/1	0.26	-	71,71,71,71	0
54	MG	AA	1639	1/1	0.33	-	88,88,88,88	0
54	MG	DA	3422	1/1	0.18	-	83,83,83,83	0
54	MG	BA	3411	1/1	0.28	-	80,80,80,80	0
54	MG	BA	3583	1/1	0.20	-	88,88,88,88	0
54	MG	AA	1652	1/1	0.38	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1623	1/1	0.07	-	142,142,142,142	0
54	MG	CA	1671	1/1	0.15	-	77,77,77,77	0
54	MG	CA	1798	1/1	0.25	-	115,115,115,115	0
54	MG	CA	1675	1/1	0.16	-	96,96,96,96	0
54	MG	AA	1688	1/1	0.41	-	118,118,118,118	0
54	MG	AA	1633	1/1	0.29	-	90,90,90,90	0
54	MG	DA	3216	1/1	0.17	-	78,78,78,78	0
54	MG	BA	3201	1/1	0.30	-	66,66,66,66	0
54	MG	BA	3140	1/1	0.42	-	47,47,47,47	0
54	MG	BA	3502	1/1	0.24	-	113,113,113,113	0
54	MG	BA	3075	1/1	0.31	-	82,82,82,82	0
54	MG	BA	3408	1/1	0.37	-	79,79,79,79	0
54	MG	BA	3387	1/1	0.31	-	90,90,90,90	0
54	MG	BA	3038	1/1	0.31	-	53,53,53,53	0
54	MG	BA	3450	1/1	0.12	-	166,166,166,166	0
54	MG	BA	3247	1/1	0.36	-	59,59,59,59	0
54	MG	AC	103	1/1	0.35	-	83,83,83,83	0
54	MG	DA	3011	1/1	0.16	-	103,103,103,103	0
54	MG	BA	3118	1/1	0.52	-	83,83,83,83	0
54	MG	DA	3225	1/1	0.34	-	57,57,57,57	0
54	MG	BA	3011	1/1	0.37	-	49,49,49,49	0
54	MG	BB	213	1/1	0.26	-	103,103,103,103	0
54	MG	DA	3316	1/1	0.24	-	76,76,76,76	0
54	MG	CA	1602	1/1	0.19	-	91,91,91,91	0
54	MG	DA	3179	1/1	0.26	-	73,73,73,73	0
54	MG	AA	1733	1/1	0.15	-	88,88,88,88	0
54	MG	DA	3030	1/1	0.09	-	64,64,64,64	0
54	MG	CA	1657	1/1	0.22	-	114,114,114,114	0
54	MG	DA	3267	1/1	0.29	-	78,78,78,78	0
54	MG	AA	1624	1/1	0.12	-	92,92,92,92	0
54	MG	AA	1710	1/1	0.14	-	118,118,118,118	0
54	MG	BA	3171	1/1	0.53	-	92,92,92,92	0
54	MG	BA	3263	1/1	0.24	-	73,73,73,73	0
54	MG	BA	3544	1/1	0.27	-	83,83,83,83	0
54	MG	AA	1824	1/1	0.20	-	93,93,93,93	0
54	MG	BA	3136	1/1	0.21	-	60,60,60,60	0
54	MG	BA	3123	1/1	0.43	-	74,74,74,74	0
54	MG	BA	3461	1/1	0.27	-	73,73,73,73	0
54	MG	BA	3049	1/1	0.21	-	59,59,59,59	0
54	MG	DA	3100	1/1	0.38	-	64,64,64,64	0
54	MG	DA	3158	1/1	0.36	-	71,71,71,71	0
54	MG	DA	3229	1/1	0.35	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3476	1/1	0.25	-	71,71,71,71	0
54	MG	BA	3161	1/1	0.39	-	70,70,70,70	0
54	MG	CA	1723	1/1	0.41	-	82,82,82,82	0
54	MG	DA	3024	1/1	0.18	-	110,110,110,110	0
54	MG	DB	208	1/1	0.26	-	94,94,94,94	0
54	MG	DA	3277	1/1	0.41	-	76,76,76,76	0
54	MG	DA	3339	1/1	0.08	-	76,76,76,76	0
54	MG	CA	1731	1/1	0.21	-	70,70,70,70	0
54	MG	BA	3002	1/1	0.34	-	58,58,58,58	0
54	MG	BA	3366	1/1	0.36	-	65,65,65,65	0
54	MG	DA	3498	1/1	0.10	-	71,71,71,71	0
54	MG	DA	3300	1/1	0.28	-	83,83,83,83	0
54	MG	DA	3455	1/1	0.44	-	80,80,80,80	0
54	MG	DA	3364	1/1	0.12	-	102,102,102,102	0
54	MG	DA	3258	1/1	0.37	-	86,86,86,86	0
54	MG	BA	3616	1/1	0.22	-	73,73,73,73	0
54	MG	BA	3434	1/1	0.16	-	86,86,86,86	0
54	MG	CA	1712	1/1	0.19	-	99,99,99,99	0
54	MG	AA	1739	1/1	0.13	-	191,191,191,191	0
54	MG	DA	3121	1/1	0.36	-	109,109,109,109	0
54	MG	BB	214	1/1	0.20	-	99,99,99,99	0
54	MG	AA	1662	1/1	0.16	-	71,71,71,71	0
54	MG	CA	1615	1/1	0.32	-	113,113,113,113	0
54	MG	BE	301	1/1	0.32	-	59,59,59,59	0
54	MG	DA	3375	1/1	0.13	-	96,96,96,96	0
54	MG	BA	3227	1/1	0.17	-	101,101,101,101	0
54	MG	BA	3573	1/1	0.21	-	87,87,87,87	0
54	MG	BA	3604	1/1	0.32	-	92,92,92,92	0
54	MG	BA	3482	1/1	0.41	-	84,84,84,84	0
54	MG	DA	3172	1/1	0.37	-	66,66,66,66	0
54	MG	DA	3403	1/1	0.12	-	62,62,62,62	0
54	MG	DA	3065	1/1	0.37	-	82,82,82,82	0
54	MG	AA	1732	1/1	0.13	-	104,104,104,104	0
54	MG	BA	3535	1/1	0.24	-	79,79,79,79	0
54	MG	DA	3022	1/1	0.23	-	61,61,61,61	0
54	MG	BA	3053	1/1	0.27	-	90,90,90,90	0
54	MG	AA	1617	1/1	0.26	-	97,97,97,97	0
54	MG	BA	3031	1/1	0.31	-	58,58,58,58	0
54	MG	DA	3135	1/1	0.16	-	79,79,79,79	0
54	MG	DA	3468	1/1	0.42	-	47,47,47,47	0
54	MG	CA	1788	1/1	0.27	-	91,91,91,91	0
54	MG	DA	3474	1/1	0.21	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1671	1/1	0.42	-	81,81,81,81	0
54	MG	AA	1717	1/1	0.28	-	87,87,87,87	0
54	MG	BA	3332	1/1	0.36	-	92,92,92,92	0
54	MG	DA	3436	1/1	0.36	-	92,92,92,92	0
54	MG	AA	1795	1/1	0.34	-	86,86,86,86	0
54	MG	BA	3028	1/1	0.38	-	59,59,59,59	0
54	MG	BA	3009	1/1	0.16	-	66,66,66,66	0
54	MG	DA	3038	1/1	0.16	-	119,119,119,119	0
54	MG	AA	1830	1/1	0.11	-	89,89,89,89	0
54	MG	BA	3611	1/1	0.23	-	55,55,55,55	0
54	MG	BA	3228	1/1	0.19	-	62,62,62,62	0
54	MG	BA	3334	1/1	0.22	-	84,84,84,84	0
54	MG	DA	3162	1/1	0.11	-	81,81,81,81	0
54	MG	AC	106	1/1	0.28	-	104,104,104,104	0
54	MG	CA	1630	1/1	0.10	-	91,91,91,91	0
54	MG	AA	1784	1/1	0.14	-	82,82,82,82	0
54	MG	DA	3263	1/1	0.41	-	62,62,62,62	0
54	MG	AA	1704	1/1	0.32	-	88,88,88,88	0
54	MG	CA	1689	1/1	0.18	-	98,98,98,98	0
54	MG	DA	3420	1/1	0.24	-	84,84,84,84	0
54	MG	CA	1697	1/1	0.36	-	95,95,95,95	0
54	MG	BA	3374	1/1	0.36	-	74,74,74,74	0
54	MG	CA	1760	1/1	0.37	-	109,109,109,109	0
54	MG	DA	3173	1/1	0.29	-	53,53,53,53	0
54	MG	DA	3088	1/1	0.31	-	110,110,110,110	0
54	MG	DA	3489	1/1	0.13	-	79,79,79,79	0
54	MG	DA	3224	1/1	0.46	-	49,49,49,49	0
54	MG	DA	3283	1/1	0.16	-	69,69,69,69	0
54	MG	DA	3002	1/1	0.17	-	87,87,87,87	0
54	MG	DA	3412	1/1	0.26	-	89,89,89,89	0
54	MG	AA	1692	1/1	0.22	-	94,94,94,94	0
54	MG	BA	3137	1/1	0.22	-	54,54,54,54	0
54	MG	BD	301	1/1	0.12	-	91,91,91,91	0
54	MG	BA	3571	1/1	0.35	-	45,45,45,45	0
54	MG	DA	3070	1/1	0.31	-	68,68,68,68	0
54	MG	BA	3464	1/1	0.38	-	101,101,101,101	0
54	MG	BA	3459	1/1	0.35	-	78,78,78,78	0
54	MG	AA	1816	1/1	0.41	-	93,93,93,93	0
54	MG	AA	1793	1/1	0.26	-	71,71,71,71	0
54	MG	AA	1701	1/1	0.11	-	96,96,96,96	0
54	MG	BA	3297	1/1	0.30	-	86,86,86,86	0
54	MG	DA	3241	1/1	0.37	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1658	1/1	0.24	-	104,104,104,104	0
54	MG	AA	1629	1/1	0.12	-	134,134,134,134	0
54	MG	BE	303	1/1	0.33	-	89,89,89,89	0
54	MG	BA	3595	1/1	0.20	-	91,91,91,91	0
54	MG	DA	3301	1/1	0.24	-	140,140,140,140	0
54	MG	BA	3231	1/1	0.25	-	89,89,89,89	0
54	MG	AA	1646	1/1	0.40	-	105,105,105,105	0
54	MG	BA	3308	1/1	0.20	-	108,108,108,108	0
54	MG	BA	3189	1/1	0.41	-	52,52,52,52	0
54	MG	BA	3064	1/1	0.29	-	63,63,63,63	0
54	MG	BA	3601	1/1	0.15	-	83,83,83,83	0
54	MG	BA	3208	1/1	0.48	-	67,67,67,67	0
54	MG	BA	3340	1/1	0.24	-	84,84,84,84	0
54	MG	DA	3482	1/1	0.31	-	54,54,54,54	0
54	MG	CA	1782	1/1	0.34	-	93,93,93,93	0
54	MG	BA	3495	1/1	0.17	-	80,80,80,80	0
54	MG	AA	1648	1/1	0.09	-	115,115,115,115	0
54	MG	BA	3177	1/1	0.21	-	87,87,87,87	0
54	MG	DA	3107	1/1	0.17	-	56,56,56,56	0
54	MG	DA	3307	1/1	0.15	-	75,75,75,75	0
54	MG	CA	1709	1/1	0.20	-	97,97,97,97	0
54	MG	DA	3348	1/1	0.27	-	90,90,90,90	0
54	MG	DA	3174	1/1	0.20	-	52,52,52,52	0
54	MG	DA	3026	1/1	0.24	-	76,76,76,76	0
54	MG	BA	3612	1/1	0.21	-	67,67,67,67	0
54	MG	CA	1732	1/1	0.28	-	108,108,108,108	0
54	MG	AA	1690	1/1	0.21	-	131,131,131,131	0
54	MG	DA	3119	1/1	0.29	-	58,58,58,58	0
54	MG	DA	3080	1/1	0.21	-	74,74,74,74	0
54	MG	CX	101	1/1	0.27	-	101,101,101,101	0
54	MG	CC	107	1/1	0.17	-	105,105,105,105	0
54	MG	AA	1703	1/1	0.29	-	61,61,61,61	0
54	MG	AA	1699	1/1	0.12	-	96,96,96,96	0
54	MG	BA	3315	1/1	0.30	-	83,83,83,83	0
54	MG	AA	1696	1/1	0.12	-	80,80,80,80	0
54	MG	DA	3176	1/1	0.37	-	58,58,58,58	0
54	MG	AA	1802	1/1	0.07	-	100,100,100,100	0
54	MG	BA	3582	1/1	0.38	-	78,78,78,78	0
54	MG	DA	3366	1/1	0.30	-	78,78,78,78	0
54	MG	BA	3078	1/1	0.43	-	63,63,63,63	0
54	MG	DA	3298	1/1	0.27	-	73,73,73,73	0
54	MG	DA	3244	1/1	0.32	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1715	1/1	0.41	-	112,112,112,112	0
54	MG	BA	3015	1/1	0.12	-	88,88,88,88	0
54	MG	DA	3328	1/1	0.15	-	98,98,98,98	0
54	MG	BA	3470	1/1	0.25	-	90,90,90,90	0
54	MG	AA	1601	1/1	0.28	-	76,76,76,76	0
54	MG	DA	3414	1/1	0.20	-	92,92,92,92	0
54	MG	DA	3397	1/1	0.43	-	52,52,52,52	0
54	MG	BA	3547	1/1	0.38	-	84,84,84,84	0
54	MG	DA	3358	1/1	0.21	-	113,113,113,113	0
54	MG	AA	1796	1/1	0.44	-	76,76,76,76	0
54	MG	AD	101	1/1	0.26	-	114,114,114,114	0
54	MG	BA	3022	1/1	0.37	-	66,66,66,66	0
54	MG	DA	3389	1/1	0.11	-	82,82,82,82	0
54	MG	CA	1713	1/1	0.21	-	109,109,109,109	0
54	MG	BA	3607	1/1	0.39	-	62,62,62,62	0
54	MG	BA	3437	1/1	0.16	-	81,81,81,81	0
54	MG	CA	1692	1/1	0.32	-	93,93,93,93	0
54	MG	BA	3168	1/1	0.40	-	85,85,85,85	0
54	MG	BB	203	1/1	0.40	-	70,70,70,70	0
54	MG	BA	3481	1/1	0.21	-	79,79,79,79	0
54	MG	BA	3147	1/1	0.36	-	73,73,73,73	0
54	MG	BA	3444	1/1	0.33	-	81,81,81,81	0
54	MG	DA	3147	1/1	0.25	-	79,79,79,79	0
54	MG	DA	3106	1/1	0.24	-	66,66,66,66	0
54	MG	DA	3214	1/1	0.26	-	69,69,69,69	0
54	MG	DA	3401	1/1	0.28	-	93,93,93,93	0
54	MG	BA	3089	1/1	0.36	-	87,87,87,87	0
54	MG	BA	3295	1/1	0.37	-	78,78,78,78	0
54	MG	DA	3373	1/1	0.36	-	107,107,107,107	0
54	MG	BA	3553	1/1	0.32	-	50,50,50,50	0
54	MG	BA	3320	1/1	0.45	-	82,82,82,82	0
54	MG	DA	3082	1/1	0.17	-	97,97,97,97	0
54	MG	BA	3609	1/1	0.24	-	80,80,80,80	0
54	MG	BA	3134	1/1	0.30	-	66,66,66,66	0
54	MG	BA	3391	1/1	0.37	-	85,85,85,85	0
54	MG	BA	3525	1/1	0.32	-	47,47,47,47	0
54	MG	DA	3090	1/1	0.22	-	119,119,119,119	0
54	MG	BA	3375	1/1	0.45	-	99,99,99,99	0
54	MG	BA	3590	1/1	0.15	-	83,83,83,83	0
54	MG	BA	3256	1/1	0.54	-	80,80,80,80	0
54	MG	AA	1603	1/1	0.20	-	89,89,89,89	0
54	MG	BA	3335	1/1	0.27	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3044	1/1	0.27	-	60,60,60,60	0
54	MG	DA	3217	1/1	0.38	-	89,89,89,89	0
54	MG	BA	3250	1/1	0.25	-	61,61,61,61	0
54	MG	BA	3484	1/1	0.31	-	76,76,76,76	0
54	MG	BA	3419	1/1	0.33	-	81,81,81,81	0
54	MG	BA	3494	1/1	0.33	-	72,72,72,72	0
54	MG	DA	3310	1/1	0.37	-	85,85,85,85	0
54	MG	AA	1620	1/1	0.08	-	140,140,140,140	0
54	MG	AA	1664	1/1	0.50	-	81,81,81,81	0
54	MG	AA	1655	1/1	0.45	-	97,97,97,97	0
54	MG	BA	3392	1/1	0.20	-	91,91,91,91	0
54	MG	DE	301	1/1	0.20	-	67,67,67,67	0
54	MG	BA	3338	1/1	0.25	-	77,77,77,77	0
54	MG	DA	3120	1/1	0.20	-	60,60,60,60	0
54	MG	DA	3153	1/1	0.33	-	88,88,88,88	0
54	MG	CA	1742	1/1	0.26	-	90,90,90,90	0
54	MG	DA	3104	1/1	0.15	-	71,71,71,71	0
54	MG	DA	3456	1/1	0.10	-	105,105,105,105	0
54	MG	DA	3494	1/1	0.26	-	72,72,72,72	0
54	MG	DA	3510	1/1	0.13	-	77,77,77,77	0
54	MG	BA	3088	1/1	0.38	-	84,84,84,84	0
54	MG	DA	3342	1/1	0.31	-	90,90,90,90	0
56	ZN	CG	303	1/1	0.26	-	139,139,139,139	0
54	MG	AA	1823	1/1	0.09	-	151,151,151,151	0
54	MG	DA	3182	1/1	0.39	-	74,74,74,74	0
54	MG	BA	3010	1/1	0.33	-	45,45,45,45	0
54	MG	BA	3436	1/1	0.30	-	75,75,75,75	0
54	MG	BB	208	1/1	0.17	-	89,89,89,89	0
54	MG	BO	202	1/1	0.16	-	68,68,68,68	0
54	MG	AC	105	1/1	0.24	-	100,100,100,100	0
54	MG	BA	3020	1/1	0.41	-	49,49,49,49	0
54	MG	DA	3338	1/1	0.48	-	105,105,105,105	0
54	MG	BA	3430	1/1	0.24	-	93,93,93,93	0
54	MG	BA	3030	1/1	0.36	-	70,70,70,70	0
54	MG	BA	3277	1/1	0.26	-	89,89,89,89	0
54	MG	DA	3291	1/1	0.41	-	84,84,84,84	0
54	MG	AN	202	1/1	0.09	-	88,88,88,88	0
54	MG	DA	3417	1/1	0.28	-	81,81,81,81	0
54	MG	DA	3057	1/1	0.31	-	70,70,70,70	0
54	MG	BA	3242	1/1	0.32	-	59,59,59,59	0
54	MG	BA	3440	1/1	0.34	-	73,73,73,73	0
54	MG	CA	1691	1/1	0.32	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3106	1/1	0.52	-	73,73,73,73	0
54	MG	CA	1764	1/1	0.23	-	89,89,89,89	0
54	MG	DA	3066	1/1	0.15	-	80,80,80,80	0
54	MG	DA	3438	1/1	0.25	-	82,82,82,82	0
54	MG	DA	3050	1/1	0.21	-	67,67,67,67	0
54	MG	DA	3433	1/1	0.38	-	91,91,91,91	0
54	MG	DA	3149	1/1	0.28	-	79,79,79,79	0
54	MG	BA	3151	1/1	0.37	-	91,91,91,91	0
54	MG	DA	3039	1/1	0.38	-	80,80,80,80	0
54	MG	AA	1709	1/1	0.25	-	106,106,106,106	0
54	MG	BA	3591	1/1	0.33	-	69,69,69,69	0
54	MG	BA	3218	1/1	0.29	-	90,90,90,90	0
54	MG	DA	3045	1/1	0.34	-	93,93,93,93	0
54	MG	BA	3241	1/1	0.13	-	70,70,70,70	0
54	MG	BA	3056	1/1	0.36	-	109,109,109,109	0
54	MG	BA	3156	1/1	0.37	-	57,57,57,57	0
54	MG	BA	3076	1/1	0.40	-	86,86,86,86	0
54	MG	DA	3118	1/1	0.13	-	57,57,57,57	0
54	MG	BA	3229	1/1	0.41	-	64,64,64,64	0
54	MG	BA	3384	1/1	0.23	-	73,73,73,73	0
54	MG	CA	1610	1/1	0.16	-	97,97,97,97	0
54	MG	BA	3169	1/1	0.13	-	65,65,65,65	0
54	MG	BA	3415	1/1	0.37	-	80,80,80,80	0
54	MG	AA	1606	1/1	0.18	-	101,101,101,101	0
54	MG	BA	3472	1/1	0.35	-	114,114,114,114	0
54	MG	BA	3326	1/1	0.31	-	89,89,89,89	0
54	MG	DA	3329	1/1	0.46	-	88,88,88,88	0
54	MG	BA	3346	1/1	0.19	-	74,74,74,74	0
54	MG	CA	1778	1/1	0.32	-	107,107,107,107	0
54	MG	CC	108	1/1	0.13	-	120,120,120,120	0
54	MG	BA	3207	1/1	0.34	-	78,78,78,78	0
54	MG	BA	3119	1/1	0.32	-	84,84,84,84	0
54	MG	DR	201	1/1	0.14	-	82,82,82,82	0
54	MG	BA	3584	1/1	0.18	-	66,66,66,66	0
54	MG	DA	3512	1/1	0.21	-	63,63,63,63	0
54	MG	AA	1760	1/1	0.23	-	87,87,87,87	0
54	MG	DA	3073	1/1	0.16	-	66,66,66,66	0
54	MG	CA	1668	1/1	0.41	-	61,61,61,61	0
54	MG	DA	3005	1/1	0.40	-	99,99,99,99	0
54	MG	BA	3388	1/1	0.49	-	82,82,82,82	0
54	MG	AA	1625	1/1	0.28	-	83,83,83,83	0
54	MG	DA	3075	1/1	0.30	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3128	1/1	0.09	-	85,85,85,85	0
54	MG	BA	3067	1/1	0.22	-	60,60,60,60	0
54	MG	AA	1804	1/1	0.40	-	81,81,81,81	0
54	MG	BA	3132	1/1	0.14	-	65,65,65,65	0
54	MG	DA	3315	1/1	0.36	-	95,95,95,95	0
54	MG	DA	3432	1/1	0.23	-	102,102,102,102	0
54	MG	CA	1637	1/1	0.10	-	97,97,97,97	0
54	MG	AA	1789	1/1	0.36	-	109,109,109,109	0
54	MG	CA	1631	1/1	0.12	-	102,102,102,102	0
54	MG	BA	3324	1/1	0.27	-	70,70,70,70	0
54	MG	BA	3181	1/1	0.31	-	64,64,64,64	0
54	MG	CA	1750	1/1	0.35	-	97,97,97,97	0
54	MG	BA	3433	1/1	0.14	-	94,94,94,94	0
54	MG	AA	1777	1/1	0.21	-	117,117,117,117	0
54	MG	DA	3431	1/1	0.07	-	81,81,81,81	0
54	MG	DA	3161	1/1	0.18	-	84,84,84,84	0
54	MG	DA	3290	1/1	0.25	-	75,75,75,75	0
54	MG	BA	3005	1/1	0.36	-	59,59,59,59	0
54	MG	DA	3514	1/1	0.23	-	92,92,92,92	0
54	MG	BA	3133	1/1	0.33	-	72,72,72,72	0
54	MG	DA	3095	1/1	0.26	-	88,88,88,88	0
54	MG	CA	1707	1/1	0.30	-	88,88,88,88	0
54	MG	DA	3168	1/1	0.12	-	69,69,69,69	0
54	MG	BA	3296	1/1	0.41	-	81,81,81,81	0
54	MG	CA	1688	1/1	0.28	-	88,88,88,88	0
54	MG	BA	3230	1/1	0.19	-	71,71,71,71	0
54	MG	BA	3504	1/1	0.16	-	90,90,90,90	0
54	MG	CA	1614	1/1	0.22	-	100,100,100,100	0
54	MG	AA	1766	1/1	0.12	-	98,98,98,98	0
54	MG	BA	3294	1/1	0.38	-	75,75,75,75	0
54	MG	DA	3445	1/1	0.08	-	96,96,96,96	0
54	MG	DA	3285	1/1	0.23	-	57,57,57,57	0
54	MG	BA	3501	1/1	0.28	-	90,90,90,90	0
54	MG	CA	1753	1/1	0.24	-	105,105,105,105	0
54	MG	BA	3261	1/1	0.21	-	65,65,65,65	0
54	MG	DA	3248	1/1	0.30	-	93,93,93,93	0
54	MG	BA	3395	1/1	0.38	-	84,84,84,84	0
54	MG	BA	3003	1/1	0.33	-	61,61,61,61	0
54	MG	BA	3054	1/1	0.27	-	100,100,100,100	0
54	MG	BA	3509	1/1	0.26	-	102,102,102,102	0
54	MG	DA	3480	1/1	0.33	-	64,64,64,64	0
54	MG	DA	3395	1/1	0.09	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3023	1/1	0.29	-	45,45,45,45	0
54	MG	DA	3040	1/1	0.26	-	103,103,103,103	0
54	MG	BA	3367	1/1	0.27	-	91,91,91,91	0
54	MG	CA	1625	1/1	0.14	-	115,115,115,115	0
54	MG	DB	210	1/1	0.27	-	95,95,95,95	0
54	MG	BA	3435	1/1	0.19	-	94,94,94,94	0
54	MG	DA	3437	1/1	0.35	-	101,101,101,101	0
54	MG	CA	1698	1/1	0.18	-	96,96,96,96	0
54	MG	CA	1642	1/1	0.13	-	116,116,116,116	0
54	MG	DA	3365	1/1	0.31	-	73,73,73,73	0
54	MG	AA	1645	1/1	0.30	-	81,81,81,81	0
54	MG	AA	1753	1/1	0.17	-	97,97,97,97	0
54	MG	DA	3286	1/1	0.21	-	63,63,63,63	0
54	MG	DA	3281	1/1	0.22	-	92,92,92,92	0
54	MG	AA	1675	1/1	0.40	-	112,112,112,112	0
54	MG	CA	1703	1/1	0.48	-	85,85,85,85	0
54	MG	DA	3284	1/1	0.29	-	76,76,76,76	0
54	MG	BA	3492	1/1	0.18	-	87,87,87,87	0
54	MG	BA	3401	1/1	0.13	-	73,73,73,73	0
54	MG	BA	3270	1/1	0.45	-	91,91,91,91	0
54	MG	AA	1781	1/1	0.12	-	103,103,103,103	0
54	MG	CA	1629	1/1	0.11	-	107,107,107,107	0
54	MG	BA	3280	1/1	0.25	-	106,106,106,106	0
54	MG	CA	1613	1/1	0.33	-	86,86,86,86	0
54	MG	BA	3071	1/1	0.25	-	90,90,90,90	0
54	MG	BA	3405	1/1	0.34	-	72,72,72,72	0
54	MG	DA	3282	1/1	0.37	-	88,88,88,88	0
54	MG	BA	3576	1/1	0.26	-	93,93,93,93	0
54	MG	DA	3097	1/1	0.21	-	89,89,89,89	0
54	MG	AA	1665	1/1	0.41	-	82,82,82,82	0
54	MG	DA	3150	1/1	0.30	-	91,91,91,91	0
54	MG	CA	1694	1/1	0.18	-	91,91,91,91	0
54	MG	DA	3276	1/1	0.24	-	91,91,91,91	0
54	MG	AA	1667	1/1	0.53	-	82,82,82,82	0
54	MG	AA	1722	1/1	0.33	-	96,96,96,96	0
54	MG	AA	1827	1/1	0.13	-	112,112,112,112	0
54	MG	AA	1801	1/1	0.29	-	113,113,113,113	0
54	MG	AA	1819	1/1	0.19	-	92,92,92,92	0
54	MG	DA	3312	1/1	0.31	-	81,81,81,81	0
54	MG	DA	3109	1/1	0.33	-	61,61,61,61	0
54	MG	AQ	101	1/1	0.16	-	94,94,94,94	0
54	MG	AA	1700	1/1	0.20	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3239	1/1	0.29	-	64,64,64,64	0
54	MG	CA	1765	1/1	0.19	-	122,122,122,122	0
54	MG	BA	3378	1/1	0.43	-	80,80,80,80	0
54	MG	DA	3243	1/1	0.31	-	71,71,71,71	0
54	MG	BA	3569	1/1	0.40	-	51,51,51,51	0
54	MG	BA	3109	1/1	0.32	-	89,89,89,89	0
54	MG	CA	1736	1/1	0.12	-	90,90,90,90	0
54	MG	DA	3006	1/1	0.38	-	95,95,95,95	0
54	MG	CA	1656	1/1	0.20	-	127,127,127,127	0
54	MG	DA	3511	1/1	0.30	-	77,77,77,77	0
54	MG	DA	3355	1/1	0.40	-	84,84,84,84	0
54	MG	DA	3204	1/1	0.35	-	71,71,71,71	0
54	MG	BB	206	1/1	0.24	-	84,84,84,84	0
54	MG	DA	3297	1/1	0.40	-	84,84,84,84	0
54	MG	AA	1695	1/1	0.13	-	76,76,76,76	0
54	MG	BA	3497	1/1	0.38	-	72,72,72,72	0
54	MG	AA	1826	1/1	0.17	-	117,117,117,117	0
54	MG	BA	3316	1/1	0.32	-	91,91,91,91	0
54	MG	DA	3321	1/1	0.29	-	78,78,78,78	0
54	MG	AA	1711	1/1	0.13	-	132,132,132,132	0
55	T1C	CA	1800	42/42	0.19	-	101,116,124,127	0
54	MG	BA	3567	1/1	0.30	-	62,62,62,62	0
54	MG	AA	1811	1/1	0.74	-	102,102,102,102	0
54	MG	BA	3266	1/1	0.34	-	72,72,72,72	0
54	MG	BA	3520	1/1	0.18	-	86,86,86,86	0
54	MG	BA	3531	1/1	0.23	-	83,83,83,83	0
54	MG	BA	3421	1/1	0.36	-	73,73,73,73	0
54	MG	BA	3345	1/1	0.32	-	91,91,91,91	0
54	MG	BA	3439	1/1	0.40	-	70,70,70,70	0
54	MG	DA	3137	1/1	0.41	-	86,86,86,86	0
54	MG	AA	1609	1/1	0.33	-	61,61,61,61	0
54	MG	AA	1694	1/1	0.31	-	87,87,87,87	0
54	MG	DA	3491	1/1	0.17	-	71,71,71,71	0
54	MG	DA	3101	1/1	0.35	-	100,100,100,100	0
54	MG	BA	3488	1/1	0.39	-	94,94,94,94	0
54	MG	BA	3376	1/1	0.23	-	84,84,84,84	0
54	MG	DA	3271	1/1	0.18	-	67,67,67,67	0
54	MG	BA	3070	1/1	0.15	-	64,64,64,64	0
54	MG	BA	3577	1/1	0.20	-	72,72,72,72	0
54	MG	CA	1683	1/1	0.39	-	86,86,86,86	0
54	MG	AA	1678	1/1	0.31	-	87,87,87,87	0
54	MG	DA	3166	1/1	0.20	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	AA	1707	1/1	0.12	-	127,127,127,127	0
54	MG	BA	3117	1/1	0.40	-	57,57,57,57	0
54	MG	BA	3409	1/1	0.26	-	73,73,73,73	0
54	MG	DA	3071	1/1	0.13	-	107,107,107,107	0
54	MG	DA	3192	1/1	0.25	-	92,92,92,92	0
54	MG	BA	3073	1/1	0.10	-	73,73,73,73	0
54	MG	AA	1736	1/1	0.28	-	92,92,92,92	0
54	MG	CC	106	1/1	0.14	-	98,98,98,98	0
54	MG	DA	3421	1/1	0.47	-	86,86,86,86	0
54	MG	BA	3124	1/1	0.39	-	85,85,85,85	0
54	MG	AA	1685	1/1	0.31	-	73,73,73,73	0
54	MG	AA	1643	1/1	0.18	-	91,91,91,91	0
54	MG	AA	1747	1/1	0.30	-	88,88,88,88	0
54	MG	DA	3460	1/1	1.07	-	100,100,100,100	0
54	MG	BA	3514	1/1	0.29	-	76,76,76,76	0
54	MG	BA	3463	1/1	0.29	-	84,84,84,84	0
54	MG	BA	3418	1/1	0.43	-	104,104,104,104	0
54	MG	BA	3046	1/1	0.29	-	60,60,60,60	0
54	MG	BA	3004	1/1	0.26	-	72,72,72,72	0
54	MG	BA	3052	1/1	0.56	-	81,81,81,81	0
54	MG	BA	3438	1/1	0.23	-	90,90,90,90	0
54	MG	DA	3085	1/1	0.42	-	89,89,89,89	0
54	MG	DA	3252	1/1	0.25	-	67,67,67,67	0
54	MG	BA	3082	1/1	0.36	-	80,80,80,80	0
54	MG	DA	3261	1/1	0.40	-	97,97,97,97	0
55	T1C	AA	1837	42/42	0.21	-	81,103,111,117	0
54	MG	CA	1634	1/1	0.19	-	87,87,87,87	0
54	MG	AG	301	1/1	0.09	-	122,122,122,122	0
54	MG	DA	3309	1/1	0.15	-	64,64,64,64	0
54	MG	BA	3225	1/1	0.26	-	75,75,75,75	0
54	MG	CA	1720	1/1	0.26	-	86,86,86,86	0
54	MG	DA	3211	1/1	0.27	-	52,52,52,52	0
54	MG	BA	3490	1/1	0.31	-	102,102,102,102	0
54	MG	CA	1718	1/1	0.12	-	100,100,100,100	0
54	MG	DB	205	1/1	0.29	-	84,84,84,84	0
54	MG	AA	1663	1/1	0.16	-	72,72,72,72	0
54	MG	BA	3344	1/1	0.18	-	91,91,91,91	0
54	MG	AA	1748	1/1	0.17	-	152,152,152,152	0
54	MG	AA	1691	1/1	0.12	-	107,107,107,107	0
54	MG	AA	1658	1/1	0.25	-	68,68,68,68	0
54	MG	DA	3032	1/1	0.20	-	79,79,79,79	0
54	MG	BA	3283	1/1	0.38	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3035	1/1	0.06	-	92,92,92,92	0
54	MG	DA	3372	1/1	0.11	-	84,84,84,84	0
54	MG	BA	3035	1/1	0.33	-	52,52,52,52	0
54	MG	AA	1723	1/1	0.23	-	82,82,82,82	0
54	MG	DA	3288	1/1	0.34	-	77,77,77,77	0
54	MG	DU	202	1/1	0.11	-	96,96,96,96	0
54	MG	BA	3630	1/1	0.20	-	93,93,93,93	0
54	MG	CG	301	1/1	0.24	-	113,113,113,113	0
54	MG	DA	3134	1/1	0.14	-	96,96,96,96	0
54	MG	DA	3296	1/1	0.20	-	104,104,104,104	0
54	MG	CA	1601	1/1	0.16	-	95,95,95,95	0
54	MG	BA	3523	1/1	0.45	-	82,82,82,82	0
54	MG	BA	3614	1/1	0.12	-	92,92,92,92	0
54	MG	BA	3558	1/1	0.34	-	58,58,58,58	0
54	MG	BA	3043	1/1	0.37	-	57,57,57,57	0
54	MG	BA	3091	1/1	0.31	-	128,128,128,128	0
54	MG	BA	3292	1/1	0.14	-	78,78,78,78	0
54	MG	DA	3477	1/1	0.12	-	67,67,67,67	0
54	MG	DA	3357	1/1	0.20	-	123,123,123,123	0
54	MG	AA	1615	1/1	0.16	-	114,114,114,114	0
54	MG	DA	3280	1/1	0.26	-	44,44,44,44	0
54	MG	BA	3599	1/1	0.35	-	85,85,85,85	0
54	MG	BA	3058	1/1	0.26	-	68,68,68,68	0
54	MG	BA	3274	1/1	0.21	-	81,81,81,81	0
54	MG	BA	3474	1/1	0.22	-	86,86,86,86	0
54	MG	AA	1605	1/1	0.08	-	103,103,103,103	0
54	MG	BA	3597	1/1	0.31	-	103,103,103,103	0
54	MG	DA	3398	1/1	0.22	-	84,84,84,84	0
54	MG	CS	101	1/1	0.21	-	95,95,95,95	0
54	MG	CA	1786	1/1	0.28	-	83,83,83,83	0
54	MG	AA	1669	1/1	0.40	-	76,76,76,76	0
54	MG	BA	3029	1/1	0.33	-	62,62,62,62	0
54	MG	BA	3145	1/1	0.44	-	61,61,61,61	0
54	MG	AA	1719	1/1	0.20	-	98,98,98,98	0
54	MG	DA	3504	1/1	0.30	-	79,79,79,79	0
54	MG	BA	3313	1/1	0.47	-	94,94,94,94	0
54	MG	BA	3317	1/1	0.29	-	87,87,87,87	0
54	MG	BA	3585	1/1	0.45	-	77,77,77,77	0
54	MG	BA	3249	1/1	0.23	-	74,74,74,74	0
54	MG	BA	3099	1/1	0.16	-	68,68,68,68	0
54	MG	CA	1727	1/1	0.09	-	128,128,128,128	0
54	MG	DA	3152	1/1	0.16	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1706	1/1	0.25	-	90,90,90,90	0
54	MG	DA	3255	1/1	0.31	-	62,62,62,62	0
54	MG	BA	3105	1/1	0.38	-	60,60,60,60	0
54	MG	DA	3509	1/1	0.27	-	64,64,64,64	0
54	MG	DA	3132	1/1	0.27	-	80,80,80,80	0
54	MG	CA	1704	1/1	0.37	-	99,99,99,99	0
54	MG	DA	3337	1/1	0.47	-	80,80,80,80	0
54	MG	AC	104	1/1	0.27	-	100,100,100,100	0
54	MG	BA	3079	1/1	0.33	-	103,103,103,103	0
54	MG	BA	3103	1/1	0.29	-	76,76,76,76	0
54	MG	BA	3069	1/1	0.27	-	68,68,68,68	0
54	MG	BA	3203	1/1	0.33	-	75,75,75,75	0
54	MG	DA	3374	1/1	0.22	-	87,87,87,87	0
54	MG	DA	3209	1/1	0.31	-	61,61,61,61	0
54	MG	BA	3477	1/1	0.27	-	92,92,92,92	0
54	MG	CA	1730	1/1	0.20	-	117,117,117,117	0
54	MG	CA	1754	1/1	0.40	-	108,108,108,108	0
54	MG	BA	3191	1/1	0.25	-	78,78,78,78	0
54	MG	BA	3557	1/1	0.37	-	44,44,44,44	0
54	MG	BA	3060	1/1	0.24	-	92,92,92,92	0
54	MG	DA	3031	1/1	0.20	-	72,72,72,72	0
54	MG	DA	3413	1/1	0.20	-	84,84,84,84	0
54	MG	AA	1833	1/1	0.12	-	98,98,98,98	0
54	MG	AA	1798	1/1	0.43	-	93,93,93,93	0
54	MG	BA	3594	1/1	0.59	-	81,81,81,81	0
54	MG	AA	1834	1/1	0.29	-	86,86,86,86	0
54	MG	BA	3282	1/1	0.45	-	60,60,60,60	0
54	MG	BA	3007	1/1	0.37	-	59,59,59,59	0
54	MG	BA	3339	1/1	0.46	-	85,85,85,85	0
54	MG	DA	3142	1/1	0.31	-	83,83,83,83	0
54	MG	DA	3513	1/1	0.34	-	81,81,81,81	0
54	MG	AN	201	1/1	0.10	-	91,91,91,91	0
54	MG	AA	1779	1/1	0.44	-	78,78,78,78	0
54	MG	DA	3154	1/1	0.17	-	102,102,102,102	0
54	MG	DA	3227	1/1	0.15	-	67,67,67,67	0
54	MG	BA	3096	1/1	0.40	-	56,56,56,56	0
54	MG	BA	3605	1/1	0.31	-	72,72,72,72	0
54	MG	BA	3081	1/1	0.15	-	72,72,72,72	0
54	MG	BA	3164	1/1	0.46	-	83,83,83,83	0
54	MG	DA	3287	1/1	0.18	-	102,102,102,102	0
54	MG	BA	3016	1/1	0.40	-	57,57,57,57	0
54	MG	BA	3166	1/1	0.27	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3578	1/1	0.30	-	73,73,73,73	0
54	MG	BA	3013	1/1	0.27	-	65,65,65,65	0
54	MG	BA	3506	1/1	0.33	-	74,74,74,74	0
54	MG	AA	1681	1/1	0.26	-	101,101,101,101	0
54	MG	BA	3489	1/1	0.21	-	84,84,84,84	0
54	MG	BA	3424	1/1	0.24	-	86,86,86,86	0
54	MG	BA	3390	1/1	0.45	-	95,95,95,95	0
54	MG	AA	1836	1/1	0.18	-	91,91,91,91	0
54	MG	DA	3335	1/1	0.28	-	91,91,91,91	0
54	MG	CA	1673	1/1	0.33	-	74,74,74,74	0
54	MG	BA	3072	1/1	0.34	-	81,81,81,81	0
54	MG	BA	3352	1/1	0.32	-	112,112,112,112	0
54	MG	BA	3347	1/1	0.41	-	86,86,86,86	0
54	MG	CA	1792	1/1	0.19	-	105,105,105,105	0
54	MG	CA	1665	1/1	0.16	-	82,82,82,82	0
54	MG	DA	3130	1/1	0.32	-	52,52,52,52	0
54	MG	CA	1741	1/1	0.20	-	114,114,114,114	0
54	MG	BO	201	1/1	0.20	-	79,79,79,79	0
54	MG	BA	3104	1/1	0.33	-	45,45,45,45	0
54	MG	CA	1737	1/1	0.18	-	93,93,93,93	0
54	MG	CA	1644	1/1	0.27	-	85,85,85,85	0
54	MG	BA	3521	1/1	0.44	-	81,81,81,81	0
54	MG	CA	1667	1/1	0.31	-	70,70,70,70	0
54	MG	DA	3240	1/1	0.16	-	86,86,86,86	0
54	MG	BA	3144	1/1	0.36	-	68,68,68,68	0
54	MG	AA	1702	1/1	0.27	-	80,80,80,80	0
54	MG	AA	1821	1/1	0.26	-	96,96,96,96	0
54	MG	BA	3245	1/1	0.32	-	67,67,67,67	0
54	MG	AA	1674	1/1	0.28	-	93,93,93,93	0
54	MG	DA	3019	1/1	0.16	-	79,79,79,79	0
54	MG	DA	3093	1/1	0.28	-	88,88,88,88	0
54	MG	BA	3146	1/1	0.31	-	75,75,75,75	0
54	MG	BA	3285	1/1	0.39	-	67,67,67,67	0
54	MG	BA	3377	1/1	0.20	-	81,81,81,81	0
54	MG	BA	3176	1/1	0.15	-	73,73,73,73	0
54	MG	BA	3024	1/1	0.34	-	56,56,56,56	0
54	MG	BU	202	1/1	0.19	-	71,71,71,71	0
54	MG	DA	3262	1/1	0.21	-	95,95,95,95	0
54	MG	BA	3516	1/1	0.51	-	90,90,90,90	0
54	MG	CA	1735	1/1	0.30	-	86,86,86,86	0
54	MG	CN	201	1/1	0.07	-	95,95,95,95	0
54	MG	DA	3156	1/1	0.33	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3289	1/1	0.34	-	110,110,110,110	0
54	MG	BA	3364	1/1	0.39	-	78,78,78,78	0
54	MG	BA	3548	1/1	0.38	-	76,76,76,76	0
54	MG	BA	3048	1/1	0.30	-	67,67,67,67	0
54	MG	DE	302	1/1	0.15	-	96,96,96,96	0
54	MG	BA	3131	1/1	0.40	-	80,80,80,80	0
54	MG	CA	1635	1/1	0.17	-	93,93,93,93	0
54	MG	BA	3223	1/1	0.17	-	84,84,84,84	0
54	MG	DA	3213	1/1	0.23	-	64,64,64,64	0
54	MG	BA	3500	1/1	0.17	-	92,92,92,92	0
54	MG	DA	3484	1/1	0.19	-	69,69,69,69	0
54	MG	DA	3076	1/1	0.28	-	93,93,93,93	0
54	MG	AA	1768	1/1	0.11	-	89,89,89,89	0
54	MG	BA	3623	1/1	0.20	-	93,93,93,93	0
54	MG	DA	3295	1/1	0.19	-	128,128,128,128	0
54	MG	AA	1831	1/1	0.26	-	91,91,91,91	0
54	MG	AA	1684	1/1	0.40	-	90,90,90,90	0
54	MG	CA	1693	1/1	0.53	-	89,89,89,89	0
54	MG	BA	3613	1/1	0.18	-	64,64,64,64	0
54	MG	BA	3039	1/1	0.28	-	76,76,76,76	0
54	MG	BA	3431	1/1	0.17	-	88,88,88,88	0
54	MG	DA	3406	1/1	0.32	-	113,113,113,113	0
54	MG	BA	3063	1/1	0.20	-	67,67,67,67	0
54	MG	BA	3404	1/1	0.33	-	90,90,90,90	0
54	MG	DA	3349	1/1	0.24	-	78,78,78,78	0
54	MG	BA	3307	1/1	0.33	-	75,75,75,75	0
54	MG	BA	3301	1/1	0.36	-	91,91,91,91	0
54	MG	CA	1608	1/1	0.17	-	94,94,94,94	0
54	MG	BA	3062	1/1	0.22	-	106,106,106,106	0
54	MG	DA	3371	1/1	0.37	-	98,98,98,98	0
54	MG	BA	3539	1/1	0.34	-	59,59,59,59	0
54	MG	DA	3029	1/1	0.16	-	96,96,96,96	0
54	MG	DA	3159	1/1	0.22	-	67,67,67,67	0
54	MG	DA	3444	1/1	0.12	-	133,133,133,133	0
54	MG	BA	3457	1/1	0.52	-	49,49,49,49	0
54	MG	BA	3185	1/1	0.55	-	62,62,62,62	0
54	MG	B2	201	1/1	0.19	-	104,104,104,104	0
54	MG	BA	3219	1/1	0.29	-	82,82,82,82	0
54	MG	BA	3244	1/1	0.34	-	53,53,53,53	0
54	MG	DA	3317	1/1	0.25	-	67,67,67,67	0
54	MG	DA	3058	1/1	0.20	-	84,84,84,84	0
56	ZN	AG	302	1/1	0.29	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3074	1/1	0.18	-	76,76,76,76	0
54	MG	BA	3204	1/1	0.40	-	106,106,106,106	0
54	MG	BA	3107	1/1	0.42	-	76,76,76,76	0
54	MG	BA	3182	1/1	0.41	-	81,81,81,81	0
54	MG	BA	3329	1/1	0.43	-	62,62,62,62	0
54	MG	CA	1728	1/1	0.31	-	76,76,76,76	0
54	MG	BA	3625	1/1	0.18	-	113,113,113,113	0
54	MG	BA	3127	1/1	0.28	-	90,90,90,90	0
54	MG	CA	1641	1/1	0.30	-	78,78,78,78	0
54	MG	DA	3047	1/1	0.17	-	91,91,91,91	0
54	MG	DA	3462	1/1	0.40	-	94,94,94,94	0
54	MG	DA	3092	1/1	0.41	-	85,85,85,85	0
54	MG	BA	3001	1/1	0.40	-	57,57,57,57	0
54	MG	DA	3062	1/1	0.30	-	60,60,60,60	0
54	MG	AA	1649	1/1	0.29	-	81,81,81,81	0
54	MG	AA	1640	1/1	0.30	-	77,77,77,77	0
54	MG	BA	3426	1/1	0.40	-	100,100,100,100	0
54	MG	BB	212	1/1	0.40	-	82,82,82,82	0
54	MG	BA	3534	1/1	0.23	-	85,85,85,85	0
54	MG	BA	3236	1/1	0.37	-	74,74,74,74	0
54	MG	DA	3238	1/1	0.20	-	65,65,65,65	0
54	MG	CA	1787	1/1	0.42	-	136,136,136,136	0
54	MG	BA	3302	1/1	0.42	-	59,59,59,59	0
54	MG	AC	108	1/1	0.17	-	95,95,95,95	0
54	MG	DA	3325	1/1	0.26	-	92,92,92,92	0
54	MG	DA	3354	1/1	0.20	-	126,126,126,126	0
54	MG	BA	3150	1/1	0.50	-	76,76,76,76	0
54	MG	BA	3574	1/1	0.20	-	60,60,60,60	0
54	MG	BA	3101	1/1	0.44	-	42,42,42,42	0
54	MG	DA	3103	1/1	0.20	-	66,66,66,66	0
54	MG	BA	3617	1/1	0.20	-	83,83,83,83	0
54	MG	AA	1727	1/1	0.18	-	88,88,88,88	0
54	MG	BA	3353	1/1	0.48	-	95,95,95,95	0
54	MG	DA	3200	1/1	0.35	-	58,58,58,58	0
54	MG	AA	1778	1/1	0.47	-	70,70,70,70	0
54	MG	DA	3404	1/1	0.24	-	86,86,86,86	0
54	MG	BA	3475	1/1	0.13	-	79,79,79,79	0
54	MG	B3	101	1/1	0.47	-	84,84,84,84	0
54	MG	DA	3488	1/1	0.14	-	77,77,77,77	0
54	MG	DA	3202	1/1	0.26	-	60,60,60,60	0
54	MG	BA	3598	1/1	0.23	-	75,75,75,75	0
54	MG	DA	3117	1/1	0.31	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3175	1/1	0.26	-	61,61,61,61	0
54	MG	BA	3503	1/1	0.46	-	117,117,117,117	0
54	MG	BA	3452	1/1	0.33	-	108,108,108,108	0
54	MG	CA	1715	1/1	0.22	-	102,102,102,102	0
54	MG	DA	3242	1/1	0.47	-	66,66,66,66	0
54	MG	CA	1716	1/1	0.42	-	103,103,103,103	0
54	MG	BA	3454	1/1	0.38	-	92,92,92,92	0
54	MG	BA	3328	1/1	0.35	-	68,68,68,68	0
54	MG	DA	3424	1/1	0.49	-	114,114,114,114	0
54	MG	DA	3473	1/1	0.21	-	70,70,70,70	0
54	MG	BA	3142	1/1	0.30	-	66,66,66,66	0
54	MG	DA	3061	1/1	0.15	-	67,67,67,67	0
54	MG	CA	1695	1/1	0.14	-	119,119,119,119	0
54	MG	BA	3287	1/1	0.47	-	70,70,70,70	0
54	MG	BA	3524	1/1	0.21	-	77,77,77,77	0
54	MG	DA	3347	1/1	0.12	-	79,79,79,79	0
54	MG	CA	1640	1/1	0.28	-	99,99,99,99	0
54	MG	BA	3251	1/1	0.37	-	48,48,48,48	0
54	MG	AA	1608	1/1	0.35	-	91,91,91,91	0
54	MG	DA	3059	1/1	0.33	-	87,87,87,87	0
54	MG	DA	3467	1/1	0.26	-	72,72,72,72	0
54	MG	DB	203	1/1	0.28	-	81,81,81,81	0
54	MG	AA	1731	1/1	0.17	-	97,97,97,97	0
54	MG	CA	1769	1/1	0.29	-	101,101,101,101	0
54	MG	DA	3018	1/1	0.12	-	90,90,90,90	0
54	MG	CA	1749	1/1	0.24	-	91,91,91,91	0
54	MG	DA	3102	1/1	0.26	-	68,68,68,68	0
54	MG	BA	3386	1/1	0.19	-	76,76,76,76	0
54	MG	AA	1805	1/1	0.41	-	91,91,91,91	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.