



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:31 PM BST

PDB ID : 4V8C
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex with paromomycin).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

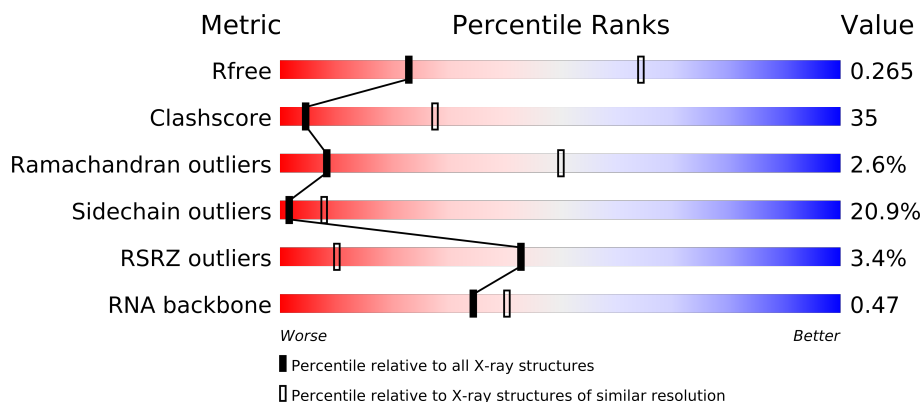
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	2912	
1	BA	2912	
2	AB	122	
2	BB	122	
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	210	
5	BF	210	
6	AG	182	
6	BG	182	

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Mol	Chain	Length	Quality of chain
7	AH	180	
7	BH	180	
8	AK	148	
8	BK	148	
9	AM	140	
9	BM	140	
10	AN	122	
10	BN	122	
11	AO	150	
11	BO	150	
12	AP	141	
12	BP	141	
13	A0	118	
13	B0	118	
14	AQ	112	
14	BQ	112	
15	AR	146	
15	BR	146	
16	A1	118	
16	B1	118	
17	A2	101	
17	B2	101	
18	AS	113	
18	BS	113	
19	AT	96	
19	BT	96	
20	AU	110	
20	BU	110	
21	AV	206	
21	BV	206	
22	A3	85	
22	B3	85	
23	AZ	98	
23	BZ	98	
24	AW	72	
24	BW	72	
25	AX	60	
25	BX	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1506	
31	DA	1506	
32	CE	256	
32	DE	256	
33	CF	239	
33	DF	239	
34	CG	208	
34	DG	208	
35	CH	162	
35	DH	162	
36	CI	101	
36	DI	101	
37	CJ	156	
37	DJ	156	
38	CK	138	
38	DK	138	
39	CL	128	
39	DL	128	
40	CM	105	
40	DM	105	
41	CN	129	
41	DN	129	
42	CO	132	
42	DO	132	
43	CP	126	
43	DP	126	
44	CQ	61	
44	DQ	61	
45	CR	89	
45	DR	89	
46	CS	88	
46	DS	88	
47	CT	105	
47	DT	105	
48	CU	88	
48	DU	88	

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Mol	Chain	Length	Quality of chain
49	CV	93	
49	DV	93	
50	CW	106	
50	DW	106	
51	CX	27	
51	DX	27	
52	CB	87	
52	DB	87	
53	CC	77	
53	CD	77	
53	DC	77	
53	DD	77	
54	C1	10	
54	D1	10	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299682 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 RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	BA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	EXPRESSION TAG	GB AP008226.1
AA	654A	A	G	CONFLICT	GB AP008226.1
AA	654E	C	G	CONFLICT	GB AP008226.1
AA	654P	G	C	CONFLICT	GB AP008226.1
AA	654T	A	C	CONFLICT	GB AP008226.1
AA	1058	U	G	CONFLICT	GB AP008226.1
AA	1080	A	C	CONFLICT	GB AP008226.1
BA	158	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

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	B0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	B3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	B4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	DE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	DH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CL	127	Total	C	N	O	0	0	0
			1010	639	197	174			
39	DL	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	DN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	DP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	DU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
49	DV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CB	87	Total	C	N	O	P	9	0	0
			1861	829	333	612	87			
52	DB	87	Total	C	N	O	P	8	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	18	C	U	CONFLICT	GB AP012306.1
CD	18	C	U	CONFLICT	GB AP012306.1
DC	18	C	U	CONFLICT	GB AP012306.1
DD	18	C	U	CONFLICT	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
54	D1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

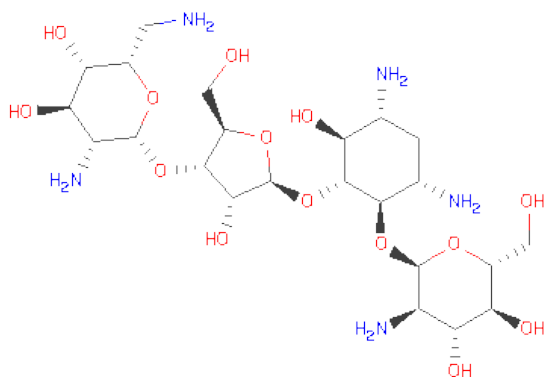
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	528	Total Mg 528 528	0	0
55	CA	240	Total Mg 240 240	0	0
55	AB	17	Total Mg 17 17	0	0
55	A6	1	Total Mg 1 1	0	0
55	BE	3	Total Mg 3 3	0	0
55	B1	1	Total Mg 1 1	0	0
55	C1	1	Total Mg 1 1	0	0
55	CD	1	Total Mg 1 1	0	0
55	BP	1	Total Mg 1 1	0	0
55	CN	2	Total Mg 2 2	0	0
55	A2	1	Total Mg 1 1	0	0
55	DC	8	Total Mg 8 8	0	0
55	B5	1	Total Mg 1 1	0	0
55	BB	15	Total Mg 15 15	0	0
55	AE	4	Total Mg 4 4	0	0
55	DG	2	Total Mg 2 2	0	0
55	AA	626	Total Mg 626 626	0	0
55	CQ	2	Total Mg 2 2	0	0
55	A5	2	Total Mg 2 2	0	0
55	CG	2	Total Mg 2 2	0	0
55	A1	1	Total Mg 1 1	0	0
55	AD	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CT	1	Total 1	Mg 1	0	0
55	DH	1	Total 1	Mg 1	0	0
55	CC	7	Total 7	Mg 7	0	0
55	DS	1	Total 1	Mg 1	0	0
55	B3	1	Total 1	Mg 1	0	0
55	BR	2	Total 2	Mg 2	0	0
55	AZ	1	Total 1	Mg 1	0	0
55	DA	204	Total 204	Mg 204	0	0
55	AU	1	Total 1	Mg 1	0	0
55	A0	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	A7	2	Total 2	Mg 2	0	0
55	BD	1	Total 1	Mg 1	0	0
55	AO	3	Total 3	Mg 3	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	3	Total 3	Mg 3	0	0
55	DB	2	Total 2	Mg 2	0	0

- Molecule 56 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	CA	1	Total	C	N	O	0	0
			42	23	5	14		
56	DA	1	Total	C	N	O	0	0
			42	23	5	14		

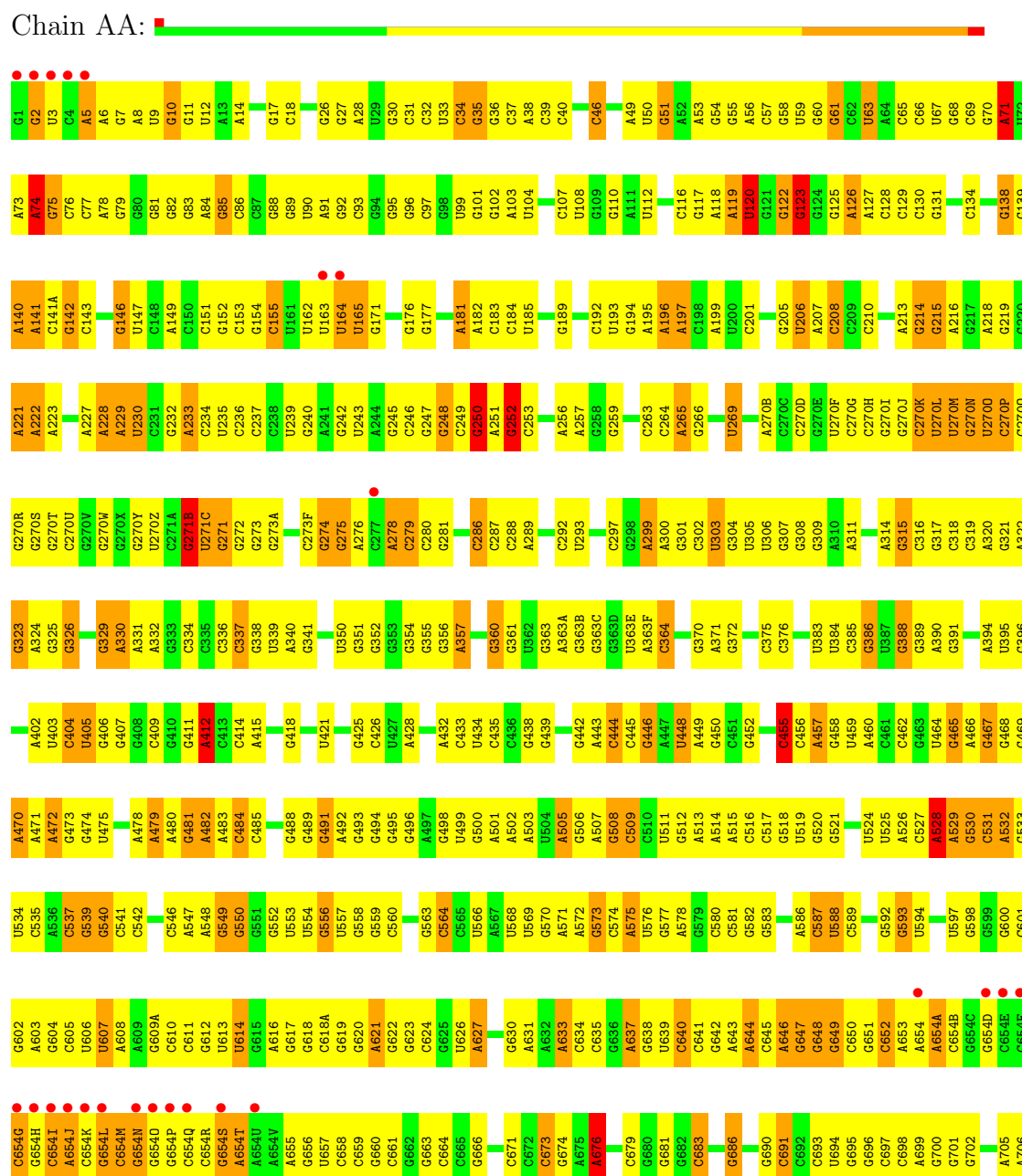
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DG	1	Total	Zn	0	0
			1	1		
57	CQ	1	Total	Zn	0	0
			1	1		
57	DQ	1	Total	Zn	0	0
			1	1		
57	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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (2912-MER)



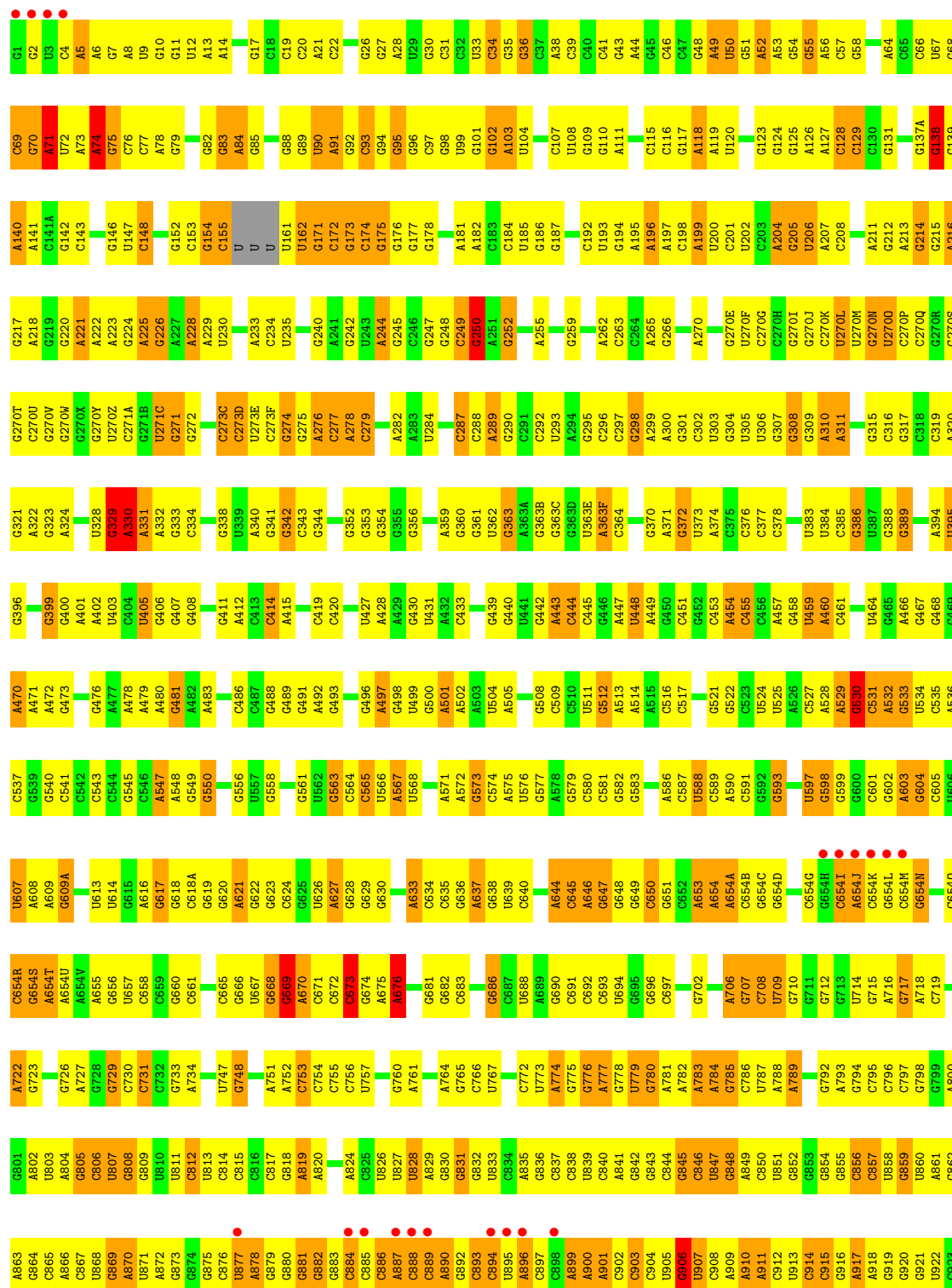
G1746	C1563	A1586	G1525	A1460	A1395	U1326	C1251	C1180	A1054	C986	A917	U851	U787	G707
G1750	A1664	A1587	G1526	G1461	U1396	U1327	G1252	C1181	G1055	G987	A918	G852	A788	C708
C1751	G1666	C1588	G1527	G1462	U1397	C1328	A1253	A1182	G1056	G988	G919	G853	A789	G710
C1752	G1667	C1589	G1528	C1463	U1398	U1329	G1257	G1184	A1057	G989	U922	G854	C790	G710
G1756	A1529	G1591	A1529	G1464	C1399	C1330	C1257	G1185	U1058	C991	C923	G855	C791	G715
A1569	G1592	C1592	G1530	G1465	G1400	A1331	G1258	G1186	C1060	C992	G924	C856	C792	G716
C1670	G1593	C1593	G1531	G1466	G1401	G1332	G1259	G1187	U1061	C993	C925	C857	A793	G717
U1757	C1594	C1594	C1532	C1467	C1402	G1333	G1260	G1188	G1062	G994	A926	U858	C794	G718
G1758	C1595	C1595	C1533	C1468	C1403	A1336	G1261	G1189	C1063	C995	G928	G859	C795	G719
A1759	G1596	C1596	G1534	G1470	C1404	G1337	A1262	A1189	C1064	A996	G929	U860	C796	C720
A1762	C1597	C1597	U1535	A1471	U1406	G1338	G1263	G1191	U1065	C997	U930	G862	C797	C720
G1763	G1598	C1598	A1536	G1472	C1407	G1339	G1264	G1192	U1066	C998	G931	A863	A800	G728
G1764	C1599	C1599	C1537	A1473	C1408	U1340	A1265	G1193	A1087	U999	G932	G864	G801	G729
G1769	G1606	C1606	G1538	G1475	C1409	U1341	G1266	G1194	G1068	A1000	A933	C865	A802	C730
G1770	U1680	C1607	G1539	C1476	G1410	U1267	G1267	G1195	A1089	A1001	G938	A866	G803	C731
C1771	G1681	A1608	G1540	A1477	C1411	A1268	A1268	G1196	A1070	G1002	U942	G867	A804	C732
G1772	C1684	A1609	G1542	G1479	G1412	G1345	A1269	G1197	G1071	G1005	A941	U871	C806	C733
A1773	C1685	A1610	G1543	G1480	G1413	G1346	C1270	C1201	C1072	C1006	G942	A872	U807	A734
C1774	C1686	C1611	C1544	G1481	G1416	A1348	G1271	C1202	A1073	C1007	G943	G873	G808	G739
U1775	G1687	C1612	A1545	G1482	C1417	A1349	A1272	G1203	G1074	G1008	G944	A874	G809	U740
G1776	U1688	G1613	A1545A	G1484	G1418	U1352	A1274	G1204	C1075	A1010	A945	A878	U810	G745
U1777	A1614	C1546	G1547	G1485	U1420	A1353	A1275	G1205	A1077	G1011	G946	G879	U811	G745
U1778	G1615	C1547	G1547	G1487	G1421	A1354	A1276	G1206	U1078	U1012	G950	G880	C812	A746
U1779	A1616	C1548	C1548	G1488	G1421	G1355	G1277	C1207	C1079	C1013	G951	G881	U813	A746
C1780	C1617	C1549	C1549	U1489	G1422	G1356	A1278	C1208	A1080	U1014	C952	G882	C814	U747
C1781	U1693	A1618	C1550	G1490	G1424	U1357	G1279	G1209	C1081	G1015	A953	G883	C815	G748
C1782	C1694	G1618	C1550	G1491	G1425	G1358	A1287	A1210	U1082	G1016	G954	C884	C816	G748
A1783	G1695	G1627	A1553	G1492	G1426	A1359	U1211	G1212	U1083	C985	C817	C885	C817	A751
A1784	A1554	C1493	A1554	C1493	A1427	A1360	U1212	G1212	A1084	U1019	C955	C886	G818	A752
A1785	C1555	A1494	C1555	A1494	C1428	G1361	C1290	G1215	A1085	A1020	G956	A887	A819	C753
C1786	C1556	G1495	C1556	G1495	G1429	A1366	C1291	G1216	A1086	A1021	A957	C888	A820	C754
A1787	A1633	C1557	C1557	A1496	C1430	A1365	U1292	G1216	G1087	G1022	U958	C889	U821	C755
C1788	G1635	A1558	C1557	U1497	U1431	A1366	U1293	C1217	A1088	U1023	A959	U822	A822	G760
A1789	C1636	G1559	G1559	C1498	C1432	A1367	U1294	G1218	G1089	G1024	A960	G892	G823	A761
C1790	G1560	C1499	G1560	U1433	U1433	G1368	G1295	G1219	U1090	U1025	C961	C893	A824	G761
A1791	C1638	G1500	G1561	A1434	A1434	G1369	C1296	A1220	G1091	U1026	G962	C894	C825	U762
G1792	C1639	C1501	A1562	C1501	G1435	U1372	C1297	A1227	C1092	A1027	U963	C897	U826	U762
C1793	C1640	U1503	G1563	G1436	C1436	A1373	G1298	G1228	U1093	A1028	C964	C898	U827	G763
U1794	A1641	C1504	C1564	U1503	C1437	G1374	U1299	G1228	U1094	U1033	C965	C899	U827	A764
C1795	G1642	C1504	C1565	U1504	U1438	C1375	U1300	G1228	A1095	U1033	C967	A899	U828	C766
U1796	G1643	C1505	A1566	C1505	A1439	U1375	A1302	G1230	U1097	G1036	C968	A900	G831	G766
C1797	C1506	G1440	C1567	G1506	G1440	A1379	G1303	G1231	A1098	G1037	C971	A901	G832	G769
U1798	A1507	G1441	G1568	A1507	G1441	G1380	G1303	G1232	C1099	G1038	C972	C902	U833	G770
G1799	C1508	G1442	A1569	G1508	G1442	G1381	G1310	C1233	G1100	G1039	C973	C903	C834	G771
C1800	G1509	G1443	A1570	C1509	G1443	G1382	G1311	U1234	U1101	C904	A973	C904	C838	A774
G1803	C1510	G1444	A1571	A1510	G1444	C1383	U1312	G1235	G1102	G1042	G974	U905	U839	G775
C1804	A1511	A1444A	C1384	A1511	A1444A	U1313	U1312	G1236	A1103	C1043	C974A	G906	C840	G776
U1805	G1512	G1448	G1385	G1512	G1448	A1384	G1314	A1237	C1104	G1044	G975	U907	A841	A777
C1806	C1513	G1449	C1386	C1513	G1449	G1385	C1315	G1238	U1105	A1045	C978	C908	G842	G778
G1807	U1514	G1449A	G1387	G1514	G1449A	C1386	C1316	G1239	G1170	U1046	G979	C909	U843	U779
A1810	C1515	G1450	G1388	C1515	G1450	G1387	U1316	U1240	G1171	A1047	G843	A909	C844	G780
C1811	U1516	G1451	G1389	G1516	G1451	A1317	A1317	G1241	G1173	G1047	A980	A910	G844	A781
G1812	G1517	A1453	G1390	G1517	A1453	G1388	G1318	A1242	U1108	C1048	C982	A911	G845	A782
C1813	C1518	G1454	U1391	U1518	G1454	U1389	G1319	G1243	C1109	C1049	C981	C912	C846	A783
G1814	G1519	G1455	U1391	G1519	G1455	U1390	C1320	G1244	G1110	A1050	C982	U913	U847	A783
C1815	U1520	C1458	A1392	U1520	C1458	U1392	A1321	G1244	G1111	G1051	A983	C915	G848	A784
G1816	G1522	G1459	A1393	G1522	G1459	A1392	A1322	U1249	G1112	C1052	A984	C915	A849	G785
			U1394	U1394	U1394	U1394	U1323	G1250	U1113	C1053	C985	G916	C850	C786

A2810	A2741	A2679	G2503	G2532	C2324	U2262	G2184	G2120	G2053	G1983	G1904	A1819
G2811	C2745	C2680	U2604	A2533	G2325	C2263	C2186	G2121	A2054	C1982	C1905	U1820
G2812	C2746	C2681	U2605	A2534	C2326	C2264	G2187	G2122	G2055	C1983	G1906	
A2813	G2747	C2682	G2606	G2535	A2327	U2265	G2188	G2123	G2056	G1984	G1907	
C2814	G2748	C2683	G2607	G2536	A2328	A2266	G2189	G2124	A2057	A1825	A1912	A1826
C2815	A2749	U2684	G2608	U2537	G2329	A2267	G2190	G2125	A2058	G1826	A1913	C1827
C2816	G2750	G2685	U2609	C2538	G2330	A2268	G2191	A2126	A2059	G1827	A1914	G1828
G2817	G2751	G2686	C2610	G2539	G2331	A2269	G2192	G2127	A2060	G1828	C1914	A1829
G2818	C2752	U2687	U2611	C2540	U2332	G2270	G2193	G2128	G2061	C1989	U1915	G1830
G2819	C2753	U2688	G2612	A2541	G2333	U2271		G2129	A2062	C1990	U1916	C1831
A2820		U2689	U2613	A2542	A2334	U2272		G2130	C2063	C1991	U1917	G1832
A2821		C2690	A2614	G2543	G2335	A2273	A2198	U2131	C2064	A1918	A1918	U1833
G2822	C2755		U2615	G2544	A2336	A2274	C2205	U2132	C2065	A1919	A1919	C1834
A2823	U2756		C2616	G2545	G2337	C2275	C2206	G2133	C2066	C1999	C1920	U1835
C2824	A2757		G2617	U2546	G2338	G2276		A2134	G2067	G2000	C1925	
C2825	U2758		G2618			G2277		G2135	U2068	A2001	U1926	G1839
	C2760		G2619	U2552				G2136	G2069	G2002		
C2829	C2761		C2620	U2553	G2341	G2280		G2137	G2070	G2003		
G2830			U2554	C2542	C2342	C2281		C2138		G2004	G1929	A1847
G2831			U2555	C2343	C2343	C2282		G2139		A2005	G1930	A1848
U2832			U2556	U2344	U2344	U2283		G2140		G2006	U1931	G1849
G2833			G2557	G2345	G2345	C2284		G2141			A1932	G1850
G2834				A2346	A2346	C2285		G2142			G1933	
U2835				G2347	G2347	C2286		G2143			C1934	
U2836				U2348	U2348	A2287		U2144				
G2837				A2422	G2349	A2288		G2145			A1937	G1856
				G2423	C2350	G2289		C2146			A1938	G1857
G2838				A2424	G2351	U2291		A2013			U1939	G1858
G2839				A2425	A2352	U2292		A2014			A1940	A1859
C2840				G2427		C2293		A2015			G1953	G1860
G2841				U2428	C2359	A2294		U2016			U1954	G1861
C2842				G2429	A2360	C2295		U2017			C1958	G1862
G2843				A2430	A2361	G2296		G2018			U1959	G1863
				U2431		C2297		A2019			U1961	U1864
G2844				A2432	C2364	U2298		A2020			A1962	U1865
G2845				A2433	A2365	C2299		C2021			G1963	A1884
G2846				G2434	A2366	G2300		A2022			G1964	A1885
U2847				A2435		G2301		G2023			A1965	C1886
U2848				G2436		G2302		U2096			G1966	C1887
U2849				U2437		G2303		G2097			C1967	A1888
A2850				U2438		G2304		U2098			G1968	A1889
A2851				A2439		A2305		U2099			A1969	A1890
G2852				G2444		G2306		G2100			U1970	G1891
						G2307		U2101			A1971	C1892
C2855				U2447		G2308		G2102			U1972	C1893
C2856				A2448		G2309		C2103			G1973	C1894
G2857				C2442		G2310		G2104			A1974	
C2858				C2443		A2311		G2105			C1975	
C2859				G2444		G2312		G2106			U1976	
						C2313		G2107			C1977	
A2860						G2314		C2108			A1978	
G2861						G2315		U2109			A1979	
G2862						G2316		G2110			C1980	
G2863						G2317		C2111				
G2864						G2318		U2112				
U2865						G2319		G2113				
U2866						G2320		A2114				
U2867						G2321		G2115				
A2734						G2322		G2116				
A2735						G2323		A2117				
G2736						A2320		C2050				
						U2390		A2051				
G2805						A2321		U2118				
G2807						A2322		C2181				
C2870						G2323		C2183				
C2871												
A2809												
G2872												



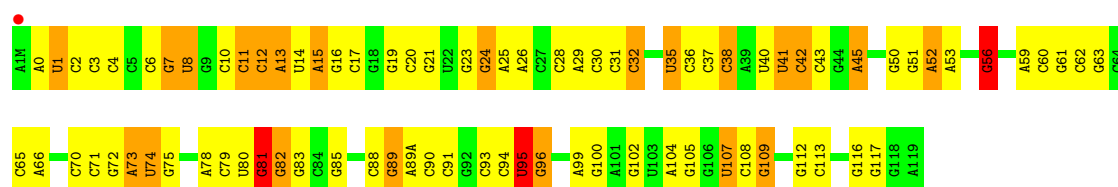
● Molecule 1: RNA (2912-MER)

Chain BA:



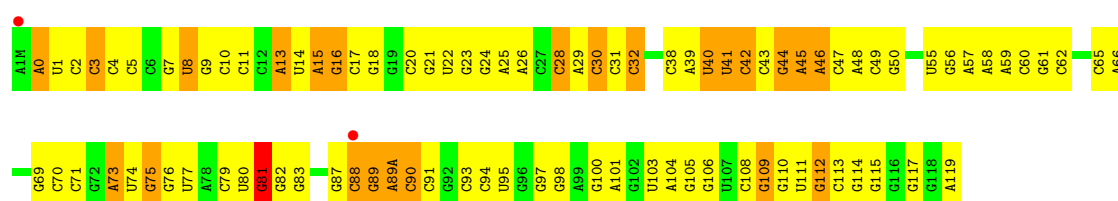


Chain AB: 



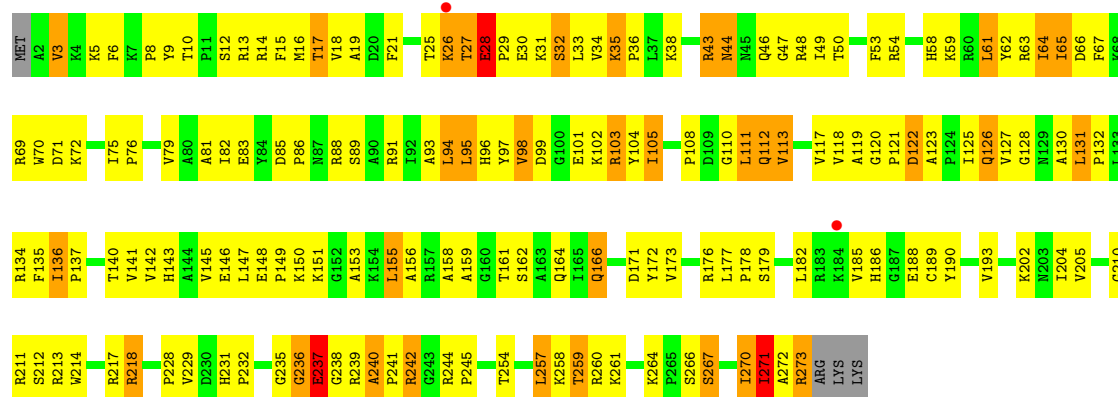
• Molecule 2: 5S RIBOSOMAL RNA

Chain BB:



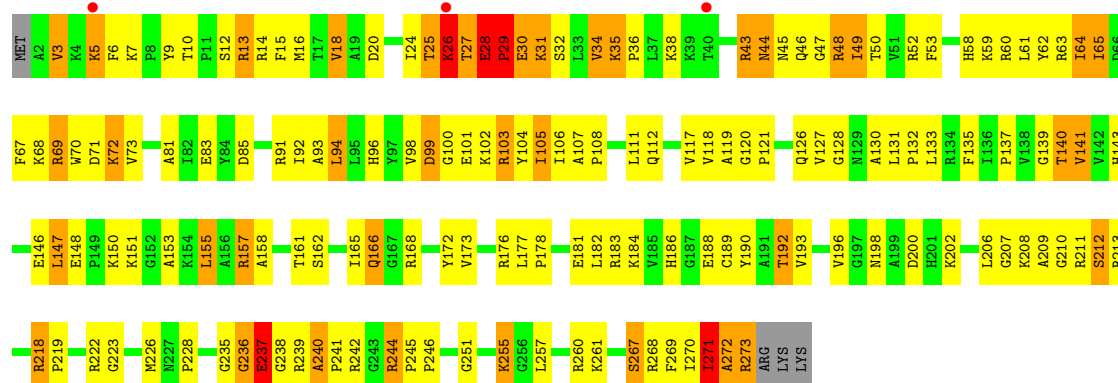
• Molecule 3: 50S ribosomal protein L2

Chain AD:



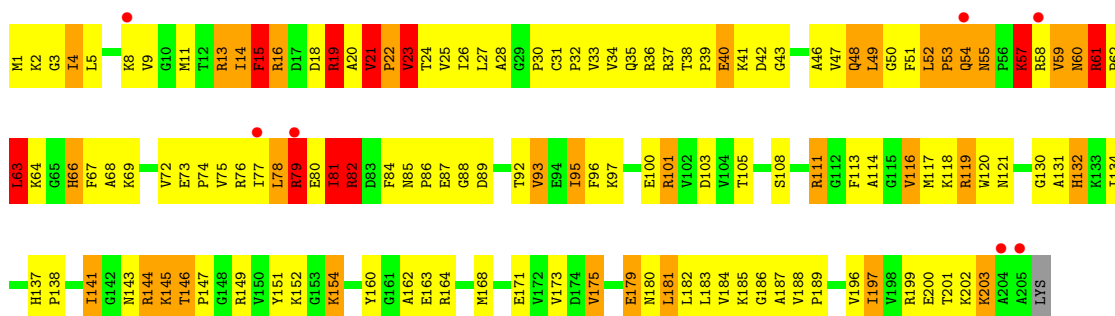
• Molecule 3: 50S ribosomal protein L2

Chain BD:



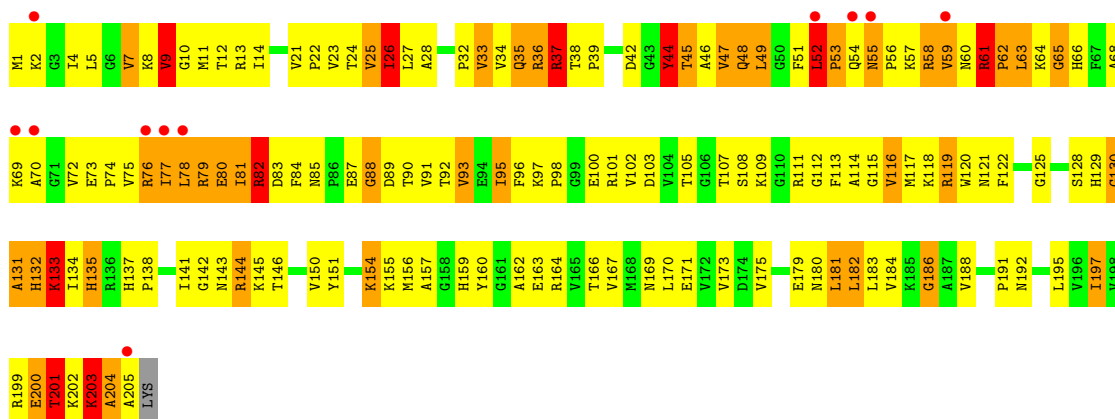
• Molecule 4: 50S ribosomal protein L3

Chain AE:



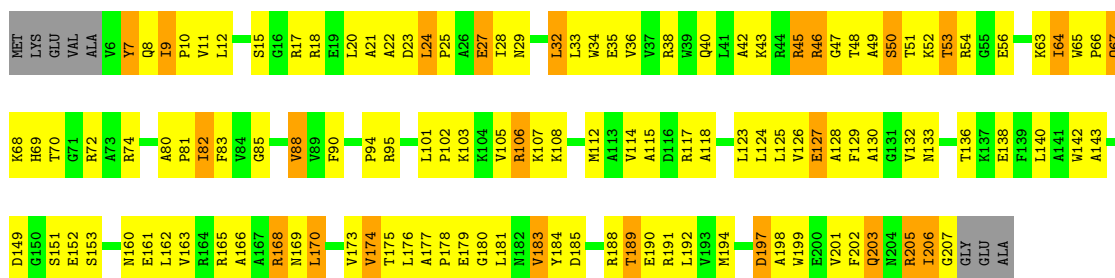
• Molecule 4: 50S ribosomal protein L3

Chain BE:



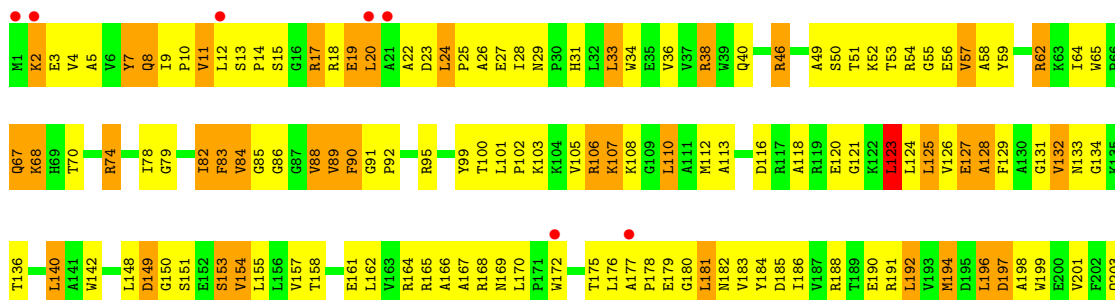
• Molecule 5: 50S ribosomal protein L4

Chain AF:



• Molecule 5: 50S ribosomal protein L4

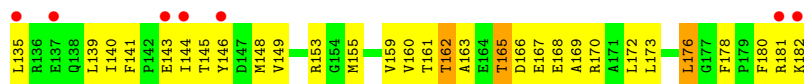
Chain BF:





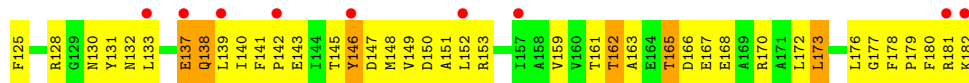
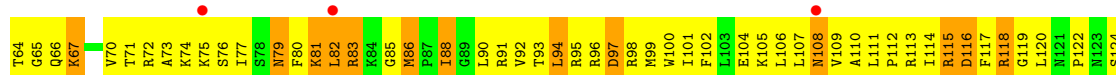
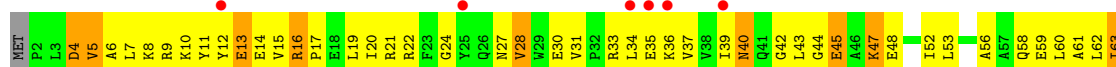
- Molecule 6: 50S ribosomal protein L5

Chain AG:



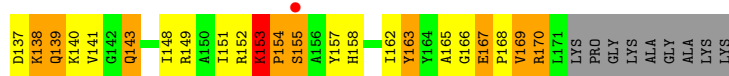
- Molecule 6: 50S ribosomal protein L5

Chain BG:



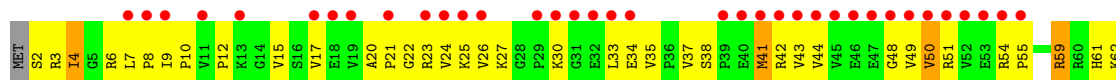
- Molecule 7: 50S ribosomal protein L6

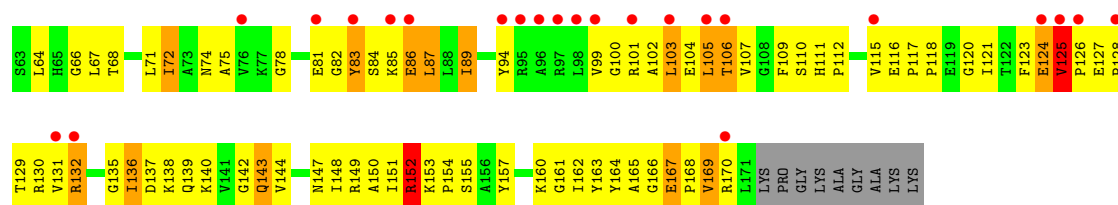
Chain AH:



- Molecule 7: 50S ribosomal protein L6

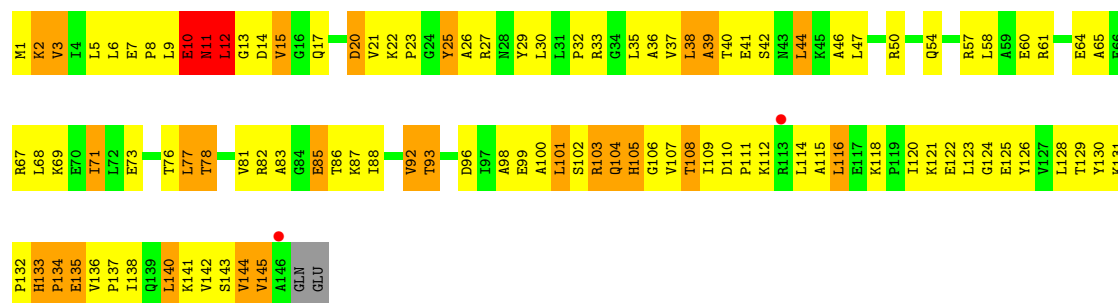
Chain BH:





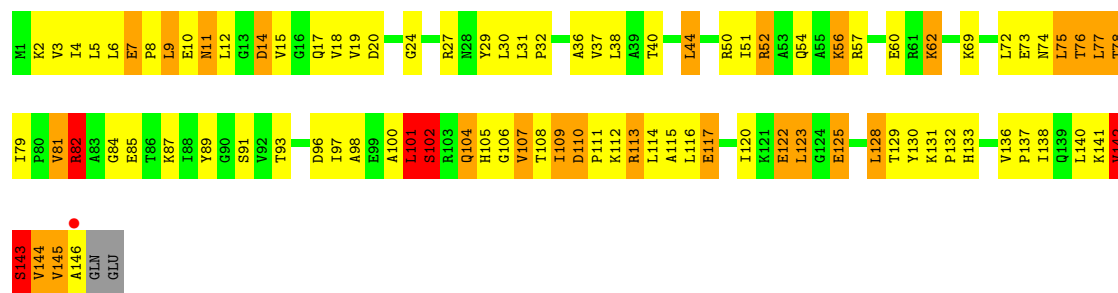
• Molecule 8: 50S ribosomal protein L9

Chain AK:



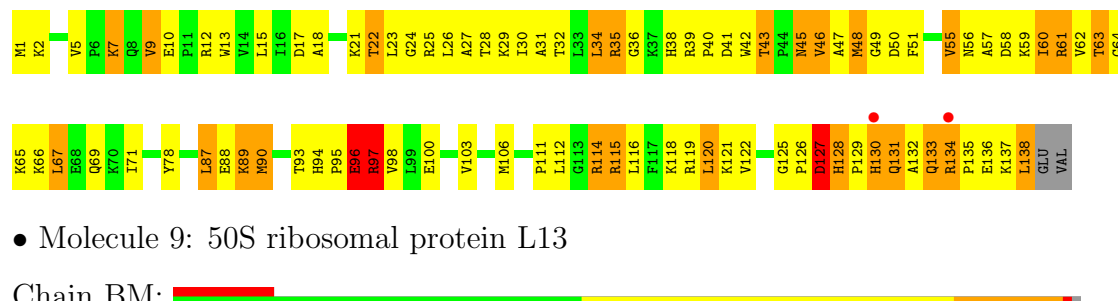
• Molecule 8: 50S ribosomal protein L9

Chain BK:



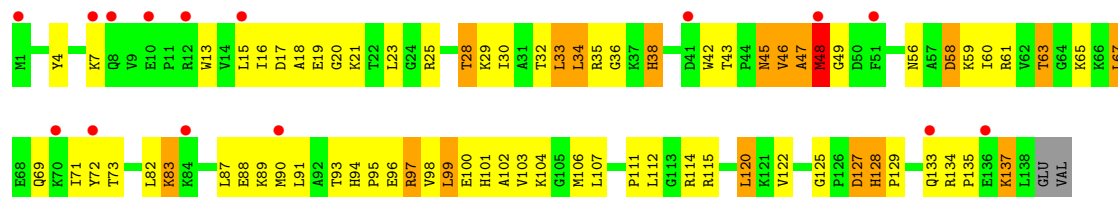
• Molecule 9: 50S ribosomal protein L13

Chain AM:

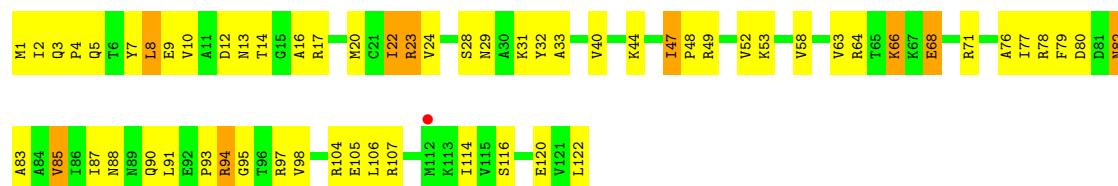


• Molecule 9: 50S ribosomal protein L13

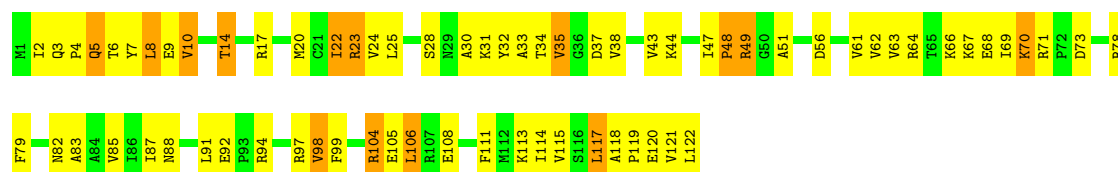
Chain BM:



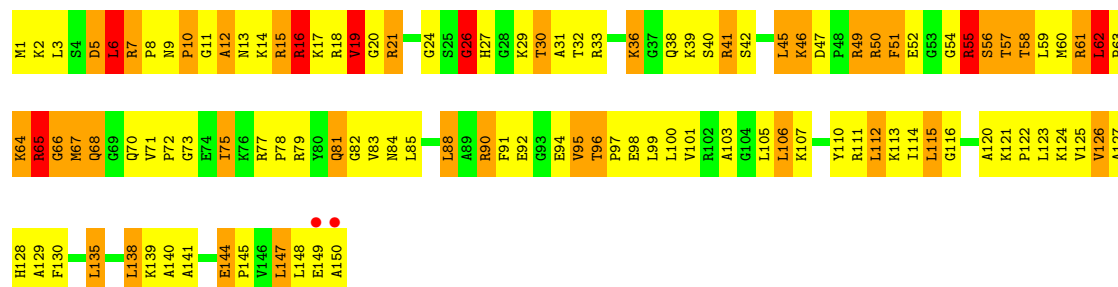
- Molecule 10: 50S ribosomal protein L14

Chain AN: 

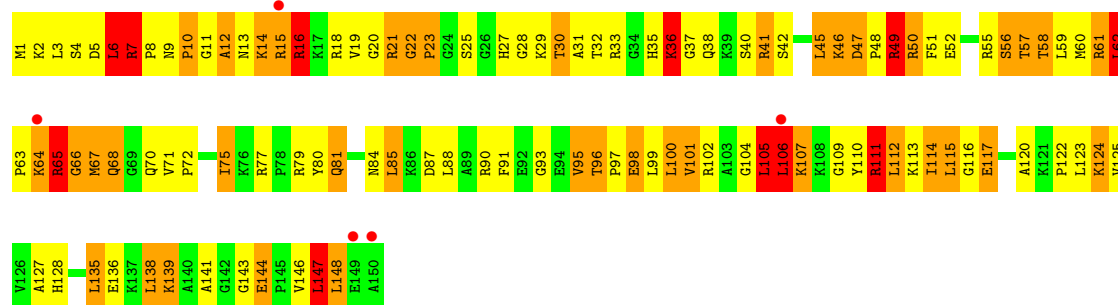
- Molecule 10: 50S ribosomal protein L14

Chain BN: 

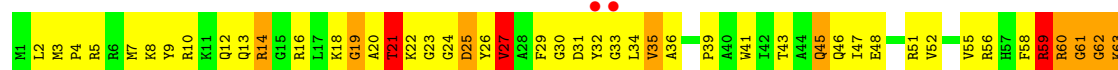
- Molecule 11: 50S ribosomal protein L15

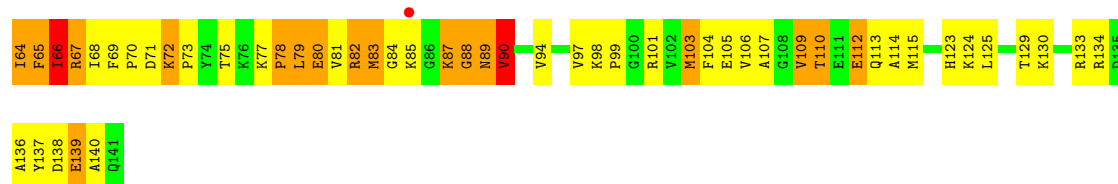
Chain AO: 

- Molecule 11: 50S ribosomal protein L15

Chain BO: 

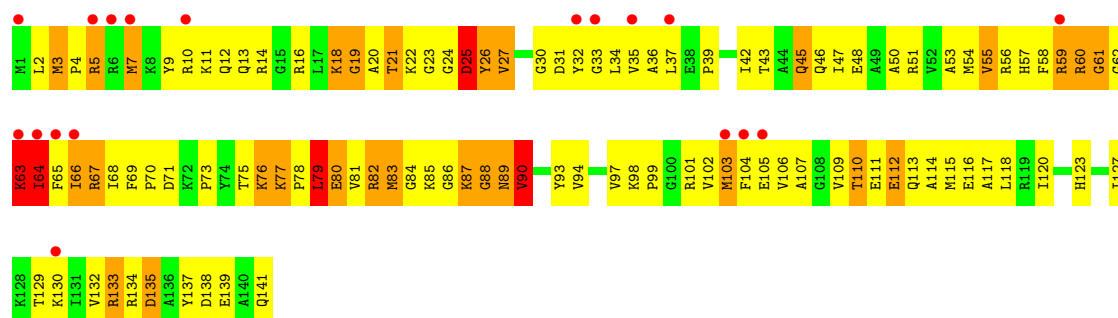
- Molecule 12: 50S ribosomal protein L16

Chain AP: 



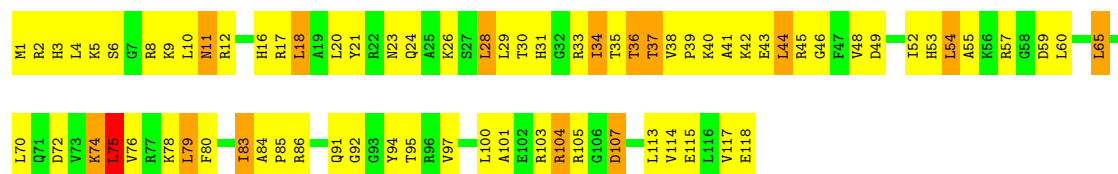
- Molecule 12: 50S ribosomal protein L16

Chain BP:



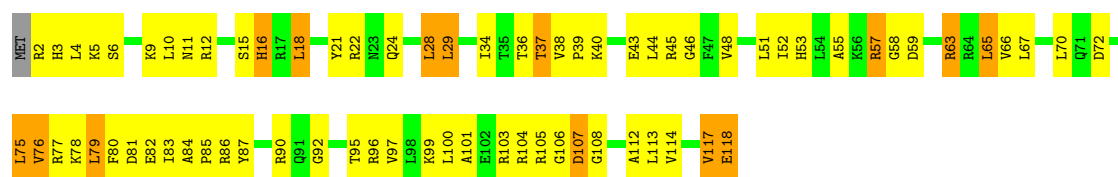
- Molecule 13: 50S ribosomal protein L17

Chain A0:



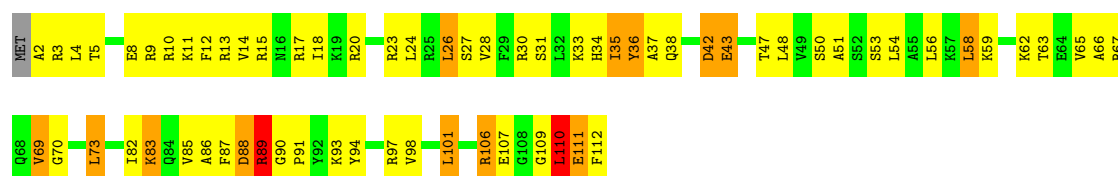
- Molecule 13: 50S ribosomal protein L17

Chain B0:



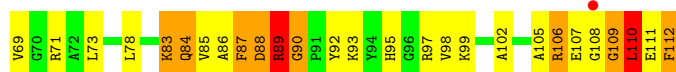
- Molecule 14: 50S ribosomal protein L18

Chain AQ:



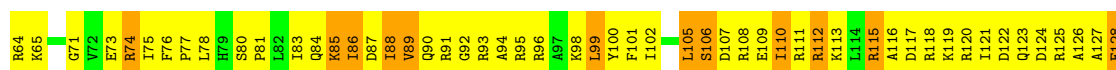
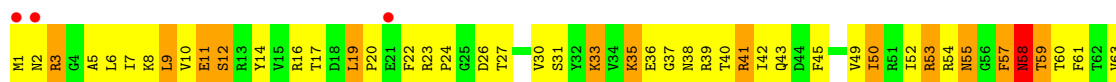
- Molecule 14: 50S ribosomal protein L18

Chain BQ:



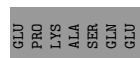
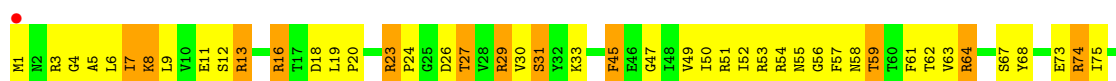
• Molecule 15: 50S ribosomal protein L19

Chain AR:



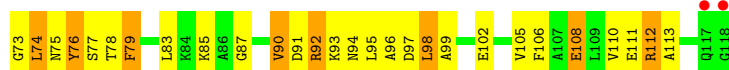
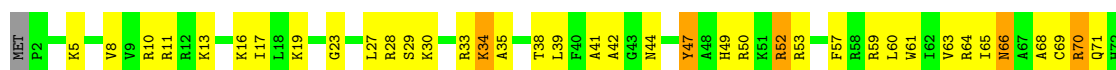
• Molecule 15: 50S ribosomal protein L19

Chain BR:



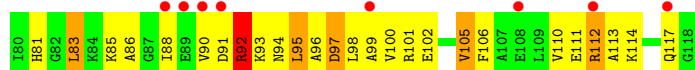
• Molecule 16: 50S ribosomal protein L20

Chain A1:



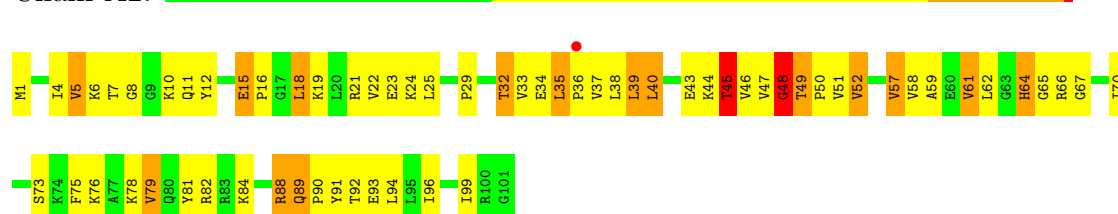
• Molecule 16: 50S ribosomal protein L20

Chain B1:



- Molecule 17: 50S ribosomal protein L21

Chain A2:



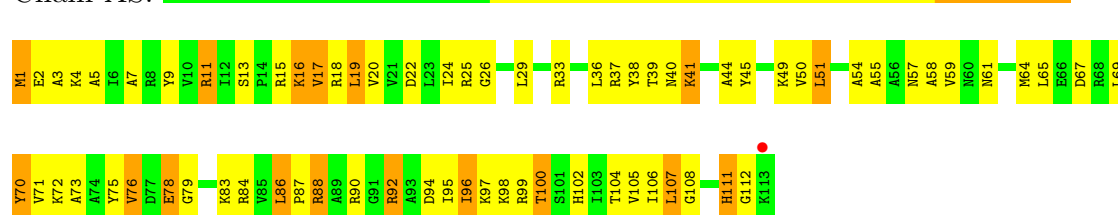
- Molecule 17: 50S ribosomal protein L21

Chain B2:



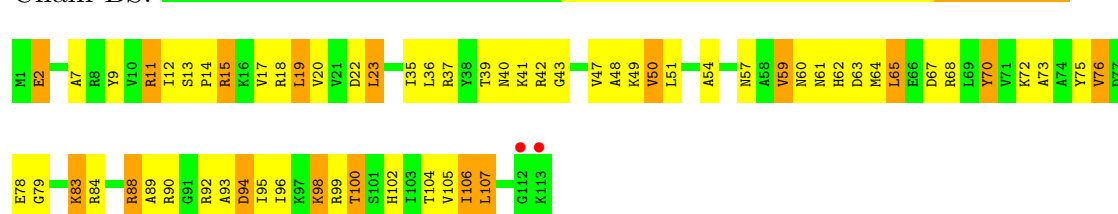
- Molecule 18: 50S ribosomal protein L22

Chain AS:



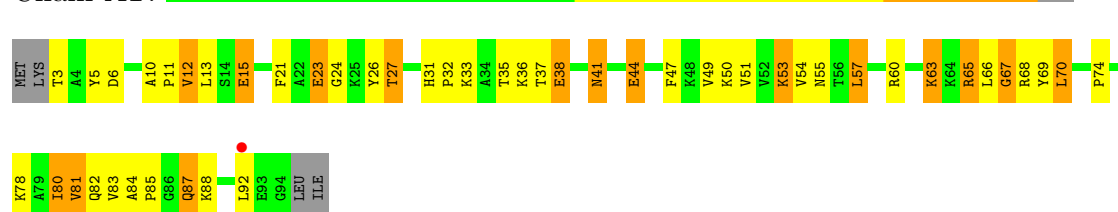
- Molecule 18: 50S ribosomal protein L22

Chain BS:



- Molecule 19: 50S ribosomal protein L23

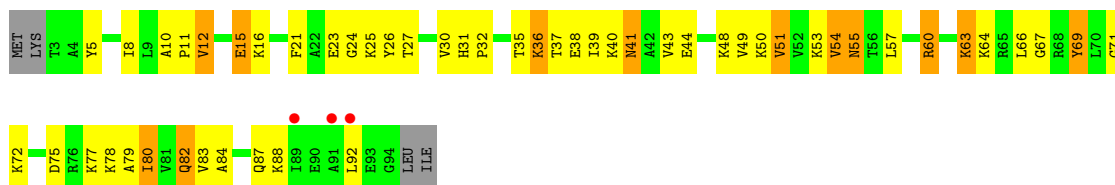
Chain AT:



- Molecule 19: 50S ribosomal protein L23

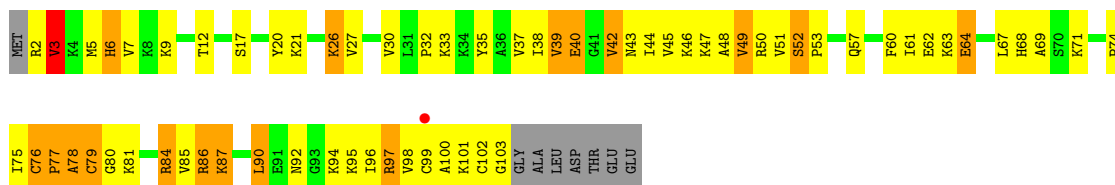
Chain BT:





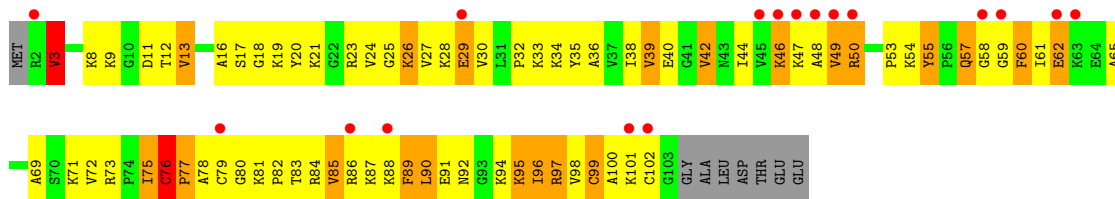
• Molecule 20: 50S ribosomal protein L24

Chain AU:



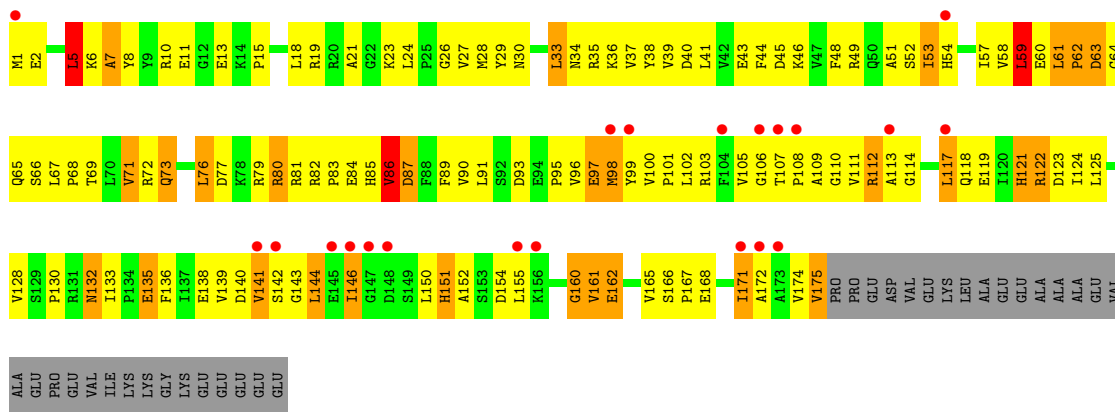
• Molecule 20: 50S ribosomal protein L24

Chain BU:



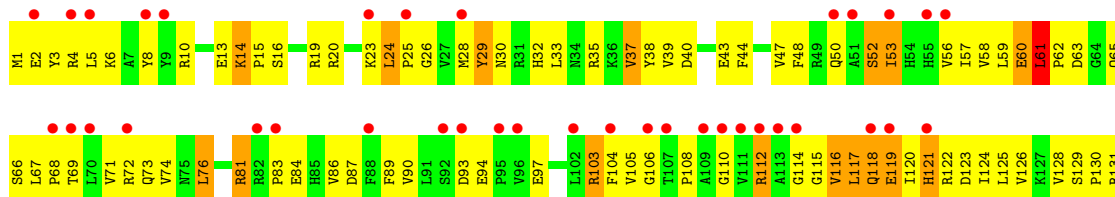
• Molecule 21: 50S ribosomal protein L25

Chain AV:



• Molecule 21: 50S ribosomal protein L25

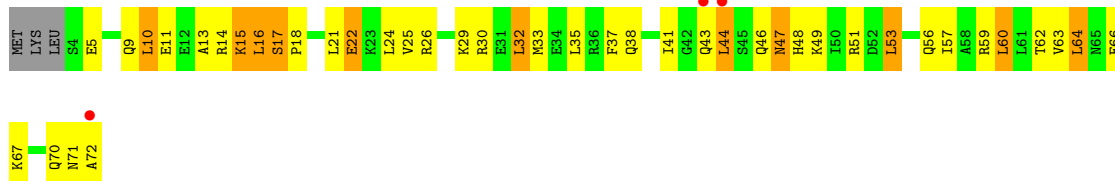
Chain BV:



GLN
ASN
ALA

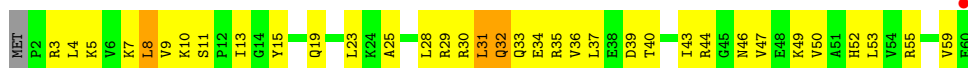
- Molecule 24: 50S ribosomal protein L29

Chain BW:



- Molecule 25: 50S ribosomal protein L30

Chain AX:



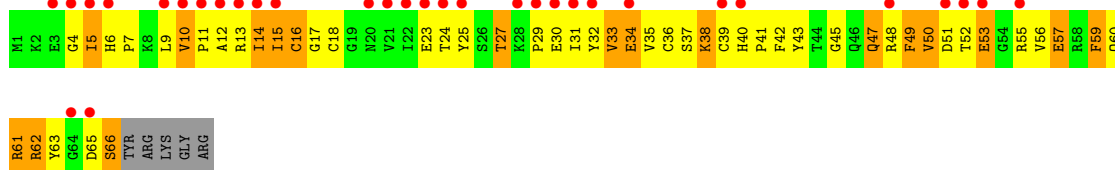
- Molecule 25: 50S ribosomal protein L30

Chain BX:



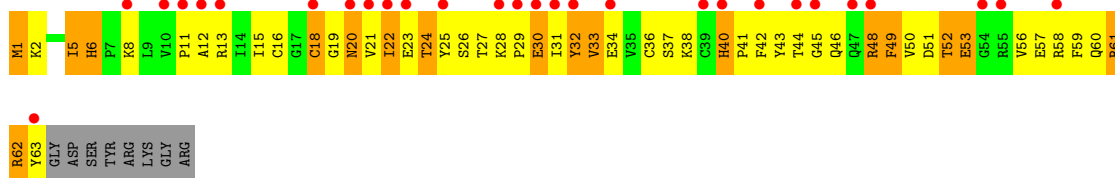
- Molecule 26: 50S ribosomal protein L31

Chain A4:



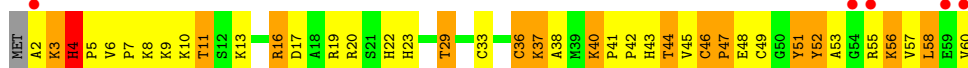
- Molecule 26: 50S ribosomal protein L31

Chain B4:



- Molecule 27: 50S ribosomal protein L32

Chain A5:



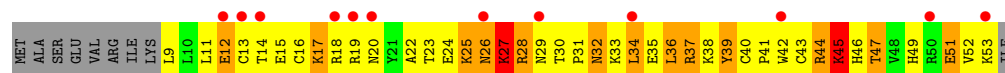
- Molecule 27: 50S ribosomal protein L32

Chain B5: 



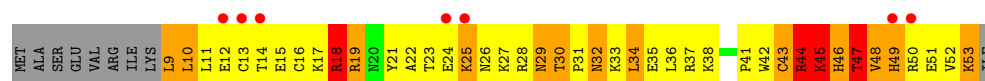
- Molecule 28: 50S ribosomal protein L33

Chain A6: 



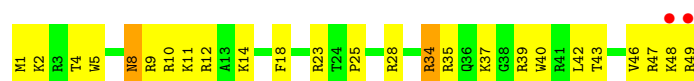
- Molecule 28: 50S ribosomal protein L33

Chain B6: 



- Molecule 29: 50S ribosomal protein L34

Chain A7: 



- Molecule 29: 50S ribosomal protein L34

Chain B7: 



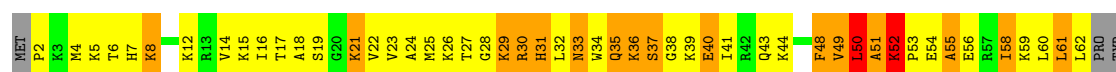
- Molecule 30: 50S ribosomal protein L35

Chain A8: 



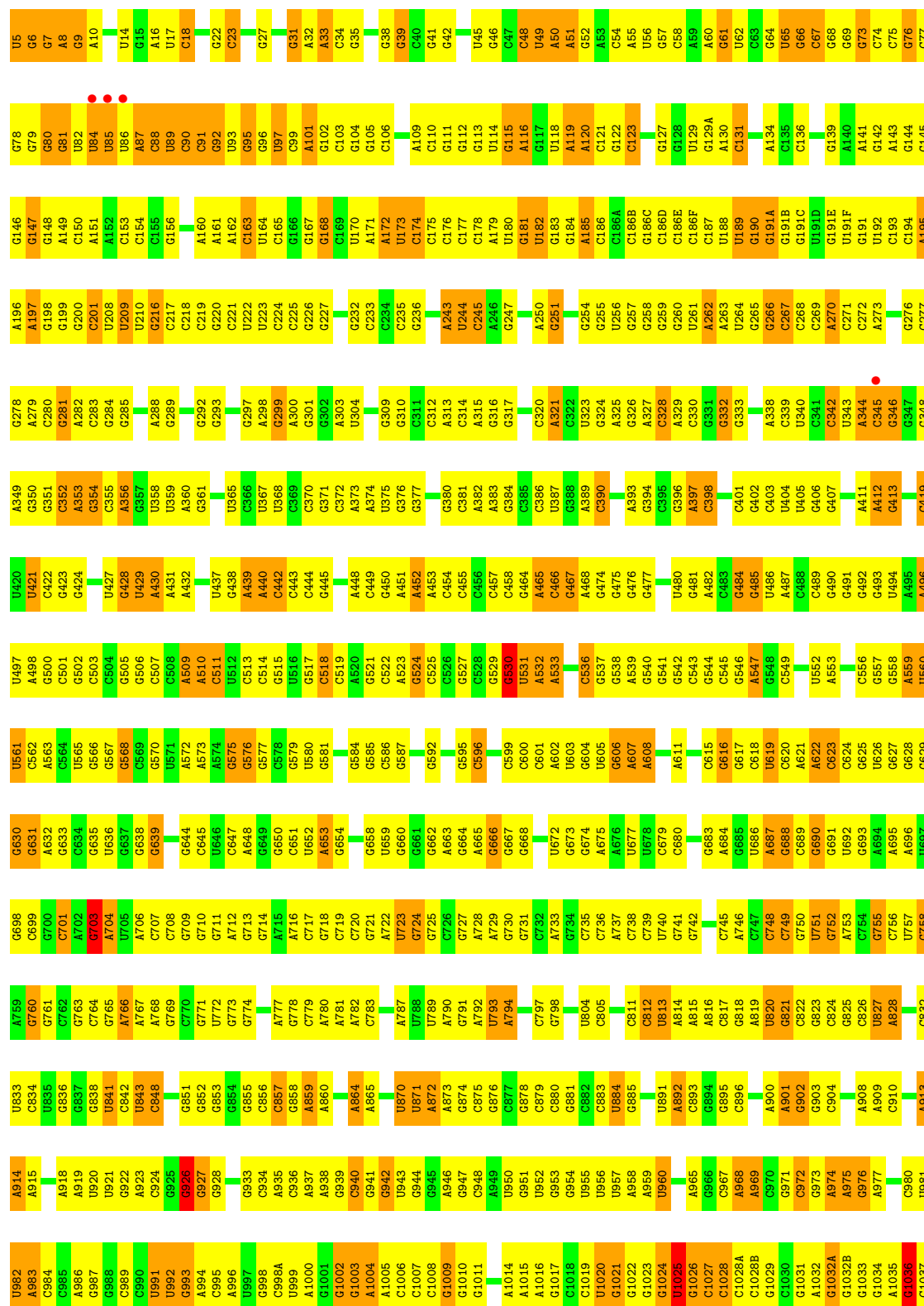
- Molecule 30: 50S ribosomal protein L35

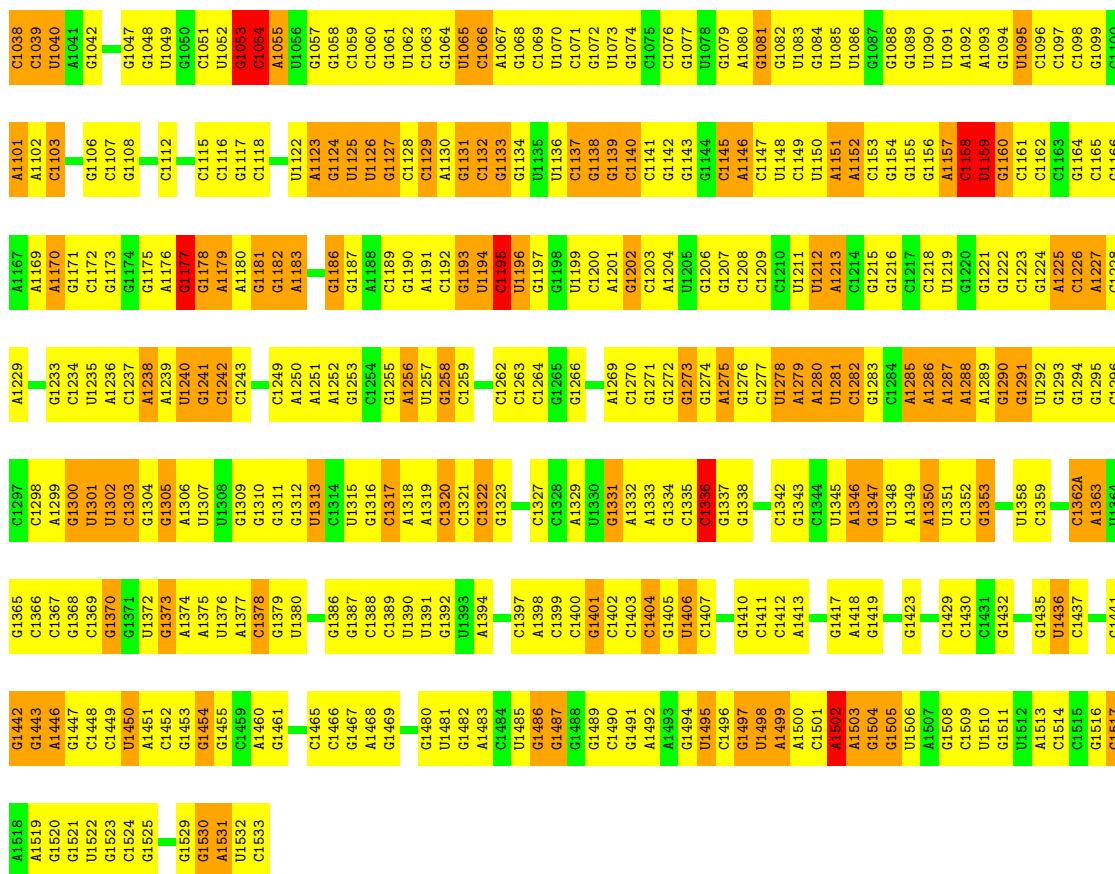
Chain B8: 



● Molecule 31: 16S ribosomal RNA

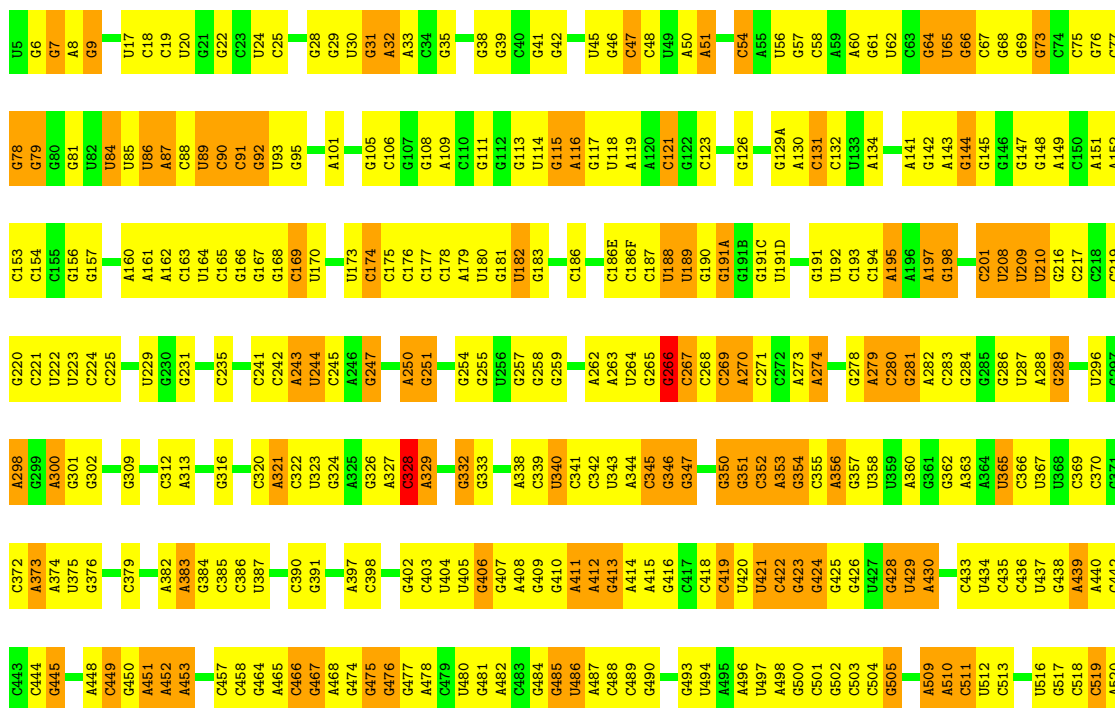
Chain CA:

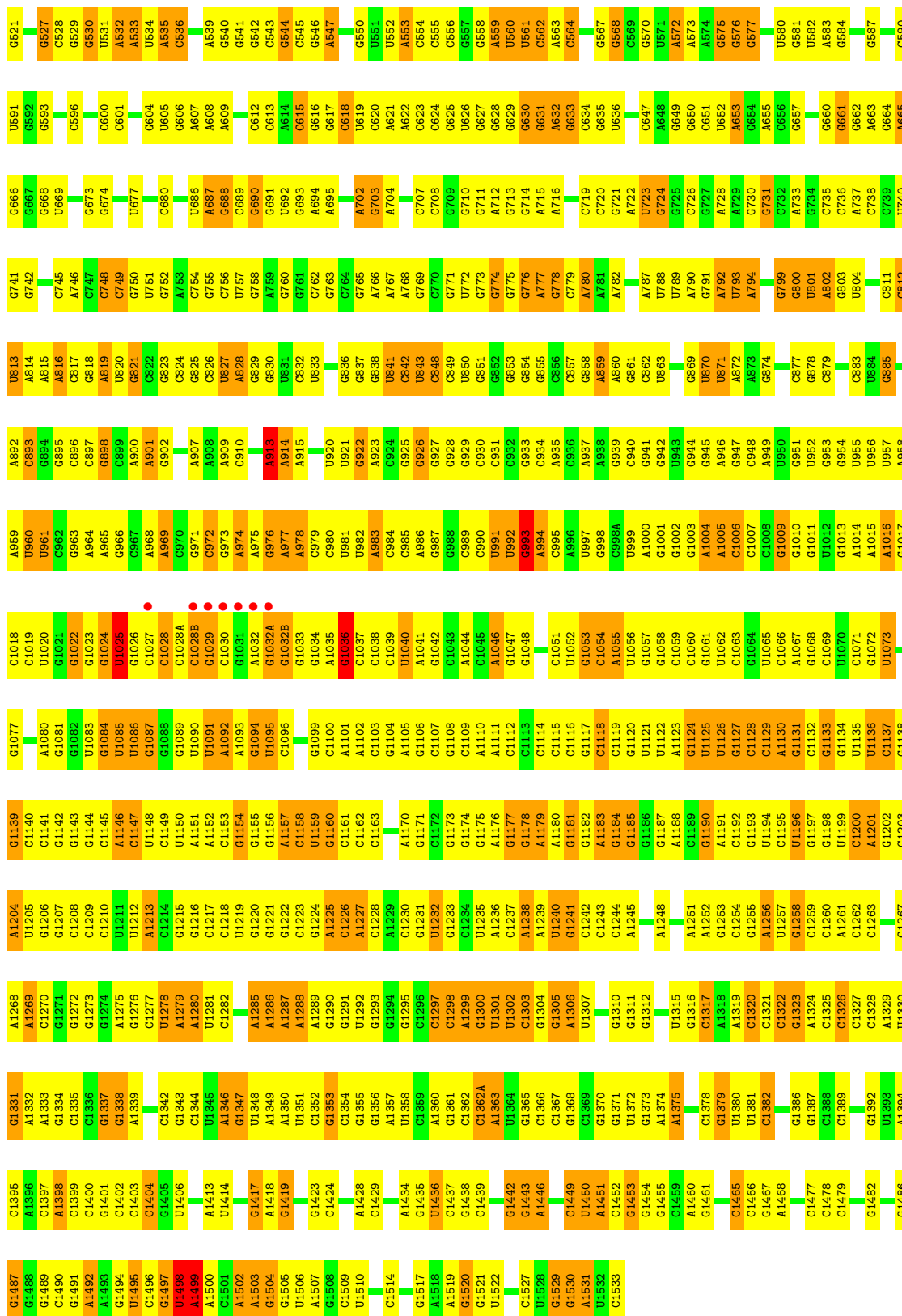




• Molecule 31: 16S ribosomal RNA

Chain DA:

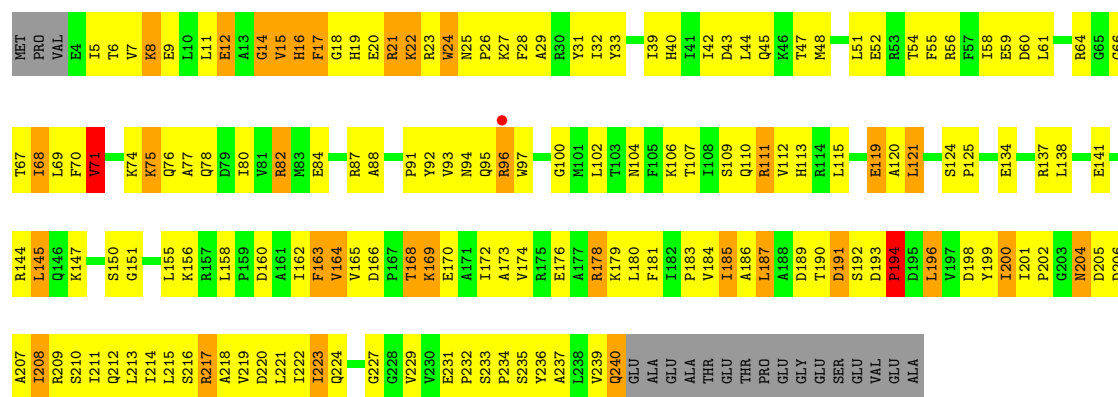




• Molecule 32: 30S RIBOSOMAL PROTEIN S2

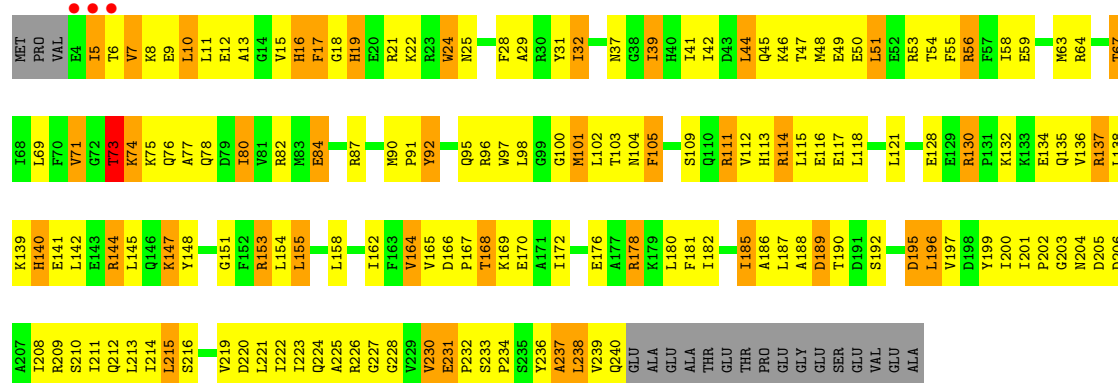
Chain CE:





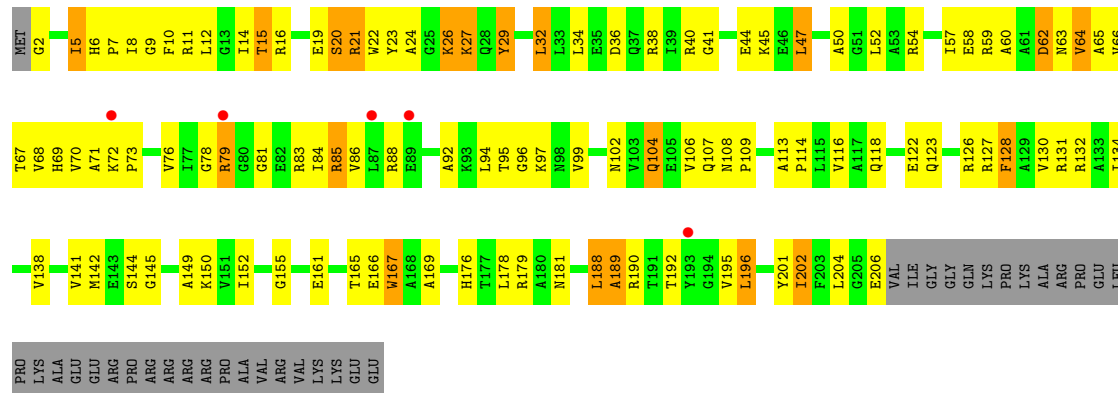
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain DE:



• Molecule 33: 30S RIBOSOMAL PROTEIN S3

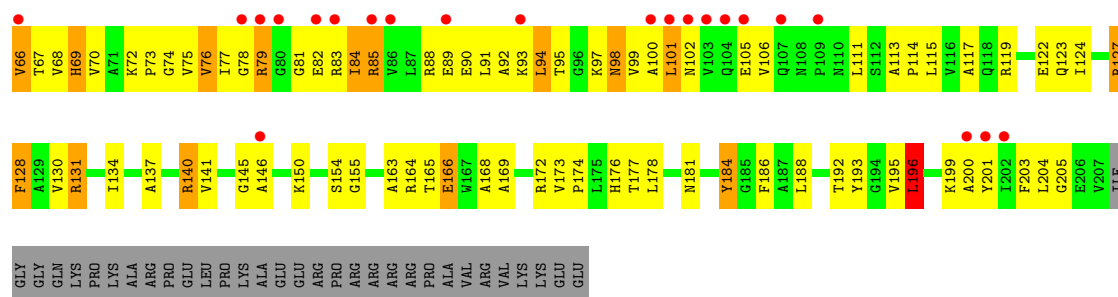
Chain CF:



• Molecule 33: 30S RIBOSOMAL PROTEIN S3

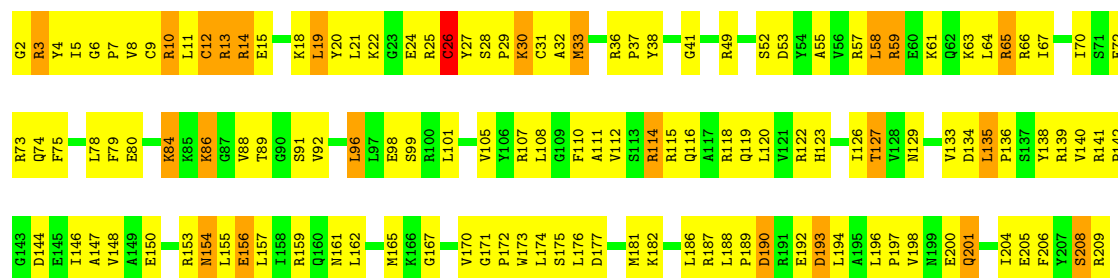
Chain DF:





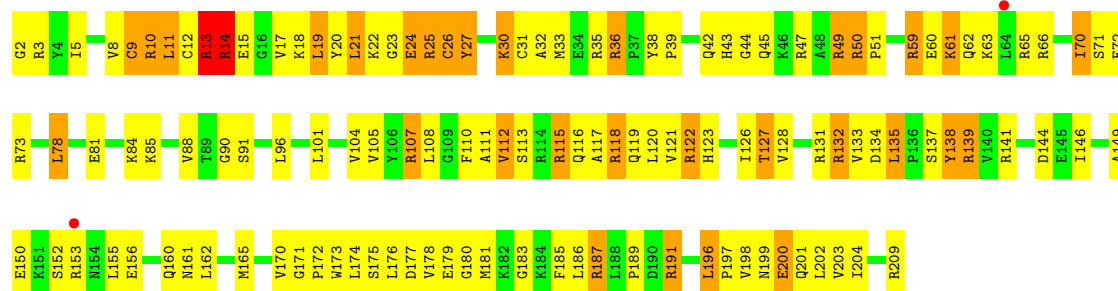
• Molecule 34: 30S RIBOSOMAL PROTEIN S4

Chain CG:



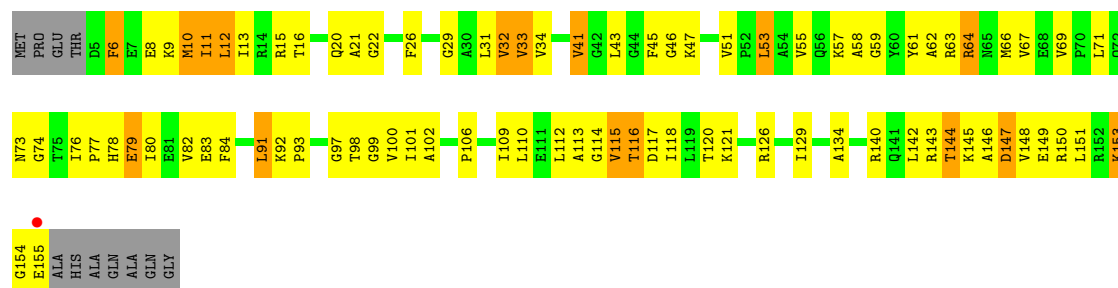
• Molecule 34: 30S RIBOSOMAL PROTEIN S4

Chain DG:



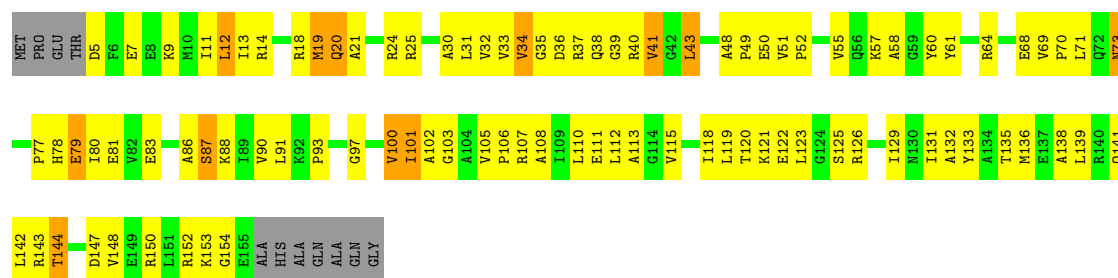
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain CH:



• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain DH:



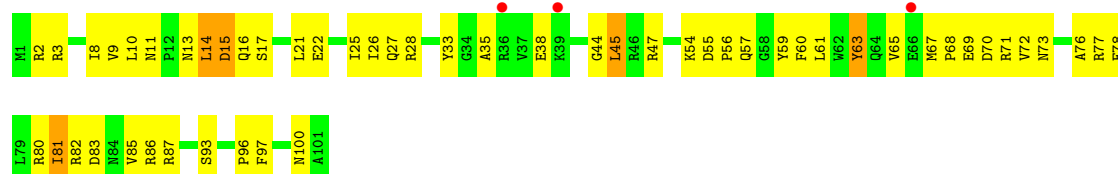
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain CI:



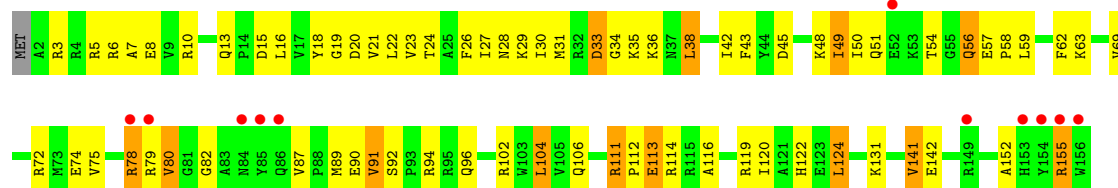
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain DI:



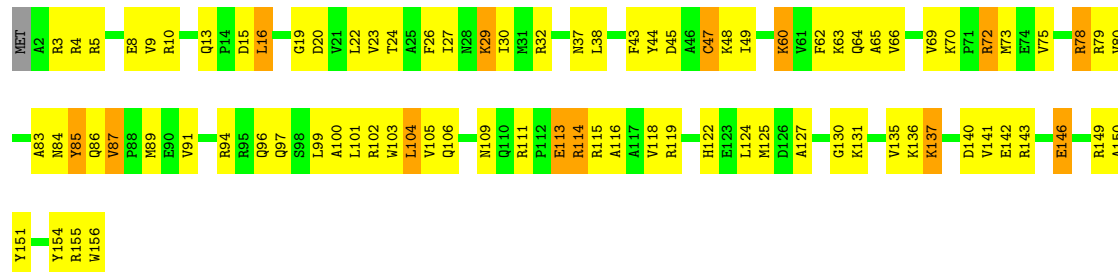
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



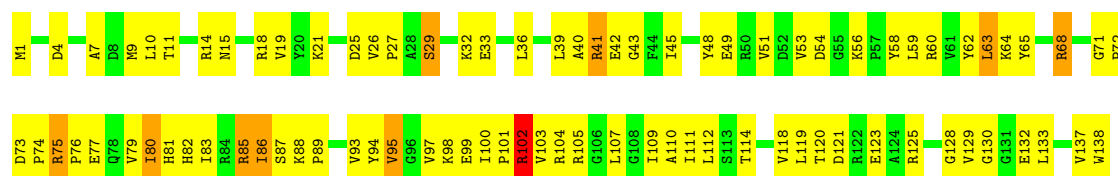
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain DJ:



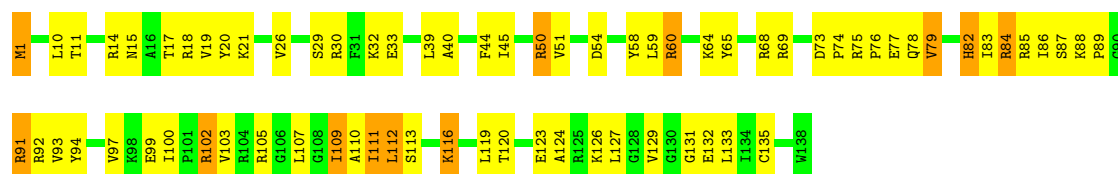
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain CK:



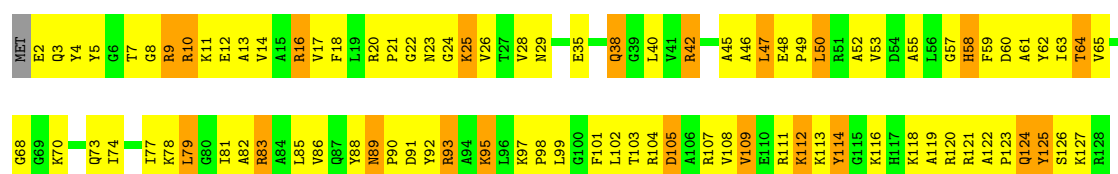
- Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain DK:



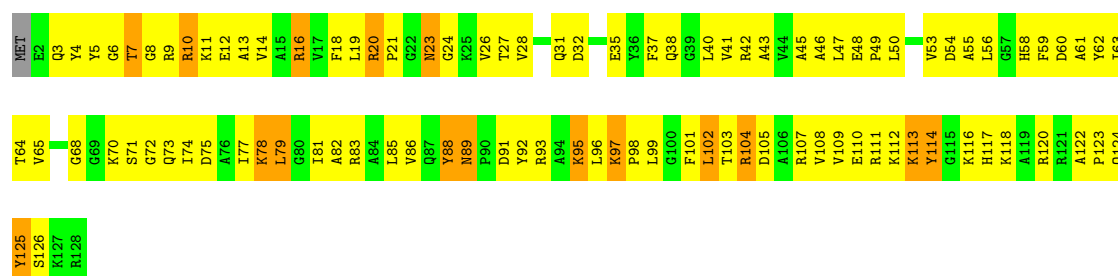
- Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain CL:



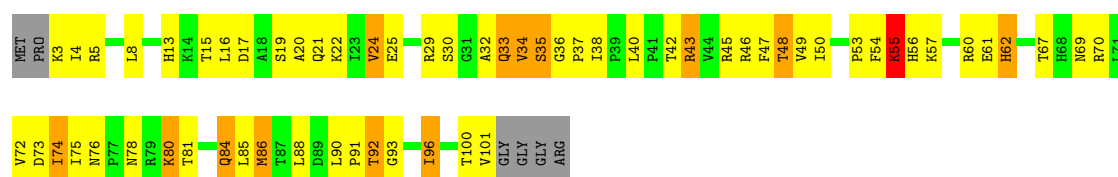
- Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain DL:



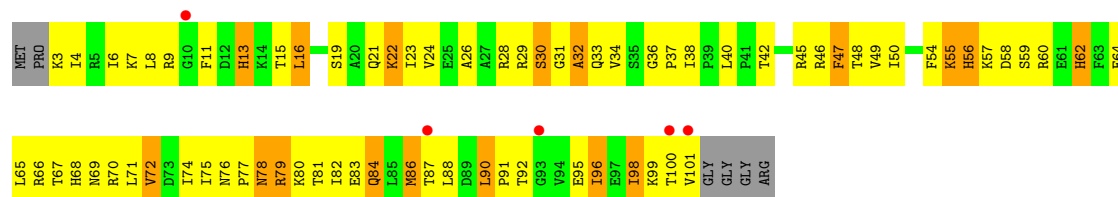
- Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain CM:



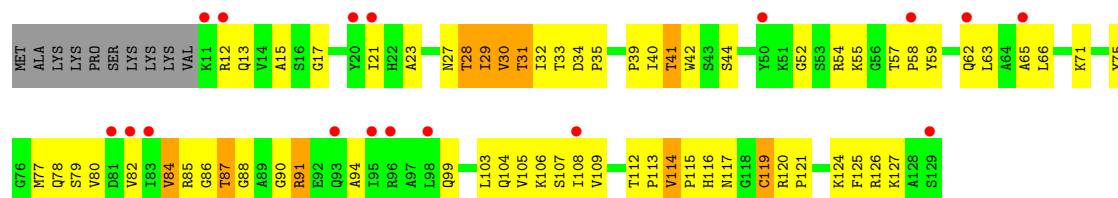
- Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain DM:



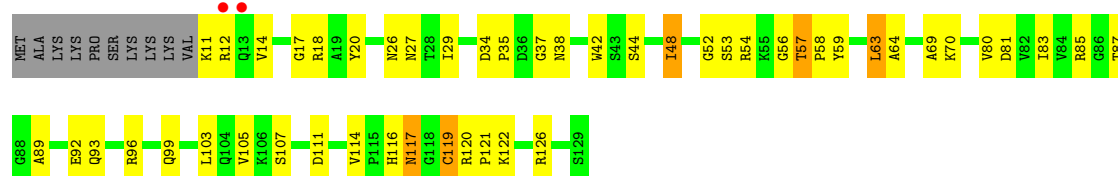
• Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain CN:



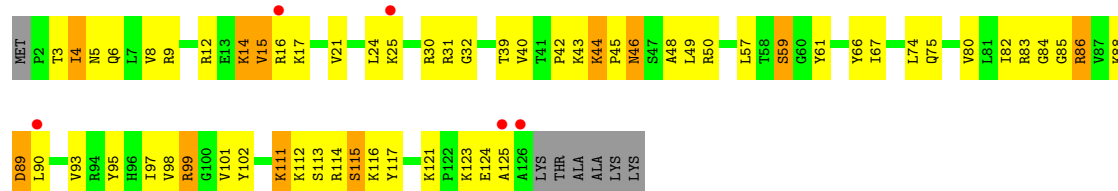
• Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain DN:



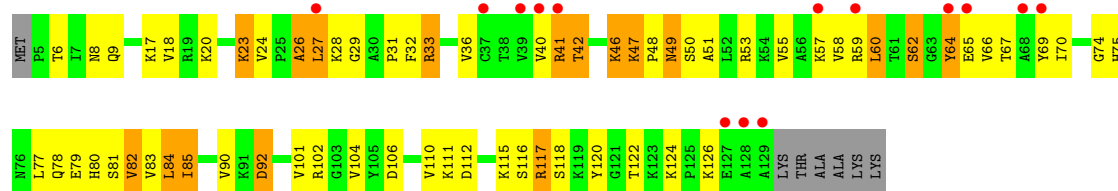
• Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain CO:



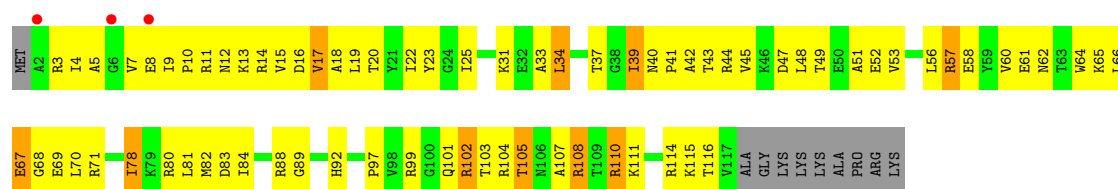
• Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain DO:



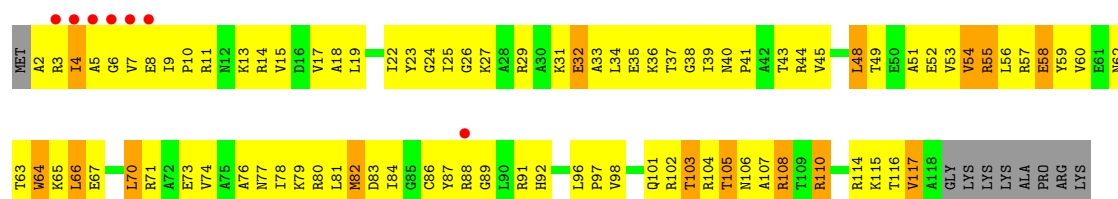
• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain CP:



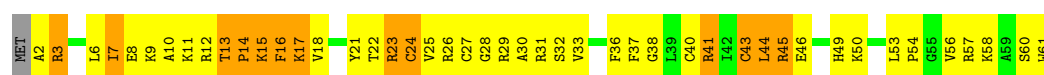
• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain DP:



• Molecule 44: 30S RIBOSOMAL PROTEIN S14

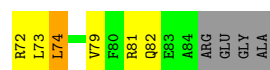
Chain CQ:





• Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain DS:



• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain CT:



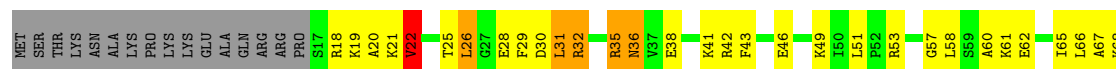
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain DT:



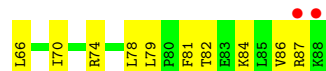
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain CU:



• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain DU:



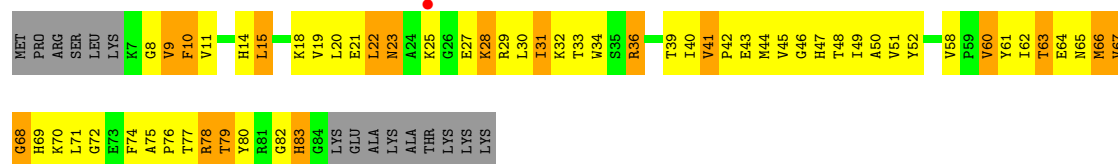
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain CV: 



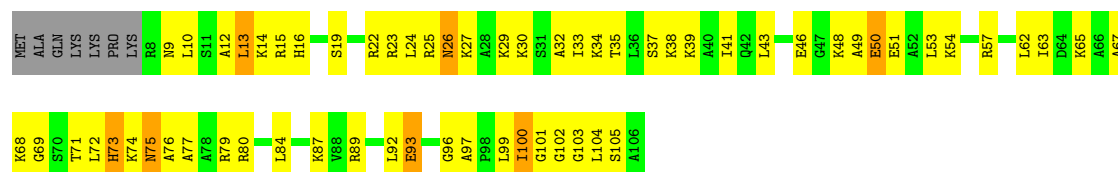
- Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain DV: 



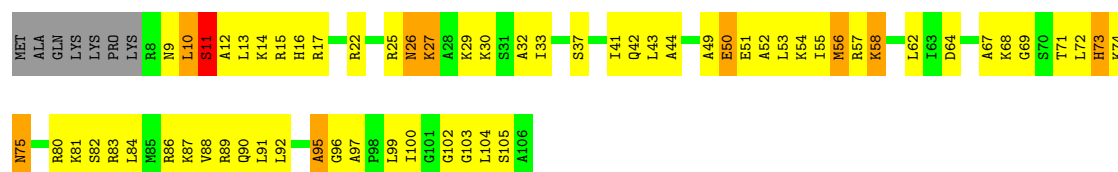
- Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain CW: 



- Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain DW: 



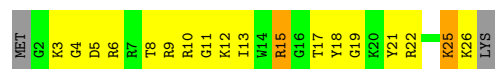
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain CX: 



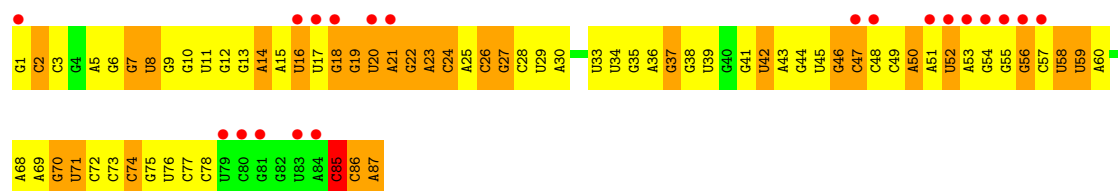
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain DX: 



- Molecule 52: TRNA-LEU

Chain CB: 



• Molecule 52: TRNA-LEU

Chain DB:



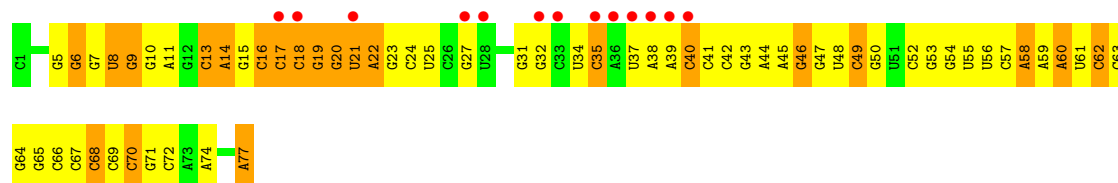
• Molecule 53: TRNA-FMET

Chain CC:



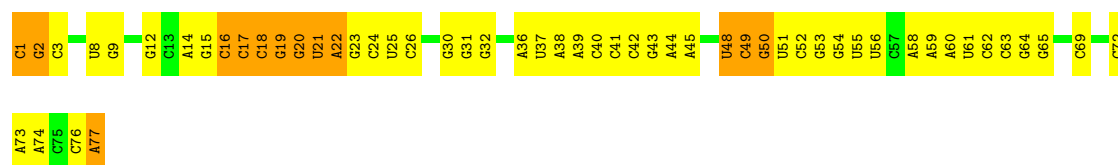
• Molecule 53: TRNA-FMET

Chain CD:



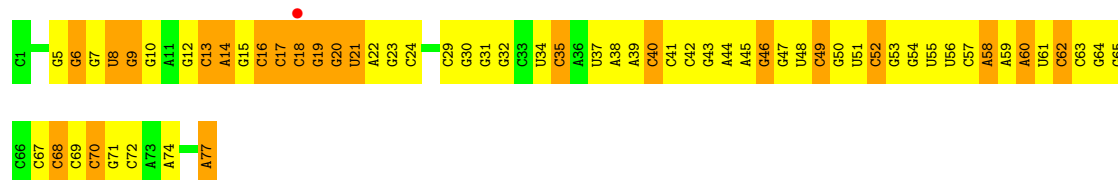
• Molecule 53: TRNA-FMET

Chain DC:



• Molecule 53: TRNA-FMET

Chain DD:



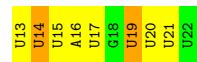
• Molecule 54: MRNA

Chain C1: 



• Molecule 54: MRNA

Chain D1: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 448.15Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.73 – 3.30 224.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (189.73-3.30) 95.4 (224.07-3.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.199 , 0.237 0.257 , 0.265	Depositor DCC
R_{free} test set	948 reflections (0.11%)	DCC
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 864978 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	299682	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, PAR

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	0.62	12/70233 (0.0%)	1.11	353/109643 (0.3%)
1	BA	0.56	6/70167 (0.0%)	1.03	240/109541 (0.2%)
2	AB	0.53	0/2928	1.07	13/4568 (0.3%)
2	BB	0.45	0/2928	0.93	6/4568 (0.1%)
3	AD	0.55	0/2165	0.81	3/2919 (0.1%)
3	BD	0.47	0/2165	0.73	1/2919 (0.0%)
4	AE	0.44	0/1601	0.73	1/2160 (0.0%)
4	BE	0.41	0/1601	0.72	1/2160 (0.0%)
5	AF	0.45	0/1620	0.72	0/2194
5	BF	0.38	0/1662	0.67	0/2249
6	AG	0.36	0/1499	0.60	0/2016
6	BG	0.30	0/1499	0.55	0/2016
7	AH	0.41	0/1332	0.71	0/1802
7	BH	0.29	0/1332	0.58	0/1802
8	AK	0.38	0/1151	0.72	1/1558 (0.1%)
8	BK	0.36	0/1151	0.66	1/1558 (0.1%)
9	AM	0.45	0/1131	0.71	0/1525
9	BM	0.32	0/1131	0.58	0/1525
10	AN	0.41	0/943	0.66	0/1269
10	BN	0.40	0/943	0.61	0/1269
11	AO	0.39	0/1162	0.71	1/1544 (0.1%)
11	BO	0.33	0/1162	0.64	1/1544 (0.1%)
12	AP	0.41	0/1143	0.59	0/1527
12	BP	0.33	0/1143	0.52	0/1527
13	A0	0.41	0/982	0.71	1/1312 (0.1%)
13	B0	0.40	0/974	0.67	0/1302
14	AQ	0.40	0/892	0.69	1/1187 (0.1%)
14	BQ	0.34	0/892	0.62	1/1187 (0.1%)
15	AR	0.45	0/1155	0.70	0/1542
15	BR	0.41	0/1155	0.63	0/1542
16	A1	0.46	0/982	0.67	0/1306
16	B1	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.44	0/790	0.71	0/1057
17	B2	0.33	0/790	0.59	0/1057
18	AS	0.43	0/911	0.69	0/1220
18	BS	0.42	0/911	0.65	0/1220
19	AT	0.52	0/739	0.69	0/993
19	BT	0.48	0/739	0.66	0/993
20	AU	0.48	0/798	0.72	0/1064
20	BU	0.43	0/798	0.72	0/1064
21	AV	0.35	0/1427	0.67	2/1935 (0.1%)
21	BV	0.28	0/1460	0.56	0/1982
22	A3	0.46	0/615	0.69	0/819
22	B3	0.40	0/621	0.64	0/827
23	AZ	0.46	0/770	0.78	0/1022
23	BZ	0.43	0/770	0.75	0/1022
24	AW	0.51	0/560	0.75	0/741
24	BW	0.40	0/583	0.62	0/771
25	AX	0.35	0/474	0.61	0/635
25	BX	0.33	0/474	0.54	0/635
26	A4	0.39	0/545	0.73	1/733 (0.1%)
26	B4	0.34	0/527	0.65	0/709
27	A5	0.45	0/473	0.67	0/639
27	B5	0.40	0/473	0.73	0/639
28	A6	0.47	0/396	0.68	0/529
28	B6	0.36	0/396	0.60	0/529
29	A7	0.50	0/438	0.71	0/575
29	B7	0.40	0/438	0.62	0/575
30	A8	0.56	0/494	0.87	0/649
30	B8	0.40	0/494	0.58	0/649
31	CA	0.49	1/36234 (0.0%)	0.94	68/56554 (0.1%)
31	DA	0.46	0/36237	0.90	64/56558 (0.1%)
32	CE	0.31	0/1959	0.55	0/2642
32	DE	0.30	0/1959	0.54	0/2642
33	CF	0.34	0/1629	0.54	0/2195
33	DF	0.32	0/1636	0.57	1/2205 (0.0%)
34	CG	0.42	1/1733 (0.1%)	0.62	0/2318
34	DG	0.38	0/1733	0.63	0/2318
35	CH	0.38	0/1171	0.58	0/1576
35	DH	0.34	0/1171	0.58	0/1576
36	CI	0.38	0/856	0.58	0/1154
36	DI	0.36	0/856	0.55	0/1154
37	CJ	0.31	0/1276	0.48	0/1709
37	DJ	0.32	0/1276	0.48	0/1709
38	CK	0.36	0/1136	0.64	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.31	0/1136	0.54	0/1527
39	CL	0.30	0/1029	0.52	0/1379
39	DL	0.29	0/1029	0.53	0/1379
40	CM	0.32	0/814	0.61	1/1095 (0.1%)
40	DM	0.31	0/814	0.59	0/1095
41	CN	0.37	0/900	0.61	0/1213
41	DN	0.36	0/900	0.59	0/1213
42	CO	0.45	0/991	0.75	1/1327 (0.1%)
42	DO	0.41	0/991	0.65	0/1327
43	CP	0.33	0/938	0.59	0/1258
43	DP	0.29	0/943	0.53	0/1265
44	CQ	0.42	1/501 (0.2%)	0.68	1/664 (0.2%)
44	DQ	0.32	0/501	0.57	0/664
45	CR	0.38	0/745	0.64	0/992
45	DR	0.35	0/745	0.53	0/992
46	CS	0.31	0/721	0.55	0/970
46	DS	0.38	0/721	0.60	0/970
47	CT	0.36	0/847	0.56	0/1131
47	DT	0.34	0/847	0.55	0/1131
48	CU	0.35	0/596	0.62	0/790
48	DU	0.36	0/596	0.57	0/790
49	CV	0.34	0/638	0.57	0/860
49	DV	0.29	0/638	0.63	0/860
50	CW	0.32	0/765	0.55	0/1007
50	DW	0.35	0/765	0.63	0/1007
51	CX	0.29	0/221	0.49	0/288
51	DX	0.27	0/221	0.48	0/288
52	CB	0.44	0/2080	0.80	1/3242 (0.0%)
52	DB	0.46	0/2080	0.80	3/3242 (0.1%)
53	CC	0.46	0/1835	0.85	0/2859
53	CD	0.28	0/1835	0.66	2/2859 (0.1%)
53	DC	0.44	0/1835	0.83	0/2859
53	DD	0.27	0/1835	0.63	1/2859 (0.0%)
54	C1	0.69	0/226	0.84	0/348
54	D1	0.58	0/226	0.81	0/348
All	All	0.51	21/324077 (0.0%)	0.93	771/485305 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	6
3	BD	0	3
4	AE	0	1
4	BE	0	6
5	BF	0	2
6	AG	0	1
6	BG	0	1
7	AH	0	2
7	BH	0	4
8	AK	0	5
8	BK	0	5
9	AM	0	1
11	AO	0	3
11	BO	0	3
13	B0	0	1
14	AQ	0	2
14	BQ	0	3
15	AR	0	2
16	A1	0	2
17	A2	0	1
20	BU	0	2
21	AV	0	3
21	BV	0	3
22	A3	0	2
24	AW	0	2
24	BW	0	1
26	A4	0	3
26	B4	0	1
27	A5	0	3
27	B5	0	1
28	A6	0	1
28	B6	0	1
30	A8	0	2
32	CE	0	3
32	DE	0	4
33	CF	0	1
33	DF	0	1
34	DG	0	1
38	CK	0	1
40	CM	0	1
40	DM	0	1
42	CO	0	2
44	CQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	DQ	0	1
45	CR	0	1
50	DW	0	1
All	All	0	98

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1143	A	N7-C5	-9.76	1.33	1.39
1	BA	1342	A	N7-C5	-8.93	1.33	1.39
1	BA	2873	A	N7-C5	-8.51	1.34	1.39
1	BA	2287	A	N9-C4	-8.15	1.32	1.37
1	AA	1021	A	N9-C4	-8.08	1.32	1.37

The worst 5 of 771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	1025	U	C5-C4-O4	-13.19	117.99	125.90
1	BA	933	A	C6-C5-N7	-12.57	123.50	132.30
1	AA	1899	G	N3-C4-N9	-12.39	118.57	126.00
1	BA	1899	G	N3-C4-N9	-12.35	118.59	126.00
1	BA	2720	U	C2-N3-C4	-11.91	119.85	127.00

There are no chirality outliers.

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	122	ASP	Peptide
3	AD	236	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	28	GLU	Peptide
3	AD	47	GLY	Peptide

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	62707	0	31613	2746	0
1	BA	62647	0	31583	2774	1
2	AB	2617	0	1328	105	0
2	BB	2617	0	1328	133	0
3	AD	2115	0	2195	263	0
3	BD	2115	0	2195	244	0
4	AE	1568	0	1634	288	0
4	BE	1568	0	1634	286	0
5	AF	1585	0	1632	143	0
5	BF	1627	0	1680	208	0
6	AG	1474	0	1535	200	0
6	BG	1474	0	1535	164	0
7	AH	1307	0	1382	158	0
7	BH	1307	0	1382	148	2
8	AK	1136	0	1223	128	0
8	BK	1136	0	1223	102	0
9	AM	1104	0	1180	139	0
9	BM	1104	0	1180	102	0
10	AN	933	0	996	53	0
10	BN	933	0	996	68	0
11	AO	1145	0	1228	245	0
11	BO	1145	0	1228	306	0
12	AP	1122	0	1179	208	0
12	BP	1122	0	1179	250	0
13	A0	968	0	1033	81	0
13	B0	960	0	1021	82	0
14	AQ	882	0	943	101	0
14	BQ	882	0	943	104	0
15	AR	1141	0	1202	128	0
15	BR	1141	0	1202	132	0
16	A1	964	0	1022	109	0
16	B1	964	0	1022	108	0
17	A2	779	0	852	98	1
17	B2	779	0	852	182	0
18	AS	900	0	964	86	0
18	BS	900	0	964	56	0
19	AT	725	0	778	60	0
19	BT	725	0	778	60	0
20	AU	785	0	878	95	0
20	BU	785	0	878	113	0
21	AV	1397	0	1430	140	0
21	BV	1428	0	1454	142	0
22	A3	607	0	628	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B3	613	0	633	59	0
23	AZ	763	0	848	61	0
23	BZ	763	0	848	59	0
24	AW	558	0	610	47	0
24	BW	581	0	629	63	0
25	AX	469	0	518	36	0
25	BX	469	0	518	33	0
26	A4	533	0	522	78	0
26	B4	515	0	510	109	0
27	A5	459	0	480	78	1
27	B5	459	0	480	72	0
28	A6	389	0	404	90	0
28	B6	389	0	404	110	0
29	A7	430	0	480	28	0
29	B7	430	0	480	32	0
30	A8	488	0	560	105	0
30	B8	488	0	560	153	0
31	CA	32369	0	16339	1550	2
31	DA	32372	0	16338	1515	1
32	CE	1924	0	1975	186	0
32	DE	1924	0	1975	206	0
33	CF	1605	0	1668	123	0
33	DF	1612	0	1677	160	0
34	CG	1703	0	1764	180	0
34	DG	1703	0	1763	158	1
35	CH	1155	0	1213	81	0
35	DH	1155	0	1213	91	0
36	CI	843	0	857	59	1
36	DI	843	0	857	48	0
37	CJ	1257	0	1296	72	0
37	DJ	1257	0	1296	90	0
38	CK	1116	0	1177	100	0
38	DK	1116	0	1177	62	0
39	CL	1010	0	1037	111	0
39	DL	1010	0	1037	130	0
40	CM	801	0	849	86	0
40	DM	801	0	849	95	0
41	CN	885	0	904	76	0
41	DN	885	0	904	45	0
42	CO	975	0	1062	63	0
42	DO	975	0	1062	89	0
43	CP	928	0	987	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DP	933	0	992	108	0
44	CQ	492	0	529	55	0
44	DQ	492	0	529	56	0
45	CR	734	0	771	55	0
45	DR	734	0	771	44	0
46	CS	705	0	725	63	0
46	DS	705	0	725	45	0
47	CT	834	0	904	79	0
47	DT	834	0	904	44	0
48	CU	591	0	662	31	0
48	DU	591	0	662	43	0
49	CV	624	0	636	74	0
49	DV	624	0	636	100	0
50	CW	763	0	861	76	0
50	DW	763	0	861	71	0
51	CX	217	0	234	20	0
51	DX	217	0	234	28	0
52	CB	1861	0	938	84	0
52	DB	1861	0	938	82	0
53	CC	1643	0	837	69	0
53	CD	1643	0	837	98	0
53	DC	1643	0	837	78	0
53	DD	1643	0	837	111	0
54	C1	205	0	103	9	0
54	D1	205	0	103	9	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	2	0	0	0	0
55	AA	626	0	0	0	0
55	AB	17	0	0	0	0
55	AD	1	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	AZ	1	0	0	0	0
55	B1	1	0	0	0	0
55	B3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B5	1	0	0	0	0
55	BA	528	0	0	0	0
55	BB	15	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BP	1	0	0	0	0
55	BR	2	0	0	0	0
55	C1	1	0	0	0	0
55	CA	240	0	0	0	0
55	CB	5	0	0	0	0
55	CC	7	0	0	0	0
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CN	2	0	0	0	0
55	CQ	2	0	0	0	0
55	CT	1	0	0	0	0
55	DA	204	0	0	0	0
55	DB	2	0	0	0	0
55	DC	8	0	0	0	0
55	DG	2	0	0	0	0
55	DH	1	0	0	0	0
55	DS	1	0	0	0	0
56	CA	42	0	45	4	0
56	DA	42	0	45	5	0
57	CG	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	299682	0	201028	17558	5

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 35.

The worst 5 of 17558 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:BO:62:LEU:CD1	30:B8:30:ARG:HH11	1.03	1.63
11:BO:71:VAL:CG1	11:BO:72:PRO:HD3	1.32	1.59
4:AE:23:VAL:HG12	4:AE:185:LYS:CA	1.33	1.59
1:BA:2015:A:C1'	27:B5:2:ALA:HA	1.42	1.48
4:BE:51:PHE:CG	4:BE:52:LEU:HB3	1.45	1.47

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:276:A:OP2	31:DA:86:U:O2'[3_555]	1.96	0.24
7:BH:100:GLY:O	31:CA:85:U:O2'[3_545]	2.02	0.18
36:CI:15:ASP:OD2	34:DG:27:TYR:OH[4_555]	2.06	0.14
7:BH:132:ARG:O	31:CA:84:U:N3[3_545]	2.18	0.02
17:A2:51:VAL:N	27:A5:60:VAL:O[4_465]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/276 (98%)	244 (90%)	20 (7%)	6 (2%)	10	55
3	BD	270/276 (98%)	246 (91%)	15 (6%)	9 (3%)	6	43
4	AE	203/206 (98%)	149 (73%)	37 (18%)	17 (8%)	1	12
4	BE	203/206 (98%)	149 (73%)	34 (17%)	20 (10%)	1	8
5	AF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
5	BF	206/210 (98%)	172 (84%)	29 (14%)	5 (2%)	9	53
6	AG	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	5	37
6	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	33	83
7	AH	168/180 (93%)	135 (80%)	25 (15%)	8 (5%)	4	30
7	BH	168/180 (93%)	129 (77%)	37 (22%)	2 (1%)	19	71
8	AK	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	3	25
8	BK	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	11	56
9	AM	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	4	32
9	BM	136/140 (97%)	120 (88%)	12 (9%)	4 (3%)	7	47
10	AN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	BN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	27	78
11	AO	148/150 (99%)	101 (68%)	31 (21%)	16 (11%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	BO	148/150 (99%)	95 (64%)	32 (22%)	21 (14%)	0	2
12	AP	139/141 (99%)	101 (73%)	19 (14%)	19 (14%)	0	2
12	BP	139/141 (99%)	88 (63%)	34 (24%)	17 (12%)	1	4
13	A0	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	25	76
13	B0	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	AQ	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	13	61
14	BQ	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	5	39
15	AR	135/146 (92%)	111 (82%)	22 (16%)	2 (2%)	15	65
15	BR	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
16	A1	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	25	76
16	B1	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	25	76
17	A2	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	7	46
17	B2	99/101 (98%)	73 (74%)	13 (13%)	13 (13%)	0	3
18	AS	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	25	76
18	BS	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
19	AT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	10	55
19	BT	90/96 (94%)	81 (90%)	8 (9%)	1 (1%)	21	73
20	AU	100/110 (91%)	84 (84%)	10 (10%)	6 (6%)	2	22
20	BU	100/110 (91%)	67 (67%)	27 (27%)	6 (6%)	2	22
21	AV	173/206 (84%)	131 (76%)	35 (20%)	7 (4%)	5	36
21	BV	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	4	32
22	A3	74/85 (87%)	68 (92%)	4 (5%)	2 (3%)	8	49
22	B3	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	AZ	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	6	43
23	BZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	21	73
24	AW	64/72 (89%)	60 (94%)	1 (2%)	3 (5%)	4	30
24	BW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	15	65
25	AX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	BX	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	A4	64/71 (90%)	42 (66%)	20 (31%)	2 (3%)	7	45
26	B4	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	A5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	13	61
27	B5	57/60 (95%)	48 (84%)	6 (10%)	3 (5%)	3	26
28	A6	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	4	30
28	B6	43/54 (80%)	26 (60%)	11 (26%)	6 (14%)	0	2
29	A7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	B7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	A8	59/65 (91%)	54 (92%)	4 (7%)	1 (2%)	14	62
30	B8	59/65 (91%)	42 (71%)	10 (17%)	7 (12%)	1	4
32	CE	235/256 (92%)	190 (81%)	44 (19%)	1 (0%)	43	89
32	DE	235/256 (92%)	186 (79%)	45 (19%)	4 (2%)	14	62
33	CF	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
33	DF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	22	74
34	CG	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	38	86
34	DG	206/208 (99%)	177 (86%)	28 (14%)	1 (0%)	38	86
35	CH	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	30	81
35	DH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
36	DI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
37	CJ	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
37	DJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
38	CK	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	30	81
38	DK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	CL	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
39	DL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	CM	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
40	DM	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	11	56
41	CN	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
41	DN	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
42	CO	123/132 (93%)	108 (88%)	13 (11%)	2 (2%)	14	64
42	DO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	14	64
43	CP	114/126 (90%)	90 (79%)	24 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DP	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	25	76
44	CQ	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	6	42
44	DQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	14	62
45	CR	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
45	DR	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
46	CS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
46	DS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	CT	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	11	58
47	DT	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
48	CU	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	16	67
48	DU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	CV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	8	50
49	DV	76/93 (82%)	58 (76%)	13 (17%)	5 (7%)	2	19
50	CW	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	22	74
50	DW	97/106 (92%)	81 (84%)	15 (16%)	1 (1%)	22	74
51	CX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
51	DX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
All	All	11336/12052 (94%)	9645 (85%)	1396 (12%)	295 (3%)	8	50

5 of 295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	237	GLU
3	AD	271	ILE
4	AE	15	PHE
4	AE	19	ARG
4	AE	23	VAL

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	
3	AD	214/218 (98%)	176 (82%)	38 (18%)	2	13
3	BD	214/218 (98%)	163 (76%)	51 (24%)	1	4
4	AE	165/166 (99%)	119 (72%)	46 (28%)	0	2
4	BE	165/166 (99%)	127 (77%)	38 (23%)	1	5
5	AF	161/166 (97%)	125 (78%)	36 (22%)	1	6
5	BF	165/166 (99%)	124 (75%)	41 (25%)	1	3
6	AG	155/156 (99%)	121 (78%)	34 (22%)	1	7
6	BG	155/156 (99%)	116 (75%)	39 (25%)	1	3
7	AH	142/148 (96%)	110 (78%)	32 (22%)	1	6
7	BH	142/148 (96%)	118 (83%)	24 (17%)	3	15
8	AK	122/124 (98%)	99 (81%)	23 (19%)	2	11
8	BK	122/124 (98%)	89 (73%)	33 (27%)	1	2
9	AM	117/119 (98%)	88 (75%)	29 (25%)	1	3
9	BM	117/119 (98%)	95 (81%)	22 (19%)	2	11
10	AN	100/100 (100%)	86 (86%)	14 (14%)	5	25
10	BN	100/100 (100%)	80 (80%)	20 (20%)	2	9
11	AO	116/116 (100%)	81 (70%)	35 (30%)	0	1
11	BO	116/116 (100%)	76 (66%)	40 (34%)	0	1
12	AP	111/111 (100%)	86 (78%)	25 (22%)	1	6
12	BP	111/111 (100%)	86 (78%)	25 (22%)	1	6
13	A0	101/101 (100%)	80 (79%)	21 (21%)	2	8
13	B0	100/101 (99%)	81 (81%)	19 (19%)	2	11
14	AQ	87/88 (99%)	69 (79%)	18 (21%)	2	8
14	BQ	87/88 (99%)	66 (76%)	21 (24%)	1	4
15	AR	120/127 (94%)	91 (76%)	29 (24%)	1	4
15	BR	120/127 (94%)	84 (70%)	36 (30%)	0	1
16	A1	93/94 (99%)	77 (83%)	16 (17%)	3	15
16	B1	93/94 (99%)	80 (86%)	13 (14%)	5	25
17	A2	82/82 (100%)	59 (72%)	23 (28%)	0	2
17	B2	82/82 (100%)	54 (66%)	28 (34%)	0	1
18	AS	92/92 (100%)	72 (78%)	20 (22%)	1	7
18	BS	92/92 (100%)	66 (72%)	26 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AT	74/78 (95%)	58 (78%)	16 (22%)	1	7
19	BT	74/78 (95%)	60 (81%)	14 (19%)	2	11
20	AU	85/91 (93%)	68 (80%)	17 (20%)	2	9
20	BU	85/91 (93%)	61 (72%)	24 (28%)	0	2
21	AV	154/179 (86%)	123 (80%)	31 (20%)	2	8
21	BV	158/179 (88%)	130 (82%)	28 (18%)	3	13
22	A3	61/67 (91%)	52 (85%)	9 (15%)	4	21
22	B3	62/67 (92%)	50 (81%)	12 (19%)	2	10
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	5	23
23	BZ	82/83 (99%)	66 (80%)	16 (20%)	2	9
24	AW	62/67 (92%)	46 (74%)	16 (26%)	1	3
24	BW	64/67 (96%)	51 (80%)	13 (20%)	2	8
25	AX	51/52 (98%)	47 (92%)	4 (8%)	18	60
25	BX	51/52 (98%)	38 (74%)	13 (26%)	1	3
26	A4	59/63 (94%)	42 (71%)	17 (29%)	0	2
26	B4	57/63 (90%)	41 (72%)	16 (28%)	0	2
27	A5	51/52 (98%)	37 (72%)	14 (28%)	0	2
27	B5	51/52 (98%)	38 (74%)	13 (26%)	1	3
28	A6	44/52 (85%)	28 (64%)	16 (36%)	0	1
28	B6	44/52 (85%)	29 (66%)	15 (34%)	0	1
29	A7	42/42 (100%)	35 (83%)	7 (17%)	3	16
29	B7	42/42 (100%)	30 (71%)	12 (29%)	0	2
30	A8	51/55 (93%)	41 (80%)	10 (20%)	2	9
30	B8	51/55 (93%)	37 (72%)	14 (28%)	0	2
32	CE	205/220 (93%)	164 (80%)	41 (20%)	2	9
32	DE	205/220 (93%)	168 (82%)	37 (18%)	2	13
33	CF	159/188 (85%)	132 (83%)	27 (17%)	3	15
33	DF	160/188 (85%)	129 (81%)	31 (19%)	2	10
34	CG	180/180 (100%)	150 (83%)	30 (17%)	3	16
34	DG	180/180 (100%)	141 (78%)	39 (22%)	1	7
35	CH	116/123 (94%)	94 (81%)	22 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DH	116/123 (94%)	97 (84%)	19 (16%)	3	16
36	CI	90/90 (100%)	78 (87%)	12 (13%)	6	27
36	DI	90/90 (100%)	78 (87%)	12 (13%)	6	27
37	CJ	126/127 (99%)	105 (83%)	21 (17%)	3	16
37	DJ	126/127 (99%)	100 (79%)	26 (21%)	2	8
38	CK	119/119 (100%)	106 (89%)	13 (11%)	9	38
38	DK	119/119 (100%)	102 (86%)	17 (14%)	5	23
39	CL	98/99 (99%)	69 (70%)	29 (30%)	0	1
39	DL	98/99 (99%)	72 (74%)	26 (26%)	1	2
40	CM	89/92 (97%)	69 (78%)	20 (22%)	1	6
40	DM	89/92 (97%)	65 (73%)	24 (27%)	1	2
41	CN	90/99 (91%)	77 (86%)	13 (14%)	5	23
41	DN	90/99 (91%)	79 (88%)	11 (12%)	7	32
42	CO	104/109 (95%)	88 (85%)	16 (15%)	4	20
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	12
43	CP	94/101 (93%)	76 (81%)	18 (19%)	2	10
43	DP	94/101 (93%)	77 (82%)	17 (18%)	2	12
44	CQ	49/50 (98%)	34 (69%)	15 (31%)	0	1
44	DQ	49/50 (98%)	37 (76%)	12 (24%)	1	3
45	CR	79/80 (99%)	69 (87%)	10 (13%)	6	30
45	DR	79/80 (99%)	68 (86%)	11 (14%)	5	25
46	CS	72/74 (97%)	58 (81%)	14 (19%)	2	10
46	DS	72/74 (97%)	58 (81%)	14 (19%)	2	10
47	CT	95/97 (98%)	83 (87%)	12 (13%)	7	31
47	DT	95/97 (98%)	88 (93%)	7 (7%)	20	63
48	CU	63/77 (82%)	51 (81%)	12 (19%)	2	11
48	DU	63/77 (82%)	50 (79%)	13 (21%)	2	8
49	CV	67/80 (84%)	50 (75%)	17 (25%)	1	3
49	DV	67/80 (84%)	53 (79%)	14 (21%)	1	8
50	CW	76/82 (93%)	64 (84%)	12 (16%)	4	18
50	DW	76/82 (93%)	62 (82%)	14 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	CX	20/22 (91%)	15 (75%)	5 (25%)	1	3
51	DX	20/22 (91%)	18 (90%)	2 (10%)	11	43
All	All	9579/9996 (96%)	7581 (79%)	1998 (21%)	1	8

5 of 1998 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	BO	101	VAL
20	BU	96	ILE
40	DM	30	SER
12	BP	83	MET
15	BR	134	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such sidechains are listed below:

Mol	Chain	Res	Type
16	B1	49	HIS
23	BZ	66	HIS
40	DM	13	HIS
17	B2	64	HIS
19	BT	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	700 (24%)	52 (1%)
1	BA	2908/2912 (99%)	711 (24%)	53 (1%)
2	AB	121/122 (99%)	29 (23%)	0
2	BB	121/122 (99%)	29 (23%)	0
31	CA	1506/1506 (100%)	346 (22%)	35 (2%)
31	DA	1505/1506 (99%)	353 (23%)	49 (3%)
52	CB	86/87 (98%)	37 (43%)	4 (4%)
52	DB	86/87 (98%)	33 (38%)	3 (3%)
53	CC	77/77 (100%)	17 (22%)	4 (5%)
53	CD	76/77 (98%)	27 (35%)	1 (1%)
53	DC	77/77 (100%)	17 (22%)	4 (5%)
53	DD	76/77 (98%)	26 (34%)	1 (1%)
54	C1	9/10 (90%)	2 (22%)	0
54	D1	9/10 (90%)	2 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9568/9582 (99%)	2329 (24%)	206 (2%)

5 of 2329 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	G
1	AA	5	A
1	AA	10	G
1	AA	34	C
1	AA	35	G

5 of 206 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2282	G
31	CA	428	G
31	DA	1305	G
1	BA	2422	A
1	BA	2893	G

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 1703 ligands modelled in this entry, 1701 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	$\# Z > 2$
56	PAR	CA	1841	-	45,45,45	0.54	0	67,67,67	1.44	11 (16%)
56	PAR	DA	1805	-	45,45,45	0.56	0	67,67,67	1.67	16 (23%)

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
56	PAR	CA	1841	-	-	0/18/94/94	0/4/4/4
56	PAR	DA	1805	-	-	0/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	1805	PAR	C13-O52-C52	-4.22	107.28	118.00
56	DA	1805	PAR	O54-C54-C64	4.03	113.64	105.97
56	DA	1805	PAR	C11-O51-C51	4.02	121.51	113.73
56	CA	1841	PAR	C41-C31-C21	-3.86	104.72	111.39
56	CA	1841	PAR	O54-C54-C64	3.84	113.28	105.97

There are no chirality outliers.

There are no torsion outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.16	38 (1%) 74 27	50, 81, 215, 247	0
1	BA	2909/2912 (99%)	-0.23	42 (1%) 72 25	60, 95, 235, 249	0
2	AB	122/122 (100%)	-0.37	1 (0%) 83 39	81, 105, 124, 182	0
2	BB	122/122 (100%)	-0.37	2 (1%) 68 22	98, 133, 156, 203	0
3	AD	272/276 (98%)	0.48	2 (0%) 84 42	47, 72, 94, 112	0
3	BD	272/276 (98%)	0.40	3 (1%) 77 30	56, 82, 103, 138	0
4	AE	205/206 (99%)	0.47	7 (3%) 43 10	55, 91, 137, 149	0
4	BE	205/206 (99%)	0.59	11 (5%) 25 6	66, 104, 153, 172	0
5	AF	202/210 (96%)	-0.06	0 100 100	52, 84, 123, 137	0
5	BF	208/210 (99%)	0.51	9 (4%) 34 8	64, 108, 166, 191	0
6	AG	181/182 (99%)	0.78	14 (7%) 13 4	95, 115, 143, 157	0
6	BG	181/182 (99%)	0.78	18 (9%) 8 2	125, 148, 169, 176	0
7	AH	170/180 (94%)	0.12	2 (1%) 75 29	89, 119, 138, 160	0
7	BH	170/180 (94%)	1.95	59 (34%) 1 0	161, 203, 224, 232	0
8	AK	146/148 (98%)	0.33	2 (1%) 72 25	85, 134, 151, 157	0
8	BK	146/148 (98%)	0.20	1 (0%) 84 42	91, 134, 158, 167	0
9	AM	138/140 (98%)	0.14	2 (1%) 72 25	70, 95, 131, 144	0
9	BM	138/140 (98%)	1.06	15 (10%) 6 2	86, 118, 148, 158	0
10	AN	122/122 (100%)	0.37	1 (0%) 83 39	63, 82, 98, 111	0
10	BN	122/122 (100%)	0.41	0 100 100	76, 98, 117, 133	0
11	AO	150/150 (100%)	0.08	2 (1%) 74 27	45, 90, 122, 167	0
11	BO	150/150 (100%)	0.33	5 (3%) 44 10	44, 101, 149, 186	0
12	AP	141/141 (100%)	0.34	3 (2%) 60 17	58, 91, 116, 142	0
12	BP	141/141 (100%)	1.03	18 (12%) 4 2	58, 107, 142, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	0.13	0 100 100	64, 90, 109, 123	0
13	B0	117/118 (99%)	0.01	0 100 100	68, 90, 113, 128	0
14	AQ	111/112 (99%)	0.38	0 100 100	83, 103, 126, 142	0
14	BQ	111/112 (99%)	0.17	2 (1%) 65 20	95, 132, 156, 175	0
15	AR	137/146 (93%)	0.47	4 (2%) 49 12	75, 97, 147, 178	0
15	BR	137/146 (93%)	0.27	1 (0%) 84 42	86, 107, 167, 187	0
16	A1	117/118 (99%)	-0.14	2 (1%) 67 21	61, 84, 116, 145	0
16	B1	117/118 (99%)	0.82	12 (10%) 7 2	71, 106, 146, 165	0
17	A2	101/101 (100%)	0.06	1 (0%) 79 33	61, 105, 126, 145	0
17	B2	101/101 (100%)	1.21	20 (19%) 2 1	73, 131, 148, 158	0
18	AS	113/113 (100%)	-0.07	1 (0%) 81 37	55, 80, 111, 163	0
18	BS	113/113 (100%)	0.42	2 (1%) 65 20	69, 84, 121, 162	0
19	AT	92/96 (95%)	0.37	1 (1%) 77 30	63, 78, 102, 118	0
19	BT	92/96 (95%)	0.58	3 (3%) 44 10	78, 96, 119, 134	0
20	AU	102/110 (92%)	0.14	1 (0%) 79 33	82, 107, 157, 172	0
20	BU	102/110 (92%)	1.00	17 (16%) 2 1	97, 123, 176, 191	0
21	AV	175/206 (84%)	0.87	21 (12%) 5 2	93, 133, 193, 198	0
21	BV	179/206 (86%)	1.83	70 (39%) 1 0	128, 166, 212, 218	0
22	A3	76/85 (89%)	0.07	1 (1%) 74 27	65, 84, 98, 137	0
22	B3	77/85 (90%)	0.18	1 (1%) 74 27	79, 101, 122, 155	0
23	AZ	97/98 (98%)	0.41	5 (5%) 26 6	61, 81, 137, 165	0
23	BZ	97/98 (98%)	0.14	0 100 100	69, 91, 141, 162	0
24	AW	66/72 (91%)	0.01	1 (1%) 70 24	69, 87, 106, 137	0
24	BW	69/72 (95%)	0.35	3 (4%) 34 8	90, 114, 148, 183	0
25	AX	59/60 (98%)	-0.04	1 (1%) 67 21	73, 90, 120, 135	0
25	BX	59/60 (98%)	0.70	1 (1%) 67 21	86, 114, 146, 166	0
26	A4	66/71 (92%)	1.97	32 (48%) 1 0	127, 161, 179, 187	0
26	B4	63/71 (88%)	2.07	28 (44%) 1 0	154, 190, 200, 207	0
27	A5	59/60 (98%)	0.37	5 (8%) 11 3	55, 95, 180, 185	0
27	B5	59/60 (98%)	0.74	8 (13%) 4 2	65, 94, 181, 192	0
28	A6	45/54 (83%)	1.50	12 (26%) 1 1	122, 152, 173, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	45/54 (83%)	1.21	7 (15%) 3 1	141, 173, 188, 192	0
29	A7	49/49 (100%)	-0.01	2 (4%) 35 8	50, 60, 106, 137	0
29	B7	49/49 (100%)	0.23	2 (4%) 35 8	60, 69, 129, 148	0
30	A8	61/65 (93%)	0.17	0 100 100	64, 78, 95, 120	0
30	B8	61/65 (93%)	0.57	0 100 100	78, 95, 110, 142	0
31	CA	1506/1506 (100%)	-0.47	4 (0%) 91 63	64, 112, 193, 248	0
31	DA	1506/1506 (100%)	-0.41	7 (0%) 88 51	76, 122, 195, 248	0
32	CE	237/256 (92%)	0.19	1 (0%) 90 57	115, 149, 188, 198	0
32	DE	237/256 (92%)	0.02	3 (1%) 74 27	127, 165, 200, 215	0
33	CF	205/239 (85%)	0.37	5 (2%) 56 15	98, 124, 158, 166	0
33	DF	206/239 (86%)	0.89	30 (14%) 3 1	128, 151, 180, 188	0
34	CG	208/208 (100%)	-0.09	0 100 100	95, 119, 143, 154	0
34	DG	208/208 (100%)	0.39	2 (0%) 79 33	91, 116, 137, 151	0
35	CH	151/162 (93%)	0.18	1 (0%) 84 42	87, 109, 132, 166	0
35	DH	151/162 (93%)	-0.08	0 100 100	104, 125, 148, 169	0
36	CI	101/101 (100%)	0.46	4 (3%) 36 8	89, 112, 130, 153	0
36	DI	101/101 (100%)	0.47	3 (2%) 48 11	87, 109, 130, 156	0
37	CJ	155/156 (99%)	0.58	11 (7%) 16 4	111, 128, 158, 167	0
37	DJ	155/156 (99%)	-0.16	0 100 100	116, 136, 164, 170	0
38	CK	138/138 (100%)	0.03	0 100 100	95, 116, 130, 137	0
38	DK	138/138 (100%)	-0.22	0 100 100	109, 129, 143, 151	0
39	CL	127/128 (99%)	-0.25	0 100 100	99, 147, 167, 173	0
39	DL	127/128 (99%)	-0.28	0 100 100	120, 158, 174, 178	0
40	CM	99/105 (94%)	-0.14	0 100 100	93, 146, 176, 179	0
40	DM	99/105 (94%)	0.34	5 (5%) 27 6	127, 164, 180, 185	0
41	CN	119/129 (92%)	1.21	17 (14%) 3 1	79, 110, 142, 169	0
41	DN	119/129 (92%)	0.35	2 (1%) 67 21	90, 116, 148, 172	0
42	CO	125/132 (94%)	0.64	5 (4%) 36 8	76, 87, 119, 164	0
42	DO	125/132 (94%)	0.86	14 (11%) 6 2	88, 112, 137, 175	0
43	CP	116/126 (92%)	0.29	3 (2%) 53 13	98, 132, 151, 160	0
43	DP	117/126 (92%)	0.38	7 (5%) 21 5	117, 160, 174, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CQ	60/61 (98%)	-0.06	0 100 100	95, 115, 129, 139	0
44	DQ	60/61 (98%)	0.27	1 (1%) 67 21	129, 146, 159, 166	0
45	CR	88/89 (98%)	0.03	0 100 100	86, 108, 129, 133	0
45	DR	88/89 (98%)	0.18	0 100 100	85, 118, 142, 148	0
46	CS	84/88 (95%)	0.12	0 100 100	104, 121, 148, 179	0
46	DS	84/88 (95%)	0.07	0 100 100	94, 111, 134, 166	0
47	CT	100/105 (95%)	0.10	1 (1%) 79 33	94, 115, 132, 146	0
47	DT	100/105 (95%)	0.11	1 (1%) 79 33	95, 117, 141, 155	0
48	CU	72/88 (81%)	0.56	3 (4%) 35 8	91, 112, 146, 173	0
48	DU	72/88 (81%)	0.27	3 (4%) 35 8	97, 120, 156, 173	0
49	CV	78/93 (83%)	0.31	1 (1%) 74 27	112, 136, 151, 158	0
49	DV	78/93 (83%)	0.30	1 (1%) 74 27	150, 167, 187, 191	0
50	CW	99/106 (93%)	-0.11	0 100 100	106, 130, 158, 169	0
50	DW	99/106 (93%)	-0.15	0 100 100	97, 124, 158, 172	0
51	CX	25/27 (92%)	-0.17	0 100 100	101, 124, 142, 160	0
51	DX	25/27 (92%)	-0.01	0 100 100	126, 149, 163, 175	0
52	CB	87/87 (100%)	1.15	20 (22%) 1 1	91, 155, 201, 213	2 (2%)
52	DB	87/87 (100%)	1.52	26 (29%) 1 1	97, 156, 203, 216	2 (2%)
53	CC	77/77 (100%)	0.15	0 100 100	82, 118, 149, 164	0
53	CD	77/77 (100%)	0.52	13 (16%) 2 1	86, 232, 246, 248	0
53	DC	77/77 (100%)	-0.27	0 100 100	87, 120, 153, 167	0
53	DD	77/77 (100%)	-0.51	1 (1%) 74 27	91, 234, 245, 249	0
54	C1	10/10 (100%)	1.29	2 (20%) 2 1	85, 102, 117, 131	0
54	D1	10/10 (100%)	-0.09	0 100 100	88, 109, 119, 137	0
All	All	21107/21634 (97%)	0.11	721 (3%) 43 10	44, 110, 191, 249	4 (0%)

The worst 5 of 721 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	654(J)	A	13.3
1	AA	654(K)	C	12.8
41	CN	11	LYS	10.5
1	BA	654(K)	C	9.3
1	AA	654(L)	G	9.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3483	1/1	0.33	-	34,34,34,34	0
55	MG	BA	3510	1/1	0.29	-	67,67,67,67	0
55	MG	BA	3205	1/1	0.26	-	70,70,70,70	0
55	MG	CN	201	1/1	0.07	-	78,78,78,78	0
55	MG	A6	101	1/1	0.27	-	111,111,111,111	0
55	MG	AA	3552	1/1	0.33	-	83,83,83,83	0
55	MG	AA	3292	1/1	0.35	-	76,76,76,76	0
55	MG	DA	1716	1/1	0.42	-	105,105,105,105	0
55	MG	AA	3579	1/1	0.25	-	39,39,39,39	0
55	MG	DA	1647	1/1	0.21	-	71,71,71,71	0
55	MG	BA	3407	1/1	0.14	-	96,96,96,96	0
55	MG	DA	1669	1/1	0.51	-	68,68,68,68	0
55	MG	BA	3060	1/1	0.18	-	51,51,51,51	0
55	MG	AA	3073	1/1	0.68	-	97,97,97,97	0
55	MG	AA	3147	1/1	0.50	-	89,89,89,89	0
55	MG	BA	3139	1/1	0.20	-	58,58,58,58	0
55	MG	AA	3078	1/1	0.76	-	88,88,88,88	0
55	MG	CA	1804	1/1	0.41	-	107,107,107,107	0
55	MG	BA	3170	1/1	0.24	-	96,96,96,96	0
55	MG	BA	3448	1/1	0.24	-	85,85,85,85	0
55	MG	AA	3537	1/1	0.22	-	105,105,105,105	0
55	MG	BR	201	1/1	0.24	-	77,77,77,77	0
55	MG	AA	3046	1/1	0.12	-	57,57,57,57	0
55	MG	CA	1626	1/1	0.29	-	88,88,88,88	0
55	MG	CA	1610	1/1	0.27	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3381	1/1	0.42	-	80,80,80,80	0
55	MG	AA	3209	1/1	0.34	-	81,81,81,81	0
55	MG	BA	3486	1/1	0.25	-	30,30,30,30	0
55	MG	CC	105	1/1	0.22	-	105,105,105,105	0
55	MG	BA	3189	1/1	0.35	-	61,61,61,61	0
55	MG	AA	3029	1/1	0.20	-	46,46,46,46	0
55	MG	AA	3563	1/1	0.40	-	52,52,52,52	0
55	MG	BA	3471	1/1	0.41	-	96,96,96,96	0
55	MG	DA	1795	1/1	0.34	-	101,101,101,101	0
55	MG	BA	3159	1/1	0.25	-	83,83,83,83	0
55	MG	BA	3031	1/1	0.34	-	60,60,60,60	0
55	MG	CA	1668	1/1	0.49	-	79,79,79,79	0
55	MG	AA	3520	1/1	0.24	-	68,68,68,68	0
55	MG	BA	3267	1/1	0.24	-	62,62,62,62	0
55	MG	AA	3522	1/1	0.47	-	97,97,97,97	0
55	MG	BA	3293	1/1	0.20	-	96,96,96,96	0
55	MG	AA	3024	1/1	0.39	-	45,45,45,45	0
55	MG	DA	1659	1/1	0.14	-	80,80,80,80	0
55	MG	BA	3366	1/1	0.30	-	76,76,76,76	0
55	MG	BA	3057	1/1	0.21	-	97,97,97,97	0
55	MG	BA	3405	1/1	0.34	-	87,87,87,87	0
55	MG	CA	1757	1/1	0.30	-	92,92,92,92	0
55	MG	BA	3043	1/1	0.19	-	108,108,108,108	0
55	MG	DA	1670	1/1	0.41	-	49,49,49,49	0
55	MG	CA	1781	1/1	0.36	-	62,62,62,62	0
55	MG	AA	3081	1/1	0.59	-	51,51,51,51	0
55	MG	AA	3501	1/1	0.32	-	99,99,99,99	0
55	MG	BA	3363	1/1	0.26	-	88,88,88,88	0
55	MG	CB	105	1/1	0.09	-	113,113,113,113	0
55	MG	BA	3003	1/1	0.57	-	99,99,99,99	0
55	MG	AA	3225	1/1	0.38	-	95,95,95,95	0
55	MG	BA	3513	1/1	0.16	-	104,104,104,104	0
55	MG	BA	3261	1/1	0.39	-	65,65,65,65	0
55	MG	AA	3319	1/1	0.35	-	94,94,94,94	0
55	MG	BA	3040	1/1	0.28	-	94,94,94,94	0
55	MG	AA	3457	1/1	0.59	-	64,64,64,64	0
55	MG	DA	1754	1/1	0.24	-	98,98,98,98	0
55	MG	AA	3007	1/1	0.28	-	42,42,42,42	0
55	MG	BA	3505	1/1	0.30	-	94,94,94,94	0
55	MG	DA	1701	1/1	0.48	-	80,80,80,80	0
55	MG	AA	3400	1/1	0.51	-	39,39,39,39	0
55	MG	CA	1792	1/1	0.27	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3208	1/1	0.26	-	57,57,57,57	0
55	MG	BA	3037	1/1	0.32	-	75,75,75,75	0
55	MG	AA	3342	1/1	0.56	-	70,70,70,70	0
55	MG	DA	1791	1/1	0.51	-	80,80,80,80	0
55	MG	BA	3200	1/1	0.43	-	65,65,65,65	0
55	MG	DA	1654	1/1	0.39	-	92,92,92,92	0
55	MG	AA	3255	1/1	0.36	-	88,88,88,88	0
55	MG	DA	1673	1/1	0.15	-	88,88,88,88	0
55	MG	AB	204	1/1	0.54	-	96,96,96,96	0
55	MG	AA	3020	1/1	0.21	-	39,39,39,39	0
55	MG	CA	1616	1/1	0.20	-	103,103,103,103	0
55	MG	AA	3535	1/1	0.16	-	103,103,103,103	0
55	MG	AA	3132	1/1	0.70	-	106,106,106,106	0
55	MG	BA	3070	1/1	0.27	-	81,81,81,81	0
55	MG	BA	3026	1/1	0.35	-	72,72,72,72	0
55	MG	BA	3465	1/1	0.32	-	97,97,97,97	0
55	MG	DA	1784	1/1	0.27	-	103,103,103,103	0
55	MG	BA	3148	1/1	0.27	-	91,91,91,91	0
55	MG	AA	3594	1/1	0.50	-	105,105,105,105	0
55	MG	DA	1642	1/1	0.25	-	110,110,110,110	0
55	MG	BA	3271	1/1	0.32	-	84,84,84,84	0
55	MG	AA	3471	1/1	0.44	-	85,85,85,85	0
55	MG	DA	1677	1/1	0.27	-	82,82,82,82	0
55	MG	DA	1770	1/1	0.38	-	95,95,95,95	0
55	MG	BA	3054	1/1	0.22	-	81,81,81,81	0
55	MG	BA	3372	1/1	0.44	-	105,105,105,105	0
55	MG	AA	3335	1/1	0.68	-	91,91,91,91	0
55	MG	BA	3222	1/1	0.20	-	54,54,54,54	0
55	MG	BA	3353	1/1	0.23	-	84,84,84,84	0
55	MG	AA	3602	1/1	0.18	-	59,59,59,59	0
55	MG	BA	3046	1/1	0.43	-	83,83,83,83	0
55	MG	BB	201	1/1	0.25	-	90,90,90,90	0
55	MG	DA	1628	1/1	0.55	-	97,97,97,97	0
55	MG	BA	3310	1/1	0.30	-	74,74,74,74	0
55	MG	DC	105	1/1	0.46	-	75,75,75,75	0
55	MG	DA	1640	1/1	0.25	-	101,101,101,101	0
55	MG	AA	3190	1/1	0.17	-	58,58,58,58	0
55	MG	DA	1686	1/1	0.32	-	97,97,97,97	0
55	MG	BA	3184	1/1	0.15	-	76,76,76,76	0
55	MG	AA	3229	1/1	0.19	-	89,89,89,89	0
55	MG	CA	1731	1/1	0.34	-	98,98,98,98	0
55	MG	BA	3318	1/1	0.32	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3473	1/1	0.37	-	77,77,77,77	0
55	MG	BA	3207	1/1	0.31	-	46,46,46,46	0
55	MG	CA	1725	1/1	0.24	-	98,98,98,98	0
55	MG	AA	3164	1/1	0.27	-	95,95,95,95	0
55	MG	AA	3571	1/1	0.18	-	52,52,52,52	0
55	MG	BA	3484	1/1	0.29	-	65,65,65,65	0
55	MG	BB	211	1/1	0.39	-	71,71,71,71	0
55	MG	BA	3515	1/1	0.23	-	59,59,59,59	0
55	MG	DA	1732	1/1	0.50	-	94,94,94,94	0
55	MG	BA	3492	1/1	0.30	-	47,47,47,47	0
55	MG	DA	1660	1/1	0.23	-	102,102,102,102	0
55	MG	AA	3008	1/1	0.40	-	44,44,44,44	0
55	MG	AA	3058	1/1	0.34	-	64,64,64,64	0
55	MG	AA	3110	1/1	0.18	-	40,40,40,40	0
55	MG	DA	1688	1/1	0.25	-	99,99,99,99	0
55	MG	BA	3004	1/1	0.24	-	105,105,105,105	0
55	MG	AA	3200	1/1	0.42	-	71,71,71,71	0
55	MG	CA	1813	1/1	0.47	-	94,94,94,94	0
55	MG	BA	3133	1/1	0.22	-	50,50,50,50	0
55	MG	AA	3351	1/1	0.50	-	82,82,82,82	0
55	MG	AA	3309	1/1	0.73	-	90,90,90,90	0
55	MG	BA	3384	1/1	0.42	-	92,92,92,92	0
55	MG	BA	3181	1/1	0.16	-	49,49,49,49	0
55	MG	BA	3171	1/1	0.30	-	63,63,63,63	0
55	MG	AA	3175	1/1	0.20	-	45,45,45,45	0
55	MG	DA	1772	1/1	0.34	-	68,68,68,68	0
55	MG	AA	3516	1/1	0.29	-	76,76,76,76	0
55	MG	AA	3233	1/1	0.31	-	55,55,55,55	0
55	MG	DA	1747	1/1	0.42	-	105,105,105,105	0
55	MG	DB	102	1/1	0.15	-	107,107,107,107	0
55	MG	AA	3048	1/1	0.38	-	86,86,86,86	0
55	MG	AA	3612	1/1	0.55	-	92,92,92,92	0
55	MG	BA	3008	1/1	0.40	-	89,89,89,89	0
55	MG	AA	3605	1/1	0.54	-	72,72,72,72	0
55	MG	BA	3270	1/1	0.30	-	81,81,81,81	0
55	MG	BA	3373	1/1	0.44	-	88,88,88,88	0
55	MG	BA	3213	1/1	0.29	-	75,75,75,75	0
55	MG	BA	3199	1/1	0.46	-	76,76,76,76	0
55	MG	BA	3214	1/1	0.29	-	77,77,77,77	0
55	MG	AA	3114	1/1	0.50	-	56,56,56,56	0
55	MG	AA	3483	1/1	0.19	-	87,87,87,87	0
55	MG	CA	1802	1/1	0.20	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3443	1/1	0.33	-	90,90,90,90	0
55	MG	AB	211	1/1	0.61	-	100,100,100,100	0
55	MG	CA	1793	1/1	0.12	-	96,96,96,96	0
55	MG	BA	3064	1/1	0.30	-	103,103,103,103	0
55	MG	BA	3206	1/1	0.29	-	98,98,98,98	0
55	MG	DA	1740	1/1	0.16	-	113,113,113,113	0
55	MG	AA	3252	1/1	0.48	-	94,94,94,94	0
55	MG	BA	3273	1/1	0.39	-	102,102,102,102	0
55	MG	DA	1621	1/1	0.52	-	99,99,99,99	0
55	MG	DA	1697	1/1	0.16	-	111,111,111,111	0
55	MG	CA	1698	1/1	0.36	-	89,89,89,89	0
55	MG	AA	3250	1/1	0.25	-	99,99,99,99	0
55	MG	CA	1808	1/1	0.22	-	67,67,67,67	0
55	MG	AA	3411	1/1	0.48	-	85,85,85,85	0
55	MG	BA	3425	1/1	0.49	-	85,85,85,85	0
55	MG	AA	3560	1/1	0.36	-	87,87,87,87	0
55	MG	AA	3297	1/1	0.32	-	69,69,69,69	0
55	MG	BA	3266	1/1	0.54	-	91,91,91,91	0
55	MG	BA	3317	1/1	0.35	-	91,91,91,91	0
55	MG	CA	1812	1/1	0.18	-	84,84,84,84	0
55	MG	BA	3224	1/1	0.30	-	51,51,51,51	0
55	MG	BA	3113	1/1	0.17	-	84,84,84,84	0
55	MG	AA	3143	1/1	0.37	-	35,35,35,35	0
55	MG	A5	101	1/1	0.21	-	51,51,51,51	0
55	MG	AE	302	1/1	0.39	-	45,45,45,45	0
55	MG	DA	1707	1/1	0.27	-	95,95,95,95	0
55	MG	CC	101	1/1	0.25	-	108,108,108,108	0
55	MG	CA	1689	1/1	0.15	-	115,115,115,115	0
55	MG	CA	1620	1/1	0.16	-	74,74,74,74	0
55	MG	AA	3238	1/1	0.57	-	82,82,82,82	0
55	MG	AA	3507	1/1	0.49	-	99,99,99,99	0
55	MG	BA	3442	1/1	0.41	-	91,91,91,91	0
55	MG	AA	3484	1/1	0.18	-	44,44,44,44	0
55	MG	BA	3289	1/1	0.50	-	70,70,70,70	0
55	MG	CA	1693	1/1	0.32	-	102,102,102,102	0
55	MG	AA	3441	1/1	0.59	-	101,101,101,101	0
55	MG	AA	3621	1/1	0.38	-	91,91,91,91	0
55	MG	BA	3395	1/1	0.22	-	89,89,89,89	0
55	MG	BA	3340	1/1	0.20	-	84,84,84,84	0
55	MG	AA	3063	1/1	0.36	-	85,85,85,85	0
55	MG	BA	3039	1/1	0.36	-	85,85,85,85	0
55	MG	AA	3317	1/1	0.37	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AB	208	1/1	0.37	-	92,92,92,92	0
55	MG	BA	3516	1/1	0.15	-	73,73,73,73	0
55	MG	DA	1756	1/1	0.43	-	106,106,106,106	0
55	MG	AA	3035	1/1	0.33	-	45,45,45,45	0
55	MG	BA	3437	1/1	0.40	-	73,73,73,73	0
55	MG	BA	3065	1/1	0.55	-	101,101,101,101	0
55	MG	AA	3161	1/1	0.29	-	42,42,42,42	0
55	MG	AA	3538	1/1	0.33	-	36,36,36,36	0
55	MG	AA	3334	1/1	0.72	-	76,76,76,76	0
55	MG	AA	3503	1/1	0.43	-	81,81,81,81	0
55	MG	AA	3609	1/1	0.26	-	62,62,62,62	0
55	MG	AA	3348	1/1	0.32	-	94,94,94,94	0
55	MG	DA	1605	1/1	0.42	-	82,82,82,82	0
55	MG	DA	1730	1/1	0.40	-	102,102,102,102	0
55	MG	AA	3458	1/1	0.26	-	70,70,70,70	0
55	MG	BA	3201	1/1	0.30	-	94,94,94,94	0
55	MG	DA	1745	1/1	0.30	-	106,106,106,106	0
55	MG	AA	3129	1/1	0.51	-	73,73,73,73	0
55	MG	AA	3251	1/1	0.29	-	68,68,68,68	0
55	MG	AA	3543	1/1	0.47	-	46,46,46,46	0
55	MG	AB	205	1/1	0.33	-	83,83,83,83	0
55	MG	DA	1627	1/1	0.18	-	105,105,105,105	0
55	MG	AA	3504	1/1	0.50	-	80,80,80,80	0
55	MG	CA	1695	1/1	0.33	-	90,90,90,90	0
55	MG	DA	1695	1/1	0.47	-	88,88,88,88	0
55	MG	DA	1667	1/1	0.30	-	82,82,82,82	0
55	MG	BA	3088	1/1	0.24	-	94,94,94,94	0
55	MG	CA	1727	1/1	0.24	-	103,103,103,103	0
55	MG	AA	3587	1/1	0.51	-	77,77,77,77	0
55	MG	BA	3074	1/1	0.24	-	83,83,83,83	0
55	MG	DA	1603	1/1	0.40	-	89,89,89,89	0
55	MG	AA	3326	1/1	0.25	-	64,64,64,64	0
55	MG	AA	3582	1/1	0.28	-	44,44,44,44	0
55	MG	CA	1681	1/1	0.30	-	80,80,80,80	0
55	MG	AA	3060	1/1	0.36	-	84,84,84,84	0
55	MG	DA	1623	1/1	0.47	-	96,96,96,96	0
55	MG	AA	3474	1/1	0.38	-	65,65,65,65	0
55	MG	BA	3042	1/1	0.21	-	86,86,86,86	0
55	MG	AA	3148	1/1	0.58	-	83,83,83,83	0
55	MG	DA	1764	1/1	0.46	-	85,85,85,85	0
55	MG	BA	3080	1/1	0.19	-	72,72,72,72	0
55	MG	AA	3312	1/1	0.43	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CB	101	1/1	0.37	-	108,108,108,108	0
55	MG	BA	3292	1/1	0.39	-	51,51,51,51	0
55	MG	CA	1603	1/1	0.20	-	73,73,73,73	0
55	MG	CA	1686	1/1	0.32	-	86,86,86,86	0
55	MG	AA	3025	1/1	0.35	-	40,40,40,40	0
55	MG	AA	3130	1/1	0.27	-	67,67,67,67	0
55	MG	BA	3231	1/1	0.26	-	47,47,47,47	0
55	MG	AA	3231	1/1	0.53	-	106,106,106,106	0
55	MG	AA	3343	1/1	0.43	-	74,74,74,74	0
55	MG	CA	1825	1/1	0.07	-	114,114,114,114	0
55	MG	AA	3027	1/1	0.36	-	45,45,45,45	0
55	MG	BA	3279	1/1	0.34	-	73,73,73,73	0
55	MG	CA	1662	1/1	0.34	-	81,81,81,81	0
55	MG	AA	3207	1/1	0.18	-	50,50,50,50	0
55	MG	CA	1823	1/1	0.12	-	110,110,110,110	0
55	MG	BD	301	1/1	0.20	-	39,39,39,39	0
55	MG	DA	1653	1/1	0.25	-	96,96,96,96	0
55	MG	BB	205	1/1	0.29	-	86,86,86,86	0
55	MG	BA	3105	1/1	0.29	-	81,81,81,81	0
55	MG	AA	3589	1/1	0.35	-	60,60,60,60	0
55	MG	AA	3472	1/1	0.62	-	80,80,80,80	0
55	MG	BA	3212	1/1	0.54	-	70,70,70,70	0
55	MG	AA	3260	1/1	0.72	-	91,91,91,91	0
55	MG	AA	3451	1/1	0.38	-	76,76,76,76	0
55	MG	BA	3226	1/1	0.48	-	82,82,82,82	0
55	MG	AA	3173	1/1	0.27	-	67,67,67,67	0
55	MG	AA	3427	1/1	0.47	-	82,82,82,82	0
55	MG	BA	3161	1/1	0.34	-	89,89,89,89	0
55	MG	BA	3098	1/1	0.27	-	106,106,106,106	0
55	MG	BA	3063	1/1	0.24	-	89,89,89,89	0
55	MG	BA	3216	1/1	0.30	-	56,56,56,56	0
55	MG	BA	3056	1/1	0.31	-	96,96,96,96	0
55	MG	AB	206	1/1	0.51	-	93,93,93,93	0
55	MG	DA	1672	1/1	0.37	-	63,63,63,63	0
55	MG	AA	3089	1/1	0.52	-	64,64,64,64	0
55	MG	AA	3528	1/1	0.52	-	76,76,76,76	0
55	MG	BA	3337	1/1	0.31	-	100,100,100,100	0
55	MG	DA	1802	1/1	0.45	-	102,102,102,102	0
55	MG	DA	1690	1/1	0.44	-	92,92,92,92	0
55	MG	BA	3364	1/1	0.25	-	76,76,76,76	0
55	MG	AA	3438	1/1	0.55	-	90,90,90,90	0
55	MG	BA	3153	1/1	0.37	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3489	1/1	0.77	-	86,86,86,86	0
55	MG	BA	3256	1/1	0.32	-	102,102,102,102	0
55	MG	AA	3440	1/1	0.47	-	87,87,87,87	0
55	MG	DA	1798	1/1	0.26	-	92,92,92,92	0
55	MG	CA	1801	1/1	0.22	-	84,84,84,84	0
55	MG	BA	3272	1/1	0.43	-	81,81,81,81	0
55	MG	BA	3092	1/1	0.26	-	95,95,95,95	0
55	MG	AA	3608	1/1	0.26	-	41,41,41,41	0
55	MG	AA	3432	1/1	0.56	-	87,87,87,87	0
55	MG	AA	3523	1/1	0.17	-	91,91,91,91	0
55	MG	BA	3474	1/1	0.51	-	88,88,88,88	0
55	MG	AA	3159	1/1	0.06	-	28,28,28,28	0
55	MG	AA	3430	1/1	0.20	-	105,105,105,105	0
55	MG	AA	3057	1/1	0.40	-	66,66,66,66	0
55	MG	AA	3064	1/1	0.12	-	79,79,79,79	0
55	MG	DA	1789	1/1	0.28	-	77,77,77,77	0
55	MG	CA	1680	1/1	0.29	-	79,79,79,79	0
55	MG	CA	1824	1/1	0.13	-	94,94,94,94	0
55	MG	CA	1746	1/1	0.21	-	98,98,98,98	0
55	MG	BA	3408	1/1	0.51	-	88,88,88,88	0
55	MG	CA	1702	1/1	0.10	-	71,71,71,71	0
55	MG	BA	3496	1/1	0.34	-	96,96,96,96	0
55	MG	BA	3304	1/1	0.40	-	91,91,91,91	0
55	MG	DA	1656	1/1	0.40	-	99,99,99,99	0
55	MG	AA	3572	1/1	0.47	-	54,54,54,54	0
55	MG	BA	3523	1/1	0.44	-	84,84,84,84	0
55	MG	BA	3103	1/1	0.25	-	82,82,82,82	0
55	MG	DA	1650	1/1	0.52	-	95,95,95,95	0
55	MG	BA	3247	1/1	0.34	-	74,74,74,74	0
55	MG	AB	212	1/1	0.50	-	94,94,94,94	0
55	MG	AA	3377	1/1	0.45	-	94,94,94,94	0
55	MG	DA	1768	1/1	0.16	-	82,82,82,82	0
55	MG	BA	3262	1/1	0.30	-	94,94,94,94	0
55	MG	AA	3360	1/1	0.32	-	63,63,63,63	0
55	MG	CA	1618	1/1	0.23	-	94,94,94,94	0
55	MG	BA	3498	1/1	0.18	-	99,99,99,99	0
55	MG	DA	1786	1/1	0.44	-	86,86,86,86	0
55	MG	BA	3018	1/1	0.33	-	83,83,83,83	0
55	MG	CN	202	1/1	0.40	-	99,99,99,99	0
55	MG	BA	3368	1/1	0.21	-	106,106,106,106	0
55	MG	AA	3135	1/1	0.26	-	66,66,66,66	0
55	MG	AU	201	1/1	0.26	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1667	1/1	0.25	-	77,77,77,77	0
55	MG	DA	1702	1/1	0.35	-	99,99,99,99	0
55	MG	BA	3110	1/1	0.39	-	92,92,92,92	0
55	MG	BA	3115	1/1	0.27	-	79,79,79,79	0
55	MG	CA	1637	1/1	0.33	-	106,106,106,106	0
55	MG	BA	3100	1/1	0.25	-	66,66,66,66	0
55	MG	AA	3316	1/1	0.29	-	83,83,83,83	0
55	MG	CC	107	1/1	0.40	-	93,93,93,93	0
55	MG	CA	1607	1/1	0.36	-	93,93,93,93	0
55	MG	BA	3311	1/1	0.28	-	82,82,82,82	0
55	MG	BA	3506	1/1	0.22	-	74,74,74,74	0
55	MG	AA	3359	1/1	0.42	-	84,84,84,84	0
55	MG	BA	3203	1/1	0.42	-	53,53,53,53	0
55	MG	CA	1778	1/1	0.42	-	95,95,95,95	0
55	MG	AA	3347	1/1	0.26	-	92,92,92,92	0
55	MG	BA	3387	1/1	0.42	-	107,107,107,107	0
55	MG	CA	1622	1/1	0.12	-	86,86,86,86	0
55	MG	BA	3303	1/1	0.43	-	89,89,89,89	0
55	MG	BA	3410	1/1	0.36	-	94,94,94,94	0
55	MG	AA	3296	1/1	0.53	-	72,72,72,72	0
55	MG	AE	304	1/1	0.19	-	87,87,87,87	0
55	MG	BA	3512	1/1	0.28	-	75,75,75,75	0
55	MG	CA	1832	1/1	0.30	-	106,106,106,106	0
55	MG	AA	3586	1/1	0.15	-	53,53,53,53	0
55	MG	AA	3111	1/1	0.51	-	36,36,36,36	0
55	MG	BA	3362	1/1	0.18	-	71,71,71,71	0
55	MG	AA	3216	1/1	0.36	-	64,64,64,64	0
55	MG	AA	3193	1/1	0.59	-	96,96,96,96	0
55	MG	BA	3169	1/1	0.27	-	56,56,56,56	0
55	MG	BA	3029	1/1	0.48	-	75,75,75,75	0
55	MG	BA	3480	1/1	0.25	-	56,56,56,56	0
55	MG	CA	1754	1/1	0.35	-	114,114,114,114	0
55	MG	BA	3033	1/1	0.31	-	94,94,94,94	0
55	MG	BA	3053	1/1	0.40	-	65,65,65,65	0
55	MG	CA	1756	1/1	0.11	-	113,113,113,113	0
55	MG	AA	3182	1/1	0.41	-	88,88,88,88	0
55	MG	AA	3283	1/1	0.46	-	91,91,91,91	0
55	MG	CA	1665	1/1	0.48	-	74,74,74,74	0
55	MG	AA	3068	1/1	0.41	-	72,72,72,72	0
55	MG	BA	3255	1/1	0.38	-	52,52,52,52	0
55	MG	CA	1608	1/1	0.22	-	68,68,68,68	0
55	MG	BA	3404	1/1	0.17	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3591	1/1	0.15	-	74,74,74,74	0
55	MG	AA	3204	1/1	0.33	-	44,44,44,44	0
55	MG	BA	3389	1/1	0.21	-	96,96,96,96	0
55	MG	BA	3356	1/1	0.23	-	84,84,84,84	0
55	MG	DA	1609	1/1	0.28	-	116,116,116,116	0
55	MG	AA	3557	1/1	0.55	-	100,100,100,100	0
55	MG	AA	3226	1/1	0.27	-	77,77,77,77	0
55	MG	DA	1769	1/1	0.32	-	79,79,79,79	0
55	MG	AA	3041	1/1	0.32	-	66,66,66,66	0
55	MG	DA	1685	1/1	0.42	-	72,72,72,72	0
55	MG	CA	1648	1/1	0.40	-	79,79,79,79	0
55	MG	AA	3179	1/1	0.27	-	53,53,53,53	0
55	MG	BA	3274	1/1	0.25	-	90,90,90,90	0
55	MG	AA	3061	1/1	0.28	-	79,79,79,79	0
55	MG	CA	1827	1/1	0.23	-	89,89,89,89	0
55	MG	BA	3454	1/1	0.33	-	105,105,105,105	0
55	MG	AA	3350	1/1	0.31	-	90,90,90,90	0
55	MG	BA	3138	1/1	0.33	-	52,52,52,52	0
55	MG	DA	1804	1/1	0.42	-	123,123,123,123	0
55	MG	AA	3150	1/1	0.56	-	59,59,59,59	0
55	MG	AA	3113	1/1	0.49	-	49,49,49,49	0
55	MG	AA	3408	1/1	0.35	-	83,83,83,83	0
55	MG	CC	106	1/1	0.18	-	92,92,92,92	0
55	MG	BB	206	1/1	0.16	-	102,102,102,102	0
55	MG	DA	1787	1/1	0.51	-	114,114,114,114	0
55	MG	AA	3269	1/1	0.48	-	55,55,55,55	0
55	MG	AA	3201	1/1	0.45	-	85,85,85,85	0
55	MG	BA	3154	1/1	0.14	-	46,46,46,46	0
55	MG	BA	3263	1/1	0.26	-	84,84,84,84	0
55	MG	DA	1750	1/1	0.25	-	84,84,84,84	0
55	MG	AA	3095	1/1	0.26	-	89,89,89,89	0
55	MG	CA	1786	1/1	0.10	-	74,74,74,74	0
55	MG	AA	3620	1/1	0.29	-	115,115,115,115	0
55	MG	CA	1736	1/1	0.27	-	88,88,88,88	0
55	MG	BA	3136	1/1	0.23	-	43,43,43,43	0
55	MG	AA	3275	1/1	0.40	-	87,87,87,87	0
55	MG	BA	3280	1/1	0.34	-	74,74,74,74	0
55	MG	DC	104	1/1	0.28	-	102,102,102,102	0
55	MG	BA	3041	1/1	0.47	-	104,104,104,104	0
55	MG	AA	3506	1/1	0.23	-	80,80,80,80	0
55	MG	AA	3302	1/1	0.35	-	104,104,104,104	0
55	MG	AA	3096	1/1	0.28	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3327	1/1	0.27	-	91,91,91,91	0
55	MG	AA	3211	1/1	0.27	-	58,58,58,58	0
55	MG	CA	1724	1/1	0.19	-	97,97,97,97	0
55	MG	AA	3236	1/1	0.66	-	96,96,96,96	0
55	MG	DA	1728	1/1	0.28	-	112,112,112,112	0
55	MG	BA	3487	1/1	0.20	-	66,66,66,66	0
55	MG	AA	3574	1/1	0.34	-	54,54,54,54	0
55	MG	BA	3370	1/1	0.32	-	98,98,98,98	0
55	MG	CA	1821	1/1	0.39	-	94,94,94,94	0
55	MG	BA	3517	1/1	0.22	-	61,61,61,61	0
55	MG	AA	3313	1/1	0.39	-	70,70,70,70	0
55	MG	BA	3186	1/1	0.31	-	52,52,52,52	0
55	MG	DA	1762	1/1	0.21	-	109,109,109,109	0
55	MG	CA	1658	1/1	0.40	-	50,50,50,50	0
55	MG	AA	3461	1/1	0.55	-	105,105,105,105	0
55	MG	AA	3305	1/1	0.35	-	80,80,80,80	0
55	MG	CA	1790	1/1	0.20	-	89,89,89,89	0
55	MG	AA	3394	1/1	0.43	-	99,99,99,99	0
55	MG	DA	1705	1/1	0.36	-	97,97,97,97	0
55	MG	BA	3361	1/1	0.21	-	88,88,88,88	0
55	MG	CA	1761	1/1	0.35	-	66,66,66,66	0
55	MG	AA	3241	1/1	0.66	-	80,80,80,80	0
55	MG	BA	3428	1/1	0.19	-	89,89,89,89	0
55	MG	AA	3248	1/1	0.61	-	74,74,74,74	0
55	MG	AA	3242	1/1	0.24	-	93,93,93,93	0
55	MG	BA	3345	1/1	0.27	-	87,87,87,87	0
55	MG	AA	3455	1/1	0.47	-	49,49,49,49	0
55	MG	CA	1611	1/1	0.18	-	97,97,97,97	0
55	MG	CD	101	1/1	0.14	-	105,105,105,105	0
55	MG	AA	3406	1/1	0.41	-	83,83,83,83	0
55	MG	CA	1789	1/1	0.07	-	71,71,71,71	0
55	MG	DA	1718	1/1	0.30	-	132,132,132,132	0
55	MG	DA	1636	1/1	0.29	-	103,103,103,103	0
55	MG	AE	301	1/1	0.13	-	65,65,65,65	0
55	MG	AA	3172	1/1	0.25	-	94,94,94,94	0
55	MG	BA	3298	1/1	0.19	-	61,61,61,61	0
55	MG	CA	1833	1/1	0.10	-	95,95,95,95	0
55	MG	BA	3518	1/1	0.45	-	74,74,74,74	0
55	MG	BA	3282	1/1	0.30	-	93,93,93,93	0
55	MG	BA	3452	1/1	0.12	-	96,96,96,96	0
55	MG	CA	1649	1/1	0.28	-	86,86,86,86	0
55	MG	CA	1654	1/1	0.37	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3346	1/1	0.52	-	99,99,99,99	0
55	MG	DA	1723	1/1	0.27	-	83,83,83,83	0
55	MG	DA	1708	1/1	0.52	-	102,102,102,102	0
55	MG	DA	1658	1/1	0.28	-	113,113,113,113	0
55	MG	AA	3356	1/1	0.57	-	86,86,86,86	0
55	MG	CA	1767	1/1	0.23	-	120,120,120,120	0
55	MG	AA	3107	1/1	0.30	-	69,69,69,69	0
55	MG	BA	3422	1/1	0.35	-	102,102,102,102	0
55	MG	AA	3056	1/1	0.62	-	98,98,98,98	0
55	MG	BA	3269	1/1	0.33	-	58,58,58,58	0
55	MG	CA	1714	1/1	0.54	-	118,118,118,118	0
55	MG	BA	3449	1/1	0.36	-	109,109,109,109	0
55	MG	AA	3564	1/1	0.32	-	76,76,76,76	0
55	MG	AA	3259	1/1	0.25	-	81,81,81,81	0
55	MG	DA	1655	1/1	0.40	-	96,96,96,96	0
55	MG	DG	301	1/1	0.34	-	94,94,94,94	0
55	MG	AA	3558	1/1	0.35	-	89,89,89,89	0
55	MG	AA	3116	1/1	0.49	-	37,37,37,37	0
55	MG	AA	3099	1/1	0.46	-	64,64,64,64	0
55	MG	AA	3001	1/1	0.47	-	44,44,44,44	0
55	MG	BA	3190	1/1	0.24	-	73,73,73,73	0
55	MG	BA	3250	1/1	0.29	-	58,58,58,58	0
55	MG	CA	1623	1/1	0.24	-	73,73,73,73	0
55	MG	BA	3488	1/1	0.14	-	59,59,59,59	0
55	MG	AA	3167	1/1	0.42	-	50,50,50,50	0
55	MG	AA	3352	1/1	0.30	-	52,52,52,52	0
55	MG	AA	3192	1/1	0.32	-	63,63,63,63	0
55	MG	DA	1635	1/1	0.31	-	79,79,79,79	0
55	MG	CA	1639	1/1	0.39	-	86,86,86,86	0
55	MG	CA	1817	1/1	0.23	-	85,85,85,85	0
55	MG	AA	3450	1/1	0.58	-	72,72,72,72	0
55	MG	BA	3241	1/1	0.34	-	52,52,52,52	0
55	MG	AA	3355	1/1	0.50	-	94,94,94,94	0
55	MG	BB	214	1/1	0.35	-	99,99,99,99	0
55	MG	AA	3466	1/1	0.60	-	100,100,100,100	0
55	MG	BA	3509	1/1	0.35	-	73,73,73,73	0
55	MG	DA	1788	1/1	0.48	-	90,90,90,90	0
55	MG	AA	3482	1/1	0.30	-	96,96,96,96	0
55	MG	AA	3071	1/1	0.53	-	56,56,56,56	0
55	MG	BA	3325	1/1	0.40	-	50,50,50,50	0
55	MG	AA	3585	1/1	0.55	-	91,91,91,91	0
55	MG	CA	1708	1/1	0.38	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1839	1/1	0.22	-	68,68,68,68	0
55	MG	DA	1726	1/1	0.51	-	79,79,79,79	0
55	MG	BA	3445	1/1	0.27	-	95,95,95,95	0
55	MG	AA	3268	1/1	0.60	-	85,85,85,85	0
55	MG	CB	102	1/1	0.31	-	106,106,106,106	0
55	MG	DC	107	1/1	0.41	-	105,105,105,105	0
55	MG	CA	1759	1/1	0.32	-	117,117,117,117	0
55	MG	AA	3393	1/1	0.55	-	98,98,98,98	0
55	MG	DA	1626	1/1	0.41	-	104,104,104,104	0
55	MG	DA	1668	1/1	0.20	-	73,73,73,73	0
55	MG	AA	3598	1/1	0.30	-	87,87,87,87	0
55	MG	AA	3449	1/1	0.30	-	63,63,63,63	0
55	MG	AA	3375	1/1	0.37	-	88,88,88,88	0
55	MG	AA	3197	1/1	0.41	-	74,74,74,74	0
55	MG	DA	1755	1/1	0.52	-	79,79,79,79	0
55	MG	CA	1678	1/1	0.26	-	69,69,69,69	0
55	MG	DA	1776	1/1	0.31	-	70,70,70,70	0
55	MG	AA	3243	1/1	0.42	-	51,51,51,51	0
55	MG	BA	3316	1/1	0.29	-	67,67,67,67	0
55	MG	AA	3595	1/1	0.36	-	79,79,79,79	0
55	MG	AA	3420	1/1	0.26	-	88,88,88,88	0
55	MG	AA	3600	1/1	0.40	-	74,74,74,74	0
55	MG	AA	3009	1/1	0.29	-	63,63,63,63	0
55	MG	AA	3426	1/1	0.44	-	80,80,80,80	0
55	MG	AA	3285	1/1	0.46	-	80,80,80,80	0
55	MG	AA	3051	1/1	0.36	-	71,71,71,71	0
55	MG	A7	102	1/1	0.50	-	68,68,68,68	0
55	MG	CA	1659	1/1	0.22	-	71,71,71,71	0
55	MG	AA	3508	1/1	0.53	-	101,101,101,101	0
55	MG	AA	3088	1/1	0.21	-	42,42,42,42	0
55	MG	CA	1703	1/1	0.18	-	103,103,103,103	0
55	MG	AA	3514	1/1	0.34	-	67,67,67,67	0
55	MG	BA	3264	1/1	0.27	-	59,59,59,59	0
55	MG	AA	3145	1/1	0.63	-	91,91,91,91	0
55	MG	AA	3019	1/1	0.30	-	55,55,55,55	0
55	MG	DA	1749	1/1	0.24	-	101,101,101,101	0
55	MG	AA	3412	1/1	0.27	-	110,110,110,110	0
55	MG	BA	3427	1/1	0.41	-	100,100,100,100	0
55	MG	DA	1731	1/1	0.42	-	70,70,70,70	0
55	MG	AA	3100	1/1	0.56	-	67,67,67,67	0
55	MG	AA	3040	1/1	0.27	-	68,68,68,68	0
55	MG	AF	301	1/1	0.25	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1741	1/1	0.45	-	93,93,93,93	0
55	MG	BA	3249	1/1	0.23	-	40,40,40,40	0
55	MG	AA	3583	1/1	0.48	-	103,103,103,103	0
55	MG	CA	1669	1/1	0.23	-	70,70,70,70	0
55	MG	BA	3457	1/1	0.33	-	99,99,99,99	0
55	MG	BA	3144	1/1	0.38	-	95,95,95,95	0
55	MG	BA	3386	1/1	0.24	-	81,81,81,81	0
55	MG	AA	3280	1/1	0.31	-	94,94,94,94	0
55	MG	AA	3536	1/1	0.42	-	92,92,92,92	0
55	MG	BA	3338	1/1	0.35	-	71,71,71,71	0
55	MG	AA	3121	1/1	0.77	-	90,90,90,90	0
55	MG	DA	1794	1/1	0.43	-	91,91,91,91	0
55	MG	AA	3102	1/1	0.28	-	90,90,90,90	0
55	MG	DA	1725	1/1	0.43	-	96,96,96,96	0
55	MG	AA	3497	1/1	0.69	-	95,95,95,95	0
55	MG	BA	3495	1/1	0.31	-	81,81,81,81	0
56	PAR	CA	1841	42/42	0.31	-	40,56,74,83	0
55	MG	CA	1733	1/1	0.16	-	107,107,107,107	0
55	MG	CA	1644	1/1	0.20	-	84,84,84,84	0
55	MG	BA	3075	1/1	0.16	-	99,99,99,99	0
55	MG	AA	3325	1/1	0.45	-	100,100,100,100	0
55	MG	CA	1642	1/1	0.27	-	69,69,69,69	0
55	MG	BA	3030	1/1	0.28	-	99,99,99,99	0
55	MG	AA	3069	1/1	0.23	-	64,64,64,64	0
55	MG	BA	3195	1/1	0.45	-	94,94,94,94	0
55	MG	AA	3445	1/1	0.32	-	95,95,95,95	0
55	MG	BA	3430	1/1	0.07	-	89,89,89,89	0
55	MG	AA	3517	1/1	0.18	-	66,66,66,66	0
55	MG	CB	103	1/1	0.19	-	110,110,110,110	0
55	MG	BA	3021	1/1	0.45	-	105,105,105,105	0
55	MG	BA	3149	1/1	0.24	-	72,72,72,72	0
55	MG	DA	1733	1/1	0.36	-	98,98,98,98	0
55	MG	AA	3033	1/1	0.37	-	49,49,49,49	0
55	MG	AA	3156	1/1	0.38	-	94,94,94,94	0
55	MG	BA	3421	1/1	0.23	-	102,102,102,102	0
55	MG	CC	104	1/1	0.22	-	97,97,97,97	0
55	MG	BA	3399	1/1	0.30	-	104,104,104,104	0
55	MG	AA	3199	1/1	0.52	-	46,46,46,46	0
55	MG	BA	3359	1/1	0.58	-	98,98,98,98	0
55	MG	DA	1752	1/1	0.35	-	89,89,89,89	0
55	MG	AA	3362	1/1	0.42	-	89,89,89,89	0
55	MG	BA	3204	1/1	0.32	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1712	1/1	0.54	-	100,100,100,100	0
55	MG	AD	301	1/1	0.22	-	99,99,99,99	0
55	MG	BA	3350	1/1	0.55	-	77,77,77,77	0
55	MG	CA	1794	1/1	0.11	-	106,106,106,106	0
55	MG	BA	3326	1/1	0.31	-	84,84,84,84	0
55	MG	AA	3500	1/1	0.33	-	103,103,103,103	0
55	MG	CA	1769	1/1	0.09	-	79,79,79,79	0
55	MG	CA	1716	1/1	0.38	-	117,117,117,117	0
55	MG	AA	3094	1/1	0.42	-	62,62,62,62	0
55	MG	AA	3240	1/1	0.30	-	80,80,80,80	0
55	MG	BA	3162	1/1	0.18	-	92,92,92,92	0
55	MG	AA	3223	1/1	0.32	-	71,71,71,71	0
55	MG	CA	1830	1/1	0.32	-	94,94,94,94	0
55	MG	DA	1651	1/1	0.29	-	72,72,72,72	0
55	MG	BA	3067	1/1	0.42	-	74,74,74,74	0
55	MG	DA	1691	1/1	0.55	-	82,82,82,82	0
55	MG	BA	3188	1/1	0.32	-	85,85,85,85	0
55	MG	AA	3105	1/1	0.39	-	61,61,61,61	0
55	MG	BA	3374	1/1	0.47	-	86,86,86,86	0
55	MG	BA	3242	1/1	0.37	-	62,62,62,62	0
55	MG	AA	3021	1/1	0.27	-	42,42,42,42	0
55	MG	AA	3119	1/1	0.43	-	75,75,75,75	0
55	MG	AA	3541	1/1	0.26	-	48,48,48,48	0
55	MG	BA	3119	1/1	0.18	-	79,79,79,79	0
55	MG	BA	3336	1/1	0.39	-	97,97,97,97	0
55	MG	CA	1601	1/1	0.17	-	56,56,56,56	0
55	MG	BA	3071	1/1	0.23	-	78,78,78,78	0
55	MG	BB	210	1/1	0.44	-	96,96,96,96	0
55	MG	AA	3083	1/1	0.40	-	34,34,34,34	0
55	MG	AA	3077	1/1	0.38	-	103,103,103,103	0
55	MG	CQ	102	1/1	0.23	-	97,97,97,97	0
55	MG	AA	3526	1/1	0.43	-	90,90,90,90	0
55	MG	BA	3482	1/1	0.22	-	65,65,65,65	0
55	MG	BA	3142	1/1	0.24	-	70,70,70,70	0
55	MG	AA	3278	1/1	0.66	-	100,100,100,100	0
55	MG	AA	3533	1/1	0.19	-	67,67,67,67	0
55	MG	B1	201	1/1	0.28	-	82,82,82,82	0
55	MG	DA	1631	1/1	0.21	-	102,102,102,102	0
55	MG	BA	3129	1/1	0.24	-	41,41,41,41	0
55	MG	AA	3217	1/1	0.17	-	64,64,64,64	0
55	MG	BA	3507	1/1	0.37	-	102,102,102,102	0
55	MG	BA	3258	1/1	0.30	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3262	1/1	0.29	-	33,33,33,33	0
55	MG	AA	3221	1/1	0.41	-	47,47,47,47	0
55	MG	BA	3493	1/1	0.28	-	39,39,39,39	0
55	MG	BA	3013	1/1	0.29	-	74,74,74,74	0
55	MG	BA	3315	1/1	0.24	-	91,91,91,91	0
55	MG	AA	3049	1/1	0.38	-	80,80,80,80	0
55	MG	CA	1805	1/1	0.31	-	75,75,75,75	0
55	MG	AA	3003	1/1	0.52	-	64,64,64,64	0
55	MG	CA	1632	1/1	0.20	-	76,76,76,76	0
55	MG	CA	1638	1/1	0.35	-	108,108,108,108	0
55	MG	CA	1749	1/1	0.25	-	62,62,62,62	0
55	MG	AA	3423	1/1	0.16	-	74,74,74,74	0
55	MG	AA	3346	1/1	0.47	-	88,88,88,88	0
55	MG	AA	3154	1/1	0.42	-	52,52,52,52	0
55	MG	BA	3297	1/1	0.13	-	63,63,63,63	0
55	MG	AA	3374	1/1	0.36	-	74,74,74,74	0
55	MG	CA	1739	1/1	0.74	-	86,86,86,86	0
55	MG	CA	1828	1/1	0.25	-	98,98,98,98	0
55	MG	DA	1799	1/1	0.39	-	68,68,68,68	0
55	MG	BA	3470	1/1	0.32	-	81,81,81,81	0
55	MG	AA	3055	1/1	0.38	-	67,67,67,67	0
55	MG	AA	3198	1/1	0.69	-	74,74,74,74	0
55	MG	BA	3173	1/1	0.41	-	50,50,50,50	0
55	MG	BA	3048	1/1	0.19	-	74,74,74,74	0
55	MG	BA	3243	1/1	0.30	-	65,65,65,65	0
55	MG	DA	1641	1/1	0.34	-	95,95,95,95	0
55	MG	BA	3376	1/1	0.39	-	65,65,65,65	0
55	MG	CA	1811	1/1	0.28	-	95,95,95,95	0
55	MG	DA	1721	1/1	0.40	-	71,71,71,71	0
55	MG	BA	3409	1/1	0.31	-	71,71,71,71	0
55	MG	AA	3546	1/1	0.24	-	74,74,74,74	0
55	MG	DA	1681	1/1	0.28	-	106,106,106,106	0
55	MG	CA	1717	1/1	0.20	-	69,69,69,69	0
55	MG	BA	3521	1/1	0.38	-	79,79,79,79	0
55	MG	AA	3462	1/1	0.35	-	85,85,85,85	0
55	MG	BA	3528	1/1	0.19	-	98,98,98,98	0
55	MG	DA	1664	1/1	0.19	-	97,97,97,97	0
55	MG	BA	3157	1/1	0.40	-	93,93,93,93	0
55	MG	DC	108	1/1	0.14	-	102,102,102,102	0
55	MG	DA	1774	1/1	0.43	-	103,103,103,103	0
55	MG	BA	3461	1/1	0.22	-	83,83,83,83	0
55	MG	AA	3566	1/1	0.28	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3467	1/1	0.42	-	93,93,93,93	0
55	MG	BA	3104	1/1	0.42	-	115,115,115,115	0
55	MG	AA	3452	1/1	0.51	-	76,76,76,76	0
55	MG	AA	3189	1/1	0.32	-	90,90,90,90	0
55	MG	DA	1652	1/1	0.17	-	85,85,85,85	0
55	MG	AA	3401	1/1	0.49	-	93,93,93,93	0
55	MG	AA	3505	1/1	0.66	-	85,85,85,85	0
55	MG	BA	3307	1/1	0.41	-	106,106,106,106	0
55	MG	BA	3278	1/1	0.28	-	92,92,92,92	0
55	MG	DA	1644	1/1	0.34	-	82,82,82,82	0
55	MG	BA	3424	1/1	0.67	-	86,86,86,86	0
55	MG	BA	3174	1/1	0.34	-	82,82,82,82	0
55	MG	AA	3498	1/1	0.62	-	95,95,95,95	0
55	MG	DA	1646	1/1	0.30	-	65,65,65,65	0
55	MG	AA	3364	1/1	0.32	-	69,69,69,69	0
55	MG	CA	1721	1/1	0.22	-	89,89,89,89	0
55	MG	BA	3006	1/1	0.09	-	47,47,47,47	0
55	MG	CA	1837	1/1	0.25	-	88,88,88,88	0
55	MG	DA	1632	1/1	0.22	-	84,84,84,84	0
55	MG	CA	1829	1/1	0.22	-	102,102,102,102	0
55	MG	BA	3268	1/1	0.19	-	59,59,59,59	0
55	MG	BA	3352	1/1	0.53	-	102,102,102,102	0
55	MG	CA	1647	1/1	0.22	-	92,92,92,92	0
55	MG	AA	3567	1/1	0.23	-	39,39,39,39	0
55	MG	CA	1614	1/1	0.25	-	101,101,101,101	0
55	MG	AA	3141	1/1	0.34	-	50,50,50,50	0
55	MG	AA	3115	1/1	0.58	-	70,70,70,70	0
55	MG	AA	3224	1/1	0.55	-	93,93,93,93	0
55	MG	CC	103	1/1	0.32	-	104,104,104,104	0
55	MG	AA	3279	1/1	0.25	-	89,89,89,89	0
55	MG	CA	1624	1/1	0.14	-	97,97,97,97	0
55	MG	C1	101	1/1	0.41	-	98,98,98,98	0
55	MG	AA	3160	1/1	0.28	-	32,32,32,32	0
55	MG	BA	3339	1/1	0.28	-	90,90,90,90	0
55	MG	BA	3172	1/1	0.35	-	85,85,85,85	0
55	MG	AA	3486	1/1	0.28	-	90,90,90,90	0
55	MG	BA	3443	1/1	0.37	-	92,92,92,92	0
55	MG	DA	1698	1/1	0.42	-	103,103,103,103	0
55	MG	AA	3465	1/1	0.30	-	71,71,71,71	0
55	MG	B3	101	1/1	0.22	-	76,76,76,76	0
55	MG	AA	3357	1/1	0.52	-	99,99,99,99	0
55	MG	AA	3065	1/1	0.50	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3447	1/1	0.65	-	75,75,75,75	0
55	MG	AA	3103	1/1	0.39	-	97,97,97,97	0
55	MG	AA	3299	1/1	0.27	-	79,79,79,79	0
55	MG	AA	3490	1/1	0.62	-	97,97,97,97	0
55	MG	CA	1800	1/1	0.12	-	104,104,104,104	0
55	MG	CA	1818	1/1	0.23	-	89,89,89,89	0
55	MG	AA	3272	1/1	0.40	-	65,65,65,65	0
55	MG	DA	1778	1/1	0.22	-	118,118,118,118	0
55	MG	BA	3027	1/1	0.28	-	107,107,107,107	0
55	MG	DA	1634	1/1	0.24	-	77,77,77,77	0
55	MG	CA	1630	1/1	0.25	-	112,112,112,112	0
55	MG	DA	1630	1/1	0.29	-	102,102,102,102	0
55	MG	AA	3290	1/1	0.46	-	72,72,72,72	0
55	MG	CA	1755	1/1	0.24	-	81,81,81,81	0
55	MG	AA	3237	1/1	0.42	-	83,83,83,83	0
55	MG	BA	3324	1/1	0.38	-	75,75,75,75	0
55	MG	DA	1706	1/1	0.63	-	90,90,90,90	0
55	MG	CA	1771	1/1	0.22	-	102,102,102,102	0
55	MG	AA	3615	1/1	0.22	-	102,102,102,102	0
55	MG	AA	3365	1/1	0.42	-	74,74,74,74	0
55	MG	DA	1665	1/1	0.37	-	82,82,82,82	0
55	MG	BA	3117	1/1	0.46	-	91,91,91,91	0
55	MG	AA	3311	1/1	0.55	-	68,68,68,68	0
55	MG	AA	3256	1/1	0.35	-	66,66,66,66	0
55	MG	BA	3511	1/1	0.23	-	68,68,68,68	0
55	MG	AA	3479	1/1	0.32	-	94,94,94,94	0
55	MG	AA	3453	1/1	0.26	-	95,95,95,95	0
55	MG	AA	3618	1/1	0.50	-	97,97,97,97	0
55	MG	AA	3448	1/1	0.45	-	106,106,106,106	0
55	MG	DA	1783	1/1	0.33	-	86,86,86,86	0
55	MG	BA	3479	1/1	0.46	-	95,95,95,95	0
55	MG	AA	3530	1/1	0.36	-	79,79,79,79	0
55	MG	AA	3502	1/1	0.80	-	96,96,96,96	0
55	MG	BA	3156	1/1	0.38	-	87,87,87,87	0
55	MG	CA	1660	1/1	0.32	-	64,64,64,64	0
55	MG	AA	3464	1/1	0.32	-	83,83,83,83	0
55	MG	AA	3013	1/1	0.32	-	44,44,44,44	0
55	MG	BA	3514	1/1	0.36	-	51,51,51,51	0
55	MG	BA	3402	1/1	0.36	-	95,95,95,95	0
55	MG	AA	3186	1/1	0.22	-	58,58,58,58	0
55	MG	BA	3455	1/1	0.31	-	92,92,92,92	0
55	MG	AA	3097	1/1	0.54	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DS	101	1/1	0.44	-	87,87,87,87	0
55	MG	BA	3111	1/1	0.16	-	82,82,82,82	0
55	MG	AA	3418	1/1	0.37	-	91,91,91,91	0
55	MG	BA	3418	1/1	0.19	-	73,73,73,73	0
55	MG	DA	1614	1/1	0.55	-	93,93,93,93	0
55	MG	CB	104	1/1	0.33	-	101,101,101,101	0
55	MG	AA	3332	1/1	0.18	-	62,62,62,62	0
55	MG	AA	3385	1/1	0.63	-	88,88,88,88	0
57	ZN	DQ	101	1/1	0.16	-	118,118,118,118	0
55	MG	BA	3240	1/1	0.33	-	72,72,72,72	0
55	MG	BA	3218	1/1	0.39	-	51,51,51,51	0
55	MG	BA	3049	1/1	0.29	-	86,86,86,86	0
55	MG	AA	3253	1/1	0.35	-	81,81,81,81	0
55	MG	BA	3283	1/1	0.22	-	43,43,43,43	0
55	MG	AA	3604	1/1	0.46	-	93,93,93,93	0
55	MG	AA	3127	1/1	0.40	-	53,53,53,53	0
55	MG	BA	3485	1/1	0.33	-	46,46,46,46	0
55	MG	AA	3625	1/1	0.30	-	89,89,89,89	0
55	MG	AA	3308	1/1	0.18	-	96,96,96,96	0
55	MG	AA	3495	1/1	0.53	-	90,90,90,90	0
55	MG	AA	3092	1/1	0.28	-	71,71,71,71	0
55	MG	AA	3493	1/1	0.35	-	92,92,92,92	0
55	MG	AA	3067	1/1	0.74	-	108,108,108,108	0
55	MG	BA	3342	1/1	0.14	-	80,80,80,80	0
55	MG	DA	1645	1/1	0.38	-	51,51,51,51	0
55	MG	AA	3166	1/1	0.39	-	53,53,53,53	0
55	MG	DA	1742	1/1	0.33	-	82,82,82,82	0
55	MG	AA	3230	1/1	0.12	-	34,34,34,34	0
55	MG	BA	3126	1/1	0.21	-	51,51,51,51	0
55	MG	CA	1816	1/1	0.16	-	95,95,95,95	0
55	MG	AA	3383	1/1	0.27	-	85,85,85,85	0
55	MG	CA	1748	1/1	0.46	-	87,87,87,87	0
55	MG	AA	3210	1/1	0.35	-	72,72,72,72	0
55	MG	BA	3081	1/1	0.26	-	91,91,91,91	0
55	MG	AA	3244	1/1	0.51	-	45,45,45,45	0
55	MG	AA	3184	1/1	0.50	-	94,94,94,94	0
55	MG	BA	3011	1/1	0.30	-	65,65,65,65	0
55	MG	AA	3339	1/1	0.31	-	85,85,85,85	0
55	MG	AA	3170	1/1	0.16	-	41,41,41,41	0
55	MG	AA	3002	1/1	0.39	-	41,41,41,41	0
55	MG	AA	3433	1/1	0.14	-	152,152,152,152	0
55	MG	CA	1807	1/1	0.36	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CG	301	1/1	0.46	-	94,94,94,94	0
55	MG	AA	3515	1/1	0.35	-	77,77,77,77	0
55	MG	AA	3005	1/1	0.28	-	25,25,25,25	0
55	MG	BA	3462	1/1	0.08	-	123,123,123,123	0
55	MG	CA	1652	1/1	0.30	-	93,93,93,93	0
55	MG	CA	1758	1/1	0.29	-	97,97,97,97	0
55	MG	BA	3109	1/1	0.17	-	75,75,75,75	0
55	MG	AA	3422	1/1	0.50	-	106,106,106,106	0
55	MG	AA	3028	1/1	0.39	-	54,54,54,54	0
55	MG	DA	1797	1/1	0.37	-	85,85,85,85	0
55	MG	CA	1745	1/1	0.37	-	95,95,95,95	0
55	MG	AA	3023	1/1	0.60	-	56,56,56,56	0
55	MG	BA	3193	1/1	0.39	-	102,102,102,102	0
55	MG	BA	3355	1/1	0.48	-	87,87,87,87	0
55	MG	DA	1748	1/1	0.52	-	91,91,91,91	0
55	MG	BA	3236	1/1	0.46	-	41,41,41,41	0
55	MG	CA	1685	1/1	0.25	-	103,103,103,103	0
55	MG	CA	1643	1/1	0.37	-	91,91,91,91	0
55	MG	AA	3414	1/1	0.52	-	94,94,94,94	0
55	MG	BA	3086	1/1	0.47	-	82,82,82,82	0
55	MG	DA	1781	1/1	0.16	-	87,87,87,87	0
55	MG	BA	3084	1/1	0.24	-	99,99,99,99	0
55	MG	AA	3310	1/1	0.24	-	65,65,65,65	0
55	MG	AA	3459	1/1	0.33	-	81,81,81,81	0
55	MG	CA	1694	1/1	0.41	-	104,104,104,104	0
55	MG	AA	3573	1/1	0.33	-	31,31,31,31	0
55	MG	DA	1602	1/1	0.30	-	85,85,85,85	0
55	MG	BA	3025	1/1	0.17	-	80,80,80,80	0
55	MG	AA	3542	1/1	0.38	-	93,93,93,93	0
55	MG	AA	3050	1/1	0.97	-	108,108,108,108	0
55	MG	CA	1740	1/1	0.37	-	72,72,72,72	0
55	MG	BA	3392	1/1	0.27	-	85,85,85,85	0
55	MG	BA	3227	1/1	0.41	-	50,50,50,50	0
55	MG	BA	3441	1/1	0.43	-	93,93,93,93	0
55	MG	CA	1688	1/1	0.20	-	77,77,77,77	0
55	MG	AA	3521	1/1	0.38	-	75,75,75,75	0
55	MG	BA	3305	1/1	0.40	-	76,76,76,76	0
55	MG	BA	3343	1/1	0.30	-	75,75,75,75	0
55	MG	DA	1757	1/1	0.39	-	104,104,104,104	0
55	MG	AA	3371	1/1	0.47	-	89,89,89,89	0
55	MG	CA	1776	1/1	0.44	-	79,79,79,79	0
55	MG	AA	3549	1/1	0.55	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1649	1/1	0.27	-	93,93,93,93	0
55	MG	CA	1711	1/1	0.27	-	98,98,98,98	0
57	ZN	DG	303	1/1	0.28	-	134,134,134,134	0
55	MG	BA	3478	1/1	0.46	-	92,92,92,92	0
55	MG	AA	3122	1/1	0.23	-	84,84,84,84	0
55	MG	DA	1694	1/1	0.64	-	84,84,84,84	0
55	MG	AB	209	1/1	0.49	-	108,108,108,108	0
55	MG	AA	3327	1/1	0.49	-	84,84,84,84	0
55	MG	BA	3450	1/1	0.31	-	99,99,99,99	0
55	MG	DA	1692	1/1	0.44	-	81,81,81,81	0
55	MG	AA	3416	1/1	0.47	-	95,95,95,95	0
55	MG	DA	1612	1/1	0.17	-	73,73,73,73	0
55	MG	BB	204	1/1	0.38	-	90,90,90,90	0
55	MG	BA	3499	1/1	0.16	-	78,78,78,78	0
55	MG	BA	3490	1/1	0.26	-	52,52,52,52	0
55	MG	AA	3597	1/1	0.16	-	91,91,91,91	0
55	MG	AA	3434	1/1	0.52	-	44,44,44,44	0
55	MG	BA	3096	1/1	0.22	-	89,89,89,89	0
55	MG	AA	3266	1/1	0.48	-	49,49,49,49	0
55	MG	BA	3319	1/1	0.42	-	68,68,68,68	0
55	MG	BA	3165	1/1	0.38	-	42,42,42,42	0
55	MG	AA	3446	1/1	0.35	-	93,93,93,93	0
55	MG	CA	1705	1/1	0.15	-	95,95,95,95	0
55	MG	BA	3382	1/1	0.28	-	89,89,89,89	0
55	MG	AA	3555	1/1	0.19	-	67,67,67,67	0
55	MG	AA	3091	1/1	0.36	-	78,78,78,78	0
55	MG	AA	3106	1/1	0.31	-	69,69,69,69	0
55	MG	AE	303	1/1	0.42	-	91,91,91,91	0
55	MG	BA	3299	1/1	0.19	-	82,82,82,82	0
55	MG	CA	1699	1/1	0.09	-	63,63,63,63	0
55	MG	BA	3314	1/1	0.37	-	71,71,71,71	0
55	MG	AA	3373	1/1	0.44	-	106,106,106,106	0
55	MG	BA	3348	1/1	0.43	-	98,98,98,98	0
55	MG	AA	3436	1/1	0.46	-	66,66,66,66	0
55	MG	BA	3463	1/1	0.31	-	114,114,114,114	0
55	MG	CA	1819	1/1	0.20	-	109,109,109,109	0
55	MG	CQ	101	1/1	0.19	-	102,102,102,102	0
55	MG	CA	1787	1/1	0.29	-	100,100,100,100	0
55	MG	DA	1782	1/1	0.40	-	94,94,94,94	0
55	MG	AA	3358	1/1	0.78	-	89,89,89,89	0
55	MG	AA	3270	1/1	0.31	-	69,69,69,69	0
55	MG	BA	3397	1/1	0.30	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1711	1/1	0.47	-	89,89,89,89	0
55	MG	DA	1684	1/1	0.27	-	92,92,92,92	0
55	MG	BA	3391	1/1	0.32	-	95,95,95,95	0
55	MG	CA	1713	1/1	0.23	-	83,83,83,83	0
55	MG	DA	1717	1/1	0.15	-	103,103,103,103	0
55	MG	AO	203	1/1	0.32	-	43,43,43,43	0
55	MG	AA	3011	1/1	0.38	-	37,37,37,37	0
55	MG	BA	3302	1/1	0.43	-	75,75,75,75	0
55	MG	CA	1683	1/1	0.31	-	104,104,104,104	0
57	ZN	CQ	103	1/1	0.13	-	144,144,144,144	0
55	MG	BA	3093	1/1	0.17	-	78,78,78,78	0
55	MG	BA	3210	1/1	0.44	-	55,55,55,55	0
55	MG	BA	3309	1/1	0.34	-	80,80,80,80	0
55	MG	CA	1687	1/1	0.26	-	78,78,78,78	0
55	MG	A2	201	1/1	0.61	-	101,101,101,101	0
55	MG	AA	3456	1/1	0.50	-	91,91,91,91	0
55	MG	AA	3366	1/1	0.47	-	92,92,92,92	0
55	MG	AA	3123	1/1	0.45	-	52,52,52,52	0
55	MG	AA	3118	1/1	0.47	-	87,87,87,87	0
55	MG	AA	3131	1/1	0.27	-	90,90,90,90	0
55	MG	DA	1687	1/1	0.39	-	72,72,72,72	0
55	MG	AA	3513	1/1	0.42	-	83,83,83,83	0
55	MG	AA	3090	1/1	0.30	-	45,45,45,45	0
55	MG	BA	3118	1/1	0.27	-	110,110,110,110	0
55	MG	CA	1770	1/1	0.32	-	90,90,90,90	0
55	MG	AA	3496	1/1	0.55	-	87,87,87,87	0
55	MG	A7	101	1/1	0.33	-	60,60,60,60	0
55	MG	BA	3101	1/1	0.37	-	94,94,94,94	0
55	MG	CA	1664	1/1	0.12	-	47,47,47,47	0
55	MG	AA	3227	1/1	0.64	-	90,90,90,90	0
55	MG	AA	3547	1/1	0.21	-	45,45,45,45	0
55	MG	BA	3257	1/1	0.53	-	86,86,86,86	0
55	MG	BA	3459	1/1	0.25	-	115,115,115,115	0
55	MG	BA	3016	1/1	0.08	-	56,56,56,56	0
55	MG	BA	3073	1/1	0.49	-	99,99,99,99	0
55	MG	CA	1625	1/1	0.15	-	71,71,71,71	0
55	MG	AA	3386	1/1	0.23	-	74,74,74,74	0
55	MG	BA	3167	1/1	0.30	-	59,59,59,59	0
55	MG	BB	213	1/1	0.34	-	97,97,97,97	0
55	MG	DG	302	1/1	0.10	-	112,112,112,112	0
55	MG	AA	3470	1/1	0.39	-	96,96,96,96	0
55	MG	AA	3424	1/1	0.45	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1613	1/1	0.14	-	94,94,94,94	0
55	MG	A3	101	1/1	0.40	-	74,74,74,74	0
55	MG	DA	1775	1/1	0.47	-	102,102,102,102	0
55	MG	BA	3005	1/1	0.31	-	70,70,70,70	0
55	MG	DA	1671	1/1	0.44	-	77,77,77,77	0
55	MG	AA	3171	1/1	0.27	-	84,84,84,84	0
55	MG	BA	3371	1/1	0.15	-	129,129,129,129	0
55	MG	CA	1780	1/1	0.33	-	55,55,55,55	0
55	MG	BA	3079	1/1	0.20	-	82,82,82,82	0
55	MG	BA	3351	1/1	0.42	-	81,81,81,81	0
55	MG	CA	1838	1/1	0.15	-	103,103,103,103	0
55	MG	DA	1715	1/1	0.37	-	92,92,92,92	0
55	MG	BA	3130	1/1	0.27	-	44,44,44,44	0
55	MG	AA	3376	1/1	0.52	-	85,85,85,85	0
55	MG	BA	3341	1/1	0.47	-	82,82,82,82	0
55	MG	BA	3308	1/1	0.20	-	108,108,108,108	0
55	MG	DA	1618	1/1	0.30	-	104,104,104,104	0
55	MG	AA	3607	1/1	0.35	-	44,44,44,44	0
55	MG	BA	3028	1/1	0.55	-	85,85,85,85	0
55	MG	BA	3502	1/1	0.22	-	91,91,91,91	0
55	MG	DA	1800	1/1	0.35	-	99,99,99,99	0
55	MG	AA	3380	1/1	0.17	-	96,96,96,96	0
55	MG	AA	3300	1/1	0.36	-	81,81,81,81	0
55	MG	AA	3289	1/1	0.54	-	84,84,84,84	0
55	MG	AA	3152	1/1	0.58	-	58,58,58,58	0
55	MG	AA	3208	1/1	0.21	-	44,44,44,44	0
55	MG	DA	1666	1/1	0.50	-	115,115,115,115	0
55	MG	AA	3596	1/1	0.37	-	93,93,93,93	0
55	MG	AA	3512	1/1	0.17	-	97,97,97,97	0
55	MG	CA	1726	1/1	0.20	-	103,103,103,103	0
55	MG	DA	1604	1/1	0.26	-	92,92,92,92	0
55	MG	BA	3396	1/1	0.38	-	91,91,91,91	0
55	MG	DA	1714	1/1	0.36	-	105,105,105,105	0
55	MG	AB	216	1/1	0.34	-	106,106,106,106	0
55	MG	BB	208	1/1	0.49	-	107,107,107,107	0
55	MG	AA	3177	1/1	0.48	-	46,46,46,46	0
55	MG	BA	3233	1/1	0.44	-	74,74,74,74	0
55	MG	BA	3022	1/1	0.27	-	75,75,75,75	0
55	MG	CA	1788	1/1	0.15	-	105,105,105,105	0
55	MG	CA	1707	1/1	0.35	-	78,78,78,78	0
55	MG	BA	3168	1/1	0.23	-	60,60,60,60	0
55	MG	BA	3330	1/1	0.44	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3251	1/1	0.28	-	81,81,81,81	0
55	MG	AA	3539	1/1	0.31	-	49,49,49,49	0
55	MG	DA	1633	1/1	0.38	-	88,88,88,88	0
55	MG	AA	3372	1/1	0.20	-	87,87,87,87	0
55	MG	BA	3329	1/1	0.22	-	66,66,66,66	0
55	MG	BA	3112	1/1	0.14	-	69,69,69,69	0
55	MG	AA	3590	1/1	0.28	-	81,81,81,81	0
55	MG	BA	3047	1/1	0.24	-	80,80,80,80	0
55	MG	CC	102	1/1	0.26	-	69,69,69,69	0
55	MG	AA	3340	1/1	0.37	-	83,83,83,83	0
55	MG	CA	1712	1/1	0.24	-	92,92,92,92	0
55	MG	AA	3075	1/1	0.61	-	85,85,85,85	0
55	MG	BA	3477	1/1	0.31	-	94,94,94,94	0
55	MG	AA	3477	1/1	0.51	-	86,86,86,86	0
55	MG	AA	3157	1/1	0.41	-	39,39,39,39	0
55	MG	DA	1601	1/1	0.22	-	107,107,107,107	0
55	MG	BA	3089	1/1	0.30	-	83,83,83,83	0
55	MG	AA	3562	1/1	0.24	-	82,82,82,82	0
55	MG	BA	3175	1/1	0.21	-	100,100,100,100	0
55	MG	BA	3106	1/1	0.07	-	85,85,85,85	0
55	MG	BA	3072	1/1	0.33	-	104,104,104,104	0
55	MG	AA	3389	1/1	0.54	-	72,72,72,72	0
55	MG	AA	3601	1/1	0.22	-	86,86,86,86	0
55	MG	CA	1814	1/1	0.24	-	86,86,86,86	0
55	MG	CA	1619	1/1	0.24	-	59,59,59,59	0
55	MG	AA	3214	1/1	0.42	-	47,47,47,47	0
55	MG	BA	3179	1/1	0.39	-	61,61,61,61	0
55	MG	AA	3294	1/1	0.90	-	93,93,93,93	0
55	MG	AA	3245	1/1	0.46	-	75,75,75,75	0
55	MG	BA	3456	1/1	0.33	-	88,88,88,88	0
55	MG	DA	1729	1/1	0.54	-	84,84,84,84	0
55	MG	BA	3182	1/1	0.20	-	47,47,47,47	0
55	MG	AA	3578	1/1	0.38	-	50,50,50,50	0
55	MG	BA	3300	1/1	0.40	-	56,56,56,56	0
55	MG	AA	3142	1/1	0.24	-	71,71,71,71	0
55	MG	AA	3354	1/1	0.31	-	84,84,84,84	0
55	MG	CA	1799	1/1	0.33	-	95,95,95,95	0
55	MG	CA	1673	1/1	0.36	-	76,76,76,76	0
55	MG	BA	3058	1/1	0.43	-	89,89,89,89	0
55	MG	AA	3337	1/1	0.37	-	99,99,99,99	0
55	MG	CA	1615	1/1	0.36	-	104,104,104,104	0
55	MG	AA	3286	1/1	0.45	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	202	1/1	0.15	-	103,103,103,103	0
55	MG	BA	3394	1/1	0.41	-	88,88,88,88	0
55	MG	BA	3475	1/1	0.29	-	90,90,90,90	0
55	MG	BA	3099	1/1	0.19	-	98,98,98,98	0
55	MG	AA	3540	1/1	0.43	-	63,63,63,63	0
55	MG	AA	3066	1/1	0.55	-	48,48,48,48	0
55	MG	DA	1675	1/1	0.44	-	60,60,60,60	0
55	MG	CA	1796	1/1	0.36	-	82,82,82,82	0
55	MG	DA	1613	1/1	0.38	-	88,88,88,88	0
55	MG	AA	3478	1/1	0.37	-	75,75,75,75	0
55	MG	AA	3080	1/1	0.73	-	104,104,104,104	0
55	MG	BB	215	1/1	0.20	-	101,101,101,101	0
55	MG	BA	3108	1/1	0.47	-	99,99,99,99	0
55	MG	AA	3454	1/1	0.49	-	94,94,94,94	0
55	MG	AA	3158	1/1	0.28	-	68,68,68,68	0
55	MG	AA	3611	1/1	0.27	-	100,100,100,100	0
55	MG	BA	3414	1/1	0.16	-	92,92,92,92	0
55	MG	BA	3194	1/1	0.44	-	70,70,70,70	0
55	MG	AA	3492	1/1	0.25	-	94,94,94,94	0
55	MG	AA	3163	1/1	0.30	-	55,55,55,55	0
55	MG	AA	3353	1/1	0.42	-	86,86,86,86	0
55	MG	BA	3472	1/1	0.44	-	83,83,83,83	0
55	MG	DA	1763	1/1	0.32	-	89,89,89,89	0
55	MG	BA	3244	1/1	0.38	-	54,54,54,54	0
55	MG	BA	3438	1/1	0.26	-	88,88,88,88	0
55	MG	AA	3581	1/1	0.12	-	36,36,36,36	0
55	MG	AA	3553	1/1	0.39	-	87,87,87,87	0
55	MG	BA	3078	1/1	0.23	-	95,95,95,95	0
55	MG	AA	3140	1/1	0.37	-	67,67,67,67	0
55	MG	BA	3217	1/1	0.32	-	39,39,39,39	0
55	MG	AA	3180	1/1	0.44	-	64,64,64,64	0
55	MG	BA	3132	1/1	0.26	-	54,54,54,54	0
55	MG	DA	1785	1/1	0.37	-	93,93,93,93	0
55	MG	AA	3321	1/1	0.39	-	65,65,65,65	0
55	MG	AA	3437	1/1	0.73	-	122,122,122,122	0
55	MG	CA	1765	1/1	0.23	-	109,109,109,109	0
55	MG	BA	3163	1/1	0.22	-	84,84,84,84	0
55	MG	CA	1612	1/1	0.21	-	102,102,102,102	0
55	MG	AA	3149	1/1	0.37	-	57,57,57,57	0
55	MG	BA	3401	1/1	0.19	-	100,100,100,100	0
55	MG	BA	3429	1/1	0.21	-	95,95,95,95	0
55	MG	DA	1661	1/1	0.55	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3476	1/1	0.57	-	79,79,79,79	0
55	MG	BA	3313	1/1	0.29	-	106,106,106,106	0
55	MG	AA	3318	1/1	0.34	-	92,92,92,92	0
55	MG	AA	3442	1/1	0.34	-	78,78,78,78	0
55	MG	BA	3085	1/1	0.39	-	74,74,74,74	0
55	MG	BA	3494	1/1	0.40	-	88,88,88,88	0
55	MG	CA	1751	1/1	0.20	-	78,78,78,78	0
55	MG	BA	3023	1/1	0.44	-	70,70,70,70	0
55	MG	CA	1696	1/1	0.32	-	90,90,90,90	0
55	MG	BA	3423	1/1	0.47	-	91,91,91,91	0
55	MG	DA	1704	1/1	0.46	-	87,87,87,87	0
55	MG	AA	3195	1/1	0.21	-	62,62,62,62	0
57	ZN	CG	303	1/1	0.32	-	95,95,95,95	0
55	MG	AA	3249	1/1	0.39	-	76,76,76,76	0
55	MG	CA	1734	1/1	0.51	-	86,86,86,86	0
55	MG	BA	3489	1/1	0.41	-	68,68,68,68	0
55	MG	AA	3215	1/1	0.32	-	79,79,79,79	0
55	MG	AA	3202	1/1	0.32	-	46,46,46,46	0
55	MG	BA	3439	1/1	0.25	-	103,103,103,103	0
55	MG	AA	3072	1/1	0.13	-	101,101,101,101	0
55	MG	DA	1724	1/1	0.49	-	72,72,72,72	0
55	MG	AA	3463	1/1	0.39	-	90,90,90,90	0
55	MG	BA	3253	1/1	0.47	-	66,66,66,66	0
55	MG	AA	3043	1/1	0.44	-	108,108,108,108	0
55	MG	DA	1771	1/1	0.20	-	114,114,114,114	0
55	MG	CA	1671	1/1	0.23	-	72,72,72,72	0
55	MG	AA	3014	1/1	0.26	-	38,38,38,38	0
55	MG	BA	3411	1/1	0.37	-	83,83,83,83	0
55	MG	CA	1762	1/1	0.10	-	89,89,89,89	0
55	MG	AA	3108	1/1	0.51	-	66,66,66,66	0
55	MG	CA	1651	1/1	0.36	-	75,75,75,75	0
55	MG	AA	3468	1/1	0.20	-	95,95,95,95	0
55	MG	CA	1795	1/1	0.27	-	68,68,68,68	0
55	MG	AA	3026	1/1	0.22	-	40,40,40,40	0
55	MG	AA	3565	1/1	0.38	-	53,53,53,53	0
55	MG	BA	3520	1/1	0.34	-	101,101,101,101	0
55	MG	DA	1619	1/1	0.41	-	77,77,77,77	0
55	MG	AA	3185	1/1	0.56	-	88,88,88,88	0
55	MG	CT	201	1/1	0.27	-	102,102,102,102	0
55	MG	AA	3397	1/1	0.54	-	95,95,95,95	0
55	MG	BP	201	1/1	0.23	-	65,65,65,65	0
55	MG	AA	3387	1/1	0.70	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1834	1/1	0.25	-	90,90,90,90	0
55	MG	AA	3036	1/1	0.20	-	39,39,39,39	0
55	MG	DA	1616	1/1	0.33	-	100,100,100,100	0
55	MG	AO	202	1/1	0.66	-	80,80,80,80	0
55	MG	BA	3051	1/1	0.35	-	90,90,90,90	0
55	MG	BA	3235	1/1	0.48	-	74,74,74,74	0
55	MG	AA	3491	1/1	0.39	-	85,85,85,85	0
55	MG	BA	3192	1/1	0.36	-	72,72,72,72	0
55	MG	BA	3306	1/1	0.23	-	86,86,86,86	0
55	MG	BA	3237	1/1	0.21	-	47,47,47,47	0
55	MG	DA	1639	1/1	0.35	-	78,78,78,78	0
55	MG	DA	1615	1/1	0.37	-	96,96,96,96	0
55	MG	AA	3511	1/1	0.82	-	98,98,98,98	0
55	MG	DA	1746	1/1	0.29	-	104,104,104,104	0
55	MG	BA	3434	1/1	0.19	-	90,90,90,90	0
55	MG	BA	3083	1/1	0.33	-	92,92,92,92	0
55	MG	BA	3140	1/1	0.28	-	42,42,42,42	0
55	MG	BA	3158	1/1	0.23	-	70,70,70,70	0
55	MG	AA	3101	1/1	0.34	-	79,79,79,79	0
55	MG	BA	3379	1/1	0.40	-	84,84,84,84	0
55	MG	AA	3125	1/1	0.46	-	55,55,55,55	0
55	MG	BA	3367	1/1	0.42	-	91,91,91,91	0
55	MG	BA	3087	1/1	0.37	-	80,80,80,80	0
55	MG	CA	1791	1/1	0.14	-	97,97,97,97	0
55	MG	CA	1737	1/1	0.22	-	92,92,92,92	0
55	MG	AA	3425	1/1	0.38	-	94,94,94,94	0
55	MG	DA	1624	1/1	0.27	-	95,95,95,95	0
55	MG	AA	3390	1/1	0.29	-	109,109,109,109	0
55	MG	BA	3413	1/1	0.45	-	94,94,94,94	0
55	MG	DA	1679	1/1	0.36	-	64,64,64,64	0
55	MG	BA	3335	1/1	0.17	-	100,100,100,100	0
55	MG	DA	1637	1/1	0.33	-	97,97,97,97	0
55	MG	AA	3525	1/1	0.15	-	73,73,73,73	0
55	MG	AA	3271	1/1	0.34	-	92,92,92,92	0
55	MG	DH	201	1/1	0.22	-	105,105,105,105	0
55	MG	CA	1700	1/1	0.07	-	72,72,72,72	0
55	MG	AA	3287	1/1	0.32	-	69,69,69,69	0
55	MG	AA	3439	1/1	0.32	-	97,97,97,97	0
55	MG	CA	1636	1/1	0.29	-	91,91,91,91	0
55	MG	AA	3084	1/1	0.26	-	43,43,43,43	0
55	MG	DA	1753	1/1	0.49	-	87,87,87,87	0
55	MG	AA	3188	1/1	0.48	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3444	1/1	0.36	-	58,58,58,58	0
55	MG	CA	1628	1/1	0.38	-	85,85,85,85	0
55	MG	AA	3419	1/1	0.66	-	89,89,89,89	0
55	MG	AA	3034	1/1	0.40	-	52,52,52,52	0
55	MG	AA	3485	1/1	0.41	-	71,71,71,71	0
55	MG	AA	3126	1/1	0.28	-	83,83,83,83	0
55	MG	BA	3135	1/1	0.36	-	52,52,52,52	0
55	MG	BA	3114	1/1	0.39	-	103,103,103,103	0
55	MG	BA	3097	1/1	0.28	-	60,60,60,60	0
55	MG	CA	1674	1/1	0.32	-	102,102,102,102	0
55	MG	BA	3010	1/1	0.27	-	68,68,68,68	0
55	MG	CA	1797	1/1	0.16	-	93,93,93,93	0
55	MG	BA	3383	1/1	0.46	-	95,95,95,95	0
55	MG	CA	1602	1/1	0.15	-	74,74,74,74	0
55	MG	CA	1738	1/1	0.38	-	103,103,103,103	0
55	MG	AA	3518	1/1	0.28	-	90,90,90,90	0
55	MG	CA	1606	1/1	0.07	-	94,94,94,94	0
55	MG	AA	3396	1/1	0.50	-	104,104,104,104	0
55	MG	CA	1835	1/1	0.12	-	87,87,87,87	0
55	MG	BA	3323	1/1	0.51	-	74,74,74,74	0
55	MG	BA	3155	1/1	0.35	-	87,87,87,87	0
55	MG	CA	1718	1/1	0.31	-	93,93,93,93	0
55	MG	BA	3415	1/1	0.41	-	109,109,109,109	0
55	MG	AA	3391	1/1	0.32	-	106,106,106,106	0
55	MG	BA	3055	1/1	0.43	-	99,99,99,99	0
55	MG	AA	3576	1/1	0.45	-	46,46,46,46	0
55	MG	CA	1720	1/1	0.30	-	102,102,102,102	0
55	MG	BA	3191	1/1	0.46	-	77,77,77,77	0
55	MG	AA	3281	1/1	0.49	-	74,74,74,74	0
55	MG	CA	1701	1/1	0.15	-	105,105,105,105	0
55	MG	BA	3497	1/1	0.28	-	63,63,63,63	0
55	MG	AA	3363	1/1	0.49	-	95,95,95,95	0
55	MG	AB	213	1/1	0.61	-	73,73,73,73	0
55	MG	AA	3324	1/1	0.22	-	92,92,92,92	0
55	MG	DA	1759	1/1	0.50	-	108,108,108,108	0
55	MG	AA	3191	1/1	0.14	-	95,95,95,95	0
55	MG	AA	3584	1/1	0.16	-	63,63,63,63	0
55	MG	AA	3093	1/1	0.52	-	65,65,65,65	0
55	MG	BA	3426	1/1	0.43	-	87,87,87,87	0
55	MG	BA	3007	1/1	0.08	-	83,83,83,83	0
55	MG	DA	1743	1/1	0.22	-	94,94,94,94	0
55	MG	BE	301	1/1	0.27	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3155	1/1	0.46	-	71,71,71,71	0
55	MG	BA	3234	1/1	0.31	-	67,67,67,67	0
55	MG	BA	3385	1/1	0.26	-	97,97,97,97	0
55	MG	BA	3369	1/1	0.39	-	69,69,69,69	0
55	MG	AA	3265	1/1	0.20	-	95,95,95,95	0
55	MG	AA	3176	1/1	0.20	-	74,74,74,74	0
55	MG	CA	1822	1/1	0.14	-	105,105,105,105	0
55	MG	DA	1739	1/1	0.17	-	113,113,113,113	0
55	MG	DA	1678	1/1	0.53	-	86,86,86,86	0
55	MG	CA	1646	1/1	0.34	-	75,75,75,75	0
55	MG	DA	1709	1/1	0.32	-	109,109,109,109	0
55	MG	AA	3004	1/1	0.39	-	40,40,40,40	0
55	MG	AA	3213	1/1	0.42	-	59,59,59,59	0
55	MG	DA	1683	1/1	0.60	-	80,80,80,80	0
55	MG	BA	3393	1/1	0.11	-	84,84,84,84	0
55	MG	BA	3147	1/1	0.27	-	63,63,63,63	0
55	MG	CA	1706	1/1	0.26	-	91,91,91,91	0
55	MG	AA	3274	1/1	0.38	-	72,72,72,72	0
55	MG	AA	3407	1/1	0.71	-	110,110,110,110	0
55	MG	BA	3277	1/1	0.27	-	109,109,109,109	0
55	MG	AA	3086	1/1	0.63	-	62,62,62,62	0
55	MG	AA	3405	1/1	0.83	-	90,90,90,90	0
55	MG	BA	3500	1/1	0.26	-	104,104,104,104	0
55	MG	BA	3312	1/1	0.42	-	98,98,98,98	0
55	MG	BA	3128	1/1	0.24	-	56,56,56,56	0
56	PAR	DA	1805	42/42	0.20	-	46,59,73,84	0
55	MG	BA	3469	1/1	0.35	-	92,92,92,92	0
55	MG	AA	3052	1/1	0.30	-	73,73,73,73	0
55	MG	BA	3094	1/1	0.24	-	79,79,79,79	0
55	MG	BA	3050	1/1	0.36	-	103,103,103,103	0
55	MG	AA	3137	1/1	0.12	-	51,51,51,51	0
55	MG	BA	3435	1/1	0.21	-	108,108,108,108	0
55	MG	AA	3534	1/1	0.42	-	49,49,49,49	0
55	MG	CA	1704	1/1	0.32	-	113,113,113,113	0
55	MG	CA	1735	1/1	0.42	-	101,101,101,101	0
55	MG	AA	3012	1/1	0.39	-	40,40,40,40	0
55	MG	AA	3037	1/1	0.36	-	69,69,69,69	0
55	MG	BA	3290	1/1	0.27	-	82,82,82,82	0
55	MG	BA	3294	1/1	0.39	-	98,98,98,98	0
55	MG	AA	3592	1/1	0.33	-	76,76,76,76	0
55	MG	BA	3002	1/1	0.29	-	66,66,66,66	0
55	MG	BA	3322	1/1	0.28	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3194	1/1	0.41	-	102,102,102,102	0
55	MG	AA	3291	1/1	0.40	-	68,68,68,68	0
55	MG	BA	3380	1/1	0.31	-	78,78,78,78	0
55	MG	AA	3222	1/1	0.47	-	54,54,54,54	0
55	MG	AA	3336	1/1	0.21	-	82,82,82,82	0
55	MG	CA	1810	1/1	0.41	-	108,108,108,108	0
55	MG	DB	101	1/1	0.26	-	103,103,103,103	0
55	MG	BA	3358	1/1	0.42	-	85,85,85,85	0
55	MG	BA	3446	1/1	0.26	-	98,98,98,98	0
55	MG	AA	3399	1/1	0.34	-	60,60,60,60	0
55	MG	BA	3229	1/1	0.34	-	50,50,50,50	0
55	MG	BA	3491	1/1	0.10	-	49,49,49,49	0
55	MG	AA	3276	1/1	0.54	-	78,78,78,78	0
55	MG	DA	1735	1/1	0.50	-	106,106,106,106	0
55	MG	BA	3453	1/1	0.24	-	93,93,93,93	0
55	MG	AB	207	1/1	0.20	-	103,103,103,103	0
55	MG	AA	3417	1/1	0.28	-	67,67,67,67	0
55	MG	CA	1621	1/1	0.47	-	107,107,107,107	0
55	MG	BA	3527	1/1	0.33	-	97,97,97,97	0
55	MG	BA	3020	1/1	0.28	-	76,76,76,76	0
55	MG	BA	3107	1/1	0.23	-	89,89,89,89	0
55	MG	BA	3146	1/1	0.25	-	86,86,86,86	0
55	MG	AA	3304	1/1	0.23	-	90,90,90,90	0
55	MG	AA	3258	1/1	0.41	-	92,92,92,92	0
55	MG	BA	3333	1/1	0.31	-	73,73,73,73	0
55	MG	DA	1682	1/1	0.53	-	96,96,96,96	0
55	MG	AA	3328	1/1	0.44	-	82,82,82,82	0
55	MG	BA	3196	1/1	0.41	-	84,84,84,84	0
55	MG	CA	1723	1/1	0.33	-	106,106,106,106	0
55	MG	AA	3070	1/1	0.31	-	68,68,68,68	0
55	MG	BA	3124	1/1	0.35	-	102,102,102,102	0
55	MG	CA	1679	1/1	0.33	-	101,101,101,101	0
55	MG	AA	3303	1/1	0.49	-	95,95,95,95	0
55	MG	AA	3480	1/1	0.63	-	86,86,86,86	0
55	MG	BA	3145	1/1	0.39	-	53,53,53,53	0
55	MG	BA	3420	1/1	0.18	-	136,136,136,136	0
55	MG	BA	3183	1/1	0.20	-	80,80,80,80	0
55	MG	BA	3501	1/1	0.20	-	88,88,88,88	0
55	MG	DA	1657	1/1	0.46	-	95,95,95,95	0
55	MG	BA	3038	1/1	0.30	-	78,78,78,78	0
55	MG	DA	1699	1/1	0.38	-	68,68,68,68	0
55	MG	CA	1692	1/1	0.09	-	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DC	102	1/1	0.17	-	74,74,74,74	0
55	MG	AA	3524	1/1	0.34	-	94,94,94,94	0
55	MG	AA	3138	1/1	0.39	-	45,45,45,45	0
55	MG	CA	1627	1/1	0.24	-	65,65,65,65	0
55	MG	BA	3121	1/1	0.44	-	99,99,99,99	0
55	MG	CA	1666	1/1	0.19	-	70,70,70,70	0
55	MG	DA	1700	1/1	0.38	-	94,94,94,94	0
55	MG	DC	106	1/1	0.20	-	111,111,111,111	0
55	MG	BA	3045	1/1	0.30	-	88,88,88,88	0
55	MG	BA	3328	1/1	0.14	-	61,61,61,61	0
55	MG	AA	3469	1/1	0.62	-	103,103,103,103	0
55	MG	AA	3153	1/1	0.24	-	48,48,48,48	0
55	MG	CA	1684	1/1	0.25	-	101,101,101,101	0
55	MG	AA	3545	1/1	0.35	-	75,75,75,75	0
55	MG	BA	3211	1/1	0.27	-	57,57,57,57	0
55	MG	BA	3198	1/1	0.28	-	44,44,44,44	0
55	MG	BA	3285	1/1	0.18	-	45,45,45,45	0
55	MG	DA	1643	1/1	0.45	-	81,81,81,81	0
55	MG	AO	201	1/1	0.45	-	65,65,65,65	0
55	MG	BA	3417	1/1	0.15	-	88,88,88,88	0
55	MG	BA	3120	1/1	0.25	-	81,81,81,81	0
55	MG	CA	1631	1/1	0.18	-	74,74,74,74	0
55	MG	BA	3076	1/1	0.38	-	91,91,91,91	0
55	MG	CA	1653	1/1	0.37	-	91,91,91,91	0
55	MG	CA	1741	1/1	0.20	-	80,80,80,80	0
55	MG	BA	3444	1/1	0.63	-	96,96,96,96	0
55	MG	BA	3378	1/1	0.23	-	78,78,78,78	0
55	MG	DA	1689	1/1	0.36	-	72,72,72,72	0
55	MG	AA	3531	1/1	0.41	-	96,96,96,96	0
55	MG	AA	3475	1/1	0.29	-	102,102,102,102	0
55	MG	CA	1773	1/1	0.33	-	101,101,101,101	0
55	MG	BA	3265	1/1	0.46	-	86,86,86,86	0
55	MG	AA	3038	1/1	0.52	-	80,80,80,80	0
55	MG	AA	3568	1/1	0.27	-	49,49,49,49	0
55	MG	CA	1803	1/1	0.62	-	94,94,94,94	0
55	MG	AA	3561	1/1	0.19	-	82,82,82,82	0
55	MG	BA	3400	1/1	0.31	-	74,74,74,74	0
55	MG	BA	3024	1/1	1.17	-	110,110,110,110	0
55	MG	AA	3293	1/1	0.19	-	77,77,77,77	0
55	MG	AA	3606	1/1	0.51	-	61,61,61,61	0
55	MG	AA	3218	1/1	0.42	-	73,73,73,73	0
55	MG	CA	1604	1/1	0.32	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3333	1/1	0.59	-	95,95,95,95	0
55	MG	AA	3017	1/1	0.44	-	64,64,64,64	0
55	MG	AA	3487	1/1	0.08	-	77,77,77,77	0
55	MG	CA	1656	1/1	0.50	-	88,88,88,88	0
55	MG	BA	3451	1/1	0.39	-	89,89,89,89	0
55	MG	AA	3554	1/1	0.46	-	74,74,74,74	0
55	MG	DA	1693	1/1	0.44	-	93,93,93,93	0
55	MG	CA	1722	1/1	0.38	-	74,74,74,74	0
55	MG	DA	1648	1/1	0.12	-	69,69,69,69	0
55	MG	BA	3180	1/1	0.32	-	57,57,57,57	0
55	MG	CA	1809	1/1	0.32	-	79,79,79,79	0
55	MG	AA	3556	1/1	0.51	-	96,96,96,96	0
55	MG	AA	3039	1/1	0.61	-	82,82,82,82	0
55	MG	CA	1715	1/1	0.31	-	115,115,115,115	0
55	MG	AA	3331	1/1	0.41	-	76,76,76,76	0
55	MG	BA	3296	1/1	0.30	-	76,76,76,76	0
55	MG	AA	3174	1/1	0.41	-	40,40,40,40	0
55	MG	AA	3410	1/1	0.36	-	95,95,95,95	0
55	MG	AA	3481	1/1	0.19	-	112,112,112,112	0
55	MG	AA	3257	1/1	0.38	-	79,79,79,79	0
55	MG	BA	3248	1/1	0.23	-	54,54,54,54	0
55	MG	AA	3532	1/1	0.41	-	88,88,88,88	0
55	MG	DA	1610	1/1	0.29	-	97,97,97,97	0
55	MG	AA	3059	1/1	0.41	-	80,80,80,80	0
55	MG	AA	3196	1/1	0.23	-	61,61,61,61	0
55	MG	CA	1730	1/1	0.27	-	107,107,107,107	0
55	MG	AA	3519	1/1	0.14	-	53,53,53,53	0
55	MG	AA	3031	1/1	0.39	-	52,52,52,52	0
55	MG	AA	3212	1/1	0.31	-	52,52,52,52	0
55	MG	AA	3509	1/1	0.33	-	95,95,95,95	0
55	MG	AB	217	1/1	0.25	-	110,110,110,110	0
55	MG	BA	3160	1/1	0.28	-	82,82,82,82	0
55	MG	BA	3466	1/1	0.11	-	73,73,73,73	0
55	MG	AA	3610	1/1	0.18	-	46,46,46,46	0
55	MG	BA	3197	1/1	0.14	-	76,76,76,76	0
55	MG	AA	3178	1/1	0.16	-	54,54,54,54	0
55	MG	AA	3577	1/1	0.18	-	52,52,52,52	0
55	MG	AA	3431	1/1	0.26	-	89,89,89,89	0
55	MG	AA	3378	1/1	0.54	-	84,84,84,84	0
55	MG	BA	3232	1/1	0.32	-	55,55,55,55	0
55	MG	AA	3575	1/1	0.39	-	42,42,42,42	0
55	MG	BA	3284	1/1	0.13	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1690	1/1	0.35	-	102,102,102,102	0
55	MG	AA	3018	1/1	0.33	-	43,43,43,43	0
55	MG	AA	3219	1/1	0.44	-	81,81,81,81	0
55	MG	BA	3406	1/1	0.39	-	97,97,97,97	0
55	MG	BA	3082	1/1	0.43	-	76,76,76,76	0
55	MG	BA	3069	1/1	0.17	-	70,70,70,70	0
55	MG	AA	3314	1/1	0.60	-	80,80,80,80	0
55	MG	CA	1806	1/1	0.15	-	62,62,62,62	0
55	MG	CA	1641	1/1	0.19	-	65,65,65,65	0
55	MG	DA	1680	1/1	0.38	-	81,81,81,81	0
55	MG	AA	3144	1/1	0.46	-	45,45,45,45	0
55	MG	AA	3254	1/1	0.68	-	85,85,85,85	0
55	MG	CA	1752	1/1	0.14	-	96,96,96,96	0
55	MG	CA	1617	1/1	0.42	-	72,72,72,72	0
55	MG	AA	3162	1/1	0.26	-	45,45,45,45	0
55	MG	AA	3109	1/1	0.38	-	53,53,53,53	0
55	MG	BA	3412	1/1	0.45	-	50,50,50,50	0
55	MG	CA	1744	1/1	0.45	-	57,57,57,57	0
55	MG	DA	1608	1/1	0.29	-	92,92,92,92	0
55	MG	CA	1677	1/1	0.19	-	90,90,90,90	0
55	MG	CA	1836	1/1	0.23	-	71,71,71,71	0
55	MG	AA	3460	1/1	0.35	-	106,106,106,106	0
55	MG	CA	1772	1/1	0.19	-	83,83,83,83	0
55	MG	AA	3616	1/1	0.28	-	95,95,95,95	0
55	MG	CA	1675	1/1	0.25	-	97,97,97,97	0
55	MG	BA	3225	1/1	0.23	-	78,78,78,78	0
55	MG	AA	3467	1/1	0.31	-	87,87,87,87	0
55	MG	AA	3124	1/1	0.53	-	47,47,47,47	0
55	MG	BA	3223	1/1	0.28	-	64,64,64,64	0
55	MG	AA	3022	1/1	0.27	-	49,49,49,49	0
55	MG	BA	3228	1/1	0.36	-	74,74,74,74	0
55	MG	AA	3062	1/1	0.35	-	86,86,86,86	0
55	MG	AA	3010	1/1	0.38	-	47,47,47,47	0
55	MG	DA	1777	1/1	0.47	-	87,87,87,87	0
55	MG	AA	3392	1/1	0.46	-	93,93,93,93	0
55	MG	CA	1779	1/1	0.11	-	113,113,113,113	0
55	MG	BA	3095	1/1	0.46	-	112,112,112,112	0
55	MG	DA	1638	1/1	0.27	-	74,74,74,74	0
55	MG	AA	3329	1/1	0.15	-	94,94,94,94	0
55	MG	CA	1710	1/1	0.29	-	81,81,81,81	0
55	MG	BA	3447	1/1	0.37	-	100,100,100,100	0
55	MG	BA	3220	1/1	0.34	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3047	1/1	0.28	-	60,60,60,60	0
55	MG	AB	210	1/1	0.45	-	65,65,65,65	0
55	MG	AA	3267	1/1	0.32	-	62,62,62,62	0
55	MG	CA	1672	1/1	0.21	-	106,106,106,106	0
55	MG	AA	3529	1/1	0.24	-	68,68,68,68	0
55	MG	AA	3330	1/1	0.42	-	60,60,60,60	0
55	MG	BA	3416	1/1	0.25	-	103,103,103,103	0
55	MG	BA	3230	1/1	0.23	-	68,68,68,68	0
55	MG	CA	1709	1/1	0.38	-	96,96,96,96	0
55	MG	AA	3187	1/1	0.45	-	87,87,87,87	0
55	MG	BA	3259	1/1	0.34	-	54,54,54,54	0
55	MG	BA	3219	1/1	0.27	-	48,48,48,48	0
55	MG	BA	3134	1/1	0.33	-	63,63,63,63	0
55	MG	CA	1729	1/1	0.34	-	94,94,94,94	0
55	MG	DA	1734	1/1	0.38	-	88,88,88,88	0
55	MG	BA	3150	1/1	0.47	-	96,96,96,96	0
55	MG	AA	3323	1/1	0.21	-	71,71,71,71	0
55	MG	CA	1657	1/1	0.27	-	63,63,63,63	0
55	MG	DA	1767	1/1	0.32	-	113,113,113,113	0
55	MG	BA	3388	1/1	0.32	-	87,87,87,87	0
55	MG	AA	3045	1/1	0.50	-	54,54,54,54	0
55	MG	DA	1765	1/1	0.29	-	93,93,93,93	0
55	MG	BA	3141	1/1	0.24	-	72,72,72,72	0
55	MG	BA	3503	1/1	0.15	-	69,69,69,69	0
55	MG	BA	3012	1/1	0.35	-	63,63,63,63	0
55	MG	DA	1607	1/1	0.36	-	92,92,92,92	0
55	MG	AA	3341	1/1	0.37	-	95,95,95,95	0
55	MG	AA	3614	1/1	0.47	-	78,78,78,78	0
55	MG	BA	3052	1/1	0.32	-	58,58,58,58	0
55	MG	BA	3014	1/1	0.34	-	72,72,72,72	0
55	MG	AA	3435	1/1	0.58	-	78,78,78,78	0
55	MG	BA	3347	1/1	0.32	-	85,85,85,85	0
55	MG	AA	3421	1/1	0.44	-	94,94,94,94	0
55	MG	AA	3428	1/1	0.20	-	120,120,120,120	0
55	MG	CA	1764	1/1	0.16	-	92,92,92,92	0
55	MG	BA	3125	1/1	1.01	-	104,104,104,104	0
55	MG	AA	3301	1/1	0.24	-	85,85,85,85	0
55	MG	AB	214	1/1	0.40	-	102,102,102,102	0
55	MG	AA	3569	1/1	0.29	-	60,60,60,60	0
55	MG	BA	3365	1/1	0.48	-	90,90,90,90	0
55	MG	BA	3009	1/1	0.28	-	48,48,48,48	0
55	MG	CA	1775	1/1	0.19	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3166	1/1	0.35	-	40,40,40,40	0
55	MG	CA	1820	1/1	0.41	-	88,88,88,88	0
55	MG	AB	201	1/1	0.72	-	96,96,96,96	0
55	MG	AF	303	1/1	0.33	-	69,69,69,69	0
55	MG	DA	1793	1/1	0.46	-	108,108,108,108	0
55	MG	AA	3322	1/1	0.51	-	68,68,68,68	0
55	MG	DA	1758	1/1	0.50	-	109,109,109,109	0
55	MG	DA	1801	1/1	0.29	-	90,90,90,90	0
55	MG	AA	3404	1/1	0.38	-	95,95,95,95	0
55	MG	BA	3349	1/1	0.35	-	93,93,93,93	0
55	MG	AA	3349	1/1	0.37	-	84,84,84,84	0
55	MG	DA	1803	1/1	0.45	-	100,100,100,100	0
55	MG	AA	3030	1/1	0.29	-	45,45,45,45	0
55	MG	BA	3301	1/1	0.31	-	106,106,106,106	0
55	MG	AA	3367	1/1	0.61	-	87,87,87,87	0
55	MG	AA	3388	1/1	0.49	-	85,85,85,85	0
55	MG	BA	3209	1/1	0.36	-	46,46,46,46	0
55	MG	BE	303	1/1	0.26	-	57,57,57,57	0
55	MG	AA	3619	1/1	0.46	-	87,87,87,87	0
55	MG	BA	3403	1/1	0.24	-	77,77,77,77	0
55	MG	AA	3228	1/1	0.46	-	79,79,79,79	0
55	MG	DC	103	1/1	0.37	-	78,78,78,78	0
55	MG	AA	3580	1/1	0.23	-	78,78,78,78	0
55	MG	BA	3464	1/1	0.39	-	104,104,104,104	0
55	MG	BA	3178	1/1	0.29	-	62,62,62,62	0
55	MG	CA	1798	1/1	0.34	-	82,82,82,82	0
55	MG	BA	3215	1/1	0.34	-	66,66,66,66	0
55	MG	BA	3431	1/1	0.21	-	84,84,84,84	0
55	MG	BA	3436	1/1	0.32	-	94,94,94,94	0
55	MG	CA	1831	1/1	0.33	-	105,105,105,105	0
55	MG	AA	3499	1/1	0.78	-	93,93,93,93	0
55	MG	AA	3112	1/1	0.59	-	45,45,45,45	0
55	MG	CA	1753	1/1	0.18	-	107,107,107,107	0
55	MG	BA	3062	1/1	0.32	-	110,110,110,110	0
55	MG	BA	3468	1/1	0.34	-	105,105,105,105	0
55	MG	AA	3548	1/1	0.32	-	54,54,54,54	0
55	MG	BA	3398	1/1	0.68	-	96,96,96,96	0
55	MG	CA	1645	1/1	0.38	-	60,60,60,60	0
55	MG	DA	1744	1/1	0.45	-	57,57,57,57	0
55	MG	AB	202	1/1	0.21	-	92,92,92,92	0
55	MG	AA	3320	1/1	0.30	-	103,103,103,103	0
55	MG	BA	3151	1/1	0.25	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3187	1/1	0.38	-	65,65,65,65	0
55	MG	BA	3131	1/1	0.18	-	49,49,49,49	0
55	MG	CA	1719	1/1	0.31	-	85,85,85,85	0
55	MG	AA	3168	1/1	0.34	-	68,68,68,68	0
55	MG	CA	1747	1/1	0.37	-	83,83,83,83	0
55	MG	BA	3116	1/1	0.30	-	107,107,107,107	0
55	MG	DA	1710	1/1	0.46	-	100,100,100,100	0
55	MG	BA	3176	1/1	0.25	-	79,79,79,79	0
55	MG	AA	3232	1/1	0.71	-	104,104,104,104	0
55	MG	AA	3623	1/1	0.28	-	74,74,74,74	0
55	MG	DA	1674	1/1	0.30	-	76,76,76,76	0
55	MG	AA	3128	1/1	0.41	-	56,56,56,56	0
55	MG	AA	3261	1/1	0.63	-	85,85,85,85	0
55	MG	DA	1796	1/1	0.30	-	97,97,97,97	0
55	MG	BE	302	1/1	0.15	-	76,76,76,76	0
55	MG	DA	1766	1/1	0.60	-	116,116,116,116	0
55	MG	AA	3134	1/1	0.38	-	79,79,79,79	0
55	MG	BA	3321	1/1	0.10	-	59,59,59,59	0
55	MG	BB	207	1/1	0.41	-	116,116,116,116	0
55	MG	BA	3360	1/1	0.34	-	83,83,83,83	0
55	MG	BA	3275	1/1	0.39	-	52,52,52,52	0
55	MG	AA	3344	1/1	0.44	-	68,68,68,68	0
55	MG	BA	3245	1/1	0.20	-	72,72,72,72	0
55	MG	CA	1784	1/1	0.42	-	101,101,101,101	0
55	MG	BA	3288	1/1	0.23	-	98,98,98,98	0
55	MG	BA	3281	1/1	0.29	-	92,92,92,92	0
55	MG	AA	3151	1/1	0.47	-	58,58,58,58	0
55	MG	DA	1629	1/1	0.21	-	92,92,92,92	0
55	MG	AA	3146	1/1	0.37	-	65,65,65,65	0
55	MG	BA	3332	1/1	0.20	-	100,100,100,100	0
55	MG	BA	3508	1/1	0.38	-	73,73,73,73	0
55	MG	AA	3617	1/1	0.41	-	92,92,92,92	0
55	MG	AA	3234	1/1	0.45	-	82,82,82,82	0
55	MG	AA	3284	1/1	0.56	-	81,81,81,81	0
55	MG	BA	3061	1/1	0.18	-	69,69,69,69	0
55	MG	BA	3001	1/1	0.29	-	64,64,64,64	0
55	MG	CA	1629	1/1	0.15	-	95,95,95,95	0
55	MG	CA	1774	1/1	0.42	-	97,97,97,97	0
55	MG	AA	3368	1/1	0.53	-	90,90,90,90	0
55	MG	DC	101	1/1	0.17	-	95,95,95,95	0
55	MG	AA	3544	1/1	0.36	-	63,63,63,63	0
55	MG	AA	3239	1/1	0.39	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1609	1/1	0.43	-	78,78,78,78	0
55	MG	BA	3059	1/1	0.28	-	50,50,50,50	0
55	MG	BA	3357	1/1	0.41	-	71,71,71,71	0
55	MG	DA	1727	1/1	0.41	-	86,86,86,86	0
55	MG	AA	3403	1/1	0.16	-	91,91,91,91	0
55	MG	BA	3164	1/1	0.21	-	99,99,99,99	0
55	MG	AA	3603	1/1	0.41	-	41,41,41,41	0
55	MG	AA	3282	1/1	0.50	-	78,78,78,78	0
55	MG	DA	1773	1/1	0.53	-	69,69,69,69	0
55	MG	CA	1743	1/1	0.15	-	112,112,112,112	0
55	MG	BA	3260	1/1	0.14	-	82,82,82,82	0
55	MG	AA	3298	1/1	0.55	-	73,73,73,73	0
55	MG	BA	3504	1/1	0.16	-	117,117,117,117	0
55	MG	BA	3122	1/1	0.32	-	95,95,95,95	0
55	MG	BA	3525	1/1	0.35	-	98,98,98,98	0
55	MG	AA	3295	1/1	0.73	-	102,102,102,102	0
55	MG	AF	302	1/1	0.36	-	93,93,93,93	0
55	MG	BA	3036	1/1	0.53	-	85,85,85,85	0
55	MG	AA	3246	1/1	0.58	-	73,73,73,73	0
55	MG	BA	3295	1/1	0.21	-	58,58,58,58	0
55	MG	CA	1783	1/1	0.78	-	106,106,106,106	0
55	MG	AA	3588	1/1	0.46	-	68,68,68,68	0
55	MG	DA	1617	1/1	0.38	-	102,102,102,102	0
55	MG	BA	3390	1/1	0.42	-	77,77,77,77	0
55	MG	AA	3382	1/1	0.56	-	102,102,102,102	0
55	MG	AA	3527	1/1	0.44	-	86,86,86,86	0
55	MG	AA	3622	1/1	0.46	-	65,65,65,65	0
55	MG	CA	1655	1/1	0.48	-	95,95,95,95	0
55	MG	BA	3377	1/1	0.30	-	81,81,81,81	0
55	MG	AB	203	1/1	0.47	-	69,69,69,69	0
55	MG	CA	1682	1/1	0.14	-	106,106,106,106	0
55	MG	DA	1606	1/1	0.33	-	95,95,95,95	0
55	MG	AA	3181	1/1	0.34	-	66,66,66,66	0
55	MG	BA	3185	1/1	0.49	-	68,68,68,68	0
55	MG	DA	1751	1/1	0.42	-	124,124,124,124	0
55	MG	BA	3286	1/1	0.29	-	85,85,85,85	0
55	MG	BA	3334	1/1	0.20	-	103,103,103,103	0
55	MG	BA	3137	1/1	0.32	-	48,48,48,48	0
55	MG	DA	1738	1/1	0.42	-	85,85,85,85	0
55	MG	BA	3433	1/1	0.26	-	88,88,88,88	0
55	MG	CA	1661	1/1	0.14	-	52,52,52,52	0
55	MG	AA	3006	1/1	0.56	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3307	1/1	0.56	-	76,76,76,76	0
55	MG	CA	1605	1/1	0.24	-	86,86,86,86	0
55	MG	BA	3473	1/1	0.27	-	78,78,78,78	0
55	MG	BA	3102	1/1	0.17	-	86,86,86,86	0
55	MG	AA	3338	1/1	0.48	-	51,51,51,51	0
55	MG	AA	3488	1/1	0.23	-	93,93,93,93	0
55	MG	BA	3246	1/1	0.14	-	99,99,99,99	0
55	MG	AA	3076	1/1	0.42	-	82,82,82,82	0
55	MG	CA	1785	1/1	0.53	-	89,89,89,89	0
55	MG	AA	3074	1/1	0.57	-	68,68,68,68	0
55	MG	DA	1792	1/1	0.22	-	81,81,81,81	0
55	MG	DA	1720	1/1	0.38	-	96,96,96,96	0
55	MG	BB	212	1/1	0.45	-	104,104,104,104	0
55	MG	DA	1713	1/1	0.44	-	111,111,111,111	0
55	MG	CA	1782	1/1	0.56	-	94,94,94,94	0
55	MG	BA	3460	1/1	0.28	-	101,101,101,101	0
55	MG	AA	3559	1/1	0.34	-	83,83,83,83	0
55	MG	AA	3613	1/1	0.30	-	76,76,76,76	0
55	MG	BA	3458	1/1	0.27	-	71,71,71,71	0
55	MG	AA	3570	1/1	0.37	-	41,41,41,41	0
55	MG	AA	3379	1/1	0.30	-	66,66,66,66	0
55	MG	CA	1766	1/1	0.54	-	108,108,108,108	0
55	MG	AA	3273	1/1	0.24	-	101,101,101,101	0
55	MG	BA	3354	1/1	0.36	-	90,90,90,90	0
55	MG	AA	3398	1/1	0.39	-	73,73,73,73	0
55	MG	AA	3235	1/1	0.50	-	84,84,84,84	0
55	MG	DA	1676	1/1	0.51	-	82,82,82,82	0
55	MG	AA	3117	1/1	0.34	-	54,54,54,54	0
55	MG	CA	1635	1/1	0.23	-	100,100,100,100	0
55	MG	DA	1736	1/1	0.46	-	65,65,65,65	0
55	MG	BA	3375	1/1	0.30	-	75,75,75,75	0
55	MG	AA	3551	1/1	0.31	-	69,69,69,69	0
55	MG	AA	3098	1/1	0.46	-	81,81,81,81	0
55	MG	AA	3369	1/1	0.60	-	93,93,93,93	0
55	MG	AA	3183	1/1	0.30	-	93,93,93,93	0
55	MG	DA	1719	1/1	0.55	-	112,112,112,112	0
55	MG	CA	1670	1/1	0.26	-	70,70,70,70	0
55	MG	DA	1703	1/1	0.38	-	115,115,115,115	0
55	MG	CA	1732	1/1	0.31	-	69,69,69,69	0
55	MG	AA	3402	1/1	0.52	-	92,92,92,92	0
55	MG	BA	3320	1/1	0.29	-	77,77,77,77	0
55	MG	AA	3409	1/1	0.44	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3139	1/1	0.25	-	54,54,54,54	0
55	MG	AA	3429	1/1	0.46	-	90,90,90,90	0
55	MG	BA	3238	1/1	0.27	-	66,66,66,66	0
55	MG	DA	1779	1/1	0.37	-	91,91,91,91	0
55	MG	BA	3524	1/1	0.48	-	105,105,105,105	0
55	MG	A5	102	1/1	0.47	-	83,83,83,83	0
55	MG	A0	201	1/1	0.21	-	62,62,62,62	0
55	MG	AA	3413	1/1	0.58	-	109,109,109,109	0
55	MG	BR	202	1/1	0.70	-	105,105,105,105	0
55	MG	AA	3415	1/1	0.41	-	87,87,87,87	0
55	MG	BA	3526	1/1	0.27	-	92,92,92,92	0
55	MG	BA	3068	1/1	0.26	-	93,93,93,93	0
55	MG	AB	215	1/1	0.41	-	93,93,93,93	0
55	MG	DA	1611	1/1	0.37	-	100,100,100,100	0
55	MG	AA	3032	1/1	0.32	-	65,65,65,65	0
55	MG	DA	1696	1/1	0.30	-	66,66,66,66	0
55	MG	CA	1650	1/1	0.37	-	73,73,73,73	0
55	MG	CA	1697	1/1	0.94	-	92,92,92,92	0
55	MG	BA	3440	1/1	0.20	-	80,80,80,80	0
55	MG	CA	1633	1/1	0.29	-	83,83,83,83	0
55	MG	DA	1625	1/1	0.21	-	105,105,105,105	0
55	MG	AA	3264	1/1	0.58	-	80,80,80,80	0
55	MG	CA	1634	1/1	0.31	-	60,60,60,60	0
55	MG	AA	3079	1/1	0.27	-	92,92,92,92	0
55	MG	BA	3419	1/1	0.17	-	99,99,99,99	0
55	MG	AA	3169	1/1	0.37	-	89,89,89,89	0
55	MG	CG	302	1/1	0.15	-	122,122,122,122	0
55	MG	AA	3599	1/1	0.29	-	87,87,87,87	0
55	MG	AA	3205	1/1	0.35	-	55,55,55,55	0
55	MG	BB	203	1/1	0.36	-	76,76,76,76	0
55	MG	AA	3624	1/1	0.31	-	111,111,111,111	0
55	MG	CA	1691	1/1	0.31	-	56,56,56,56	0
55	MG	AA	3085	1/1	0.43	-	34,34,34,34	0
55	MG	AA	3381	1/1	0.77	-	90,90,90,90	0
55	MG	CA	1840	1/1	0.29	-	69,69,69,69	0
55	MG	DA	1662	1/1	0.51	-	78,78,78,78	0
55	MG	AA	3306	1/1	0.43	-	65,65,65,65	0
55	MG	CA	1777	1/1	0.36	-	92,92,92,92	0
55	MG	CA	1728	1/1	0.29	-	117,117,117,117	0
55	MG	AA	3593	1/1	0.49	-	95,95,95,95	0
55	MG	DA	1622	1/1	0.11	-	98,98,98,98	0
55	MG	A1	201	1/1	0.40	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1760	1/1	0.40	-	100,100,100,100	0
55	MG	DA	1620	1/1	0.39	-	85,85,85,85	0
55	MG	BA	3254	1/1	0.52	-	69,69,69,69	0
55	MG	AA	3054	1/1	0.28	-	62,62,62,62	0
55	MG	AA	3247	1/1	0.48	-	74,74,74,74	0
55	MG	AA	3510	1/1	0.61	-	84,84,84,84	0
55	MG	BA	3035	1/1	0.28	-	103,103,103,103	0
55	MG	BA	3476	1/1	0.21	-	68,68,68,68	0
55	MG	BA	3287	1/1	0.35	-	87,87,87,87	0
55	MG	AA	3361	1/1	0.42	-	93,93,93,93	0
55	MG	BA	3331	1/1	0.20	-	101,101,101,101	0
55	MG	BA	3202	1/1	0.29	-	69,69,69,69	0
55	MG	DA	1780	1/1	0.55	-	107,107,107,107	0
55	MG	AA	3203	1/1	0.49	-	65,65,65,65	0
55	MG	AA	3345	1/1	0.64	-	93,93,93,93	0
55	MG	BA	3019	1/1	0.26	-	100,100,100,100	0
55	MG	BA	3123	1/1	0.20	-	77,77,77,77	0
55	MG	AA	3550	1/1	0.52	-	39,39,39,39	0
55	MG	BA	3291	1/1	0.25	-	67,67,67,67	0
55	MG	BA	3090	1/1	0.44	-	109,109,109,109	0
55	MG	CA	1763	1/1	0.35	-	81,81,81,81	0
55	MG	AA	3288	1/1	0.60	-	90,90,90,90	0
55	MG	BA	3344	1/1	0.38	-	101,101,101,101	0
55	MG	AA	3384	1/1	0.63	-	87,87,87,87	0
55	MG	AA	3220	1/1	0.36	-	70,70,70,70	0
55	MG	DA	1722	1/1	0.24	-	106,106,106,106	0
55	MG	BA	3127	1/1	0.41	-	55,55,55,55	0
55	MG	AA	3120	1/1	0.38	-	86,86,86,86	0
55	MG	AA	3370	1/1	0.23	-	106,106,106,106	0
55	MG	BA	3015	1/1	0.23	-	71,71,71,71	0
55	MG	AA	3494	1/1	0.54	-	88,88,88,88	0
55	MG	BA	3519	1/1	0.26	-	107,107,107,107	0
55	MG	AA	3315	1/1	0.50	-	70,70,70,70	0
55	MG	AA	3165	1/1	0.44	-	82,82,82,82	0
55	MG	DA	1761	1/1	0.44	-	84,84,84,84	0
55	MG	AA	3395	1/1	0.47	-	80,80,80,80	0
55	MG	AZ	101	1/1	0.26	-	77,77,77,77	0
55	MG	BA	3221	1/1	0.28	-	37,37,37,37	0
55	MG	CA	1676	1/1	0.30	-	76,76,76,76	0
55	MG	BA	3017	1/1	0.34	-	50,50,50,50	0
55	MG	BA	3091	1/1	0.37	-	86,86,86,86	0
55	MG	AA	3044	1/1	0.40	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1815	1/1	0.26	-	91,91,91,91	0
55	MG	AA	3015	1/1	0.36	-	44,44,44,44	0
55	MG	CA	1750	1/1	0.59	-	104,104,104,104	0
55	MG	DA	1790	1/1	0.44	-	100,100,100,100	0
55	MG	AA	3104	1/1	0.33	-	80,80,80,80	0
55	MG	BA	3034	1/1	0.34	-	81,81,81,81	0
55	MG	BA	3143	1/1	0.21	-	63,63,63,63	0
55	MG	AA	3136	1/1	0.14	-	61,61,61,61	0
55	MG	BA	3032	1/1	0.38	-	110,110,110,110	0
55	MG	B5	101	1/1	0.24	-	61,61,61,61	0
55	MG	BA	3432	1/1	0.42	-	88,88,88,88	0
55	MG	BA	3077	1/1	0.26	-	101,101,101,101	0
55	MG	BA	3177	1/1	0.26	-	75,75,75,75	0
55	MG	AA	3263	1/1	0.32	-	51,51,51,51	0
55	MG	AA	3053	1/1	0.63	-	67,67,67,67	0
55	MG	CA	1663	1/1	0.21	-	52,52,52,52	0
55	MG	AA	3626	1/1	0.59	-	96,96,96,96	0
55	MG	BA	3044	1/1	0.46	-	104,104,104,104	0
55	MG	CA	1742	1/1	0.13	-	115,115,115,115	0
55	MG	CA	1826	1/1	0.23	-	81,81,81,81	0
55	MG	BB	209	1/1	0.38	-	95,95,95,95	0
55	MG	DA	1737	1/1	0.38	-	74,74,74,74	0
55	MG	CA	1640	1/1	0.34	-	85,85,85,85	0
55	MG	CA	1768	1/1	0.33	-	105,105,105,105	0
55	MG	AA	3206	1/1	0.14	-	51,51,51,51	0
55	MG	BA	3481	1/1	0.29	-	49,49,49,49	0
55	MG	AA	3133	1/1	0.50	-	46,46,46,46	0
55	MG	DA	1663	1/1	0.30	-	103,103,103,103	0
55	MG	BA	3066	1/1	0.23	-	86,86,86,86	0
55	MG	AA	3016	1/1	0.28	-	48,48,48,48	0
55	MG	BA	3276	1/1	0.16	-	88,88,88,88	0
55	MG	BA	3252	1/1	0.40	-	86,86,86,86	0
55	MG	CA	1760	1/1	0.18	-	91,91,91,91	0
55	MG	AA	3042	1/1	0.17	-	77,77,77,77	0
55	MG	AA	3087	1/1	0.51	-	76,76,76,76	0
55	MG	AA	3082	1/1	0.37	-	50,50,50,50	0
55	MG	BA	3522	1/1	0.43	-	84,84,84,84	0
55	MG	BA	3239	1/1	0.24	-	80,80,80,80	0
55	MG	AA	3277	1/1	0.26	-	82,82,82,82	0
55	MG	BA	3152	1/1	0.19	-	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.