



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:27 PM BST

PDB ID : 4V87
Title : Crystal structure analysis of ribosomal decoding.
Authors : Demeshkina, N.; Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-09-20
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

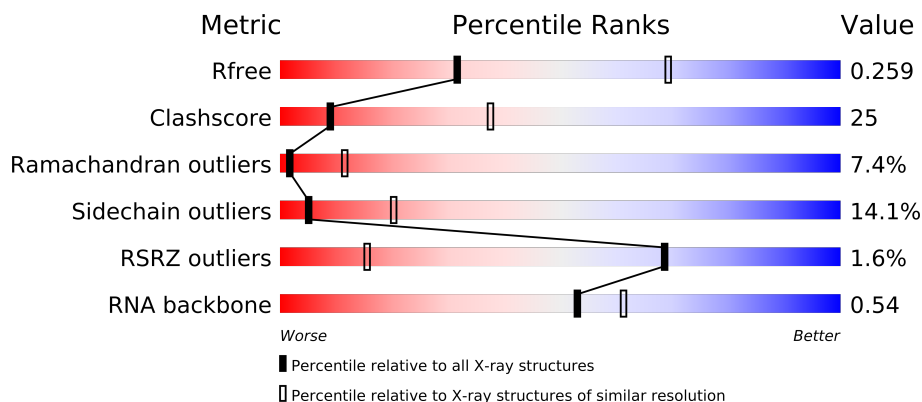
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	DA	2912	
2	AB	122	
2	DB	122	
3	AD	272	
3	DD	272	
4	AE	205	
4	DE	205	
5	AF	202	
6	AG	181	
6	DG	181	
7	AH	170	

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Mol	Chain	Length	Quality of chain
7	DH	170	
8	AK	146	
8	DK	146	
9	AM	138	
9	DM	138	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
14	AQ	111	
14	DQ	111	
15	AR	137	
15	DR	137	
16	A1	117	
16	D1	117	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	92	
19	DT	92	
20	AU	102	
20	DU	102	
21	AV	175	
22	A3	76	
23	AZ	97	
23	DZ	97	
24	AW	66	
25	AX	59	
25	DX	59	
26	A4	66	
27	A5	59	
27	D5	59	
28	A6	45	
28	D6	45	
29	A7	49	
29	D7	49	
30	A8	61	
30	D8	61	

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Mol	Chain	Length	Quality of chain
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	

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Mol	Chain	Length	Quality of chain
52	BB	87	
52	CB	87	
53	BC	77	
53	BD	77	
53	CC	77	
53	CD	77	
54	B1	10	
54	C1	10	
55	DF	208	
56	D0	117	
57	DV	179	
58	D3	77	
59	DW	69	
60	D4	63	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299628 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 (2909-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	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

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

- Molecule 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	DB	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
			2116	1335	420	358	3			
3	DD	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
			1569	991	300	272	6			
4	DE	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
			1586	1011	297	276	2			

- 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	DG	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
			1308	829	245	233	1			
7	DH	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
			1137	726	201	209	1			
8	DK	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
			1105	712	206	183	4			
9	DM	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	DN	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	DO	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	DP	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			

- 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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	DQ	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
			1142	710	234	197	1			
15	DR	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	D1	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	D2	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	DS	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
			726	471	131	124			
19	DT	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
			786	505	150	126	5			
20	DU	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			

- 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			

- 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	DZ	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			

- 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	DX	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			

- 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	D5	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
			390	241	79	66	4			
28	D6	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	D7	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	D8	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	BA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
31	CA	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	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	CE	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	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	CF	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	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	CG	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	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	CH	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	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	CI	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	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	CJ	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	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	CK	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	BL	127	Total	C	N	O	0	0	0
			1010	639	197	174			
39	CL	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	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
40	CM	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	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	CN	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	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	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	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	CP	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	BQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
44	CQ	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	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	CR	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	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	CS	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	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	CT	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	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	CU	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	BV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
49	CV	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	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	CW	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	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	CX	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	BB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
52	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	10	Total 205	C 92	N 28	O 75	P 10	0	0	0
54	C1	10	Total 205	C 92	N 28	O 75	P 10	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	DF	208	Total 1627	C 1037	N 304	O 283	S 3	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	D0	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 57 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DV	179	Total 1428	C 911	N 255	O 259	S 3	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 59 is a protein called 50S ribosomal protein L29.

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

- Molecule 60 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BA	244	Total	Mg	0	0
			244	244		
61	CA	209	Total	Mg	0	0
			209	209		
61	AB	17	Total	Mg	0	0
			17	17		
61	A6	1	Total	Mg	0	0
			1	1		
61	DU	1	Total	Mg	0	0
			1	1		
61	B1	2	Total	Mg	0	0
			2	2		
61	A2	1	Total	Mg	0	0
			1	1		
61	BB	8	Total	Mg	0	0
			8	8		
61	AE	4	Total	Mg	0	0
			4	4		
61	D3	1	Total	Mg	0	0
			1	1		
61	AA	630	Total	Mg	0	0
			630	630		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BQ	2	Total 2	Mg 2	0	0
61	A5	2	Total 2	Mg 2	0	0
61	CH	1	Total 1	Mg 1	0	0
61	BC	9	Total 9	Mg 9	0	0
61	CG	3	Total 3	Mg 3	0	0
61	A1	1	Total 1	Mg 1	0	0
61	AD	2	Total 2	Mg 2	0	0
61	BN	2	Total 2	Mg 2	0	0
61	D0	1	Total 1	Mg 1	0	0
61	BG	1	Total 1	Mg 1	0	0
61	CC	8	Total 8	Mg 8	0	0
61	DA	528	Total 528	Mg 528	0	0
61	AU	1	Total 1	Mg 1	0	0
61	A0	1	Total 1	Mg 1	0	0
61	DE	3	Total 3	Mg 3	0	0
61	D1	2	Total 2	Mg 2	0	0
61	CB	5	Total 5	Mg 5	0	0
61	DP	1	Total 1	Mg 1	0	0
61	A7	1	Total 1	Mg 1	0	0
61	D5	1	Total 1	Mg 1	0	0
61	BD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AO	3	Total 3	Mg 3	0	0
61	CS	1	Total 1	Mg 1	0	0
61	A3	1	Total 1	Mg 1	0	0
61	AF	3	Total 3	Mg 3	0	0
61	DB	14	Total 14	Mg 14	0	0

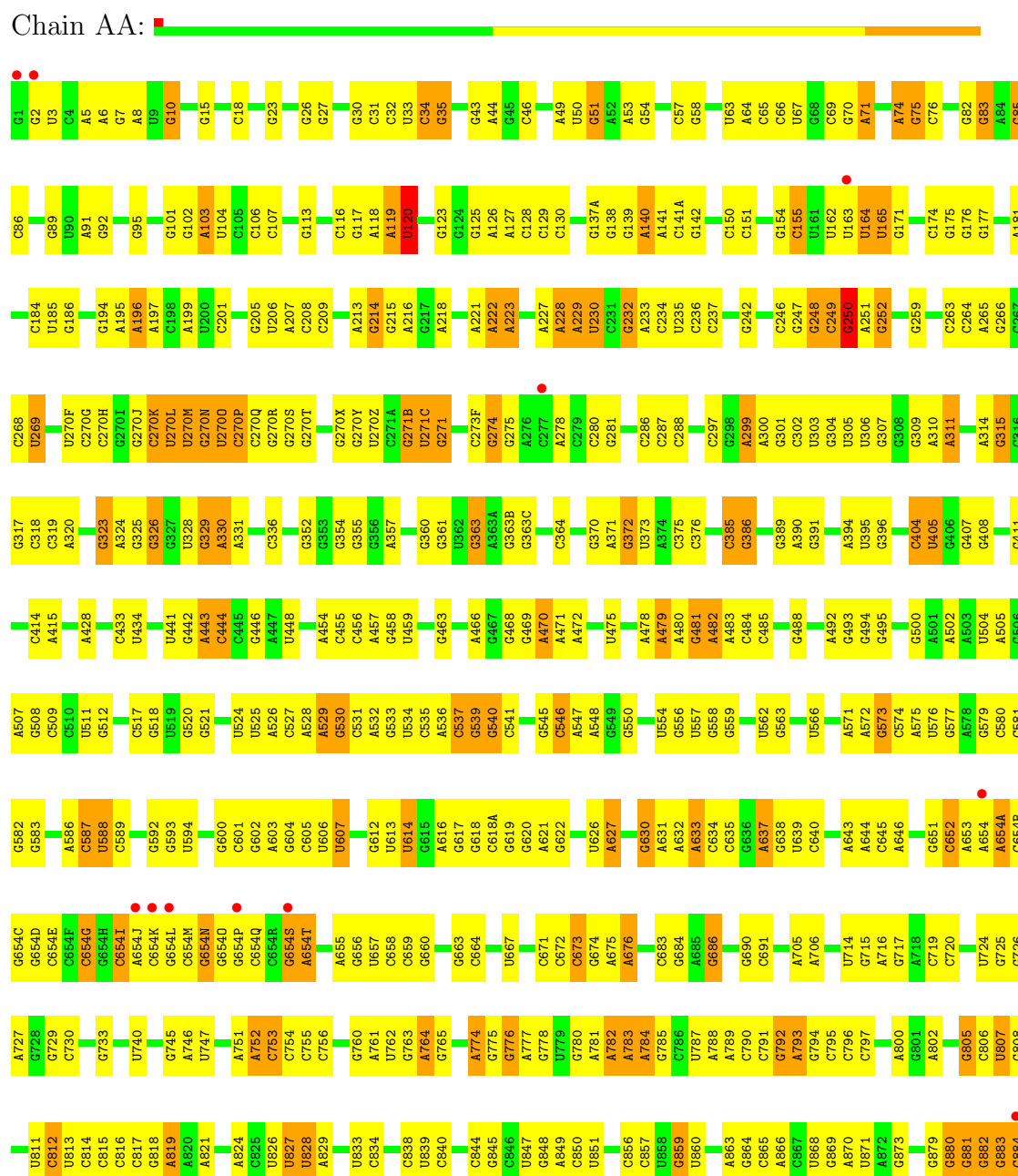
- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	BG	1	Total 1	Zn 1	0	0
62	BQ	1	Total 1	Zn 1	0	0
62	CQ	1	Total 1	Zn 1	0	0
62	CG	1	Total 1	Zn 1	0	0

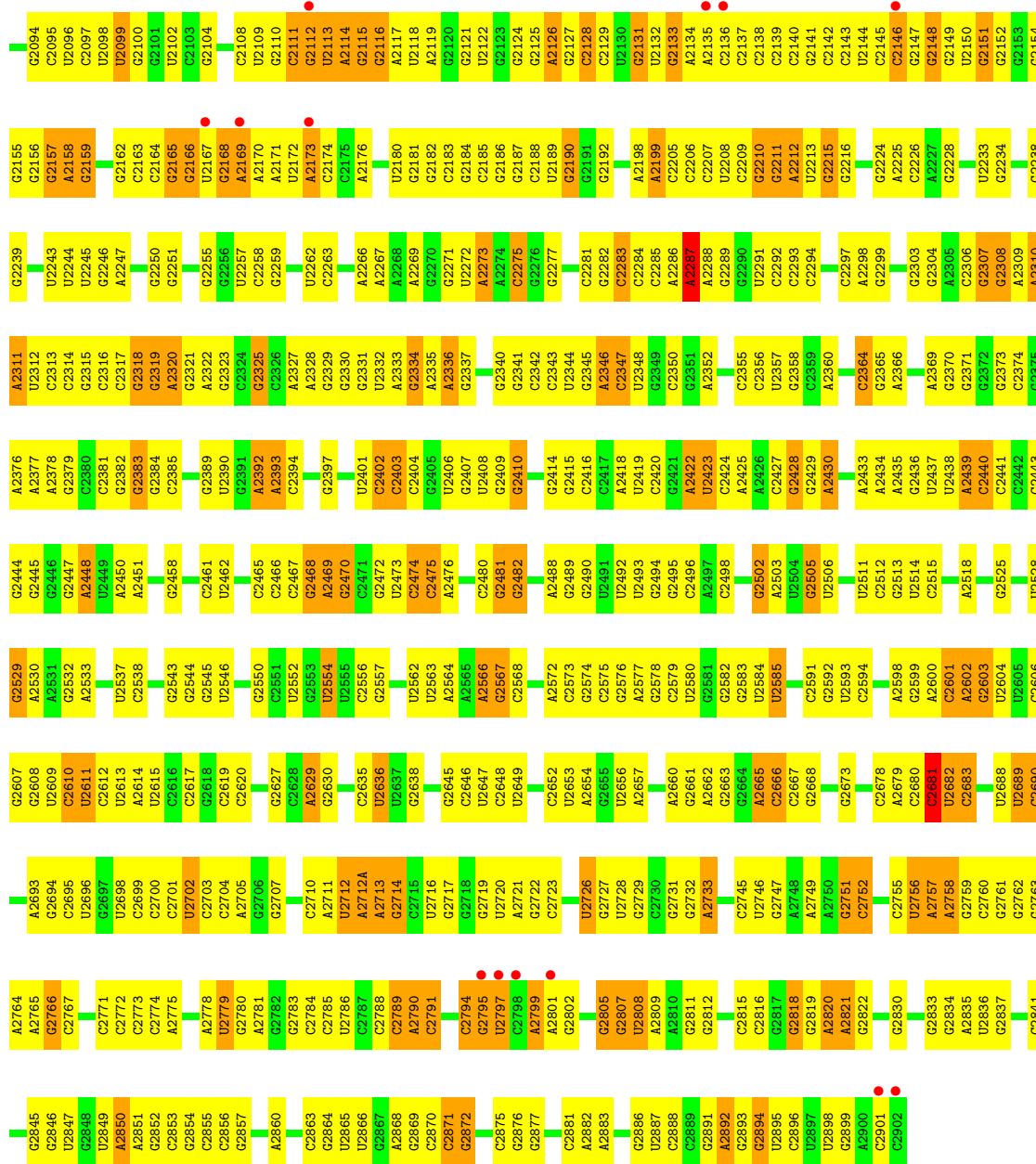
3 Residue-property plots

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

• Molecule 1: RNA (2909-MER)

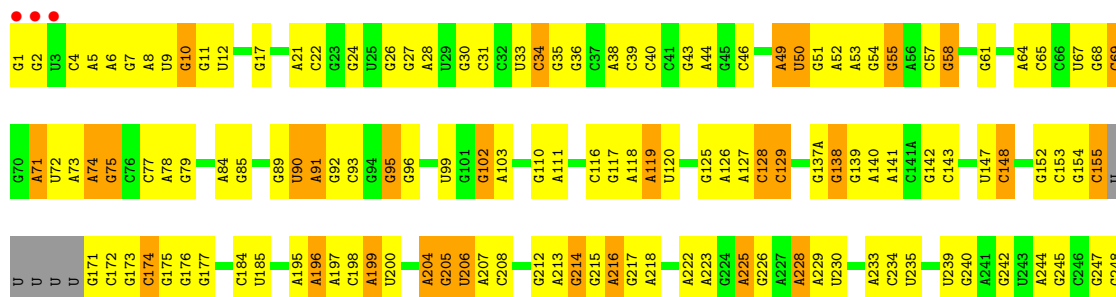


G2012	A1918	G1733	A1641	U1541	G1403	U1323	A1237	G1162	A1095	U1033	G966	C985
A2013	A1919	C1734	G1642	G1542	C1404	G1324	U1240	U1165	A1096	G1036	C967	C986
A2014	C1735	C1741	G1643	A1543	U1406	G1325	A1241	C1166	U1097	G1037	G968	C987
A2015	A1545	A1545	G1648	A1545	U1406	U1326	U1241	U1166	A1098	C1038	C969	C988
U2016	C1742	G1743	G1649	C1547	C1408	C1327	G1244	U1167	G1099	C1039	C970	A890
U2017	G1743	A1749	G1650	C1548	C1409	U1329	G1244	G1168	C1100	G1042	G972	G992
G2018	A1927	G1750	G1651	C1549	G1410	C1330	A1247	G1170	A1101	G1043	C973	C993
A2019	C1750	C1750	G1652	C1550	C1411	A1331	G1250	G1171	C1102	C1043	G974	C994
A2020	C1751	C1751	G1653	C1551	U1412	C1332	G1251	G1172	C1103	G1044	C975	C995
C2021	C1752	C1752	G1654	C1552	G1413	C1333	G1252	A1174	U1105	A1045	G976	U895
U2022	G1755	G1755	G1655	A1554	G1414	G1337	U1253	U1175	G1106	A1046	C977	C997
G2023	G1756	G1756	G1656	G1555	U1415	G1338	A1254	G1176	G1110	G1047	G978	C998
G2024	U1757	G1757	G1657	C1556	G1416	U1339	A1255	A1177	A1111	A1048	G979	A899
C2025	G1758	G1758	G1658	C1557	C1417	U1340	G1256	C1178	A1112	C1049	G980	A900
C2026	C1843	C1843	A1665	A1558	G1418	U1341	U1267	C1179	A1113	A1050	G981	A901
A2030	A1847	G1763	G1666	G1559	A1419	G1344	G1264	C1180	U1116	C1052	G982	C902
G2032	G1764	G1667	G1667	G1560	U1420	C1345	A1265	C1181	C1116	C1053	G983	C903
A2033	U1851	A1668	G1668	G1568	G1421	C1346	G1266	A1182	C1117	A1054	G984	C904
C2036	G1769	A1669	G1669	A1569	G1424	U1348	U1267	C1185	C1118	G1055	G986	U905
G2037	U1770	C1670	G1670	A1570	G1425	A1349	A1268	G1186	C1119	G1056	G987	G906
G2038	A1772	G1674	G1674	G1571	G1426	U1352	A1269	G1187	U1122	U1058	G988	C907
C2039	G1773	G1678	G1678	C1575	A1427	A1353	G1270	U1188	G1123	C1223	A990	A909
C1958	U1778	G1681	G1681	U1576	G1429	A1354	A1272	G1190	C1124	U1061	C991	A910
G1963	U1779	G1686	G1686	U1577	C1430	G1355	U1273	G1191	G1125	G1062	C992	A911
C2043	A1780	G1687	G1687	A1579	U1431	U1356	A1274	G1195	A1126	G1063	C993	C915
G2050	G1783	C1688	G1688	A1580	C1432	U1357	A1275	G1199	A1127	G1064	C994	G916
A2051	A1784	U1688	U1688	G1581	U1433	A1358	A1276	C1201	U1130	U1065	A996	A917
G2052	G1785	A1689	A1689	C1582	G1435	A1359	G1277	G1202	G1131	A1066	A1000	A918
A2054	C1787	A1690	A1690	A1583	G1436	A1360	U1278	G1203	C1131	A1067	A1001	G919
C2055	U1788	C1691	C1691	U1585	C1437	G1364	U1288	G1204	C1135	A1068	A1002	G929
G2056	A1789	G1692	G1692	A1586	G1441	A1365	C1289	U1205	G1136	G1069	G1003	G932
C1973	C1790	U1693	U1693	A1587	G1442	G1368	C1290	G1206	G1137	A1070	G1004	A933
C1974	G1791	G1694	G1694	C1588	G1443	G1369	C1291	C1207	G1138	G1071	G1005	A933
A2059	A1792	C1695	C1695	U1589	G1444	U1372	U1292	C1208	G1139	C1072	C1006	G938
A2060	G1793	A1696	A1696	U1590	A1444A	U1373	U1293	G1209	C1140	A1073	C1007	G938
G2061	C1794	G1698	G1698	G1591	G1448	A1374	C1297	U1210	U1141	G1074	G1011	A941
C2062	U1795	A1701	A1701	C1592	U1449	G1375	C1298	U1211	U1142	C1075	U1012	G942
C2064	G1796	G1702	G1702	G1593	G1449A	C1376	G1299	G1212	A1143	C1076	G1013	U943
C2065	C1797	G1705	G1705	G1594	G1453	G1377	U1300	G1215	G1144	U1077	U1014	G944
C2066	U1798	U1706	U1706	G1595	G1454	U1378	U1301	G1216	C1145	C1079	G1015	A945
G2067	G1799	G1707	G1707	C1600	G1455	A1379	G1309	C1217	C1146	A1080	G1016	G946
U2068	C1800	C1800	C1800	G1601	G1456	G1380	G1310	G1218	C1147	U1081	G1017	G950
G2069	G1801	A1802	A1802	C1607	G1458	G1381	G1311	G1219	A1148	U1082	G1018	C951
A2077	A1803	C1710	C1710	A1608	G1459	G1382	U1312	A1220	G1150	U1083	U1019	G952
C2078	G1804	G1718	G1718	A1609	G1460	C1383	U1313	C1221	C1151	A1084	A1020	G952
U2079	U1805	G1725	G1725	A1610	G1461	A1384	C1314	C1222	C1152	A1085	A1021	A953
G2080	C1810	G1726	G1726	C1617	G1464	C1385	C1315	G1228	C1153	A1086	G1022	G954
C2081	A1811	U1727	U1727	G1618	G1465	G1387	U1316	A1227	G1154	G1087	U1023	C955
A2082	G1812	G1728	G1728	A1618	G1466	C1388	A1317	G1230	A1155	A1088	G1024	G956
G2083	C1914	A1729	A1729	A1637	G1467	G1389	G1318	G1231	C1158	G1089	G1025	A957
C2084	U1915	U1730	U1730	C1638	G1468	U1396	G1319	G1235	C1159	U1090	U1026	U958
C2085	G1813	G1731	G1731	U1639	C1469	U1396	A1321	G1236	G1160	G1091	A1027	A959
U2086	G1816	A1732	A1732	C1640	A1469	U1396	A1322	G1236	C1161	C1092	A1029	C960



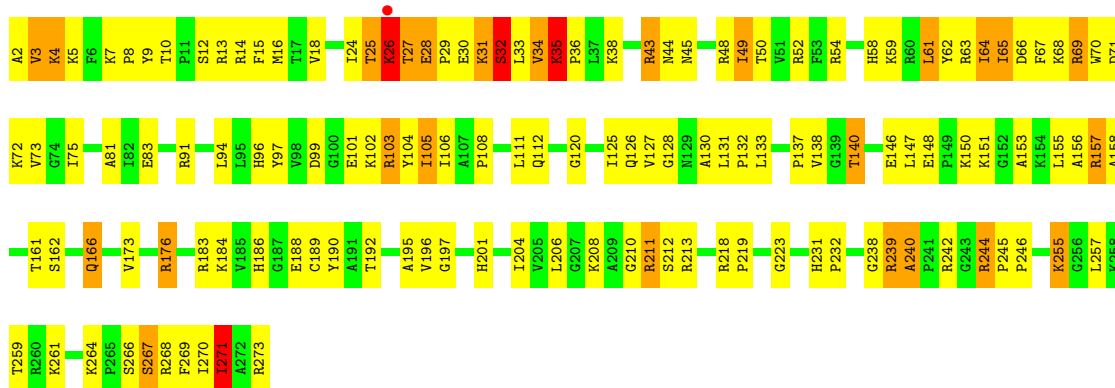
• Molecule 1: RNA (2909-MER)

Chain DA:



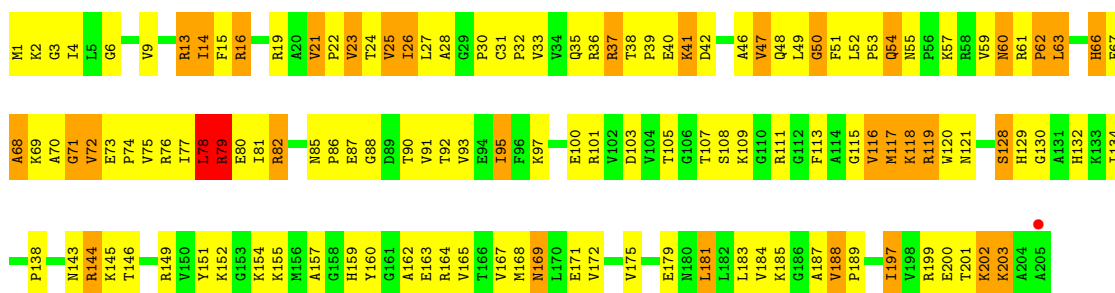
A1317	G1244	G1154	G1089	U1023	U958	C889	U827	C756	G669	G625	G556	A480	U383	C296	C249
G1318	A1155	A1156	U1090	G1024	A959	A890	U828	U757	A670	U626	U557	G461	U384	C297	G260
C1320	A1246	A1156	G1091	U1025	A960	C892	A829	C758	C671	A627	G558	A482	C385	C298	G252
A1321	A1247	G1160	U1093	U1026	C961	C893	G830	G759	C672	G628	G561	A483	G386	A299	
A1322	G1248	C1161	U1094	A1027	G962	C894	G831	G760	C673	G629	G562	C466	G389	A300	A255
U1323	U1249	C1161	A1095	U1033	U963	U895	G832	A761	G674	A631	G563	C467	G392	A256	A257
G1324	G1250	G1164	A1096	G1034	C965	C897	C834	A764	A676	A632	G564	G488	C393	G307	G258
U1325	G1251	U1165	U1097	U1035	G966	C898	C835	G765	C675	A633	C565	G489	G394	G308	G259
U1326	C1166	C1166	A1098	G1036		A899	G836	G769	C679	C634	U566	G491	A394	G309	
C1327	A1253	C1169	A900		C970	A900	C837	G769	G680	C635	G570	A492	U395	A310	C260
G1328	U1254	G1169	A901	U1039	C971	C838	G838	A774	G684	G636	G571	C493	U405	A265	A266
U1329	U1255	G1170	C902	G1040	G972	U839	U839	G775	A685	A637	A572	G495	G406	G315	
C1330	G1256	G1171	C903	C1041	A973	C840	C840	G776	A686	G638	G573	G496	U409	C316	U269
A1331	C1257	G1173	U904	G1042	G974	A841	A841	A777	G686	C639	C574	G497	C409	A270	A270A
G1332	A1174	A1174	U905	C1043	C974A	G842	G842	G778	G690	C641	U576	G498	G410	A320	
A1336	G1260	U1175	G906	G1044	G975	G843	G844	U779	G691	G642	U576	G498	G411	A321	U270F
C1337	G1261	A1177	U907	A1045	C976	G845	G845	G780	G691	A643	G577	A501	A412	A322	
G1338	A1262	C1178	C908	G1046	G977	G846	G846	A781	G696	A644	A578	A502		A323	
G1339	A1111	C1179	A909	G1047	G978	G847	G847	A782	C897	G644	G578	A503	C420	A324	
U1340	A1265	C1180	A910	A1048	G979	A782	A782	A783	C898	A646	G579	A504	C420	C270G	
U1341	G1266	C1181	A911	C1049	A980	A783	G848	A784	C899	A647	C580	U504	U421	C270H	
A1342	U1267	C1182	C912	A1050		A784	A849	A784	A699	G647	C581	A505		C270I	
C1345	U1268	G1115	U913	G1051	A983	G785	G850	G786	G700	G648	G582	G506	A428	C270J	
G1346	A1269	C1116	C914	C1052		C786	C851	U787	G701	G649	G583	A507		C270K	
G1347	C1270	G1187	G915	G1053	C986	U788	U851		G702	C650		G508	C433	C270L	
A1348	G1271	U1188	G916	A1054	G987	A789	G854	A789	A705	G651	A586	C509	U434	U270M	
G1349	A1272	A1189	A917	G1056	A988	A789	G855	A789	A706	G652	C510	C510	G333	C270N	
A1274	G1190	G1122	G918	U1057	G989	G856	G857	G792	A707	A653	U511	G334	A443	U270O	
A1274	G1191		G919	C991	A990	G858	U858	G793	C708	A654	C588	A513	C444	C270P	
A1278	U1198	G1125	G920	U1058	C992	G859	G859	G794	U709	C654B	G592		C445	C270Q	
G1283	C1201	A1129	G921	G1059	G993	U860	G860	G795	G710	C654C	G593	C517	U448	C270R	
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G1285	G1203	G1131	G923	U1061	C995	G862	G862	C797	G717	C654E	G599	G520	C451	U270Z	
A1286	A1204	A1132	G928	G1062	A996	A863	A863	G798	A718	C654F			C452	C271A	
U1287	U1205	G1135	G929	G1063	C997	G864	G864	G799	G723	C654G	G602	U524	C453	G271B	
G1356	G1283	C1136	G932	U1064	C998	C865	C865	G800		C654H	A603	U525	A454	G271C	
U1357	G1284	G1137	G933	U1065	C999	A866	A866	G801	G726	C654I	G604	A526	C455	G271	
G1358	G1285	G1138	G934	U1066	A1000	A867	A867	A802	A727	C654J	C805	C527	C456	C273C	
A1359	A1286	G1139	G935	G1068	G1002	G868	G868		G728	C654K	U606	A528	A457	G354	
A1360	U1287	G1137	C936	G1069	G1003	A870	G870	C805	G729	C654L	U607	A529	G458	G355	
G1361	C1289	G1138	U937	G1070	C1004	U871	U871	U807	C730	C654M	A608	G530	U459	G356	
A1365	U1292	G1212	G938	C1071	G1005	A872	A872	G808	C731	C654N	A609	C531	A460		
G1368	C1293	C1217	G941	C1072	C1006	G873	G873	G809		C654O	G609A	A532	C461	U362	
G1369	C1297	A1220	G942	A1073	C1007			U810	A734	C654P	G612	G533	C462	G274	
U1372	G1299	G1226	G943	C1075	G1011	U877	U877	U811	U740	C654Q	U613	U534	G463	G275	
A1379	U1300	C1225	G944	A1077	G1012	A878	A878	U813		C654R	U614	C535	G466	A276	
G1380	A1301	G1226	G945	A1078	G1013	G879	G879	U814	G745	A654T	G615	A536	A466	A278	
A1384	G1309	C1228	G946	U1080	G1014	G880	G880	C814	A746	A655	C543	G543	G467	C280	
C1385	G1310	G1228	G947	U1081	G1015	G881	G881	G818	U747	C656	C544	G469	G469	G281	
C1386	G1311	C1147	G948	U1082	G1016	G882	G882	A819	G748	U657	G545	A470	A470	A282	
C1387	G1312	G1231	G949	U1083	G1017	G883	G883	A820	G619	C658	C546	A471	A471	G370	
G1388	U1313	G1232	G952	A1084	G1018	A821	A821	A751	G620	A547	A548	A472	A472	C286	
G1389	U1314	C1239	G953	A1085	U1019	C885	C885	A752	A621	C659	G622	A549	A476	C287	
U1390	C1315	U1240	G954	A1086	U1019	C886	C886	C753	G623	G660	G549	G549	G476	C288	
U1391	U1316	C1153	A957	A1088	G1022	A887	A887	C754	C755	G666	C624			A289	

G2557	C2474	C2395	A2327	A2267	U2172	C2111	A2033	A1937	A1829	G1756	G1642	A1543	G1473	A1392
G2558	C2475	G2396	A2328	A2268	A2173	G2112	U2034	A1938	U1833	U1757	G1645	C1544	C1474	A1393
C2559	A2476	A2269	G2329	A2268	C2174	U2113	C2036	C1942	U1834	G1758	C1646	A1545	C1475	U1396
U2563	C2477	G2402	G2330	A2269	C2175	A2114	C2036	U1946	G1835	A1760	G1647	C1547	A1477	U1397
A2564	G2481	C2403	G2331	G2270	A2176	G2116	C2039	U1947	C1837	G1761	G1648	C1548	A1478	G1479
A2565	G2482	U2406	A2332	G2271	C2177	G2117	C2040	C1947	C1838	A1762	G1649	C1549	A1479	G1401
A2566	G2483	G2410	A2333	U2272	U2180	A2118	U2041	C1952	C1839	G1763	G1650	C1557	A1480	C1402
G2567	C2484	A2411	A2335	A2273	G2181	U2119	C2043	U1956	A1847	G1764	G1651	A1558	U1482	G1401
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		U2473	A2392	A2392	U2262	A2169	C2108	A2030	G1935	G1827			G1542	
			C2394	C2394	C2263	A2171		G2032	A1936	G1828				



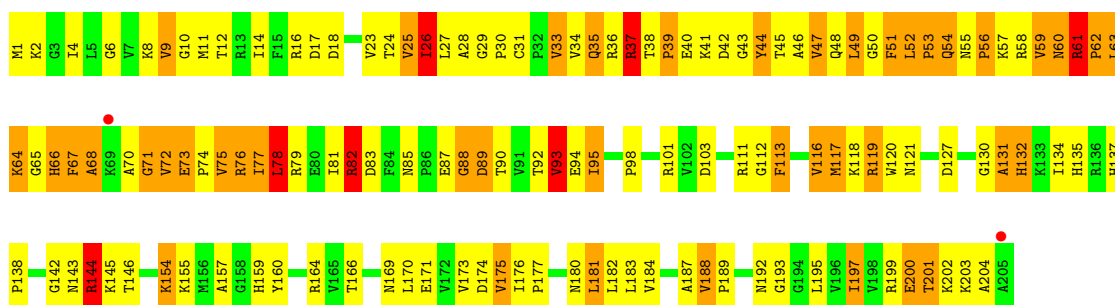
• Molecule 4: 50S ribosomal protein L3

Chain AE:



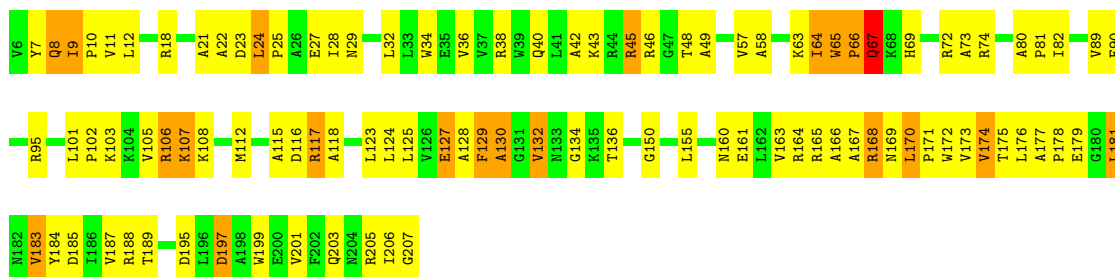
• Molecule 4: 50S ribosomal protein L3

Chain DE:



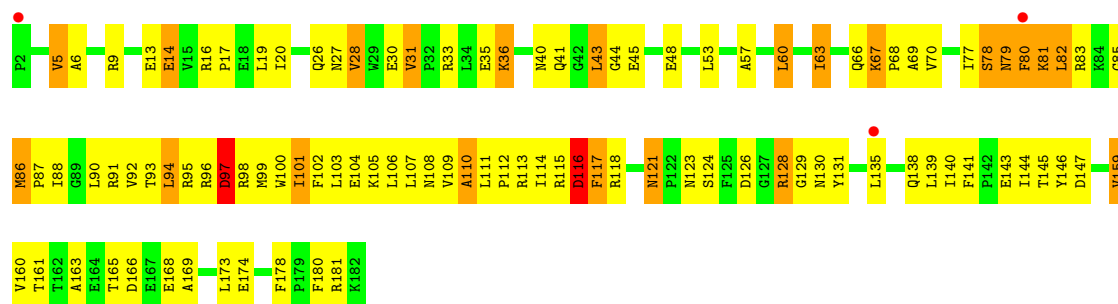
• Molecule 5: 50S ribosomal protein L4

Chain AF:



• Molecule 6: 50S ribosomal protein L5

Chain AG:



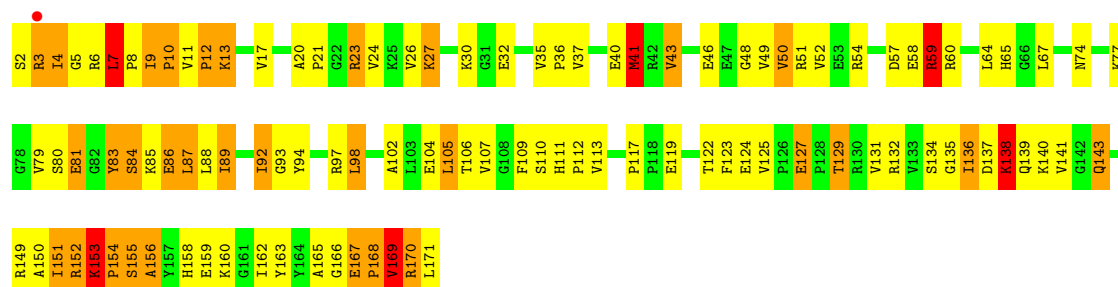
- Molecule 6: 50S ribosomal protein L5

Chain DG:



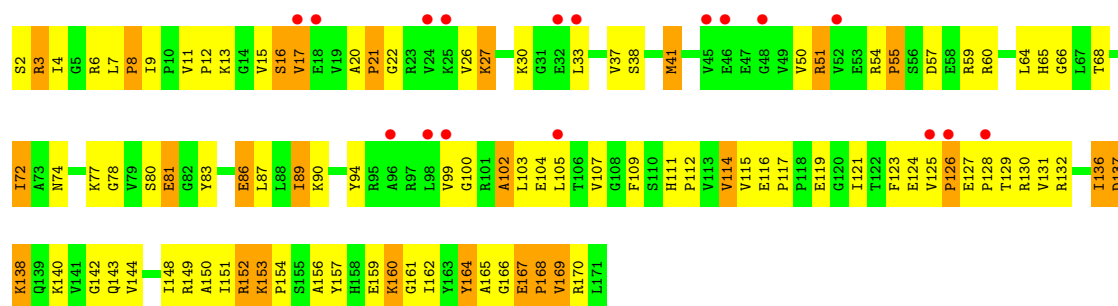
- Molecule 7: 50S ribosomal protein L6

Chain AH:



- Molecule 7: 50S ribosomal protein L6

Chain DH:



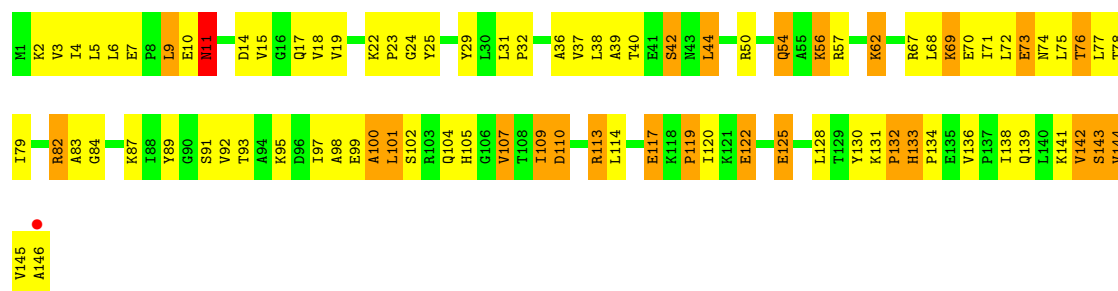
- Molecule 8: 50S ribosomal protein L9

Chain AK:



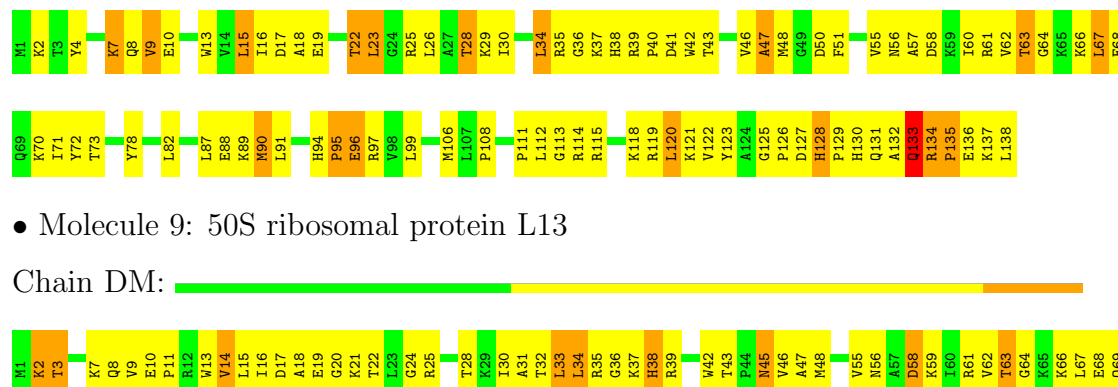
- Molecule 8: 50S ribosomal protein L9

Chain DK:



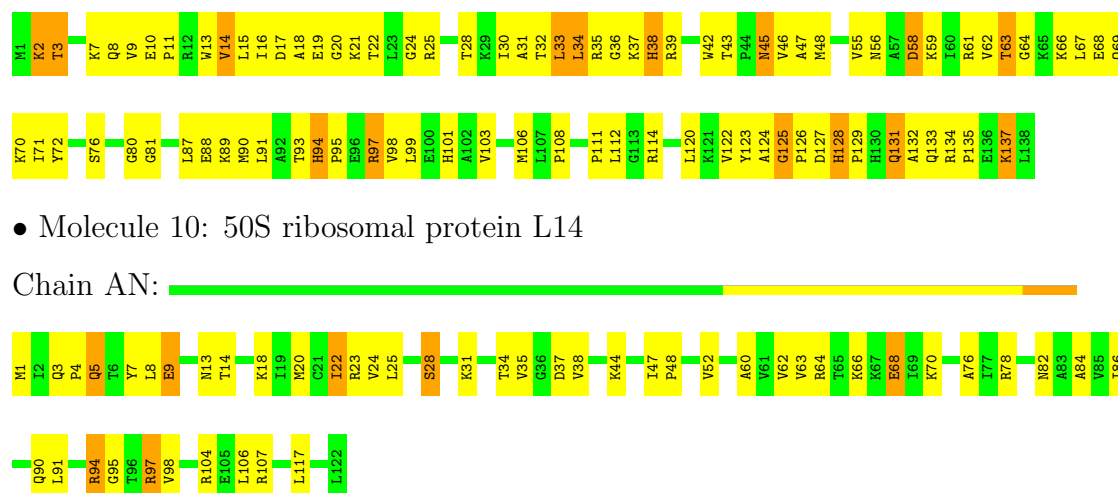
- Molecule 9: 50S ribosomal protein L13

Chain AM:



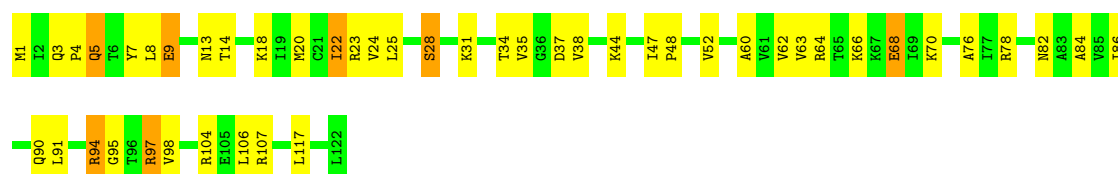
- Molecule 9: 50S ribosomal protein L13

Chain DM:



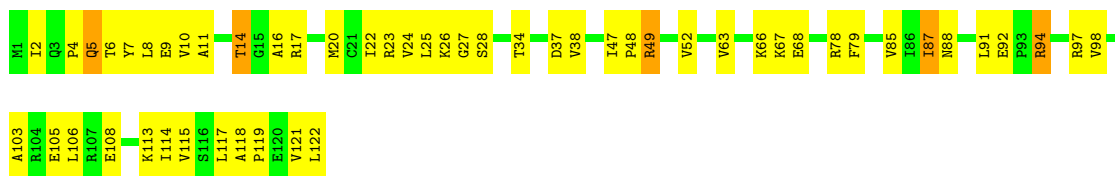
- Molecule 10: 50S ribosomal protein L14

Chain AN:



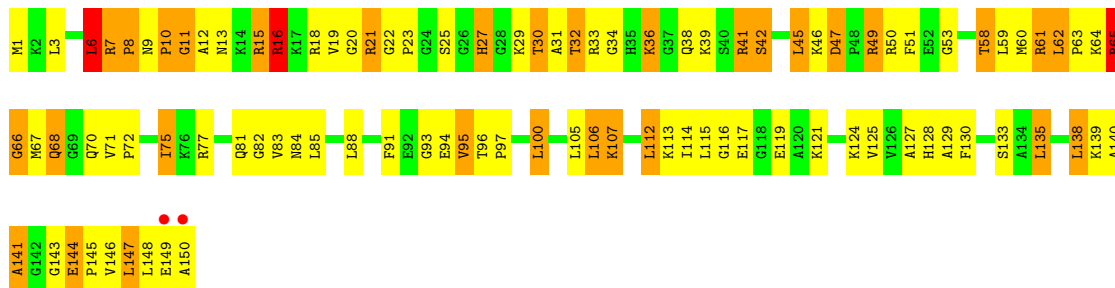
- Molecule 10: 50S ribosomal protein L14

Chain DN:



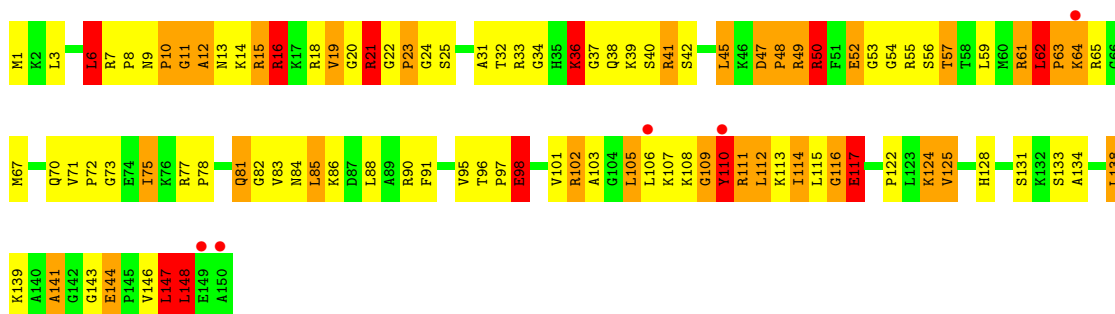
- Molecule 11: 50S ribosomal protein L15

Chain AO:



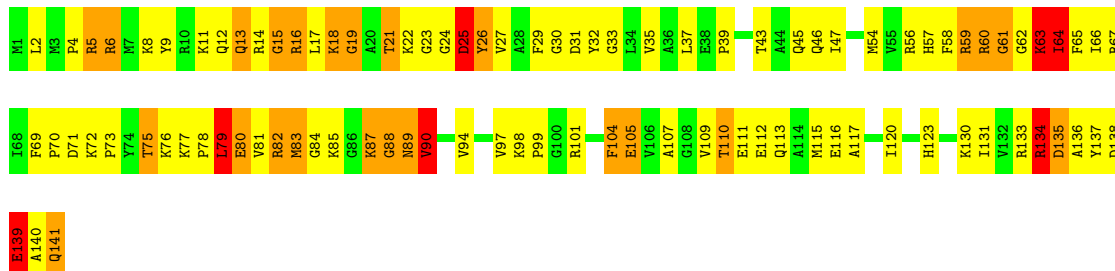
- Molecule 11: 50S ribosomal protein L15

Chain DO:



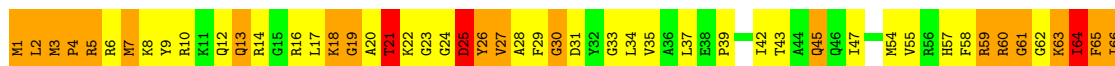
- Molecule 12: 50S ribosomal protein L16

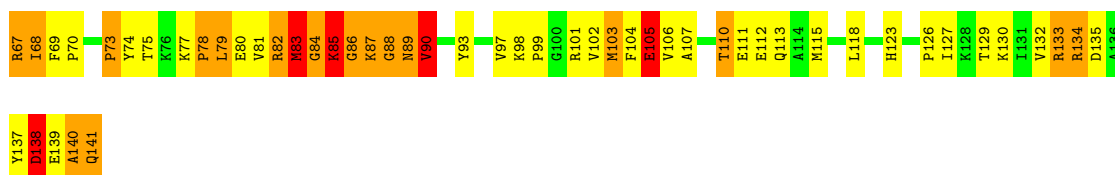
Chain AP:



- Molecule 12: 50S ribosomal protein L16

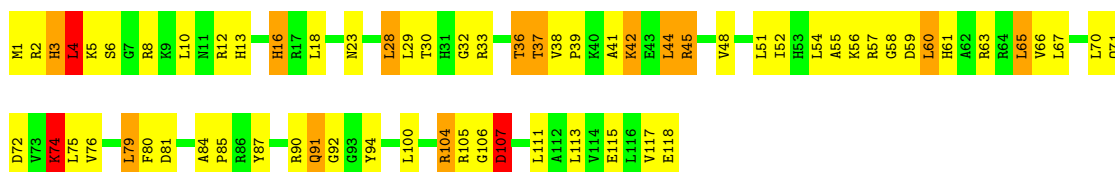
Chain DP:





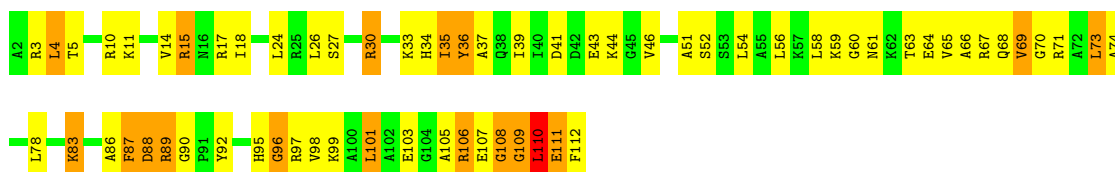
- Molecule 13: 50S ribosomal protein L17

Chain A0:



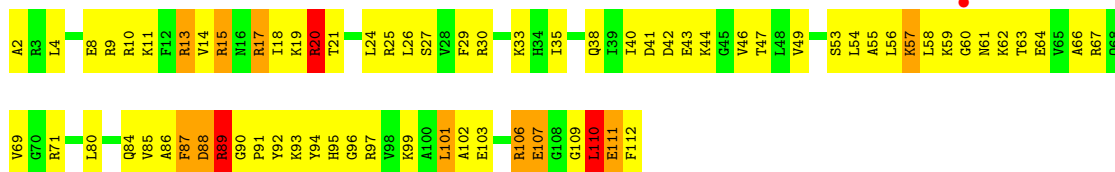
- Molecule 14: 50S ribosomal protein L18

Chain AQ:



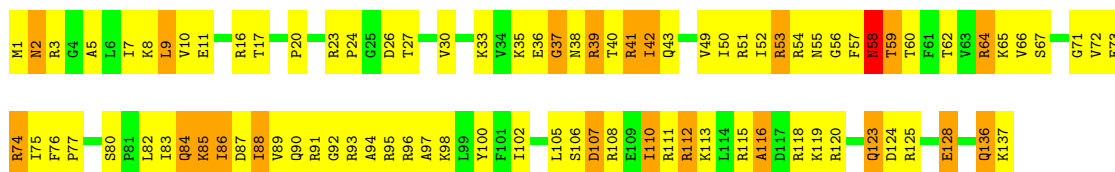
- Molecule 14: 50S ribosomal protein L18

Chain DQ:



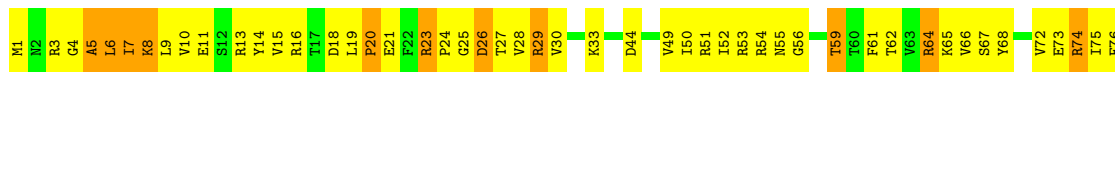
- Molecule 15: 50S ribosomal protein L19

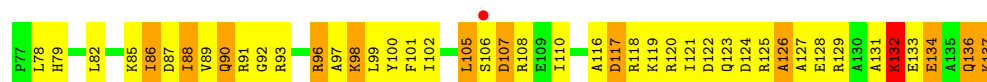
Chain AR:



- Molecule 15: 50S ribosomal protein L19

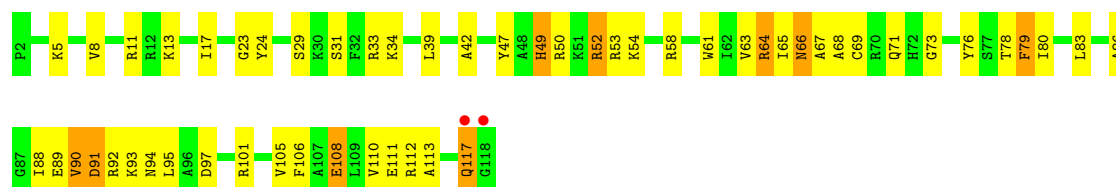
Chain DR:





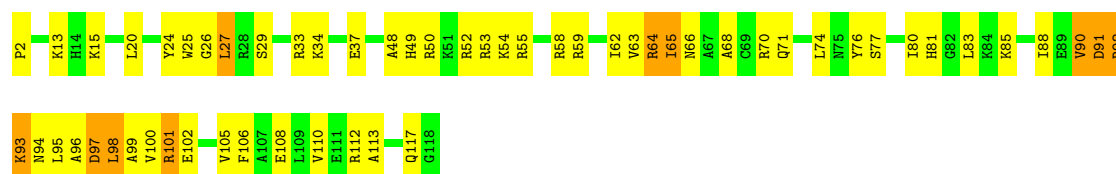
- Molecule 16: 50S ribosomal protein L20

Chain A1:



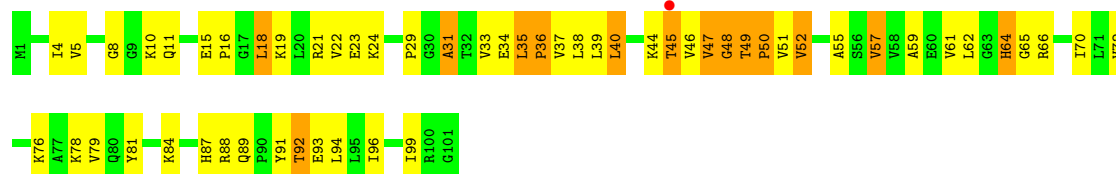
- Molecule 16: 50S ribosomal protein L20

Chain D1:



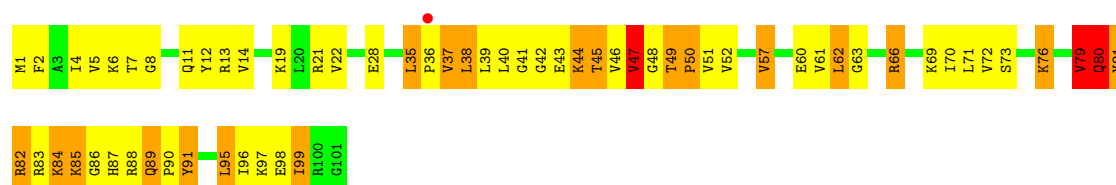
- Molecule 17: 50S ribosomal protein L21

Chain A2:



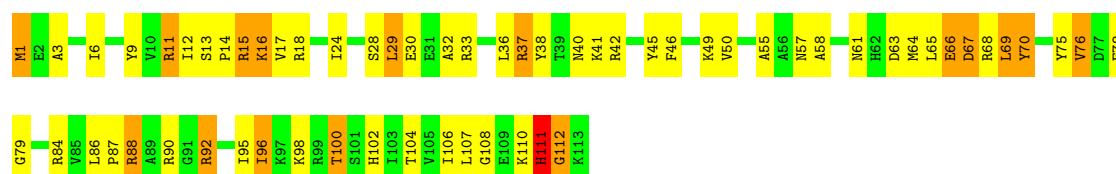
- Molecule 17: 50S ribosomal protein L21

Chain D2:



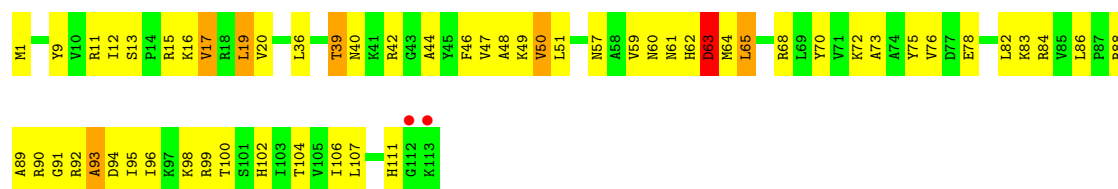
- Molecule 18: 50S ribosomal protein L22

Chain AS:



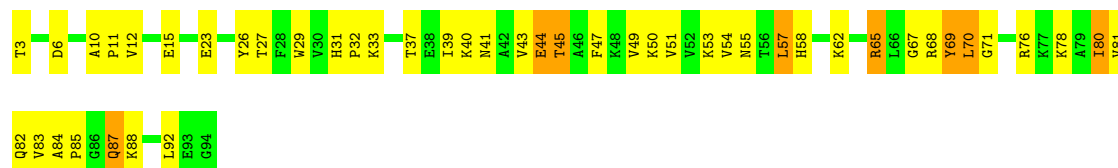
- Molecule 18: 50S ribosomal protein L22

Chain DS:



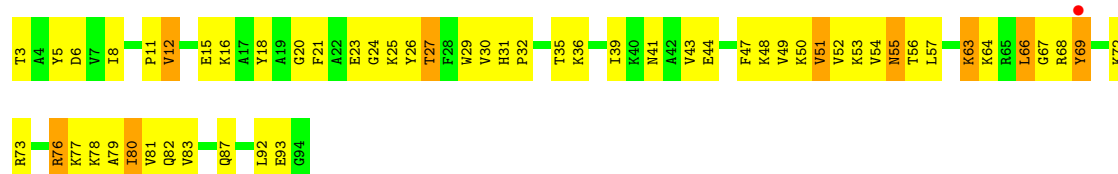
- Molecule 19: 50S ribosomal protein L23

Chain AT:



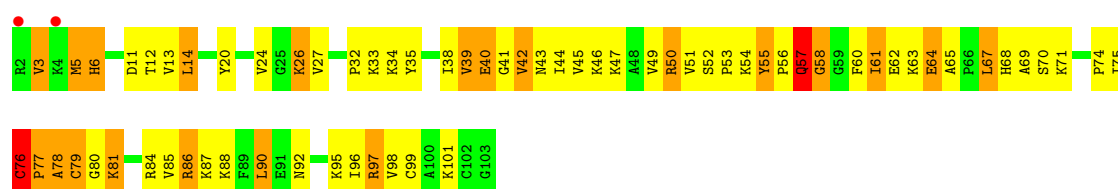
- Molecule 19: 50S ribosomal protein L23

Chain DT:



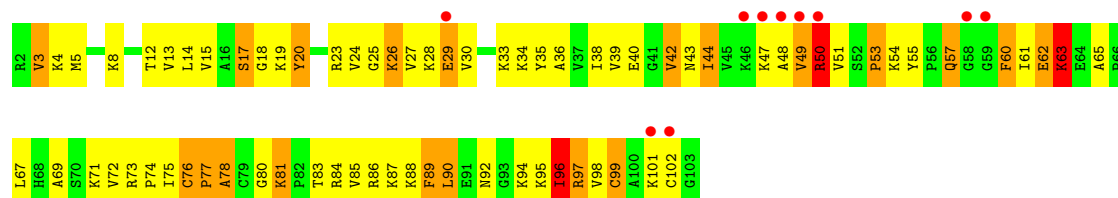
- Molecule 20: 50S ribosomal protein L24

Chain AU:



- Molecule 20: 50S ribosomal protein L24

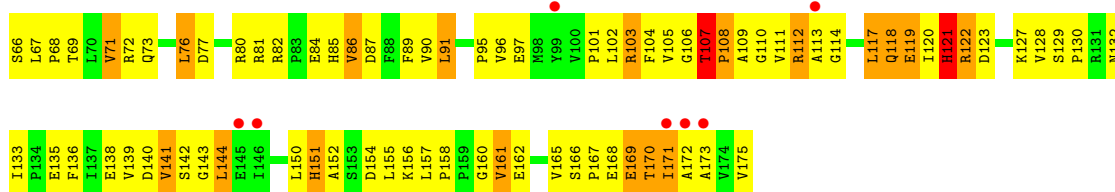
Chain DU:



- Molecule 21: 50S ribosomal protein L25

Chain AV:





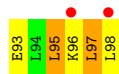
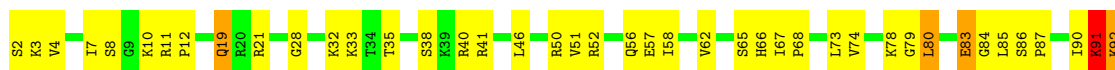
- Molecule 22: 50S ribosomal protein L27

Chain A3:



- Molecule 23: 50S ribosomal protein L28

Chain AZ:



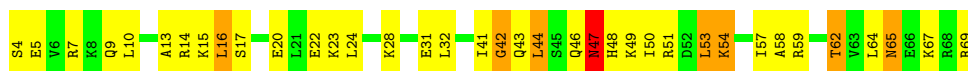
- Molecule 23: 50S ribosomal protein L28

Chain DZ:



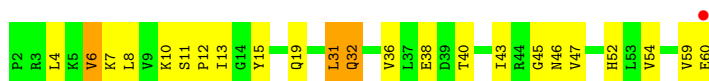
- Molecule 24: 50S ribosomal protein L29

Chain AW:



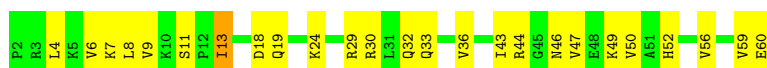
- Molecule 25: 50S ribosomal protein L30

Chain AX:

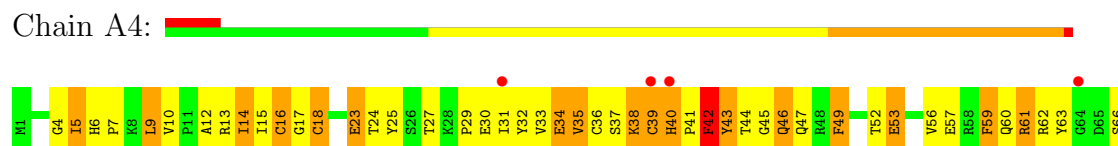


- Molecule 25: 50S ribosomal protein L30

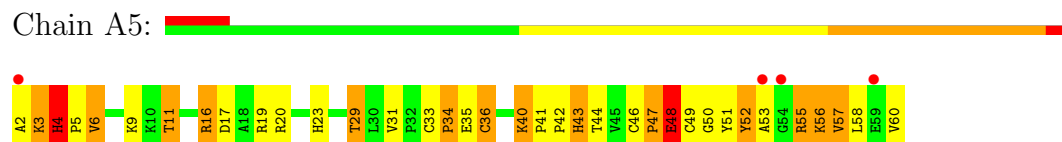
Chain DX:



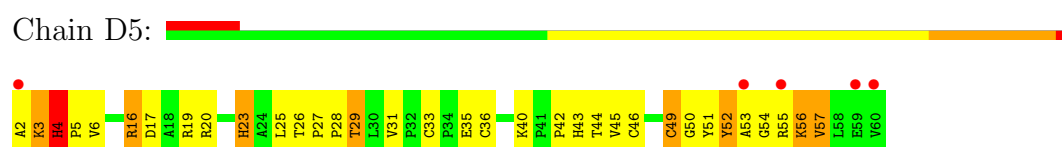
- Molecule 26: 50S ribosomal protein L31



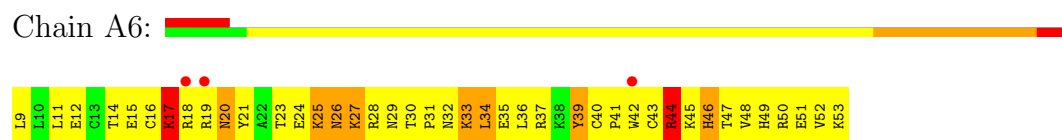
- Molecule 27: 50S ribosomal protein L32



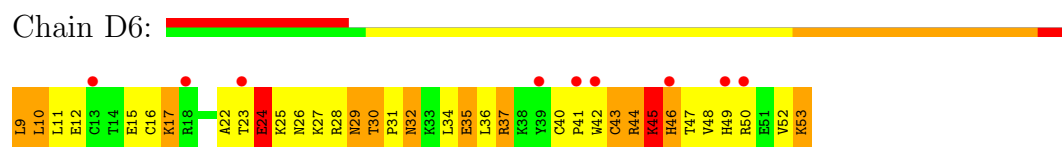
- Molecule 27: 50S ribosomal protein L32



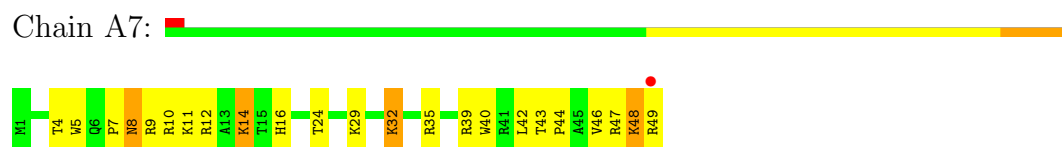
- Molecule 28: 50S ribosomal protein L33



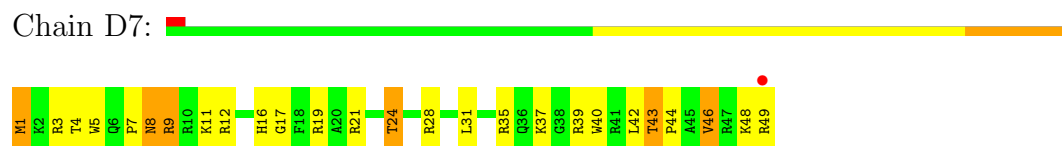
- Molecule 28: 50S ribosomal protein L33



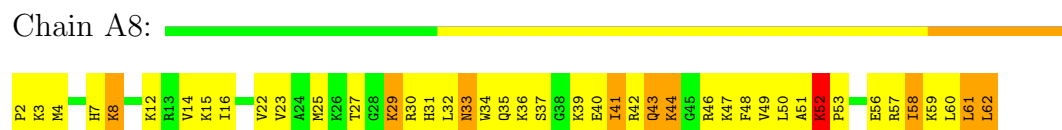
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



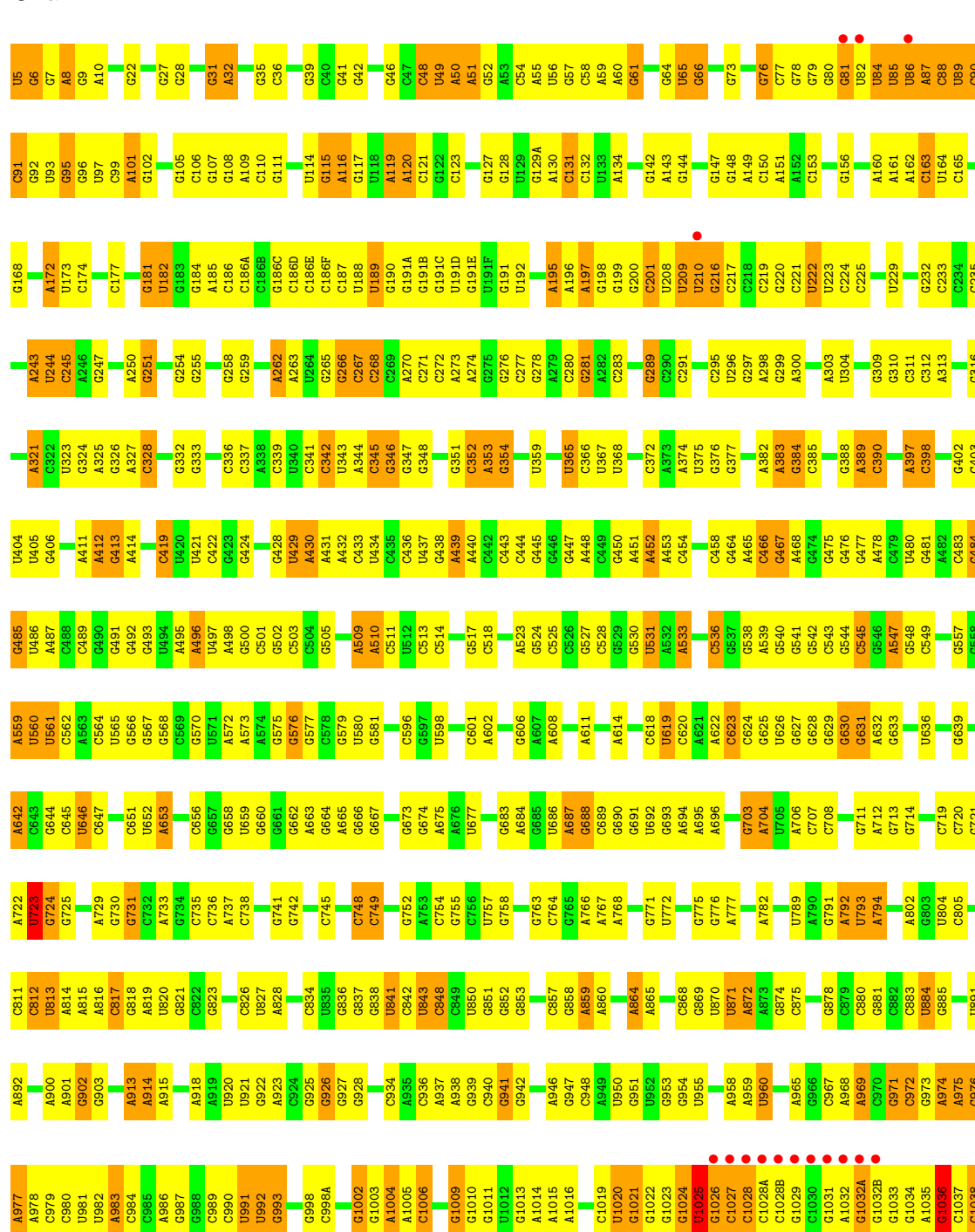
• Molecule 30: 50S ribosomal protein L35

Chain D8:

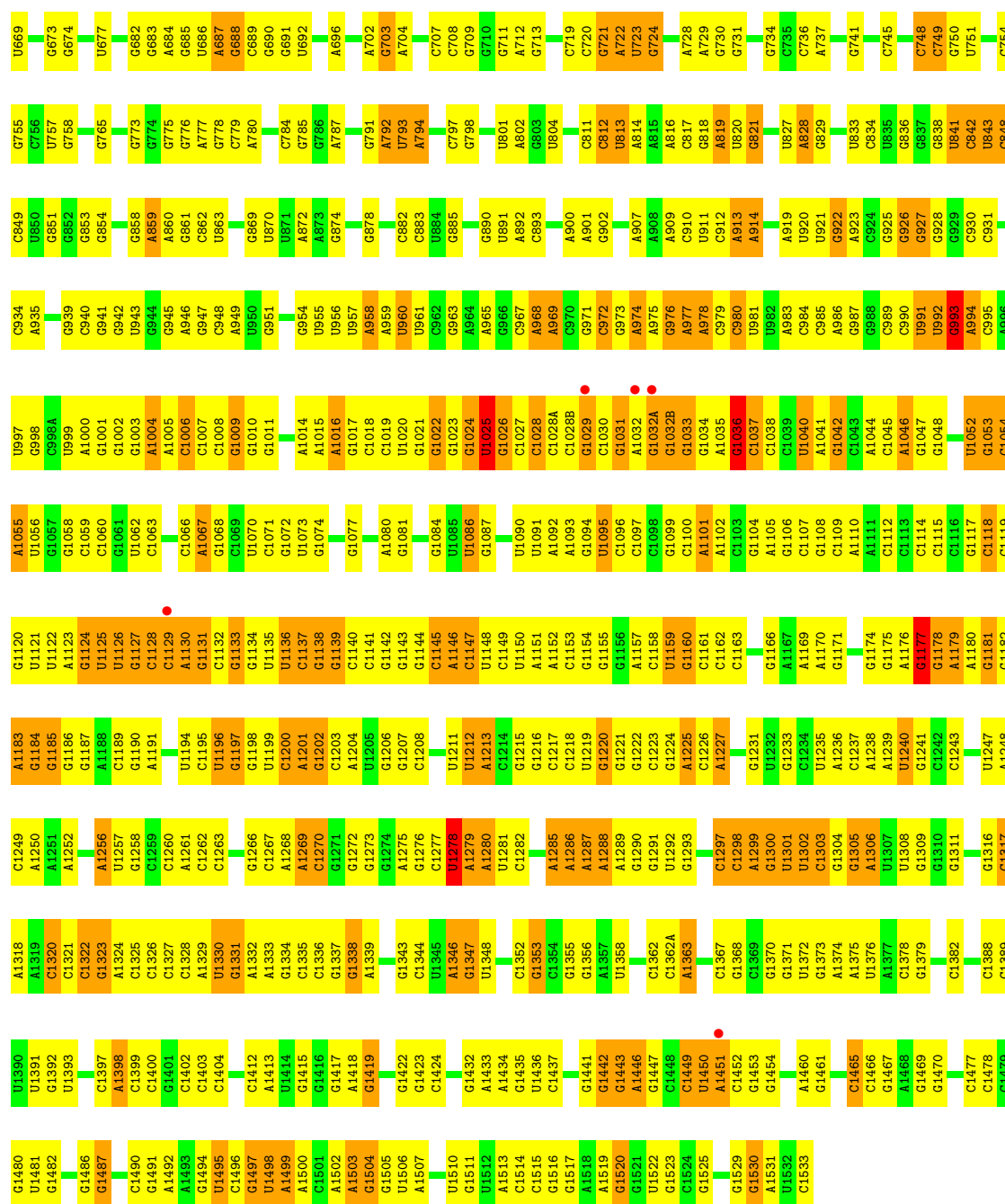


• Molecule 31: 16S ribosomal RNA

Chain BA:

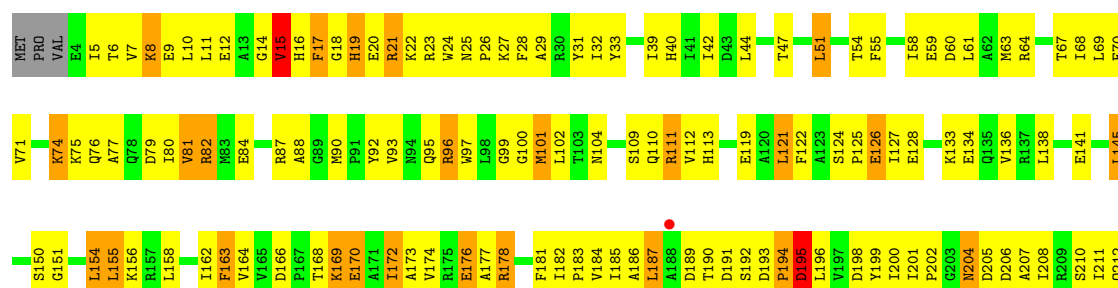


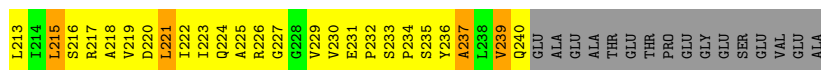




• Molecule 32: 30S RIBOSOMAL PROTEIN S2

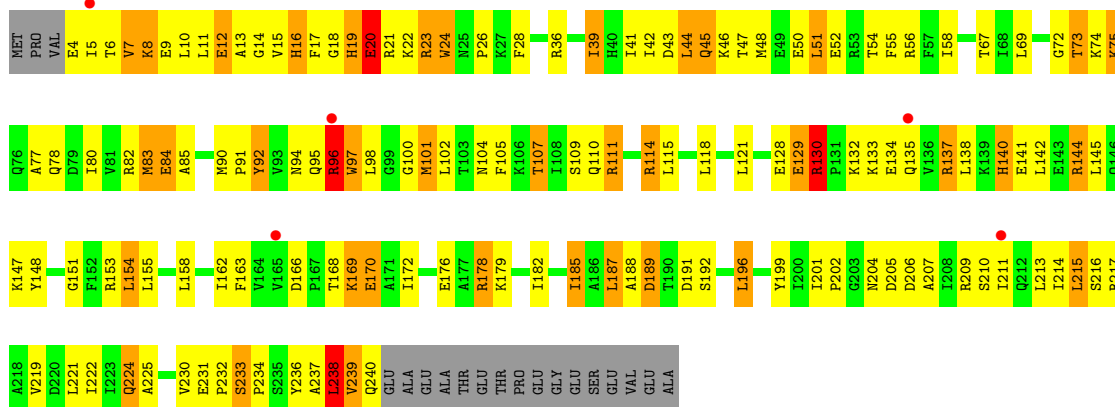
Chain BE:





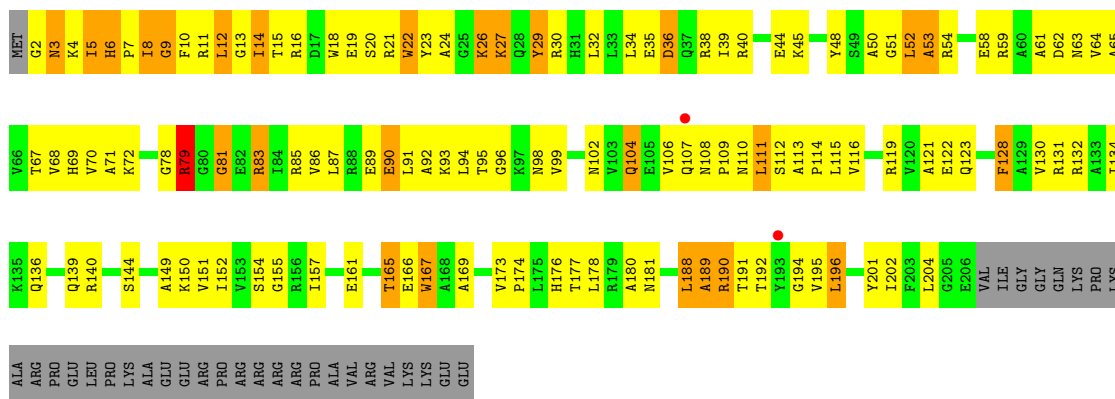
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain CE:



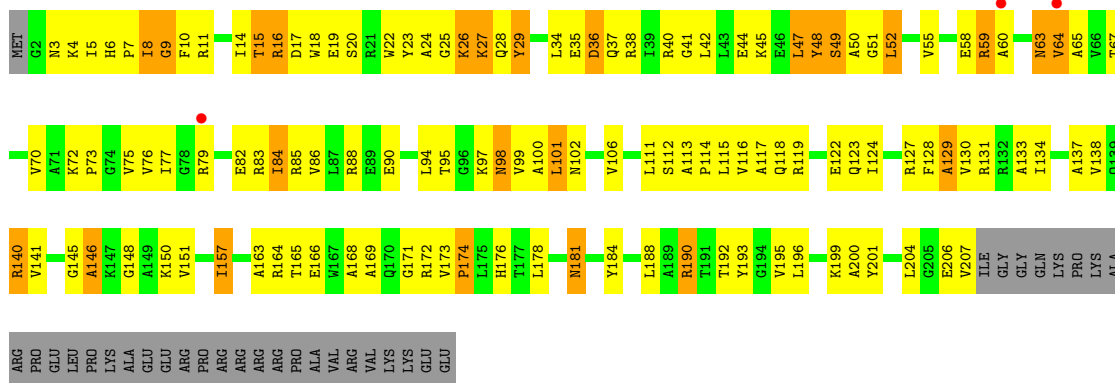
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain BF:



• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain CF:

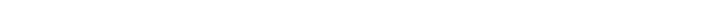


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

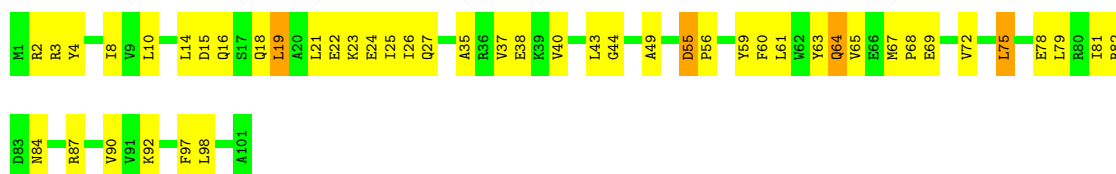
Frequency	Percentage
Daily	60%
Weekly	30%
Monthly	10%



Frequency	Percentage
Daily	65%
Weekly	25%
Monthly	10%

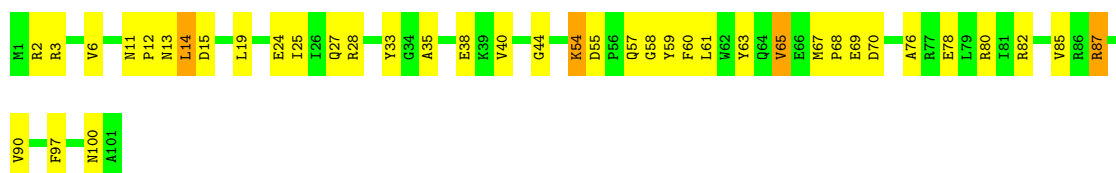


Frequency	Percentage
Daily	65%
Weekly	25%
Monthly	10%



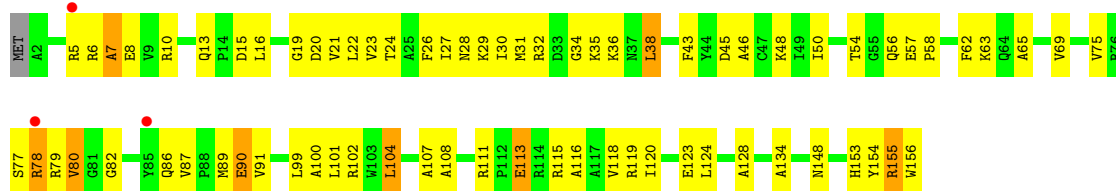
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain CI:



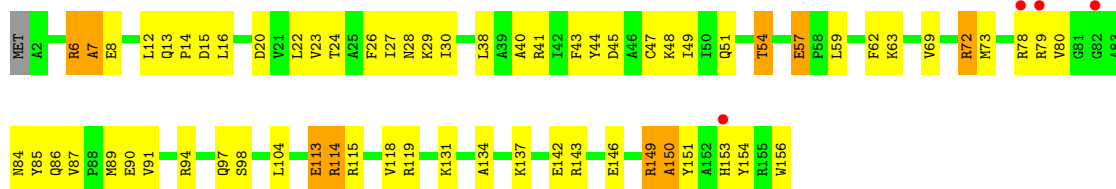
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ:



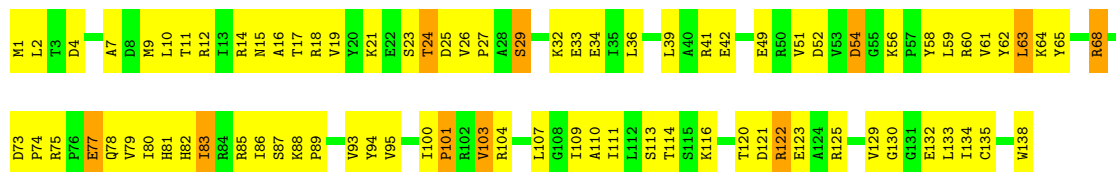
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK:



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain CK:





• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL:



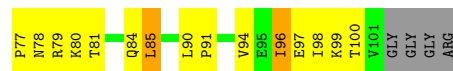
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain CL:



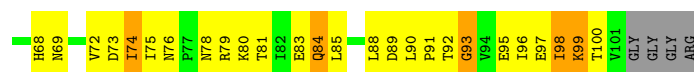
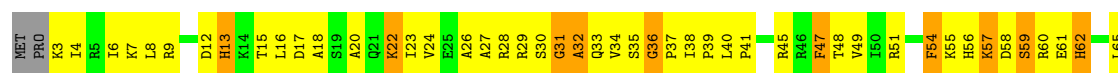
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain BM:



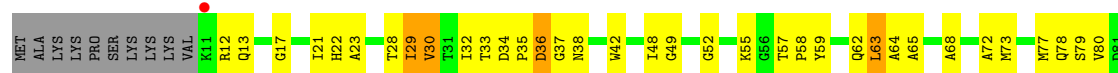
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain CM:



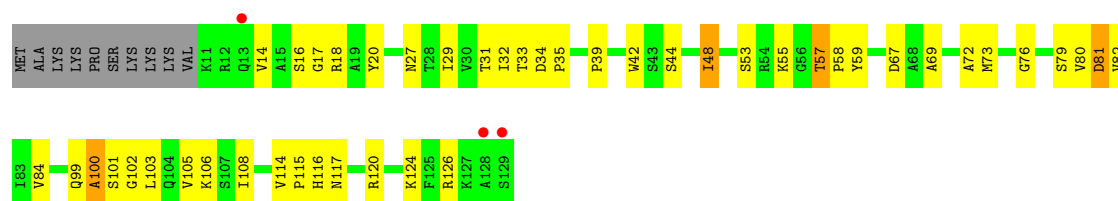
• Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain BN:



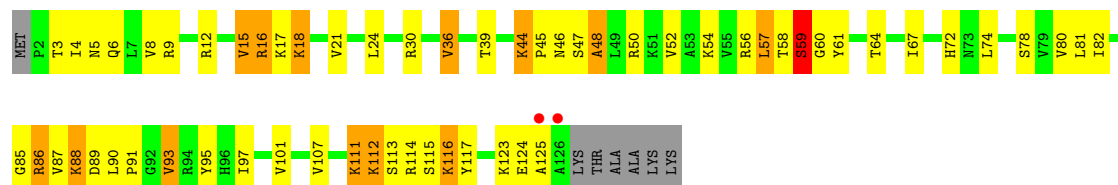
- Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain CN:



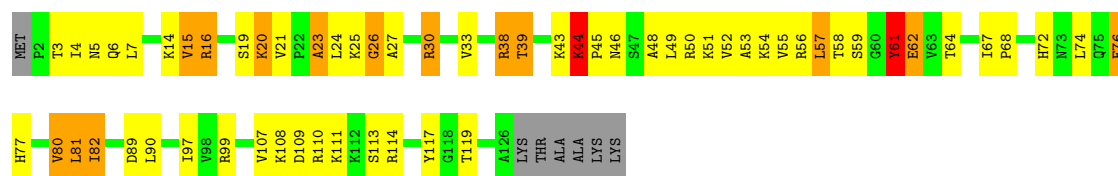
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain BO:



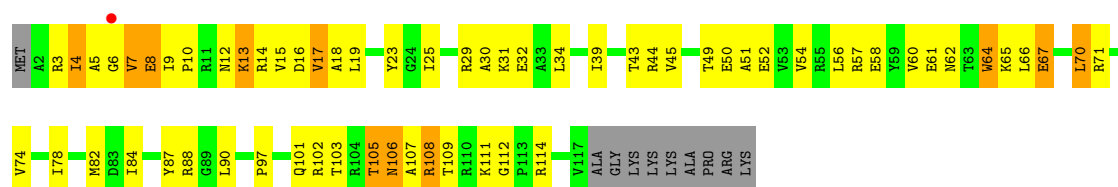
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain CO:



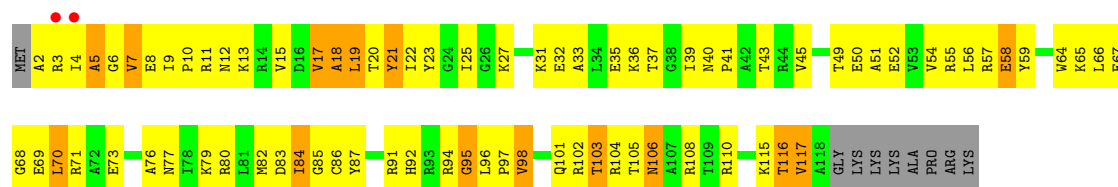
- Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain BP:



- Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain CP:



- Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain BQ:



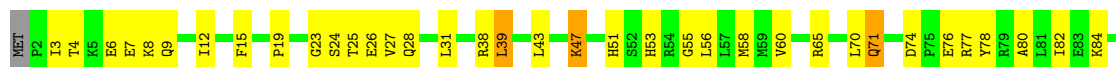
- Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain BR:



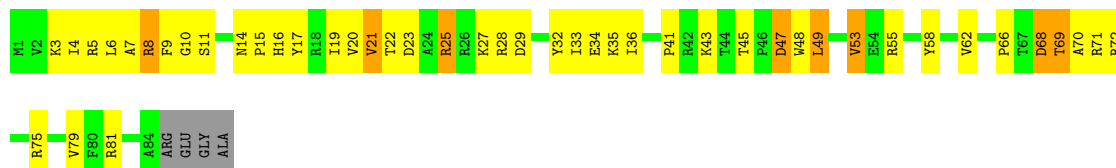
- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain CR:



- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS:



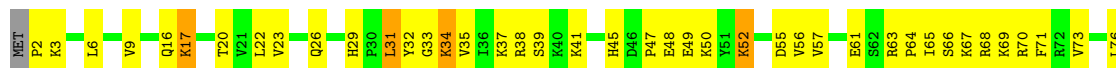
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain CS:



- Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT:



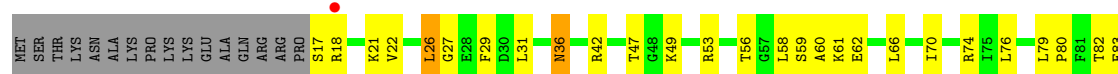
- Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain CT:



- Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain BU:



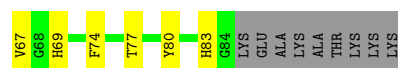
- Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain CU:



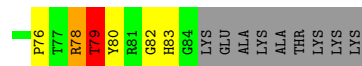
- Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain BV:



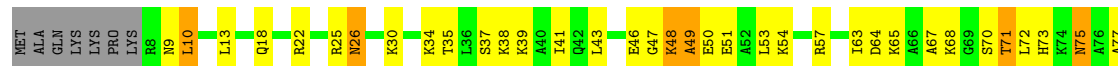
- Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain CV:



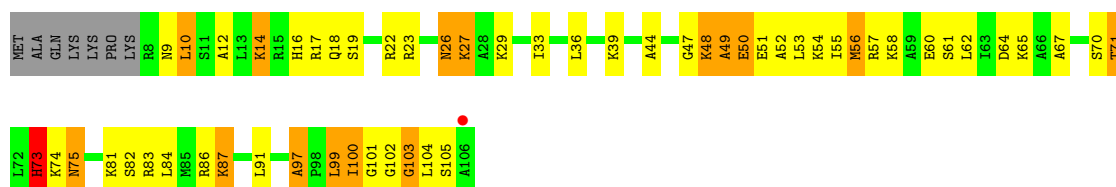
- Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain BW:



- Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain CW:



• Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain BX:



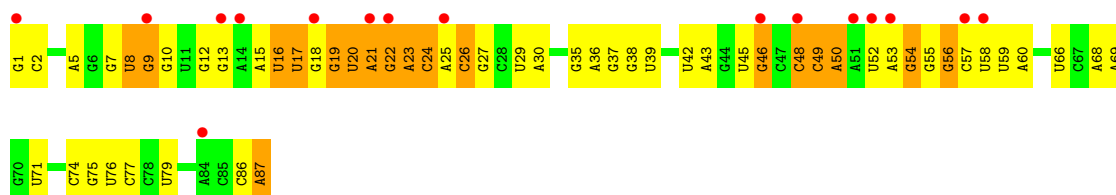
• Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain CX:



• Molecule 52: TRNA-LEU

Chain BB:



• Molecule 52: TRNA-LEU

Chain CB:



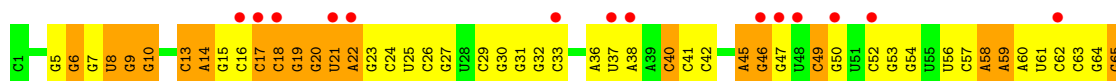
• Molecule 53: TRNA-FMET

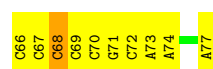
Chain BC:



• Molecule 53: TRNA-FMET

Chain BD:





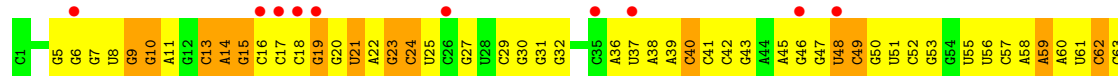
- Molecule 53: TRNA-FMET

Chain CC:



- Molecule 53: TRNA-FMET

Chain CD:



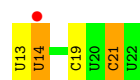
- Molecule 54: MRNA

Chain B1:



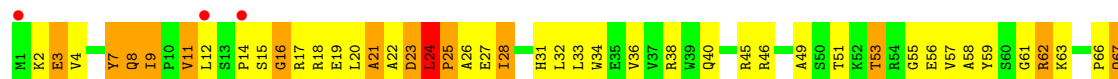
- Molecule 54: MRNA

Chain C1:



- Molecule 55: 50S ribosomal protein L4

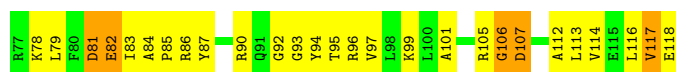
Chain DF:



- Molecule 56: 50S ribosomal protein L17

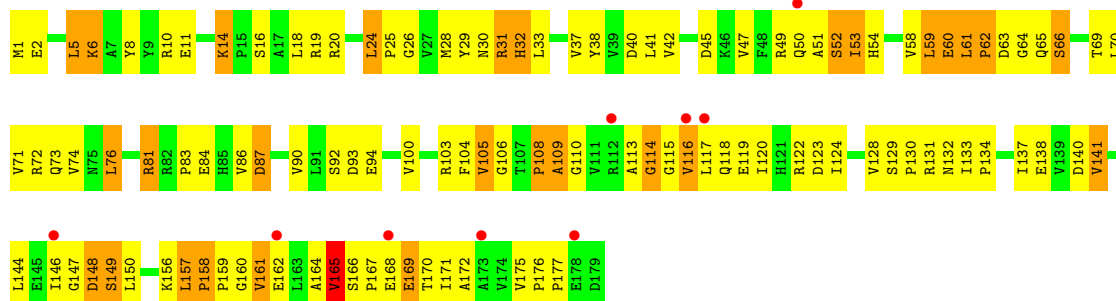
Chain D0:





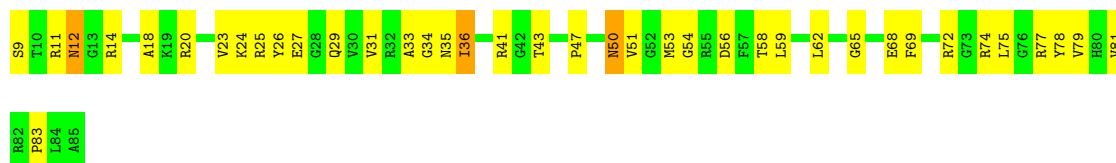
• Molecule 57: 50S ribosomal protein L25

Chain DV:



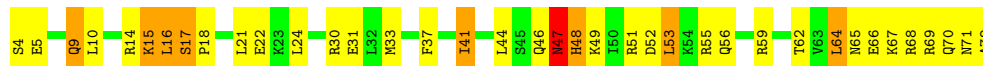
• Molecule 58: 50S ribosomal protein L27

Chain D3:



• Molecule 59: 50S ribosomal protein L29

Chain DW:



• Molecule 60: 50S ribosomal protein L31

Chain D4:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.19Å 451.05Å 621.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.76 – 3.10 122.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.76-3.10) 91.7 (122.29-3.00)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.201 , 0.240 0.244 , 0.259	Depositor DCC
R_{free} test set	833 reflections (0.08%)	DCC
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1157389 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299628	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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

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	0.37	0/70233	0.74	48/109643 (0.0%)
1	DA	0.33	1/70122 (0.0%)	0.71	58/109469 (0.1%)
2	AB	0.31	0/2928	0.72	6/4568 (0.1%)
2	DB	0.27	0/2928	0.71	2/4568 (0.0%)
3	AD	0.31	0/2166	0.55	0/2919
3	DD	0.29	0/2165	0.52	0/2919
4	AE	0.27	0/1602	0.53	0/2160
4	DE	0.27	0/1601	0.54	0/2160
5	AF	0.29	0/1621	0.50	0/2194
6	AG	0.24	0/1499	0.42	0/2016
6	DG	0.22	0/1499	0.41	0/2016
7	AH	0.25	0/1333	0.50	0/1802
7	DH	0.21	0/1332	0.48	0/1802
8	AK	0.24	0/1152	0.49	0/1558
8	DK	0.23	0/1151	0.49	0/1558
9	AM	0.26	0/1132	0.47	0/1525
9	DM	0.23	0/1131	0.45	0/1525
10	AN	0.27	0/943	0.46	0/1269
10	DN	0.26	0/943	0.46	0/1269
11	AO	0.29	0/1162	0.57	0/1544
11	DO	0.26	0/1162	0.56	0/1544
12	AP	0.26	0/1143	0.41	0/1527
12	DP	0.58	1/1143 (0.1%)	0.40	0/1527
13	A0	0.26	0/982	0.50	0/1312
14	AQ	0.27	0/892	0.53	0/1187
14	DQ	0.23	0/892	0.46	0/1187
15	AR	0.28	0/1156	0.51	0/1542
15	DR	0.26	0/1155	0.45	0/1542
16	A1	0.29	0/982	0.48	0/1306
16	D1	0.24	0/982	0.43	0/1306
17	A2	0.27	0/790	0.52	0/1057
17	D2	0.28	0/790	0.51	0/1057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	AS	0.26	0/911	0.48	0/1220
18	DS	0.26	0/911	0.46	0/1220
19	AT	0.32	0/740	0.48	0/993
19	DT	0.31	0/739	0.46	0/993
20	AU	0.30	0/799	0.52	0/1064
20	DU	0.27	0/798	0.49	0/1064
21	AV	0.22	0/1427	0.48	0/1935
22	A3	0.29	0/615	0.49	0/819
23	AZ	0.28	0/770	0.52	0/1022
23	DZ	0.27	0/770	0.49	0/1022
24	AW	0.30	0/560	0.54	0/741
25	AX	0.25	0/474	0.44	0/635
25	DX	0.22	0/474	0.42	0/635
26	A4	0.24	0/545	0.48	0/733
27	A5	0.29	0/473	0.55	0/639
27	D5	0.27	0/473	0.57	0/639
28	A6	0.28	0/397	0.52	0/529
28	D6	0.25	0/396	0.51	0/529
29	A7	0.31	0/438	0.44	0/575
29	D7	0.26	0/438	0.43	0/575
30	A8	0.33	0/494	0.60	0/649
30	D8	0.34	0/494	0.68	0/649
31	BA	0.28	0/36234	0.65	19/56554 (0.0%)
31	CA	0.28	0/36237	0.65	15/56558 (0.0%)
32	BE	0.22	0/1959	0.42	0/2642
32	CE	0.22	0/1959	0.43	0/2642
33	BF	0.22	0/1629	0.41	0/2195
33	CF	0.21	0/1636	0.40	0/2205
34	BG	0.28	0/1733	0.45	0/2318
34	CG	0.26	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	CH	0.24	0/1171	0.44	0/1576
36	BI	0.23	0/856	0.43	0/1154
36	CI	0.24	0/856	0.43	0/1154
37	BJ	0.22	0/1276	0.39	0/1709
37	CJ	0.22	0/1276	0.38	0/1709
38	BK	0.23	0/1136	0.44	0/1527
38	CK	0.22	0/1136	0.43	0/1527
39	BL	0.22	0/1029	0.42	0/1379
39	CL	0.22	0/1029	0.41	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	CM	0.21	0/814	0.43	0/1095
41	BN	0.24	0/900	0.45	0/1213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	CN	0.23	0/900	0.42	0/1213
42	BO	0.27	0/991	0.49	0/1327
42	CO	0.25	0/991	0.46	0/1327
43	BP	0.22	0/938	0.44	0/1258
43	CP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/501	0.49	0/664
44	CQ	0.23	0/501	0.43	0/664
45	BR	0.24	0/745	0.41	0/992
45	CR	0.23	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	CS	0.24	0/721	0.43	0/970
47	BT	0.24	0/847	0.43	0/1131
47	CT	0.24	0/847	0.42	0/1131
48	BU	0.24	0/596	0.44	0/790
48	CU	0.24	0/596	0.43	0/790
49	BV	0.23	0/680	0.47	0/915
49	CV	0.22	0/638	0.44	0/860
50	BW	0.22	0/765	0.43	0/1007
50	CW	0.24	0/765	0.45	0/1007
51	BX	0.22	0/221	0.40	0/288
51	CX	0.21	0/221	0.41	0/288
52	BB	0.21	0/2080	0.51	0/3242
52	CB	0.20	0/2080	0.49	0/3242
53	BC	0.25	0/1835	0.56	0/2859
53	BD	0.16	0/1835	0.46	0/2859
53	CC	0.24	0/1835	0.57	0/2859
53	CD	0.16	0/1835	0.47	0/2859
54	B1	0.27	0/226	0.50	0/348
54	C1	0.37	0/226	0.73	1/348 (0.3%)
55	DF	0.25	0/1662	0.50	0/2249
56	D0	0.25	0/974	0.45	0/1302
57	DV	0.21	0/1460	0.43	0/1982
58	D3	0.26	0/621	0.43	0/827
59	DW	0.25	0/583	0.48	0/771
60	D4	0.24	0/527	0.48	0/709
All	All	0.30	2/324084 (0.0%)	0.64	149/485288 (0.0%)

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
7	AH	0	1
42	BO	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	DP	141	GLN	C-OXT	17.97	1.57	1.23
1	DA	1342	A	N7-C5	-5.40	1.36	1.39

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	933	A	C4-N9-C1'	10.03	144.35	126.30
1	DA	933	A	C6-C5-N7	-10.02	125.28	132.30
1	AA	673	C	C2-N3-C4	-9.52	115.14	119.90
1	DA	933	A	C8-N9-C1'	-9.44	110.72	127.70
31	BA	1025	U	C5-C4-O4	-9.10	120.44	125.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AH	153	LYS	Peptide
42	BO	44	LYS	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	31614	1928	1
1	DA	62607	0	31565	1969	1
2	AB	2617	0	1328	93	0
2	DB	2617	0	1328	98	0
3	AD	2116	0	2195	197	0
3	DD	2115	0	2195	178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AE	1569	0	1634	163	0
4	DE	1568	0	1634	175	0
5	AF	1586	0	1632	111	0
6	AG	1474	0	1535	127	0
6	DG	1474	0	1535	99	0
7	AH	1308	0	1382	143	0
7	DH	1307	0	1382	102	1
8	AK	1137	0	1223	93	0
8	DK	1136	0	1223	92	0
9	AM	1105	0	1180	98	0
9	DM	1104	0	1180	84	0
10	AN	933	0	996	40	0
10	DN	933	0	996	38	0
11	AO	1145	0	1228	157	0
11	DO	1145	0	1228	169	0
12	AP	1122	0	1179	184	0
12	DP	1122	0	1179	204	0
13	A0	968	0	1033	63	0
14	AQ	882	0	943	85	0
14	DQ	882	0	943	73	0
15	AR	1142	0	1202	92	0
15	DR	1141	0	1202	96	0
16	A1	964	0	1022	76	0
16	D1	964	0	1022	88	0
17	A2	779	0	852	75	0
17	D2	779	0	852	117	0
18	AS	900	0	964	61	0
18	DS	900	0	964	41	0
19	AT	726	0	778	52	0
19	DT	725	0	778	56	0
20	AU	786	0	878	77	0
20	DU	785	0	878	97	0
21	AV	1397	0	1430	120	0
22	A3	607	0	628	41	0
23	AZ	763	0	848	40	0
23	DZ	763	0	848	50	0
24	AW	558	0	610	29	0
25	AX	469	0	518	21	0
25	DX	469	0	518	22	0
26	A4	533	0	522	79	0
27	A5	459	0	480	53	0
27	D5	459	0	480	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A6	390	0	404	64	0
28	D6	389	0	404	50	0
29	A7	430	0	480	19	0
29	D7	430	0	480	28	0
30	A8	488	0	560	80	0
30	D8	488	0	560	86	0
31	BA	32369	0	16339	1082	1
31	CA	32372	0	16338	1075	2
32	BE	1924	0	1975	154	0
32	CE	1924	0	1975	162	0
33	BF	1605	0	1668	114	0
33	CF	1612	0	1677	115	0
34	BG	1703	0	1764	120	0
34	CG	1703	0	1763	94	1
35	BH	1155	0	1213	64	0
35	CH	1155	0	1213	75	0
36	BI	843	0	857	41	1
36	CI	843	0	857	38	0
37	BJ	1257	0	1296	65	0
37	CJ	1257	0	1296	62	0
38	BK	1116	0	1177	68	0
38	CK	1116	0	1177	50	0
39	BL	1010	0	1037	84	0
39	CL	1010	0	1037	96	0
40	BM	801	0	849	74	0
40	CM	801	0	849	70	0
41	BN	885	0	904	57	0
41	CN	885	0	904	34	0
42	BO	975	0	1062	52	0
42	CO	975	0	1062	67	0
43	BP	928	0	987	62	0
43	CP	933	0	992	71	0
44	BQ	492	0	529	46	0
44	CQ	492	0	530	38	0
45	BR	734	0	771	34	0
45	CR	734	0	771	34	0
46	BS	705	0	725	41	0
46	CS	705	0	725	32	0
47	BT	834	0	904	47	0
47	CT	834	0	904	31	0
48	BU	591	0	662	24	0
48	CU	591	0	662	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	BV	665	0	686	66	0
49	CV	624	0	636	65	0
50	BW	763	0	861	56	0
50	CW	763	0	861	47	0
51	BX	217	0	234	16	0
51	CX	217	0	234	20	0
52	BB	1861	0	938	50	0
52	CB	1861	0	938	62	0
53	BC	1643	0	837	48	0
53	BD	1643	0	837	65	0
53	CC	1643	0	837	50	0
53	CD	1643	0	837	79	0
54	B1	205	0	105	7	0
54	C1	205	0	105	5	0
55	DF	1627	0	1680	126	0
56	D0	960	0	1021	69	0
57	DV	1428	0	1454	100	0
58	D3	613	0	633	45	0
59	DW	581	0	629	49	0
60	D4	515	0	510	83	0
61	A0	1	0	0	0	0
61	A1	1	0	0	0	0
61	A2	1	0	0	0	0
61	A3	1	0	0	0	0
61	A5	2	0	0	0	0
61	A6	1	0	0	0	0
61	A7	1	0	0	0	0
61	AA	630	0	0	0	0
61	AB	17	0	0	0	0
61	AD	2	0	0	0	0
61	AE	4	0	0	0	0
61	AF	3	0	0	0	0
61	AO	3	0	0	0	0
61	AU	1	0	0	0	0
61	B1	2	0	0	0	0
61	BA	244	0	0	0	0
61	BB	8	0	0	0	0
61	BC	9	0	0	0	0
61	BD	1	0	0	0	0
61	BG	1	0	0	0	0
61	BN	2	0	0	0	0
61	BQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	CA	209	0	0	0	0
61	CB	5	0	0	0	0
61	CC	8	0	0	0	0
61	CG	3	0	0	0	0
61	CH	1	0	0	0	0
61	CS	1	0	0	0	0
61	D0	1	0	0	0	0
61	D1	2	0	0	0	0
61	D3	1	0	0	0	0
61	D5	1	0	0	0	0
61	DA	528	0	0	0	0
61	DB	14	0	0	0	0
61	DE	3	0	0	0	0
61	DP	1	0	0	0	0
61	DU	1	0	0	0	0
62	BG	1	0	0	0	0
62	BQ	1	0	0	0	0
62	CG	1	0	0	0	0
62	CQ	1	0	0	0	0
All	All	299628	0	200976	12579	4

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 25.

The worst 5 of 12579 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:AG:108:ASN:HA	26:A4:38:LYS:CG	1.41	1.51
6:AG:108:ASN:CA	26:A4:38:LYS:HG2	1.46	1.45
1:AA:1056:G:H21	1:AA:1103:A:N6	1.13	1.45
1:DA:226:G:H21	1:DA:228:A:N6	0.93	1.41
1:DA:226:G:N2	1:DA:228:A:H61	1.15	1.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:BA:85:U:O2'	7:DH:100:GLY:O[3_555]	1.87	0.33
1:AA:2137:C:OP1	31:CA:999:U:O2'[4_555]	1.89	0.31
36:BI:15:ASP:OD2	34:CG:27:TYR:OH[4_555]	2.05	0.15
31:CA:86:U:O2'	1:DA:276:A:OP2[3_545]	2.15	0.05

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	270/272 (99%)	226 (84%)	31 (12%)	13 (5%)	4	23
3	DD	270/272 (99%)	231 (86%)	25 (9%)	14 (5%)	3	21
4	AE	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1	8
4	DE	203/205 (99%)	128 (63%)	41 (20%)	34 (17%)	0	0
5	AF	200/202 (99%)	177 (88%)	12 (6%)	11 (6%)	3	19
6	AG	179/181 (99%)	147 (82%)	21 (12%)	11 (6%)	2	16
6	DG	179/181 (99%)	141 (79%)	27 (15%)	11 (6%)	2	16
7	AH	168/170 (99%)	116 (69%)	22 (13%)	30 (18%)	0	0
7	DH	168/170 (99%)	108 (64%)	37 (22%)	23 (14%)	0	2
8	AK	144/146 (99%)	97 (67%)	27 (19%)	20 (14%)	0	2
8	DK	144/146 (99%)	106 (74%)	26 (18%)	12 (8%)	1	9
9	AM	136/138 (99%)	105 (77%)	18 (13%)	13 (10%)	1	7
9	DM	136/138 (99%)	108 (79%)	20 (15%)	8 (6%)	2	17
10	AN	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	14	54
10	DN	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	27	74
11	AO	148/150 (99%)	106 (72%)	25 (17%)	17 (12%)	1	4
11	DO	148/150 (99%)	92 (62%)	28 (19%)	28 (19%)	0	0
12	AP	139/141 (99%)	95 (68%)	25 (18%)	19 (14%)	0	2
12	DP	139/141 (99%)	91 (66%)	20 (14%)	28 (20%)	0	0
13	A0	116/118 (98%)	93 (80%)	15 (13%)	8 (7%)	2	13
14	AQ	109/111 (98%)	77 (71%)	24 (22%)	8 (7%)	2	12
14	DQ	109/111 (98%)	78 (72%)	21 (19%)	10 (9%)	1	7
15	AR	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	2	11
15	DR	135/137 (98%)	103 (76%)	23 (17%)	9 (7%)	2	14
16	A1	115/117 (98%)	101 (88%)	7 (6%)	7 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	D1	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	2	16
17	A2	99/101 (98%)	83 (84%)	9 (9%)	7 (7%)	2	12
17	D2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	1	4
18	AS	111/113 (98%)	92 (83%)	14 (13%)	5 (4%)	4	24
18	DS	111/113 (98%)	99 (89%)	10 (9%)	2 (2%)	13	52
19	AT	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	21	65
19	DT	90/92 (98%)	75 (83%)	12 (13%)	3 (3%)	6	33
20	AU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	3
20	DU	100/102 (98%)	61 (61%)	22 (22%)	17 (17%)	0	0
21	AV	173/175 (99%)	112 (65%)	36 (21%)	25 (14%)	0	2
22	A3	74/76 (97%)	57 (77%)	15 (20%)	2 (3%)	8	39
23	AZ	95/97 (98%)	78 (82%)	10 (10%)	7 (7%)	2	11
23	DZ	95/97 (98%)	77 (81%)	7 (7%)	11 (12%)	1	4
24	AW	64/66 (97%)	56 (88%)	3 (5%)	5 (8%)	1	11
25	AX	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	DX	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	52
26	A4	64/66 (97%)	38 (59%)	16 (25%)	10 (16%)	0	1
27	A5	57/59 (97%)	40 (70%)	10 (18%)	7 (12%)	1	3
27	D5	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	2	13
28	A6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	2
28	D6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	2
29	A7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	48
29	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	A8	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	2	14
30	D8	59/61 (97%)	39 (66%)	11 (19%)	9 (15%)	0	1
32	BE	235/256 (92%)	170 (72%)	47 (20%)	18 (8%)	1	11
32	CE	235/256 (92%)	188 (80%)	23 (10%)	24 (10%)	1	6
33	BF	203/239 (85%)	141 (70%)	46 (23%)	16 (8%)	1	11
33	CF	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	2	11
34	BG	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	3	21
34	CG	206/208 (99%)	171 (83%)	30 (15%)	5 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BH	149/162 (92%)	129 (87%)	14 (9%)	6 (4%)	5	28
35	CH	149/162 (92%)	134 (90%)	11 (7%)	4 (3%)	8	39
36	BI	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	11	49
36	CI	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	22	68
37	BJ	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	30	76
37	CJ	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	11	49
38	BK	136/138 (99%)	115 (85%)	14 (10%)	7 (5%)	3	22
38	CK	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	10	46
39	BL	125/128 (98%)	100 (80%)	22 (18%)	3 (2%)	9	43
39	CL	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	6	35
40	BM	97/105 (92%)	76 (78%)	19 (20%)	2 (2%)	11	48
40	CM	97/105 (92%)	75 (77%)	13 (13%)	9 (9%)	1	7
41	BN	117/129 (91%)	97 (83%)	15 (13%)	5 (4%)	4	26
41	CN	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	8	41
42	BO	123/132 (93%)	101 (82%)	13 (11%)	9 (7%)	2	12
42	CO	123/132 (93%)	96 (78%)	19 (15%)	8 (6%)	2	15
43	BP	114/126 (90%)	86 (75%)	20 (18%)	8 (7%)	2	13
43	CP	115/126 (91%)	83 (72%)	22 (19%)	10 (9%)	1	9
44	BQ	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	1	9
44	CQ	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	1	6
45	BR	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
45	CR	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	19	62
46	BS	82/88 (93%)	65 (79%)	14 (17%)	3 (4%)	5	31
46	CS	82/88 (93%)	69 (84%)	13 (16%)	0	100	100
47	BT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	11	49
47	CT	98/105 (93%)	92 (94%)	4 (4%)	2 (2%)	11	49
48	BU	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	7	38
48	CU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	BV	81/93 (87%)	63 (78%)	11 (14%)	7 (9%)	1	9
49	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	7
50	BW	97/106 (92%)	75 (77%)	12 (12%)	10 (10%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	CW	97/106 (92%)	73 (75%)	13 (13%)	11 (11%)	1	4
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	4	26
51	CX	23/27 (85%)	19 (83%)	0	4 (17%)	0	0
55	DF	206/208 (99%)	162 (79%)	25 (12%)	19 (9%)	1	7
56	D0	115/117 (98%)	93 (81%)	17 (15%)	5 (4%)	4	26
57	DV	177/179 (99%)	120 (68%)	27 (15%)	30 (17%)	0	0
58	D3	75/77 (97%)	62 (83%)	13 (17%)	0	100	100
59	DW	67/69 (97%)	56 (84%)	5 (8%)	6 (9%)	1	8
60	D4	61/63 (97%)	24 (39%)	25 (41%)	12 (20%)	0	0
All	All	11341/11826 (96%)	8910 (79%)	1589 (14%)	842 (7%)	2	11

5 of 842 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	26	LYS
3	AD	28	GLU
3	AD	33	LEU
3	AD	122	ASP
3	AD	237	GLU

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	214/214 (100%)	182 (85%)	32 (15%)	4	17
3	DD	214/214 (100%)	179 (84%)	35 (16%)	3	12
4	AE	165/165 (100%)	133 (81%)	32 (19%)	2	8
4	DE	165/165 (100%)	138 (84%)	27 (16%)	3	12
5	AF	161/161 (100%)	139 (86%)	22 (14%)	5	21
6	AG	155/155 (100%)	134 (86%)	21 (14%)	6	22
6	DG	155/155 (100%)	135 (87%)	20 (13%)	6	24
7	AH	142/142 (100%)	118 (83%)	24 (17%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	DH	142/142 (100%)	130 (92%)	12 (8%)	15	51
8	AK	122/122 (100%)	106 (87%)	16 (13%)	6	23
8	DK	122/122 (100%)	103 (84%)	19 (16%)	4	14
9	AM	117/117 (100%)	99 (85%)	18 (15%)	4	15
9	DM	117/117 (100%)	98 (84%)	19 (16%)	3	13
10	AN	100/100 (100%)	91 (91%)	9 (9%)	14	47
10	DN	100/100 (100%)	89 (89%)	11 (11%)	9	34
11	AO	116/116 (100%)	87 (75%)	29 (25%)	1	3
11	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	87 (78%)	24 (22%)	1	6
12	DP	111/111 (100%)	85 (77%)	26 (23%)	1	5
13	A0	101/101 (100%)	82 (81%)	19 (19%)	2	9
14	AQ	87/87 (100%)	68 (78%)	19 (22%)	1	6
14	DQ	87/87 (100%)	76 (87%)	11 (13%)	7	24
15	AR	120/120 (100%)	100 (83%)	20 (17%)	3	11
15	DR	120/120 (100%)	91 (76%)	29 (24%)	1	4
16	A1	93/93 (100%)	82 (88%)	11 (12%)	8	29
16	D1	93/93 (100%)	88 (95%)	5 (5%)	31	72
17	A2	82/82 (100%)	71 (87%)	11 (13%)	6	22
17	D2	82/82 (100%)	68 (83%)	14 (17%)	3	11
18	AS	92/92 (100%)	74 (80%)	18 (20%)	2	8
18	DS	92/92 (100%)	77 (84%)	15 (16%)	3	12
19	AT	74/74 (100%)	62 (84%)	12 (16%)	3	13
19	DT	74/74 (100%)	63 (85%)	11 (15%)	4	17
20	AU	85/85 (100%)	70 (82%)	15 (18%)	3	10
20	DU	85/85 (100%)	67 (79%)	18 (21%)	1	7
21	AV	154/154 (100%)	130 (84%)	24 (16%)	4	14
22	A3	61/61 (100%)	57 (93%)	4 (7%)	24	64
23	AZ	82/82 (100%)	72 (88%)	10 (12%)	7	26
23	DZ	82/82 (100%)	71 (87%)	11 (13%)	6	22
24	AW	62/62 (100%)	50 (81%)	12 (19%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AX	51/51 (100%)	46 (90%)	5 (10%)	12	40
25	DX	51/51 (100%)	48 (94%)	3 (6%)	28	68
26	A4	59/59 (100%)	49 (83%)	10 (17%)	3	11
27	A5	51/51 (100%)	39 (76%)	12 (24%)	1	5
27	D5	51/51 (100%)	41 (80%)	10 (20%)	2	8
28	A6	44/44 (100%)	37 (84%)	7 (16%)	4	13
28	D6	44/44 (100%)	34 (77%)	10 (23%)	1	5
29	A7	42/42 (100%)	35 (83%)	7 (17%)	3	11
29	D7	42/42 (100%)	34 (81%)	8 (19%)	2	9
30	A8	51/51 (100%)	40 (78%)	11 (22%)	1	6
30	D8	51/51 (100%)	44 (86%)	7 (14%)	5	21
32	BE	205/220 (93%)	174 (85%)	31 (15%)	4	16
32	CE	205/220 (93%)	174 (85%)	31 (15%)	4	16
33	BF	159/188 (85%)	137 (86%)	22 (14%)	5	21
33	CF	160/188 (85%)	139 (87%)	21 (13%)	6	23
34	BG	180/180 (100%)	161 (89%)	19 (11%)	10	35
34	CG	180/180 (100%)	152 (84%)	28 (16%)	4	14
35	BH	116/123 (94%)	101 (87%)	15 (13%)	6	24
35	CH	116/123 (94%)	101 (87%)	15 (13%)	6	24
36	BI	90/90 (100%)	82 (91%)	8 (9%)	14	47
36	CI	90/90 (100%)	85 (94%)	5 (6%)	30	70
37	BJ	126/127 (99%)	113 (90%)	13 (10%)	10	36
37	CJ	126/127 (99%)	107 (85%)	19 (15%)	4	16
38	BK	119/119 (100%)	109 (92%)	10 (8%)	16	52
38	CK	119/119 (100%)	109 (92%)	10 (8%)	16	52
39	BL	98/99 (99%)	81 (83%)	17 (17%)	3	11
39	CL	98/99 (99%)	85 (87%)	13 (13%)	6	22
40	BM	89/92 (97%)	79 (89%)	10 (11%)	9	33
40	CM	89/92 (97%)	78 (88%)	11 (12%)	7	25
41	BN	90/99 (91%)	81 (90%)	9 (10%)	11	38
41	CN	90/99 (91%)	82 (91%)	8 (9%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BO	104/109 (95%)	87 (84%)	17 (16%)	3	12
42	CO	104/109 (95%)	92 (88%)	12 (12%)	8	31
43	BP	94/101 (93%)	85 (90%)	9 (10%)	12	42
43	CP	94/101 (93%)	80 (85%)	14 (15%)	4	17
44	BQ	49/50 (98%)	40 (82%)	9 (18%)	2	9
44	CQ	49/50 (98%)	47 (96%)	2 (4%)	41	82
45	BR	79/80 (99%)	76 (96%)	3 (4%)	44	84
45	CR	79/80 (99%)	72 (91%)	7 (9%)	14	47
46	BS	72/74 (97%)	64 (89%)	8 (11%)	9	33
46	CS	72/74 (97%)	63 (88%)	9 (12%)	7	25
47	BT	95/97 (98%)	86 (90%)	9 (10%)	12	42
47	CT	95/97 (98%)	91 (96%)	4 (4%)	40	81
48	BU	63/77 (82%)	58 (92%)	5 (8%)	18	55
48	CU	63/77 (82%)	56 (89%)	7 (11%)	9	33
49	BV	72/80 (90%)	60 (83%)	12 (17%)	3	11
49	CV	67/80 (84%)	55 (82%)	12 (18%)	2	10
50	BW	76/82 (93%)	67 (88%)	9 (12%)	8	29
50	CW	76/82 (93%)	66 (87%)	10 (13%)	6	23
51	BX	20/22 (91%)	19 (95%)	1 (5%)	34	75
51	CX	20/22 (91%)	20 (100%)	0	100	100
55	DF	165/165 (100%)	142 (86%)	23 (14%)	5	21
56	D0	100/100 (100%)	85 (85%)	15 (15%)	4	17
57	DV	158/158 (100%)	146 (92%)	12 (8%)	19	58
58	D3	62/62 (100%)	58 (94%)	4 (6%)	24	65
59	DW	64/64 (100%)	56 (88%)	8 (12%)	7	25
60	D4	57/57 (100%)	50 (88%)	7 (12%)	7	26
All	All	9584/9814 (98%)	8234 (86%)	1350 (14%)	5	20

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BO	17	LYS
34	CG	84	LYS

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Mol	Chain	Res	Type
19	DT	63	LYS
43	BP	70	LEU
50	BW	73	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 259 such sidechains are listed below:

Mol	Chain	Res	Type
42	BO	46	ASN
34	CG	43	HIS
57	DV	65	GLN
43	BP	101	GLN
49	BV	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	555 (19%)	51 (1%)
1	DA	2905/2912 (99%)	601 (20%)	50 (1%)
2	AB	121/122 (99%)	24 (19%)	0
2	DB	121/122 (99%)	28 (23%)	0
31	BA	1506/1506 (100%)	291 (19%)	32 (2%)
31	CA	1505/1506 (99%)	315 (20%)	42 (2%)
52	BB	86/87 (98%)	26 (30%)	4 (4%)
52	CB	86/87 (98%)	30 (34%)	3 (3%)
53	BC	77/77 (100%)	12 (15%)	3 (3%)
53	BD	76/77 (98%)	25 (32%)	2 (2%)
53	CC	76/77 (98%)	14 (18%)	3 (3%)
53	CD	76/77 (98%)	16 (21%)	2 (2%)
54	B1	9/10 (90%)	2 (22%)	0
54	C1	9/10 (90%)	2 (22%)	0
All	All	9564/9582 (99%)	1941 (20%)	192 (2%)

5 of 1941 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	15	G
1	AA	23	G
1	AA	34	C
1	AA	35	G

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BB	23	A
31	CA	560	U
1	DA	2210	G
53	BC	48	U
31	CA	209	U

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 1720 ligands modelled in this entry, 1720 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.03	32 (1%) 77 22	38, 71, 209, 243	0
1	DA	2907/2912 (99%)	0.08	62 (2%) 60 11	49, 82, 229, 246	0
2	AB	122/122 (100%)	-0.27	0 100 100	73, 98, 119, 180	0
2	DB	122/122 (100%)	-0.20	1 (0%) 83 28	87, 121, 145, 200	0
3	AD	272/272 (100%)	-0.04	0 100 100	38, 61, 83, 107	0
3	DD	272/272 (100%)	-0.04	1 (0%) 90 45	45, 69, 94, 125	0
4	AE	205/205 (100%)	-0.04	1 (0%) 88 39	44, 82, 133, 147	0
4	DE	205/205 (100%)	0.04	2 (0%) 79 23	51, 90, 144, 167	0
5	AF	202/202 (100%)	-0.08	0 100 100	40, 74, 116, 133	0
6	AG	181/181 (100%)	0.31	3 (1%) 67 15	91, 110, 140, 149	0
6	DG	181/181 (100%)	0.35	3 (1%) 67 15	112, 138, 161, 171	0
7	AH	170/170 (100%)	0.04	1 (0%) 86 36	80, 110, 129, 154	0
7	DH	170/170 (100%)	0.81	17 (10%) 8 2	150, 196, 217, 230	0
8	AK	146/146 (100%)	0.13	0 100 100	75, 124, 142, 149	0
8	DK	146/146 (100%)	0.13	1 (0%) 84 32	76, 127, 150, 154	0
9	AM	138/138 (100%)	-0.09	0 100 100	63, 86, 124, 137	0
9	DM	138/138 (100%)	-0.10	0 100 100	74, 105, 136, 148	0
10	AN	122/122 (100%)	-0.00	0 100 100	54, 74, 92, 103	0
10	DN	122/122 (100%)	-0.04	0 100 100	62, 84, 106, 123	0
11	AO	150/150 (100%)	0.01	2 (1%) 74 19	45, 82, 112, 166	0
11	DO	150/150 (100%)	0.22	5 (3%) 44 6	50, 100, 140, 180	0
12	AP	141/141 (100%)	0.10	0 100 100	58, 85, 110, 134	0
12	DP	141/141 (100%)	0.17	0 100 100	58, 101, 131, 154	0
13	A0	118/118 (100%)	-0.07	0 100 100	55, 80, 102, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	AQ	111/111 (100%)	-0.01	0 100 100	75, 96, 120, 136	0
14	DQ	111/111 (100%)	0.05	1 (0%) 81 25	80, 118, 143, 165	0
15	AR	137/137 (100%)	-0.04	0 100 100	69, 89, 140, 171	0
15	DR	137/137 (100%)	0.11	1 (0%) 84 32	70, 94, 158, 186	0
16	A1	117/117 (100%)	0.01	2 (1%) 67 15	46, 74, 108, 149	0
16	D1	117/117 (100%)	-0.02	0 100 100	59, 95, 138, 157	0
17	A2	101/101 (100%)	-0.00	1 (0%) 79 23	47, 96, 125, 142	0
17	D2	101/101 (100%)	0.07	1 (0%) 79 23	57, 121, 140, 151	0
18	AS	113/113 (100%)	-0.07	0 100 100	46, 70, 106, 155	0
18	DS	113/113 (100%)	-0.03	2 (1%) 65 14	61, 74, 107, 155	0
19	AT	92/92 (100%)	-0.08	0 100 100	54, 68, 98, 112	0
19	DT	92/92 (100%)	-0.03	1 (1%) 77 22	64, 86, 112, 128	0
20	AU	102/102 (100%)	0.10	2 (1%) 62 12	70, 97, 148, 168	0
20	DU	102/102 (100%)	0.54	10 (9%) 8 2	85, 113, 163, 184	0
21	AV	175/175 (100%)	0.50	7 (4%) 36 5	87, 125, 190, 195	0
22	A3	76/76 (100%)	-0.06	0 100 100	56, 75, 95, 135	0
23	AZ	97/97 (100%)	0.08	2 (2%) 60 11	50, 69, 126, 161	0
23	DZ	97/97 (100%)	0.09	2 (2%) 60 11	52, 78, 131, 156	0
24	AW	66/66 (100%)	-0.10	0 100 100	60, 77, 97, 134	0
25	AX	59/59 (100%)	0.14	1 (1%) 67 15	63, 80, 112, 127	0
25	DX	59/59 (100%)	0.05	0 100 100	74, 100, 138, 162	0
26	A4	66/66 (100%)	0.71	4 (6%) 21 3	117, 153, 177, 184	0
27	A5	59/59 (100%)	0.18	4 (6%) 17 3	43, 85, 167, 172	0
27	D5	59/59 (100%)	0.29	5 (8%) 11 2	55, 83, 177, 186	0
28	A6	45/45 (100%)	0.53	3 (6%) 17 3	107, 136, 159, 163	0
28	D6	45/45 (100%)	1.22	9 (20%) 2 0	121, 158, 176, 182	0
29	A7	49/49 (100%)	-0.02	1 (2%) 62 12	38, 47, 95, 123	0
29	D7	49/49 (100%)	0.08	1 (2%) 62 12	49, 58, 115, 133	0
30	A8	61/61 (100%)	-0.05	0 100 100	55, 68, 85, 108	0
30	D8	61/61 (100%)	0.16	1 (1%) 68 15	65, 81, 103, 120	0
31	BA	1506/1506 (100%)	-0.04	16 (1%) 77 22	54, 103, 187, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
31	CA	1506/1506 (100%)	-0.05	8 (0%)	88 39	59, 109, 187, 245	0
32	BE	237/256 (92%)	0.17	1 (0%)	90 45	107, 142, 181, 191	0
32	CE	237/256 (92%)	0.33	5 (2%)	60 11	117, 158, 190, 208	0
33	BF	205/239 (85%)	0.13	2 (0%)	79 23	88, 118, 150, 162	0
33	CF	206/239 (86%)	0.27	3 (1%)	70 16	119, 143, 172, 183	0
34	BG	208/208 (100%)	0.08	1 (0%)	88 39	84, 110, 135, 149	0
34	CG	208/208 (100%)	-0.05	0	100 100	74, 101, 128, 142	0
35	BH	151/162 (93%)	0.01	0	100 100	79, 101, 129, 159	0
35	CH	151/162 (93%)	0.08	0	100 100	90, 114, 139, 162	0
36	BI	101/101 (100%)	-0.05	0	100 100	77, 102, 122, 143	0
36	CI	101/101 (100%)	-0.15	0	100 100	73, 98, 121, 149	0
37	BJ	155/156 (99%)	0.07	3 (1%)	64 13	101, 122, 156, 167	0
37	CJ	155/156 (99%)	0.15	4 (2%)	53 8	105, 127, 158, 165	0
38	BK	138/138 (100%)	-0.07	0	100 100	84, 108, 123, 132	0
38	CK	138/138 (100%)	-0.04	0	100 100	93, 118, 131, 141	0
39	BL	127/128 (99%)	0.14	1 (0%)	83 28	91, 141, 160, 169	0
39	CL	127/128 (99%)	0.35	3 (2%)	56 9	107, 151, 168, 172	0
40	BM	99/105 (94%)	0.29	0	100 100	87, 140, 171, 176	0
40	CM	99/105 (94%)	0.39	0	100 100	113, 154, 173, 176	0
41	BN	119/129 (92%)	0.06	2 (1%)	67 15	63, 101, 133, 162	0
41	CN	119/129 (92%)	0.15	3 (2%)	54 9	77, 103, 141, 166	0
42	BO	125/132 (94%)	0.07	2 (1%)	68 15	61, 78, 116, 162	0
42	CO	125/132 (94%)	0.06	0	100 100	70, 97, 130, 168	0
43	BP	116/126 (92%)	0.10	1 (0%)	81 25	87, 124, 144, 158	0
43	CP	117/126 (92%)	0.23	2 (1%)	67 15	105, 152, 166, 174	0
44	BQ	60/61 (98%)	0.08	1 (1%)	67 15	84, 107, 124, 134	0
44	CQ	60/61 (98%)	0.48	2 (3%)	44 6	120, 136, 153, 161	0
45	BR	88/89 (98%)	0.03	1 (1%)	77 22	73, 97, 120, 126	0
45	CR	88/89 (98%)	-0.05	0	100 100	75, 105, 129, 135	0
46	BS	84/88 (95%)	0.06	0	100 100	98, 113, 141, 173	0
46	CS	84/88 (95%)	-0.04	0	100 100	79, 96, 122, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BT	100/105 (95%)	0.07	0 100 100	85, 105, 123, 137	0
47	CT	100/105 (95%)	0.15	1 (1%) 79 23	81, 104, 126, 143	0
48	BU	72/88 (81%)	0.14	1 (1%) 72 17	75, 102, 140, 169	0
48	CU	72/88 (81%)	0.11	1 (1%) 72 17	86, 109, 150, 165	0
49	BV	83/93 (89%)	0.23	1 (1%) 75 20	103, 129, 145, 156	0
49	CV	78/93 (83%)	0.50	0 100 100	137, 160, 180, 183	0
50	BW	99/106 (93%)	0.12	0 100 100	101, 123, 152, 162	0
50	CW	99/106 (93%)	0.10	1 (1%) 79 23	79, 110, 149, 164	0
51	BX	25/27 (92%)	0.34	0 100 100	93, 114, 133, 155	0
51	CX	25/27 (92%)	0.45	2 (8%) 12 2	110, 134, 152, 170	0
52	BB	87/87 (100%)	1.12	16 (18%) 2 0	83, 164, 192, 209	0
52	CB	87/87 (100%)	1.11	24 (27%) 1 0	99, 167, 196, 209	0
53	BC	77/77 (100%)	0.08	0 100 100	66, 101, 139, 152	0
53	BD	77/77 (100%)	1.04	14 (18%) 2 0	75, 226, 239, 242	0
53	CC	77/77 (100%)	0.07	1 (1%) 74 19	77, 110, 148, 162	0
53	CD	77/77 (100%)	1.20	11 (14%) 3 1	78, 227, 239, 242	0
54	B1	10/10 (100%)	0.45	1 (10%) 8 2	73, 80, 132, 141	0
54	C1	10/10 (100%)	0.57	1 (10%) 8 2	81, 98, 145, 150	0
55	DF	208/208 (100%)	0.19	4 (1%) 64 13	54, 96, 161, 183	0
56	D0	117/117 (100%)	-0.13	0 100 100	58, 78, 100, 119	0
57	DV	179/179 (100%)	0.65	9 (5%) 28 4	112, 156, 209, 216	0
58	D3	77/77 (100%)	-0.07	0 100 100	66, 88, 113, 152	0
59	DW	69/69 (100%)	0.10	0 100 100	79, 105, 134, 172	0
60	D4	63/63 (100%)	0.86	4 (6%) 19 3	143, 184, 193, 201	0
All	All	21110/21408 (98%)	0.09	345 (1%) 68 15	38, 99, 184, 246	0

The worst 5 of 345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	654(J)	A	7.2
16	A1	118	GLY	7.1
52	CB	17	U	7.1
55	DF	1	MET	6.7
1	AA	654(K)	C	6.4

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
61	MG	BA	1795	1/1	0.43	-	66,66,66,66	0
61	MG	AA	3529	1/1	0.32	-	78,78,78,78	0
61	MG	BA	1703	1/1	0.50	-	118,118,118,118	0
61	MG	DA	3222	1/1	0.44	-	57,57,57,57	0
61	MG	BA	1630	1/1	0.25	-	105,105,105,105	0
61	MG	CA	1601	1/1	0.27	-	95,95,95,95	0
61	MG	CA	1634	1/1	0.76	-	90,90,90,90	0
61	MG	AA	3255	1/1	0.18	-	61,61,61,61	0
61	MG	DA	3056	1/1	0.62	-	100,100,100,100	0
61	MG	AA	3181	1/1	0.26	-	92,92,92,92	0
61	MG	BA	1706	1/1	0.66	-	55,55,55,55	0
61	MG	DA	3202	1/1	0.36	-	65,65,65,65	0
61	MG	AA	3208	1/1	0.17	-	66,66,66,66	0
61	MG	AA	3448	1/1	0.17	-	85,85,85,85	0
61	MG	DA	3196	1/1	0.47	-	82,82,82,82	0
61	MG	AA	3461	1/1	0.34	-	78,78,78,78	0
61	MG	AA	3543	1/1	0.52	-	61,61,61,61	0
61	MG	AA	3067	1/1	0.25	-	61,61,61,61	0
61	MG	DA	3519	1/1	0.36	-	114,114,114,114	0
61	MG	AA	3511	1/1	0.32	-	51,51,51,51	0
61	MG	BA	1812	1/1	0.32	-	76,76,76,76	0
61	MG	AA	3417	1/1	0.34	-	78,78,78,78	0
61	MG	DA	3314	1/1	0.35	-	78,78,78,78	0
61	MG	AA	3541	1/1	0.65	-	94,94,94,94	0
61	MG	CA	1780	1/1	0.22	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1738	1/1	0.39	-	73,73,73,73	0
61	MG	CA	1662	1/1	0.28	-	102,102,102,102	0
61	MG	DA	3238	1/1	0.25	-	80,80,80,80	0
61	MG	AA	3470	1/1	0.23	-	59,59,59,59	0
61	MG	AA	3508	1/1	0.41	-	96,96,96,96	0
61	MG	CA	1678	1/1	0.13	-	67,67,67,67	0
61	MG	DA	3320	1/1	0.24	-	73,73,73,73	0
61	MG	DA	3465	1/1	0.56	-	51,51,51,51	0
61	MG	DA	3254	1/1	0.30	-	84,84,84,84	0
61	MG	AA	3182	1/1	0.14	-	77,77,77,77	0
61	MG	DA	3248	1/1	0.23	-	98,98,98,98	0
61	MG	DA	3287	1/1	0.52	-	62,62,62,62	0
61	MG	CA	1661	1/1	0.24	-	105,105,105,105	0
61	MG	DA	3199	1/1	0.37	-	49,49,49,49	0
61	MG	AA	3184	1/1	0.34	-	90,90,90,90	0
61	MG	AA	3537	1/1	0.45	-	39,39,39,39	0
61	MG	AA	3419	1/1	0.19	-	102,102,102,102	0
61	MG	AA	3145	1/1	0.51	-	98,98,98,98	0
61	MG	CA	1685	1/1	0.37	-	85,85,85,85	0
61	MG	DA	3520	1/1	0.14	-	99,99,99,99	0
61	MG	DA	3291	1/1	0.43	-	70,70,70,70	0
61	MG	AA	3586	1/1	0.29	-	80,80,80,80	0
61	MG	DA	3229	1/1	0.45	-	109,109,109,109	0
61	MG	BA	1785	1/1	0.72	-	91,91,91,91	0
61	MG	AB	216	1/1	0.21	-	112,112,112,112	0
61	MG	CA	1670	1/1	0.47	-	54,54,54,54	0
61	MG	AA	3061	1/1	0.13	-	75,75,75,75	0
61	MG	AA	3428	1/1	0.36	-	106,106,106,106	0
61	MG	BA	1674	1/1	0.21	-	113,113,113,113	0
61	MG	AB	213	1/1	0.21	-	54,54,54,54	0
61	MG	DA	3284	1/1	0.78	-	81,81,81,81	0
61	MG	CA	1652	1/1	0.27	-	70,70,70,70	0
61	MG	BA	1741	1/1	0.24	-	124,124,124,124	0
61	MG	CG	301	1/1	0.43	-	86,86,86,86	0
61	MG	DA	3507	1/1	0.17	-	88,88,88,88	0
61	MG	DA	3399	1/1	0.34	-	97,97,97,97	0
61	MG	AA	3516	1/1	0.49	-	57,57,57,57	0
61	MG	CA	1688	1/1	0.42	-	75,75,75,75	0
61	MG	BA	1830	1/1	0.42	-	96,96,96,96	0
61	MG	AA	3050	1/1	0.21	-	69,69,69,69	0
61	MG	DA	3207	1/1	0.35	-	61,61,61,61	0
61	MG	AA	3445	1/1	0.42	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1639	1/1	0.24	-	94,94,94,94	0
61	MG	DA	3113	1/1	0.29	-	44,44,44,44	0
61	MG	AA	3532	1/1	0.31	-	89,89,89,89	0
61	MG	CA	1667	1/1	0.13	-	144,144,144,144	0
61	MG	AA	3299	1/1	0.20	-	94,94,94,94	0
61	MG	AA	3284	1/1	0.47	-	80,80,80,80	0
61	MG	BA	1743	1/1	0.34	-	58,58,58,58	0
61	MG	BA	1828	1/1	0.51	-	85,85,85,85	0
61	MG	DA	3114	1/1	0.44	-	70,70,70,70	0
61	MG	DA	3060	1/1	0.42	-	85,85,85,85	0
61	MG	DA	3481	1/1	0.43	-	45,45,45,45	0
61	MG	AA	3630	1/1	0.45	-	92,92,92,92	0
61	MG	DA	3025	1/1	0.18	-	111,111,111,111	0
61	MG	BQ	101	1/1	0.22	-	99,99,99,99	0
61	MG	CA	1733	1/1	0.33	-	66,66,66,66	0
61	MG	AA	3113	1/1	0.46	-	55,55,55,55	0
61	MG	CA	1710	1/1	0.11	-	105,105,105,105	0
61	MG	DA	3181	1/1	0.40	-	48,48,48,48	0
61	MG	DA	3409	1/1	0.15	-	70,70,70,70	0
61	MG	BA	1638	1/1	0.10	-	123,123,123,123	0
61	MG	AA	3008	1/1	0.40	-	42,42,42,42	0
61	MG	CA	1709	1/1	0.36	-	81,81,81,81	0
61	MG	DB	204	1/1	0.30	-	102,102,102,102	0
61	MG	DA	3132	1/1	0.32	-	56,56,56,56	0
61	MG	AA	3367	1/1	0.39	-	101,101,101,101	0
61	MG	BB	108	1/1	0.20	-	106,106,106,106	0
61	MG	BA	1736	1/1	0.93	-	89,89,89,89	0
61	MG	BA	1729	1/1	0.12	-	85,85,85,85	0
61	MG	BA	1807	1/1	0.48	-	70,70,70,70	0
61	MG	DA	3047	1/1	0.30	-	84,84,84,84	0
61	MG	DA	3230	1/1	0.23	-	68,68,68,68	0
61	MG	BA	1602	1/1	0.24	-	65,65,65,65	0
61	MG	BA	1607	1/1	0.14	-	87,87,87,87	0
61	MG	AA	3584	1/1	0.25	-	94,94,94,94	0
61	MG	DA	3294	1/1	0.25	-	93,93,93,93	0
61	MG	AA	3278	1/1	0.84	-	81,81,81,81	0
61	MG	DA	3374	1/1	0.60	-	72,72,72,72	0
61	MG	AA	3454	1/1	0.23	-	78,78,78,78	0
61	MG	BA	1760	1/1	0.53	-	67,67,67,67	0
61	MG	AA	3170	1/1	0.36	-	34,34,34,34	0
61	MG	CA	1712	1/1	0.23	-	86,86,86,86	0
61	MG	DA	3220	1/1	0.47	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3353	1/1	0.41	-	105,105,105,105	0
61	MG	AA	3402	1/1	0.34	-	94,94,94,94	0
61	MG	AA	3553	1/1	0.60	-	100,100,100,100	0
61	MG	BA	1650	1/1	0.46	-	78,78,78,78	0
61	MG	AD	301	1/1	0.77	-	100,100,100,100	0
61	MG	DA	3050	1/1	0.63	-	78,78,78,78	0
61	MG	AA	3179	1/1	0.52	-	70,70,70,70	0
61	MG	BA	1769	1/1	0.34	-	86,86,86,86	0
61	MG	CA	1766	1/1	0.21	-	75,75,75,75	0
61	MG	B1	102	1/1	0.39	-	69,69,69,69	0
61	MG	DA	3262	1/1	0.26	-	39,39,39,39	0
61	MG	AA	3307	1/1	0.88	-	75,75,75,75	0
61	MG	BA	1744	1/1	0.42	-	93,93,93,93	0
61	MG	DA	3347	1/1	0.46	-	66,66,66,66	0
61	MG	AA	3166	1/1	0.37	-	63,63,63,63	0
61	MG	AA	3542	1/1	0.41	-	40,40,40,40	0
61	MG	AA	3477	1/1	0.18	-	65,65,65,65	0
61	MG	BA	1660	1/1	0.67	-	64,64,64,64	0
61	MG	AA	3139	1/1	0.35	-	42,42,42,42	0
61	MG	AA	3288	1/1	0.71	-	73,73,73,73	0
61	MG	DA	3326	1/1	0.50	-	63,63,63,63	0
61	MG	DA	3011	1/1	0.46	-	68,68,68,68	0
61	MG	DA	3189	1/1	0.42	-	43,43,43,43	0
61	MG	DA	3214	1/1	0.47	-	70,70,70,70	0
61	MG	BA	1754	1/1	0.30	-	80,80,80,80	0
61	MG	CA	1617	1/1	0.30	-	91,91,91,91	0
61	MG	DA	3064	1/1	0.40	-	54,54,54,54	0
61	MG	AA	3409	1/1	0.74	-	98,98,98,98	0
61	MG	AA	3335	1/1	0.14	-	90,90,90,90	0
61	MG	AA	3130	1/1	0.18	-	59,59,59,59	0
61	MG	AA	3016	1/1	0.29	-	53,53,53,53	0
61	MG	DA	3308	1/1	0.12	-	95,95,95,95	0
61	MG	BA	1814	1/1	0.28	-	86,86,86,86	0
61	MG	AE	301	1/1	0.24	-	52,52,52,52	0
61	MG	AA	3281	1/1	0.23	-	67,67,67,67	0
61	MG	AA	3399	1/1	0.36	-	71,71,71,71	0
62	ZN	BQ	103	1/1	0.08	-	129,129,129,129	0
61	MG	AA	3295	1/1	0.28	-	70,70,70,70	0
61	MG	DA	3394	1/1	0.39	-	70,70,70,70	0
61	MG	BA	1819	1/1	0.13	-	107,107,107,107	0
61	MG	DA	3361	1/1	0.46	-	102,102,102,102	0
61	MG	D1	201	1/1	0.47	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3515	1/1	0.32	-	52,52,52,52	0
61	MG	DA	3125	1/1	0.20	-	86,86,86,86	0
61	MG	CA	1784	1/1	0.29	-	102,102,102,102	0
61	MG	DA	3476	1/1	0.54	-	76,76,76,76	0
61	MG	AA	3112	1/1	0.50	-	48,48,48,48	0
61	MG	AA	3105	1/1	0.27	-	64,64,64,64	0
61	MG	DA	3407	1/1	0.11	-	80,80,80,80	0
61	MG	AA	3277	1/1	0.74	-	98,98,98,98	0
61	MG	BA	1679	1/1	0.32	-	86,86,86,86	0
61	MG	BA	1764	1/1	0.36	-	93,93,93,93	0
61	MG	DA	3237	1/1	0.91	-	84,84,84,84	0
61	MG	BB	105	1/1	0.32	-	115,115,115,115	0
61	MG	AA	3374	1/1	0.48	-	96,96,96,96	0
61	MG	DA	3505	1/1	0.52	-	87,87,87,87	0
61	MG	DA	3223	1/1	0.16	-	83,83,83,83	0
61	MG	DA	3273	1/1	0.53	-	108,108,108,108	0
61	MG	AA	3264	1/1	0.53	-	74,74,74,74	0
61	MG	DB	206	1/1	0.32	-	122,122,122,122	0
61	MG	DA	3401	1/1	0.37	-	75,75,75,75	0
61	MG	AA	3491	1/1	0.12	-	93,93,93,93	0
61	MG	AA	3333	1/1	0.23	-	80,80,80,80	0
61	MG	BA	1753	1/1	0.13	-	91,91,91,91	0
61	MG	CA	1731	1/1	0.56	-	85,85,85,85	0
61	MG	CA	1800	1/1	0.14	-	102,102,102,102	0
61	MG	DA	3318	1/1	0.62	-	93,93,93,93	0
61	MG	BA	1737	1/1	0.13	-	102,102,102,102	0
61	MG	BA	1653	1/1	0.32	-	91,91,91,91	0
61	MG	BA	1672	1/1	0.36	-	104,104,104,104	0
61	MG	AA	3039	1/1	0.24	-	80,80,80,80	0
61	MG	DA	3431	1/1	0.15	-	93,93,93,93	0
61	MG	DA	3482	1/1	0.40	-	56,56,56,56	0
61	MG	DA	3345	1/1	0.25	-	75,75,75,75	0
61	MG	DA	3439	1/1	0.49	-	92,92,92,92	0
61	MG	BA	1704	1/1	0.35	-	87,87,87,87	0
61	MG	AA	3120	1/1	0.34	-	92,92,92,92	0
61	MG	AA	3334	1/1	0.12	-	73,73,73,73	0
61	MG	AA	3251	1/1	0.47	-	97,97,97,97	0
61	MG	AA	3097	1/1	0.27	-	65,65,65,65	0
61	MG	AA	3575	1/1	0.33	-	40,40,40,40	0
61	MG	AA	3029	1/1	0.29	-	50,50,50,50	0
61	MG	AA	3020	1/1	0.41	-	31,31,31,31	0
61	MG	BA	1820	1/1	0.42	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3383	1/1	0.08	-	70,70,70,70	0
61	MG	DA	3444	1/1	0.10	-	82,82,82,82	0
61	MG	DA	3246	1/1	0.21	-	66,66,66,66	0
61	MG	DA	3042	1/1	0.36	-	84,84,84,84	0
61	MG	AA	3356	1/1	0.30	-	72,72,72,72	0
61	MG	AA	3236	1/1	0.29	-	93,93,93,93	0
61	MG	CA	1636	1/1	0.34	-	80,80,80,80	0
61	MG	BA	1676	1/1	0.43	-	81,81,81,81	0
61	MG	CA	1799	1/1	0.50	-	95,95,95,95	0
61	MG	AB	209	1/1	0.13	-	103,103,103,103	0
61	MG	AA	3371	1/1	0.51	-	69,69,69,69	0
61	MG	AA	3556	1/1	0.58	-	85,85,85,85	0
61	MG	DA	3074	1/1	0.36	-	89,89,89,89	0
61	MG	DA	3381	1/1	0.25	-	89,89,89,89	0
61	MG	DA	3357	1/1	0.29	-	89,89,89,89	0
61	MG	CA	1742	1/1	0.34	-	93,93,93,93	0
61	MG	AA	3015	1/1	0.43	-	30,30,30,30	0
61	MG	DA	3316	1/1	0.18	-	87,87,87,87	0
61	MG	A6	101	1/1	0.83	-	121,121,121,121	0
61	MG	AA	3293	1/1	0.58	-	87,87,87,87	0
61	MG	BA	1671	1/1	0.28	-	74,74,74,74	0
61	MG	DA	3268	1/1	0.39	-	82,82,82,82	0
61	MG	DA	3363	1/1	0.39	-	73,73,73,73	0
61	MG	DA	3348	1/1	0.50	-	77,77,77,77	0
61	MG	AA	3206	1/1	0.33	-	53,53,53,53	0
61	MG	AA	3025	1/1	0.57	-	46,46,46,46	0
61	MG	DA	3004	1/1	0.29	-	91,91,91,91	0
61	MG	AA	3574	1/1	0.38	-	29,29,29,29	0
61	MG	AA	3300	1/1	0.24	-	77,77,77,77	0
61	MG	DA	3052	1/1	0.29	-	84,84,84,84	0
61	MG	AA	3392	1/1	0.62	-	94,94,94,94	0
61	MG	AA	3193	1/1	0.15	-	94,94,94,94	0
61	MG	DA	3383	1/1	0.54	-	79,79,79,79	0
61	MG	BA	1818	1/1	0.19	-	82,82,82,82	0
61	MG	DA	3014	1/1	0.30	-	62,62,62,62	0
61	MG	AA	3297	1/1	0.47	-	63,63,63,63	0
61	MG	CA	1715	1/1	0.20	-	99,99,99,99	0
61	MG	DA	3489	1/1	0.51	-	57,57,57,57	0
61	MG	AA	3600	1/1	0.14	-	79,79,79,79	0
61	MG	BA	1643	1/1	0.35	-	80,80,80,80	0
61	MG	BA	1686	1/1	0.38	-	94,94,94,94	0
61	MG	AA	3545	1/1	0.38	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1729	1/1	0.84	-	81,81,81,81	0
61	MG	DA	3019	1/1	0.66	-	66,66,66,66	0
61	MG	CA	1684	1/1	0.57	-	77,77,77,77	0
61	MG	AA	3433	1/1	0.42	-	77,77,77,77	0
61	MG	CA	1657	1/1	0.12	-	94,94,94,94	0
61	MG	AA	3118	1/1	0.26	-	74,74,74,74	0
61	MG	DA	3402	1/1	0.71	-	73,73,73,73	0
61	MG	AA	3256	1/1	0.32	-	65,65,65,65	0
61	MG	AA	3366	1/1	0.42	-	78,78,78,78	0
61	MG	DA	3184	1/1	0.27	-	71,71,71,71	0
61	MG	CA	1619	1/1	0.57	-	62,62,62,62	0
61	MG	BA	1826	1/1	0.40	-	73,73,73,73	0
61	MG	BA	1702	1/1	0.23	-	98,98,98,98	0
61	MG	AA	3610	1/1	0.31	-	34,34,34,34	0
61	MG	DA	3283	1/1	0.35	-	78,78,78,78	0
61	MG	AA	3321	1/1	0.70	-	68,68,68,68	0
61	MG	AA	3342	1/1	0.25	-	65,65,65,65	0
61	MG	BA	1742	1/1	0.09	-	133,133,133,133	0
61	MG	DA	3083	1/1	0.31	-	108,108,108,108	0
61	MG	AA	3345	1/1	0.32	-	78,78,78,78	0
61	MG	BA	1790	1/1	0.39	-	83,83,83,83	0
61	MG	BA	1606	1/1	0.21	-	88,88,88,88	0
61	MG	AA	3391	1/1	0.19	-	90,90,90,90	0
61	MG	AA	3404	1/1	0.25	-	89,89,89,89	0
61	MG	DA	3329	1/1	0.84	-	80,80,80,80	0
61	MG	CA	1604	1/1	0.22	-	78,78,78,78	0
61	MG	AA	3084	1/1	0.44	-	40,40,40,40	0
61	MG	BA	1689	1/1	0.11	-	110,110,110,110	0
61	MG	CA	1602	1/1	0.21	-	81,81,81,81	0
61	MG	CA	1713	1/1	0.30	-	109,109,109,109	0
61	MG	CA	1707	1/1	0.48	-	88,88,88,88	0
61	MG	BA	1797	1/1	0.26	-	89,89,89,89	0
61	MG	AB	204	1/1	0.19	-	94,94,94,94	0
61	MG	AA	3121	1/1	0.55	-	93,93,93,93	0
61	MG	DA	3305	1/1	0.30	-	83,83,83,83	0
61	MG	AA	3046	1/1	0.19	-	54,54,54,54	0
61	MG	AA	3126	1/1	0.19	-	63,63,63,63	0
61	MG	BC	108	1/1	0.58	-	101,101,101,101	0
61	MG	AA	3465	1/1	0.32	-	88,88,88,88	0
61	MG	AA	3598	1/1	0.30	-	84,84,84,84	0
61	MG	CA	1637	1/1	0.30	-	97,97,97,97	0
61	MG	DA	3048	1/1	0.59	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3412	1/1	0.47	-	97,97,97,97	0
61	MG	DA	3217	1/1	0.53	-	51,51,51,51	0
61	MG	AA	3282	1/1	0.30	-	87,87,87,87	0
61	MG	AA	3551	1/1	0.51	-	73,73,73,73	0
61	MG	AA	3096	1/1	0.16	-	75,75,75,75	0
61	MG	AA	3257	1/1	0.22	-	84,84,84,84	0
61	MG	DA	3169	1/1	0.68	-	68,68,68,68	0
61	MG	AA	3488	1/1	0.43	-	94,94,94,94	0
61	MG	DA	3366	1/1	0.34	-	97,97,97,97	0
61	MG	DA	3312	1/1	0.18	-	101,101,101,101	0
61	MG	AA	3525	1/1	0.29	-	67,67,67,67	0
61	MG	AB	214	1/1	0.10	-	88,88,88,88	0
61	MG	BA	1755	1/1	0.57	-	106,106,106,106	0
61	MG	DA	3382	1/1	0.23	-	84,84,84,84	0
61	MG	AA	3361	1/1	0.34	-	88,88,88,88	0
61	MG	BA	1629	1/1	0.19	-	100,100,100,100	0
61	MG	DA	3093	1/1	0.34	-	51,51,51,51	0
61	MG	AA	3060	1/1	0.19	-	57,57,57,57	0
61	MG	DE	302	1/1	0.19	-	75,75,75,75	0
61	MG	AA	3301	1/1	0.81	-	113,113,113,113	0
61	MG	CA	1706	1/1	0.33	-	77,77,77,77	0
61	MG	AA	3460	1/1	0.23	-	89,89,89,89	0
61	MG	DA	3203	1/1	0.67	-	52,52,52,52	0
61	MG	CA	1673	1/1	0.66	-	65,65,65,65	0
61	MG	DA	3226	1/1	0.37	-	57,57,57,57	0
61	MG	AE	304	1/1	0.28	-	85,85,85,85	0
61	MG	AA	3358	1/1	0.45	-	79,79,79,79	0
61	MG	CA	1751	1/1	0.32	-	102,102,102,102	0
61	MG	AA	3310	1/1	0.39	-	74,74,74,74	0
61	MG	AA	3114	1/1	0.44	-	41,41,41,41	0
61	MG	AA	3289	1/1	0.41	-	62,62,62,62	0
61	MG	AA	3316	1/1	0.63	-	87,87,87,87	0
61	MG	BA	1813	1/1	0.39	-	80,80,80,80	0
61	MG	AA	3583	1/1	0.55	-	44,44,44,44	0
61	MG	AA	3319	1/1	0.22	-	61,61,61,61	0
61	MG	CA	1624	1/1	0.26	-	83,83,83,83	0
61	MG	BA	1711	1/1	0.40	-	86,86,86,86	0
61	MG	AA	3527	1/1	0.20	-	77,77,77,77	0
61	MG	DA	3508	1/1	0.60	-	77,77,77,77	0
61	MG	BA	1761	1/1	0.15	-	85,85,85,85	0
61	MG	BA	1654	1/1	0.24	-	74,74,74,74	0
61	MG	BA	1617	1/1	0.49	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
62	ZN	CG	304	1/1	0.26	-	112,112,112,112	0
61	MG	DA	3127	1/1	0.65	-	44,44,44,44	0
61	MG	DA	3256	1/1	0.43	-	82,82,82,82	0
61	MG	AA	3474	1/1	0.24	-	93,93,93,93	0
61	MG	CA	1730	1/1	0.09	-	118,118,118,118	0
61	MG	AA	3429	1/1	0.28	-	85,85,85,85	0
61	MG	A1	201	1/1	0.34	-	49,49,49,49	0
61	MG	BA	1695	1/1	0.17	-	101,101,101,101	0
61	MG	AA	3191	1/1	0.31	-	61,61,61,61	0
61	MG	AA	3194	1/1	0.15	-	54,54,54,54	0
61	MG	BA	1669	1/1	0.37	-	76,76,76,76	0
61	MG	AA	3497	1/1	0.24	-	105,105,105,105	0
61	MG	BA	1662	1/1	0.62	-	80,80,80,80	0
61	MG	DA	3003	1/1	0.43	-	70,70,70,70	0
61	MG	AA	3028	1/1	0.40	-	51,51,51,51	0
61	MG	AA	3080	1/1	0.47	-	52,52,52,52	0
61	MG	AA	3405	1/1	0.96	-	86,86,86,86	0
61	MG	CA	1769	1/1	0.20	-	109,109,109,109	0
61	MG	AB	212	1/1	0.29	-	76,76,76,76	0
61	MG	BA	1782	1/1	0.28	-	88,88,88,88	0
61	MG	DA	3524	1/1	1.13	-	99,99,99,99	0
61	MG	DA	3448	1/1	0.36	-	75,75,75,75	0
61	MG	DA	3102	1/1	0.24	-	72,72,72,72	0
61	MG	BA	1735	1/1	0.25	-	80,80,80,80	0
61	MG	DA	3389	1/1	0.61	-	85,85,85,85	0
61	MG	DA	3304	1/1	0.39	-	106,106,106,106	0
61	MG	AA	3560	1/1	0.56	-	84,84,84,84	0
61	MG	AA	3077	1/1	0.46	-	94,94,94,94	0
61	MG	BA	1823	1/1	0.36	-	93,93,93,93	0
61	MG	CA	1804	1/1	0.19	-	81,81,81,81	0
61	MG	BA	1601	1/1	0.36	-	65,65,65,65	0
61	MG	DA	3406	1/1	0.74	-	72,72,72,72	0
61	MG	BA	1693	1/1	0.18	-	80,80,80,80	0
61	MG	DA	3512	1/1	0.31	-	70,70,70,70	0
61	MG	DA	3212	1/1	0.41	-	70,70,70,70	0
61	MG	CA	1651	1/1	0.14	-	79,79,79,79	0
61	MG	BA	1810	1/1	0.19	-	110,110,110,110	0
61	MG	DA	3377	1/1	0.88	-	92,92,92,92	0
61	MG	BA	1811	1/1	0.17	-	86,86,86,86	0
61	MG	CA	1740	1/1	0.43	-	75,75,75,75	0
61	MG	AA	3603	1/1	0.36	-	65,65,65,65	0
61	MG	AA	3167	1/1	0.32	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3462	1/1	0.56	-	67,67,67,67	0
61	MG	BA	1683	1/1	0.14	-	112,112,112,112	0
61	MG	DA	3288	1/1	0.72	-	82,82,82,82	0
61	MG	DA	3397	1/1	0.45	-	150,150,150,150	0
61	MG	DA	3516	1/1	0.28	-	60,60,60,60	0
61	MG	CA	1671	1/1	0.56	-	51,51,51,51	0
61	MG	AF	301	1/1	0.11	-	75,75,75,75	0
61	MG	DA	3257	1/1	0.18	-	75,75,75,75	0
61	MG	AA	3416	1/1	0.27	-	70,70,70,70	0
61	MG	CA	1704	1/1	0.57	-	129,129,129,129	0
61	MG	DA	3274	1/1	0.49	-	80,80,80,80	0
61	MG	AA	3141	1/1	0.49	-	37,37,37,37	0
61	MG	DA	3224	1/1	0.36	-	59,59,59,59	0
61	MG	CA	1774	1/1	0.29	-	72,72,72,72	0
61	MG	CA	1607	1/1	0.28	-	77,77,77,77	0
61	MG	AA	3619	1/1	0.28	-	94,94,94,94	0
61	MG	AA	3156	1/1	0.34	-	87,87,87,87	0
61	MG	CA	1692	1/1	0.30	-	75,75,75,75	0
61	MG	CA	1677	1/1	0.28	-	68,68,68,68	0
61	MG	DA	3358	1/1	0.22	-	90,90,90,90	0
61	MG	BA	1832	1/1	0.28	-	100,100,100,100	0
61	MG	BA	1673	1/1	0.28	-	80,80,80,80	0
61	MG	AA	3506	1/1	0.51	-	73,73,73,73	0
61	MG	BA	1839	1/1	0.27	-	61,61,61,61	0
61	MG	AA	3614	1/1	0.28	-	91,91,91,91	0
61	MG	DA	3213	1/1	0.17	-	94,94,94,94	0
61	MG	BA	1747	1/1	0.19	-	97,97,97,97	0
61	MG	CA	1793	1/1	0.46	-	78,78,78,78	0
61	MG	BA	1778	1/1	0.23	-	93,93,93,93	0
61	MG	AA	3041	1/1	0.20	-	62,62,62,62	0
61	MG	DA	3388	1/1	0.39	-	85,85,85,85	0
61	MG	DA	3130	1/1	0.50	-	64,64,64,64	0
61	MG	CA	1629	1/1	0.29	-	82,82,82,82	0
61	MG	DA	3195	1/1	0.21	-	73,73,73,73	0
61	MG	BA	1829	1/1	0.31	-	102,102,102,102	0
61	MG	CA	1803	1/1	0.26	-	87,87,87,87	0
61	MG	CA	1646	1/1	0.44	-	56,56,56,56	0
61	MG	AB	211	1/1	0.07	-	105,105,105,105	0
61	MG	AA	3027	1/1	0.47	-	49,49,49,49	0
61	MG	DA	3457	1/1	0.42	-	62,62,62,62	0
61	MG	DA	3309	1/1	0.34	-	69,69,69,69	0
61	MG	CA	1741	1/1	0.27	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3185	1/1	0.37	-	64,64,64,64	0
61	MG	BQ	102	1/1	0.51	-	89,89,89,89	0
61	MG	CA	1781	1/1	0.33	-	92,92,92,92	0
61	MG	BA	1717	1/1	0.77	-	79,79,79,79	0
61	MG	AA	3153	1/1	0.39	-	33,33,33,33	0
61	MG	BA	1696	1/1	0.38	-	90,90,90,90	0
61	MG	DA	3522	1/1	0.47	-	85,85,85,85	0
61	MG	DA	3473	1/1	0.22	-	103,103,103,103	0
61	MG	CA	1632	1/1	0.17	-	77,77,77,77	0
61	MG	DA	3073	1/1	0.14	-	69,69,69,69	0
61	MG	AA	3040	1/1	0.35	-	67,67,67,67	0
61	MG	DA	3334	1/1	0.57	-	95,95,95,95	0
61	MG	CA	1690	1/1	0.37	-	74,74,74,74	0
61	MG	DA	3404	1/1	1.10	-	91,91,91,91	0
61	MG	BA	1603	1/1	0.34	-	63,63,63,63	0
61	MG	CA	1737	1/1	0.23	-	109,109,109,109	0
61	MG	CA	1689	1/1	0.31	-	87,87,87,87	0
61	MG	AA	3161	1/1	0.55	-	41,41,41,41	0
61	MG	DB	211	1/1	0.20	-	104,104,104,104	0
61	MG	CA	1801	1/1	0.55	-	71,71,71,71	0
61	MG	DA	3215	1/1	0.51	-	50,50,50,50	0
61	MG	AA	3001	1/1	0.58	-	49,49,49,49	0
61	MG	AB	205	1/1	0.16	-	75,75,75,75	0
61	MG	DA	3190	1/1	0.44	-	46,46,46,46	0
61	MG	AA	3436	1/1	0.33	-	82,82,82,82	0
61	MG	DA	3298	1/1	0.38	-	95,95,95,95	0
61	MG	AA	3026	1/1	0.50	-	35,35,35,35	0
61	MG	CA	1791	1/1	0.59	-	70,70,70,70	0
61	MG	AA	3086	1/1	0.27	-	70,70,70,70	0
61	MG	AA	3062	1/1	0.36	-	73,73,73,73	0
61	MG	DA	3153	1/1	0.44	-	54,54,54,54	0
61	MG	AA	3056	1/1	0.21	-	64,64,64,64	0
61	MG	DA	3120	1/1	0.29	-	78,78,78,78	0
61	MG	AA	3136	1/1	0.20	-	40,40,40,40	0
61	MG	DA	3469	1/1	0.30	-	64,64,64,64	0
61	MG	DA	3066	1/1	0.29	-	83,83,83,83	0
61	MG	AA	3350	1/1	0.58	-	59,59,59,59	0
61	MG	AA	3165	1/1	0.26	-	71,71,71,71	0
61	MG	DA	3390	1/1	0.16	-	81,81,81,81	0
61	MG	DA	3478	1/1	0.54	-	99,99,99,99	0
61	MG	AA	3162	1/1	0.52	-	45,45,45,45	0
61	MG	AA	3115	1/1	0.37	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3625	1/1	0.57	-	70,70,70,70	0
61	MG	AA	3243	1/1	0.33	-	52,52,52,52	0
61	MG	AA	3518	1/1	0.24	-	71,71,71,71	0
61	MG	CA	1611	1/1	0.54	-	76,76,76,76	0
61	MG	DA	3436	1/1	0.22	-	69,69,69,69	0
61	MG	DA	3075	1/1	0.42	-	80,80,80,80	0
61	MG	DA	3058	1/1	0.36	-	75,75,75,75	0
61	MG	DA	3342	1/1	0.34	-	96,96,96,96	0
61	MG	CA	1641	1/1	0.20	-	101,101,101,101	0
61	MG	AA	3222	1/1	0.35	-	59,59,59,59	0
61	MG	DA	3192	1/1	0.38	-	51,51,51,51	0
61	MG	DA	3007	1/1	0.27	-	75,75,75,75	0
61	MG	AA	3292	1/1	0.45	-	80,80,80,80	0
61	MG	DA	3452	1/1	0.26	-	91,91,91,91	0
61	MG	DA	3143	1/1	0.48	-	69,69,69,69	0
61	MG	D5	101	1/1	0.42	-	50,50,50,50	0
61	MG	DA	3245	1/1	0.30	-	80,80,80,80	0
61	MG	AA	3265	1/1	0.52	-	42,42,42,42	0
61	MG	BA	1699	1/1	0.26	-	58,58,58,58	0
61	MG	AA	3309	1/1	0.35	-	64,64,64,64	0
61	MG	AA	3479	1/1	0.17	-	97,97,97,97	0
61	MG	DA	3337	1/1	0.79	-	75,75,75,75	0
61	MG	BA	1751	1/1	0.16	-	122,122,122,122	0
61	MG	CA	1736	1/1	1.06	-	90,90,90,90	0
61	MG	AA	3623	1/1	0.21	-	107,107,107,107	0
61	MG	AA	3539	1/1	0.53	-	54,54,54,54	0
61	MG	AA	3006	1/1	0.53	-	60,60,60,60	0
61	MG	CA	1747	1/1	0.32	-	114,114,114,114	0
61	MG	CB	101	1/1	0.34	-	102,102,102,102	0
61	MG	AA	3324	1/1	0.75	-	60,60,60,60	0
61	MG	AA	3393	1/1	0.23	-	91,91,91,91	0
61	MG	CA	1768	1/1	0.22	-	115,115,115,115	0
61	MG	AA	3432	1/1	0.59	-	41,41,41,41	0
61	MG	BA	1802	1/1	0.40	-	69,69,69,69	0
61	MG	AA	3174	1/1	0.47	-	43,43,43,43	0
61	MG	CA	1649	1/1	0.12	-	70,70,70,70	0
61	MG	AA	3125	1/1	0.45	-	49,49,49,49	0
61	MG	AA	3226	1/1	0.81	-	85,85,85,85	0
61	MG	AA	3494	1/1	0.46	-	88,88,88,88	0
61	MG	DA	3355	1/1	0.32	-	93,93,93,93	0
61	MG	BA	1645	1/1	0.43	-	52,52,52,52	0
61	MG	DA	3458	1/1	0.57	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1620	1/1	0.22	-	58,58,58,58	0
61	MG	AA	3042	1/1	0.13	-	67,67,67,67	0
61	MG	DA	3470	1/1	0.39	-	75,75,75,75	0
61	MG	CA	1794	1/1	0.37	-	72,72,72,72	0
61	MG	CA	1628	1/1	0.13	-	86,86,86,86	0
61	MG	AA	3010	1/1	0.31	-	52,52,52,52	0
61	MG	DA	3428	1/1	0.35	-	79,79,79,79	0
61	MG	AA	3422	1/1	0.78	-	73,73,73,73	0
61	MG	BA	1625	1/1	0.39	-	61,61,61,61	0
61	MG	AA	3260	1/1	0.22	-	70,70,70,70	0
61	MG	AA	3303	1/1	0.41	-	91,91,91,91	0
61	MG	AA	3244	1/1	0.25	-	69,69,69,69	0
61	MG	DA	3154	1/1	0.55	-	59,59,59,59	0
61	MG	DB	205	1/1	0.10	-	90,90,90,90	0
61	MG	CA	1748	1/1	0.47	-	91,91,91,91	0
61	MG	AA	3571	1/1	0.40	-	48,48,48,48	0
61	MG	BA	1779	1/1	0.39	-	105,105,105,105	0
61	MG	CC	105	1/1	0.36	-	74,74,74,74	0
61	MG	AA	3362	1/1	0.54	-	86,86,86,86	0
61	MG	AA	3509	1/1	0.96	-	80,80,80,80	0
61	MG	CA	1658	1/1	0.21	-	78,78,78,78	0
61	MG	DA	3067	1/1	0.24	-	75,75,75,75	0
61	MG	BA	1726	1/1	0.69	-	98,98,98,98	0
61	MG	BA	1715	1/1	0.27	-	69,69,69,69	0
61	MG	DA	3211	1/1	0.44	-	49,49,49,49	0
61	MG	AE	303	1/1	0.64	-	91,91,91,91	0
61	MG	AA	3076	1/1	0.08	-	109,109,109,109	0
61	MG	DA	3443	1/1	0.70	-	94,94,94,94	0
61	MG	DA	3033	1/1	0.07	-	94,94,94,94	0
61	MG	AA	3476	1/1	0.63	-	94,94,94,94	0
61	MG	AA	3435	1/1	0.26	-	137,137,137,137	0
61	MG	AA	3489	1/1	0.80	-	93,93,93,93	0
61	MG	BA	1801	1/1	0.07	-	93,93,93,93	0
61	MG	AA	3178	1/1	0.38	-	49,49,49,49	0
61	MG	AA	3225	1/1	0.24	-	69,69,69,69	0
61	MG	AA	3385	1/1	0.17	-	75,75,75,75	0
61	MG	BA	1622	1/1	0.17	-	84,84,84,84	0
61	MG	DA	3255	1/1	0.21	-	83,83,83,83	0
61	MG	BA	1763	1/1	0.23	-	93,93,93,93	0
61	MG	AA	3534	1/1	0.40	-	100,100,100,100	0
61	MG	DA	3081	1/1	0.17	-	73,73,73,73	0
61	MG	AA	3621	1/1	0.18	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3415	1/1	0.18	-	84,84,84,84	0
61	MG	CA	1615	1/1	0.30	-	92,92,92,92	0
61	MG	BA	1636	1/1	0.18	-	92,92,92,92	0
61	MG	AA	3159	1/1	0.28	-	30,30,30,30	0
61	MG	AA	3604	1/1	0.38	-	84,84,84,84	0
61	MG	AA	3369	1/1	0.50	-	85,85,85,85	0
61	MG	AA	3569	1/1	0.51	-	40,40,40,40	0
61	MG	BA	1838	1/1	0.44	-	101,101,101,101	0
61	MG	BA	1675	1/1	0.47	-	89,89,89,89	0
61	MG	AA	3498	1/1	0.42	-	86,86,86,86	0
61	MG	CA	1630	1/1	0.27	-	76,76,76,76	0
61	MG	DA	3367	1/1	0.35	-	85,85,85,85	0
61	MG	AA	3368	1/1	0.40	-	83,83,83,83	0
61	MG	DA	3352	1/1	0.27	-	77,77,77,77	0
61	MG	BB	104	1/1	0.28	-	103,103,103,103	0
61	MG	BA	1690	1/1	0.13	-	109,109,109,109	0
61	MG	AA	3325	1/1	0.13	-	78,78,78,78	0
61	MG	DA	3408	1/1	0.24	-	61,61,61,61	0
61	MG	DA	3387	1/1	0.52	-	45,45,45,45	0
61	MG	DA	3141	1/1	0.53	-	44,44,44,44	0
61	MG	AA	3011	1/1	0.44	-	38,38,38,38	0
61	MG	CA	1608	1/1	0.30	-	81,81,81,81	0
61	MG	AA	3068	1/1	0.36	-	49,49,49,49	0
61	MG	A5	102	1/1	0.38	-	75,75,75,75	0
61	MG	DA	3281	1/1	0.30	-	75,75,75,75	0
61	MG	AA	3245	1/1	0.32	-	81,81,81,81	0
61	MG	AB	201	1/1	0.09	-	91,91,91,91	0
61	MG	AA	3215	1/1	0.33	-	55,55,55,55	0
61	MG	DA	3280	1/1	0.18	-	80,80,80,80	0
61	MG	DA	3008	1/1	0.66	-	76,76,76,76	0
61	MG	DA	3071	1/1	0.17	-	74,74,74,74	0
61	MG	CA	1779	1/1	0.17	-	82,82,82,82	0
61	MG	BG	301	1/1	0.18	-	110,110,110,110	0
61	MG	AA	3228	1/1	0.30	-	89,89,89,89	0
61	MG	DA	3461	1/1	0.37	-	50,50,50,50	0
61	MG	DA	3049	1/1	0.85	-	72,72,72,72	0
61	MG	DA	3193	1/1	0.29	-	49,49,49,49	0
61	MG	AA	3312	1/1	0.28	-	88,88,88,88	0
61	MG	BA	1612	1/1	0.23	-	90,90,90,90	0
61	MG	AA	3588	1/1	0.51	-	63,63,63,63	0
61	MG	DB	209	1/1	0.60	-	103,103,103,103	0
61	MG	AA	3049	1/1	0.68	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1659	1/1	0.76	-	70,70,70,70	0
61	MG	CA	1771	1/1	0.24	-	64,64,64,64	0
61	MG	DA	3518	1/1	0.47	-	63,63,63,63	0
61	MG	AA	3054	1/1	0.32	-	52,52,52,52	0
61	MG	DA	3386	1/1	0.20	-	88,88,88,88	0
61	MG	AA	3250	1/1	0.22	-	73,73,73,73	0
61	MG	AA	3408	1/1	0.70	-	70,70,70,70	0
61	MG	BA	1604	1/1	0.29	-	77,77,77,77	0
61	MG	A7	101	1/1	0.43	-	69,69,69,69	0
61	MG	CG	302	1/1	0.13	-	83,83,83,83	0
61	MG	BA	1799	1/1	0.34	-	85,85,85,85	0
61	MG	BA	1722	1/1	0.22	-	90,90,90,90	0
61	MG	CA	1681	1/1	0.30	-	71,71,71,71	0
61	MG	AA	3616	1/1	0.30	-	69,69,69,69	0
61	MG	BA	1641	1/1	0.56	-	62,62,62,62	0
61	MG	DA	3249	1/1	0.16	-	87,87,87,87	0
61	MG	BA	1789	1/1	0.20	-	69,69,69,69	0
61	MG	AA	3002	1/1	0.42	-	40,40,40,40	0
61	MG	AB	206	1/1	0.24	-	97,97,97,97	0
61	MG	AA	3318	1/1	0.46	-	120,120,120,120	0
61	MG	BA	1749	1/1	0.34	-	95,95,95,95	0
61	MG	BA	1667	1/1	0.30	-	78,78,78,78	0
61	MG	AA	3576	1/1	0.31	-	36,36,36,36	0
61	MG	BA	1644	1/1	0.14	-	78,78,78,78	0
61	MG	AA	3279	1/1	0.60	-	81,81,81,81	0
61	MG	AA	3438	1/1	0.21	-	77,77,77,77	0
61	MG	DA	3188	1/1	0.54	-	48,48,48,48	0
61	MG	DA	3128	1/1	0.26	-	66,66,66,66	0
61	MG	DA	3373	1/1	0.55	-	90,90,90,90	0
61	MG	DA	3279	1/1	0.28	-	66,66,66,66	0
61	MG	CA	1753	1/1	0.52	-	129,129,129,129	0
61	MG	CS	101	1/1	0.24	-	84,84,84,84	0
61	MG	DA	3385	1/1	0.45	-	90,90,90,90	0
61	MG	AA	3414	1/1	0.35	-	68,68,68,68	0
61	MG	DA	3258	1/1	0.46	-	56,56,56,56	0
61	MG	AA	3268	1/1	0.66	-	47,47,47,47	0
61	MG	CA	1705	1/1	0.29	-	86,86,86,86	0
61	MG	CA	1650	1/1	0.20	-	90,90,90,90	0
61	MG	BA	1774	1/1	0.26	-	98,98,98,98	0
61	MG	DA	3070	1/1	0.12	-	73,73,73,73	0
61	MG	AA	3523	1/1	0.35	-	87,87,87,87	0
61	MG	DA	3167	1/1	0.23	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3339	1/1	0.48	-	77,77,77,77	0
61	MG	AA	3622	1/1	0.16	-	71,71,71,71	0
61	MG	BA	1670	1/1	0.34	-	62,62,62,62	0
61	MG	DA	3332	1/1	0.50	-	90,90,90,90	0
61	MG	AA	3499	1/1	0.52	-	79,79,79,79	0
61	MG	CA	1735	1/1	0.14	-	86,86,86,86	0
61	MG	A5	101	1/1	0.48	-	49,49,49,49	0
61	MG	CA	1665	1/1	0.17	-	101,101,101,101	0
61	MG	AA	3258	1/1	0.12	-	80,80,80,80	0
61	MG	AA	3098	1/1	0.46	-	71,71,71,71	0
61	MG	DA	3006	1/1	0.44	-	78,78,78,78	0
61	MG	DA	3016	1/1	0.72	-	105,105,105,105	0
61	MG	BA	1740	1/1	0.19	-	72,72,72,72	0
61	MG	CA	1700	1/1	0.35	-	60,60,60,60	0
61	MG	AA	3274	1/1	0.22	-	77,77,77,77	0
61	MG	DA	3405	1/1	0.09	-	97,97,97,97	0
61	MG	AA	3513	1/1	0.37	-	73,73,73,73	0
61	MG	AA	3504	1/1	0.30	-	103,103,103,103	0
61	MG	BC	105	1/1	0.36	-	95,95,95,95	0
61	MG	DA	3013	1/1	0.54	-	55,55,55,55	0
61	MG	DA	3252	1/1	0.34	-	45,45,45,45	0
61	MG	BA	1816	1/1	0.36	-	87,87,87,87	0
61	MG	DA	3110	1/1	0.18	-	84,84,84,84	0
61	MG	DA	3466	1/1	0.55	-	78,78,78,78	0
61	MG	DA	3236	1/1	0.53	-	57,57,57,57	0
61	MG	BA	1792	1/1	0.16	-	94,94,94,94	0
61	MG	AA	3519	1/1	0.15	-	91,91,91,91	0
61	MG	BB	106	1/1	0.48	-	120,120,120,120	0
61	MG	AA	3411	1/1	0.18	-	84,84,84,84	0
61	MG	AA	3085	1/1	0.35	-	62,62,62,62	0
61	MG	AA	3398	1/1	0.21	-	91,91,91,91	0
61	MG	AA	3357	1/1	0.52	-	61,61,61,61	0
61	MG	AA	3580	1/1	0.71	-	44,44,44,44	0
61	MG	AA	3143	1/1	0.42	-	40,40,40,40	0
61	MG	DA	3523	1/1	0.61	-	86,86,86,86	0
61	MG	DB	208	1/1	0.55	-	114,114,114,114	0
61	MG	BA	1697	1/1	0.33	-	84,84,84,84	0
61	MG	CA	1761	1/1	0.35	-	96,96,96,96	0
61	MG	AA	3535	1/1	0.29	-	82,82,82,82	0
61	MG	DA	3430	1/1	0.31	-	102,102,102,102	0
61	MG	CA	1656	1/1	0.22	-	87,87,87,87	0
61	MG	DA	3349	1/1	0.22	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3160	1/1	0.51	-	31,31,31,31	0
61	MG	AA	3473	1/1	0.35	-	70,70,70,70	0
61	MG	DA	3333	1/1	0.37	-	85,85,85,85	0
61	MG	DA	3106	1/1	0.33	-	46,46,46,46	0
61	MG	AA	3133	1/1	0.51	-	38,38,38,38	0
61	MG	DA	3146	1/1	0.48	-	38,38,38,38	0
61	MG	DA	3208	1/1	0.45	-	40,40,40,40	0
61	MG	DA	3210	1/1	0.37	-	51,51,51,51	0
61	MG	AA	3157	1/1	0.53	-	41,41,41,41	0
61	MG	DA	3018	1/1	0.53	-	85,85,85,85	0
61	MG	DA	3126	1/1	0.56	-	39,39,39,39	0
61	MG	AA	3568	1/1	0.49	-	29,29,29,29	0
61	MG	DA	3078	1/1	0.18	-	87,87,87,87	0
61	MG	AA	3134	1/1	0.45	-	59,59,59,59	0
61	MG	DA	3330	1/1	0.13	-	74,74,74,74	0
61	MG	BA	1682	1/1	0.18	-	98,98,98,98	0
61	MG	AA	3424	1/1	0.41	-	77,77,77,77	0
61	MG	BA	1701	1/1	0.23	-	73,73,73,73	0
61	MG	AA	3095	1/1	0.19	-	75,75,75,75	0
61	MG	AA	3452	1/1	0.21	-	95,95,95,95	0
61	MG	AA	3273	1/1	0.70	-	63,63,63,63	0
61	MG	DA	3057	1/1	0.51	-	81,81,81,81	0
61	MG	DA	3076	1/1	0.20	-	96,96,96,96	0
61	MG	DA	3163	1/1	0.21	-	97,97,97,97	0
61	MG	AA	3565	1/1	1.02	-	81,81,81,81	0
61	MG	BA	1803	1/1	0.21	-	81,81,81,81	0
61	MG	AA	3626	1/1	0.34	-	63,63,63,63	0
61	MG	CA	1718	1/1	0.13	-	78,78,78,78	0
61	MG	DA	3293	1/1	0.25	-	67,67,67,67	0
61	MG	CA	1675	1/1	0.52	-	65,65,65,65	0
61	MG	AA	3533	1/1	0.42	-	89,89,89,89	0
61	MG	DA	3200	1/1	0.40	-	66,66,66,66	0
61	MG	BA	1825	1/1	0.11	-	104,104,104,104	0
61	MG	BA	1773	1/1	0.34	-	79,79,79,79	0
61	MG	DA	3240	1/1	0.34	-	80,80,80,80	0
61	MG	BA	1800	1/1	0.26	-	101,101,101,101	0
61	MG	BA	1677	1/1	0.26	-	92,92,92,92	0
61	MG	CA	1721	1/1	0.28	-	94,94,94,94	0
61	MG	BA	1815	1/1	0.53	-	81,81,81,81	0
61	MG	CA	1767	1/1	0.41	-	94,94,94,94	0
61	MG	AA	3210	1/1	0.64	-	58,58,58,58	0
61	MG	AA	3441	1/1	0.17	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3074	1/1	0.42	-	81,81,81,81	0
61	MG	BA	1796	1/1	0.30	-	78,78,78,78	0
61	MG	AA	3439	1/1	0.18	-	93,93,93,93	0
61	MG	BA	1770	1/1	0.20	-	106,106,106,106	0
61	MG	DA	3121	1/1	0.41	-	99,99,99,99	0
61	MG	DB	207	1/1	0.28	-	98,98,98,98	0
61	MG	AA	3538	1/1	0.37	-	37,37,37,37	0
61	MG	DA	3039	1/1	0.32	-	82,82,82,82	0
61	MG	AA	3033	1/1	0.29	-	46,46,46,46	0
61	MG	DA	3266	1/1	0.24	-	97,97,97,97	0
61	MG	DA	3479	1/1	1.16	-	87,87,87,87	0
61	MG	AA	3449	1/1	0.19	-	76,76,76,76	0
61	MG	AA	3480	1/1	0.20	-	77,77,77,77	0
61	MG	DA	3336	1/1	0.21	-	68,68,68,68	0
61	MG	BA	1817	1/1	0.35	-	92,92,92,92	0
61	MG	CA	1691	1/1	0.31	-	69,69,69,69	0
61	MG	AA	3140	1/1	0.38	-	53,53,53,53	0
61	MG	CC	103	1/1	0.87	-	72,72,72,72	0
61	MG	BA	1628	1/1	0.27	-	86,86,86,86	0
61	MG	AA	3248	1/1	0.40	-	53,53,53,53	0
61	MG	DA	3158	1/1	0.29	-	77,77,77,77	0
61	MG	AA	3420	1/1	0.21	-	107,107,107,107	0
61	MG	AA	3078	1/1	0.19	-	84,84,84,84	0
61	MG	AA	3221	1/1	0.41	-	51,51,51,51	0
61	MG	AA	3351	1/1	0.90	-	84,84,84,84	0
61	MG	DA	3315	1/1	0.26	-	82,82,82,82	0
61	MG	AA	3347	1/1	0.40	-	92,92,92,92	0
61	MG	AA	3035	1/1	0.26	-	46,46,46,46	0
61	MG	DA	3290	1/1	0.40	-	59,59,59,59	0
61	MG	AA	3180	1/1	0.40	-	56,56,56,56	0
61	MG	AA	3612	1/1	0.19	-	38,38,38,38	0
61	MG	AA	3510	1/1	0.17	-	73,73,73,73	0
61	MG	DA	3119	1/1	0.26	-	80,80,80,80	0
61	MG	AA	3415	1/1	0.23	-	86,86,86,86	0
61	MG	BA	1776	1/1	0.35	-	84,84,84,84	0
61	MG	AA	3055	1/1	0.20	-	100,100,100,100	0
61	MG	DA	3395	1/1	0.48	-	80,80,80,80	0
61	MG	AA	3064	1/1	0.32	-	77,77,77,77	0
61	MG	AA	3102	1/1	0.22	-	108,108,108,108	0
61	MG	AA	3052	1/1	0.62	-	74,74,74,74	0
61	MG	AA	3154	1/1	0.56	-	55,55,55,55	0
61	MG	DA	3046	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
61	MG	DA	3494	1/1	0.63	-	81,81,81,81	0
61	MG	DA	3166	1/1	0.54	-	86,86,86,86	0
61	MG	CA	1805	1/1	0.21	-	81,81,81,81	0
61	MG	AA	3286	1/1	0.45	-	69,69,69,69	0
61	MG	BA	1723	1/1	0.45	-	95,95,95,95	0
61	MG	AA	3490	1/1	0.22	-	88,88,88,88	0
61	MG	DA	3112	1/1	0.14	-	70,70,70,70	0
61	MG	AA	3088	1/1	0.60	-	60,60,60,60	0
61	MG	BA	1635	1/1	0.13	-	87,87,87,87	0
61	MG	CA	1743	1/1	0.35	-	71,71,71,71	0
61	MG	DA	3510	1/1	0.60	-	67,67,67,67	0
61	MG	CA	1809	1/1	0.19	-	100,100,100,100	0
61	MG	CA	1760	1/1	0.27	-	103,103,103,103	0
61	MG	AA	3239	1/1	0.10	-	70,70,70,70	0
61	MG	BA	1806	1/1	0.23	-	75,75,75,75	0
61	MG	DA	3379	1/1	0.43	-	99,99,99,99	0
61	MG	DA	3502	1/1	0.28	-	96,96,96,96	0
61	MG	AA	3168	1/1	0.27	-	64,64,64,64	0
61	MG	BA	1710	1/1	0.27	-	99,99,99,99	0
61	MG	BA	1700	1/1	0.99	-	97,97,97,97	0
61	MG	DA	3475	1/1	0.91	-	81,81,81,81	0
61	MG	CA	1653	1/1	0.20	-	73,73,73,73	0
61	MG	AA	3007	1/1	0.24	-	33,33,33,33	0
61	MG	BA	1618	1/1	0.27	-	94,94,94,94	0
61	MG	DA	3094	1/1	0.46	-	45,45,45,45	0
61	MG	AA	3104	1/1	0.42	-	54,54,54,54	0
61	MG	BA	1694	1/1	0.24	-	99,99,99,99	0
61	MG	AA	3081	1/1	0.58	-	41,41,41,41	0
61	MG	DA	3432	1/1	0.32	-	89,89,89,89	0
61	MG	CA	1798	1/1	0.09	-	96,96,96,96	0
61	MG	DA	3499	1/1	0.70	-	78,78,78,78	0
61	MG	AA	3348	1/1	0.31	-	92,92,92,92	0
61	MG	CA	1789	1/1	0.16	-	117,117,117,117	0
61	MG	AA	3271	1/1	0.44	-	68,68,68,68	0
61	MG	AA	3444	1/1	0.27	-	87,87,87,87	0
61	MG	BA	1794	1/1	0.82	-	94,94,94,94	0
61	MG	DA	3235	1/1	0.31	-	53,53,53,53	0
61	MG	DA	3045	1/1	0.57	-	79,79,79,79	0
61	MG	AA	3594	1/1	0.24	-	97,97,97,97	0
61	MG	CA	1777	1/1	0.38	-	95,95,95,95	0
61	MG	AA	3044	1/1	0.30	-	54,54,54,54	0
61	MG	AA	3397	1/1	0.38	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BB	103	1/1	0.37	-	87,87,87,87	0
61	MG	DA	3241	1/1	0.22	-	85,85,85,85	0
61	MG	CC	106	1/1	0.52	-	115,115,115,115	0
61	MG	DA	3362	1/1	0.54	-	86,86,86,86	0
61	MG	DA	3364	1/1	0.37	-	85,85,85,85	0
61	MG	AA	3388	1/1	2.06	-	119,119,119,119	0
61	MG	BA	1691	1/1	0.70	-	60,60,60,60	0
61	MG	AA	3059	1/1	0.12	-	84,84,84,84	0
61	MG	BA	1681	1/1	0.16	-	79,79,79,79	0
61	MG	AA	3218	1/1	0.56	-	77,77,77,77	0
61	MG	DA	3328	1/1	0.34	-	83,83,83,83	0
61	MG	DA	3378	1/1	0.25	-	56,56,56,56	0
61	MG	AA	3122	1/1	0.73	-	87,87,87,87	0
61	MG	DA	3109	1/1	0.26	-	97,97,97,97	0
61	MG	AA	3446	1/1	0.10	-	93,93,93,93	0
61	MG	DA	3380	1/1	0.78	-	74,74,74,74	0
61	MG	DA	3311	1/1	0.22	-	80,80,80,80	0
61	MG	AA	3401	1/1	0.21	-	98,98,98,98	0
61	MG	DB	201	1/1	0.19	-	77,77,77,77	0
61	MG	AA	3024	1/1	0.41	-	35,35,35,35	0
61	MG	DA	3063	1/1	0.35	-	86,86,86,86	0
61	MG	AA	3410	1/1	0.13	-	99,99,99,99	0
61	MG	AA	3203	1/1	0.47	-	53,53,53,53	0
61	MG	DA	3267	1/1	0.44	-	74,74,74,74	0
61	MG	BA	1623	1/1	0.72	-	68,68,68,68	0
61	MG	CA	1659	1/1	0.17	-	111,111,111,111	0
61	MG	AA	3283	1/1	0.36	-	74,74,74,74	0
61	MG	AA	3406	1/1	0.15	-	99,99,99,99	0
61	MG	AA	3246	1/1	0.31	-	73,73,73,73	0
61	MG	AA	3322	1/1	0.11	-	83,83,83,83	0
61	MG	CA	1702	1/1	0.30	-	74,74,74,74	0
61	MG	AA	3572	1/1	0.42	-	40,40,40,40	0
61	MG	AA	3578	1/1	0.44	-	52,52,52,52	0
61	MG	DA	3376	1/1	0.14	-	88,88,88,88	0
61	MG	CA	1738	1/1	0.38	-	75,75,75,75	0
61	MG	BA	1833	1/1	0.29	-	88,88,88,88	0
61	MG	DA	3089	1/1	0.30	-	46,46,46,46	0
61	MG	AA	3075	1/1	0.24	-	71,71,71,71	0
61	MG	D0	201	1/1	0.20	-	78,78,78,78	0
61	MG	AA	3305	1/1	0.35	-	62,62,62,62	0
61	MG	CA	1723	1/1	0.07	-	93,93,93,93	0
61	MG	DA	3206	1/1	0.24	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1716	1/1	0.31	-	90,90,90,90	0
61	MG	AA	3101	1/1	0.16	-	69,69,69,69	0
61	MG	CA	1745	1/1	0.12	-	87,87,87,87	0
61	MG	AA	3524	1/1	0.25	-	72,72,72,72	0
61	MG	CA	1770	1/1	0.39	-	75,75,75,75	0
61	MG	CC	107	1/1	0.91	-	102,102,102,102	0
61	MG	AA	3592	1/1	0.45	-	69,69,69,69	0
61	MG	CA	1788	1/1	0.60	-	68,68,68,68	0
61	MG	DA	3375	1/1	0.55	-	82,82,82,82	0
61	MG	BA	1786	1/1	0.36	-	72,72,72,72	0
61	MG	BA	1609	1/1	0.51	-	84,84,84,84	0
61	MG	DA	3079	1/1	0.23	-	83,83,83,83	0
61	MG	DA	3504	1/1	0.16	-	119,119,119,119	0
61	MG	CA	1772	1/1	0.44	-	76,76,76,76	0
61	MG	CA	1703	1/1	0.09	-	88,88,88,88	0
61	MG	CA	1699	1/1	0.19	-	106,106,106,106	0
61	MG	DA	3438	1/1	0.57	-	102,102,102,102	0
61	MG	AA	3211	1/1	0.49	-	43,43,43,43	0
61	MG	AA	3464	1/1	0.54	-	83,83,83,83	0
61	MG	DA	3426	1/1	0.17	-	94,94,94,94	0
61	MG	AA	3280	1/1	0.45	-	65,65,65,65	0
61	MG	AA	3030	1/1	0.46	-	51,51,51,51	0
61	MG	AA	3196	1/1	0.33	-	60,60,60,60	0
61	MG	BA	1772	1/1	0.21	-	89,89,89,89	0
61	MG	BA	1739	1/1	0.26	-	79,79,79,79	0
61	MG	BA	1634	1/1	0.34	-	68,68,68,68	0
61	MG	DA	3117	1/1	0.21	-	68,68,68,68	0
61	MG	DA	3183	1/1	0.35	-	59,59,59,59	0
61	MG	AA	3425	1/1	0.29	-	70,70,70,70	0
61	MG	AA	3327	1/1	0.17	-	82,82,82,82	0
61	MG	DA	3265	1/1	0.21	-	63,63,63,63	0
61	MG	CA	1711	1/1	0.30	-	88,88,88,88	0
61	MG	AA	3564	1/1	0.50	-	54,54,54,54	0
61	MG	DA	3506	1/1	0.23	-	80,80,80,80	0
61	MG	CA	1622	1/1	0.14	-	74,74,74,74	0
61	MG	AA	3609	1/1	0.32	-	39,39,39,39	0
61	MG	AA	3566	1/1	0.58	-	73,73,73,73	0
61	MG	DA	3450	1/1	0.16	-	86,86,86,86	0
61	MG	AA	3458	1/1	0.26	-	105,105,105,105	0
61	MG	AA	3372	1/1	0.14	-	77,77,77,77	0
61	MG	DA	3077	1/1	0.46	-	82,82,82,82	0
61	MG	DA	3175	1/1	0.27	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3430	1/1	0.44	-	88,88,88,88	0
61	MG	AA	3437	1/1	0.14	-	105,105,105,105	0
61	MG	BA	1631	1/1	0.22	-	67,67,67,67	0
61	MG	AA	3579	1/1	0.41	-	35,35,35,35	0
61	MG	AA	3467	1/1	0.26	-	83,83,83,83	0
61	MG	DA	3270	1/1	0.47	-	73,73,73,73	0
61	MG	AA	3455	1/1	0.45	-	61,61,61,61	0
61	MG	DA	3414	1/1	0.32	-	74,74,74,74	0
61	MG	AA	3453	1/1	0.33	-	47,47,47,47	0
61	MG	AA	3036	1/1	0.34	-	34,34,34,34	0
61	MG	BA	1748	1/1	0.70	-	61,61,61,61	0
61	MG	DA	3098	1/1	0.32	-	41,41,41,41	0
61	MG	AA	3253	1/1	0.41	-	82,82,82,82	0
61	MG	DA	3219	1/1	0.51	-	79,79,79,79	0
61	MG	BC	102	1/1	0.31	-	100,100,100,100	0
61	MG	CA	1603	1/1	0.36	-	75,75,75,75	0
61	MG	AA	3083	1/1	0.27	-	47,47,47,47	0
61	MG	AA	3254	1/1	0.40	-	97,97,97,97	0
61	MG	DA	3289	1/1	0.14	-	47,47,47,47	0
61	MG	DA	3292	1/1	0.64	-	56,56,56,56	0
61	MG	BA	1663	1/1	0.19	-	47,47,47,47	0
61	MG	BA	1720	1/1	0.30	-	71,71,71,71	0
61	MG	CA	1620	1/1	0.61	-	70,70,70,70	0
61	MG	BA	1834	1/1	0.78	-	86,86,86,86	0
61	MG	CA	1639	1/1	0.25	-	64,64,64,64	0
61	MG	CA	1776	1/1	0.29	-	91,91,91,91	0
61	MG	AA	3311	1/1	0.27	-	58,58,58,58	0
61	MG	AA	3155	1/1	0.66	-	61,61,61,61	0
61	MG	DA	3425	1/1	0.48	-	88,88,88,88	0
61	MG	AA	3373	1/1	0.74	-	71,71,71,71	0
61	MG	BC	104	1/1	0.93	-	106,106,106,106	0
61	MG	DA	3468	1/1	0.37	-	53,53,53,53	0
61	MG	DA	3012	1/1	0.44	-	64,64,64,64	0
61	MG	BA	1837	1/1	0.64	-	88,88,88,88	0
61	MG	DA	3260	1/1	0.39	-	82,82,82,82	0
61	MG	CA	1763	1/1	0.23	-	96,96,96,96	0
61	MG	AA	3597	1/1	0.47	-	67,67,67,67	0
61	MG	DA	3137	1/1	0.29	-	78,78,78,78	0
61	MG	DA	3253	1/1	0.30	-	83,83,83,83	0
61	MG	AA	3379	1/1	0.68	-	88,88,88,88	0
61	MG	BA	1730	1/1	0.28	-	97,97,97,97	0
61	MG	CA	1716	1/1	0.35	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BC	109	1/1	0.48	-	92,92,92,92	0
61	MG	DA	3286	1/1	0.68	-	86,86,86,86	0
61	MG	DA	3278	1/1	0.40	-	116,116,116,116	0
61	MG	AO	202	1/1	0.28	-	74,74,74,74	0
61	MG	BA	1680	1/1	0.31	-	71,71,71,71	0
61	MG	DA	3191	1/1	0.58	-	47,47,47,47	0
61	MG	CA	1785	1/1	0.32	-	81,81,81,81	0
61	MG	DA	3087	1/1	0.48	-	48,48,48,48	0
61	MG	DA	3488	1/1	0.20	-	45,45,45,45	0
61	MG	DA	3147	1/1	0.12	-	16,16,16,16	0
61	MG	BA	1687	1/1	0.25	-	74,74,74,74	0
61	MG	CA	1783	1/1	0.23	-	72,72,72,72	0
61	MG	BA	1614	1/1	0.19	-	93,93,93,93	0
61	MG	AA	3090	1/1	0.41	-	68,68,68,68	0
61	MG	DA	3034	1/1	0.20	-	72,72,72,72	0
61	MG	DA	3429	1/1	0.41	-	94,94,94,94	0
61	MG	DA	3517	1/1	0.27	-	62,62,62,62	0
61	MG	AA	3375	1/1	0.18	-	74,74,74,74	0
61	MG	BA	1610	1/1	0.45	-	53,53,53,53	0
61	MG	BA	1731	1/1	0.39	-	67,67,67,67	0
61	MG	DA	3391	1/1	0.21	-	86,86,86,86	0
61	MG	CB	103	1/1	0.34	-	110,110,110,110	0
61	MG	AA	3163	1/1	0.37	-	48,48,48,48	0
61	MG	AA	3323	1/1	0.10	-	93,93,93,93	0
61	MG	DA	3124	1/1	0.78	-	111,111,111,111	0
61	MG	BA	1831	1/1	0.50	-	116,116,116,116	0
61	MG	AA	3547	1/1	0.33	-	45,45,45,45	0
61	MG	DA	3335	1/1	0.33	-	72,72,72,72	0
61	MG	BA	1642	1/1	0.40	-	69,69,69,69	0
61	MG	DA	3164	1/1	0.19	-	65,65,65,65	0
61	MG	DA	3323	1/1	0.60	-	85,85,85,85	0
61	MG	DA	3463	1/1	0.59	-	44,44,44,44	0
61	MG	DA	3194	1/1	0.32	-	59,59,59,59	0
61	MG	DA	3122	1/1	0.06	-	71,71,71,71	0
61	MG	AA	3540	1/1	0.29	-	44,44,44,44	0
61	MG	DA	3419	1/1	0.60	-	90,90,90,90	0
61	MG	DA	3232	1/1	0.29	-	75,75,75,75	0
61	MG	AA	3079	1/1	0.34	-	100,100,100,100	0
61	MG	AA	3514	1/1	0.50	-	59,59,59,59	0
61	MG	DA	3411	1/1	0.15	-	77,77,77,77	0
61	MG	DA	3338	1/1	0.89	-	75,75,75,75	0
61	MG	AA	3058	1/1	0.11	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1719	1/1	0.15	-	157,157,157,157	0
61	MG	DA	3149	1/1	0.56	-	60,60,60,60	0
61	MG	DA	3054	1/1	0.55	-	105,105,105,105	0
61	MG	DA	3423	1/1	0.39	-	102,102,102,102	0
61	MG	AA	3070	1/1	0.63	-	66,66,66,66	0
61	MG	AA	3223	1/1	0.59	-	72,72,72,72	0
61	MG	AA	3482	1/1	0.53	-	82,82,82,82	0
61	MG	DA	3092	1/1	0.39	-	47,47,47,47	0
61	MG	DA	3072	1/1	0.27	-	98,98,98,98	0
61	MG	AA	3354	1/1	0.48	-	79,79,79,79	0
61	MG	AA	3164	1/1	0.33	-	102,102,102,102	0
61	MG	AA	3217	1/1	0.34	-	58,58,58,58	0
61	MG	AA	3107	1/1	0.34	-	56,56,56,56	0
61	MG	DA	3297	1/1	0.32	-	70,70,70,70	0
61	MG	CA	1625	1/1	0.11	-	85,85,85,85	0
61	MG	BA	1624	1/1	0.40	-	92,92,92,92	0
61	MG	DA	3104	1/1	0.55	-	38,38,38,38	0
61	MG	AA	3063	1/1	0.13	-	64,64,64,64	0
61	MG	DA	3216	1/1	0.59	-	47,47,47,47	0
61	MG	AA	3521	1/1	0.31	-	87,87,87,87	0
61	MG	AA	3607	1/1	0.32	-	54,54,54,54	0
61	MG	BA	1784	1/1	0.27	-	106,106,106,106	0
61	MG	BA	1824	1/1	0.16	-	97,97,97,97	0
61	MG	DB	213	1/1	0.27	-	90,90,90,90	0
61	MG	AA	3109	1/1	0.28	-	33,33,33,33	0
61	MG	DA	3242	1/1	0.61	-	61,61,61,61	0
61	MG	DA	3313	1/1	0.48	-	75,75,75,75	0
61	MG	AA	3262	1/1	0.33	-	71,71,71,71	0
61	MG	DA	3299	1/1	0.30	-	92,92,92,92	0
61	MG	BA	1714	1/1	0.22	-	127,127,127,127	0
61	MG	AA	3213	1/1	0.52	-	50,50,50,50	0
61	MG	DA	3173	1/1	0.63	-	59,59,59,59	0
61	MG	CA	1797	1/1	0.26	-	94,94,94,94	0
61	MG	DA	3456	1/1	0.29	-	83,83,83,83	0
61	MG	DA	3317	1/1	0.38	-	87,87,87,87	0
61	MG	CA	1717	1/1	0.34	-	106,106,106,106	0
61	MG	CA	1726	1/1	0.63	-	82,82,82,82	0
61	MG	AA	3147	1/1	0.52	-	77,77,77,77	0
61	MG	DA	3131	1/1	0.80	-	93,93,93,93	0
61	MG	AA	3376	1/1	0.28	-	67,67,67,67	0
61	MG	DA	3151	1/1	0.69	-	75,75,75,75	0
61	MG	AA	3528	1/1	0.18	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AB	203	1/1	0.24	-	70,70,70,70	0
61	MG	AA	3332	1/1	0.61	-	82,82,82,82	0
61	MG	AA	3012	1/1	0.44	-	45,45,45,45	0
61	MG	AA	3185	1/1	0.23	-	43,43,43,43	0
61	MG	DA	3493	1/1	0.60	-	46,46,46,46	0
61	MG	DA	3091	1/1	0.45	-	52,52,52,52	0
61	MG	DA	3310	1/1	0.44	-	80,80,80,80	0
61	MG	DA	3513	1/1	0.14	-	103,103,103,103	0
62	ZN	BG	302	1/1	0.32	-	95,95,95,95	0
61	MG	AA	3238	1/1	0.57	-	48,48,48,48	0
61	MG	AA	3219	1/1	0.28	-	60,60,60,60	0
61	MG	BC	103	1/1	0.44	-	65,65,65,65	0
61	MG	AA	3091	1/1	0.26	-	69,69,69,69	0
61	MG	DA	3142	1/1	0.62	-	51,51,51,51	0
61	MG	BA	1727	1/1	0.14	-	125,125,125,125	0
61	MG	BA	1685	1/1	0.19	-	82,82,82,82	0
61	MG	DA	3116	1/1	0.09	-	96,96,96,96	0
61	MG	AA	3188	1/1	0.35	-	72,72,72,72	0
61	MG	DA	3472	1/1	0.53	-	85,85,85,85	0
61	MG	AA	3624	1/1	0.17	-	80,80,80,80	0
61	MG	AA	3456	1/1	0.56	-	70,70,70,70	0
61	MG	DA	3403	1/1	0.14	-	78,78,78,78	0
61	MG	BA	1775	1/1	0.20	-	100,100,100,100	0
61	MG	BA	1771	1/1	0.17	-	100,100,100,100	0
61	MG	AA	3128	1/1	0.30	-	54,54,54,54	0
61	MG	AA	3224	1/1	0.33	-	77,77,77,77	0
61	MG	AA	3263	1/1	0.28	-	56,56,56,56	0
61	MG	DA	3269	1/1	0.41	-	86,86,86,86	0
61	MG	CA	1660	1/1	0.16	-	76,76,76,76	0
61	MG	DB	214	1/1	0.17	-	99,99,99,99	0
61	MG	AA	3043	1/1	0.24	-	83,83,83,83	0
61	MG	CA	1790	1/1	0.18	-	75,75,75,75	0
61	MG	CA	1752	1/1	0.21	-	70,70,70,70	0
61	MG	AA	3326	1/1	0.32	-	81,81,81,81	0
61	MG	AA	3585	1/1	0.07	-	46,46,46,46	0
61	MG	BA	1640	1/1	0.33	-	80,80,80,80	0
61	MG	AA	3175	1/1	0.48	-	70,70,70,70	0
61	MG	CA	1645	1/1	0.33	-	71,71,71,71	0
61	MG	AA	3031	1/1	0.54	-	44,44,44,44	0
61	MG	DB	203	1/1	0.21	-	71,71,71,71	0
61	MG	DA	3139	1/1	0.49	-	51,51,51,51	0
61	MG	DA	3420	1/1	0.75	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3380	1/1	0.53	-	84,84,84,84	0
61	MG	DA	3369	1/1	0.49	-	61,61,61,61	0
61	MG	AA	3389	1/1	0.81	-	89,89,89,89	0
61	MG	DA	3209	1/1	0.55	-	54,54,54,54	0
61	MG	BA	1844	1/1	0.39	-	95,95,95,95	0
61	MG	AA	3544	1/1	0.77	-	67,67,67,67	0
61	MG	AA	3427	1/1	0.22	-	78,78,78,78	0
61	MG	BA	1713	1/1	0.09	-	107,107,107,107	0
61	MG	AA	3261	1/1	0.26	-	30,30,30,30	0
61	MG	DA	3218	1/1	0.67	-	75,75,75,75	0
61	MG	AA	3302	1/1	0.30	-	84,84,84,84	0
61	MG	AA	3259	1/1	0.29	-	91,91,91,91	0
61	MG	AA	3536	1/1	0.73	-	102,102,102,102	0
61	MG	BA	1718	1/1	0.19	-	104,104,104,104	0
61	MG	AA	3072	1/1	0.49	-	75,75,75,75	0
61	MG	DA	3028	1/1	0.29	-	71,71,71,71	0
61	MG	DA	3107	1/1	0.36	-	89,89,89,89	0
61	MG	DA	3068	1/1	0.19	-	100,100,100,100	0
62	ZN	CQ	101	1/1	0.17	-	113,113,113,113	0
61	MG	DA	3447	1/1	0.53	-	86,86,86,86	0
61	MG	DA	3350	1/1	0.30	-	79,79,79,79	0
61	MG	AA	3298	1/1	0.43	-	80,80,80,80	0
61	MG	CA	1627	1/1	0.39	-	102,102,102,102	0
61	MG	AA	3017	1/1	0.42	-	59,59,59,59	0
61	MG	DA	3001	1/1	0.27	-	58,58,58,58	0
61	MG	CA	1786	1/1	0.16	-	97,97,97,97	0
61	MG	DA	3327	1/1	0.41	-	85,85,85,85	0
61	MG	DA	3359	1/1	0.14	-	75,75,75,75	0
61	MG	AA	3530	1/1	0.16	-	65,65,65,65	0
61	MG	CC	101	1/1	0.24	-	110,110,110,110	0
61	MG	AB	217	1/1	0.68	-	109,109,109,109	0
61	MG	DA	3082	1/1	0.23	-	83,83,83,83	0
61	MG	AA	3176	1/1	0.53	-	38,38,38,38	0
61	MG	BA	1835	1/1	0.60	-	82,82,82,82	0
61	MG	AA	3618	1/1	0.39	-	76,76,76,76	0
61	MG	AA	3131	1/1	0.38	-	88,88,88,88	0
61	MG	DA	3225	1/1	0.32	-	64,64,64,64	0
61	MG	DA	3023	1/1	0.10	-	107,107,107,107	0
61	MG	AA	3290	1/1	0.81	-	62,62,62,62	0
61	MG	BA	1656	1/1	0.27	-	78,78,78,78	0
61	MG	CA	1642	1/1	0.32	-	78,78,78,78	0
61	MG	BA	1732	1/1	0.29	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3392	1/1	0.29	-	106,106,106,106	0
61	MG	AA	3082	1/1	0.48	-	39,39,39,39	0
61	MG	AA	3149	1/1	0.36	-	49,49,49,49	0
61	MG	DA	3201	1/1	0.44	-	75,75,75,75	0
61	MG	DA	3101	1/1	0.30	-	57,57,57,57	0
61	MG	AA	3038	1/1	0.19	-	70,70,70,70	0
61	MG	DA	3344	1/1	0.28	-	93,93,93,93	0
61	MG	CA	1744	1/1	0.22	-	70,70,70,70	0
61	MG	DA	3090	1/1	0.24	-	47,47,47,47	0
61	MG	AA	3100	1/1	0.15	-	79,79,79,79	0
61	MG	DE	303	1/1	0.52	-	52,52,52,52	0
61	MG	AA	3559	1/1	0.38	-	93,93,93,93	0
61	MG	BA	1766	1/1	0.51	-	116,116,116,116	0
61	MG	DA	3144	1/1	0.85	-	68,68,68,68	0
61	MG	AA	3512	1/1	0.32	-	71,71,71,71	0
61	MG	AA	3492	1/1	0.34	-	84,84,84,84	0
61	MG	AA	3048	1/1	0.17	-	63,63,63,63	0
61	MG	BA	1719	1/1	0.33	-	91,91,91,91	0
61	MG	AA	3382	1/1	0.40	-	83,83,83,83	0
61	MG	DA	3032	1/1	0.45	-	73,73,73,73	0
61	MG	CC	102	1/1	0.47	-	69,69,69,69	0
61	MG	DA	3040	1/1	0.37	-	92,92,92,92	0
61	MG	DA	3138	1/1	0.22	-	71,71,71,71	0
61	MG	AO	201	1/1	0.25	-	39,39,39,39	0
61	MG	AA	3617	1/1	0.42	-	92,92,92,92	0
61	MG	DA	3491	1/1	0.27	-	43,43,43,43	0
61	MG	BA	1788	1/1	0.13	-	108,108,108,108	0
61	MG	DA	3324	1/1	1.26	-	89,89,89,89	0
61	MG	CA	1644	1/1	0.21	-	59,59,59,59	0
61	MG	AA	3065	1/1	0.41	-	52,52,52,52	0
61	MG	CA	1643	1/1	0.17	-	97,97,97,97	0
61	MG	AA	3613	1/1	0.62	-	104,104,104,104	0
61	MG	AA	3412	1/1	0.77	-	88,88,88,88	0
61	MG	DA	3480	1/1	0.68	-	56,56,56,56	0
61	MG	AA	3563	1/1	0.66	-	75,75,75,75	0
61	MG	CA	1623	1/1	0.10	-	98,98,98,98	0
61	MG	AA	3426	1/1	0.14	-	123,123,123,123	0
61	MG	BA	1725	1/1	0.58	-	82,82,82,82	0
61	MG	AA	3431	1/1	0.48	-	197,197,197,197	0
61	MG	CA	1655	1/1	0.32	-	87,87,87,87	0
61	MG	AA	3558	1/1	0.51	-	110,110,110,110	0
61	MG	DA	3002	1/1	0.64	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1618	1/1	0.14	-	89,89,89,89	0
61	MG	DA	3159	1/1	0.32	-	52,52,52,52	0
61	MG	AA	3595	1/1	0.40	-	90,90,90,90	0
61	MG	DA	3500	1/1	0.56	-	100,100,100,100	0
61	MG	AA	3135	1/1	0.33	-	66,66,66,66	0
61	MG	DA	3346	1/1	0.24	-	83,83,83,83	0
61	MG	CA	1775	1/1	0.38	-	66,66,66,66	0
61	MG	DA	3455	1/1	0.47	-	95,95,95,95	0
61	MG	AA	3377	1/1	0.33	-	85,85,85,85	0
61	MG	AF	303	1/1	0.43	-	77,77,77,77	0
61	MG	DA	3485	1/1	0.49	-	40,40,40,40	0
61	MG	DA	3413	1/1	0.46	-	96,96,96,96	0
61	MG	DA	3115	1/1	0.23	-	76,76,76,76	0
61	MG	CA	1610	1/1	0.15	-	75,75,75,75	0
61	MG	BA	1767	1/1	0.25	-	101,101,101,101	0
61	MG	AA	3172	1/1	0.48	-	102,102,102,102	0
61	MG	DA	3303	1/1	0.72	-	61,61,61,61	0
61	MG	CA	1778	1/1	0.29	-	69,69,69,69	0
61	MG	DA	3103	1/1	0.47	-	82,82,82,82	0
61	MG	AA	3605	1/1	0.47	-	45,45,45,45	0
61	MG	AA	3515	1/1	1.02	-	67,67,67,67	0
61	MG	BA	1791	1/1	0.14	-	89,89,89,89	0
61	MG	DA	3301	1/1	0.30	-	91,91,91,91	0
61	MG	DA	3417	1/1	0.20	-	83,83,83,83	0
61	MG	BA	1621	1/1	0.34	-	116,116,116,116	0
61	MG	DA	3396	1/1	0.19	-	89,89,89,89	0
61	MG	AA	3418	1/1	0.80	-	85,85,85,85	0
61	MG	AA	3053	1/1	0.35	-	59,59,59,59	0
61	MG	CA	1698	1/1	0.32	-	104,104,104,104	0
61	MG	DA	3271	1/1	0.33	-	76,76,76,76	0
61	MG	AA	3520	1/1	0.20	-	97,97,97,97	0
61	MG	DA	3371	1/1	0.28	-	82,82,82,82	0
61	MG	BC	107	1/1	0.22	-	88,88,88,88	0
61	MG	AA	3199	1/1	0.36	-	66,66,66,66	0
61	MG	DA	3174	1/1	0.36	-	49,49,49,49	0
61	MG	CA	1708	1/1	0.28	-	91,91,91,91	0
61	MG	DA	3243	1/1	0.23	-	83,83,83,83	0
61	MG	DA	3467	1/1	0.32	-	49,49,49,49	0
61	MG	DA	3496	1/1	0.25	-	85,85,85,85	0
61	MG	AA	3627	1/1	1.01	-	108,108,108,108	0
61	MG	AA	3611	1/1	0.37	-	54,54,54,54	0
61	MG	AA	3517	1/1	0.35	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1664	1/1	0.24	-	97,97,97,97	0
61	MG	DA	3296	1/1	0.21	-	56,56,56,56	0
61	MG	DA	3418	1/1	0.36	-	81,81,81,81	0
61	MG	CA	1638	1/1	0.32	-	93,93,93,93	0
61	MG	DA	3250	1/1	0.32	-	54,54,54,54	0
61	MG	AA	3005	1/1	0.47	-	38,38,38,38	0
61	MG	AA	3495	1/1	0.37	-	98,98,98,98	0
61	MG	DA	3487	1/1	0.46	-	59,59,59,59	0
61	MG	DA	3446	1/1	0.28	-	98,98,98,98	0
61	MG	CA	1605	1/1	0.27	-	72,72,72,72	0
61	MG	AA	3363	1/1	0.30	-	80,80,80,80	0
61	MG	AA	3457	1/1	0.20	-	73,73,73,73	0
61	MG	CA	1669	1/1	0.21	-	67,67,67,67	0
61	MG	AA	3602	1/1	0.16	-	70,70,70,70	0
61	MG	DA	3319	1/1	0.40	-	68,68,68,68	0
61	MG	AB	207	1/1	0.07	-	97,97,97,97	0
61	MG	AA	3330	1/1	0.13	-	61,61,61,61	0
61	MG	CA	1720	1/1	0.42	-	108,108,108,108	0
61	MG	AO	203	1/1	0.50	-	63,63,63,63	0
61	MG	DA	3168	1/1	0.43	-	49,49,49,49	0
61	MG	AA	3381	1/1	0.33	-	88,88,88,88	0
61	MG	DA	3424	1/1	0.30	-	79,79,79,79	0
61	MG	CA	1686	1/1	0.34	-	68,68,68,68	0
61	MG	CA	1682	1/1	0.41	-	97,97,97,97	0
61	MG	AA	3216	1/1	0.26	-	56,56,56,56	0
61	MG	AA	3111	1/1	0.58	-	43,43,43,43	0
61	MG	CA	1782	1/1	0.45	-	104,104,104,104	0
61	MG	AA	3317	1/1	0.62	-	95,95,95,95	0
61	MG	AA	3442	1/1	0.36	-	49,49,49,49	0
61	MG	DA	3435	1/1	0.34	-	104,104,104,104	0
61	MG	BA	1611	1/1	0.34	-	97,97,97,97	0
61	MG	BA	1657	1/1	0.44	-	44,44,44,44	0
61	MG	AA	3413	1/1	0.32	-	82,82,82,82	0
61	MG	AA	3434	1/1	0.39	-	65,65,65,65	0
61	MG	CA	1734	1/1	0.26	-	92,92,92,92	0
61	MG	DA	3020	1/1	0.51	-	51,51,51,51	0
61	MG	AA	3249	1/1	0.23	-	92,92,92,92	0
61	MG	DA	3030	1/1	0.22	-	66,66,66,66	0
61	MG	DA	3503	1/1	0.29	-	52,52,52,52	0
61	MG	AA	3234	1/1	0.43	-	83,83,83,83	0
61	MG	AA	3103	1/1	0.41	-	75,75,75,75	0
61	MG	CA	1755	1/1	0.49	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3503	1/1	0.16	-	72,72,72,72	0
61	MG	AA	3150	1/1	0.54	-	58,58,58,58	0
61	MG	DA	3370	1/1	0.16	-	85,85,85,85	0
61	MG	DA	3285	1/1	0.37	-	109,109,109,109	0
61	MG	DA	3177	1/1	0.46	-	51,51,51,51	0
61	MG	AA	3127	1/1	0.28	-	47,47,47,47	0
61	MG	DA	3176	1/1	0.60	-	78,78,78,78	0
61	MG	AA	3137	1/1	0.20	-	43,43,43,43	0
61	MG	DA	3263	1/1	0.34	-	88,88,88,88	0
61	MG	AA	3177	1/1	0.18	-	45,45,45,45	0
61	MG	BA	1768	1/1	0.40	-	86,86,86,86	0
61	MG	DA	3521	1/1	0.45	-	89,89,89,89	0
61	MG	DA	3123	1/1	0.12	-	73,73,73,73	0
61	MG	DA	3156	1/1	0.49	-	62,62,62,62	0
61	MG	AA	3214	1/1	0.47	-	66,66,66,66	0
61	MG	CC	108	1/1	0.59	-	110,110,110,110	0
61	MG	DA	3043	1/1	0.24	-	81,81,81,81	0
61	MG	AA	3590	1/1	0.41	-	56,56,56,56	0
61	MG	BA	1781	1/1	0.42	-	57,57,57,57	0
61	MG	AA	3315	1/1	0.63	-	68,68,68,68	0
61	MG	AA	3106	1/1	0.59	-	65,65,65,65	0
61	MG	BB	101	1/1	0.16	-	88,88,88,88	0
61	MG	BC	106	1/1	0.19	-	80,80,80,80	0
61	MG	DA	3080	1/1	0.07	-	114,114,114,114	0
61	MG	AF	302	1/1	0.68	-	80,80,80,80	0
61	MG	BA	1842	1/1	0.28	-	88,88,88,88	0
61	MG	BA	1733	1/1	0.30	-	88,88,88,88	0
61	MG	AA	3269	1/1	0.28	-	72,72,72,72	0
61	MG	DA	3053	1/1	0.54	-	86,86,86,86	0
61	MG	AA	3496	1/1	0.35	-	91,91,91,91	0
61	MG	BA	1836	1/1	0.51	-	73,73,73,73	0
61	MG	AA	3469	1/1	0.39	-	76,76,76,76	0
61	MG	DA	3099	1/1	0.29	-	51,51,51,51	0
61	MG	AA	3233	1/1	0.22	-	74,74,74,74	0
61	MG	AA	3116	1/1	0.36	-	43,43,43,43	0
61	MG	AA	3151	1/1	0.50	-	61,61,61,61	0
61	MG	CA	1697	1/1	0.31	-	56,56,56,56	0
61	MG	CA	1701	1/1	0.34	-	77,77,77,77	0
61	MG	DE	301	1/1	0.40	-	43,43,43,43	0
61	MG	AA	3328	1/1	0.47	-	71,71,71,71	0
61	MG	DA	3421	1/1	0.27	-	76,76,76,76	0
61	MG	BA	1745	1/1	0.53	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3021	1/1	0.57	-	61,61,61,61	0
61	MG	DA	3437	1/1	0.26	-	140,140,140,140	0
61	MG	DA	3027	1/1	0.43	-	93,93,93,93	0
61	MG	DA	3498	1/1	1.21	-	90,90,90,90	0
61	MG	CA	1714	1/1	1.14	-	115,115,115,115	0
61	MG	DA	3062	1/1	0.19	-	85,85,85,85	0
61	MG	AA	3123	1/1	0.38	-	47,47,47,47	0
61	MG	BA	1809	1/1	1.11	-	88,88,88,88	0
61	MG	AA	3484	1/1	0.24	-	86,86,86,86	0
61	MG	AA	3108	1/1	0.70	-	79,79,79,79	0
61	MG	CA	1725	1/1	0.23	-	75,75,75,75	0
61	MG	AD	302	1/1	0.30	-	44,44,44,44	0
61	MG	CA	1765	1/1	0.34	-	97,97,97,97	0
61	MG	DA	3239	1/1	0.54	-	75,75,75,75	0
61	MG	DA	3182	1/1	0.61	-	72,72,72,72	0
61	MG	AA	3423	1/1	0.24	-	69,69,69,69	0
61	MG	AA	3329	1/1	0.27	-	77,77,77,77	0
61	MG	DA	3365	1/1	0.55	-	89,89,89,89	0
61	MG	CA	1759	1/1	0.22	-	100,100,100,100	0
61	MG	AA	3270	1/1	0.21	-	96,96,96,96	0
61	MG	CA	1762	1/1	0.30	-	105,105,105,105	0
61	MG	AA	3019	1/1	0.33	-	35,35,35,35	0
61	MG	AA	3200	1/1	0.33	-	80,80,80,80	0
61	MG	DA	3514	1/1	0.52	-	49,49,49,49	0
61	MG	CG	303	1/1	0.12	-	100,100,100,100	0
61	MG	AA	3198	1/1	0.62	-	57,57,57,57	0
61	MG	CA	1680	1/1	0.50	-	68,68,68,68	0
61	MG	DA	3471	1/1	0.57	-	89,89,89,89	0
61	MG	AA	3092	1/1	0.45	-	59,59,59,59	0
61	MG	CA	1808	1/1	0.21	-	73,73,73,73	0
61	MG	AA	3599	1/1	0.60	-	84,84,84,84	0
61	MG	A0	201	1/1	0.24	-	46,46,46,46	0
61	MG	DA	3307	1/1	0.48	-	77,77,77,77	0
61	MG	DA	3108	1/1	0.30	-	69,69,69,69	0
61	MG	CH	201	1/1	0.15	-	96,96,96,96	0
61	MG	AA	3009	1/1	0.28	-	48,48,48,48	0
61	MG	AA	3387	1/1	0.35	-	102,102,102,102	0
61	MG	DA	3051	1/1	0.40	-	81,81,81,81	0
61	MG	DA	3464	1/1	0.34	-	55,55,55,55	0
61	MG	AA	3501	1/1	0.35	-	73,73,73,73	0
61	MG	DA	3088	1/1	0.50	-	49,49,49,49	0
61	MG	BA	1616	1/1	0.16	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3302	1/1	0.65	-	91,91,91,91	0
61	MG	CA	1796	1/1	0.34	-	81,81,81,81	0
61	MG	AA	3451	1/1	0.33	-	85,85,85,85	0
61	MG	BA	1734	1/1	0.60	-	96,96,96,96	0
61	MG	AA	3500	1/1	0.41	-	32,32,32,32	0
61	MG	AA	3341	1/1	0.23	-	63,63,63,63	0
61	MG	AA	3275	1/1	0.37	-	65,65,65,65	0
61	MG	BA	1780	1/1	0.45	-	58,58,58,58	0
61	MG	DA	3353	1/1	0.58	-	70,70,70,70	0
61	MG	CA	1696	1/1	0.14	-	79,79,79,79	0
61	MG	BA	1627	1/1	0.31	-	62,62,62,62	0
61	MG	AA	3124	1/1	0.61	-	56,56,56,56	0
61	MG	DA	3272	1/1	0.26	-	117,117,117,117	0
61	MG	CB	104	1/1	0.26	-	114,114,114,114	0
61	MG	AA	3365	1/1	0.24	-	83,83,83,83	0
61	MG	AA	3285	1/1	0.32	-	77,77,77,77	0
61	MG	AA	3057	1/1	0.26	-	52,52,52,52	0
61	MG	DA	3372	1/1	0.45	-	108,108,108,108	0
61	MG	AA	3195	1/1	0.12	-	62,62,62,62	0
61	MG	DA	3085	1/1	0.25	-	89,89,89,89	0
61	MG	AA	3336	1/1	0.44	-	48,48,48,48	0
61	MG	DA	3322	1/1	0.56	-	83,83,83,83	0
61	MG	AA	3189	1/1	0.32	-	57,57,57,57	0
61	MG	DA	3416	1/1	0.25	-	75,75,75,75	0
61	MG	BA	1750	1/1	0.41	-	79,79,79,79	0
61	MG	AA	3355	1/1	0.56	-	87,87,87,87	0
61	MG	BA	1668	1/1	0.52	-	73,73,73,73	0
61	MG	AA	3570	1/1	0.25	-	49,49,49,49	0
61	MG	BA	1615	1/1	0.34	-	104,104,104,104	0
61	MG	AA	3403	1/1	0.10	-	74,74,74,74	0
61	MG	CA	1749	1/1	0.15	-	106,106,106,106	0
61	MG	AA	3099	1/1	0.36	-	64,64,64,64	0
61	MG	DA	3024	1/1	0.79	-	100,100,100,100	0
61	MG	BA	1698	1/1	0.42	-	73,73,73,73	0
61	MG	BA	1613	1/1	0.47	-	96,96,96,96	0
61	MG	AA	3475	1/1	0.30	-	67,67,67,67	0
61	MG	AA	3227	1/1	0.37	-	66,66,66,66	0
61	MG	BA	1665	1/1	0.62	-	66,66,66,66	0
61	MG	AB	202	1/1	0.16	-	86,86,86,86	0
61	MG	AU	201	1/1	0.24	-	74,74,74,74	0
61	MG	AA	3018	1/1	0.51	-	38,38,38,38	0
61	MG	DA	3161	1/1	0.44	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	BA	1840	1/1	0.46	-	80,80,80,80	0
61	MG	AA	3343	1/1	0.30	-	94,94,94,94	0
61	MG	BA	1708	1/1	0.19	-	78,78,78,78	0
61	MG	DA	3037	1/1	0.19	-	84,84,84,84	0
61	MG	CA	1722	1/1	0.33	-	63,63,63,63	0
61	MG	BC	101	1/1	0.42	-	58,58,58,58	0
61	MG	CA	1640	1/1	0.34	-	78,78,78,78	0
61	MG	AA	3552	1/1	0.69	-	75,75,75,75	0
61	MG	DA	3511	1/1	0.34	-	65,65,65,65	0
61	MG	AA	3073	1/1	0.44	-	76,76,76,76	0
61	MG	BA	1822	1/1	0.52	-	107,107,107,107	0
61	MG	AA	3207	1/1	0.51	-	44,44,44,44	0
61	MG	AA	3235	1/1	0.39	-	86,86,86,86	0
61	MG	AA	3522	1/1	0.24	-	67,67,67,67	0
61	MG	DA	3434	1/1	0.49	-	75,75,75,75	0
61	MG	CA	1633	1/1	0.42	-	79,79,79,79	0
61	MG	DA	3105	1/1	0.30	-	72,72,72,72	0
61	MG	DA	3022	1/1	0.70	-	66,66,66,66	0
61	MG	DA	3227	1/1	0.29	-	81,81,81,81	0
61	MG	BA	1783	1/1	0.52	-	91,91,91,91	0
61	MG	BA	1752	1/1	0.17	-	116,116,116,116	0
61	MG	DA	3044	1/1	0.17	-	66,66,66,66	0
61	MG	AA	3478	1/1	0.11	-	93,93,93,93	0
61	MG	AA	3396	1/1	0.29	-	58,58,58,58	0
61	MG	DA	3069	1/1	0.36	-	82,82,82,82	0
61	MG	AA	3205	1/1	0.28	-	43,43,43,43	0
61	MG	AA	3276	1/1	0.50	-	59,59,59,59	0
61	MG	AA	3466	1/1	0.65	-	106,106,106,106	0
61	MG	AA	3220	1/1	0.27	-	44,44,44,44	0
61	MG	DA	3097	1/1	0.34	-	42,42,42,42	0
61	MG	DA	3460	1/1	0.47	-	45,45,45,45	0
61	MG	AA	3047	1/1	0.22	-	87,87,87,87	0
61	MG	AA	3339	1/1	0.22	-	95,95,95,95	0
61	MG	BA	1661	1/1	0.29	-	49,49,49,49	0
61	MG	BB	107	1/1	0.19	-	97,97,97,97	0
61	MG	AA	3183	1/1	0.25	-	79,79,79,79	0
61	MG	AA	3287	1/1	0.12	-	88,88,88,88	0
61	MG	BA	1647	1/1	0.23	-	93,93,93,93	0
61	MG	D3	101	1/1	0.34	-	68,68,68,68	0
61	MG	DA	3065	1/1	0.54	-	95,95,95,95	0
61	MG	DA	3282	1/1	0.46	-	55,55,55,55	0
61	MG	AA	3596	1/1	0.22	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3209	1/1	0.69	-	71,71,71,71	0
61	MG	BA	1655	1/1	0.22	-	89,89,89,89	0
61	MG	AA	3187	1/1	0.57	-	65,65,65,65	0
61	MG	AA	3242	1/1	0.35	-	58,58,58,58	0
61	MG	BA	1798	1/1	0.31	-	89,89,89,89	0
61	MG	DA	3162	1/1	0.25	-	70,70,70,70	0
61	MG	DA	3341	1/1	0.47	-	62,62,62,62	0
61	MG	AA	3071	1/1	0.16	-	99,99,99,99	0
61	MG	AA	3119	1/1	0.18	-	64,64,64,64	0
61	MG	DA	3228	1/1	0.41	-	71,71,71,71	0
61	MG	DA	3005	1/1	0.37	-	83,83,83,83	0
61	MG	AA	3308	1/1	0.25	-	58,58,58,58	0
61	MG	BA	1688	1/1	0.20	-	76,76,76,76	0
61	MG	AA	3589	1/1	0.29	-	72,72,72,72	0
61	MG	AA	3360	1/1	0.41	-	89,89,89,89	0
61	MG	AA	3378	1/1	0.68	-	86,86,86,86	0
61	MG	AA	3606	1/1	0.21	-	77,77,77,77	0
61	MG	DA	3086	1/1	1.65	-	98,98,98,98	0
61	MG	DA	3484	1/1	0.53	-	46,46,46,46	0
61	MG	AA	3266	1/1	0.18	-	47,47,47,47	0
61	MG	DA	3129	1/1	0.29	-	55,55,55,55	0
61	MG	CA	1676	1/1	0.43	-	55,55,55,55	0
61	MG	AA	3240	1/1	0.37	-	76,76,76,76	0
61	MG	BA	1712	1/1	0.44	-	125,125,125,125	0
61	MG	DB	212	1/1	0.33	-	94,94,94,94	0
61	MG	AA	3562	1/1	0.31	-	96,96,96,96	0
61	MG	BD	101	1/1	0.38	-	108,108,108,108	0
61	MG	AB	215	1/1	0.10	-	92,92,92,92	0
61	MG	AA	3337	1/1	0.75	-	88,88,88,88	0
61	MG	DA	3205	1/1	0.34	-	60,60,60,60	0
61	MG	CB	105	1/1	0.26	-	80,80,80,80	0
61	MG	DA	3009	1/1	0.25	-	88,88,88,88	0
61	MG	AA	3421	1/1	0.20	-	64,64,64,64	0
61	MG	AA	3370	1/1	0.19	-	103,103,103,103	0
61	MG	DA	3059	1/1	0.57	-	104,104,104,104	0
61	MG	AA	3202	1/1	0.43	-	55,55,55,55	0
61	MG	BA	1684	1/1	0.29	-	100,100,100,100	0
61	MG	BA	1759	1/1	0.22	-	97,97,97,97	0
61	MG	DA	3140	1/1	0.69	-	49,49,49,49	0
61	MG	DA	3010	1/1	0.38	-	121,121,121,121	0
61	MG	AA	3386	1/1	0.33	-	74,74,74,74	0
61	MG	AA	3346	1/1	0.38	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1609	1/1	0.18	-	108,108,108,108	0
61	MG	DA	3038	1/1	0.27	-	102,102,102,102	0
61	MG	DA	3247	1/1	0.40	-	71,71,71,71	0
61	MG	CA	1732	1/1	0.17	-	93,93,93,93	0
61	MG	CA	1807	1/1	0.84	-	121,121,121,121	0
61	MG	DA	3231	1/1	0.30	-	55,55,55,55	0
61	MG	AA	3192	1/1	0.19	-	90,90,90,90	0
61	MG	CA	1654	1/1	0.15	-	88,88,88,88	0
61	MG	BA	1757	1/1	0.32	-	88,88,88,88	0
61	MG	DA	3055	1/1	0.65	-	80,80,80,80	0
61	MG	DA	3340	1/1	0.26	-	107,107,107,107	0
61	MG	BA	1793	1/1	0.17	-	82,82,82,82	0
61	MG	DA	3442	1/1	0.25	-	96,96,96,96	0
61	MG	DA	3528	1/1	0.33	-	87,87,87,87	0
61	MG	DA	3445	1/1	0.24	-	72,72,72,72	0
61	MG	DA	3483	1/1	0.71	-	45,45,45,45	0
61	MG	DA	3178	1/1	0.33	-	45,45,45,45	0
61	MG	AA	3229	1/1	0.11	-	18,18,18,18	0
61	MG	AA	3110	1/1	0.24	-	39,39,39,39	0
61	MG	BA	1762	1/1	0.56	-	85,85,85,85	0
61	MG	DA	3251	1/1	0.14	-	50,50,50,50	0
61	MG	BA	1724	1/1	0.23	-	100,100,100,100	0
61	MG	DA	3036	1/1	0.33	-	87,87,87,87	0
61	MG	AA	3463	1/1	0.74	-	108,108,108,108	0
61	MG	DA	3264	1/1	0.18	-	76,76,76,76	0
61	MG	BA	1633	1/1	0.28	-	75,75,75,75	0
61	MG	AA	3320	1/1	0.42	-	70,70,70,70	0
61	MG	AA	3573	1/1	0.37	-	47,47,47,47	0
61	MG	DA	3451	1/1	0.58	-	65,65,65,65	0
61	MG	BA	1692	1/1	0.27	-	132,132,132,132	0
61	MG	CA	1679	1/1	0.40	-	84,84,84,84	0
61	MG	D1	202	1/1	0.60	-	102,102,102,102	0
61	MG	AA	3601	1/1	0.31	-	79,79,79,79	0
61	MG	A2	201	1/1	0.34	-	81,81,81,81	0
61	MG	BA	1649	1/1	0.26	-	85,85,85,85	0
61	MG	AA	3087	1/1	0.26	-	45,45,45,45	0
61	MG	DA	3187	1/1	0.54	-	40,40,40,40	0
61	MG	AA	3014	1/1	0.53	-	41,41,41,41	0
61	MG	AA	3608	1/1	0.52	-	69,69,69,69	0
61	MG	AA	3169	1/1	0.19	-	74,74,74,74	0
61	MG	CB	102	1/1	0.42	-	94,94,94,94	0
61	MG	AA	3554	1/1	0.43	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3356	1/1	0.32	-	80,80,80,80	0
61	MG	AB	210	1/1	0.29	-	71,71,71,71	0
61	MG	AA	3129	1/1	0.29	-	75,75,75,75	0
61	MG	DA	3155	1/1	0.48	-	49,49,49,49	0
61	MG	AA	3089	1/1	0.37	-	44,44,44,44	0
61	MG	DA	3449	1/1	0.55	-	96,96,96,96	0
61	MG	AA	3272	1/1	0.12	-	86,86,86,86	0
61	MG	DA	3300	1/1	0.37	-	71,71,71,71	0
61	MG	BA	1646	1/1	0.32	-	70,70,70,70	0
61	MG	BA	1678	1/1	0.31	-	75,75,75,75	0
61	MG	CA	1693	1/1	0.59	-	73,73,73,73	0
61	MG	DA	3179	1/1	0.48	-	56,56,56,56	0
61	MG	CA	1674	1/1	0.28	-	76,76,76,76	0
61	MG	BA	1804	1/1	0.47	-	80,80,80,80	0
61	MG	BA	1619	1/1	0.28	-	67,67,67,67	0
61	MG	AA	3550	1/1	0.60	-	52,52,52,52	0
61	MG	DU	201	1/1	0.22	-	72,72,72,72	0
61	MG	DA	3525	1/1	0.32	-	88,88,88,88	0
61	MG	AA	3462	1/1	0.35	-	69,69,69,69	0
61	MG	DA	3321	1/1	0.27	-	81,81,81,81	0
61	MG	BN	201	1/1	0.18	-	67,67,67,67	0
61	MG	AA	3190	1/1	0.15	-	83,83,83,83	0
61	MG	AA	3146	1/1	0.37	-	62,62,62,62	0
61	MG	DA	3096	1/1	0.35	-	47,47,47,47	0
61	MG	AA	3557	1/1	0.54	-	68,68,68,68	0
61	MG	DA	3133	1/1	0.31	-	77,77,77,77	0
61	MG	AA	3344	1/1	0.49	-	71,71,71,71	0
61	MG	DA	3061	1/1	0.45	-	67,67,67,67	0
61	MG	CA	1606	1/1	0.28	-	96,96,96,96	0
61	MG	AA	3138	1/1	0.64	-	41,41,41,41	0
61	MG	AA	3212	1/1	0.53	-	56,56,56,56	0
61	MG	CA	1802	1/1	0.10	-	107,107,107,107	0
61	MG	DA	3398	1/1	0.23	-	107,107,107,107	0
61	MG	DA	3261	1/1	0.41	-	89,89,89,89	0
61	MG	CA	1757	1/1	0.24	-	83,83,83,83	0
61	MG	AA	3247	1/1	0.47	-	76,76,76,76	0
61	MG	BA	1605	1/1	0.20	-	69,69,69,69	0
61	MG	DA	3509	1/1	0.45	-	65,65,65,65	0
61	MG	AA	3450	1/1	0.35	-	84,84,84,84	0
61	MG	CA	1683	1/1	0.52	-	84,84,84,84	0
61	MG	DA	3157	1/1	0.42	-	51,51,51,51	0
61	MG	AA	3013	1/1	0.35	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3034	1/1	0.30	-	61,61,61,61	0
61	MG	BA	1664	1/1	0.32	-	52,52,52,52	0
61	MG	AA	3487	1/1	0.16	-	78,78,78,78	0
61	MG	BA	1608	1/1	0.32	-	63,63,63,63	0
61	MG	BA	1827	1/1	0.38	-	85,85,85,85	0
61	MG	DA	3198	1/1	0.54	-	68,68,68,68	0
61	MG	AA	3493	1/1	0.40	-	89,89,89,89	0
61	MG	BA	1666	1/1	0.51	-	74,74,74,74	0
61	MG	AA	3481	1/1	0.61	-	66,66,66,66	0
61	MG	CA	1792	1/1	0.24	-	91,91,91,91	0
61	MG	CA	1694	1/1	0.24	-	94,94,94,94	0
61	MG	AA	3440	1/1	0.26	-	83,83,83,83	0
61	MG	DA	3306	1/1	0.78	-	73,73,73,73	0
61	MG	DA	3118	1/1	0.19	-	72,72,72,72	0
61	MG	AA	3173	1/1	0.54	-	70,70,70,70	0
61	MG	CA	1621	1/1	0.43	-	84,84,84,84	0
61	MG	AA	3204	1/1	0.30	-	56,56,56,56	0
61	MG	DA	3275	1/1	0.38	-	81,81,81,81	0
61	MG	AB	208	1/1	0.18	-	87,87,87,87	0
61	MG	CA	1626	1/1	0.25	-	103,103,103,103	0
61	MG	DA	3492	1/1	0.57	-	48,48,48,48	0
61	MG	DA	3454	1/1	0.14	-	108,108,108,108	0
61	MG	DA	3440	1/1	0.25	-	92,92,92,92	0
61	MG	AA	3051	1/1	0.40	-	51,51,51,51	0
61	MG	AA	3142	1/1	0.17	-	61,61,61,61	0
61	MG	DA	3495	1/1	0.60	-	65,65,65,65	0
61	MG	AA	3230	1/1	0.15	-	112,112,112,112	0
61	MG	DA	3393	1/1	0.21	-	93,93,93,93	0
61	MG	AA	3241	1/1	0.17	-	101,101,101,101	0
61	MG	AA	3022	1/1	0.33	-	43,43,43,43	0
61	MG	CA	1666	1/1	0.18	-	76,76,76,76	0
61	MG	AA	3331	1/1	0.35	-	79,79,79,79	0
61	MG	DA	3171	1/1	0.28	-	81,81,81,81	0
61	MG	AA	3069	1/1	0.18	-	64,64,64,64	0
61	MG	AA	3231	1/1	0.48	-	120,120,120,120	0
61	MG	BB	102	1/1	0.32	-	86,86,86,86	0
61	MG	CA	1635	1/1	0.26	-	87,87,87,87	0
61	MG	AA	3620	1/1	0.29	-	99,99,99,99	0
61	MG	AA	3472	1/1	0.10	-	81,81,81,81	0
61	MG	AA	3158	1/1	0.64	-	66,66,66,66	0
61	MG	CA	1739	1/1	0.48	-	69,69,69,69	0
61	MG	DA	3259	1/1	0.73	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3160	1/1	0.32	-	65,65,65,65	0
61	MG	DA	3095	1/1	0.34	-	45,45,45,45	0
61	MG	AE	302	1/1	0.44	-	38,38,38,38	0
61	MG	DA	3427	1/1	0.43	-	78,78,78,78	0
61	MG	AA	3340	1/1	0.42	-	61,61,61,61	0
61	MG	CA	1728	1/1	0.39	-	58,58,58,58	0
61	MG	DB	210	1/1	0.16	-	76,76,76,76	0
61	MG	AA	3471	1/1	0.22	-	69,69,69,69	0
61	MG	DA	3422	1/1	0.20	-	96,96,96,96	0
61	MG	DA	3172	1/1	0.34	-	59,59,59,59	0
61	MG	AA	3267	1/1	0.24	-	80,80,80,80	0
61	MG	AA	3093	1/1	0.17	-	55,55,55,55	0
61	MG	BA	1637	1/1	0.13	-	93,93,93,93	0
61	MG	DA	3015	1/1	0.18	-	83,83,83,83	0
61	MG	DA	3497	1/1	0.19	-	62,62,62,62	0
61	MG	AA	3045	1/1	0.27	-	50,50,50,50	0
61	MG	DA	3197	1/1	0.60	-	52,52,52,52	0
61	MG	DA	3152	1/1	0.17	-	44,44,44,44	0
61	MG	DA	3351	1/1	0.35	-	70,70,70,70	0
61	MG	BA	1777	1/1	0.09	-	88,88,88,88	0
61	MG	DA	3084	1/1	0.44	-	87,87,87,87	0
61	MG	AA	3152	1/1	0.46	-	53,53,53,53	0
61	MG	DA	3325	1/1	0.29	-	70,70,70,70	0
61	MG	AA	3232	1/1	0.22	-	47,47,47,47	0
61	MG	DA	3170	1/1	0.77	-	66,66,66,66	0
61	MG	AA	3023	1/1	0.49	-	52,52,52,52	0
61	MG	BA	1707	1/1	0.33	-	94,94,94,94	0
61	MG	CA	1758	1/1	0.31	-	64,64,64,64	0
61	MG	DA	3233	1/1	0.87	-	84,84,84,84	0
61	MG	AA	3486	1/1	0.27	-	96,96,96,96	0
61	MG	CA	1787	1/1	0.37	-	84,84,84,84	0
61	MG	AA	3390	1/1	0.36	-	73,73,73,73	0
61	MG	AA	3132	1/1	0.29	-	89,89,89,89	0
61	MG	BA	1705	1/1	0.34	-	70,70,70,70	0
61	MG	CA	1756	1/1	0.55	-	93,93,93,93	0
61	MG	BA	1787	1/1	0.26	-	107,107,107,107	0
61	MG	BA	1843	1/1	0.64	-	87,87,87,87	0
61	MG	DA	3486	1/1	0.59	-	46,46,46,46	0
61	MG	AA	3561	1/1	0.14	-	88,88,88,88	0
61	MG	AA	3171	1/1	0.31	-	81,81,81,81	0
61	MG	DA	3186	1/1	0.43	-	56,56,56,56	0
61	MG	AA	3548	1/1	0.22	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	CA	1754	1/1	0.30	-	84,84,84,84	0
61	MG	DA	3244	1/1	0.42	-	106,106,106,106	0
61	MG	AA	3384	1/1	0.51	-	79,79,79,79	0
61	MG	DA	3360	1/1	0.24	-	96,96,96,96	0
61	MG	AA	3447	1/1	0.18	-	51,51,51,51	0
61	MG	DA	3134	1/1	0.51	-	56,56,56,56	0
61	MG	DA	3433	1/1	0.43	-	110,110,110,110	0
61	MG	AA	3304	1/1	0.31	-	59,59,59,59	0
61	MG	AA	3117	1/1	0.31	-	62,62,62,62	0
61	MG	AA	3291	1/1	0.64	-	70,70,70,70	0
61	MG	AA	3459	1/1	0.46	-	110,110,110,110	0
61	MG	AA	3306	1/1	0.37	-	63,63,63,63	0
61	MG	AA	3066	1/1	0.82	-	103,103,103,103	0
61	MG	CA	1613	1/1	0.17	-	84,84,84,84	0
61	MG	DA	3453	1/1	0.56	-	94,94,94,94	0
61	MG	AA	3359	1/1	0.51	-	60,60,60,60	0
61	MG	DA	3400	1/1	0.52	-	82,82,82,82	0
61	MG	BA	1805	1/1	0.51	-	62,62,62,62	0
61	MG	BA	1648	1/1	0.24	-	77,77,77,77	0
61	MG	AA	3037	1/1	0.13	-	50,50,50,50	0
61	MG	DA	3234	1/1	0.49	-	55,55,55,55	0
61	MG	AA	3526	1/1	0.28	-	57,57,57,57	0
61	MG	DA	3354	1/1	0.21	-	92,92,92,92	0
61	MG	DA	3490	1/1	0.41	-	49,49,49,49	0
61	MG	BA	1632	1/1	0.23	-	72,72,72,72	0
61	MG	DA	3459	1/1	0.52	-	49,49,49,49	0
61	MG	AA	3296	1/1	0.13	-	75,75,75,75	0
61	MG	DA	3150	1/1	0.72	-	76,76,76,76	0
61	MG	DA	3026	1/1	0.43	-	82,82,82,82	0
61	MG	DA	3165	1/1	0.28	-	73,73,73,73	0
61	MG	DA	3276	1/1	0.13	-	86,86,86,86	0
61	MG	AA	3294	1/1	0.46	-	99,99,99,99	0
61	MG	AA	3003	1/1	0.44	-	43,43,43,43	0
61	MG	AA	3186	1/1	0.32	-	77,77,77,77	0
61	MG	AA	3338	1/1	0.28	-	72,72,72,72	0
61	MG	CA	1695	1/1	0.36	-	77,77,77,77	0
61	MG	AA	3531	1/1	0.57	-	53,53,53,53	0
61	MG	BA	1626	1/1	0.63	-	76,76,76,76	0
61	MG	DA	3277	1/1	0.35	-	77,77,77,77	0
61	MG	AA	3507	1/1	0.24	-	62,62,62,62	0
61	MG	DA	3148	1/1	0.41	-	42,42,42,42	0
61	MG	AA	3593	1/1	0.37	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3314	1/1	0.45	-	82,82,82,82	0
61	MG	BA	1709	1/1	0.25	-	101,101,101,101	0
61	MG	AA	3582	1/1	0.26	-	33,33,33,33	0
61	MG	AA	3237	1/1	0.28	-	81,81,81,81	0
61	MG	DA	3035	1/1	0.62	-	102,102,102,102	0
61	MG	CA	1687	1/1	0.25	-	99,99,99,99	0
61	MG	AA	3628	1/1	0.26	-	89,89,89,89	0
61	MG	DA	3135	1/1	0.19	-	64,64,64,64	0
61	MG	AA	3407	1/1	0.30	-	84,84,84,84	0
61	MG	BA	1808	1/1	0.40	-	69,69,69,69	0
61	MG	CA	1773	1/1	0.29	-	115,115,115,115	0
61	MG	BA	1821	1/1	0.23	-	78,78,78,78	0
61	MG	DA	3368	1/1	0.47	-	87,87,87,87	0
61	MG	AA	3032	1/1	0.34	-	60,60,60,60	0
61	MG	DA	3527	1/1	0.44	-	96,96,96,96	0
61	MG	CA	1795	1/1	0.25	-	110,110,110,110	0
61	MG	BA	1728	1/1	0.70	-	90,90,90,90	0
61	MG	AA	3485	1/1	0.50	-	96,96,96,96	0
61	MG	AA	3400	1/1	0.64	-	86,86,86,86	0
61	MG	CC	104	1/1	0.45	-	90,90,90,90	0
61	MG	AA	3349	1/1	0.17	-	79,79,79,79	0
61	MG	DA	3136	1/1	0.19	-	97,97,97,97	0
61	MG	CA	1746	1/1	0.57	-	59,59,59,59	0
61	MG	BA	1841	1/1	0.28	-	105,105,105,105	0
61	MG	AA	3395	1/1	0.16	-	57,57,57,57	0
61	MG	DB	202	1/1	0.13	-	101,101,101,101	0
61	MG	AA	3502	1/1	0.38	-	81,81,81,81	0
61	MG	DA	3384	1/1	0.55	-	64,64,64,64	0
61	MG	AA	3021	1/1	0.39	-	38,38,38,38	0
61	MG	DA	3221	1/1	0.51	-	66,66,66,66	0
61	MG	BA	1758	1/1	0.23	-	110,110,110,110	0
61	MG	AA	3352	1/1	0.43	-	91,91,91,91	0
61	MG	AA	3549	1/1	0.55	-	41,41,41,41	0
61	MG	AA	3094	1/1	0.34	-	81,81,81,81	0
61	MG	DA	3041	1/1	0.48	-	91,91,91,91	0
61	MG	DA	3474	1/1	0.61	-	103,103,103,103	0
61	MG	CA	1647	1/1	0.40	-	65,65,65,65	0
61	MG	CA	1672	1/1	0.53	-	76,76,76,76	0
61	MG	AA	3197	1/1	0.54	-	63,63,63,63	0
61	MG	DA	3029	1/1	0.26	-	92,92,92,92	0
61	MG	DA	3017	1/1	0.57	-	88,88,88,88	0
61	MG	DA	3180	1/1	0.45	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	DA	3111	1/1	0.17	-	67,67,67,67	0
61	MG	DA	3145	1/1	0.50	-	54,54,54,54	0
61	MG	CA	1614	1/1	0.46	-	95,95,95,95	0
61	MG	DA	3410	1/1	0.49	-	99,99,99,99	0
61	MG	A3	101	1/1	0.43	-	80,80,80,80	0
61	MG	AA	3555	1/1	0.41	-	68,68,68,68	0
61	MG	DA	3100	1/1	0.24	-	62,62,62,62	0
61	MG	AA	3546	1/1	0.27	-	33,33,33,33	0
61	MG	AA	3629	1/1	0.51	-	107,107,107,107	0
61	MG	DA	3331	1/1	0.25	-	76,76,76,76	0
61	MG	AA	3201	1/1	0.42	-	42,42,42,42	0
61	MG	CA	1727	1/1	0.15	-	84,84,84,84	0
61	MG	CA	1764	1/1	0.48	-	67,67,67,67	0
61	MG	AA	3567	1/1	0.49	-	38,38,38,38	0
61	MG	DA	3343	1/1	0.44	-	145,145,145,145	0
61	MG	AA	3483	1/1	0.24	-	70,70,70,70	0
61	MG	CA	1612	1/1	0.40	-	91,91,91,91	0
61	MG	AA	3144	1/1	0.68	-	51,51,51,51	0
61	MG	CA	1616	1/1	0.14	-	90,90,90,90	0
61	MG	DA	3441	1/1	0.10	-	67,67,67,67	0
61	MG	AA	3252	1/1	0.22	-	68,68,68,68	0
61	MG	AA	3505	1/1	0.24	-	103,103,103,103	0
61	MG	DA	3477	1/1	0.59	-	125,125,125,125	0
61	MG	AA	3004	1/1	0.40	-	37,37,37,37	0
61	MG	AA	3587	1/1	0.15	-	28,28,28,28	0
61	MG	BA	1651	1/1	0.43	-	73,73,73,73	0
61	MG	BA	1658	1/1	0.71	-	54,54,54,54	0
61	MG	BA	1652	1/1	0.29	-	86,86,86,86	0
61	MG	CA	1631	1/1	0.22	-	95,95,95,95	0
61	MG	AA	3581	1/1	0.48	-	67,67,67,67	0
61	MG	DA	3031	1/1	0.27	-	69,69,69,69	0
61	MG	DA	3526	1/1	0.27	-	92,92,92,92	0
61	MG	BA	1756	1/1	0.57	-	96,96,96,96	0
61	MG	BA	1721	1/1	0.38	-	109,109,109,109	0
61	MG	DA	3295	1/1	0.42	-	66,66,66,66	0
61	MG	CA	1648	1/1	0.26	-	65,65,65,65	0
61	MG	CA	1668	1/1	0.36	-	75,75,75,75	0
61	MG	AA	3615	1/1	0.32	-	84,84,84,84	0
61	MG	AA	3443	1/1	0.20	-	95,95,95,95	0
61	MG	CA	1663	1/1	0.25	-	72,72,72,72	0
61	MG	DA	3204	1/1	0.40	-	50,50,50,50	0
61	MG	AA	3591	1/1	1.22	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	MG	AA	3468	1/1	0.49	-	92,92,92,92	0
61	MG	AA	3394	1/1	0.16	-	85,85,85,85	0
61	MG	CA	1806	1/1	0.27	-	115,115,115,115	0
61	MG	AA	3148	1/1	0.42	-	70,70,70,70	0
61	MG	BN	202	1/1	0.46	-	104,104,104,104	0
61	MG	CA	1724	1/1	0.53	-	88,88,88,88	0
61	MG	BA	1746	1/1	0.43	-	95,95,95,95	0
61	MG	BA	1765	1/1	0.28	-	99,99,99,99	0
61	MG	AA	3577	1/1	0.41	-	42,42,42,42	0
61	MG	B1	101	1/1	0.23	-	64,64,64,64	0
61	MG	CA	1750	1/1	0.49	-	91,91,91,91	0
61	MG	DP	201	1/1	0.28	-	63,63,63,63	0
61	MG	AA	3313	1/1	0.33	-	62,62,62,62	0
61	MG	AA	3364	1/1	0.50	-	89,89,89,89	0
61	MG	DA	3501	1/1	0.40	-	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.