



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:55 PM BST

PDB ID : 4V8B  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-06  
Resolution : 3.00 Å(reported)

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

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

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

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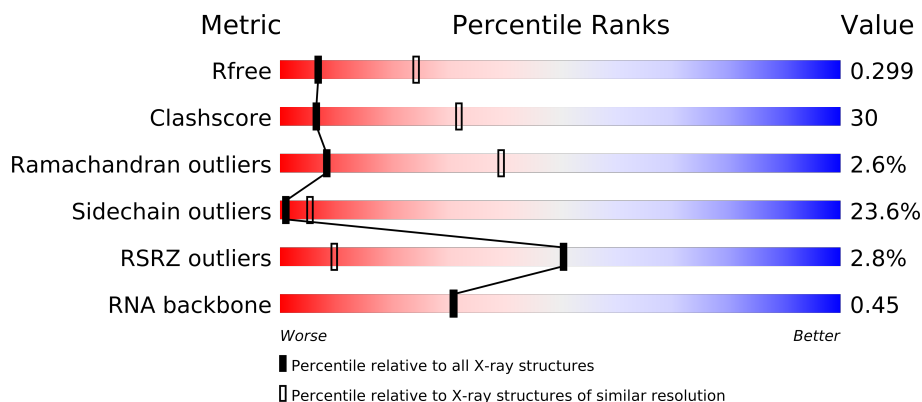
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	
1	CA	1506	
2	AE	256	
2	CE	256	
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	

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Mol	Chain	Length	Quality of chain
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	87	
22	CB	87	
23	AC	77	
23	AD	77	
23	CC	77	
23	CD	77	
24	A1	10	
24	C1	10	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

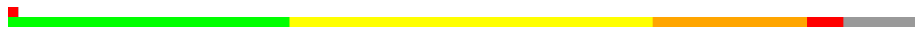
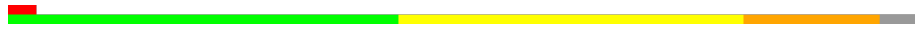


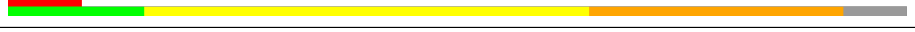
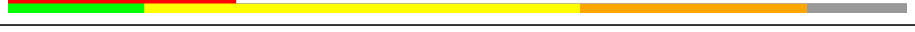
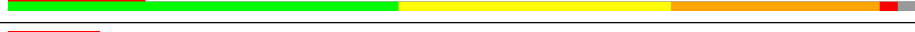



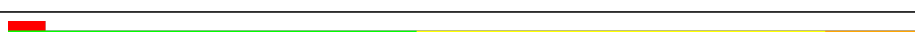
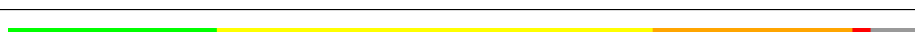
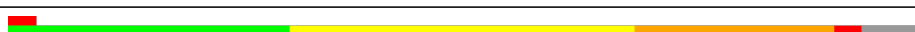
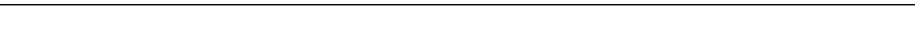
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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	

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Mol	Chain	Length	Quality of chain
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299552 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

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

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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



- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

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

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
22	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	AD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
24	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 25 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2912	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
25	DA	2907	Total 62607	C 27866	N 11712	O 20123	P 2906	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	EXPRESSION TAG	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	168	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			



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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	623	Total 623	Mg 623	0	0
55	CA	207	Total 207	Mg 207	0	0
55	AB	5	Total 5	Mg 5	0	0
55	B8	1	Total 1	Mg 1	0	0
55	BE	5	Total 5	Mg 5	0	0
55	DU	1	Total 1	Mg 1	0	0
55	B1	1	Total 1	Mg 1	0	0
55	AN	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	BB	17	Total 17	Mg 17	0	0
55	D3	1	Total 1	Mg 1	0	0
55	BF	3	Total 3	Mg 3	0	0
55	DR	1	Total 1	Mg 1	0	0
55	B2	1	Total 1	Mg 1	0	0
55	AA	242	Total 242	Mg 242	0	0
55	CG	2	Total 2	Mg 2	0	0
55	BU	2	Total 2	Mg 2	0	0
55	A1	2	Total 2	Mg 2	0	0
55	AD	1	Total 1	Mg 1	0	0
55	CC	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	Mg 3	0	0
55	B3	1	Total 1	Mg 1	0	0
55	DA	526	Total 526	Mg 526	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	1	Total 1	Mg 1	0	0
55	BO	2	Total 2	Mg 2	0	0
55	AQ	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	AH	1	Total 1	Mg 1	0	0
55	DP	1	Total 1	Mg 1	0	0
55	AC	9	Total 9	Mg 9	0	0
55	CB	3	Total 3	Mg 3	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B0	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	DB	14	Total 14	Mg 14	0	0

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

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

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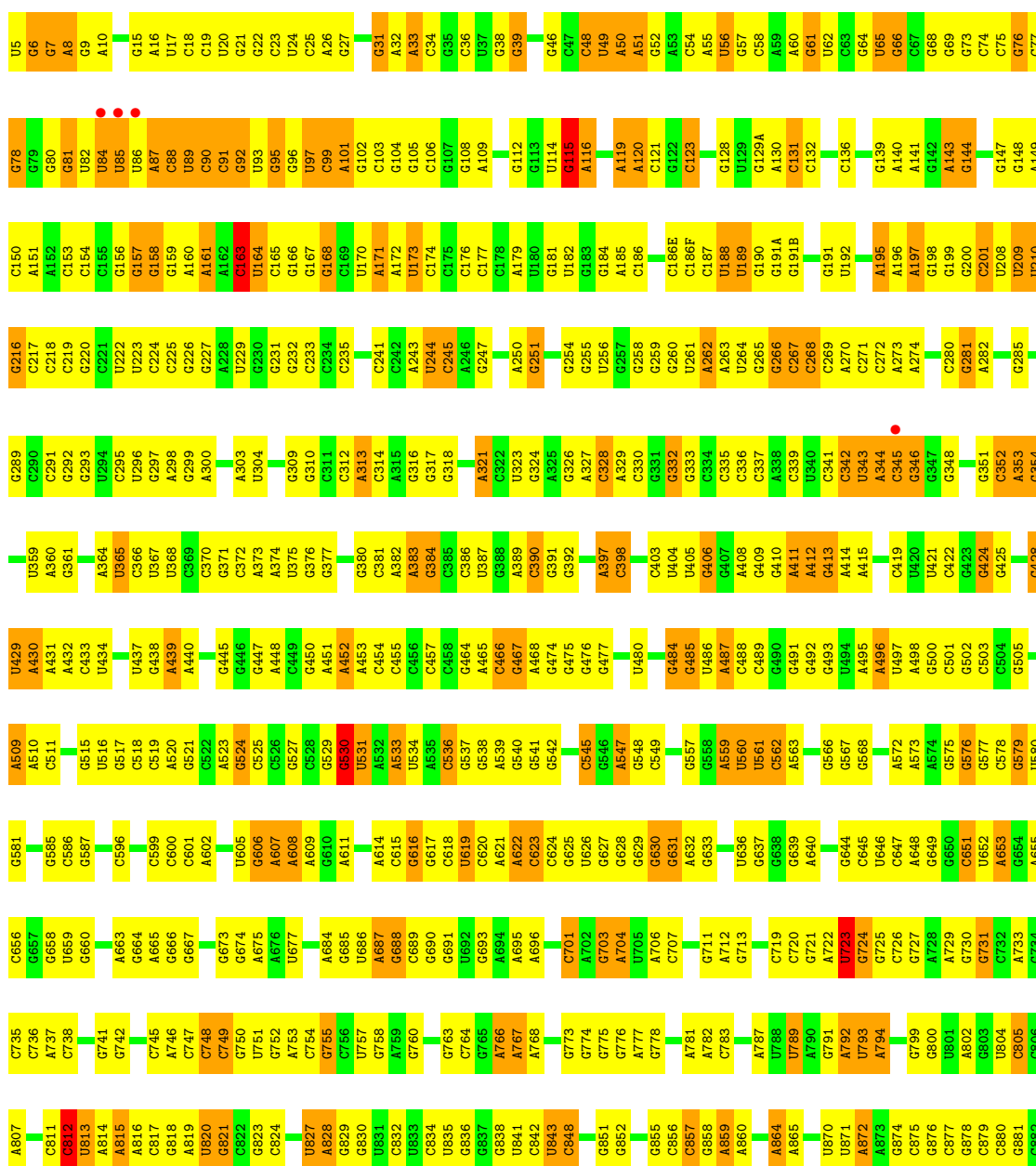
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

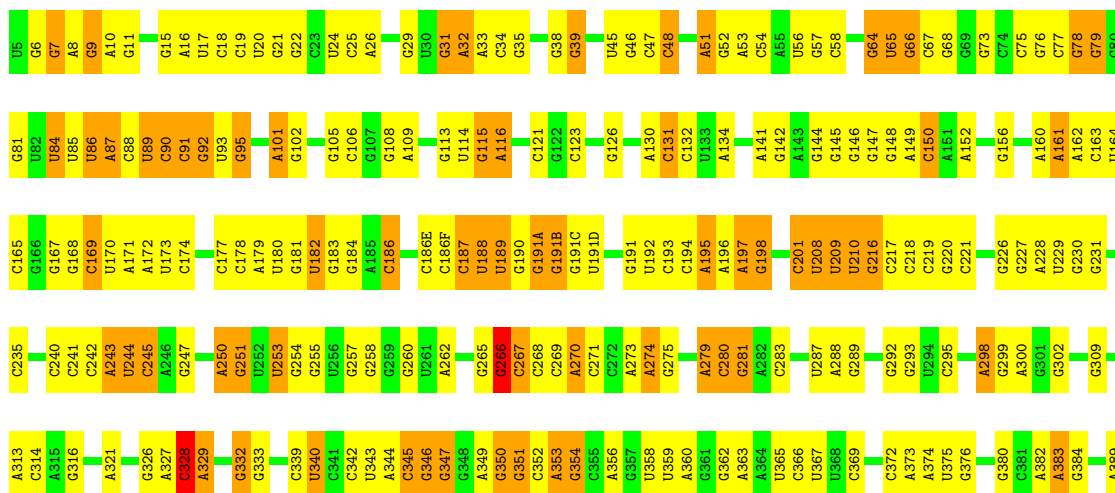
### 3 Residue-property plots

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: 16S ribosomal RNA

Chain AA:



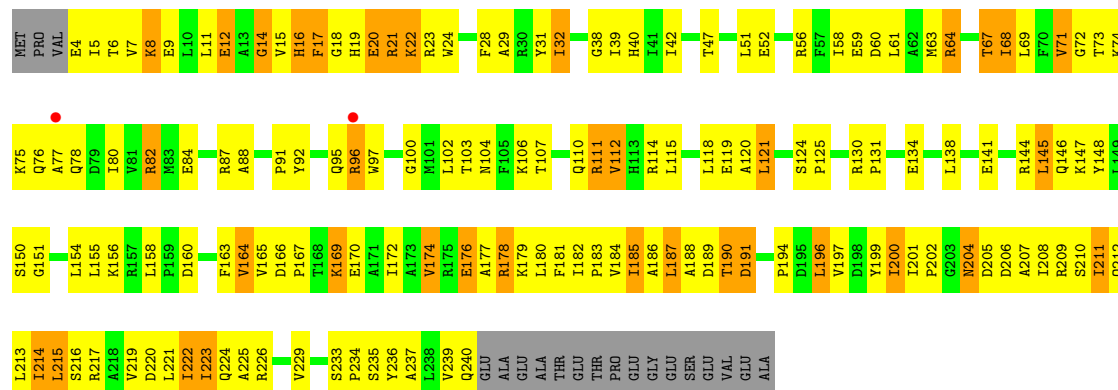


G1416	A1350	G1287	C1223	G1160	G1034	A978	G917	G755	G682	G612	G541	G467	C390
G1417	U1351	A1288	G1224	C1161	A1035	C979	A918	C756	G683	G613	G542	A468	G391
G1418	C1352	A1289	A1225	C1162	G1036	C980	A919	U757	A684	G616	C543	G474	G392
G1419	G1353	C1290	C1226	C1163	C1037	C981	U920	G758	G685	U981	G544	G475	A393
	C1354	A1291	A1227	C1164	C1038	C982	U921		U686	G617	C545	G476	G394
G1423	G1355	U1292	C1228	C1165	G1039	A983	G836	G763	A687	C618	G546	G477	C395
G1424	G1356	C1293		G1166	C1040	C984	G938	C764	G688	U619	A547	A478	G396
	A1357	G1294	G1231	G1106	A1041	C985	U941	C765	C689	C620	G548		A397
C1429	U1358	G1295	U1232	G1107	G1042	A986	G926	A766	C690	A621	C549	G481	C398
C1430		C1296	G1233	G1108	C1043	C987	G927		G691	G624	U551	A482	U404
	G1361	C1297	C1234	C1109	G1044	C988	G928	G769	U692	G625	U552	G484	U405
A1434	C1362	U1298	U1235	A1110	G1045	C989	G929	G773	G693	U626	A553	G485	G406
G1435	C1362A	A1299	G1173	A1111	C1046	C990	C930	G774	A694	G627	C554	U486	G407
U1436	A1363	G1300	G1174	C1112	U991	U992	C931	G775	A695	G628	C555	A487	A408
C1437	G1364	U1301	A1176	C1113	G1047	C993	G932	G776	A696	G629	C556	C488	G409
G1438	G1365	C1302	G1177		G1048	C994	G933			G630		C489	G410
C1439	C1366	C1303	G1178	C1116	U1052	A994	C934	A777	G700	G631	A559		A411
	C1367	G1304	A1179	G1117	G1053	C995	A935	G778	C701	A632	U560	A495	A412
G1442	G1368	A1305	C1242	C1118	C1054	A996	C936	C779	A702	G633	U561	U496	G413
G1443	C1369	A1306	C1243	C1119	A1055	U997	A937	A780	G703	C634	C562	U497	A414
	G1370		C1244	G1120	U1056	G998	A938			G635			
	G1371	G1309		U1121	U1057	C998A	A939	G783	U705	A640	U565	G501	U420
	U1372	G1310	U1247	U1122	G1058	U999	G940	C784	A706	G641	C564	G500	U421
C1448	G1373	G1311	A1248	A1123	C1059	U999	G941	G785	C707	U642	G566	G502	C422
	U1450	G1374	G1186	G1124	C1060	G1001	G942	G786		A641	G567	C503	G423
A1451	A1375	U1313	C1249	U1125	G1061	G1002	U943	A787	G710	A642	G568	C504	G424
C1452	U1376	G1314	U1250	U1126	U1062	G1003	G944	U788	G711	G643	C569	G505	G425
G1453	A1377	C1315	A1189	G1127	C1063	A1004	G945		A712	G644	C570	G506	G426
G1454	C1378	G1316	G1184	C1128	G1064	A1005	A946	G791	G713	G645	C571		
	U1379	C1317	G1185	A1129	U1065	G1006	G947	A792	U723	U646	U571		U427
	A1380	A1318	G1186	U1130	C1066	C1007	G948	U793	G718	C647	A572	A509	G428
C1465	U1381	C1319	G1187	C1131	C1067	C1008	A949	A794	C719	A648	A573	A510	U429
C1466	G1382	C1320	A1189	U1132	G1068	G1009	U950	G795	G720	G649	A574	C511	A430
A1468		C1321	C1195	G1133	C1069	G1010	U951	C796	G575	G650	G576	U512	A431
G1469	G1386	C1322	U1196	G1134	U1070		U952	C797	A722	C651	G577	C513	A432
	G1387	G1323	G1197	U1135	C1071	G1013	G953	G798	U724	U652	C578	G514	C433
	C1388	A1324	G1198	U1136	G1072	A1014	G954	G799		A653	C579	G515	U434
		C1325	U1199	C1137	U1073	A1015	U955	G800		G654	G579	U516	C435
			C1200	G1138	G1074	A1016	U956	U801	A728	A655	U580	G517	C436
	U1391	C1326	A1201	G1139		G1017	U957	A802	A729	G656	G581	C518	U437
C1479	G1392	G1202	C1203	C1140	C1075	C1018	A958	G803	U730		U582	C519	G438
U1481	C1393	C1267	C1204	C1141	C1076	C1019	A959	U804	G731	G660	A583	A520	A439
G1482	A1394	U1330	A1268	G1142	G1077	U1020	U960	C805		G661	G584	G521	A440
A1483	C1395	C1330	A1269	G1143		G1021	U961		C736	G662	G585	C522	
	A1396	G1331	C1205	C1144	A1080	G1022	C962	C810	A737	A663	C586		C444
G1486	C1397	A1332	C1270	G1145	G1081	G1023	G963	C811		G664	C587	C526	G445
G1487	A1398	C1333	G1271	C1146	U1082	G1024	A964	C812	U740	A665	G588	G527	G446
G1488	C1399	G1334	G1272	A1146	G1083	U1025	A965	C813	G741		C589	C528	G447
G1489	C1400	C1335	C1273	C1147	U1084	G1026	G966	U813	G742	G668		G529	A448
C1490	G1401	G1337	G1274	U1148	U1085	C1027	U967	A814		U669	G593	G530	C449
G1491	C1402	A1338	A1275	C1149	U1086	C1028	A968	A815	C745	G670		U531	G450
A1492	C1403	A1339	G1276	U1150		C1028A	A969	A816		G671	C600	A532	A451
	C1404		C1277	A1151	G1089	C1028B	C970	C817	A746	U672	C601	A533	A452
	G1494	C1342	U1278	A1152	U1090	C1029	G971	G818	C747	G673	U534	A453	
U1495	U1406	G1343	G1216	C1153	U1091	C1030	G972	A819	C748	G674	G504	A535	C457
C1496	C1496	C1344	C1217	G1154	A1092	G1031	G973	U820	C749	A675	G605	C536	G458
G1497		U1345	U1281	G1155	A1093	G1032	G974	G821	G750	A676	G606	G537	G459
U1498		A1346	C1218	C1156	G1094	A1032	A974		U751		A607	G538	A464
A1499		G1347	U1219	G1157	U1095	G1032A	A975	U827	A752	U677	A608	A539	A465
		C1158	G1220	A1157	C1096	G1032B	A976	A828	A753		A609	G540	C466
A1502	G1415	A1349	G1222	U1159	C1097	G1033	A977	G829	C754	C681			



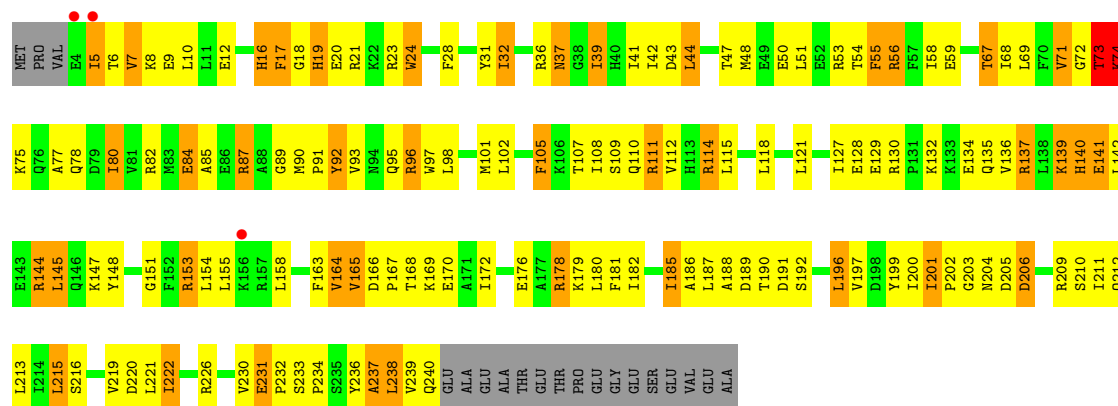
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AE:



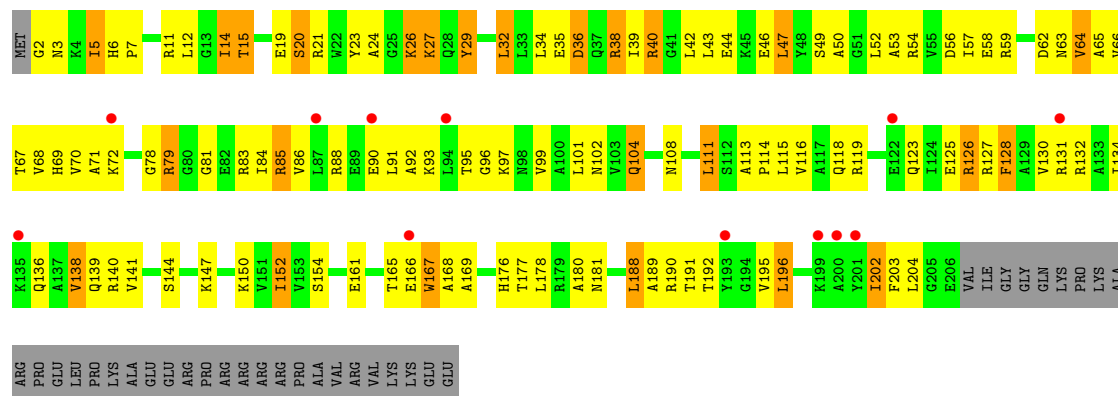
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CE:



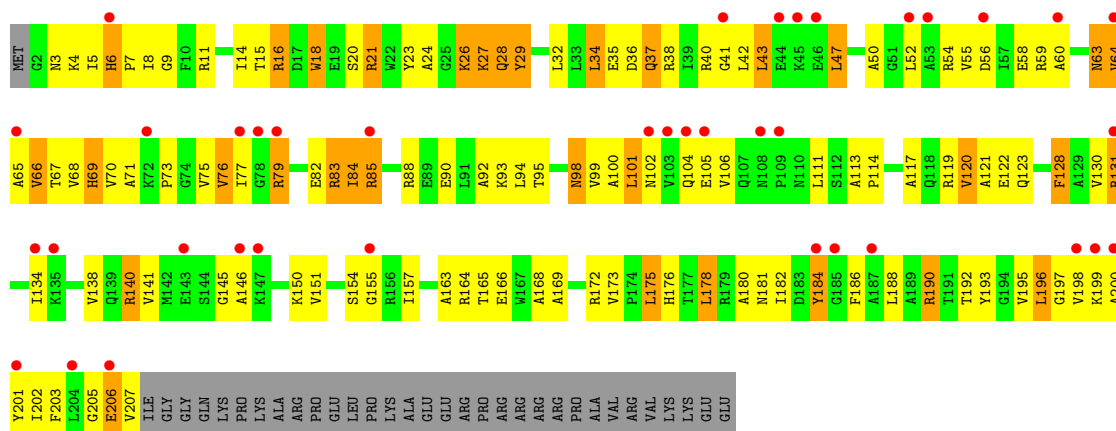
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF:



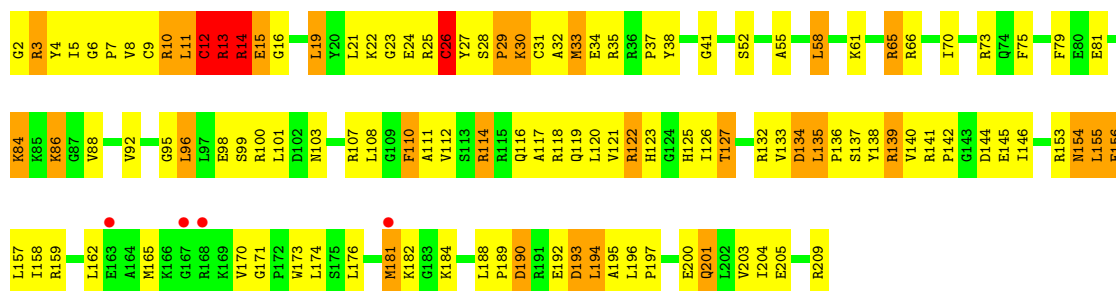
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



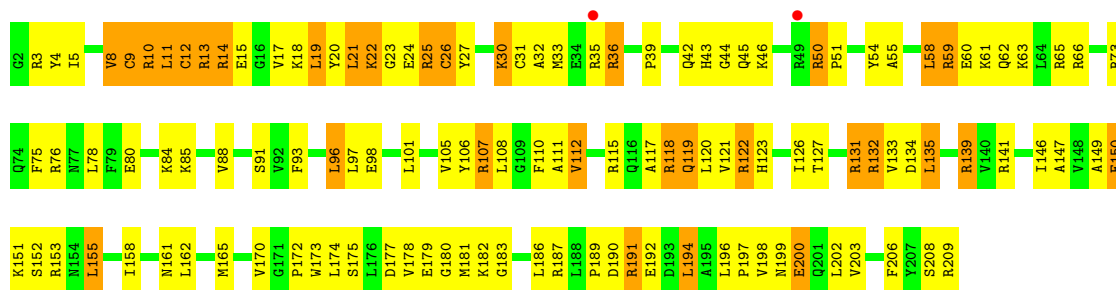
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG:



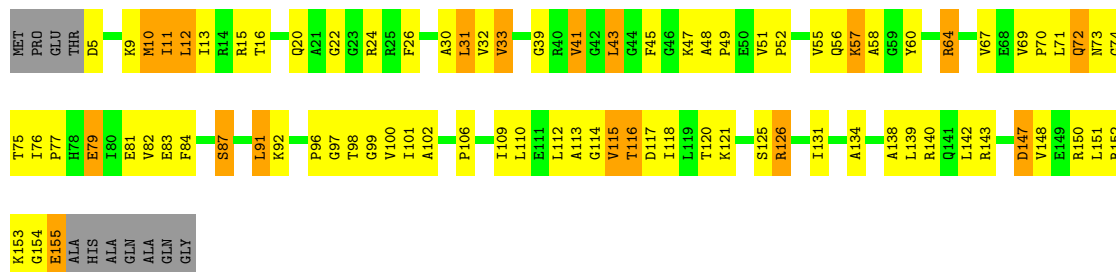
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

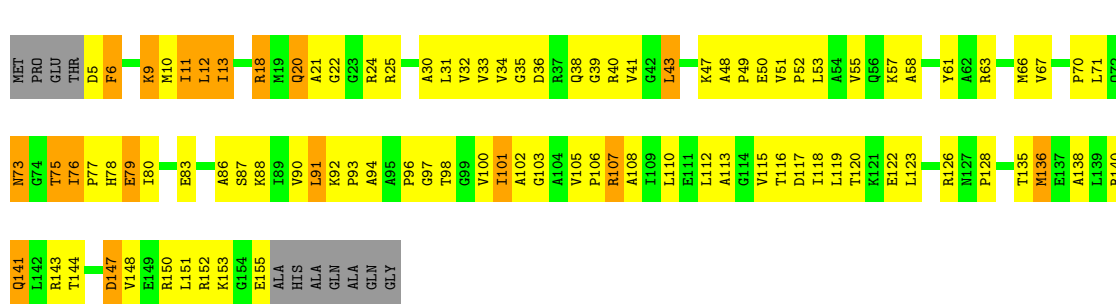
Chain AH:





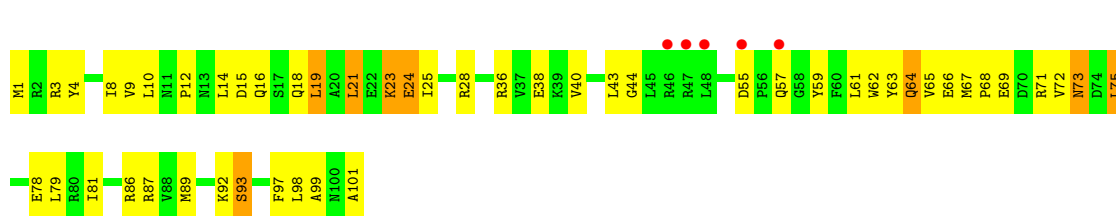
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



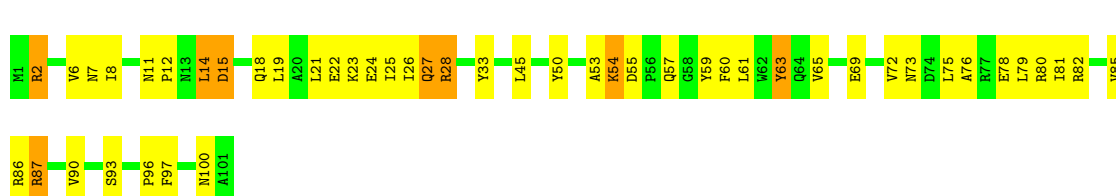
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



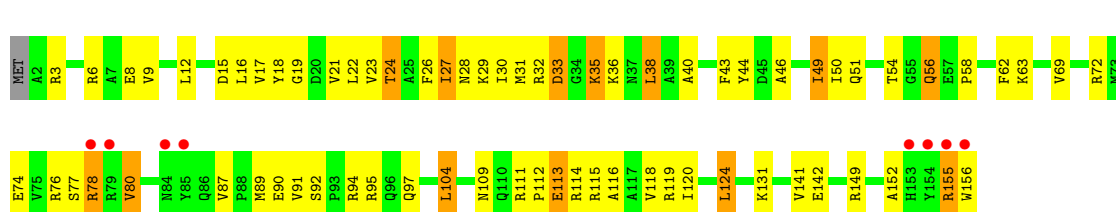
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



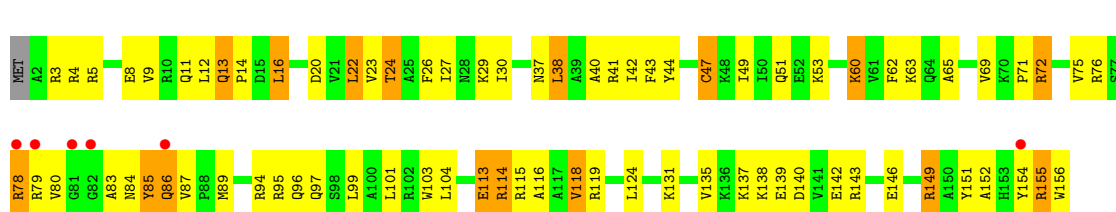
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



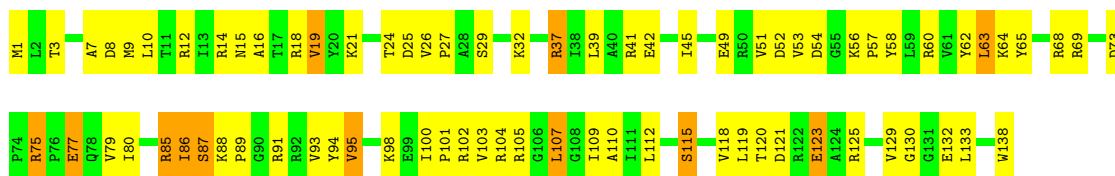
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



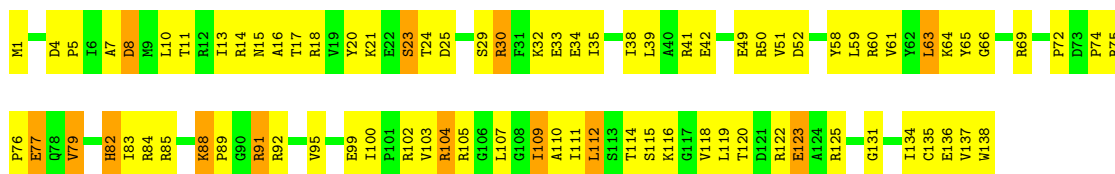
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



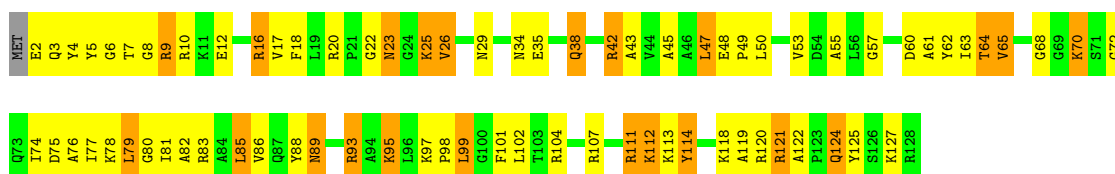
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



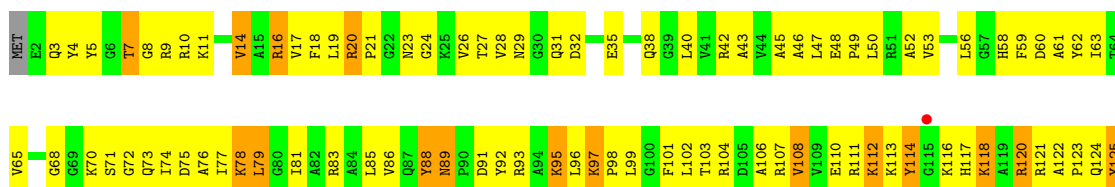
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



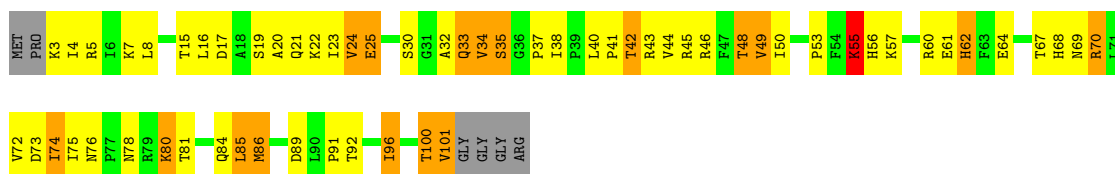
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

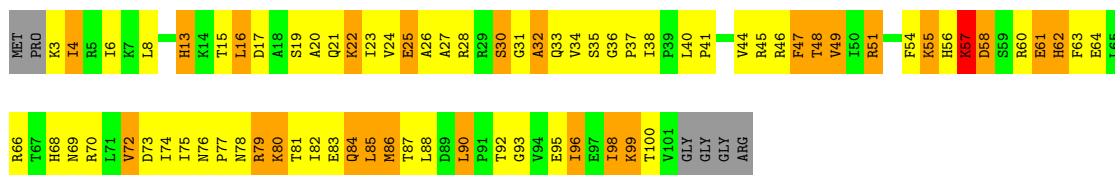
Chain AM:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

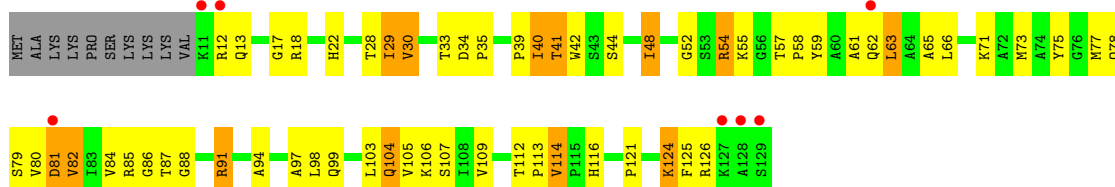
Chain CM:





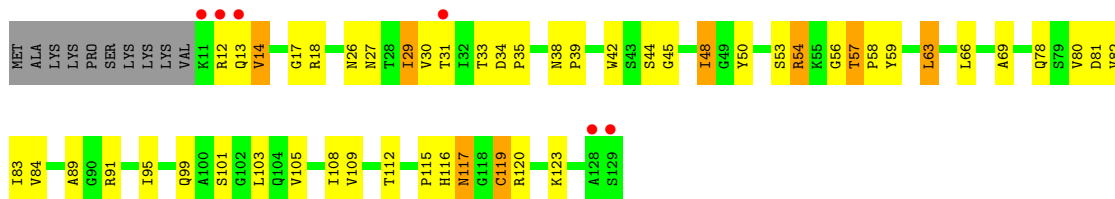
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AN:



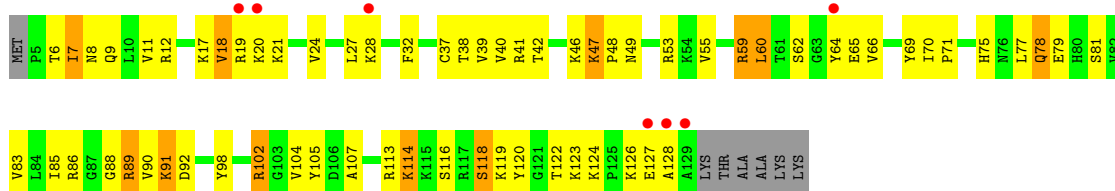
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN:



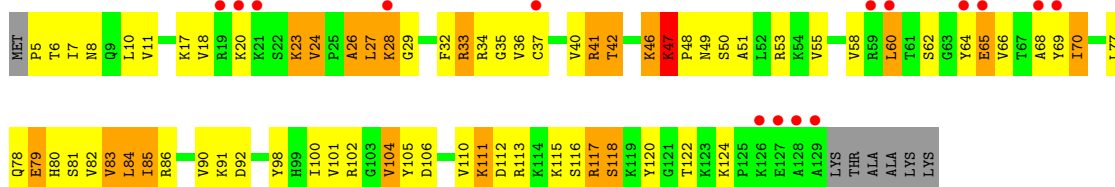
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO:



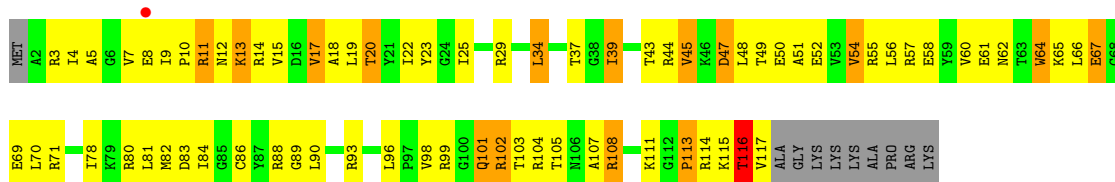
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



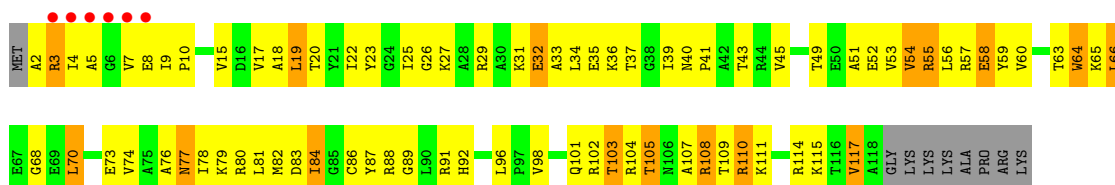
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AP:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



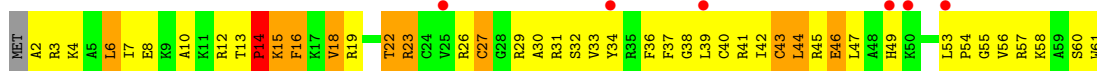
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



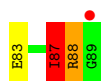
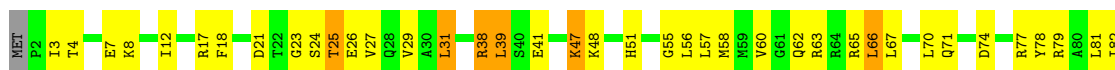
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



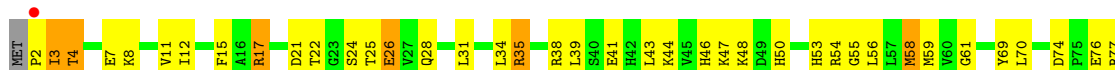
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



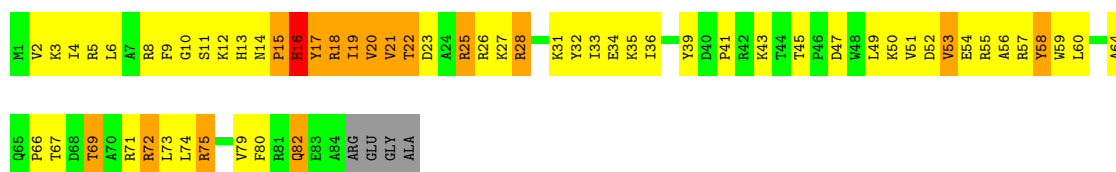
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:



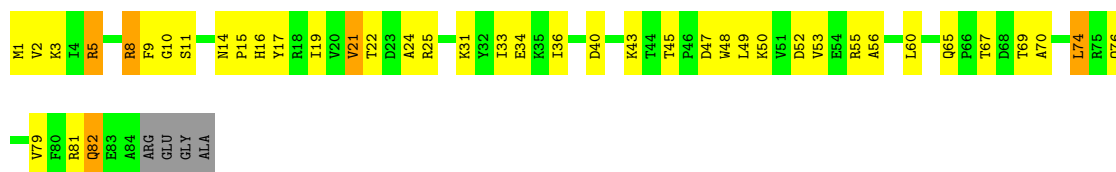
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:



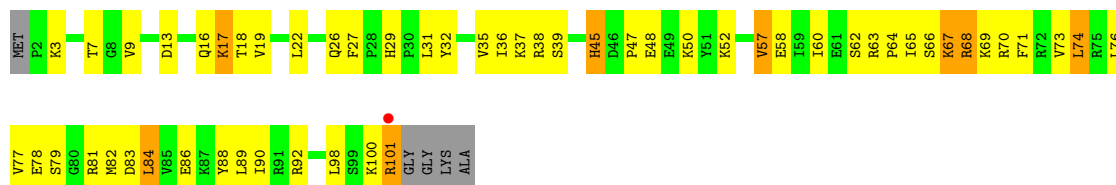
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:



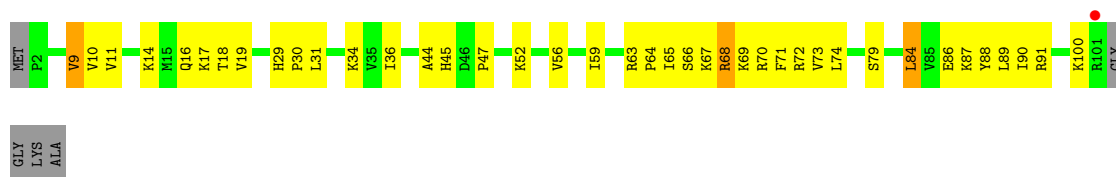
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:



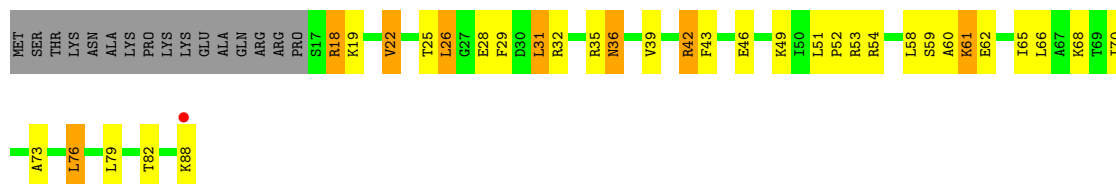
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

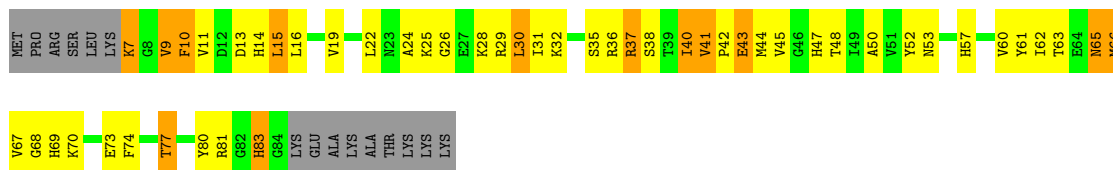
Chain CU:





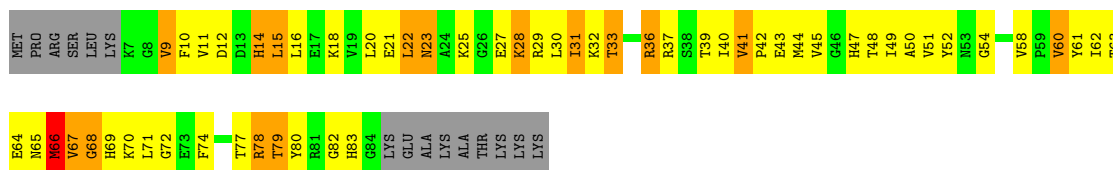
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AV:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV:



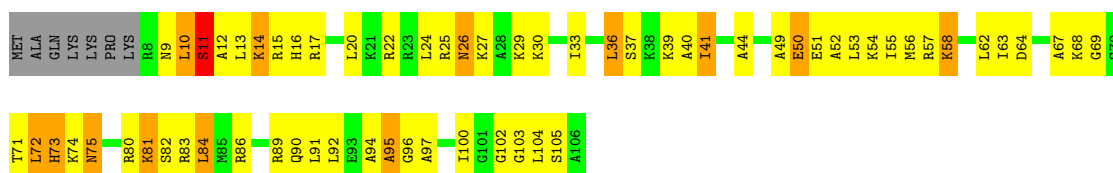
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



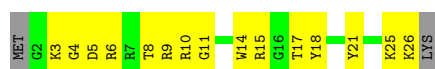
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



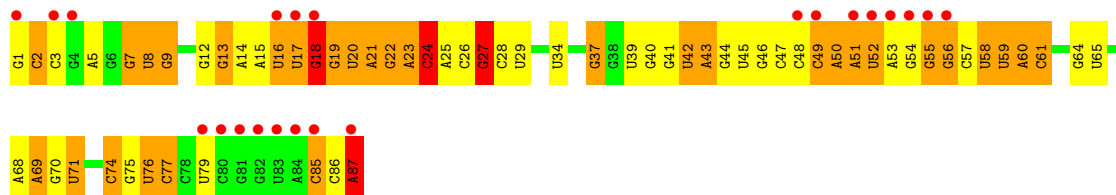
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



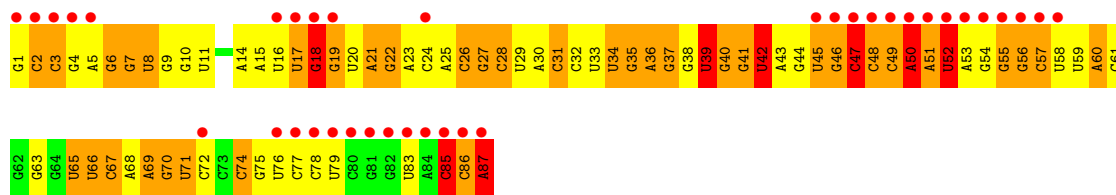
• Molecule 22: TRNA-LEU

Chain AB:



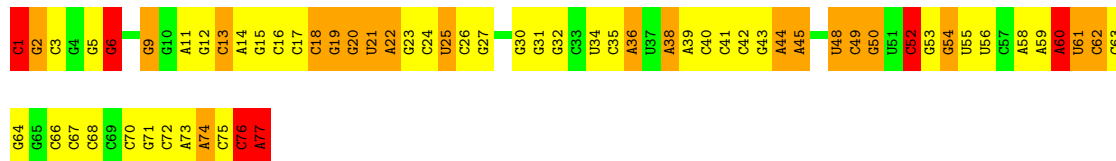
• Molecule 22: TRNA-LEU

Chain CB:



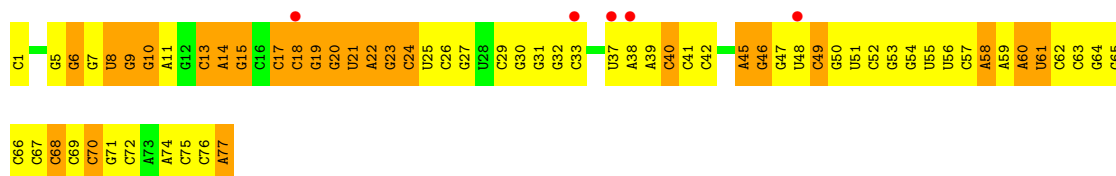
• Molecule 23: TRNA-FMET

Chain AC:



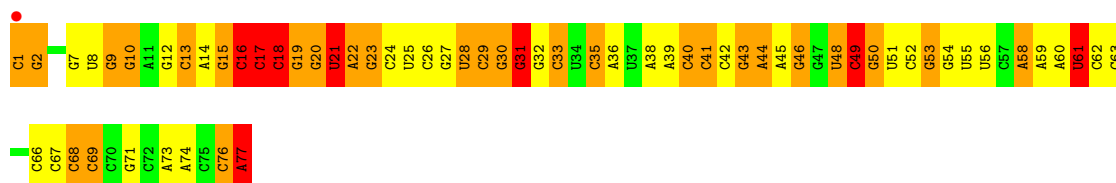
• Molecule 23: TRNA-FMET

Chain AD:



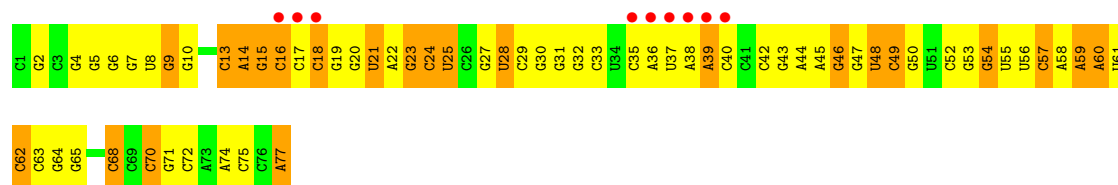
• Molecule 23: TRNA-FMET

Chain CC:



• Molecule 23: TRNA-FMET

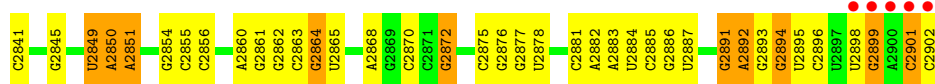
Chain CD: 





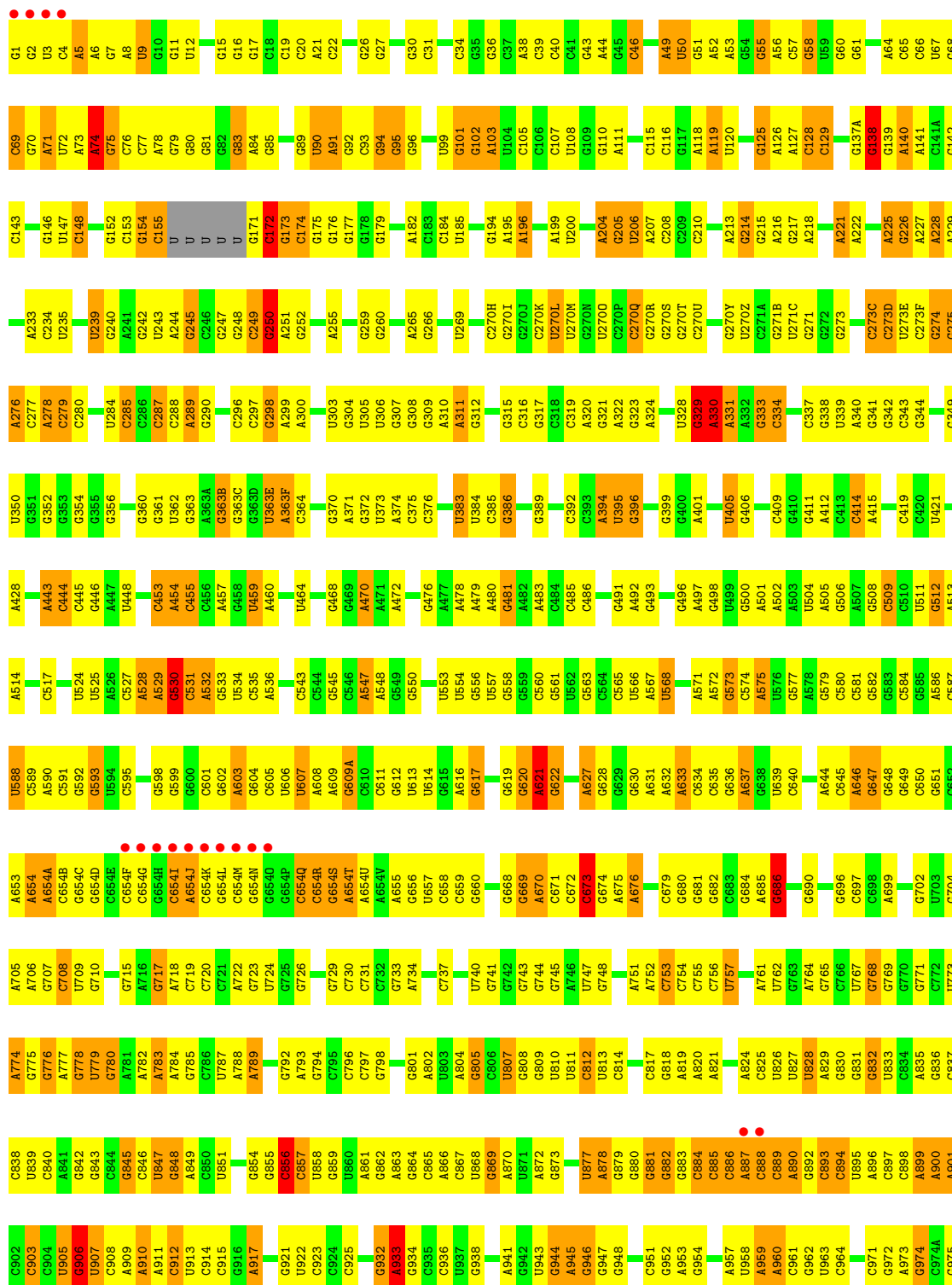
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U1390	U1391	C1464	C1465	C1466	C1467	C1468	A1469	G1470	A1471	A1472	A1473	C1474	C1475	C1476	A1477	C1478	C1479	A1480	A1481	A1482	C1483	A1486	G1487	G1488	U1489	A1490	C1493	A1494	A1495	A1496	U1497	C1498	C1502	U1503	C1504	C1505	C1506	A1507	A1508	C1509	A1510	A1511	U1514	C1515	U1516	C1517	C1518	C1519	U1520	G1521	C1522	G1525	C1526	A1527	A1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	A1554	C1555	C1556	C1557	A1558	C1559	C1560	G1561	C1564	C1565	C1566	A1567	C1568	C1569	A1570	A1571	C1575	U1576	C1577	C1578	A1579	A1580	G1581	C1582	A1583	C1584	A1585	C1586	A1587	C1588	C1589	U1590	C1591	C1592	C1593	G1594	C1595	G1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	U1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	A1627	C1628	C1629	C1630	A1631	A1632	A1633	C1634	C1635	C1636	A1637	C1638	U1639	C1640	A1643	C1644	C1645	A1646	C1647	C1648	C1649	C1650	C1651	C1652	A1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	U1667	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1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WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

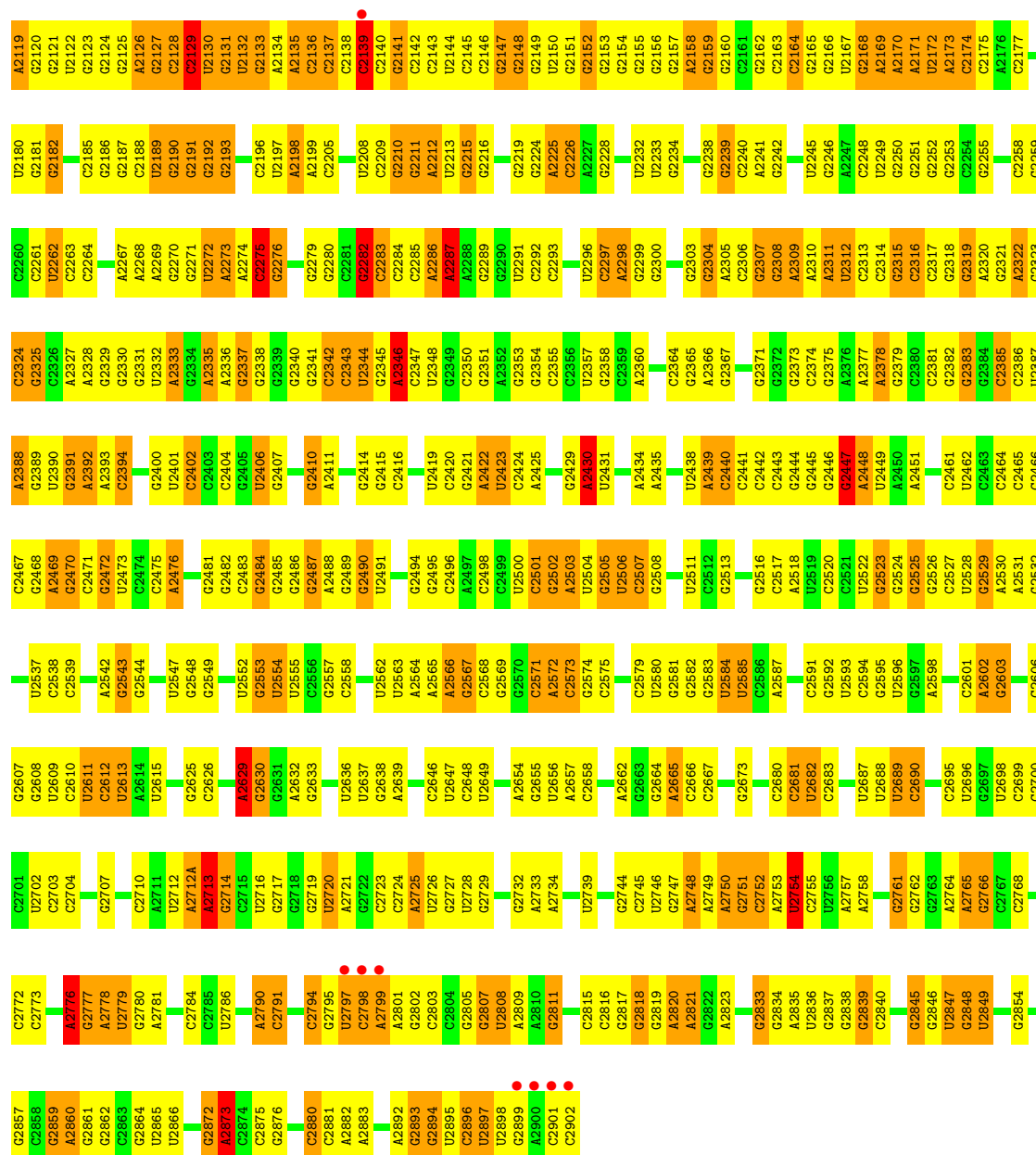


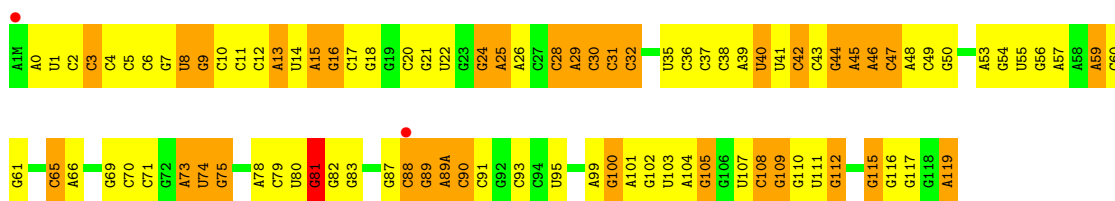
• Molecule 25: RNA (2912-MER)

Chain DA:



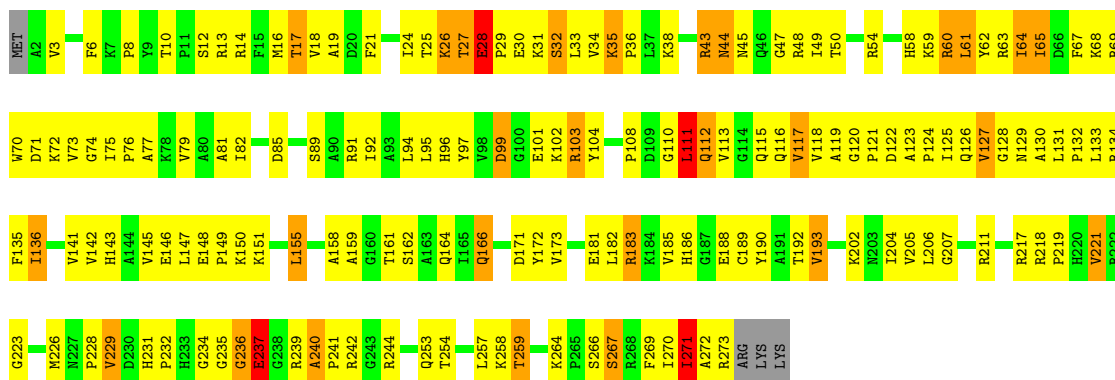
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G2041	U1955	A1884	G1601	G1704	G1624	A1545A	C1476	U1405	U1526	U1249	A1174	A1103	C1041	G977
C2043	U1956	G1888	A1802	U1706	G1625	C1546	A1477	U1406	G1327	G1250	U1175	U1105	C1042	G978
C2044	C1957	A1889	U1806	U1716	U1629	C1548	G1478	C1408	G1328	G1251	G1176	U1104	C1043	G979
G2048	C1958	A1890	U1807	G1717	G1630	A1553	U1482	A1412	G1479	G1252	A1177	G1106	C1044	A980
G2049	U1963	G1896	U1808	G1718	G1633	A1554	G1483	G1413	C1549	G1253	C1178	G1107	A1045	A981
G2052	G1964	G1897	A1809	G1725	G1634	C1557	G1484	G1416	A1336	U1262	C1180	U1108	A1046	C982
G2053	C1965	U1898	G1810	G1726	A1634	C1558	G1485	C1417	G1337	U1263	A1181	G1109	G1047	A983
A2054	A1966	G1899	G1811	U1727	G1635	G1559	A1486	G1418	G1338	G1264	A1182	G1112	A1049	C986
G2055	C1967	A1900	A1812	G1728	C1638	G1560	G1487	A1419	G1339	U1265	A1183	U1113	A1050	G987
G2056	G1968	A1901	U1808	G1729	U1639	A1561	G1488	U1420	U1340	C1266	G1188	G1114	G1051	A988
A2057	A1969	C1902	G1816	U1730	U1639	G1566	U1489	G1421	U1341	U1267	C1189	G1115	A1054	A990
A2058	A1970	G1903	G1817	G1731	C1640	A1567	G1490	G1422	A1342	U1268	G1191	C1116	G1055	C991
A2059	A1971	U1818	A1819	C1741	C1648	G1568	G1491	G1423	A1343	U1269	G1198	U1126	A1057	C994
A2060	A1972	G1906	U1820	G1742	C1651	A1570	C1493	G1424	C1345	A1268	U1199	A1127	U1058	C995
G2061	G1973	G1907	A1821	G1743	G1652	A1571	A1495	G1425	G1346	C1270	U1200	A1128	U1060	A996
A2062	C1974	C1908	U1821	G1743	G1652	A1571	A1496	G1426	G1347	G1271	C1201	A1129	U1061	C998
C2063	U1977	C1909	G1826	G1750	G1653	C1575	C1499	A1427	G1348	G1272	U1205	U1133	U1065	A1000
C2064	A1978	A1913	C1827	C1751	A1654	U1576	C1500	G1428	G1349	U1272	U1206	C1135	U1066	G1003
C2065	A1978	C1914	G1828	C1751	A1655	U1577	G1500	G1429	A1350	A1273	U1211	U1136	A1067	G1004
G2066	C1979	U1915	A1829	G1756	C1656	U1578	C1501	U1430	C1351	G1274	G1203	G1131	G1068	C1005
G2067	G1980	A1916	U1830	U1757	C1657	U1579	C1502	U1431	U1352	A1275	A1204	G1132	G1069	C1006
U2068	A1981	U1917	G1831	G1758	C1658	A1580	C1503	C1432	U1356	A1276	U1205	U1133	U1070	C1007
G2069	U1918	A1918	C1832	C1759	C1659	U1581	U1504	U1433	G1357	G1277	U1206	C1136	C1072	A1009
G2070	A1919	C1920	U1833	A1759	C1660	G1582	C1505	U1434	G1358	U1278	U1212	U1137	A1010	G1011
A2071	U1921	U1834	G1835	G1762	G1661	A1583	C1506	G1435	A1359	G1279	C1202	U1130	G1074	U1012
U2074	G1992	G1921	G1835	G1763	G1661	C1585	A1507	G1436	A1360	G1283	G1218	G1139	C1075	U1013
U2075	U1993	G1922	C1836	G1764	C1666	A1586	A1508	U1437	U1365	A1284	C1219	C1140	C1076	G1008
U2076	C1994	U1923	C1837	G1764	C1666	A1587	A1509	U1438	A1365	U1285	U1210	U1141	C1077	A1009
A2082	C1999	C1925	G1839	C1767	G1667	U1587	C1509	A1439	U1368	A1287	U1216	U1142	G1074	G1011
G2087	U1926	U1926	U1839	G1769	A1668	C1588	A1510	G1443	G1368	U1288	G1219	G1144	C1075	U1012
U2092	A1927	A1927	C1844	G1770	C1670	C1589	C1515	G1444	G1371	U1292	A1220	C1145	A1077	G1013
G2093	G1930	G1929	A1847	G1772	G1672	G1593	G1519	A1444A	U1372	C1293	C1221	C1146	A1080	G1016
A2014	U1931	C1932	A1853	C1773	U1673	G1594	G1520	C1445	A1378	C1298	C1223	C1147	U1081	G1017
A2015	A1932	A1854	A1854	U1774	G1674	A1596	G1521	G1446	A1379	G1299	C1224	C1150	U1019	C1018
U2016	G1933	G1855	G1855	U1775	A1676	C1598	G1522	U1449A	A1384	U1300	C1225	C1151	A1084	A1020
U2017	C1934	G1856	G1856	G1776	A1677	C1600	G1527	C1450	C1385	U1301	G1226	C1152	A1085	A1021
G2018	G1935	G1857	G1858	U1778	G1678	G1601	A1528	A1451	C1386	A1301	C1229	G1154	A1086	G1022
G2023	A1936	C1858	C1858	U1779	C1686	U1602	G1530	U1454	G1387	C1304	G1229A	A1156	A1088	U1023
G2024	A1937	C1859	G1860	C1781	G1687	C1606	C1532	G1459	G1388	G1309	G1235	G1160	U1090	G1025
C2025	A1938	G1861	G1861	C1782	G1688	C1607	C1533	G1460	U1390	G1310	G1236	G1163	G1091	A1027
C2026	U1939	G1862	G1862	A1783	A1689	A1608	G1534	G1461	U1391	G1311	A1237	G1093	A1028	A1029
G2027	C1941	G1863	G1863	U1784	C1689	A1609	U1535	C1464	A1392	U1312	G1238	G1164	U1094	U1033
A2030	C1942	U1864	G1869	A1785	C1694	A1609	A1536	G1465	A1393	U1313	G1239	U1165	A1095	G1034
A2031	U1943	C1870	G1870	A1786	G1695	A1610	C1537	G1466	U1394	C1314	U1240	C1166	A1096	G1035
G2032	G1945	A1871	G1871	A1791	G1696	C1612	G1538	C1467	A1395	U1319	A1241	U1167	U1097	G1036
A2033	U1946	A1872	G1872	U1794	G1697	G1613	G1539	C1467	U1396	G1320	G1244	G1168	A1088	G1037
C2036	C1947	G1878	G1878	U1794	G1698	A1614	G1540	U1471	U1397	A1321	G1245	G1169	C1100	G1038
G2037	G1948	C1879	C1879	C1795	G1699	G1615	U1541	A1472	G1401	A1322	A1246	G1170	G1099	G1039
G2038	G1949	C1880	C1880	U1796	A1700	A1616	A1542	G1473	C1402	U1323	A1246	G1171	C1100	G1039
C2039	U1951	G1881	C1881	C1797	G1702	G1619	C1544	C1474	C1403	G1324	A1247		U1101	





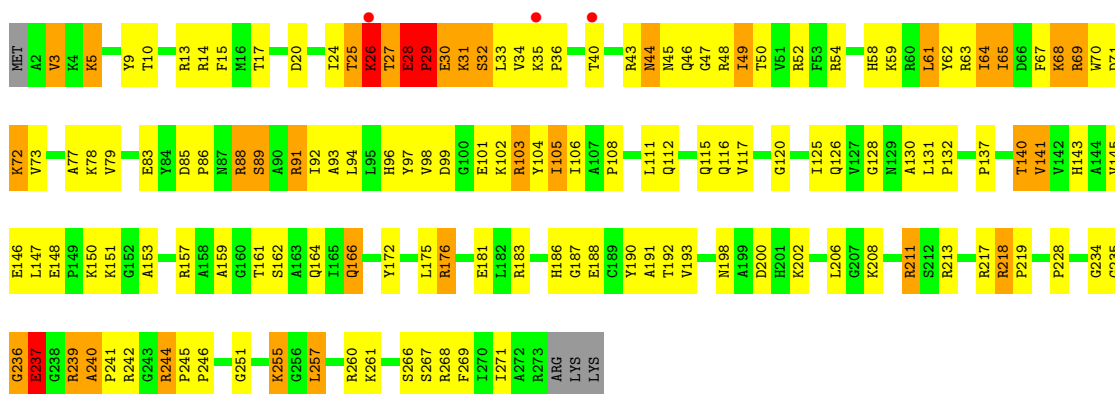
• Molecule 27: 50S ribosomal protein L2

Chain BD:



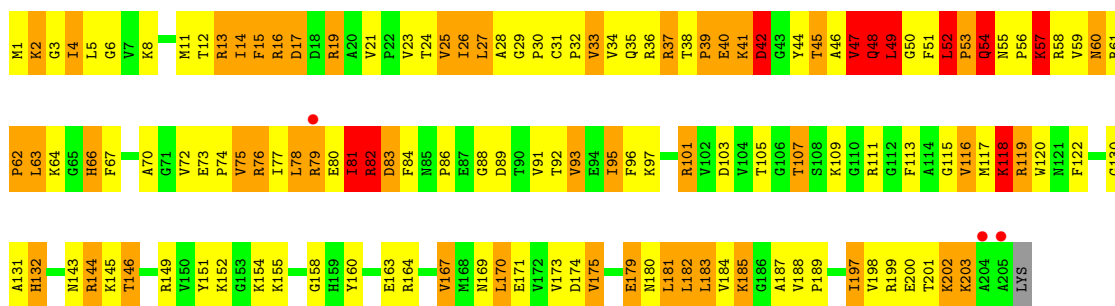
• Molecule 27: 50S ribosomal protein L2

Chain DD:



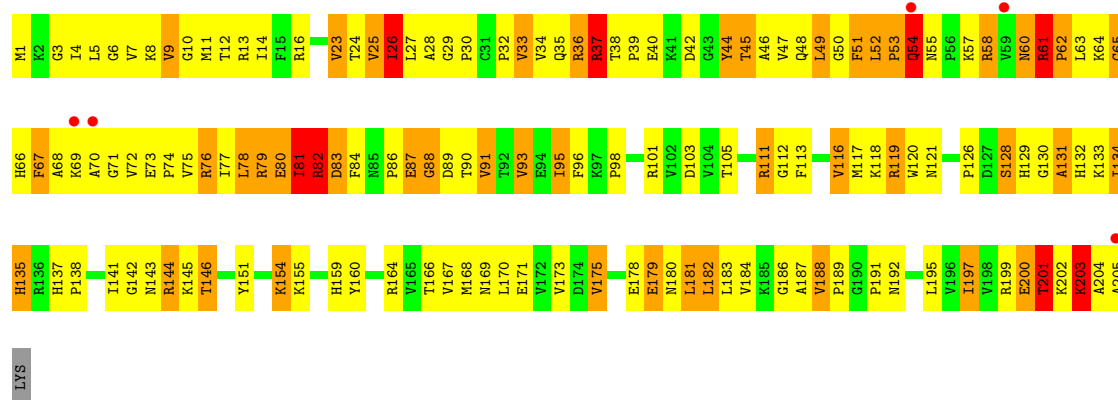
• Molecule 28: 50S ribosomal protein L3

Chain BE:



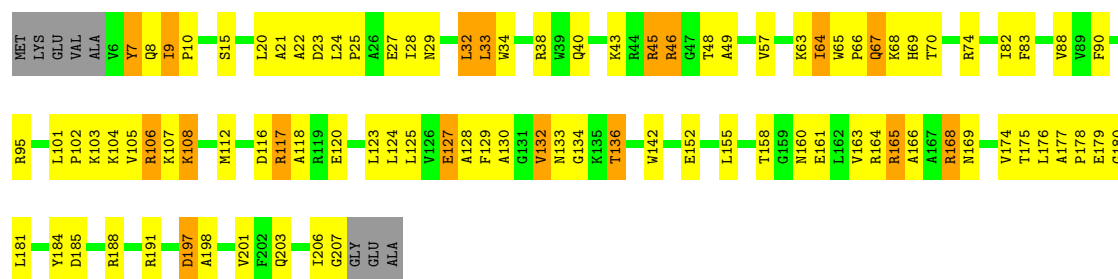
• Molecule 28: 50S ribosomal protein L3

Chain DE:



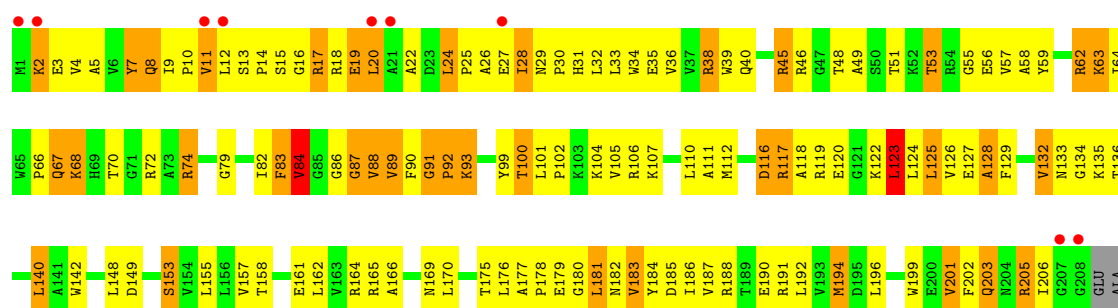
- Molecule 29: 50S ribosomal protein L4

Chain BF:



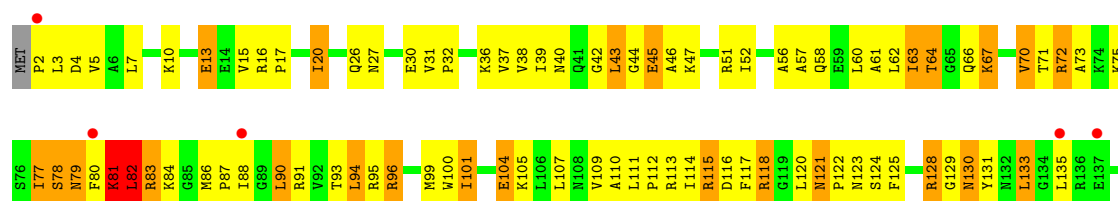
- Molecule 29: 50S ribosomal protein L4

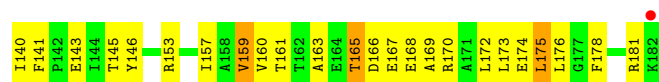
Chain DF:



- Molecule 30: 50S ribosomal protein L5

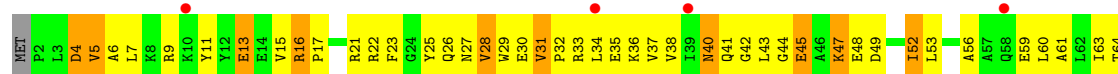
Chain BG:





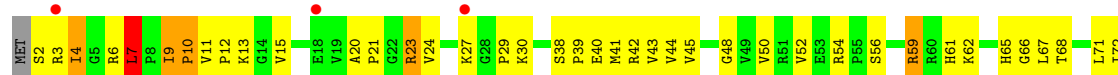
- Molecule 30: 50S ribosomal protein L5

Chain DG:

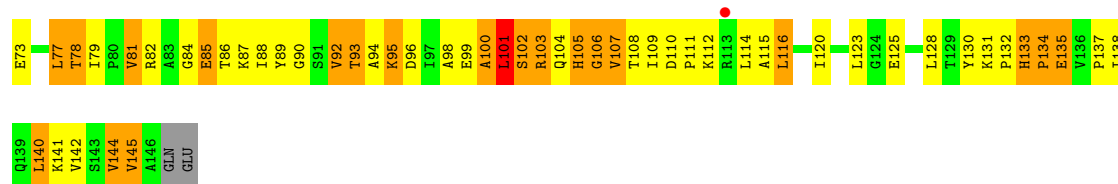


- Molecule 31: 50S ribosomal protein L6

Chain BH:

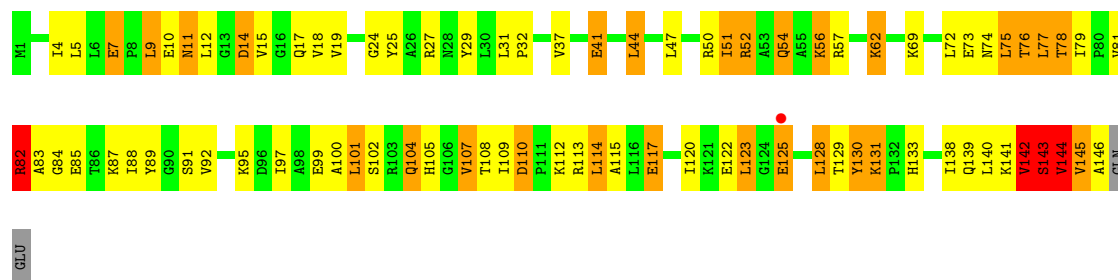






- Molecule 32: 50S ribosomal protein L9

Chain DK:



- Molecule 33: 50S ribosomal protein L13

Chain BM:



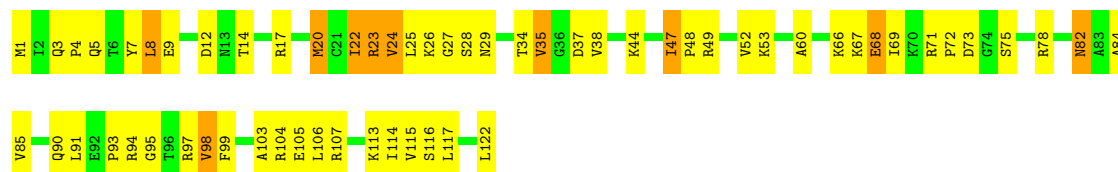
- Molecule 33: 50S ribosomal protein L13

Chain DM:



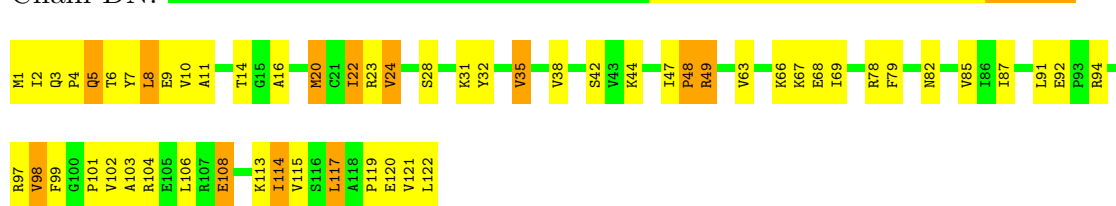
- Molecule 34: 50S ribosomal protein L14

Chain BN:



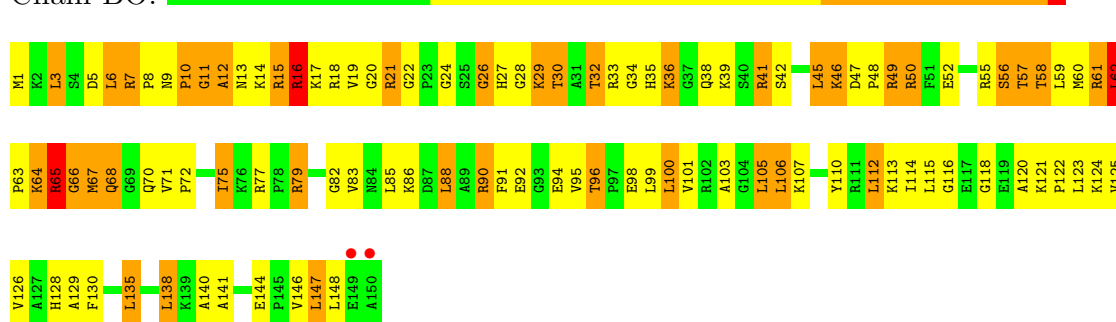
- Molecule 34: 50S ribosomal protein L14

Chain DN:



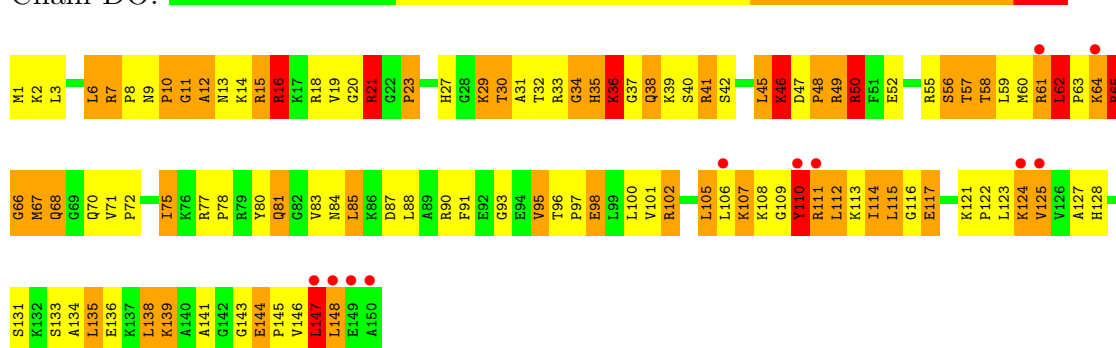
- Molecule 35: 50S ribosomal protein L15

Chain BO:



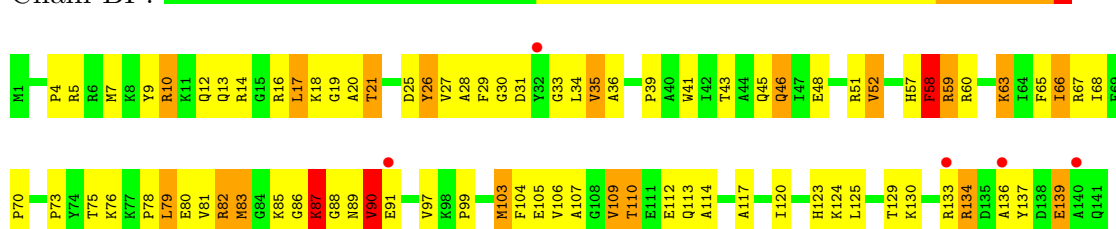
- Molecule 35: 50S ribosomal protein L15

Chain DO:



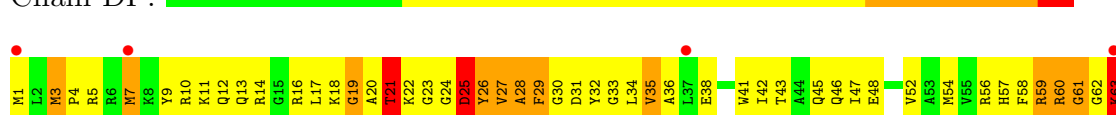
- Molecule 36: 50S ribosomal protein L16

Chain BP:



- Molecule 36: 50S ribosomal protein L16

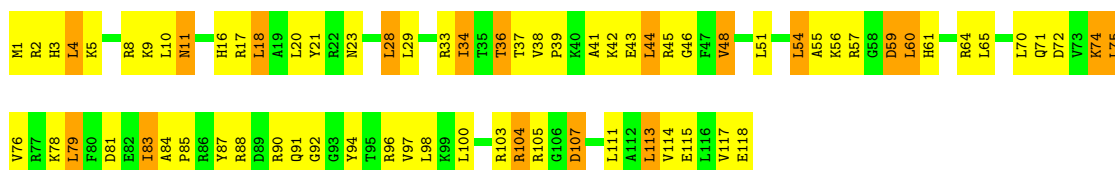
Chain DP:





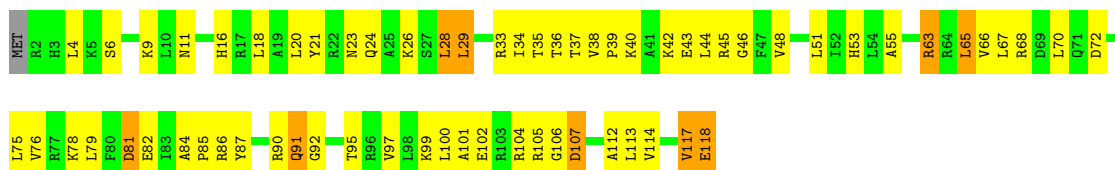
- Molecule 37: 50S ribosomal protein L17

Chain B0:



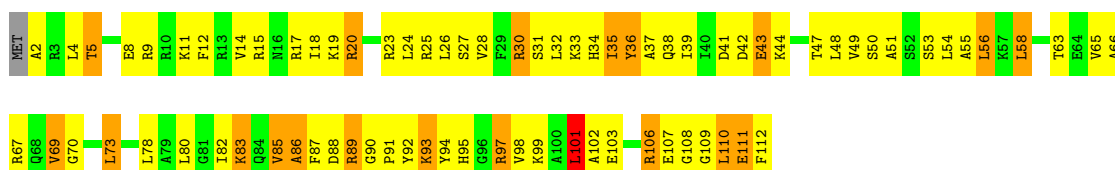
- Molecule 37: 50S ribosomal protein L17

Chain D0:



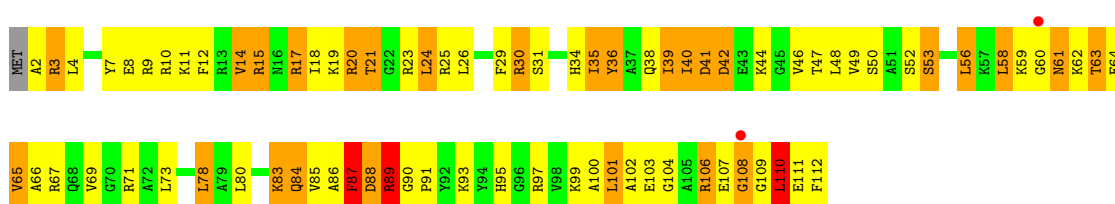
- Molecule 38: 50S ribosomal protein L18

Chain BQ:



- Molecule 38: 50S ribosomal protein L18

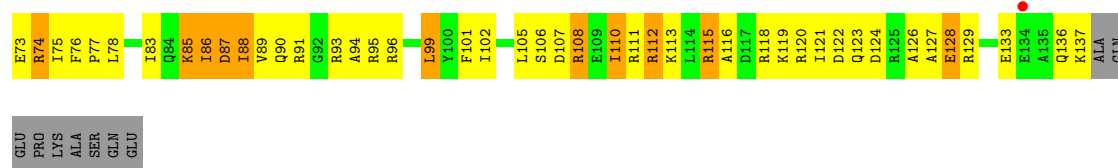
Chain DQ:



- Molecule 39: 50S ribosomal protein L19

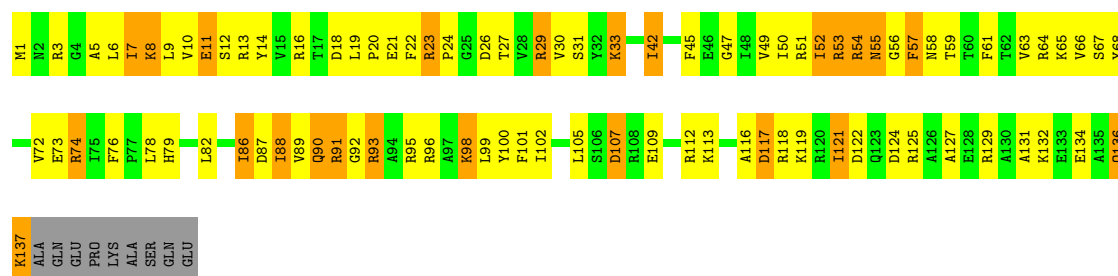
Chain BR:





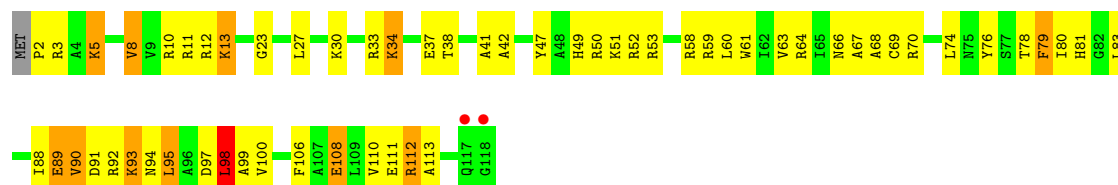
• Molecule 39: 50S ribosomal protein L19

Chain DR:



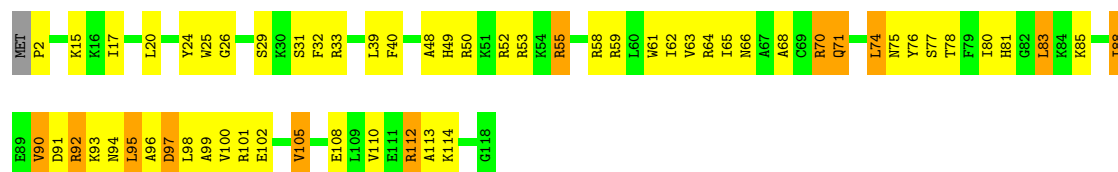
• Molecule 40: 50S ribosomal protein L20

Chain B1:



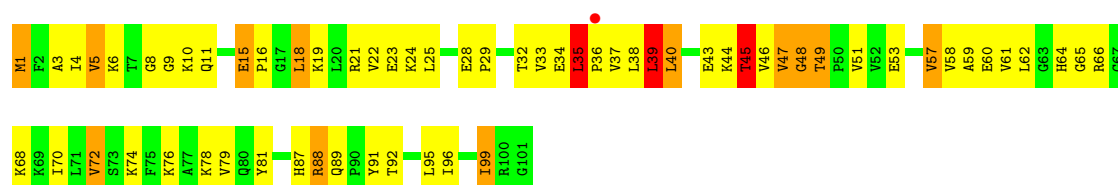
• Molecule 40: 50S ribosomal protein L20

Chain D1:



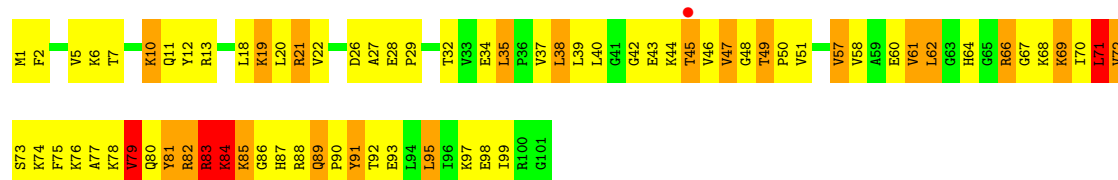
• Molecule 41: 50S ribosomal protein L21

Chain B2:



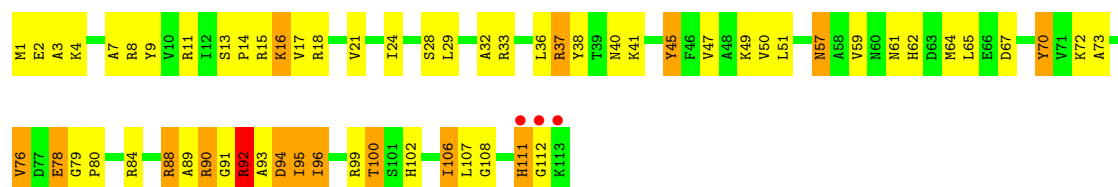
• Molecule 41: 50S ribosomal protein L21

Chain D2:



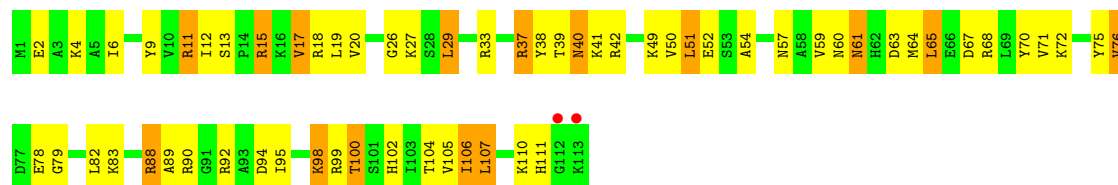
• Molecule 42: 50S ribosomal protein L22

Chain BS:



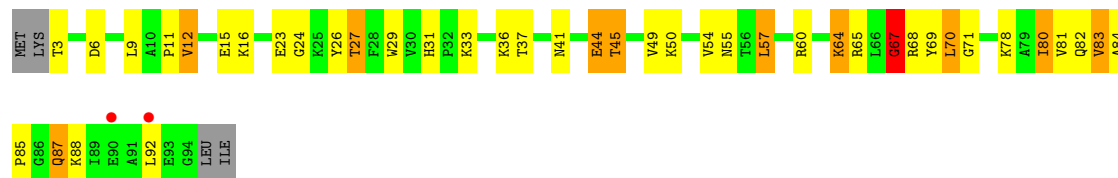
• Molecule 42: 50S ribosomal protein L22

Chain DS:



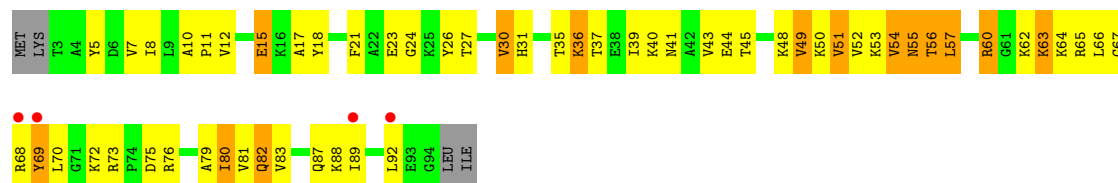
• Molecule 43: 50S ribosomal protein L23

Chain BT:



• Molecule 43: 50S ribosomal protein L23

Chain DT:



• Molecule 44: 50S ribosomal protein L24

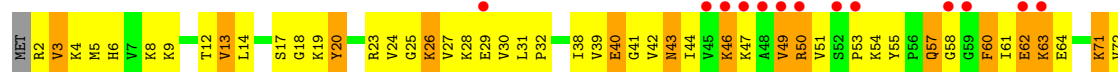
Chain BU:





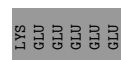
- Molecule 44: 50S ribosomal protein L24

Chain DU:



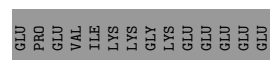
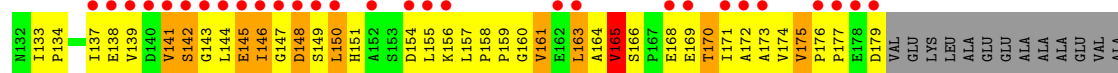
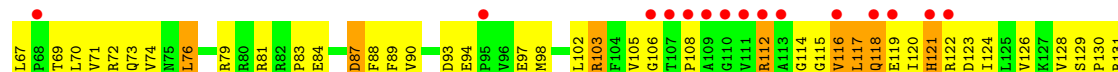
- Molecule 45: 50S ribosomal protein L25

Chain BV:



- Molecule 45: 50S ribosomal protein L25

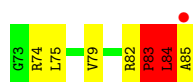
Chain DV:



- Molecule 46: 50S ribosomal protein L27

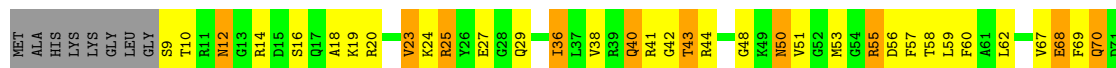
Chain B3:





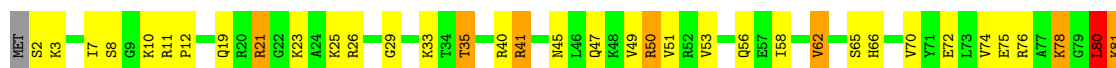
- Molecule 46: 50S ribosomal protein L27

Chain D3:



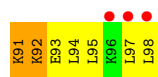
- Molecule 47: 50S ribosomal protein L28

Chain BZ:



- Molecule 47: 50S ribosomal protein L28

Chain DZ:



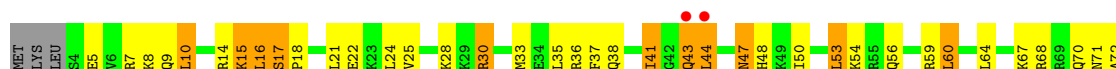
- Molecule 48: 50S ribosomal protein L29

Chain BW:



- Molecule 48: 50S ribosomal protein L29

Chain DW:



- Molecule 49: 50S ribosomal protein L30

Chain BX:



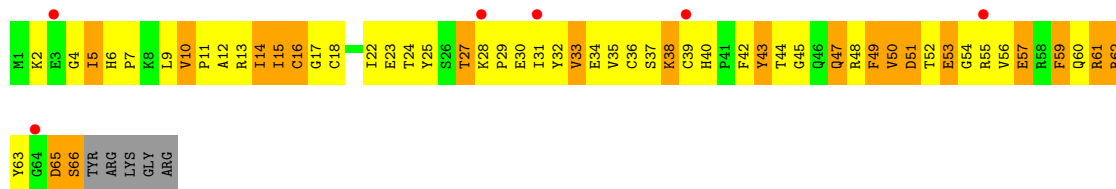
- Molecule 49: 50S ribosomal protein L30

Chain DX:



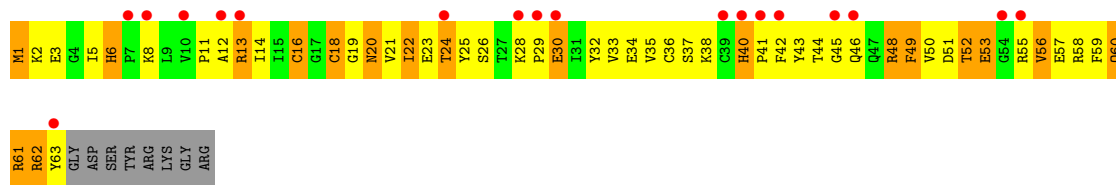
- Molecule 50: 50S ribosomal protein L31

Chain B4:



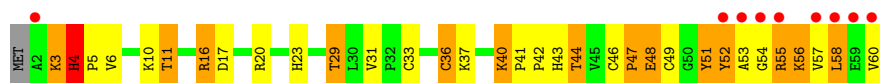
- Molecule 50: 50S ribosomal protein L31

Chain D4:



- Molecule 51: 50S ribosomal protein L32

Chain B5:



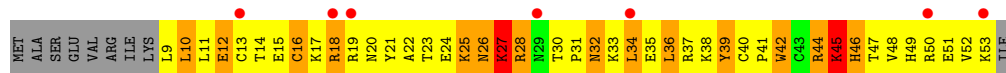
- Molecule 51: 50S ribosomal protein L32

Chain D5:



- Molecule 52: 50S ribosomal protein L33

Chain B6:



- Molecule 52: 50S ribosomal protein L33

Chain D6:





- Molecule 53: 50S ribosomal protein L34

Chain B7:



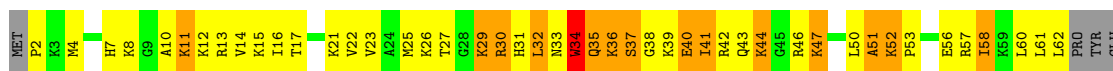
- Molecule 53: 50S ribosomal protein L34

Chain D7:



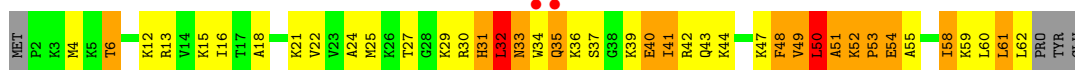
- Molecule 54: 50S ribosomal protein L35

Chain B8:



- Molecule 54: 50S ribosomal protein L35

Chain D8:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.211 , 0.272 0.246 , 0.299	Depositor DCC
$R_{free}$ test set	928 reflections (0.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1160172 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	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.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.44	5/36234 (0.0%)	0.91	68/56554 (0.1%)
1	CA	0.42	1/36237 (0.0%)	0.90	79/56558 (0.1%)
2	AE	0.29	0/1959	0.56	0/2642
2	CE	0.28	0/1959	0.53	0/2642
3	AF	0.33	0/1629	0.53	0/2195
3	CF	0.31	0/1636	0.54	0/2205
4	AG	0.49	2/1733 (0.1%)	0.62	1/2318 (0.0%)
4	CG	0.38	0/1733	0.61	0/2318
5	AH	0.35	0/1171	0.58	0/1576
5	CH	0.34	0/1171	0.56	0/1576
6	AI	0.33	0/856	0.55	0/1154
6	CI	0.32	0/856	0.54	0/1154
7	AJ	0.29	0/1276	0.50	0/1709
7	CJ	0.28	0/1276	0.45	0/1709
8	AK	0.33	0/1136	0.60	0/1527
8	CK	0.27	0/1136	0.51	0/1527
9	AL	0.29	0/1029	0.52	0/1379
9	CL	0.29	0/1029	0.53	0/1379
10	AM	0.31	0/814	0.59	1/1095 (0.1%)
10	CM	0.28	0/814	0.54	0/1095
11	AN	0.33	0/900	0.57	0/1213
11	CN	0.31	0/900	0.56	0/1213
12	AO	0.40	0/991	0.68	1/1327 (0.1%)
12	CO	0.35	0/991	0.60	0/1327
13	AP	0.30	0/938	0.57	0/1258
13	CP	0.28	0/943	0.52	0/1265
14	AQ	0.42	0/501	0.66	1/664 (0.2%)
14	CQ	0.29	0/501	0.58	0/664
15	AR	0.35	0/745	0.58	0/992
15	CR	0.30	0/745	0.51	0/992
16	AS	0.29	0/721	0.53	0/970
16	CS	0.31	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.35	0/847	0.54	0/1131
17	CT	0.31	0/847	0.51	0/1131
18	AU	0.34	0/596	0.64	0/790
18	CU	0.35	0/596	0.59	0/790
19	AV	0.33	0/638	0.59	0/860
19	CV	0.31	0/638	0.65	0/860
20	AW	0.29	0/765	0.52	0/1007
20	CW	0.32	0/765	0.63	0/1007
21	AX	0.28	0/221	0.55	0/288
21	CX	0.28	0/221	0.49	0/288
22	AB	1.15	2/2080 (0.1%)	1.41	25/3242 (0.8%)
22	CB	1.34	6/2080 (0.3%)	1.41	36/3242 (1.1%)
23	AC	1.12	3/1835 (0.2%)	1.69	56/2859 (2.0%)
23	AD	0.57	0/1835	0.97	7/2859 (0.2%)
23	CC	1.08	1/1835 (0.1%)	1.52	44/2859 (1.5%)
23	CD	0.61	0/1835	0.98	5/2859 (0.2%)
24	A1	1.43	2/226 (0.9%)	1.60	7/348 (2.0%)
24	C1	1.57	1/226 (0.4%)	1.73	5/348 (1.4%)
25	BA	0.59	15/70233 (0.0%)	1.07	285/109643 (0.3%)
25	DA	0.52	13/70122 (0.0%)	1.00	265/109469 (0.2%)
26	BB	0.49	0/2928	0.97	9/4568 (0.2%)
26	DB	0.44	0/2928	0.96	7/4568 (0.2%)
27	BD	0.50	0/2165	0.80	2/2919 (0.1%)
27	DD	0.46	0/2165	0.72	0/2919
28	BE	0.38	0/1601	0.67	2/2160 (0.1%)
28	DE	0.38	0/1601	0.69	0/2160
29	BF	0.43	0/1620	0.67	0/2194
29	DF	0.36	0/1662	0.65	0/2249
30	BG	0.36	0/1499	0.60	0/2016
30	DG	0.29	0/1499	0.54	0/2016
31	BH	0.36	0/1332	0.67	1/1802 (0.1%)
31	DH	0.28	0/1332	0.55	0/1802
32	BK	0.34	0/1151	0.68	1/1558 (0.1%)
32	DK	0.33	0/1151	0.66	1/1558 (0.1%)
33	BM	0.42	0/1131	0.69	0/1525
33	DM	0.29	0/1131	0.59	0/1525
34	BN	0.40	0/943	0.64	0/1269
34	DN	0.36	0/943	0.60	0/1269
35	BO	0.39	0/1162	0.76	0/1544
35	DO	0.32	0/1162	0.65	1/1544 (0.1%)
36	BP	0.52	0/1143	0.80	0/1527
36	DP	0.32	0/1143	0.54	0/1527
37	B0	0.39	0/982	0.69	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	D0	0.37	0/974	0.64	0/1302
38	BQ	0.42	0/892	0.70	1/1187 (0.1%)
38	DQ	0.30	0/892	0.62	1/1187 (0.1%)
39	BR	0.40	0/1155	0.66	0/1542
39	DR	0.37	0/1155	0.59	0/1542
40	B1	0.42	0/982	0.67	1/1306 (0.1%)
40	D1	0.34	0/982	0.57	0/1306
41	B2	0.42	0/790	0.74	2/1057 (0.2%)
41	D2	0.32	0/790	0.59	0/1057
42	BS	0.37	0/911	0.62	0/1220
42	DS	0.38	0/911	0.64	0/1220
43	BT	0.50	0/739	0.68	0/993
43	DT	0.47	0/739	0.62	0/993
44	BU	0.45	0/798	0.68	0/1064
44	DU	0.41	0/798	0.72	0/1064
45	BV	0.32	0/1427	0.63	0/1935
45	DV	0.28	0/1460	0.56	0/1982
46	B3	0.44	0/615	0.67	0/819
46	D3	0.39	0/621	0.61	0/827
47	BZ	0.42	0/770	0.73	1/1022 (0.1%)
47	DZ	0.39	0/770	0.70	0/1022
48	BW	0.53	0/560	0.72	0/741
48	DW	0.37	0/583	0.63	0/771
49	BX	0.36	0/474	0.64	1/635 (0.2%)
49	DX	0.32	0/474	0.53	0/635
50	B4	0.34	0/545	0.72	1/733 (0.1%)
50	D4	0.32	0/527	0.67	0/709
51	B5	0.43	0/473	0.69	0/639
51	D5	0.34	0/468	0.70	0/632
52	B6	0.43	0/396	0.70	0/529
52	D6	0.33	0/396	0.63	0/529
53	B7	0.46	0/438	0.68	0/575
53	D7	0.40	0/438	0.59	0/575
54	B8	0.52	0/494	0.71	0/649
54	D8	0.38	0/494	0.71	1/649 (0.2%)
All	All	0.51	51/324027 (0.0%)	0.93	919/485226 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AE	0	3
2	CE	0	5
3	CF	0	1
4	AG	0	1
8	AK	0	1
10	AM	0	1
12	AO	0	2
14	AQ	0	1
14	CQ	0	2
15	AR	0	1
19	CV	0	1
20	CW	0	1
27	BD	0	6
27	DD	0	3
28	BE	0	1
28	DE	0	6
29	DF	0	2
30	BG	0	1
30	DG	0	1
31	BH	0	2
31	DH	0	2
32	BK	0	3
32	DK	0	4
33	BM	0	1
35	BO	0	4
35	DO	0	3
36	BP	0	3
37	D0	0	2
38	BQ	0	1
38	DQ	0	2
39	BR	0	2
40	B1	0	1
40	D1	0	1
41	B2	0	1
43	BT	0	1
44	DU	0	2
45	BV	0	3
45	DV	0	2
46	B3	0	2
48	BW	0	2
48	DW	0	1
50	B4	0	4
50	D4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
51	B5	0	1
51	D5	0	1
52	B6	0	1
52	D6	0	1
53	B7	0	1
54	B8	0	2
54	D8	0	1
All	All	0	99

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	1143	A	N7-C5	-11.10	1.32	1.39
4	AG	12	CYS	CB-SG	10.86	2.00	1.82
25	DA	2873	A	N7-C5	-10.30	1.33	1.39
25	DA	1342	A	N7-C5	-9.87	1.33	1.39
25	BA	2430	A	N9-C4	-9.40	1.32	1.37

The worst 5 of 919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1899	G	N3-C4-N9	-15.77	116.54	126.00
1	AA	1025	U	C5-C4-O4	-15.29	116.72	125.90
1	AA	1177	G	N9-C4-C5	14.63	111.25	105.40
1	AA	1177	G	C4-C5-N7	-14.21	105.12	110.80
25	DA	1899	G	N3-C4-N9	-13.25	118.05	126.00

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AE	14	GLY	Peptide
2	AE	194	PRO	Peptide
2	AE	71	VAL	Peptide
4	AG	29	PRO	Peptide
8	AK	102	ARG	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	32369	0	16339	1207	1
1	CA	32372	0	16338	1298	1
2	AE	1924	0	1975	158	0
2	CE	1924	0	1975	180	0
3	AF	1605	0	1668	111	0
3	CF	1612	0	1677	144	0
4	AG	1703	0	1764	146	0
4	CG	1703	0	1763	140	1
5	AH	1155	0	1213	74	0
5	CH	1155	0	1213	91	0
6	AI	843	0	857	39	1
6	CI	843	0	857	45	0
7	AJ	1257	0	1296	68	0
7	CJ	1257	0	1296	74	0
8	AK	1116	0	1177	75	0
8	CK	1116	0	1177	66	0
9	AL	1010	0	1037	99	0
9	CL	1010	0	1037	121	0
10	AM	801	0	849	78	0
10	CM	801	0	849	114	0
11	AN	885	0	904	65	0
11	CN	885	0	904	45	0
12	AO	975	0	1062	62	0
12	CO	975	0	1062	75	0
13	AP	928	0	987	66	0
13	CP	933	0	992	107	0
14	AQ	492	0	529	47	0
14	CQ	492	0	531	68	0
15	AR	734	0	771	38	0
15	CR	734	0	771	35	0
16	AS	705	0	725	79	0
16	CS	705	0	725	45	0
17	AT	834	0	904	55	0
17	CT	834	0	904	41	0
18	AU	591	0	662	30	0
18	CU	591	0	662	47	0
19	AV	624	0	636	71	0
19	CV	624	0	636	91	0
20	AW	763	0	859	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	CW	763	0	861	56	0
21	AX	217	0	234	17	0
21	CX	217	0	234	23	0
22	AB	1861	0	938	85	0
22	CB	1861	0	938	99	0
23	AC	1643	0	837	75	0
23	AD	1643	0	837	97	0
23	CC	1643	0	837	91	0
23	CD	1643	0	837	108	0
24	A1	205	0	103	12	0
24	C1	205	0	103	10	0
25	BA	62707	0	31613	2105	0
25	DA	62607	0	31565	2108	1
26	BB	2617	0	1328	94	0
26	DB	2617	0	1328	135	0
27	BD	2115	0	2195	238	0
27	DD	2115	0	2195	211	0
28	BE	1568	0	1634	334	0
28	DE	1568	0	1634	256	0
29	BF	1585	0	1632	119	0
29	DF	1627	0	1680	184	0
30	BG	1474	0	1535	171	0
30	DG	1474	0	1535	148	0
31	BH	1307	0	1382	135	0
31	DH	1307	0	1382	156	1
32	BK	1136	0	1223	99	0
32	DK	1136	0	1223	84	0
33	BM	1104	0	1180	142	0
33	DM	1104	0	1180	87	0
34	BN	933	0	996	63	0
34	DN	933	0	996	51	0
35	BO	1145	0	1228	200	0
35	DO	1145	0	1227	240	0
36	BP	1122	0	1179	95	0
36	DP	1122	0	1179	208	0
37	B0	968	0	1033	78	0
37	D0	960	0	1021	60	0
38	BQ	882	0	943	106	0
38	DQ	882	0	943	120	0
39	BR	1141	0	1202	116	0
39	DR	1141	0	1202	125	0
40	B1	964	0	1022	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	D1	964	0	1022	94	0
41	B2	779	0	852	80	0
41	D2	779	0	852	129	0
42	BS	900	0	964	71	0
42	DS	900	0	964	42	0
43	BT	725	0	778	53	0
43	DT	725	0	778	75	0
44	BU	785	0	878	75	0
44	DU	785	0	878	98	0
45	BV	1397	0	1430	120	0
45	DV	1428	0	1454	162	0
46	B3	607	0	628	50	0
46	D3	613	0	633	52	0
47	BZ	763	0	848	50	0
47	DZ	763	0	848	46	0
48	BW	558	0	610	44	0
48	DW	581	0	629	49	0
49	BX	469	0	518	35	0
49	DX	469	0	518	24	0
50	B4	533	0	522	84	0
50	D4	515	0	510	84	0
51	B5	459	0	480	54	0
51	D5	454	0	475	44	0
52	B6	389	0	404	80	0
52	D6	389	0	404	84	0
53	B7	430	0	480	30	0
53	D7	430	0	480	36	0
54	B8	488	0	558	110	0
54	D8	488	0	558	113	0
55	A1	2	0	0	0	0
55	AA	242	0	0	0	0
55	AB	5	0	0	0	0
55	AC	9	0	0	0	0
55	AD	1	0	0	0	0
55	AG	1	0	0	0	0
55	AH	1	0	0	0	0
55	AN	2	0	0	0	0
55	AQ	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	1	0	0	0	0
55	B2	1	0	0	0	0
55	B3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B5	1	0	0	0	0
55	B7	1	0	0	0	0
55	B8	1	0	0	0	0
55	BA	623	0	0	0	0
55	BB	17	0	0	0	0
55	BD	1	0	0	0	0
55	BE	5	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BU	2	0	0	0	0
55	CA	207	0	0	0	0
55	CB	3	0	0	0	0
55	CC	8	0	0	0	0
55	CG	2	0	0	0	0
55	CN	1	0	0	0	0
55	CS	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	526	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DR	1	0	0	0	0
55	DU	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299552	0	200910	14872	3

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 30.

The worst 5 of 14872 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:625:G:H4'	16:AS:16:HIS:CD2	1.33	1.61
28:DE:46:ALA:CB	28:DE:82:ARG:HA	1.37	1.55
30:BG:83:ARG:H	30:BG:86:MET:CE	1.24	1.47
36:DP:26:TYR:CE1	36:DP:139:GLU:HB2	1.48	1.45
25:BA:1056:G:N2	25:BA:1103:A:H62	1.13	1.44

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:85:U:O2'	31:DH:100:GLY:O[3.555]	1.90	0.30
1:CA:86:U:O2'	25:DA:276:A:OP2[3.545]	2.02	0.18
6:AI:15:ASP:OD2	4:CG:27:TYR:OH[4.555]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	14	54
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	22	70
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	15	58
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	22	70
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	18	62
5	CH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	AI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	CI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	AJ	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	CJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	AK	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	30	78
8	CK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	AL	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	CL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	AM	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
10	CM	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	25	73
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	14	56
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	9	42
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	13	53
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	14	54
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	14	54
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	19	64
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	5	28
16	CS	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	AT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	CT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	AU	70/88 (80%)	64 (91%)	5 (7%)	1 (1%)	16	60
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	8	39
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	3	18
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	22	70
21	AX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	CX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	BD	270/276 (98%)	243 (90%)	22 (8%)	5 (2%)	12	51
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	8	39
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	1	2
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	1	5
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	5	26
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	8	37
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	33	81
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	4	20
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	2	9
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	11	47
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	3	18
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	15	58
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	27	76
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	1	4
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0	1
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	10	45
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	1	3
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	14	54
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	8	37
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	8	37
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	15	58
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	25	73
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	11	48
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	2	9
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	5	29
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	10	45
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	10	45
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	3	19
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	2	14
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	5	25
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	3	16
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	8	38
46	D3	75/85 (88%)	69 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BZ	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	6	33
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	21	67
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	7	34
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	15	58
49	BX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	DX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	B4	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	7	34
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	14	56
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	13	53
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	13	53
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	4	21
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	1	5
53	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
53	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
54	B8	59/65 (91%)	47 (80%)	7 (12%)	5 (8%)	1	6
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	1	2
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	8	39

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AG	13	ARG
4	AG	14	ARG
11	AN	82	VAL
16	AS	17	TYR
18	AU	22	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	155 (76%)	50 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1	7
3	AF	159/188 (85%)	120 (76%)	39 (24%)	1	5
3	CF	160/188 (85%)	124 (78%)	36 (22%)	1	7
4	AG	180/180 (100%)	144 (80%)	36 (20%)	2	10
4	CG	180/180 (100%)	140 (78%)	40 (22%)	1	7
5	AH	116/123 (94%)	88 (76%)	28 (24%)	1	5
5	CH	116/123 (94%)	89 (77%)	27 (23%)	1	6
6	AI	90/90 (100%)	76 (84%)	14 (16%)	4	18
6	CI	90/90 (100%)	74 (82%)	16 (18%)	2	14
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	3	14
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0	2
8	AK	119/119 (100%)	100 (84%)	19 (16%)	3	17
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1	8
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0	3
9	CL	98/99 (99%)	69 (70%)	29 (30%)	0	2
10	AM	89/92 (97%)	66 (74%)	23 (26%)	1	4
10	CM	89/92 (97%)	60 (67%)	29 (33%)	0	2
11	AN	90/99 (91%)	74 (82%)	16 (18%)	2	14
11	CN	90/99 (91%)	73 (81%)	17 (19%)	2	12
12	AO	104/109 (95%)	88 (85%)	16 (15%)	4	19
12	CO	104/109 (95%)	80 (77%)	24 (23%)	1	6
13	AP	94/101 (93%)	71 (76%)	23 (24%)	1	5
13	CP	94/101 (93%)	75 (80%)	19 (20%)	2	10
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0	2
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	2	9
15	AR	79/80 (99%)	68 (86%)	11 (14%)	5	23
15	CR	79/80 (99%)	66 (84%)	13 (16%)	3	16
16	AS	72/74 (97%)	53 (74%)	19 (26%)	1	4
16	CS	72/74 (97%)	62 (86%)	10 (14%)	5	23
17	AT	95/97 (98%)	82 (86%)	13 (14%)	5	24
17	CT	95/97 (98%)	89 (94%)	6 (6%)	25	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	63/77 (82%)	50 (79%)	13 (21%)	2	9
18	CU	63/77 (82%)	48 (76%)	15 (24%)	1	5
19	AV	67/80 (84%)	47 (70%)	20 (30%)	0	2
19	CV	67/80 (84%)	53 (79%)	14 (21%)	1	8
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1	8
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0	3
21	AX	20/22 (91%)	17 (85%)	3 (15%)	4	20
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	2	11
27	DD	214/218 (98%)	162 (76%)	52 (24%)	1	5
28	BE	165/166 (99%)	114 (69%)	51 (31%)	0	2
28	DE	165/166 (99%)	121 (73%)	44 (27%)	1	4
29	BF	161/166 (97%)	129 (80%)	32 (20%)	2	10
29	DF	165/166 (99%)	122 (74%)	43 (26%)	1	4
30	BG	155/156 (99%)	115 (74%)	40 (26%)	1	4
30	DG	155/156 (99%)	113 (73%)	42 (27%)	1	3
31	BH	142/148 (96%)	107 (75%)	35 (25%)	1	4
31	DH	142/148 (96%)	110 (78%)	32 (22%)	1	7
32	BK	122/124 (98%)	91 (75%)	31 (25%)	1	4
32	DK	122/124 (98%)	84 (69%)	38 (31%)	0	2
33	BM	117/119 (98%)	87 (74%)	30 (26%)	1	4
33	DM	117/119 (98%)	96 (82%)	21 (18%)	2	13
34	BN	100/100 (100%)	83 (83%)	17 (17%)	3	15
34	DN	100/100 (100%)	78 (78%)	22 (22%)	1	7
35	BO	116/116 (100%)	78 (67%)	38 (33%)	0	2
35	DO	116/116 (100%)	72 (62%)	44 (38%)	0	1
36	BP	111/111 (100%)	84 (76%)	27 (24%)	1	5
36	DP	111/111 (100%)	85 (77%)	26 (23%)	1	5
37	B0	101/101 (100%)	78 (77%)	23 (23%)	1	6
37	D0	100/101 (99%)	80 (80%)	20 (20%)	2	10
38	BQ	87/88 (99%)	65 (75%)	22 (25%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DQ	87/88 (99%)	53 (61%)	34 (39%)	0	1
39	BR	120/127 (94%)	92 (77%)	28 (23%)	1	6
39	DR	120/127 (94%)	84 (70%)	36 (30%)	0	2
40	B1	93/94 (99%)	76 (82%)	17 (18%)	2	13
40	D1	93/94 (99%)	80 (86%)	13 (14%)	5	23
41	B2	82/82 (100%)	61 (74%)	21 (26%)	1	4
41	D2	82/82 (100%)	50 (61%)	32 (39%)	0	1
42	BS	92/92 (100%)	72 (78%)	20 (22%)	1	8
42	DS	92/92 (100%)	65 (71%)	27 (29%)	0	2
43	BT	74/78 (95%)	61 (82%)	13 (18%)	3	14
43	DT	74/78 (95%)	57 (77%)	17 (23%)	1	6
44	BU	85/91 (93%)	65 (76%)	20 (24%)	1	5
44	DU	85/91 (93%)	51 (60%)	34 (40%)	0	0
45	BV	154/179 (86%)	116 (75%)	38 (25%)	1	4
45	DV	158/179 (88%)	124 (78%)	34 (22%)	1	8
46	B3	61/67 (91%)	54 (88%)	7 (12%)	8	32
46	D3	62/67 (92%)	47 (76%)	15 (24%)	1	5
47	BZ	82/83 (99%)	64 (78%)	18 (22%)	1	7
47	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	7
48	BW	62/67 (92%)	42 (68%)	20 (32%)	0	2
48	DW	64/67 (96%)	50 (78%)	14 (22%)	1	7
49	BX	51/52 (98%)	41 (80%)	10 (20%)	2	11
49	DX	51/52 (98%)	42 (82%)	9 (18%)	3	14
50	B4	59/63 (94%)	41 (70%)	18 (30%)	0	2
50	D4	57/63 (90%)	38 (67%)	19 (33%)	0	2
51	B5	51/52 (98%)	35 (69%)	16 (31%)	0	2
51	D5	51/52 (98%)	37 (72%)	14 (28%)	0	3
52	B6	44/52 (85%)	27 (61%)	17 (39%)	0	1
52	D6	44/52 (85%)	31 (70%)	13 (30%)	0	2
53	B7	42/42 (100%)	34 (81%)	8 (19%)	2	12
53	D7	42/42 (100%)	32 (76%)	10 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	B8	51/55 (93%)	40 (78%)	11 (22%)	<b>1</b> <b>8</b>
54	D8	51/55 (93%)	41 (80%)	10 (20%)	<b>2</b> <b>11</b>
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	<b>1</b> <b>5</b>

5 of 2262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BX	53	LEU
7	CJ	13	GLN
44	DU	62	GLU
51	B5	48	GLU
3	CF	28	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 255 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	65	ASN
6	CI	32	ASN
46	D3	12	ASN
49	BX	46	ASN
2	CE	78	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	375 (24%)	32 (2%)
1	CA	1505/1506 (99%)	409 (27%)	41 (2%)
22	AB	86/87 (98%)	40 (46%)	5 (5%)
22	CB	86/87 (98%)	46 (53%)	2 (2%)
23	AC	77/77 (100%)	23 (29%)	6 (7%)
23	AD	76/77 (98%)	28 (36%)	1 (1%)
23	CC	77/77 (100%)	21 (27%)	5 (6%)
23	CD	76/77 (98%)	26 (34%)	1 (1%)
24	A1	9/10 (90%)	3 (33%)	1 (11%)
24	C1	9/10 (90%)	3 (33%)	0
25	BA	2911/2912 (99%)	713 (24%)	57 (1%)
25	DA	2905/2912 (99%)	763 (26%)	57 (1%)
26	BB	121/122 (99%)	30 (24%)	0
26	DB	121/122 (99%)	39 (32%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9564/9582 (99%)	2519 (26%)	208 (2%)

5 of 2519 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	32	A
1	AA	33	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2439	A
1	CA	412	A
25	DA	2275	C
25	BA	2610	C
1	CA	115	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1700 ligands modelled in this entry, 1700 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1506/1506 (100%)	-0.57	4 (0%) 91 48	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.58	2 (0%) 93 63	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.08	2 (0%) 83 26	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.24	3 (1%) 74 19	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.64	12 (5%) 22 5	84, 111, 144, 153	0
3	CF	206/239 (86%)	1.16	38 (18%) 2 1	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.14	4 (1%) 64 13	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.17	2 (0%) 79 22	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.09	0 100 100	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.12	0 100 100	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.45	5 (4%) 28 6	76, 99, 115, 137	0
6	CI	101/101 (100%)	0.36	0 100 100	74, 95, 116, 141	0
7	AJ	155/156 (99%)	0.26	8 (5%) 26 6	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.22	6 (3%) 37 7	102, 122, 149, 156	0
8	AK	138/138 (100%)	-0.12	0 100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	-0.24	0 100 100	94, 116, 128, 136	0
9	AL	127/128 (99%)	-0.33	0 100 100	85, 133, 153, 160	0
9	CL	127/128 (99%)	-0.06	2 (1%) 68 16	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.14	0 100 100	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.26	0 100 100	111, 149, 165, 170	0
11	AN	119/129 (92%)	0.72	7 (5%) 22 5	64, 97, 128, 154	0
11	CN	119/129 (92%)	0.71	6 (5%) 28 6	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.44	7 (5%) 24 5	63, 73, 105, 151	0
12	CO	125/132 (94%)	0.82	15 (12%) 5 1	75, 98, 124, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	116/126 (92%)	0.00	1 (0%) 81 24	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.20	6 (5%) 27 6	106, 146, 161, 164	0
14	AQ	60/61 (98%)	-0.04	0 100 100	86, 101, 115, 126	0
14	CQ	60/61 (98%)	0.73	6 (10%) 8 2	118, 132, 146, 153	0
15	AR	88/89 (98%)	-0.02	1 (1%) 77 21	72, 93, 114, 117	0
15	CR	88/89 (98%)	0.06	1 (1%) 77 21	73, 104, 127, 133	0
16	AS	84/88 (95%)	-0.16	0 100 100	90, 107, 133, 165	0
16	CS	84/88 (95%)	-0.23	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	-0.04	1 (1%) 79 22	82, 100, 118, 130	0
17	CT	100/105 (95%)	0.00	1 (1%) 79 22	82, 102, 125, 137	0
18	AU	72/88 (81%)	0.37	1 (1%) 72 18	78, 99, 132, 159	0
18	CU	72/88 (81%)	0.32	5 (6%) 17 4	85, 106, 144, 157	0
19	AV	78/93 (83%)	-0.11	0 100 100	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.01	0 100 100	136, 154, 174, 177	0
20	AW	99/106 (93%)	-0.11	0 100 100	93, 115, 144, 155	0
20	CW	99/106 (93%)	0.01	0 100 100	83, 109, 143, 157	0
21	AX	25/27 (92%)	-0.38	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	0.11	0 100 100	112, 133, 148, 160	0
22	AB	87/87 (100%)	1.20	22 (25%) 1 1	78, 145, 185, 196	0
22	CB	87/87 (100%)	2.80	37 (42%) 1 0	92, 148, 188, 200	0
23	AC	77/77 (100%)	-0.24	0 100 100	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.21	5 (6%) 18 4	71, 218, 232, 234	0
23	CC	77/77 (100%)	-0.16	1 (1%) 74 19	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.36	9 (11%) 5 2	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.89	2 (20%) 2 1	67, 81, 112, 112	0
24	C1	10/10 (100%)	0.78	2 (20%) 2 1	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.37	31 (1%) 77 21	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.32	34 (1%) 75 20	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.64	1 (0%) 83 26	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.53	2 (1%) 68 16	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.08	0 100 100	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	272/276 (98%)	0.21	3 (1%) 77 21	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.20	3 (1%) 70 16	43, 77, 123, 132	0
28	DE	205/206 (99%)	0.18	5 (2%) 56 11	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.08	0 100 100	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.39	9 (4%) 34 7	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.36	6 (3%) 44 8	81, 101, 130, 142	0
30	DG	181/182 (99%)	0.71	14 (7%) 13 3	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.25	4 (2%) 56 11	74, 104, 121, 146	0
31	DH	170/180 (94%)	0.76	15 (8%) 10 3	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.13	1 (0%) 84 28	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.32	1 (0%) 84 28	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.14	1 (0%) 84 28	57, 81, 116, 129	0
33	DM	138/140 (98%)	-0.07	0 100 100	71, 102, 133, 143	0
34	BN	122/122 (100%)	0.21	0 100 100	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.33	0 100 100	62, 82, 102, 118	0
35	BO	150/150 (100%)	-0.00	2 (1%) 74 19	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.64	11 (7%) 15 3	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.35	5 (3%) 42 8	52, 78, 99, 125	0
36	DP	141/141 (100%)	0.65	10 (7%) 16 4	58, 98, 129, 148	0
37	B0	118/118 (100%)	0.15	0 100 100	50, 76, 94, 110	0
37	D0	117/118 (99%)	-0.04	0 100 100	50, 75, 97, 113	0
38	BQ	111/112 (99%)	0.07	0 100 100	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.17	2 (1%) 65 14	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.16	3 (2%) 59 12	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.18	0 100 100	69, 93, 154, 174	0
40	B1	117/118 (99%)	-0.15	2 (1%) 67 15	44, 70, 101, 132	0
40	D1	117/118 (99%)	-0.03	0 100 100	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.01	1 (0%) 79 22	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.29	1 (0%) 79 22	58, 115, 133, 142	0
42	BS	113/113 (100%)	0.07	3 (2%) 52 10	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.33	2 (1%) 65 14	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BT	92/96 (95%)	0.06	2 (2%) 59 12	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.27	4 (4%) 34 7	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.37	6 (5%) 22 5	67, 92, 142, 159	0
44	DU	102/110 (92%)	0.79	16 (15%) 3 1	82, 109, 160, 176	0
45	BV	175/206 (84%)	1.09	28 (16%) 3 1	80, 117, 179, 183	0
45	DV	179/206 (86%)	1.52	50 (27%) 1 0	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.14	1 (1%) 74 19	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.23	1 (1%) 74 19	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.27	6 (6%) 20 5	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.41	3 (3%) 47 9	54, 77, 126, 148	0
48	BW	66/72 (91%)	0.04	1 (1%) 70 16	55, 73, 90, 120	0
48	DW	69/72 (95%)	0.05	2 (2%) 49 9	77, 100, 130, 167	0
49	BX	59/60 (98%)	0.14	1 (1%) 67 15	60, 75, 105, 120	0
49	DX	59/60 (98%)	0.10	1 (1%) 67 15	73, 98, 130, 153	0
50	B4	66/71 (92%)	0.88	6 (9%) 9 2	111, 146, 164, 173	0
50	D4	63/71 (88%)	1.46	18 (28%) 1 0	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.66	9 (15%) 3 1	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.46	6 (10%) 7 2	52, 78, 167, 178	0
52	B6	45/54 (83%)	1.19	7 (15%) 3 1	105, 134, 156, 160	0
52	D6	45/54 (83%)	1.94	21 (46%) 1 0	121, 156, 173, 176	0
53	B7	49/49 (100%)	0.02	2 (4%) 35 7	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.25	2 (4%) 35 7	44, 54, 112, 131	0
54	B8	61/65 (93%)	0.06	0 100 100	51, 64, 81, 102	0
54	D8	61/65 (93%)	0.73	2 (3%) 44 8	65, 79, 94, 123	0
All	All	21104/21634 (97%)	-0.01	591 (2%) 50 10	35, 96, 177, 235	0

The worst 5 of 591 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	CB	54	G	13.6
22	CB	52	U	12.9
22	CB	53	A	12.8
22	CB	82	G	12.2
22	CB	51	A	11.4

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	BA	3156	1/1	0.27	-	40,40,40,40	0
55	MG	CA	1653	1/1	0.14	-	77,77,77,77	0
55	MG	BA	3079	1/1	0.41	-	55,55,55,55	0
55	MG	DA	3218	1/1	0.46	-	62,62,62,62	0
55	MG	BD	301	1/1	0.55	-	85,85,85,85	0
55	MG	BA	3115	1/1	0.33	-	87,87,87,87	0
55	MG	DA	3437	1/1	0.21	-	87,87,87,87	0
55	MG	BA	3102	1/1	0.31	-	66,66,66,66	0
55	MG	DA	3520	1/1	0.87	-	76,76,76,76	0
55	MG	BA	3061	1/1	0.57	-	61,61,61,61	0
55	MG	DA	3184	1/1	0.65	-	61,61,61,61	0
55	MG	BA	3110	1/1	0.54	-	59,59,59,59	0
55	MG	BA	3409	1/1	0.20	-	68,68,68,68	0
55	MG	AA	1619	1/1	0.39	-	63,63,63,63	0
55	MG	AA	1708	1/1	0.44	-	91,91,91,91	0
55	MG	DA	3113	1/1	0.57	-	43,43,43,43	0
55	MG	AA	1669	1/1	0.43	-	68,68,68,68	0
55	MG	BA	3506	1/1	0.44	-	78,78,78,78	0
55	MG	AA	1662	1/1	0.62	-	81,81,81,81	0
55	MG	BA	3158	1/1	0.27	-	41,41,41,41	0
55	MG	BA	3016	1/1	0.52	-	39,39,39,39	0
55	MG	DA	3122	1/1	0.47	-	46,46,46,46	0
55	MG	CB	101	1/1	0.22	-	101,101,101,101	0
55	MG	AA	1842	1/1	0.48	-	59,59,59,59	0
55	MG	CA	1750	1/1	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1689	1/1	0.24	-	115,115,115,115	0
55	MG	DA	3191	1/1	0.57	-	46,46,46,46	0
55	MG	DA	3196	1/1	0.46	-	50,50,50,50	0
55	MG	AA	1797	1/1	0.15	-	99,99,99,99	0
55	MG	DA	3398	1/1	0.43	-	74,74,74,74	0
55	MG	BA	3491	1/1	0.53	-	42,42,42,42	0
55	MG	BA	3045	1/1	0.39	-	45,45,45,45	0
55	MG	BA	3007	1/1	0.53	-	53,53,53,53	0
55	MG	AA	1706	1/1	0.51	-	74,74,74,74	0
55	MG	DA	3338	1/1	0.33	-	86,86,86,86	0
55	MG	DA	3313	1/1	0.32	-	85,85,85,85	0
55	MG	CA	1608	1/1	0.33	-	81,81,81,81	0
55	MG	CA	1723	1/1	0.08	-	86,86,86,86	0
55	MG	BA	3056	1/1	0.22	-	54,54,54,54	0
55	MG	BA	3225	1/1	0.23	-	65,65,65,65	0
55	MG	DA	3262	1/1	0.45	-	48,48,48,48	0
55	MG	AA	1687	1/1	0.38	-	72,72,72,72	0
55	MG	DA	3222	1/1	0.55	-	60,60,60,60	0
55	MG	DA	3306	1/1	0.53	-	65,65,65,65	0
55	MG	AA	1841	1/1	0.42	-	59,59,59,59	0
55	MG	BA	3338	1/1	0.38	-	71,71,71,71	0
55	MG	AA	1612	1/1	0.14	-	91,91,91,91	0
55	MG	BA	3030	1/1	0.53	-	44,44,44,44	0
55	MG	BA	3205	1/1	0.39	-	80,80,80,80	0
55	MG	BA	3333	1/1	0.53	-	80,80,80,80	0
55	MG	AA	1664	1/1	0.21	-	45,45,45,45	0
55	MG	BA	3324	1/1	0.56	-	73,73,73,73	0
55	MG	CA	1632	1/1	0.33	-	95,95,95,95	0
55	MG	DA	3308	1/1	0.40	-	97,97,97,97	0
55	MG	CA	1768	1/1	0.56	-	84,84,84,84	0
55	MG	BA	3385	1/1	0.15	-	87,87,87,87	0
55	MG	CA	1650	1/1	0.23	-	102,102,102,102	0
55	MG	AA	1690	1/1	0.20	-	96,96,96,96	0
55	MG	CA	1625	1/1	0.25	-	90,90,90,90	0
55	MG	BA	3431	1/1	0.71	-	88,88,88,88	0
55	MG	BO	202	1/1	0.22	-	37,37,37,37	0
55	MG	DA	3400	1/1	0.49	-	89,89,89,89	0
55	MG	AA	1793	1/1	0.42	-	73,73,73,73	0
55	MG	CS	101	1/1	0.31	-	87,87,87,87	0
55	MG	BA	3276	1/1	0.16	-	74,74,74,74	0
55	MG	DA	3447	1/1	0.45	-	82,82,82,82	0
55	MG	BA	3050	1/1	0.47	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1658	1/1	0.64	-	49,49,49,49	0
55	MG	BA	3085	1/1	0.17	-	73,73,73,73	0
55	MG	BA	3223	1/1	0.35	-	92,92,92,92	0
55	MG	DA	3168	1/1	0.31	-	49,49,49,49	0
55	MG	BA	3398	1/1	0.49	-	70,70,70,70	0
55	MG	DA	3438	1/1	0.38	-	87,87,87,87	0
55	MG	BA	3548	1/1	0.49	-	76,76,76,76	0
55	MG	DA	3219	1/1	0.30	-	70,70,70,70	0
55	MG	DA	3453	1/1	0.21	-	66,66,66,66	0
55	MG	DA	3024	1/1	0.36	-	108,108,108,108	0
55	MG	DA	3462	1/1	0.80	-	107,107,107,107	0
55	MG	CA	1748	1/1	0.21	-	87,87,87,87	0
55	MG	BA	3043	1/1	0.22	-	32,32,32,32	0
55	MG	DA	3157	1/1	0.70	-	47,47,47,47	0
55	MG	CA	1728	1/1	0.68	-	69,69,69,69	0
55	MG	BA	3394	1/1	0.20	-	81,81,81,81	0
55	MG	BA	3559	1/1	0.21	-	81,81,81,81	0
55	MG	BA	3162	1/1	0.53	-	45,45,45,45	0
55	MG	BA	3512	1/1	0.33	-	69,69,69,69	0
55	MG	AA	1671	1/1	0.16	-	67,67,67,67	0
55	MG	DA	3390	1/1	0.38	-	75,75,75,75	0
55	MG	DA	3446	1/1	0.51	-	75,75,75,75	0
55	MG	BA	3033	1/1	0.39	-	38,38,38,38	0
55	MG	DA	3280	1/1	0.55	-	46,46,46,46	0
55	MG	BA	3528	1/1	0.47	-	76,76,76,76	0
55	MG	BA	3329	1/1	0.42	-	65,65,65,65	0
55	MG	BA	3238	1/1	0.57	-	41,41,41,41	0
55	MG	DA	3507	1/1	0.43	-	91,91,91,91	0
55	MG	CA	1757	1/1	0.26	-	97,97,97,97	0
55	MG	DA	3472	1/1	0.68	-	71,71,71,71	0
55	MG	BA	3179	1/1	0.44	-	64,64,64,64	0
55	MG	CA	1631	1/1	0.13	-	81,81,81,81	0
55	MG	CA	1777	1/1	0.33	-	88,88,88,88	0
55	MG	AA	1692	1/1	0.17	-	115,115,115,115	0
55	MG	BB	207	1/1	0.27	-	83,83,83,83	0
55	MG	AA	1642	1/1	0.67	-	72,72,72,72	0
55	MG	DA	3522	1/1	0.48	-	78,78,78,78	0
55	MG	BA	3485	1/1	0.33	-	80,80,80,80	0
55	MG	AA	1634	1/1	0.28	-	62,62,62,62	0
55	MG	BA	3567	1/1	0.31	-	80,80,80,80	0
55	MG	CA	1656	1/1	0.35	-	92,92,92,92	0
55	MG	BA	3584	1/1	0.24	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1821	1/1	0.28	-	75,75,75,75	0
55	MG	DA	3480	1/1	0.44	-	63,63,63,63	0
55	MG	DA	3246	1/1	0.43	-	53,53,53,53	0
55	MG	CA	1660	1/1	0.18	-	85,85,85,85	0
55	MG	BA	3382	1/1	0.37	-	43,43,43,43	0
55	MG	DA	3416	1/1	0.48	-	59,59,59,59	0
55	MG	DA	3002	1/1	0.34	-	93,93,93,93	0
55	MG	DA	3368	1/1	0.69	-	73,73,73,73	0
55	MG	BA	3224	1/1	0.15	-	55,55,55,55	0
55	MG	DA	3328	1/1	0.32	-	47,47,47,47	0
55	MG	BA	3002	1/1	0.47	-	43,43,43,43	0
55	MG	CA	1772	1/1	0.30	-	72,72,72,72	0
55	MG	BA	3017	1/1	0.48	-	25,25,25,25	0
55	MG	BA	3010	1/1	0.42	-	46,46,46,46	0
55	MG	BA	3312	1/1	0.51	-	57,57,57,57	0
55	MG	BA	3400	1/1	0.51	-	80,80,80,80	0
55	MG	DA	3212	1/1	0.60	-	48,48,48,48	0
55	MG	BA	3293	1/1	0.29	-	65,65,65,65	0
55	MG	AA	1780	1/1	0.31	-	86,86,86,86	0
55	MG	AA	1654	1/1	0.46	-	75,75,75,75	0
55	MG	CC	103	1/1	0.98	-	72,72,72,72	0
55	MG	DA	3127	1/1	0.43	-	74,74,74,74	0
55	MG	DA	3164	1/1	0.43	-	47,47,47,47	0
55	MG	BA	3289	1/1	0.57	-	60,60,60,60	0
55	MG	BA	3336	1/1	0.45	-	66,66,66,66	0
55	MG	AA	1750	1/1	0.53	-	62,62,62,62	0
55	MG	DA	3171	1/1	0.38	-	63,63,63,63	0
55	MG	AA	1726	1/1	0.49	-	81,81,81,81	0
55	MG	DA	3495	1/1	0.17	-	63,63,63,63	0
55	MG	BU	201	1/1	0.22	-	81,81,81,81	0
55	MG	CA	1677	1/1	0.47	-	73,73,73,73	0
55	MG	BA	3561	1/1	0.38	-	74,74,74,74	0
55	MG	BA	3255	1/1	0.37	-	46,46,46,46	0
55	MG	CA	1670	1/1	0.52	-	56,56,56,56	0
55	MG	CA	1703	1/1	0.30	-	94,94,94,94	0
55	MG	BA	3254	1/1	0.32	-	43,43,43,43	0
55	MG	DA	3117	1/1	0.42	-	78,78,78,78	0
55	MG	BA	3490	1/1	0.15	-	166,166,166,166	0
55	MG	CA	1610	1/1	0.23	-	97,97,97,97	0
55	MG	BA	3285	1/1	0.40	-	72,72,72,72	0
55	MG	BA	3534	1/1	0.36	-	79,79,79,79	0
55	MG	AA	1740	1/1	0.18	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3424	1/1	0.72	-	70,70,70,70	0
55	MG	BA	3147	1/1	0.21	-	55,55,55,55	0
55	MG	DA	3483	1/1	0.19	-	90,90,90,90	0
55	MG	BA	3301	1/1	0.34	-	76,76,76,76	0
55	MG	DA	3475	1/1	0.40	-	88,88,88,88	0
55	MG	BA	3211	1/1	0.47	-	39,39,39,39	0
55	MG	BA	3437	1/1	0.44	-	67,67,67,67	0
55	MG	DA	3329	1/1	0.36	-	44,44,44,44	0
55	MG	CA	1720	1/1	0.49	-	102,102,102,102	0
55	MG	BA	3186	1/1	0.41	-	36,36,36,36	0
55	MG	BA	3618	1/1	0.43	-	73,73,73,73	0
55	MG	DA	3419	1/1	0.48	-	84,84,84,84	0
55	MG	DA	3060	1/1	0.83	-	73,73,73,73	0
55	MG	BA	3601	1/1	0.29	-	85,85,85,85	0
55	MG	CA	1645	1/1	0.22	-	86,86,86,86	0
55	MG	DA	3521	1/1	0.62	-	69,69,69,69	0
55	MG	BA	3096	1/1	0.53	-	56,56,56,56	0
55	MG	DA	3020	1/1	0.33	-	85,85,85,85	0
55	MG	BA	3105	1/1	0.38	-	75,75,75,75	0
55	MG	DA	3013	1/1	0.51	-	56,56,56,56	0
55	MG	BA	3101	1/1	0.65	-	63,63,63,63	0
55	MG	DA	3134	1/1	0.32	-	72,72,72,72	0
55	MG	AA	1756	1/1	0.27	-	69,69,69,69	0
55	MG	BA	3015	1/1	0.36	-	38,38,38,38	0
55	MG	BA	3434	1/1	0.55	-	75,75,75,75	0
55	MG	DA	3243	1/1	0.55	-	79,79,79,79	0
55	MG	DA	3285	1/1	0.26	-	50,50,50,50	0
55	MG	BA	3337	1/1	0.40	-	72,72,72,72	0
55	MG	BA	3215	1/1	0.52	-	74,74,74,74	0
55	MG	BA	3082	1/1	0.39	-	64,64,64,64	0
55	MG	DA	3384	1/1	0.36	-	65,65,65,65	0
55	MG	AA	1680	1/1	0.35	-	80,80,80,80	0
55	MG	BA	3454	1/1	0.40	-	92,92,92,92	0
55	MG	BA	3425	1/1	0.58	-	91,91,91,91	0
55	MG	CC	106	1/1	0.67	-	96,96,96,96	0
55	MG	CN	201	1/1	0.21	-	74,74,74,74	0
55	MG	BA	3112	1/1	0.29	-	77,77,77,77	0
55	MG	BA	3614	1/1	0.19	-	69,69,69,69	0
55	MG	BA	3071	1/1	0.28	-	70,70,70,70	0
55	MG	AA	1751	1/1	0.39	-	98,98,98,98	0
55	MG	CC	108	1/1	0.55	-	106,106,106,106	0
55	MG	BA	3503	1/1	0.22	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1655	1/1	0.37	-	87,87,87,87	0
55	MG	BA	3525	1/1	0.35	-	77,77,77,77	0
55	MG	BA	3540	1/1	0.29	-	61,61,61,61	0
55	MG	DA	3353	1/1	0.77	-	93,93,93,93	0
55	MG	BA	3523	1/1	0.63	-	70,70,70,70	0
55	MG	DA	3116	1/1	0.48	-	74,74,74,74	0
55	MG	CA	1764	1/1	0.54	-	72,72,72,72	0
55	MG	DA	3233	1/1	0.42	-	52,52,52,52	0
55	MG	DA	3478	1/1	0.33	-	80,80,80,80	0
55	MG	CA	1796	1/1	0.48	-	102,102,102,102	0
55	MG	DA	3186	1/1	0.33	-	60,60,60,60	0
55	MG	DA	3514	1/1	0.64	-	59,59,59,59	0
55	MG	DA	3155	1/1	0.44	-	46,46,46,46	0
55	MG	DA	3056	1/1	0.40	-	81,81,81,81	0
55	MG	DA	3396	1/1	0.33	-	82,82,82,82	0
55	MG	BB	215	1/1	0.33	-	82,82,82,82	0
55	MG	BA	3320	1/1	0.29	-	62,62,62,62	0
55	MG	BA	3586	1/1	0.38	-	63,63,63,63	0
55	MG	BA	3510	1/1	0.27	-	108,108,108,108	0
55	MG	CA	1604	1/1	0.20	-	81,81,81,81	0
55	MG	AA	1716	1/1	0.24	-	92,92,92,92	0
55	MG	BA	3258	1/1	0.27	-	45,45,45,45	0
55	MG	AA	1681	1/1	0.34	-	80,80,80,80	0
55	MG	AB	105	1/1	0.33	-	110,110,110,110	0
55	MG	BA	3369	1/1	0.37	-	73,73,73,73	0
55	MG	BA	3371	1/1	0.38	-	70,70,70,70	0
55	MG	BA	3331	1/1	0.40	-	65,65,65,65	0
55	MG	AA	1636	1/1	0.31	-	87,87,87,87	0
55	MG	AA	1805	1/1	0.34	-	65,65,65,65	0
55	MG	DA	3082	1/1	0.44	-	91,91,91,91	0
55	MG	BA	3390	1/1	0.32	-	60,60,60,60	0
55	MG	BA	3150	1/1	0.44	-	36,36,36,36	0
55	MG	CA	1724	1/1	0.51	-	84,84,84,84	0
55	MG	BA	3449	1/1	0.46	-	80,80,80,80	0
55	MG	AA	1800	1/1	0.32	-	82,82,82,82	0
55	MG	BA	3198	1/1	0.18	-	45,45,45,45	0
55	MG	CA	1705	1/1	0.49	-	80,80,80,80	0
55	MG	BA	3461	1/1	0.27	-	91,91,91,91	0
55	MG	DA	3345	1/1	0.39	-	64,64,64,64	0
55	MG	AA	1646	1/1	0.47	-	67,67,67,67	0
55	MG	BA	3302	1/1	0.40	-	26,26,26,26	0
55	MG	BA	3533	1/1	0.56	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3008	1/1	0.22	-	70,70,70,70	0
55	MG	CA	1800	1/1	0.36	-	78,78,78,78	0
55	MG	BA	3571	1/1	0.43	-	92,92,92,92	0
55	MG	DA	3322	1/1	0.53	-	70,70,70,70	0
55	MG	BA	3222	1/1	0.41	-	89,89,89,89	0
55	MG	CA	1702	1/1	0.43	-	78,78,78,78	0
55	MG	DA	3268	1/1	0.53	-	69,69,69,69	0
55	MG	DA	3241	1/1	0.48	-	46,46,46,46	0
55	MG	A1	101	1/1	0.16	-	66,66,66,66	0
55	MG	AA	1609	1/1	0.41	-	78,78,78,78	0
55	MG	DA	3348	1/1	0.63	-	73,73,73,73	0
55	MG	BA	3317	1/1	0.75	-	89,89,89,89	0
55	MG	CA	1718	1/1	0.10	-	92,92,92,92	0
55	MG	BA	3551	1/1	0.45	-	87,87,87,87	0
55	MG	DA	3482	1/1	0.45	-	81,81,81,81	0
55	MG	BA	3578	1/1	0.42	-	81,81,81,81	0
55	MG	BA	3422	1/1	0.34	-	78,78,78,78	0
55	MG	DA	3010	1/1	0.53	-	97,97,97,97	0
55	MG	AA	1629	1/1	0.14	-	86,86,86,86	0
55	MG	DA	3455	1/1	0.31	-	69,69,69,69	0
55	MG	CA	1669	1/1	0.20	-	60,60,60,60	0
55	MG	AB	104	1/1	0.45	-	82,82,82,82	0
55	MG	BA	3504	1/1	0.34	-	45,45,45,45	0
55	MG	BA	3546	1/1	0.24	-	87,87,87,87	0
55	MG	BA	3153	1/1	0.42	-	52,52,52,52	0
55	MG	BA	3114	1/1	0.18	-	74,74,74,74	0
55	MG	BA	3563	1/1	0.26	-	82,82,82,82	0
55	MG	DA	3276	1/1	0.52	-	68,68,68,68	0
55	MG	CA	1675	1/1	0.45	-	62,62,62,62	0
55	MG	BA	3305	1/1	0.41	-	70,70,70,70	0
55	MG	CA	1634	1/1	0.42	-	77,77,77,77	0
55	MG	DE	301	1/1	0.35	-	41,41,41,41	0
55	MG	BA	3442	1/1	0.38	-	76,76,76,76	0
55	MG	DA	3170	1/1	0.49	-	68,68,68,68	0
55	MG	DA	3140	1/1	0.38	-	78,78,78,78	0
55	MG	DA	3150	1/1	0.33	-	68,68,68,68	0
55	MG	AA	1832	1/1	0.40	-	94,94,94,94	0
55	MG	DA	3247	1/1	0.24	-	87,87,87,87	0
55	MG	BA	3025	1/1	0.37	-	42,42,42,42	0
55	MG	DA	3110	1/1	0.32	-	58,58,58,58	0
55	MG	CA	1792	1/1	0.60	-	70,70,70,70	0
55	MG	AA	1738	1/1	0.59	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3174	1/1	0.60	-	44,44,44,44	0
55	MG	AA	1767	1/1	0.20	-	96,96,96,96	0
55	MG	BA	3031	1/1	0.38	-	33,33,33,33	0
55	MG	DA	3092	1/1	0.41	-	68,68,68,68	0
55	MG	BA	3247	1/1	0.48	-	70,70,70,70	0
55	MG	DA	3187	1/1	0.45	-	42,42,42,42	0
55	MG	DA	3190	1/1	0.58	-	61,61,61,61	0
55	MG	BA	3412	1/1	0.48	-	78,78,78,78	0
55	MG	DA	3253	1/1	0.24	-	87,87,87,87	0
55	MG	BA	3615	1/1	0.41	-	81,81,81,81	0
55	MG	BA	3487	1/1	0.22	-	94,94,94,94	0
55	MG	BA	3119	1/1	0.39	-	62,62,62,62	0
55	MG	BA	3622	1/1	0.48	-	59,59,59,59	0
55	MG	AA	1768	1/1	0.37	-	101,101,101,101	0
55	MG	BU	202	1/1	0.13	-	55,55,55,55	0
55	MG	BA	3274	1/1	0.16	-	46,46,46,46	0
55	MG	AD	101	1/1	0.38	-	101,101,101,101	0
55	MG	CA	1804	1/1	0.28	-	75,75,75,75	0
55	MG	CA	1717	1/1	0.22	-	106,106,106,106	0
55	MG	BA	3348	1/1	0.32	-	61,61,61,61	0
55	MG	BA	3028	1/1	0.43	-	46,46,46,46	0
55	MG	DA	3457	1/1	0.80	-	65,65,65,65	0
55	MG	BA	3078	1/1	0.38	-	65,65,65,65	0
55	MG	BA	3323	1/1	0.32	-	66,66,66,66	0
55	MG	CA	1737	1/1	0.28	-	99,99,99,99	0
55	MG	DA	3375	1/1	0.86	-	88,88,88,88	0
55	MG	D5	2001	1/1	0.37	-	46,46,46,46	0
55	MG	BA	3168	1/1	0.37	-	49,49,49,49	0
55	MG	DA	3005	1/1	0.53	-	77,77,77,77	0
55	MG	DA	3097	1/1	0.30	-	52,52,52,52	0
55	MG	DA	3316	1/1	0.36	-	61,61,61,61	0
55	MG	AA	1665	1/1	0.72	-	70,70,70,70	0
55	MG	AA	1712	1/1	0.38	-	78,78,78,78	0
55	MG	DA	3166	1/1	0.44	-	58,58,58,58	0
55	MG	DA	3234	1/1	0.43	-	52,52,52,52	0
55	MG	AA	1702	1/1	0.23	-	93,93,93,93	0
55	MG	BA	3460	1/1	0.25	-	83,83,83,83	0
55	MG	CA	1686	1/1	0.43	-	73,73,73,73	0
55	MG	BA	3206	1/1	0.43	-	75,75,75,75	0
55	MG	DA	3524	1/1	0.31	-	105,105,105,105	0
55	MG	AN	202	1/1	0.38	-	82,82,82,82	0
55	MG	BA	3335	1/1	0.38	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1655	1/1	0.47	-	88,88,88,88	0
55	MG	CA	1700	1/1	0.53	-	77,77,77,77	0
55	MG	DA	3050	1/1	0.68	-	66,66,66,66	0
55	MG	BA	3462	1/1	0.33	-	87,87,87,87	0
55	MG	BA	3290	1/1	0.45	-	97,97,97,97	0
55	MG	DA	3303	1/1	0.42	-	70,70,70,70	0
55	MG	BA	3516	1/1	0.95	-	78,78,78,78	0
55	MG	CA	1644	1/1	0.32	-	120,120,120,120	0
55	MG	CA	1769	1/1	0.38	-	105,105,105,105	0
55	MG	DA	3374	1/1	0.43	-	62,62,62,62	0
55	MG	BA	3244	1/1	0.34	-	58,58,58,58	0
55	MG	AA	1713	1/1	0.49	-	115,115,115,115	0
55	MG	DA	3063	1/1	0.54	-	75,75,75,75	0
55	MG	DA	3519	1/1	0.30	-	85,85,85,85	0
55	MG	DA	3176	1/1	0.62	-	65,65,65,65	0
55	MG	DA	3105	1/1	0.35	-	45,45,45,45	0
55	MG	DA	3015	1/1	0.67	-	89,89,89,89	0
55	MG	BA	3064	1/1	0.28	-	49,49,49,49	0
55	MG	DA	3473	1/1	0.51	-	96,96,96,96	0
55	MG	DA	3380	1/1	0.15	-	139,139,139,139	0
55	MG	BA	3526	1/1	0.45	-	86,86,86,86	0
55	MG	DA	3095	1/1	0.40	-	49,49,49,49	0
55	MG	CA	1797	1/1	0.34	-	87,87,87,87	0
55	MG	BA	3001	1/1	0.49	-	47,47,47,47	0
55	MG	DA	3510	1/1	0.42	-	85,85,85,85	0
55	MG	BA	3355	1/1	0.60	-	46,46,46,46	0
55	MG	BA	3620	1/1	0.31	-	68,68,68,68	0
55	MG	DA	3021	1/1	0.51	-	51,51,51,51	0
55	MG	DA	3018	1/1	0.31	-	77,77,77,77	0
55	MG	DA	3161	1/1	0.45	-	45,45,45,45	0
55	MG	BA	3300	1/1	0.45	-	88,88,88,88	0
55	MG	DA	3132	1/1	0.34	-	53,53,53,53	0
55	MG	CA	1649	1/1	0.29	-	64,64,64,64	0
55	MG	DA	3047	1/1	0.47	-	76,76,76,76	0
55	MG	BA	3436	1/1	0.28	-	59,59,59,59	0
55	MG	CA	1651	1/1	0.38	-	90,90,90,90	0
55	MG	DA	3204	1/1	0.36	-	51,51,51,51	0
55	MG	CA	1693	1/1	0.52	-	76,76,76,76	0
55	MG	DA	3200	1/1	0.44	-	44,44,44,44	0
55	MG	BA	3235	1/1	0.41	-	54,54,54,54	0
55	MG	DA	3226	1/1	0.43	-	62,62,62,62	0
55	MG	AA	1674	1/1	0.38	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3579	1/1	0.20	-	92,92,92,92	0
55	MG	BA	3054	1/1	0.34	-	80,80,80,80	0
55	MG	BA	3034	1/1	0.35	-	41,41,41,41	0
55	MG	BA	3428	1/1	0.41	-	68,68,68,68	0
55	MG	CA	1739	1/1	0.53	-	75,75,75,75	0
55	MG	AA	1766	1/1	0.18	-	79,79,79,79	0
55	MG	DA	3467	1/1	0.42	-	61,61,61,61	0
55	MG	DA	3195	1/1	0.81	-	70,70,70,70	0
55	MG	BA	3583	1/1	0.20	-	86,86,86,86	0
55	MG	BA	3505	1/1	0.55	-	96,96,96,96	0
55	MG	AA	1779	1/1	0.36	-	72,72,72,72	0
55	MG	BA	3429	1/1	0.11	-	75,75,75,75	0
55	MG	BA	3543	1/1	0.49	-	80,80,80,80	0
55	MG	BA	3319	1/1	0.34	-	65,65,65,65	0
55	MG	AC	108	1/1	0.48	-	85,85,85,85	0
55	MG	CA	1659	1/1	0.21	-	110,110,110,110	0
55	MG	BA	3210	1/1	0.20	-	74,74,74,74	0
55	MG	DA	3331	1/1	0.52	-	50,50,50,50	0
55	MG	BA	3575	1/1	0.37	-	71,71,71,71	0
55	MG	AA	1697	1/1	0.27	-	84,84,84,84	0
55	MG	BA	3268	1/1	0.57	-	67,67,67,67	0
55	MG	BA	3012	1/1	0.30	-	45,45,45,45	0
55	MG	BA	3482	1/1	0.48	-	57,57,57,57	0
55	MG	CA	1806	1/1	0.53	-	96,96,96,96	0
55	MG	DA	3383	1/1	0.51	-	87,87,87,87	0
55	MG	DA	3271	1/1	0.50	-	58,58,58,58	0
55	MG	BA	3204	1/1	0.42	-	78,78,78,78	0
55	MG	CA	1665	1/1	0.23	-	83,83,83,83	0
55	MG	BA	3271	1/1	0.19	-	35,35,35,35	0
55	MG	CA	1663	1/1	0.41	-	81,81,81,81	0
55	MG	AA	1688	1/1	0.28	-	72,72,72,72	0
55	MG	BA	3354	1/1	0.26	-	72,72,72,72	0
55	MG	BA	3192	1/1	0.34	-	34,34,34,34	0
55	MG	DB	208	1/1	0.27	-	90,90,90,90	0
55	MG	DA	3290	1/1	0.31	-	79,79,79,79	0
55	MG	CA	1664	1/1	0.29	-	99,99,99,99	0
55	MG	DA	3444	1/1	0.16	-	73,73,73,73	0
55	MG	AA	1645	1/1	0.48	-	50,50,50,50	0
55	MG	BA	3202	1/1	0.42	-	51,51,51,51	0
55	MG	AA	1614	1/1	0.26	-	91,91,91,91	0
55	MG	DA	3034	1/1	0.34	-	62,62,62,62	0
55	MG	DA	3372	1/1	0.33	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1648	1/1	0.53	-	78,78,78,78	0
55	MG	AA	1635	1/1	0.21	-	86,86,86,86	0
55	MG	CA	1617	1/1	0.28	-	93,93,93,93	0
55	MG	BA	3304	1/1	0.29	-	56,56,56,56	0
55	MG	BA	3474	1/1	0.48	-	80,80,80,80	0
55	MG	BA	3493	1/1	0.38	-	63,63,63,63	0
55	MG	DA	3245	1/1	0.55	-	60,60,60,60	0
55	MG	BA	3019	1/1	0.46	-	66,66,66,66	0
55	MG	CA	1654	1/1	0.26	-	99,99,99,99	0
55	MG	CA	1775	1/1	0.39	-	72,72,72,72	0
55	MG	BA	3151	1/1	0.28	-	83,83,83,83	0
55	MG	BA	3549	1/1	0.29	-	68,68,68,68	0
55	MG	BA	3527	1/1	0.59	-	93,93,93,93	0
55	MG	CA	1674	1/1	0.11	-	70,70,70,70	0
55	MG	BA	3190	1/1	0.35	-	63,63,63,63	0
55	MG	BA	3086	1/1	0.30	-	95,95,95,95	0
55	MG	CA	1725	1/1	0.22	-	86,86,86,86	0
55	MG	AA	1676	1/1	0.39	-	70,70,70,70	0
55	MG	DA	3279	1/1	0.30	-	84,84,84,84	0
55	MG	BA	3044	1/1	0.39	-	62,62,62,62	0
55	MG	BA	3568	1/1	0.48	-	83,83,83,83	0
55	MG	DA	3363	1/1	0.77	-	79,79,79,79	0
55	MG	DA	3324	1/1	0.27	-	78,78,78,78	0
55	MG	BA	3414	1/1	0.19	-	72,72,72,72	0
55	MG	BA	3489	1/1	0.27	-	70,70,70,70	0
55	MG	AA	1777	1/1	0.48	-	90,90,90,90	0
55	MG	DA	3089	1/1	0.55	-	82,82,82,82	0
55	MG	DA	3461	1/1	0.27	-	84,84,84,84	0
55	MG	DA	3357	1/1	0.39	-	96,96,96,96	0
55	MG	DA	3220	1/1	0.42	-	66,66,66,66	0
55	MG	AA	1820	1/1	0.29	-	75,75,75,75	0
55	MG	CA	1692	1/1	0.52	-	82,82,82,82	0
55	MG	DA	3182	1/1	0.79	-	44,44,44,44	0
55	MG	DA	3469	1/1	0.61	-	80,80,80,80	0
55	MG	DA	3273	1/1	0.20	-	99,99,99,99	0
55	MG	BA	3212	1/1	0.61	-	43,43,43,43	0
55	MG	BA	3591	1/1	0.50	-	64,64,64,64	0
55	MG	BA	3457	1/1	0.90	-	88,88,88,88	0
55	MG	DA	3141	1/1	0.53	-	38,38,38,38	0
55	MG	BA	3481	1/1	0.60	-	69,69,69,69	0
55	MG	DA	3045	1/1	0.60	-	94,94,94,94	0
55	MG	DA	3439	1/1	0.33	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3466	1/1	0.51	-	97,97,97,97	0
55	MG	DA	3202	1/1	0.45	-	47,47,47,47	0
55	MG	AA	1667	1/1	0.32	-	68,68,68,68	0
55	MG	BA	3262	1/1	0.56	-	33,33,33,33	0
55	MG	BA	3278	1/1	0.45	-	81,81,81,81	0
55	MG	BE	305	1/1	0.42	-	71,71,71,71	0
55	MG	DA	3493	1/1	0.59	-	82,82,82,82	0
55	MG	DA	3334	1/1	0.45	-	68,68,68,68	0
55	MG	DA	3409	1/1	0.60	-	76,76,76,76	0
55	MG	AA	1719	1/1	0.57	-	79,79,79,79	0
55	MG	AA	1728	1/1	0.22	-	108,108,108,108	0
55	MG	DA	3377	1/1	0.27	-	98,98,98,98	0
55	MG	DA	3036	1/1	0.25	-	99,99,99,99	0
55	MG	AA	1826	1/1	0.16	-	101,101,101,101	0
55	MG	DA	3443	1/1	0.43	-	80,80,80,80	0
55	MG	AA	1799	1/1	0.36	-	78,78,78,78	0
55	MG	BA	3325	1/1	0.46	-	76,76,76,76	0
55	MG	DA	3123	1/1	0.34	-	83,83,83,83	0
55	MG	CA	1698	1/1	0.09	-	107,107,107,107	0
55	MG	CA	1716	1/1	0.22	-	79,79,79,79	0
55	MG	BA	3594	1/1	0.60	-	79,79,79,79	0
55	MG	BA	3366	1/1	1.17	-	94,94,94,94	0
55	MG	DB	207	1/1	0.35	-	115,115,115,115	0
55	MG	CA	1641	1/1	0.28	-	66,66,66,66	0
55	MG	BA	3226	1/1	0.43	-	50,50,50,50	0
55	MG	BA	3125	1/1	0.55	-	52,52,52,52	0
55	MG	DA	3498	1/1	0.27	-	85,85,85,85	0
55	MG	DA	3434	1/1	0.13	-	74,74,74,74	0
55	MG	DA	3474	1/1	0.54	-	83,83,83,83	0
55	MG	AA	1701	1/1	0.21	-	70,70,70,70	0
55	MG	DA	3428	1/1	0.60	-	84,84,84,84	0
55	MG	BA	3280	1/1	0.54	-	50,50,50,50	0
55	MG	CA	1784	1/1	0.20	-	81,81,81,81	0
55	MG	DA	3240	1/1	0.54	-	42,42,42,42	0
55	MG	CA	1719	1/1	0.25	-	129,129,129,129	0
55	MG	BA	3138	1/1	0.47	-	46,46,46,46	0
55	MG	DA	3325	1/1	0.58	-	73,73,73,73	0
55	MG	AA	1601	1/1	0.35	-	56,56,56,56	0
55	MG	AA	1775	1/1	0.18	-	79,79,79,79	0
55	MG	DA	3030	1/1	0.36	-	74,74,74,74	0
55	MG	CA	1612	1/1	0.45	-	82,82,82,82	0
55	MG	BA	3577	1/1	0.19	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3108	1/1	0.33	-	54,54,54,54	0
55	MG	BA	3246	1/1	0.43	-	68,68,68,68	0
55	MG	AA	1773	1/1	0.27	-	87,87,87,87	0
55	MG	CA	1687	1/1	0.24	-	89,89,89,89	0
55	MG	DA	3022	1/1	0.57	-	60,60,60,60	0
55	MG	AA	1778	1/1	0.19	-	106,106,106,106	0
55	MG	DA	3275	1/1	0.37	-	76,76,76,76	0
55	MG	DA	3121	1/1	0.20	-	64,64,64,64	0
55	MG	BA	3494	1/1	0.76	-	76,76,76,76	0
55	MG	BA	3188	1/1	0.36	-	60,60,60,60	0
55	MG	BA	3589	1/1	0.33	-	41,41,41,41	0
55	MG	AA	1782	1/1	0.17	-	96,96,96,96	0
55	MG	DA	3355	1/1	0.54	-	77,77,77,77	0
55	MG	DA	3088	1/1	0.27	-	96,96,96,96	0
55	MG	CA	1787	1/1	0.17	-	87,87,87,87	0
55	MG	AA	1616	1/1	0.19	-	94,94,94,94	0
55	MG	DA	3131	1/1	0.23	-	79,79,79,79	0
55	MG	BA	3587	1/1	0.33	-	64,64,64,64	0
55	MG	BA	3448	1/1	0.48	-	100,100,100,100	0
55	MG	AA	1657	1/1	0.44	-	50,50,50,50	0
55	MG	BA	3435	1/1	0.33	-	65,65,65,65	0
55	MG	AA	1801	1/1	0.54	-	84,84,84,84	0
55	MG	DA	3158	1/1	0.62	-	44,44,44,44	0
55	MG	AA	1684	1/1	0.22	-	90,90,90,90	0
55	MG	BA	3605	1/1	0.49	-	47,47,47,47	0
55	MG	BA	3131	1/1	0.35	-	59,59,59,59	0
55	MG	AA	1823	1/1	0.52	-	77,77,77,77	0
55	MG	DA	3042	1/1	0.57	-	81,81,81,81	0
55	MG	BA	3090	1/1	0.48	-	49,49,49,49	0
55	MG	BA	3196	1/1	0.32	-	33,33,33,33	0
55	MG	AA	1714	1/1	0.40	-	107,107,107,107	0
55	MG	BA	3445	1/1	0.47	-	79,79,79,79	0
55	MG	CA	1760	1/1	0.26	-	91,91,91,91	0
55	MG	BA	3252	1/1	0.47	-	67,67,67,67	0
55	MG	DA	3244	1/1	0.51	-	71,71,71,71	0
55	MG	BA	3327	1/1	0.28	-	70,70,70,70	0
55	MG	AA	1741	1/1	0.32	-	67,67,67,67	0
55	MG	CA	1766	1/1	0.32	-	85,85,85,85	0
55	MG	BA	3597	1/1	0.23	-	79,79,79,79	0
55	MG	BA	3189	1/1	0.43	-	49,49,49,49	0
55	MG	DA	3485	1/1	0.20	-	81,81,81,81	0
55	MG	CC	104	1/1	0.63	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3072	1/1	0.44	-	112,112,112,112	0
55	MG	AA	1695	1/1	0.27	-	90,90,90,90	0
55	MG	AA	1737	1/1	0.59	-	83,83,83,83	0
55	MG	AA	1678	1/1	0.38	-	74,74,74,74	0
55	MG	BA	3391	1/1	0.45	-	86,86,86,86	0
55	MG	AA	1839	1/1	0.35	-	74,74,74,74	0
55	MG	AA	1707	1/1	0.60	-	50,50,50,50	0
55	MG	AA	1731	1/1	0.31	-	103,103,103,103	0
55	MG	AA	1620	1/1	0.27	-	66,66,66,66	0
55	MG	DA	3422	1/1	0.36	-	84,84,84,84	0
55	MG	BA	3057	1/1	0.15	-	70,70,70,70	0
55	MG	BA	3379	1/1	0.49	-	82,82,82,82	0
55	MG	AA	1781	1/1	0.44	-	94,94,94,94	0
55	MG	DA	3229	1/1	0.47	-	62,62,62,62	0
55	MG	BA	3187	1/1	0.49	-	73,73,73,73	0
55	MG	BA	3288	1/1	0.49	-	76,76,76,76	0
55	MG	BA	3165	1/1	0.59	-	61,61,61,61	0
55	MG	BA	3607	1/1	0.38	-	96,96,96,96	0
55	MG	BA	3277	1/1	0.31	-	86,86,86,86	0
55	MG	BA	3450	1/1	0.17	-	54,54,54,54	0
55	MG	DA	3426	1/1	0.40	-	58,58,58,58	0
55	MG	BA	3585	1/1	0.34	-	60,60,60,60	0
55	MG	CA	1639	1/1	0.30	-	95,95,95,95	0
55	MG	BA	3060	1/1	0.16	-	64,64,64,64	0
55	MG	DA	3283	1/1	0.43	-	61,61,61,61	0
55	MG	BA	3368	1/1	0.34	-	88,88,88,88	0
55	MG	BA	3339	1/1	0.67	-	88,88,88,88	0
55	MG	CA	1732	1/1	0.23	-	109,109,109,109	0
55	MG	BA	3612	1/1	0.53	-	66,66,66,66	0
55	MG	DA	3382	1/1	0.52	-	78,78,78,78	0
55	MG	CA	1795	1/1	0.33	-	76,76,76,76	0
55	MG	BA	3536	1/1	0.67	-	73,73,73,73	0
55	MG	DA	3028	1/1	0.30	-	101,101,101,101	0
55	MG	DA	3165	1/1	0.58	-	65,65,65,65	0
55	MG	DA	3096	1/1	0.61	-	53,53,53,53	0
55	MG	DA	3342	1/1	0.43	-	82,82,82,82	0
55	MG	DA	3347	1/1	0.11	-	75,75,75,75	0
55	MG	BA	3569	1/1	0.59	-	85,85,85,85	0
55	MG	DA	3448	1/1	0.69	-	79,79,79,79	0
55	MG	BA	3014	1/1	0.48	-	53,53,53,53	0
55	MG	DA	3238	1/1	0.43	-	60,60,60,60	0
55	MG	DA	3526	1/1	0.32	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3035	1/1	0.24	-	62,62,62,62	0
55	MG	CA	1742	1/1	0.18	-	97,97,97,97	0
55	MG	CA	1609	1/1	0.18	-	115,115,115,115	0
55	MG	BA	3350	1/1	0.27	-	55,55,55,55	0
55	MG	BA	3026	1/1	0.31	-	47,47,47,47	0
55	MG	AA	1606	1/1	0.08	-	91,91,91,91	0
55	MG	DA	3237	1/1	0.22	-	83,83,83,83	0
55	MG	DA	3180	1/1	0.62	-	52,52,52,52	0
55	MG	BA	3476	1/1	0.33	-	81,81,81,81	0
55	MG	CA	1691	1/1	0.34	-	78,78,78,78	0
55	MG	DA	3114	1/1	0.57	-	54,54,54,54	0
55	MG	BA	3438	1/1	0.45	-	91,91,91,91	0
55	MG	DA	3077	1/1	0.15	-	64,64,64,64	0
55	MG	BA	3243	1/1	0.49	-	48,48,48,48	0
55	MG	DU	201	1/1	0.16	-	72,72,72,72	0
55	MG	DA	3402	1/1	0.40	-	101,101,101,101	0
55	MG	CA	1779	1/1	0.37	-	72,72,72,72	0
55	MG	DA	3391	1/1	0.28	-	78,78,78,78	0
55	MG	DA	3370	1/1	0.11	-	67,67,67,67	0
55	MG	B2	201	1/1	0.46	-	85,85,85,85	0
55	MG	BA	3144	1/1	0.31	-	48,48,48,48	0
55	MG	DA	3433	1/1	0.55	-	57,57,57,57	0
55	MG	DA	3252	1/1	0.36	-	64,64,64,64	0
55	MG	BA	3395	1/1	0.26	-	72,72,72,72	0
55	MG	AA	1608	1/1	0.24	-	64,64,64,64	0
55	MG	BA	3451	1/1	0.50	-	65,65,65,65	0
55	MG	CA	1602	1/1	0.33	-	80,80,80,80	0
55	MG	BA	3447	1/1	0.48	-	71,71,71,71	0
55	MG	BF	302	1/1	0.21	-	72,72,72,72	0
55	MG	DA	3463	1/1	0.26	-	73,73,73,73	0
55	MG	BA	3123	1/1	0.21	-	51,51,51,51	0
55	MG	CA	1759	1/1	0.40	-	103,103,103,103	0
55	MG	DA	3145	1/1	0.53	-	60,60,60,60	0
55	MG	CA	1780	1/1	0.31	-	88,88,88,88	0
55	MG	DA	3356	1/1	0.31	-	67,67,67,67	0
55	MG	DA	3091	1/1	0.36	-	92,92,92,92	0
55	MG	BA	3208	1/1	0.10	-	45,45,45,45	0
55	MG	BA	3143	1/1	0.68	-	72,72,72,72	0
55	MG	BA	3452	1/1	0.42	-	41,41,41,41	0
55	MG	CA	1636	1/1	0.32	-	78,78,78,78	0
55	MG	BA	3175	1/1	0.49	-	69,69,69,69	0
55	MG	DA	3477	1/1	0.65	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3378	1/1	0.55	-	76,76,76,76	0
55	MG	DA	3151	1/1	0.25	-	85,85,85,85	0
55	MG	AA	1723	1/1	0.33	-	84,84,84,84	0
55	MG	DA	3025	1/1	1.41	-	84,84,84,84	0
55	MG	DA	3162	1/1	0.30	-	66,66,66,66	0
55	MG	AA	1729	1/1	0.44	-	113,113,113,113	0
55	MG	BA	3408	1/1	0.48	-	87,87,87,87	0
55	MG	CA	1626	1/1	0.19	-	93,93,93,93	0
55	MG	DA	3078	1/1	0.42	-	89,89,89,89	0
55	MG	DA	3312	1/1	0.30	-	85,85,85,85	0
55	MG	B8	101	1/1	0.19	-	97,97,97,97	0
55	MG	AA	1717	1/1	0.44	-	74,74,74,74	0
55	MG	DA	3274	1/1	0.28	-	87,87,87,87	0
55	MG	DA	3211	1/1	0.49	-	42,42,42,42	0
55	MG	DA	3142	1/1	0.52	-	40,40,40,40	0
55	MG	BA	3236	1/1	0.44	-	52,52,52,52	0
55	MG	CA	1763	1/1	0.50	-	91,91,91,91	0
55	MG	CA	1615	1/1	0.27	-	81,81,81,81	0
55	MG	BA	3149	1/1	0.23	-	80,80,80,80	0
55	MG	DA	3518	1/1	0.41	-	83,83,83,83	0
55	MG	BA	3593	1/1	0.35	-	80,80,80,80	0
55	MG	DA	3417	1/1	0.24	-	81,81,81,81	0
55	MG	DA	3516	1/1	0.34	-	105,105,105,105	0
55	MG	DA	3489	1/1	0.19	-	71,71,71,71	0
55	MG	DA	3304	1/1	0.39	-	85,85,85,85	0
55	MG	DA	3511	1/1	0.42	-	76,76,76,76	0
55	MG	BA	3133	1/1	0.31	-	66,66,66,66	0
55	MG	CA	1671	1/1	0.59	-	49,49,49,49	0
55	MG	DA	3249	1/1	0.42	-	72,72,72,72	0
55	MG	BA	3292	1/1	0.39	-	85,85,85,85	0
55	MG	CA	1640	1/1	0.34	-	81,81,81,81	0
55	MG	CA	1638	1/1	0.32	-	101,101,101,101	0
55	MG	AA	1622	1/1	0.20	-	76,76,76,76	0
55	MG	DA	3464	1/1	0.52	-	98,98,98,98	0
55	MG	DA	3152	1/1	0.13	-	67,67,67,67	0
55	MG	BA	3218	1/1	0.55	-	48,48,48,48	0
55	MG	DA	3327	1/1	0.38	-	61,61,61,61	0
55	MG	BA	3351	1/1	1.00	-	78,78,78,78	0
55	MG	CA	1647	1/1	0.52	-	61,61,61,61	0
55	MG	AA	1607	1/1	0.24	-	89,89,89,89	0
55	MG	CA	1614	1/1	0.42	-	86,86,86,86	0
55	MG	BA	3146	1/1	0.38	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3216	1/1	0.33	-	49,49,49,49	0
55	MG	DA	3431	1/1	0.40	-	91,91,91,91	0
55	MG	DA	3484	1/1	0.42	-	83,83,83,83	0
55	MG	AA	1630	1/1	0.15	-	101,101,101,101	0
55	MG	BA	3380	1/1	0.23	-	65,65,65,65	0
55	MG	BA	3432	1/1	0.39	-	80,80,80,80	0
55	MG	CA	1696	1/1	0.39	-	91,91,91,91	0
55	MG	CA	1740	1/1	0.29	-	68,68,68,68	0
55	MG	AA	1734	1/1	0.27	-	96,96,96,96	0
55	MG	BA	3389	1/1	0.27	-	59,59,59,59	0
55	MG	BA	3041	1/1	0.32	-	46,46,46,46	0
55	MG	BA	3353	1/1	0.45	-	52,52,52,52	0
55	MG	BA	3364	1/1	0.47	-	82,82,82,82	0
55	MG	AA	1670	1/1	0.43	-	63,63,63,63	0
55	MG	DB	213	1/1	0.18	-	94,94,94,94	0
55	MG	BA	3213	1/1	0.55	-	49,49,49,49	0
55	MG	AA	1816	1/1	0.23	-	81,81,81,81	0
55	MG	DA	3201	1/1	0.25	-	47,47,47,47	0
55	MG	BA	3063	1/1	0.14	-	43,43,43,43	0
55	MG	BA	3576	1/1	0.42	-	74,74,74,74	0
55	MG	DA	3300	1/1	0.31	-	81,81,81,81	0
55	MG	BA	3413	1/1	0.55	-	78,78,78,78	0
55	MG	DA	3298	1/1	0.41	-	77,77,77,77	0
55	MG	DA	3221	1/1	0.73	-	63,63,63,63	0
55	MG	BA	3458	1/1	0.19	-	82,82,82,82	0
55	MG	DA	3208	1/1	0.44	-	74,74,74,74	0
55	MG	DA	3210	1/1	0.44	-	63,63,63,63	0
55	MG	AA	1611	1/1	0.23	-	92,92,92,92	0
55	MG	CC	102	1/1	0.48	-	73,73,73,73	0
55	MG	CG	302	1/1	0.16	-	101,101,101,101	0
55	MG	DA	3264	1/1	0.64	-	59,59,59,59	0
55	MG	AA	1602	1/1	0.28	-	79,79,79,79	0
55	MG	DA	3103	1/1	0.35	-	50,50,50,50	0
55	MG	BA	3558	1/1	0.12	-	63,63,63,63	0
55	MG	DA	3515	1/1	0.65	-	82,82,82,82	0
55	MG	DA	3496	1/1	0.31	-	83,83,83,83	0
55	MG	BA	3163	1/1	0.59	-	50,50,50,50	0
55	MG	DA	3346	1/1	0.51	-	75,75,75,75	0
55	MG	DA	3386	1/1	0.52	-	61,61,61,61	0
55	MG	DB	210	1/1	0.39	-	71,71,71,71	0
55	MG	AA	1838	1/1	0.36	-	61,61,61,61	0
55	MG	DA	3017	1/1	0.39	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3265	1/1	0.73	-	60,60,60,60	0
55	MG	DA	3037	1/1	0.22	-	98,98,98,98	0
55	MG	DA	3414	1/1	0.32	-	85,85,85,85	0
55	MG	DA	3491	1/1	0.60	-	103,103,103,103	0
55	MG	BA	3117	1/1	0.49	-	60,60,60,60	0
55	MG	AA	1627	1/1	0.31	-	53,53,53,53	0
55	MG	DA	3064	1/1	0.58	-	101,101,101,101	0
55	MG	DA	3487	1/1	0.45	-	95,95,95,95	0
55	MG	CA	1652	1/1	0.34	-	71,71,71,71	0
55	MG	AA	1798	1/1	0.24	-	58,58,58,58	0
55	MG	DA	3027	1/1	0.21	-	77,77,77,77	0
55	MG	BA	3200	1/1	0.42	-	62,62,62,62	0
55	MG	DA	3069	1/1	0.40	-	60,60,60,60	0
55	MG	BA	3545	1/1	0.35	-	69,69,69,69	0
55	MG	CA	1709	1/1	0.53	-	108,108,108,108	0
55	MG	AA	1610	1/1	0.50	-	51,51,51,51	0
55	MG	BA	3038	1/1	0.40	-	56,56,56,56	0
55	MG	CA	1657	1/1	0.30	-	95,95,95,95	0
55	MG	AC	105	1/1	0.48	-	93,93,93,93	0
55	MG	DA	3407	1/1	0.45	-	73,73,73,73	0
55	MG	DA	3044	1/1	0.29	-	73,73,73,73	0
55	MG	BA	3182	1/1	0.31	-	43,43,43,43	0
55	MG	BA	3107	1/1	0.42	-	36,36,36,36	0
55	MG	BA	3453	1/1	0.59	-	60,60,60,60	0
55	MG	AA	1748	1/1	0.39	-	84,84,84,84	0
55	MG	DA	3352	1/1	0.66	-	64,64,64,64	0
55	MG	AA	1818	1/1	0.60	-	76,76,76,76	0
55	MG	BA	3299	1/1	0.54	-	89,89,89,89	0
55	MG	BA	3307	1/1	0.46	-	39,39,39,39	0
55	MG	BA	3237	1/1	0.52	-	57,57,57,57	0
55	MG	AA	1827	1/1	0.34	-	87,87,87,87	0
55	MG	CA	1721	1/1	0.24	-	80,80,80,80	0
55	MG	CA	1803	1/1	0.33	-	96,96,96,96	0
56	ZN	CQ	101	1/1	0.11	-	120,120,120,120	0
55	MG	BA	3067	1/1	0.21	-	48,48,48,48	0
55	MG	DA	3094	1/1	0.29	-	94,94,94,94	0
55	MG	BA	3467	1/1	0.35	-	78,78,78,78	0
55	MG	D1	201	1/1	0.44	-	71,71,71,71	0
55	MG	DA	3309	1/1	0.23	-	94,94,94,94	0
55	MG	BA	3124	1/1	0.53	-	45,45,45,45	0
55	MG	BA	3517	1/1	0.55	-	70,70,70,70	0
55	MG	DA	3509	1/1	0.41	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1617	1/1	0.52	-	69,69,69,69	0
55	MG	BB	213	1/1	0.47	-	66,66,66,66	0
55	MG	BA	3532	1/1	0.22	-	85,85,85,85	0
55	MG	BA	3177	1/1	0.52	-	57,57,57,57	0
55	MG	BB	211	1/1	0.37	-	92,92,92,92	0
55	MG	D1	202	1/1	0.42	-	89,89,89,89	0
55	MG	AA	1743	1/1	0.13	-	107,107,107,107	0
55	MG	BA	3282	1/1	0.12	-	83,83,83,83	0
55	MG	BA	3209	1/1	0.49	-	39,39,39,39	0
55	MG	BA	3242	1/1	0.45	-	50,50,50,50	0
55	MG	AA	1783	1/1	0.61	-	67,67,67,67	0
55	MG	BA	3318	1/1	0.55	-	75,75,75,75	0
55	MG	CA	1601	1/1	0.32	-	96,96,96,96	0
55	MG	AC	109	1/1	0.39	-	82,82,82,82	0
55	MG	DA	3106	1/1	0.40	-	48,48,48,48	0
55	MG	AA	1615	1/1	0.65	-	105,105,105,105	0
55	MG	DA	3135	1/1	0.40	-	49,49,49,49	0
55	MG	DA	3041	1/1	0.47	-	86,86,86,86	0
55	MG	BA	3421	1/1	0.37	-	62,62,62,62	0
55	MG	CA	1799	1/1	0.34	-	96,96,96,96	0
55	MG	BA	3479	1/1	0.50	-	82,82,82,82	0
55	MG	DA	3213	1/1	0.47	-	41,41,41,41	0
55	MG	BA	3048	1/1	0.57	-	77,77,77,77	0
55	MG	CA	1689	1/1	0.32	-	89,89,89,89	0
55	MG	AA	1715	1/1	0.32	-	115,115,115,115	0
55	MG	CA	1701	1/1	0.40	-	88,88,88,88	0
55	MG	AA	1730	1/1	0.37	-	78,78,78,78	0
55	MG	BA	3259	1/1	0.26	-	40,40,40,40	0
55	MG	BA	3424	1/1	0.64	-	72,72,72,72	0
55	MG	BA	3497	1/1	0.24	-	71,71,71,71	0
55	MG	CA	1733	1/1	0.44	-	69,69,69,69	0
55	MG	DA	3209	1/1	0.49	-	66,66,66,66	0
55	MG	AA	1746	1/1	0.47	-	84,84,84,84	0
55	MG	DA	3427	1/1	0.32	-	76,76,76,76	0
55	MG	BA	3495	1/1	0.34	-	123,123,123,123	0
55	MG	AA	1694	1/1	0.14	-	91,91,91,91	0
55	MG	DA	3456	1/1	0.43	-	83,83,83,83	0
55	MG	BA	3359	1/1	0.49	-	79,79,79,79	0
55	MG	BA	3116	1/1	0.36	-	73,73,73,73	0
55	MG	DA	3004	1/1	0.51	-	99,99,99,99	0
55	MG	BA	3161	1/1	0.25	-	56,56,56,56	0
55	MG	DA	3296	1/1	0.64	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3272	1/1	0.21	-	94,94,94,94	0
55	MG	DA	3341	1/1	0.53	-	84,84,84,84	0
55	MG	BA	3330	1/1	0.33	-	79,79,79,79	0
55	MG	DA	3120	1/1	0.30	-	90,90,90,90	0
55	MG	BA	3076	1/1	0.34	-	68,68,68,68	0
55	MG	DA	3205	1/1	0.52	-	67,67,67,67	0
55	MG	B3	101	1/1	0.55	-	71,71,71,71	0
55	MG	DA	3154	1/1	0.34	-	69,69,69,69	0
55	MG	BA	3352	1/1	0.38	-	76,76,76,76	0
55	MG	BA	3228	1/1	0.63	-	72,72,72,72	0
55	MG	DA	3272	1/1	0.28	-	64,64,64,64	0
55	MG	BA	3251	1/1	0.44	-	68,68,68,68	0
55	MG	DB	202	1/1	0.20	-	98,98,98,98	0
55	MG	BA	3127	1/1	0.59	-	53,53,53,53	0
55	MG	BA	3199	1/1	0.44	-	49,49,49,49	0
55	MG	BA	3126	1/1	0.42	-	46,46,46,46	0
55	MG	BA	3455	1/1	0.27	-	76,76,76,76	0
55	MG	AA	1791	1/1	0.15	-	109,109,109,109	0
55	MG	BA	3553	1/1	0.31	-	78,78,78,78	0
55	MG	BA	3194	1/1	0.45	-	68,68,68,68	0
55	MG	BA	3283	1/1	0.37	-	49,49,49,49	0
55	MG	DA	3385	1/1	0.71	-	62,62,62,62	0
55	MG	DA	3148	1/1	0.48	-	75,75,75,75	0
55	MG	BA	3311	1/1	0.42	-	83,83,83,83	0
55	MG	CA	1668	1/1	0.42	-	79,79,79,79	0
55	MG	BA	3498	1/1	0.44	-	85,85,85,85	0
55	MG	BA	3345	1/1	0.71	-	73,73,73,73	0
55	MG	D3	101	1/1	0.46	-	66,66,66,66	0
55	MG	AA	1696	1/1	0.26	-	88,88,88,88	0
55	MG	DA	3436	1/1	0.43	-	98,98,98,98	0
55	MG	DA	3405	1/1	0.40	-	79,79,79,79	0
55	MG	AA	1771	1/1	0.11	-	70,70,70,70	0
55	MG	BA	3502	1/1	0.23	-	67,67,67,67	0
55	MG	BA	3021	1/1	0.51	-	41,41,41,41	0
55	MG	CA	1681	1/1	0.55	-	72,72,72,72	0
55	MG	CA	1642	1/1	0.28	-	91,91,91,91	0
55	MG	CA	1753	1/1	0.33	-	123,123,123,123	0
55	MG	BA	3004	1/1	0.44	-	35,35,35,35	0
55	MG	BA	3316	1/1	0.49	-	69,69,69,69	0
55	MG	BA	3346	1/1	0.38	-	51,51,51,51	0
55	MG	DA	3503	1/1	0.66	-	80,80,80,80	0
55	MG	BA	3468	1/1	0.34	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1743	1/1	0.50	-	80,80,80,80	0
55	MG	BA	3606	1/1	0.37	-	77,77,77,77	0
55	MG	AA	1769	1/1	0.19	-	104,104,104,104	0
55	MG	AA	1628	1/1	0.37	-	69,69,69,69	0
55	MG	DA	3476	1/1	0.38	-	107,107,107,107	0
55	MG	DB	205	1/1	0.39	-	69,69,69,69	0
55	MG	DA	3087	1/1	0.50	-	63,63,63,63	0
55	MG	BA	3358	1/1	0.36	-	74,74,74,74	0
55	MG	CA	1715	1/1	0.30	-	104,104,104,104	0
55	MG	DA	3230	1/1	0.17	-	59,59,59,59	0
55	MG	DA	3048	1/1	0.54	-	75,75,75,75	0
55	MG	BA	3018	1/1	0.34	-	54,54,54,54	0
55	MG	DA	3361	1/1	0.71	-	79,79,79,79	0
55	MG	BA	3514	1/1	0.33	-	71,71,71,71	0
55	MG	BA	3073	1/1	0.43	-	82,82,82,82	0
55	MG	BA	3480	1/1	0.53	-	50,50,50,50	0
55	MG	BF	303	1/1	0.41	-	66,66,66,66	0
55	MG	BA	3399	1/1	0.63	-	90,90,90,90	0
55	MG	AA	1700	1/1	0.20	-	99,99,99,99	0
55	MG	DA	3267	1/1	0.38	-	64,64,64,64	0
55	MG	DA	3019	1/1	0.94	-	90,90,90,90	0
55	MG	CA	1707	1/1	0.60	-	98,98,98,98	0
55	MG	DA	3172	1/1	0.28	-	88,88,88,88	0
55	MG	CA	1736	1/1	0.82	-	79,79,79,79	0
55	MG	AA	1641	1/1	0.37	-	57,57,57,57	0
55	MG	DA	3012	1/1	0.48	-	66,66,66,66	0
55	MG	AA	1691	1/1	0.50	-	50,50,50,50	0
55	MG	DA	3007	1/1	0.35	-	74,74,74,74	0
55	MG	DB	214	1/1	0.17	-	96,96,96,96	0
55	MG	BA	3270	1/1	0.20	-	76,76,76,76	0
55	MG	CA	1662	1/1	0.26	-	90,90,90,90	0
55	MG	BA	3500	1/1	0.28	-	97,97,97,97	0
55	MG	DA	3343	1/1	0.46	-	95,95,95,95	0
55	MG	AA	1785	1/1	0.43	-	96,96,96,96	0
55	MG	BA	3486	1/1	0.48	-	80,80,80,80	0
55	MG	BA	3440	1/1	0.48	-	74,74,74,74	0
55	MG	CA	1710	1/1	0.28	-	106,106,106,106	0
55	MG	BA	3600	1/1	0.41	-	66,66,66,66	0
55	MG	BA	3373	1/1	0.50	-	64,64,64,64	0
55	MG	DA	3104	1/1	0.41	-	43,43,43,43	0
55	MG	DA	3101	1/1	0.34	-	43,43,43,43	0
55	MG	CA	1734	1/1	0.24	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3333	1/1	0.58	-	87,87,87,87	0
55	MG	BA	3513	1/1	0.44	-	90,90,90,90	0
55	MG	BA	3349	1/1	0.44	-	97,97,97,97	0
55	MG	BA	3170	1/1	0.50	-	55,55,55,55	0
55	MG	BA	3184	1/1	0.23	-	39,39,39,39	0
55	MG	BA	3397	1/1	0.30	-	81,81,81,81	0
55	MG	DA	3289	1/1	0.48	-	90,90,90,90	0
55	MG	B0	201	1/1	0.32	-	51,51,51,51	0
55	MG	AA	1808	1/1	0.62	-	76,76,76,76	0
55	MG	DA	3291	1/1	0.57	-	65,65,65,65	0
55	MG	BA	3023	1/1	0.36	-	45,45,45,45	0
55	MG	BA	3531	1/1	0.32	-	53,53,53,53	0
55	MG	AA	1677	1/1	0.33	-	87,87,87,87	0
55	MG	BA	3522	1/1	0.53	-	82,82,82,82	0
55	MG	DA	3420	1/1	0.33	-	67,67,67,67	0
55	MG	AA	1837	1/1	0.50	-	73,73,73,73	0
55	MG	DA	3179	1/1	0.31	-	70,70,70,70	0
55	MG	DA	3350	1/1	0.29	-	91,91,91,91	0
55	MG	DA	3001	1/1	0.48	-	67,67,67,67	0
55	MG	BA	3383	1/1	0.21	-	71,71,71,71	0
55	MG	BA	3469	1/1	0.27	-	60,60,60,60	0
55	MG	BA	3191	1/1	0.21	-	81,81,81,81	0
55	MG	DA	3156	1/1	0.68	-	48,48,48,48	0
55	MG	AA	1693	1/1	0.17	-	87,87,87,87	0
55	MG	CA	1712	1/1	0.56	-	86,86,86,86	0
55	MG	DA	3259	1/1	0.28	-	72,72,72,72	0
55	MG	DA	3281	1/1	0.84	-	76,76,76,76	0
55	MG	DA	3239	1/1	0.31	-	45,45,45,45	0
55	MG	CA	1699	1/1	0.15	-	97,97,97,97	0
55	MG	AA	1762	1/1	0.27	-	80,80,80,80	0
55	MG	DA	3362	1/1	0.61	-	53,53,53,53	0
55	MG	DA	3153	1/1	0.36	-	70,70,70,70	0
55	MG	BA	3130	1/1	0.46	-	44,44,44,44	0
55	MG	BA	3217	1/1	0.29	-	52,52,52,52	0
55	MG	BA	3604	1/1	0.17	-	61,61,61,61	0
55	MG	BA	3291	1/1	0.44	-	72,72,72,72	0
55	MG	BA	3515	1/1	0.21	-	72,72,72,72	0
55	MG	DA	3058	1/1	0.34	-	76,76,76,76	0
55	MG	BA	3084	1/1	0.54	-	82,82,82,82	0
55	MG	DA	3423	1/1	0.91	-	75,75,75,75	0
55	MG	DA	3071	1/1	0.31	-	81,81,81,81	0
55	MG	CA	1648	1/1	0.44	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3370	1/1	0.46	-	56,56,56,56	0
55	MG	AA	1811	1/1	0.51	-	67,67,67,67	0
55	MG	DA	3286	1/1	0.14	-	47,47,47,47	0
55	MG	BA	3214	1/1	0.69	-	67,67,67,67	0
55	MG	DA	3425	1/1	0.28	-	81,81,81,81	0
55	MG	AA	1784	1/1	0.47	-	66,66,66,66	0
55	MG	AA	1637	1/1	0.23	-	98,98,98,98	0
55	MG	AA	1831	1/1	0.51	-	90,90,90,90	0
55	MG	DB	209	1/1	0.16	-	92,92,92,92	0
55	MG	DA	3207	1/1	0.54	-	66,66,66,66	0
55	MG	BA	3072	1/1	0.35	-	77,77,77,77	0
55	MG	DA	3282	1/1	0.43	-	69,69,69,69	0
55	MG	CA	1704	1/1	0.33	-	99,99,99,99	0
55	MG	CA	1790	1/1	0.26	-	110,110,110,110	0
55	MG	DA	3039	1/1	0.45	-	85,85,85,85	0
55	MG	BA	3166	1/1	0.64	-	72,72,72,72	0
55	MG	DA	3189	1/1	0.49	-	41,41,41,41	0
55	MG	BA	3566	1/1	0.37	-	88,88,88,88	0
55	MG	CA	1683	1/1	0.34	-	87,87,87,87	0
55	MG	DA	3254	1/1	0.54	-	50,50,50,50	0
55	MG	AA	1759	1/1	0.34	-	77,77,77,77	0
55	MG	DA	3335	1/1	0.26	-	61,61,61,61	0
55	MG	BA	3142	1/1	0.39	-	51,51,51,51	0
55	MG	CA	1611	1/1	0.87	-	93,93,93,93	0
55	MG	AA	1788	1/1	0.51	-	77,77,77,77	0
55	MG	CA	1622	1/1	0.33	-	95,95,95,95	0
55	MG	BA	3239	1/1	0.31	-	74,74,74,74	0
55	MG	AN	201	1/1	0.20	-	68,68,68,68	0
55	MG	B5	101	1/1	0.31	-	45,45,45,45	0
55	MG	DA	3315	1/1	0.35	-	108,108,108,108	0
55	MG	DA	3075	1/1	0.36	-	79,79,79,79	0
55	MG	AA	1817	1/1	0.22	-	85,85,85,85	0
55	MG	DA	3512	1/1	0.51	-	75,75,75,75	0
55	MG	DA	3016	1/1	0.47	-	78,78,78,78	0
55	MG	CA	1735	1/1	0.21	-	89,89,89,89	0
55	MG	DA	3003	1/1	0.36	-	64,64,64,64	0
55	MG	BA	3013	1/1	0.43	-	34,34,34,34	0
55	MG	DA	3294	1/1	0.32	-	64,64,64,64	0
55	MG	CA	1637	1/1	0.34	-	79,79,79,79	0
55	MG	AA	1618	1/1	0.29	-	82,82,82,82	0
55	MG	BA	3419	1/1	0.53	-	85,85,85,85	0
55	MG	BA	3221	1/1	0.41	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3396	1/1	0.23	-	82,82,82,82	0
55	MG	BA	3535	1/1	0.46	-	80,80,80,80	0
55	MG	CA	1629	1/1	0.19	-	98,98,98,98	0
55	MG	DA	3093	1/1	0.38	-	80,80,80,80	0
55	MG	CA	1676	1/1	0.46	-	55,55,55,55	0
55	MG	DA	3051	1/1	0.27	-	85,85,85,85	0
55	MG	CA	1643	1/1	0.58	-	82,82,82,82	0
55	MG	BA	3256	1/1	0.40	-	61,61,61,61	0
55	MG	BA	3009	1/1	0.33	-	36,36,36,36	0
55	MG	BA	3361	1/1	0.42	-	64,64,64,64	0
55	MG	CA	1620	1/1	0.49	-	64,64,64,64	0
55	MG	BA	3181	1/1	0.34	-	39,39,39,39	0
55	MG	CA	1771	1/1	0.43	-	76,76,76,76	0
55	MG	CA	1793	1/1	0.41	-	91,91,91,91	0
55	MG	DA	3408	1/1	0.15	-	73,73,73,73	0
55	MG	BA	3356	1/1	0.48	-	70,70,70,70	0
55	MG	AA	1772	1/1	0.60	-	85,85,85,85	0
55	MG	BA	3281	1/1	0.56	-	72,72,72,72	0
55	MG	BA	3040	1/1	0.41	-	54,54,54,54	0
55	MG	DA	3441	1/1	0.10	-	137,137,137,137	0
55	MG	DA	3468	1/1	0.51	-	92,92,92,92	0
55	MG	BA	3091	1/1	0.55	-	35,35,35,35	0
55	MG	AA	1833	1/1	0.50	-	88,88,88,88	0
55	MG	BA	3137	1/1	0.37	-	47,47,47,47	0
55	MG	AB	101	1/1	0.29	-	90,90,90,90	0
55	MG	AA	1679	1/1	0.36	-	86,86,86,86	0
55	MG	BA	3070	1/1	0.12	-	63,63,63,63	0
55	MG	CA	1738	1/1	0.43	-	63,63,63,63	0
55	MG	DA	3317	1/1	0.27	-	81,81,81,81	0
55	MG	BA	3599	1/1	0.49	-	69,69,69,69	0
55	MG	DA	3465	1/1	0.37	-	74,74,74,74	0
55	MG	DA	3293	1/1	0.55	-	75,75,75,75	0
55	MG	DA	3429	1/1	0.40	-	99,99,99,99	0
55	MG	CA	1755	1/1	0.55	-	92,92,92,92	0
55	MG	DA	3517	1/1	0.49	-	84,84,84,84	0
55	MG	BA	3488	1/1	0.43	-	80,80,80,80	0
55	MG	BA	3344	1/1	0.39	-	55,55,55,55	0
55	MG	BA	3266	1/1	0.43	-	77,77,77,77	0
55	MG	BA	3417	1/1	0.30	-	99,99,99,99	0
55	MG	DA	3379	1/1	0.39	-	85,85,85,85	0
55	MG	DA	3310	1/1	0.50	-	71,71,71,71	0
55	MG	AC	102	1/1	0.67	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	210	1/1	0.44	-	64,64,64,64	0
55	MG	BA	3099	1/1	0.55	-	67,67,67,67	0
55	MG	AA	1803	1/1	0.42	-	91,91,91,91	0
55	MG	BA	3197	1/1	0.52	-	46,46,46,46	0
55	MG	DA	3169	1/1	0.32	-	69,69,69,69	0
55	MG	AB	103	1/1	0.47	-	111,111,111,111	0
55	MG	BA	3357	1/1	0.53	-	81,81,81,81	0
55	MG	BA	3169	1/1	0.63	-	63,63,63,63	0
55	MG	BE	301	1/1	0.34	-	59,59,59,59	0
55	MG	AA	1666	1/1	0.50	-	62,62,62,62	0
55	MG	BA	3308	1/1	0.35	-	61,61,61,61	0
55	MG	BA	3118	1/1	0.44	-	61,61,61,61	0
55	MG	DA	3403	1/1	0.50	-	76,76,76,76	0
55	MG	BA	3402	1/1	0.38	-	91,91,91,91	0
55	MG	DA	3332	1/1	0.47	-	76,76,76,76	0
55	MG	BA	3544	1/1	0.43	-	72,72,72,72	0
55	MG	BA	3520	1/1	0.48	-	44,44,44,44	0
55	MG	DA	3319	1/1	0.42	-	74,74,74,74	0
55	MG	BA	3027	1/1	0.54	-	36,36,36,36	0
55	MG	BA	3047	1/1	0.47	-	74,74,74,74	0
55	MG	AA	1699	1/1	0.23	-	64,64,64,64	0
55	MG	DA	3098	1/1	0.47	-	68,68,68,68	0
55	MG	CA	1801	1/1	0.32	-	89,89,89,89	0
55	MG	AC	106	1/1	0.60	-	89,89,89,89	0
55	MG	CA	1782	1/1	0.41	-	93,93,93,93	0
55	MG	CA	1783	1/1	0.49	-	100,100,100,100	0
55	MG	BA	3128	1/1	0.50	-	46,46,46,46	0
55	MG	DA	3292	1/1	0.26	-	89,89,89,89	0
55	MG	DA	3471	1/1	0.51	-	80,80,80,80	0
55	MG	AA	1757	1/1	0.10	-	110,110,110,110	0
55	MG	DA	3026	1/1	0.50	-	95,95,95,95	0
55	MG	BA	3167	1/1	0.40	-	73,73,73,73	0
55	MG	CA	1713	1/1	0.64	-	102,102,102,102	0
55	MG	CA	1749	1/1	0.29	-	89,89,89,89	0
55	MG	BA	3087	1/1	0.34	-	77,77,77,77	0
55	MG	AA	1647	1/1	0.47	-	88,88,88,88	0
55	MG	AA	1672	1/1	0.46	-	87,87,87,87	0
55	MG	AA	1668	1/1	0.64	-	76,76,76,76	0
55	MG	AA	1626	1/1	0.47	-	69,69,69,69	0
55	MG	BA	3596	1/1	0.57	-	55,55,55,55	0
55	MG	DA	3040	1/1	0.20	-	81,81,81,81	0
55	MG	CA	1603	1/1	0.39	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3344	1/1	0.37	-	95,95,95,95	0
55	MG	DA	3337	1/1	0.51	-	89,89,89,89	0
55	MG	DA	3288	1/1	0.37	-	47,47,47,47	0
55	MG	DA	3389	1/1	0.79	-	64,64,64,64	0
55	MG	BA	3573	1/1	0.55	-	83,83,83,83	0
55	MG	CA	1754	1/1	0.34	-	86,86,86,86	0
55	MG	DA	3248	1/1	0.53	-	75,75,75,75	0
55	MG	DA	3440	1/1	0.49	-	86,86,86,86	0
55	MG	BA	3386	1/1	0.53	-	59,59,59,59	0
55	MG	DB	206	1/1	0.31	-	90,90,90,90	0
55	MG	DA	3090	1/1	0.39	-	86,86,86,86	0
55	MG	BA	3094	1/1	0.60	-	78,78,78,78	0
55	MG	BA	3178	1/1	0.35	-	36,36,36,36	0
55	MG	BA	3588	1/1	0.36	-	83,83,83,83	0
55	MG	AA	1698	1/1	0.29	-	72,72,72,72	0
55	MG	BA	3427	1/1	0.39	-	65,65,65,65	0
55	MG	BA	3465	1/1	0.47	-	93,93,93,93	0
55	MG	DA	3043	1/1	0.28	-	82,82,82,82	0
55	MG	CA	1695	1/1	0.51	-	87,87,87,87	0
55	MG	BA	3229	1/1	0.15	-	50,50,50,50	0
55	MG	BA	3129	1/1	0.47	-	52,52,52,52	0
55	MG	BA	3036	1/1	0.56	-	44,44,44,44	0
55	MG	BA	3219	1/1	0.50	-	76,76,76,76	0
55	MG	AA	1625	1/1	0.44	-	57,57,57,57	0
55	MG	AA	1830	1/1	0.31	-	73,73,73,73	0
55	MG	BA	3049	1/1	0.42	-	68,68,68,68	0
55	MG	BA	3459	1/1	0.45	-	70,70,70,70	0
55	MG	BA	3623	1/1	0.41	-	60,60,60,60	0
55	MG	AA	1787	1/1	0.48	-	96,96,96,96	0
55	MG	BA	3557	1/1	0.47	-	77,77,77,77	0
55	MG	DE	302	1/1	0.27	-	65,65,65,65	0
55	MG	CA	1746	1/1	0.64	-	57,57,57,57	0
55	MG	BA	3562	1/1	0.35	-	79,79,79,79	0
55	MG	BA	3441	1/1	0.15	-	86,86,86,86	0
55	MG	DB	204	1/1	0.23	-	82,82,82,82	0
55	MG	BB	217	1/1	0.16	-	98,98,98,98	0
55	MG	AA	1705	1/1	0.29	-	83,83,83,83	0
55	MG	DA	3432	1/1	0.34	-	69,69,69,69	0
55	MG	BA	3069	1/1	0.49	-	77,77,77,77	0
55	MG	BA	3264	1/1	0.22	-	30,30,30,30	0
55	MG	BA	3286	1/1	0.34	-	66,66,66,66	0
55	MG	DA	3406	1/1	0.78	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	201	1/1	0.49	-	92,92,92,92	0
55	MG	BA	3227	1/1	0.41	-	91,91,91,91	0
55	MG	DA	3038	1/1	0.56	-	97,97,97,97	0
55	MG	DA	3076	1/1	0.45	-	86,86,86,86	0
55	MG	DA	3163	1/1	0.56	-	62,62,62,62	0
55	MG	DA	3494	1/1	0.28	-	75,75,75,75	0
55	MG	DA	3378	1/1	0.50	-	63,63,63,63	0
55	MG	CA	1646	1/1	0.36	-	76,76,76,76	0
55	MG	BA	3478	1/1	0.25	-	63,63,63,63	0
55	MG	DA	3206	1/1	0.49	-	65,65,65,65	0
55	MG	AA	1770	1/1	0.32	-	102,102,102,102	0
55	MG	DB	203	1/1	0.35	-	66,66,66,66	0
55	MG	DA	3305	1/1	0.34	-	77,77,77,77	0
55	MG	BA	3326	1/1	0.34	-	52,52,52,52	0
55	MG	DA	3192	1/1	0.48	-	62,62,62,62	0
55	MG	DA	3251	1/1	0.31	-	74,74,74,74	0
55	MG	BB	202	1/1	0.16	-	79,79,79,79	0
55	MG	BA	3471	1/1	0.34	-	72,72,72,72	0
55	MG	CA	1684	1/1	0.59	-	85,85,85,85	0
55	MG	BA	3621	1/1	0.17	-	63,63,63,63	0
55	MG	AA	1727	1/1	0.91	-	87,87,87,87	0
55	MG	DA	3228	1/1	0.46	-	44,44,44,44	0
55	MG	DA	3137	1/1	0.28	-	82,82,82,82	0
55	MG	AA	1819	1/1	0.34	-	87,87,87,87	0
55	MG	BA	3309	1/1	0.29	-	68,68,68,68	0
55	MG	BA	3062	1/1	0.27	-	56,56,56,56	0
55	MG	BA	3176	1/1	0.49	-	48,48,48,48	0
55	MG	BA	3496	1/1	0.30	-	96,96,96,96	0
55	MG	BA	3005	1/1	0.47	-	43,43,43,43	0
55	MG	BA	3121	1/1	0.46	-	57,57,57,57	0
55	MG	AA	1653	1/1	0.55	-	81,81,81,81	0
55	MG	DA	3079	1/1	0.37	-	54,54,54,54	0
55	MG	BA	3321	1/1	0.46	-	77,77,77,77	0
55	MG	CA	1694	1/1	0.48	-	97,97,97,97	0
55	MG	AA	1776	1/1	0.20	-	82,82,82,82	0
55	MG	AA	1660	1/1	0.62	-	53,53,53,53	0
55	MG	BA	3032	1/1	0.51	-	49,49,49,49	0
55	MG	AA	1631	1/1	0.21	-	66,66,66,66	0
55	MG	BA	3524	1/1	0.20	-	66,66,66,66	0
55	MG	CA	1791	1/1	0.31	-	79,79,79,79	0
55	MG	AA	1834	1/1	0.53	-	97,97,97,97	0
55	MG	BA	3279	1/1	0.12	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3479	1/1	0.17	-	99,99,99,99	0
55	MG	BA	3401	1/1	0.42	-	62,62,62,62	0
55	MG	AA	1824	1/1	0.65	-	86,86,86,86	0
55	MG	CA	1778	1/1	0.40	-	96,96,96,96	0
55	MG	BA	3294	1/1	0.32	-	72,72,72,72	0
55	MG	CA	1685	1/1	0.37	-	93,93,93,93	0
55	MG	AA	1604	1/1	0.30	-	67,67,67,67	0
55	MG	BA	3155	1/1	0.18	-	45,45,45,45	0
55	MG	BA	3122	1/1	0.30	-	37,37,37,37	0
55	MG	CA	1756	1/1	0.39	-	81,81,81,81	0
55	MG	BA	3477	1/1	0.51	-	95,95,95,95	0
55	MG	AA	1650	1/1	0.50	-	71,71,71,71	0
55	MG	DA	3126	1/1	0.22	-	41,41,41,41	0
55	MG	CA	1605	1/1	0.41	-	76,76,76,76	0
55	MG	DA	3278	1/1	0.50	-	42,42,42,42	0
55	MG	AA	1683	1/1	0.28	-	87,87,87,87	0
55	MG	AA	1806	1/1	0.28	-	81,81,81,81	0
55	MG	BA	3347	1/1	0.49	-	68,68,68,68	0
55	MG	DA	3490	1/1	0.10	-	126,126,126,126	0
55	MG	DB	201	1/1	0.41	-	81,81,81,81	0
55	MG	BA	3381	1/1	0.54	-	90,90,90,90	0
55	MG	BA	3171	1/1	0.57	-	61,61,61,61	0
55	MG	BA	3003	1/1	0.44	-	47,47,47,47	0
55	MG	BA	3377	1/1	0.74	-	62,62,62,62	0
55	MG	DA	3365	1/1	0.51	-	58,58,58,58	0
55	MG	DA	3481	1/1	0.48	-	96,96,96,96	0
55	MG	CA	1781	1/1	0.07	-	117,117,117,117	0
55	MG	BA	3120	1/1	0.42	-	56,56,56,56	0
55	MG	BB	205	1/1	0.40	-	74,74,74,74	0
55	MG	BA	3501	1/1	0.23	-	55,55,55,55	0
55	MG	BA	3610	1/1	0.46	-	61,61,61,61	0
55	MG	DA	3232	1/1	0.40	-	44,44,44,44	0
55	MG	AA	1735	1/1	0.50	-	79,79,79,79	0
55	MG	AA	1686	1/1	0.41	-	85,85,85,85	0
55	MG	DA	3394	1/1	0.22	-	90,90,90,90	0
55	MG	BA	3342	1/1	0.30	-	66,66,66,66	0
55	MG	DA	3415	1/1	0.55	-	96,96,96,96	0
55	MG	AA	1796	1/1	0.14	-	75,75,75,75	0
55	MG	BA	3322	1/1	0.66	-	64,64,64,64	0
55	MG	DP	201	1/1	0.35	-	65,65,65,65	0
55	MG	CA	1679	1/1	0.40	-	85,85,85,85	0
55	MG	BA	3077	1/1	0.41	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3318	1/1	0.37	-	63,63,63,63	0
55	MG	BA	3141	1/1	0.47	-	35,35,35,35	0
55	MG	CA	1667	1/1	0.23	-	102,102,102,102	0
55	MG	CA	1682	1/1	0.39	-	86,86,86,86	0
55	MG	DA	3109	1/1	0.26	-	65,65,65,65	0
55	MG	BA	3269	1/1	0.45	-	61,61,61,61	0
55	MG	AA	1652	1/1	0.49	-	81,81,81,81	0
55	MG	DA	3450	1/1	0.42	-	88,88,88,88	0
55	MG	BA	3248	1/1	0.40	-	53,53,53,53	0
55	MG	BB	203	1/1	0.44	-	65,65,65,65	0
55	MG	AA	1829	1/1	0.54	-	77,77,77,77	0
55	MG	CA	1635	1/1	0.77	-	86,86,86,86	0
55	MG	DA	3373	1/1	0.51	-	79,79,79,79	0
55	MG	DA	3470	1/1	0.19	-	80,80,80,80	0
55	MG	AA	1774	1/1	0.18	-	91,91,91,91	0
55	MG	DA	3188	1/1	0.60	-	56,56,56,56	0
55	MG	DA	3297	1/1	0.26	-	83,83,83,83	0
55	MG	DA	3130	1/1	0.20	-	60,60,60,60	0
55	MG	DB	211	1/1	0.48	-	93,93,93,93	0
55	MG	DA	3029	1/1	0.31	-	79,79,79,79	0
55	MG	DA	3430	1/1	0.57	-	62,62,62,62	0
55	MG	DA	3435	1/1	0.09	-	72,72,72,72	0
55	MG	BA	3616	1/1	0.49	-	58,58,58,58	0
55	MG	BA	3037	1/1	0.38	-	44,44,44,44	0
55	MG	DA	3459	1/1	0.38	-	86,86,86,86	0
55	MG	DA	3295	1/1	0.34	-	50,50,50,50	0
55	MG	CA	1607	1/1	0.43	-	85,85,85,85	0
55	MG	DA	3054	1/1	0.68	-	58,58,58,58	0
55	MG	CA	1680	1/1	0.60	-	68,68,68,68	0
55	MG	DA	3388	1/1	0.43	-	74,74,74,74	0
55	MG	AA	1815	1/1	0.51	-	84,84,84,84	0
55	MG	DA	3393	1/1	0.52	-	69,69,69,69	0
55	MG	DA	3074	1/1	0.21	-	70,70,70,70	0
55	MG	DA	3242	1/1	0.59	-	63,63,63,63	0
55	MG	DA	3143	1/1	0.31	-	58,58,58,58	0
55	MG	AA	1673	1/1	0.51	-	78,78,78,78	0
55	MG	AA	1755	1/1	0.55	-	104,104,104,104	0
55	MG	DA	3360	1/1	0.55	-	65,65,65,65	0
55	MG	CA	1722	1/1	0.37	-	75,75,75,75	0
55	MG	AC	103	1/1	0.36	-	66,66,66,66	0
55	MG	BA	3384	1/1	0.29	-	73,73,73,73	0
55	MG	DA	3031	1/1	0.25	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1814	1/1	0.35	-	83,83,83,83	0
55	MG	BA	3006	1/1	0.41	-	38,38,38,38	0
55	MG	BA	3470	1/1	0.35	-	88,88,88,88	0
55	MG	AA	1813	1/1	0.33	-	107,107,107,107	0
55	MG	CA	1794	1/1	0.29	-	74,74,74,74	0
55	MG	BA	3538	1/1	0.52	-	66,66,66,66	0
55	MG	CA	1630	1/1	0.46	-	91,91,91,91	0
55	MG	BA	3314	1/1	0.56	-	64,64,64,64	0
55	MG	DA	3508	1/1	0.72	-	80,80,80,80	0
55	MG	DA	3178	1/1	0.77	-	59,59,59,59	0
55	MG	DA	3442	1/1	0.25	-	91,91,91,91	0
55	MG	CC	101	1/1	0.43	-	92,92,92,92	0
55	MG	BB	209	1/1	0.43	-	102,102,102,102	0
55	MG	CA	1727	1/1	0.49	-	94,94,94,94	0
55	MG	BA	3095	1/1	0.47	-	37,37,37,37	0
55	MG	BA	3164	1/1	0.71	-	86,86,86,86	0
55	MG	BA	3404	1/1	0.17	-	60,60,60,60	0
55	MG	BA	3418	1/1	0.39	-	78,78,78,78	0
55	MG	AA	1623	1/1	0.72	-	65,65,65,65	0
55	MG	BA	3375	1/1	0.26	-	50,50,50,50	0
55	MG	DA	3257	1/1	0.35	-	49,49,49,49	0
55	MG	BA	3132	1/1	0.45	-	71,71,71,71	0
55	MG	BA	3603	1/1	0.57	-	63,63,63,63	0
55	MG	AA	1632	1/1	0.25	-	67,67,67,67	0
55	MG	BA	3555	1/1	0.22	-	38,38,38,38	0
55	MG	DA	3492	1/1	0.42	-	88,88,88,88	0
55	MG	DA	3160	1/1	0.42	-	49,49,49,49	0
55	MG	DA	3223	1/1	0.48	-	52,52,52,52	0
55	MG	BA	3295	1/1	0.45	-	81,81,81,81	0
55	MG	CA	1770	1/1	0.25	-	102,102,102,102	0
55	MG	DA	3488	1/1	0.61	-	86,86,86,86	0
55	MG	AC	101	1/1	0.48	-	53,53,53,53	0
55	MG	AA	1763	1/1	0.57	-	53,53,53,53	0
55	MG	DA	3387	1/1	0.32	-	92,92,92,92	0
55	MG	DA	3263	1/1	0.83	-	82,82,82,82	0
55	MG	DA	3046	1/1	0.34	-	65,65,65,65	0
55	MG	AA	1804	1/1	0.17	-	74,74,74,74	0
55	MG	BA	3303	1/1	0.38	-	72,72,72,72	0
55	MG	DA	3133	1/1	0.38	-	42,42,42,42	0
55	MG	DA	3287	1/1	0.63	-	65,65,65,65	0
55	MG	DA	3299	1/1	0.35	-	38,38,38,38	0
55	MG	BA	3230	1/1	0.59	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3173	1/1	0.29	-	60,60,60,60	0
55	MG	BA	3341	1/1	0.38	-	81,81,81,81	0
55	MG	BA	3405	1/1	0.46	-	56,56,56,56	0
55	MG	CA	1621	1/1	0.41	-	66,66,66,66	0
55	MG	CA	1678	1/1	0.24	-	70,70,70,70	0
55	MG	BA	3108	1/1	0.50	-	86,86,86,86	0
55	MG	BA	3159	1/1	0.48	-	58,58,58,58	0
55	MG	BA	3392	1/1	0.39	-	70,70,70,70	0
55	MG	BB	214	1/1	0.29	-	86,86,86,86	0
55	MG	BA	3220	1/1	0.49	-	44,44,44,44	0
55	MG	AA	1745	1/1	0.59	-	67,67,67,67	0
56	ZN	CG	303	1/1	0.31	-	118,118,118,118	0
55	MG	BA	3148	1/1	0.41	-	32,32,32,32	0
55	MG	BA	3313	1/1	0.19	-	88,88,88,88	0
55	MG	BA	3160	1/1	0.41	-	42,42,42,42	0
55	MG	BA	3554	1/1	0.46	-	45,45,45,45	0
55	MG	DA	3059	1/1	0.82	-	106,106,106,106	0
55	MG	DA	3023	1/1	0.46	-	57,57,57,57	0
55	MG	BA	3241	1/1	0.51	-	60,60,60,60	0
55	MG	AA	1822	1/1	0.11	-	107,107,107,107	0
55	MG	DA	3260	1/1	0.60	-	41,41,41,41	0
55	MG	AA	1749	1/1	0.24	-	81,81,81,81	0
55	MG	AA	1661	1/1	0.32	-	48,48,48,48	0
55	MG	BA	3416	1/1	0.28	-	87,87,87,87	0
55	MG	DA	3418	1/1	0.46	-	78,78,78,78	0
55	MG	DA	3506	1/1	0.54	-	78,78,78,78	0
55	MG	CA	1658	1/1	0.47	-	91,91,91,91	0
55	MG	AA	1633	1/1	0.25	-	74,74,74,74	0
55	MG	CA	1773	1/1	0.80	-	92,92,92,92	0
55	MG	BA	3340	1/1	0.26	-	77,77,77,77	0
55	MG	CA	1708	1/1	0.12	-	97,97,97,97	0
55	MG	BA	3443	1/1	0.15	-	77,77,77,77	0
55	MG	DA	3084	1/1	0.34	-	88,88,88,88	0
55	MG	DA	3349	1/1	0.32	-	63,63,63,63	0
55	MG	BA	3403	1/1	0.68	-	93,93,93,93	0
55	MG	DA	3197	1/1	0.69	-	70,70,70,70	0
55	MG	BA	3083	1/1	0.13	-	62,62,62,62	0
55	MG	CA	1627	1/1	0.35	-	88,88,88,88	0
55	MG	BA	3509	1/1	0.30	-	83,83,83,83	0
55	MG	DA	3340	1/1	0.26	-	85,85,85,85	0
55	MG	AC	104	1/1	0.47	-	56,56,56,56	0
55	MG	CA	1807	1/1	0.30	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	212	1/1	0.31	-	88,88,88,88	0
55	MG	DA	3053	1/1	0.62	-	62,62,62,62	0
55	MG	AA	1643	1/1	0.70	-	85,85,85,85	0
55	MG	DA	3413	1/1	0.36	-	94,94,94,94	0
55	MG	DA	3339	1/1	0.29	-	66,66,66,66	0
55	MG	BA	3024	1/1	0.37	-	27,27,27,27	0
55	MG	DA	3061	1/1	0.57	-	74,74,74,74	0
55	MG	BA	3232	1/1	0.32	-	72,72,72,72	0
55	MG	BA	3410	1/1	0.75	-	62,62,62,62	0
55	MG	CA	1767	1/1	0.52	-	77,77,77,77	0
55	MG	A1	102	1/1	0.29	-	86,86,86,86	0
55	MG	CA	1751	1/1	0.30	-	94,94,94,94	0
55	MG	CA	1761	1/1	0.41	-	92,92,92,92	0
55	MG	AA	1621	1/1	0.25	-	108,108,108,108	0
55	MG	BA	3261	1/1	0.62	-	52,52,52,52	0
55	MG	AA	1659	1/1	0.73	-	69,69,69,69	0
55	MG	AA	1794	1/1	0.20	-	84,84,84,84	0
55	MG	AA	1732	1/1	0.29	-	92,92,92,92	0
55	MG	AA	1624	1/1	0.28	-	79,79,79,79	0
55	MG	DA	3006	1/1	0.59	-	71,71,71,71	0
55	MG	CA	1623	1/1	0.12	-	90,90,90,90	0
55	MG	AA	1753	1/1	0.10	-	108,108,108,108	0
55	MG	CB	103	1/1	0.63	-	103,103,103,103	0
55	MG	BA	3334	1/1	0.59	-	96,96,96,96	0
55	MG	BA	3042	1/1	0.34	-	41,41,41,41	0
55	MG	BA	3530	1/1	0.30	-	81,81,81,81	0
55	MG	BA	3529	1/1	0.46	-	68,68,68,68	0
55	MG	BA	3613	1/1	0.32	-	93,93,93,93	0
55	MG	AA	1640	1/1	0.33	-	90,90,90,90	0
55	MG	DA	3505	1/1	0.52	-	81,81,81,81	0
55	MG	BA	3253	1/1	0.26	-	51,51,51,51	0
55	MG	BA	3157	1/1	0.59	-	45,45,45,45	0
55	MG	CA	1697	1/1	0.33	-	65,65,65,65	0
55	MG	CA	1741	1/1	0.17	-	106,106,106,106	0
55	MG	DA	3067	1/1	0.45	-	94,94,94,94	0
55	MG	DA	3277	1/1	0.31	-	89,89,89,89	0
55	MG	BA	3234	1/1	0.48	-	86,86,86,86	0
55	MG	BA	3552	1/1	0.39	-	102,102,102,102	0
55	MG	BA	3245	1/1	0.56	-	49,49,49,49	0
55	MG	DA	3146	1/1	0.60	-	92,92,92,92	0
55	MG	BA	3376	1/1	0.44	-	73,73,73,73	0
55	MG	AA	1725	1/1	0.19	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3193	1/1	0.70	-	63,63,63,63	0
55	MG	DA	3445	1/1	0.39	-	78,78,78,78	0
55	MG	BA	3374	1/1	0.44	-	71,71,71,71	0
55	MG	AA	1709	1/1	0.23	-	70,70,70,70	0
55	MG	AA	1744	1/1	0.15	-	117,117,117,117	0
55	MG	DA	3499	1/1	0.26	-	61,61,61,61	0
55	MG	BA	3267	1/1	0.25	-	61,61,61,61	0
55	MG	BA	3250	1/1	0.20	-	60,60,60,60	0
55	MG	BA	3542	1/1	0.51	-	72,72,72,72	0
55	MG	DA	3083	1/1	0.48	-	85,85,85,85	0
55	MG	BA	3602	1/1	0.27	-	67,67,67,67	0
55	MG	BA	3068	1/1	0.35	-	75,75,75,75	0
55	MG	DA	3323	1/1	0.17	-	42,42,42,42	0
55	MG	BA	3473	1/1	0.52	-	76,76,76,76	0
55	MG	DA	3183	1/1	0.53	-	57,57,57,57	0
55	MG	BA	3582	1/1	0.46	-	86,86,86,86	0
55	MG	DA	3369	1/1	0.30	-	74,74,74,74	0
55	MG	BA	3287	1/1	0.40	-	62,62,62,62	0
55	MG	BA	3415	1/1	0.40	-	84,84,84,84	0
55	MG	BA	3619	1/1	0.36	-	69,69,69,69	0
55	MG	BA	3183	1/1	0.28	-	47,47,47,47	0
55	MG	AA	1711	1/1	0.32	-	89,89,89,89	0
55	MG	DA	3525	1/1	0.80	-	79,79,79,79	0
55	MG	BA	3092	1/1	0.45	-	32,32,32,32	0
55	MG	CA	1785	1/1	0.30	-	105,105,105,105	0
55	MG	BA	3109	1/1	0.34	-	70,70,70,70	0
55	MG	DA	3358	1/1	0.55	-	88,88,88,88	0
55	MG	BA	3426	1/1	0.48	-	85,85,85,85	0
55	MG	DA	3081	1/1	0.53	-	64,64,64,64	0
55	MG	DA	3052	1/1	0.41	-	71,71,71,71	0
55	MG	DA	3513	1/1	0.76	-	67,67,67,67	0
55	MG	BA	3306	1/1	0.30	-	67,67,67,67	0
55	MG	CA	1711	1/1	0.39	-	90,90,90,90	0
55	MG	BA	3135	1/1	0.54	-	72,72,72,72	0
55	MG	BA	3407	1/1	0.31	-	59,59,59,59	0
55	MG	DA	3099	1/1	0.27	-	40,40,40,40	0
55	MG	BA	3430	1/1	0.28	-	57,57,57,57	0
55	MG	AA	1638	1/1	0.29	-	104,104,104,104	0
55	MG	AA	1810	1/1	0.49	-	67,67,67,67	0
55	MG	BB	208	1/1	0.29	-	74,74,74,74	0
55	MG	BA	3608	1/1	0.39	-	39,39,39,39	0
55	MG	AA	1710	1/1	0.34	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3521	1/1	0.63	-	79,79,79,79	0
55	MG	BA	3360	1/1	0.28	-	84,84,84,84	0
55	MG	DA	3194	1/1	0.42	-	73,73,73,73	0
55	MG	BA	3519	1/1	0.34	-	80,80,80,80	0
55	MG	CA	1730	1/1	0.28	-	106,106,106,106	0
55	MG	AA	1809	1/1	0.38	-	63,63,63,63	0
55	MG	AH	201	1/1	0.44	-	99,99,99,99	0
55	MG	AA	1840	1/1	0.51	-	87,87,87,87	0
55	MG	CA	1789	1/1	0.57	-	71,71,71,71	0
55	MG	AA	1704	1/1	0.12	-	83,83,83,83	0
55	MG	BA	3174	1/1	0.79	-	71,71,71,71	0
55	MG	BA	3180	1/1	0.39	-	37,37,37,37	0
55	MG	DA	3065	1/1	0.46	-	74,74,74,74	0
55	MG	BA	3035	1/1	0.27	-	37,37,37,37	0
55	MG	CA	1714	1/1	0.55	-	92,92,92,92	0
55	MG	DA	3381	1/1	0.51	-	99,99,99,99	0
55	MG	BA	3172	1/1	0.36	-	34,34,34,34	0
55	MG	AA	1747	1/1	0.48	-	88,88,88,88	0
55	MG	BA	3240	1/1	0.69	-	88,88,88,88	0
55	MG	BA	3298	1/1	0.30	-	65,65,65,65	0
55	MG	DA	3367	1/1	0.41	-	82,82,82,82	0
55	MG	DA	3167	1/1	0.42	-	70,70,70,70	0
55	MG	BA	3203	1/1	0.50	-	85,85,85,85	0
55	MG	CA	1752	1/1	0.18	-	70,70,70,70	0
55	MG	BA	3231	1/1	0.51	-	73,73,73,73	0
55	MG	CA	1706	1/1	0.44	-	87,87,87,87	0
55	MG	AA	1752	1/1	0.28	-	78,78,78,78	0
55	MG	BA	3022	1/1	0.44	-	30,30,30,30	0
55	MG	CA	1758	1/1	0.44	-	78,78,78,78	0
55	MG	BA	3609	1/1	0.64	-	70,70,70,70	0
55	MG	BA	3134	1/1	0.22	-	81,81,81,81	0
55	MG	BA	3195	1/1	0.48	-	47,47,47,47	0
55	MG	DA	3086	1/1	0.25	-	114,114,114,114	0
55	MG	CA	1606	1/1	0.41	-	87,87,87,87	0
55	MG	BA	3617	1/1	0.74	-	71,71,71,71	0
55	MG	DA	3410	1/1	0.47	-	78,78,78,78	0
55	MG	DA	3068	1/1	0.20	-	91,91,91,91	0
55	MG	DA	3454	1/1	0.49	-	92,92,92,92	0
55	MG	BA	3420	1/1	0.38	-	94,94,94,94	0
55	MG	AA	1802	1/1	0.48	-	85,85,85,85	0
55	MG	BA	3484	1/1	0.28	-	117,117,117,117	0
55	MG	BA	3296	1/1	0.38	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1703	1/1	0.33	-	92,92,92,92	0
55	MG	BA	3518	1/1	0.27	-	70,70,70,70	0
55	MG	DA	3266	1/1	0.52	-	55,55,55,55	0
55	MG	BA	3564	1/1	0.63	-	84,84,84,84	0
55	MG	DA	3177	1/1	0.39	-	74,74,74,74	0
55	MG	DA	3125	1/1	0.41	-	45,45,45,45	0
55	MG	DA	3107	1/1	0.34	-	53,53,53,53	0
55	MG	CA	1690	1/1	0.38	-	68,68,68,68	0
55	MG	CA	1765	1/1	0.30	-	101,101,101,101	0
55	MG	AA	1685	1/1	0.38	-	88,88,88,88	0
55	MG	BA	3065	1/1	0.40	-	91,91,91,91	0
55	MG	DA	3111	1/1	0.29	-	52,52,52,52	0
55	MG	BA	3423	1/1	0.56	-	61,61,61,61	0
55	MG	CA	1666	1/1	0.30	-	71,71,71,71	0
55	MG	BA	3492	1/1	0.50	-	77,77,77,77	0
55	MG	AA	1736	1/1	0.62	-	90,90,90,90	0
55	MG	CA	1774	1/1	0.18	-	104,104,104,104	0
55	MG	DA	3351	1/1	0.39	-	79,79,79,79	0
55	MG	DA	3009	1/1	0.53	-	68,68,68,68	0
55	MG	DA	3070	1/1	0.34	-	78,78,78,78	0
55	MG	DA	3376	1/1	0.49	-	82,82,82,82	0
55	MG	DA	3231	1/1	0.42	-	72,72,72,72	0
55	MG	AA	1836	1/1	0.58	-	79,79,79,79	0
55	MG	DA	3214	1/1	0.42	-	40,40,40,40	0
55	MG	DA	3354	1/1	0.48	-	73,73,73,73	0
55	MG	DA	3203	1/1	0.29	-	48,48,48,48	0
55	MG	AA	1795	1/1	0.22	-	73,73,73,73	0
55	MG	AA	1721	1/1	0.32	-	77,77,77,77	0
55	MG	AA	1644	1/1	0.20	-	62,62,62,62	0
55	MG	BA	3433	1/1	0.20	-	70,70,70,70	0
55	MG	BA	3483	1/1	0.37	-	68,68,68,68	0
55	MG	BE	303	1/1	0.39	-	44,44,44,44	0
55	MG	DA	3032	1/1	0.16	-	76,76,76,76	0
55	MG	CA	1688	1/1	0.35	-	71,71,71,71	0
55	MG	BA	3464	1/1	0.51	-	77,77,77,77	0
55	MG	BA	3499	1/1	0.38	-	68,68,68,68	0
55	MG	DA	3411	1/1	0.21	-	70,70,70,70	0
55	MG	BA	3598	1/1	0.30	-	77,77,77,77	0
55	MG	DA	3199	1/1	0.53	-	61,61,61,61	0
55	MG	DA	3451	1/1	0.48	-	75,75,75,75	0
55	MG	BA	3263	1/1	0.64	-	54,54,54,54	0
55	MG	AA	1761	1/1	0.42	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3363	1/1	0.59	-	67,67,67,67	0
55	MG	BA	3081	1/1	0.31	-	75,75,75,75	0
55	MG	DA	3458	1/1	0.57	-	92,92,92,92	0
55	MG	DA	3256	1/1	0.42	-	49,49,49,49	0
55	MG	BA	3104	1/1	0.23	-	57,57,57,57	0
55	MG	BA	3201	1/1	0.65	-	66,66,66,66	0
55	MG	AA	1656	1/1	0.47	-	87,87,87,87	0
55	MG	CA	1731	1/1	0.56	-	72,72,72,72	0
55	MG	DA	3284	1/1	0.33	-	56,56,56,56	0
55	MG	BA	3098	1/1	0.25	-	48,48,48,48	0
55	MG	DA	3066	1/1	0.56	-	65,65,65,65	0
55	MG	DA	3397	1/1	0.34	-	60,60,60,60	0
55	MG	DA	3500	1/1	0.35	-	92,92,92,92	0
55	MG	DA	3112	1/1	0.19	-	81,81,81,81	0
55	MG	BA	3387	1/1	0.42	-	73,73,73,73	0
55	MG	DA	3227	1/1	0.74	-	50,50,50,50	0
55	MG	DA	3014	1/1	0.55	-	74,74,74,74	0
55	MG	BE	304	1/1	0.36	-	80,80,80,80	0
55	MG	BA	3145	1/1	0.39	-	74,74,74,74	0
55	MG	DA	3144	1/1	0.28	-	60,60,60,60	0
55	MG	CA	1672	1/1	0.76	-	75,75,75,75	0
55	MG	DA	3321	1/1	0.55	-	66,66,66,66	0
55	MG	AA	1739	1/1	0.16	-	93,93,93,93	0
55	MG	BA	3029	1/1	0.41	-	35,35,35,35	0
55	MG	BA	3139	1/1	0.40	-	35,35,35,35	0
55	MG	BA	3372	1/1	0.32	-	73,73,73,73	0
55	MG	BA	3152	1/1	0.51	-	40,40,40,40	0
55	MG	DA	3404	1/1	0.28	-	61,61,61,61	0
55	MG	BA	3080	1/1	0.17	-	91,91,91,91	0
55	MG	BA	3595	1/1	0.22	-	65,65,65,65	0
55	MG	DA	3326	1/1	0.40	-	70,70,70,70	0
55	MG	BA	3020	1/1	0.47	-	41,41,41,41	0
55	MG	BA	3328	1/1	0.70	-	69,69,69,69	0
55	MG	AC	107	1/1	0.29	-	94,94,94,94	0
55	MG	BA	3058	1/1	0.34	-	62,62,62,62	0
55	MG	DA	3401	1/1	0.20	-	71,71,71,71	0
56	ZN	AQ	102	1/1	0.10	-	122,122,122,122	0
55	MG	AA	1807	1/1	0.49	-	98,98,98,98	0
55	MG	BA	3193	1/1	0.54	-	85,85,85,85	0
55	MG	DA	3258	1/1	0.29	-	37,37,37,37	0
55	MG	BA	3051	1/1	0.23	-	74,74,74,74	0
55	MG	BA	3088	1/1	0.17	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1764	1/1	0.16	-	79,79,79,79	0
55	MG	AA	1812	1/1	0.61	-	73,73,73,73	0
55	MG	BA	3074	1/1	0.46	-	49,49,49,49	0
55	MG	DA	3102	1/1	0.34	-	51,51,51,51	0
55	MG	AA	1720	1/1	0.24	-	93,93,93,93	0
55	MG	DA	3371	1/1	0.51	-	82,82,82,82	0
55	MG	BA	3093	1/1	0.30	-	57,57,57,57	0
55	MG	AA	1825	1/1	0.23	-	93,93,93,93	0
55	MG	BA	3547	1/1	0.43	-	77,77,77,77	0
55	MG	DA	3136	1/1	0.39	-	76,76,76,76	0
55	MG	BA	3511	1/1	0.18	-	89,89,89,89	0
55	MG	BE	302	1/1	0.22	-	56,56,56,56	0
55	MG	CA	1776	1/1	0.55	-	71,71,71,71	0
55	MG	DA	3250	1/1	0.42	-	63,63,63,63	0
55	MG	BA	3257	1/1	0.25	-	64,64,64,64	0
55	MG	BB	204	1/1	0.33	-	78,78,78,78	0
55	MG	BA	3136	1/1	0.10	-	74,74,74,74	0
55	MG	DA	3080	1/1	0.56	-	75,75,75,75	0
55	MG	DA	3261	1/1	0.49	-	58,58,58,58	0
55	MG	DA	3501	1/1	0.92	-	88,88,88,88	0
55	MG	BA	3310	1/1	0.37	-	57,57,57,57	0
55	MG	CA	1802	1/1	0.50	-	74,74,74,74	0
55	MG	BA	3011	1/1	0.31	-	42,42,42,42	0
55	MG	BA	3008	1/1	0.47	-	37,37,37,37	0
55	MG	BA	3362	1/1	0.26	-	48,48,48,48	0
55	MG	DA	3311	1/1	0.42	-	73,73,73,73	0
55	MG	BA	3406	1/1	0.64	-	82,82,82,82	0
55	MG	AA	1675	1/1	0.43	-	80,80,80,80	0
55	MG	AA	1742	1/1	0.17	-	78,78,78,78	0
55	MG	B7	101	1/1	0.45	-	67,67,67,67	0
55	MG	AA	1754	1/1	0.22	-	95,95,95,95	0
55	MG	BA	3233	1/1	0.39	-	48,48,48,48	0
55	MG	CA	1805	1/1	0.32	-	94,94,94,94	0
55	MG	DA	3502	1/1	0.52	-	97,97,97,97	0
55	MG	DA	3139	1/1	0.47	-	80,80,80,80	0
55	MG	DA	3185	1/1	0.35	-	74,74,74,74	0
55	MG	DA	3128	1/1	0.38	-	77,77,77,77	0
55	MG	BA	3592	1/1	0.46	-	89,89,89,89	0
55	MG	CA	1747	1/1	0.30	-	94,94,94,94	0
55	MG	BA	3444	1/1	0.54	-	78,78,78,78	0
55	MG	CA	1619	1/1	0.47	-	61,61,61,61	0
55	MG	DA	3062	1/1	0.25	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3011	1/1	0.23	-	65,65,65,65	0
55	MG	BA	3446	1/1	0.24	-	92,92,92,92	0
55	MG	BA	3103	1/1	0.52	-	52,52,52,52	0
55	MG	DA	3236	1/1	0.33	-	55,55,55,55	0
55	MG	CA	1798	1/1	0.25	-	85,85,85,85	0
55	MG	DA	3270	1/1	0.35	-	83,83,83,83	0
55	MG	CA	1628	1/1	0.23	-	101,101,101,101	0
55	MG	CA	1661	1/1	0.19	-	87,87,87,87	0
55	MG	BA	3075	1/1	0.31	-	110,110,110,110	0
55	MG	CC	105	1/1	0.58	-	82,82,82,82	0
55	MG	CA	1616	1/1	0.31	-	88,88,88,88	0
55	MG	AA	1724	1/1	0.22	-	84,84,84,84	0
55	MG	DA	3449	1/1	0.47	-	87,87,87,87	0
55	MG	BA	3343	1/1	0.30	-	60,60,60,60	0
55	MG	BA	3059	1/1	0.39	-	91,91,91,91	0
55	MG	BA	3580	1/1	0.19	-	71,71,71,71	0
55	MG	DA	3235	1/1	0.43	-	48,48,48,48	0
55	MG	DA	3198	1/1	0.30	-	47,47,47,47	0
55	MG	BA	3100	1/1	0.35	-	42,42,42,42	0
55	MG	BA	3140	1/1	0.25	-	58,58,58,58	0
55	MG	DA	3412	1/1	0.38	-	89,89,89,89	0
55	MG	DA	3073	1/1	0.52	-	80,80,80,80	0
55	MG	DA	3504	1/1	0.42	-	65,65,65,65	0
55	MG	DR	201	1/1	0.17	-	71,71,71,71	0
55	MG	DA	3033	1/1	0.29	-	62,62,62,62	0
55	MG	BA	3111	1/1	0.37	-	59,59,59,59	0
55	MG	BA	3411	1/1	0.37	-	68,68,68,68	0
55	MG	BA	3046	1/1	0.37	-	39,39,39,39	0
55	MG	DA	3497	1/1	0.32	-	74,74,74,74	0
55	MG	BA	3113	1/1	0.53	-	57,57,57,57	0
55	MG	DA	3364	1/1	0.35	-	71,71,71,71	0
55	MG	AA	1613	1/1	0.07	-	85,85,85,85	0
55	MG	CA	1613	1/1	0.28	-	68,68,68,68	0
55	MG	AB	102	1/1	0.24	-	86,86,86,86	0
55	MG	DA	3149	1/1	0.65	-	57,57,57,57	0
55	MG	BA	3508	1/1	0.41	-	59,59,59,59	0
55	MG	CB	102	1/1	0.30	-	87,87,87,87	0
55	MG	DA	3265	1/1	0.39	-	50,50,50,50	0
55	MG	BB	206	1/1	0.42	-	86,86,86,86	0
55	MG	BA	3365	1/1	0.31	-	50,50,50,50	0
55	MG	AQ	101	1/1	0.16	-	88,88,88,88	0
55	MG	BA	3297	1/1	0.24	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3217	1/1	0.44	-	55,55,55,55	0
55	MG	DA	3466	1/1	0.64	-	78,78,78,78	0
55	MG	CG	301	1/1	0.38	-	83,83,83,83	0
55	MG	BA	3550	1/1	0.34	-	93,93,93,93	0
55	MG	AA	1722	1/1	0.49	-	68,68,68,68	0
55	MG	DA	3421	1/1	0.32	-	62,62,62,62	0
55	MG	DA	3175	1/1	0.39	-	83,83,83,83	0
55	MG	BA	3456	1/1	0.53	-	78,78,78,78	0
55	MG	AA	1835	1/1	0.23	-	87,87,87,87	0
55	MG	CC	107	1/1	0.60	-	99,99,99,99	0
55	MG	AA	1760	1/1	0.68	-	78,78,78,78	0
55	MG	AA	1663	1/1	0.27	-	47,47,47,47	0
55	MG	BA	3106	1/1	0.37	-	75,75,75,75	0
55	MG	DE	303	1/1	0.34	-	56,56,56,56	0
55	MG	BA	3284	1/1	0.47	-	56,56,56,56	0
55	MG	BA	3097	1/1	0.41	-	59,59,59,59	0
55	MG	BA	3216	1/1	0.34	-	33,33,33,33	0
55	MG	CA	1673	1/1	0.56	-	64,64,64,64	0
55	MG	DA	3359	1/1	0.30	-	76,76,76,76	0
55	MG	BA	3039	1/1	0.30	-	42,42,42,42	0
55	MG	BO	201	1/1	0.37	-	62,62,62,62	0
56	ZN	AG	302	1/1	0.34	-	95,95,95,95	0
55	MG	BA	3574	1/1	0.49	-	78,78,78,78	0
55	MG	BA	3154	1/1	0.27	-	55,55,55,55	0
55	MG	BA	3570	1/1	0.44	-	87,87,87,87	0
55	MG	DA	3055	1/1	0.61	-	68,68,68,68	0
55	MG	CA	1762	1/1	0.35	-	96,96,96,96	0
55	MG	AA	1639	1/1	0.33	-	91,91,91,91	0
55	MG	BA	3556	1/1	0.49	-	58,58,58,58	0
55	MG	BF	301	1/1	0.07	-	73,73,73,73	0
55	MG	DA	3330	1/1	0.22	-	81,81,81,81	0
55	MG	AG	301	1/1	0.62	-	81,81,81,81	0
55	MG	BA	3089	1/1	0.29	-	88,88,88,88	0
55	MG	CA	1618	1/1	0.19	-	93,93,93,93	0
55	MG	AA	1786	1/1	0.17	-	86,86,86,86	0
55	MG	BA	3052	1/1	0.25	-	64,64,64,64	0
55	MG	DA	3129	1/1	0.27	-	82,82,82,82	0
55	MG	DA	3314	1/1	0.49	-	76,76,76,76	0
55	MG	DA	3452	1/1	0.21	-	83,83,83,83	0
55	MG	BA	3332	1/1	0.37	-	61,61,61,61	0
55	MG	DA	3255	1/1	0.30	-	75,75,75,75	0
55	MG	BA	3539	1/1	0.20	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3486	1/1	0.34	-	68,68,68,68	0
55	MG	DA	3302	1/1	0.59	-	95,95,95,95	0
55	MG	BA	3463	1/1	0.27	-	72,72,72,72	0
55	MG	BA	3541	1/1	0.32	-	96,96,96,96	0
55	MG	DA	3395	1/1	0.49	-	69,69,69,69	0
55	MG	CA	1786	1/1	0.30	-	73,73,73,73	0
55	MG	DA	3269	1/1	0.48	-	84,84,84,84	0
55	MG	CA	1624	1/1	0.37	-	88,88,88,88	0
55	MG	DA	3118	1/1	0.38	-	71,71,71,71	0
55	MG	AA	1790	1/1	0.25	-	98,98,98,98	0
55	MG	AA	1605	1/1	0.38	-	82,82,82,82	0
55	MG	CA	1744	1/1	0.30	-	79,79,79,79	0
55	MG	BA	3590	1/1	0.38	-	63,63,63,63	0
55	MG	DA	3119	1/1	0.46	-	98,98,98,98	0
55	MG	DA	3225	1/1	0.54	-	73,73,73,73	0
55	MG	DA	3159	1/1	0.28	-	37,37,37,37	0
55	MG	BA	3439	1/1	0.39	-	71,71,71,71	0
55	MG	BA	3275	1/1	0.25	-	73,73,73,73	0
55	MG	BA	3537	1/1	0.49	-	89,89,89,89	0
55	MG	BA	3173	1/1	0.59	-	52,52,52,52	0
55	MG	BA	3066	1/1	0.31	-	62,62,62,62	0
55	MG	BA	3611	1/1	0.51	-	87,87,87,87	0
55	MG	DA	3523	1/1	0.92	-	81,81,81,81	0
55	MG	BA	3207	1/1	0.59	-	41,41,41,41	0
55	MG	AA	1718	1/1	0.48	-	82,82,82,82	0
55	MG	BA	3185	1/1	0.38	-	76,76,76,76	0
55	MG	AA	1603	1/1	0.32	-	63,63,63,63	0
55	MG	BA	3388	1/1	0.53	-	88,88,88,88	0
55	MG	CA	1729	1/1	0.85	-	77,77,77,77	0
55	MG	BA	3507	1/1	0.30	-	89,89,89,89	0
55	MG	AA	1682	1/1	0.17	-	91,91,91,91	0
55	MG	DA	3085	1/1	0.45	-	91,91,91,91	0
55	MG	DA	3057	1/1	0.45	-	83,83,83,83	0
55	MG	DA	3100	1/1	0.45	-	44,44,44,44	0
55	MG	AA	1765	1/1	0.60	-	84,84,84,84	0
55	MG	BA	3053	1/1	0.33	-	95,95,95,95	0
55	MG	AA	1792	1/1	0.22	-	55,55,55,55	0
55	MG	CA	1726	1/1	0.59	-	75,75,75,75	0
55	MG	BA	3055	1/1	0.44	-	57,57,57,57	0
55	MG	CA	1633	1/1	0.30	-	91,91,91,91	0
55	MG	BA	3393	1/1	0.57	-	81,81,81,81	0
55	MG	B1	201	1/1	0.31	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3560	1/1	0.61	-	78,78,78,78	0
55	MG	DA	3215	1/1	0.44	-	42,42,42,42	0
55	MG	BA	3565	1/1	0.39	-	77,77,77,77	0
55	MG	DA	3307	1/1	0.25	-	77,77,77,77	0
55	MG	DA	3366	1/1	0.47	-	83,83,83,83	0
55	MG	DA	3124	1/1	0.55	-	54,54,54,54	0
55	MG	DA	3181	1/1	0.48	-	50,50,50,50	0
55	MG	DA	3301	1/1	0.41	-	63,63,63,63	0
55	MG	DA	3224	1/1	0.51	-	66,66,66,66	0
55	MG	BA	3581	1/1	0.37	-	69,69,69,69	0
55	MG	BB	212	1/1	0.48	-	81,81,81,81	0
55	MG	DA	3392	1/1	0.47	-	68,68,68,68	0
55	MG	AA	1733	1/1	0.60	-	71,71,71,71	0
55	MG	DA	3320	1/1	0.16	-	76,76,76,76	0
55	MG	DA	3460	1/1	0.45	-	72,72,72,72	0
55	MG	AA	1649	1/1	0.37	-	79,79,79,79	0
55	MG	DA	3399	1/1	0.51	-	76,76,76,76	0
55	MG	CA	1788	1/1	0.30	-	84,84,84,84	0
55	MG	AA	1651	1/1	0.57	-	71,71,71,71	0
55	MG	BA	3367	1/1	0.36	-	82,82,82,82	0
55	MG	BA	3475	1/1	0.33	-	83,83,83,83	0
55	MG	AA	1758	1/1	0.36	-	85,85,85,85	0
55	MG	AA	1789	1/1	0.35	-	74,74,74,74	0
55	MG	DA	3115	1/1	0.54	-	49,49,49,49	0
55	MG	BA	3273	1/1	0.34	-	94,94,94,94	0
55	MG	CA	1745	1/1	0.14	-	91,91,91,91	0
55	MG	BB	216	1/1	0.28	-	94,94,94,94	0
55	MG	DA	3147	1/1	0.42	-	53,53,53,53	0
55	MG	BA	3472	1/1	0.57	-	89,89,89,89	0
55	MG	DA	3138	1/1	0.27	-	70,70,70,70	0
55	MG	BA	3260	1/1	0.41	-	47,47,47,47	0
55	MG	DA	3336	1/1	0.49	-	87,87,87,87	0
55	MG	BA	3249	1/1	0.25	-	30,30,30,30	0
55	MG	DA	3049	1/1	0.37	-	74,74,74,74	0
55	MG	BA	3572	1/1	0.38	-	87,87,87,87	0
55	MG	AA	1828	1/1	0.14	-	105,105,105,105	0
55	MG	BA	3315	1/1	0.34	-	78,78,78,78	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.