



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 08:45 PM BST

PDB ID : 4V8D
Title : Structure analysis of ribosomal decoding (cognate tRNA-tyr complex).
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Deposited on : 2011-12-07
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

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

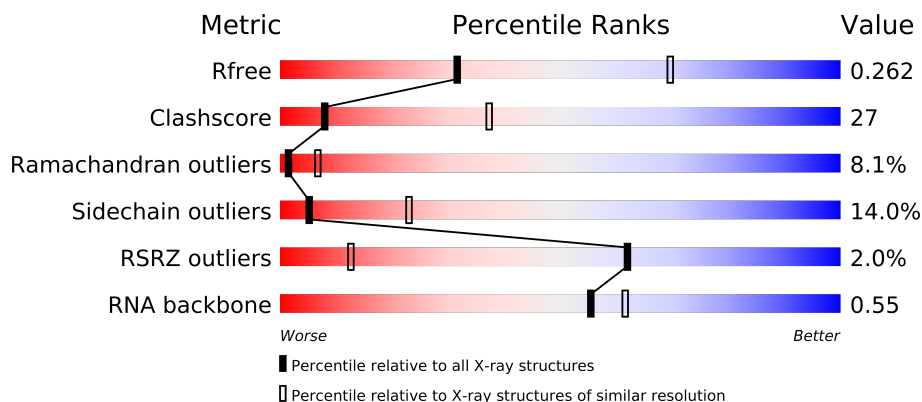
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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 ≥ 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	85	
22	AD	85	
22	CB	85	
22	CD	85	
23	AC	77	
23	CC	77	
24	A1	16	
24	C1	16	
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 299676 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	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
1	CA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

- 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	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
14	CQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	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-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	AB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	AD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

- 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	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			
24	C1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			

- 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	-	INSERTION	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	166	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 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	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	59	Total	C	N	O	S	0	0	0
			459	288	90	76	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	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
53	D7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
54	D8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	568	Total 568	Mg 568	2	0
55	CA	219	Total 219	Mg 219	0	0
55	AB	4	Total 4	Mg 4	0	0
55	BE	3	Total 3	Mg 3	0	0
55	B1	2	Total 2	Mg 2	0	0
55	AN	1	Total 1	Mg 1	0	0
55	CR	1	Total 1	Mg 1	0	0
55	AS	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	BB	18	Total 18	Mg 18	0	0
55	DO	1	Total 1	Mg 1	0	0
55	D8	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	BF	3	Total 3	Mg 3	0	0
55	B2	1	Total 1	Mg 1	0	0
55	AA	220	Total 220	Mg 220	1	0
55	D7	1	Total 1	Mg 1	0	0
55	AR	1	Total 1	Mg 1	0	0
55	B6	1	Total 1	Mg 1	0	0
55	CG	2	Total 2	Mg 2	0	0
55	A1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AD	3	Total 3	Mg 3	0	0
55	DD	3	Total 3	Mg 3	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	9	Total 9	Mg 9	0	0
55	DE	1	Total 1	Mg 1	0	0
55	B3	3	Total 3	Mg 3	0	0
55	DA	488	Total 488	Mg 488	0	0
55	D5	2	Total 2	Mg 2	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	2	Total 2	Mg 2	0	0
55	BO	2	Total 2	Mg 2	0	0
55	D1	1	Total 1	Mg 1	0	0
55	CB	4	Total 4	Mg 4	0	0
55	AC	8	Total 8	Mg 8	0	0
55	CD	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	BW	1	Total 1	Mg 1	0	0
55	CK	1	Total 1	Mg 1	0	0
55	DB	20	Total 20	Mg 20	0	0

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

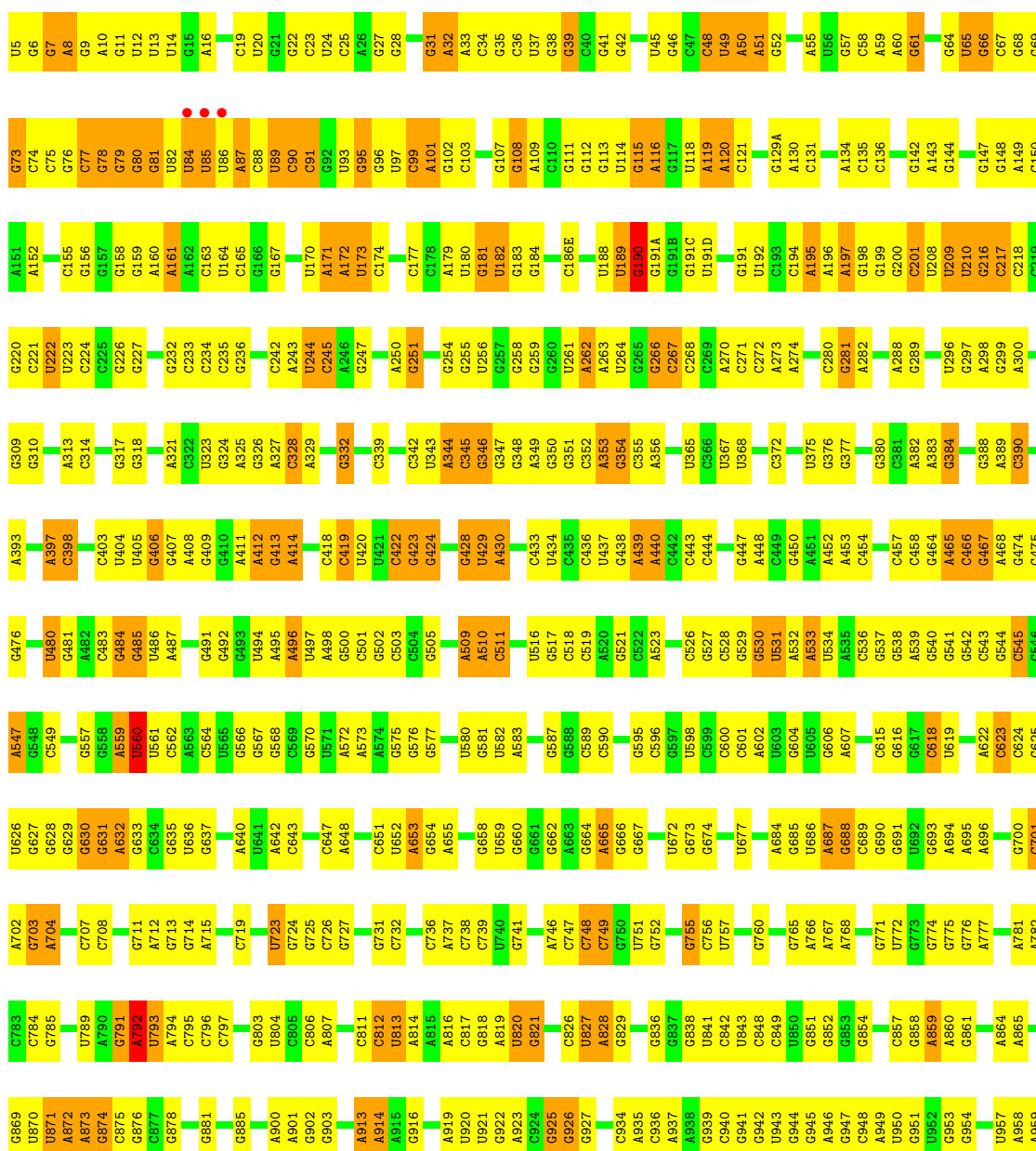
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

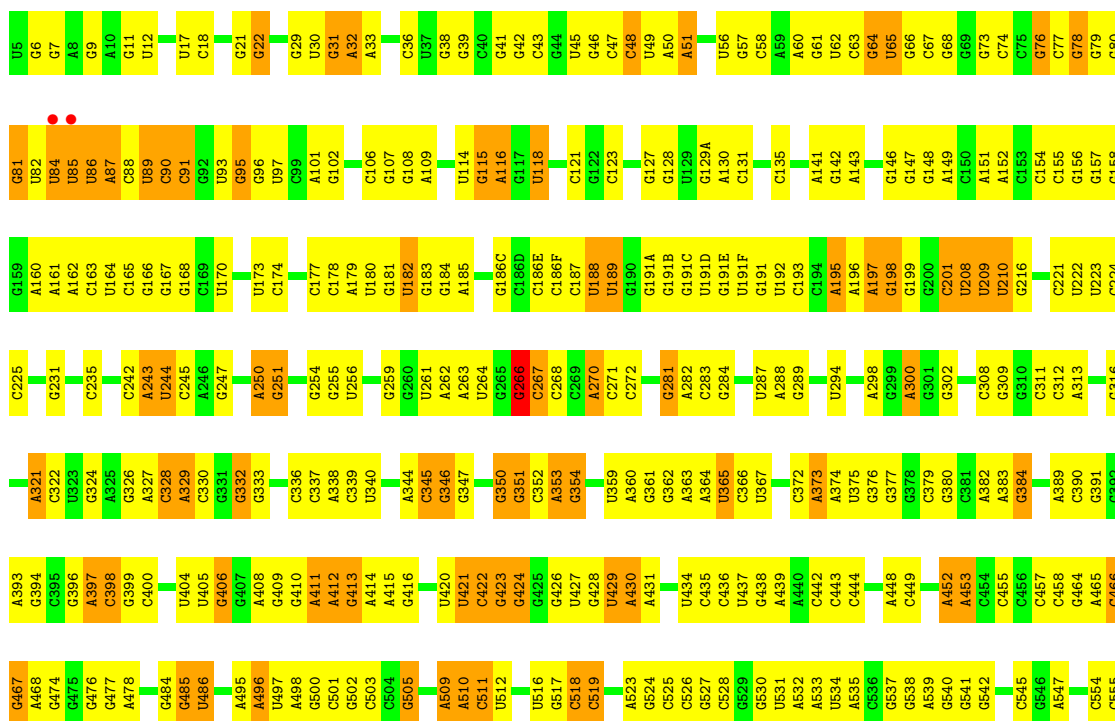
3 Residue-property plots

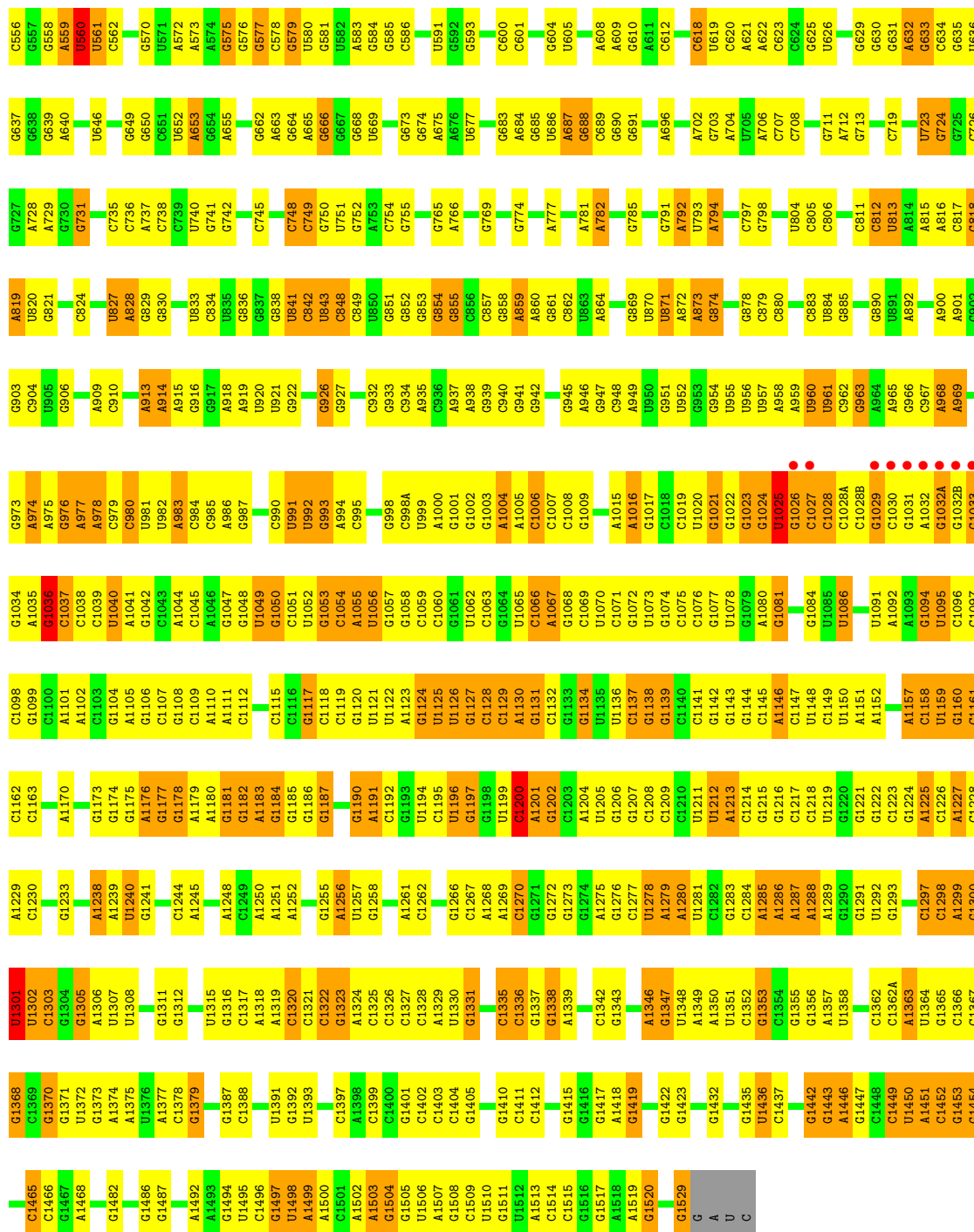
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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:



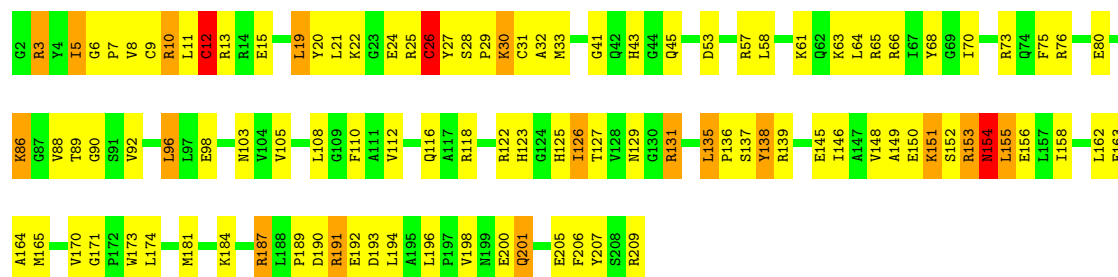





LYS
ALA
ARG
PRO
GLU
LEU
PRO
LYS
ALA
GLU
GLU
ARG
PRO
ARG
ARG
ARG
PRO
PRO
ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG: 




• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG: 



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH: 



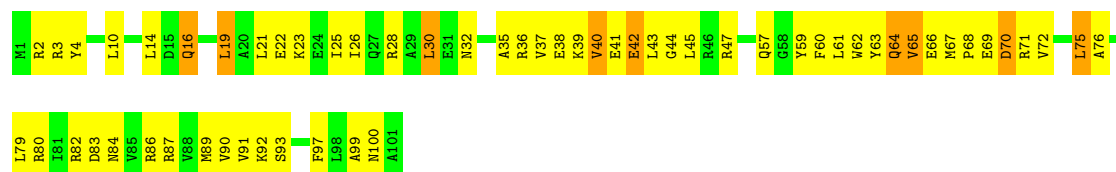
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH: 



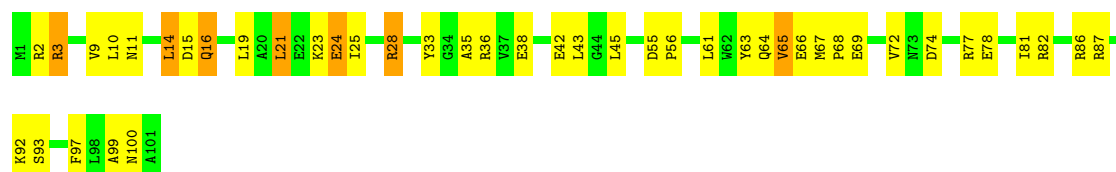
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



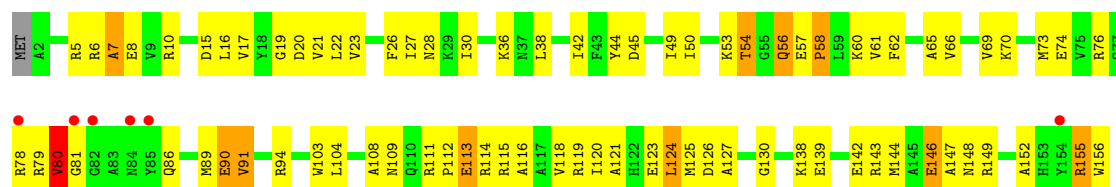
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



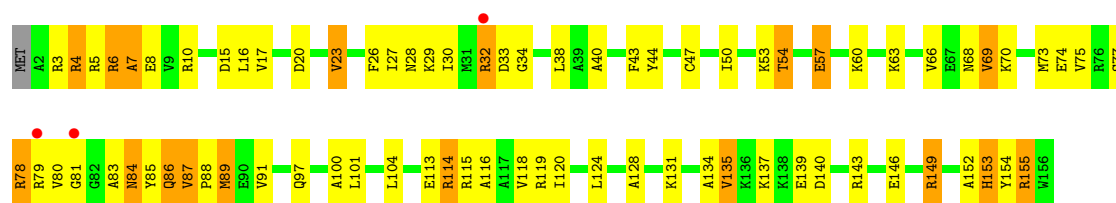
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



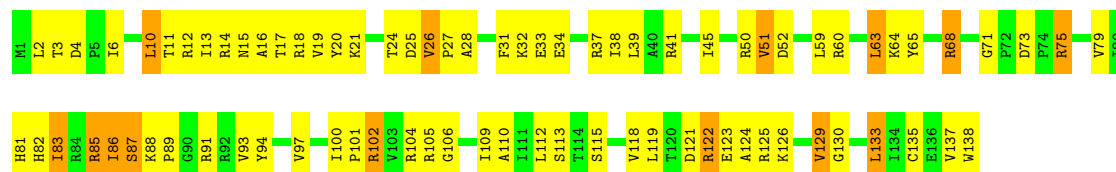
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



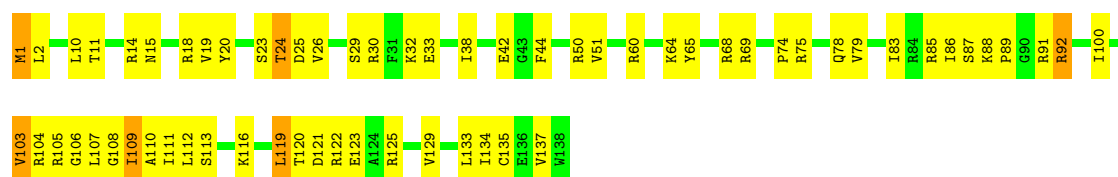
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



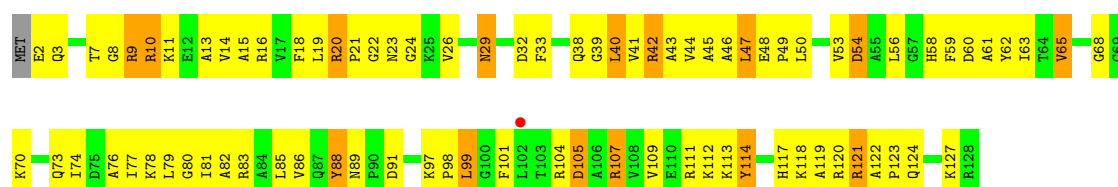
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



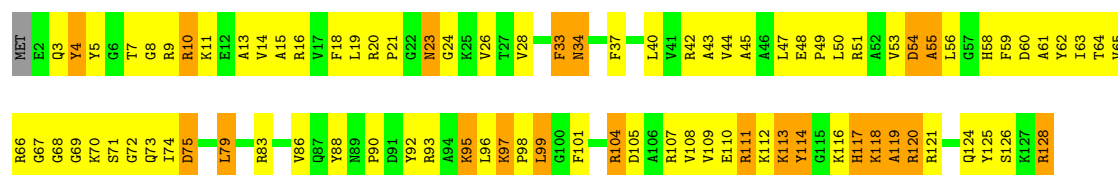
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



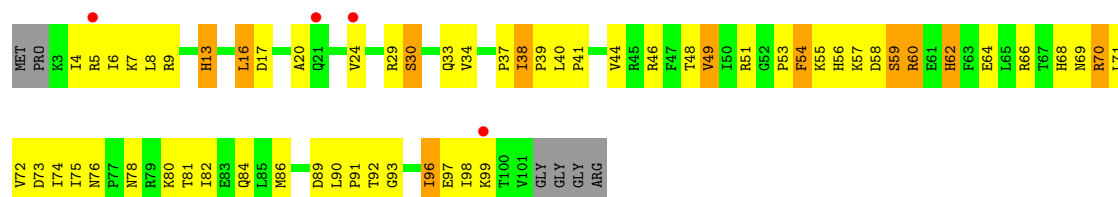
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



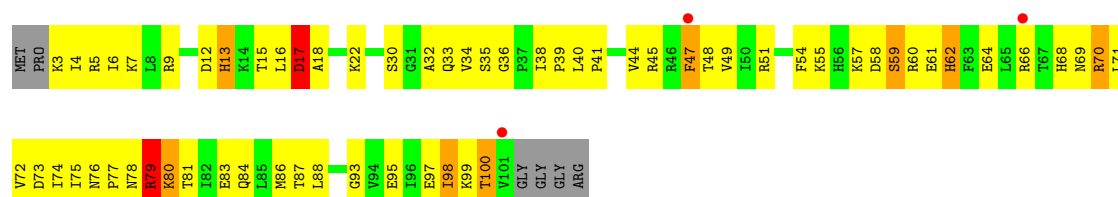
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



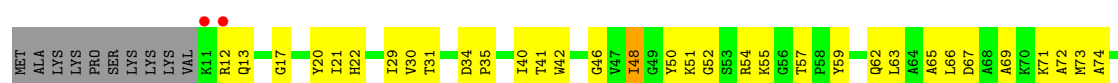
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

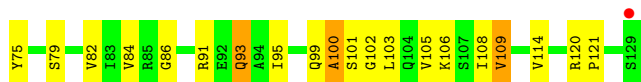
Chain AN:





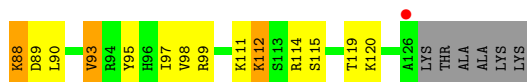
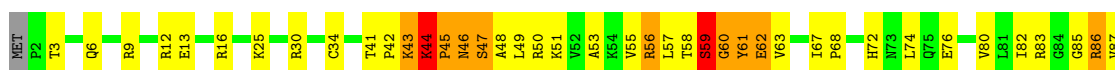
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN:



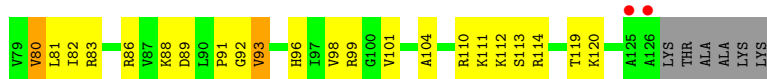
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AP:



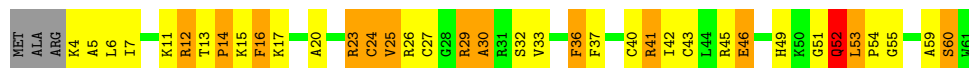
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



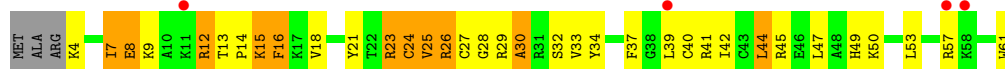
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ: 



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ: 



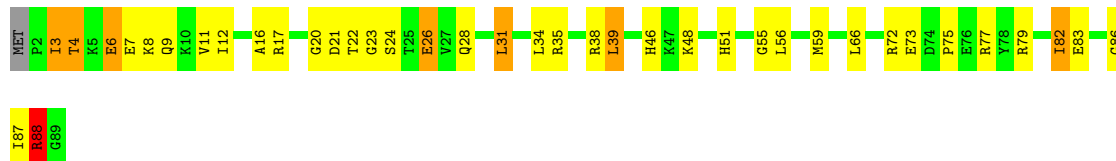
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR: 



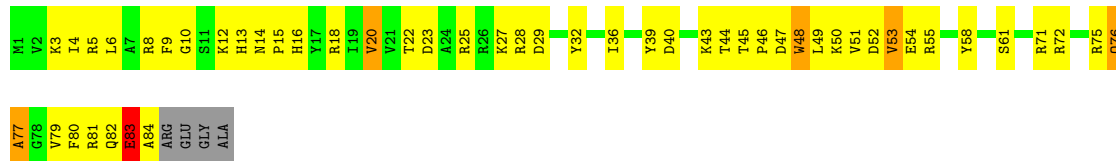
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR: 



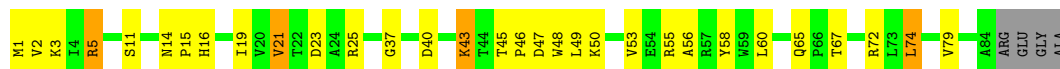
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS: 



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

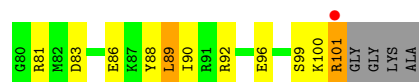
Chain CS: 



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

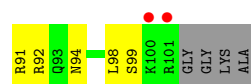
Chain AT: 





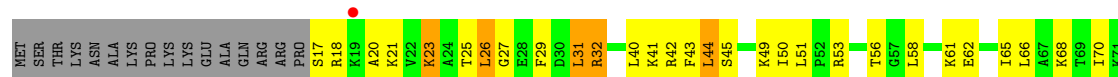
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



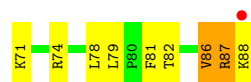
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



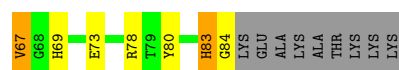
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CU:



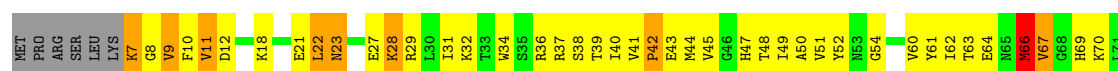
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AV:



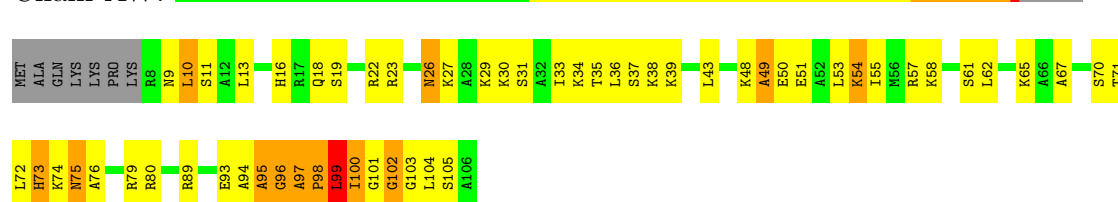
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV:



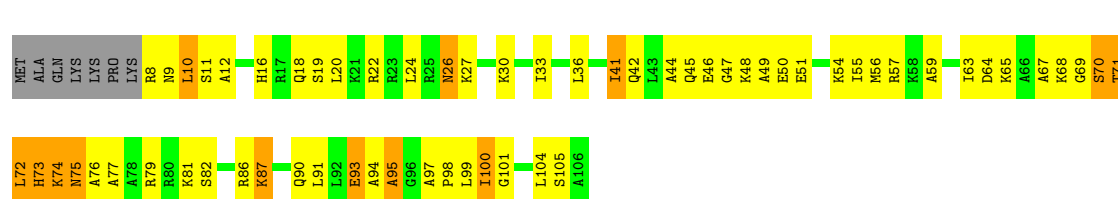
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



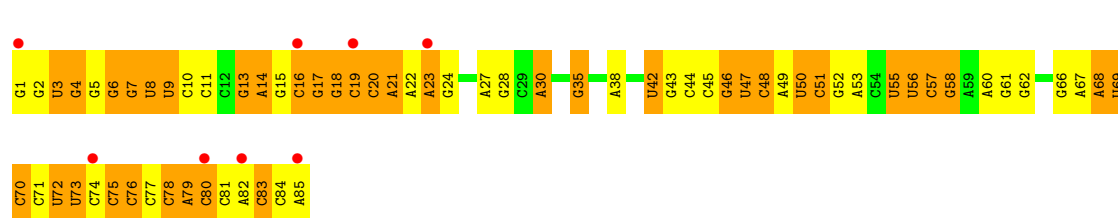
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



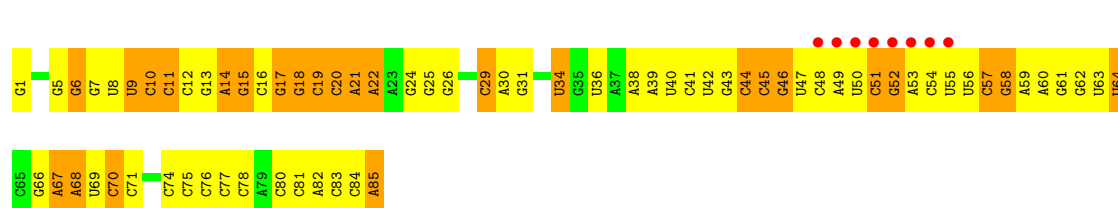
- Molecule 22: TRNA-TYR

Chain AB:



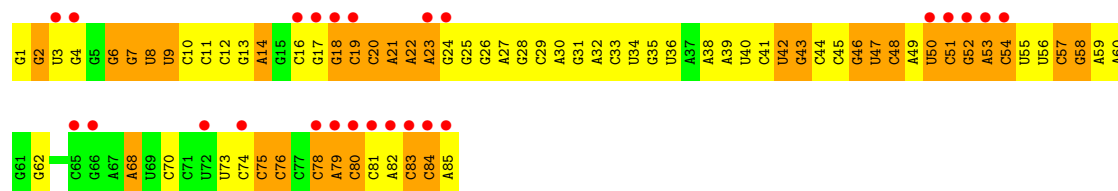
- Molecule 22: TRNA-TYR

Chain AD:



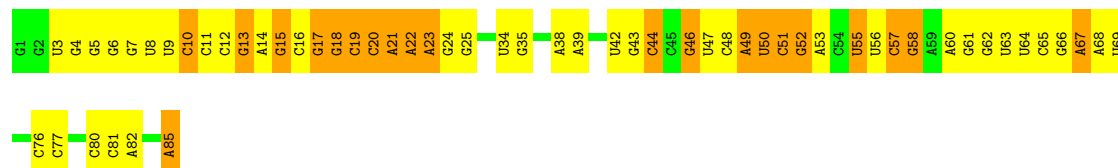
- Molecule 22: TRNA-TYR

Chain CB:



- Molecule 22: TRNA-TYR

Chain CD:



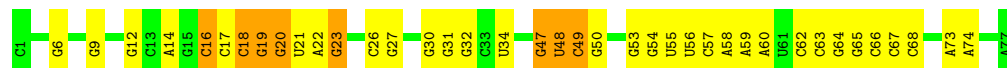
- Molecule 23: TRNA-FMET

Chain AC:



- Molecule 23: TRNA-FMET

Chain CC:



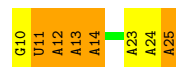
- Molecule 24: MRNA

Chain A1:



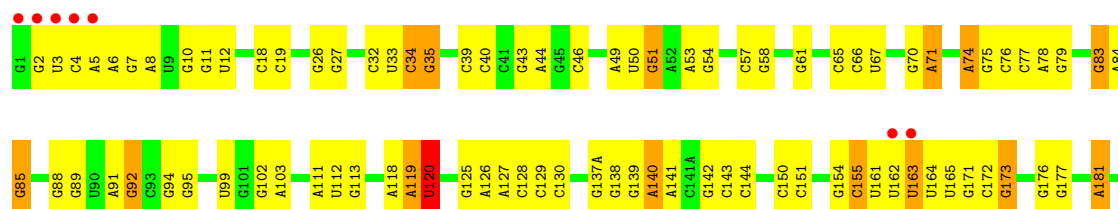
- Molecule 24: MRNA

Chain C1:



- Molecule 25: RNA (2912-MER)

Chain BA:



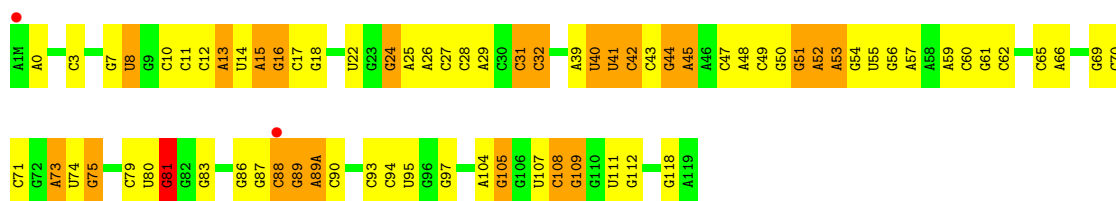
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A1331	C1261	A1174	C1000	U1033	A957	G879	A802	A722	A586	U441	G326	U270M	U185
G1332	G1252	G1176	U1101	G1034	U958	G880	A902	U724	C587	G442	G327	G270N	
U1340	A1253	C1102	C1102	G1042	A959	G881	G805	U725	U588	A443	G329	U270O	A195
U1341	G1256	A1177	A1103	G1043	A960	G882	G806	G726	C599	C444	G330	C270P	A196
G1348	C1261	C1180	C1104	G1044	C961	C884	U807		C591	U448	A331	C270Q	A197
A1349	A1262	G1106	U1105	A1045	G966	C885		C730	C592		A332	C270R	C198
U1352	U1263	G1107	G1107	A1046	C967	C886	U811		C593	C455	A333	G270S	A199
A1353	G1264	U1107	U1108	A1047	G968	C887	C812	G733	U524	U457	G334	G270T	U200
A1354	A1265	G1108	G1109	G1048	U969	C888	U813		U525	C456	C335	C270U	G205
G1355	G1266	A1110	G1110	A1049	U970	C889	C614	G738	A526	G458	C336	G270V	U206
		A1111	A1111	A1050	C971	C890		U740	A528	U459	C337	G270X	A207
A1269	U1269	G1112	U1112	G1051	G972	C891	C617		A529	A460	G338	G270Y	C208
C1270	G1271	U1113	U1113	G1052	A973	C892	G818	G743	G530	G463	A347	C271A	A213
A1272	U1272	G1114	A1114	G1053	G974	C893	A819	G744	C531	G471	G349	G271B	G214
U1273	U1273	G1115	A1115	G1054	C974A	C894	A820	G745	A532	A466	U350	U271C	G215
		C1121	C1121	G1055	G975	C895	A821	A746	U534	U475	G351	G271	A216
		G1122	G1122	G1056		C896	U826	U747	C535	G469	G352		G217
		U1125	U1125	A1057	G978	C897	U827	G748	A536	A470			A218
		A1126	A1126	A1058		C898	U828		A537	A471	G356		A222
		G1127	G1127	U1059	A983	A900	A829	A751	G537	G472			A223
		A1128	A1128	U1060	C986	C902	G830	A752	G540		G361		
		U1129	U1129	U1061	G987	C903	G831	C753	C542	U476	U862		
		U1130	U1130	G1062	A988	C904	G832	C754	C543	A478	G363		A227
		G1131	G1131	G1063	U989	C905	G833	C755	C544	A479	A363A		A228
		C1203	C1203	G1064	G989	U906	U834	C756	G545	A480	G363B		A229
		A1204	A1204	U1065	A990	C907	C834		G546	G481			U230
		U1205	U1205	U1066	C991	U908			A547	A482			C231
		G1136	G1136	U1067	C992	C909	U839	G760	A548		C364		C231
		U1137	U1137	G1068	C993	A910		A761	A549	A483			C232
		G1138	G1138	U1069	C994	A911	C844	A764	G549	A484	G370		A233
		A1139	A1139	A1070	C995	G912	G845	G765	G550	C485	A371		C234
		C1140	C1140	G1071	A996	C913	U847	C766	G551		G372		U235
		U1141	U1141	U1072	G1003	C914	G848		G552	G488	U373		
		U1142	U1142	C1073	C1004	C915	A849	U773	U553	G489	A374		G245
		A1142A	A1142A	G1074	C1005	C916	C850	A774	U554	G491	C375		G246
		U1143	U1143	C1075	C1006	A917	U851	G775	G556	G492	C376		G247
		G1144	G1144	U1076	U1006	A918	G852	G776	U557	G493			G248
		C1145	C1145	A1077	G1007	C919	G853	A777	G558	G494			C249
		U1146	U1146	U1078	A1009	G919		G778	G559	G495	U383		G250
		C1147	C1147	C1079	U1010		C856		G560	G496	C384		A251
		A1148	A1148	A1080	G1011	C925	C857	U779	G561	A497	C385		G252
		G1151	G1151	U1081	U1012	G932	C858	G780	U562	G498	C386		
		C1152	C1152	U1082	C1013	A933	U858	A761	A637	G499			G259
		C1153	C1153	U1083	U1014	C934	U860	A782	G563	U499	G389		
		A1156	A1156	A1084	G1015	G938	A861	A783	C564	G500			A265
		G1157	G1157	U1085	G1016		G862	G784	U565	A501	C404		G266
		U1236	U1236	A1086	U1019	A941	A863	G785	C641	A502	U405		
		C1237	C1237	G1087	U1020	G942	G864	C786	G642	A503			U269
		G1238	G1238	A1088	A1021	U943	C865	U787	A643	U504	G411		
		C1161	C1161	G1089	U1022	G944	A866	A788	A644	A505	A412		C270D
		U1240	U1240	U1090	G1022	A945	C867	G789	C645	G506	G317		G270E
		A1241	A1241	G1091	U1023	G946	U868	C790	A646	A507	C318		U270F
		G1163	G1163	C1092	G1024		U869	G791	G647	G508	C319		C270G
		U1242	U1242	G1093	G1025	G950	A870	G792	C680	C510	A428		C270H
		U1165	U1165	U1094	U1026	C951		A793		U511			G270I
		C1166	C1166	A1027	A1027	G952	G873	G794	A653	U512			G270J
		G1171	G1171	A1095	U1028	A953		C796	A654	A513	G439		C270K





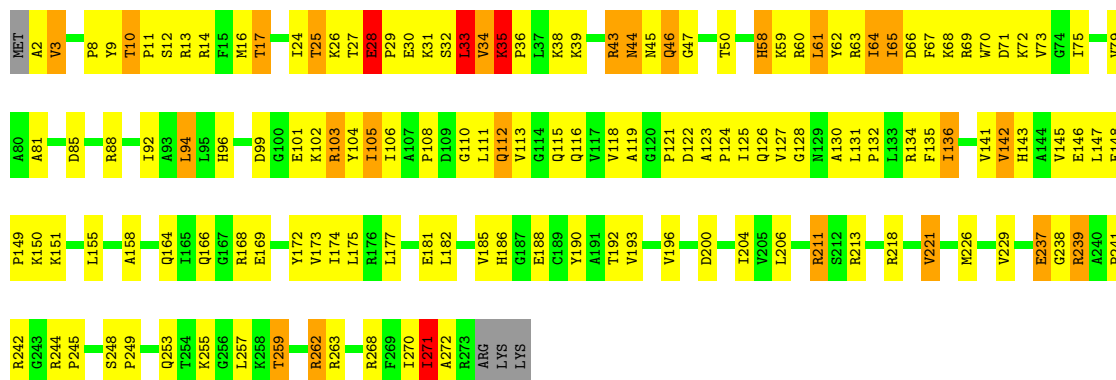
A2019	C884	C951	U1019	A1086	G1151	C1224	G1310	G1389	G1455	C1533	G1622	G1718	G1813	U1926
A2020	C885	G952	A1020	G1087	C1152	G1224	G1311	G1392	G1458	G1534	C1625	G1725	G1814	A1927
C2021	A887	A953	A1021	A1088	C1153	G1225	U1312	A1393	C1459	U1535	C1635	G1728	A1816	A1928
U2022	G955	G954	G1022	G1089	G1154	G1226	U1313	A1394	A1460	C1537	G1638	U1729	G1817	G1929
G2023	C888	C956	G1023	A1090	A1155	G1227	C1314	A1395	A1461	G1538	U1639	U1730	A1818	G1930
G2024	C889	A957	G1024	G1091	A1156	G1228	C1315	U1396	C1464	G1539	U1638	G1731	A1819	A1936
C2025	A890	A958	G1025	C1092	U1159	G1229	U1316	U1397	C1467	G1542	U1639	A1732	U1820	A1937
G2026	G892	U968	U1026	G1093	G1160	G1230	A1317	C1398	C1468	C1544	C1640	C1735	A1821	A1938
G2027	C893	A959	A1027	A1096	C1161	G1231	G1318	U1399	C1469	A1543	G1645	C1741	G1826	U1939
A2030	U896	G962	G1030	A1097	G1162	G1232	G1319	C1401	C1470	A1545	G1646	C1742	G1827	U1940
A2031	C897	U969	U1035	A1098	G1163	A1241	U1323	G1402	A1468	C1548	G1647	G1748	A1829	C1941
C2032	C898	C970	G1036	G1099	G1164	G1248	U1324	C1403	A1469	C1549	G1648	A1749	C1830	U1942
G2033	A899	C971	A1037	U1101	U1165	U1249	G1325	C1404	A1471	C1548	C1649	G1753	G1831	U1943
A2034	A901	G972	C1038	G1104	G1166	G1250	U1326	U1405	A1472	C1550	G1650	G1753	U1944	U1945
U2035	C902	A973	G1039	C1104	G1168	G1251	G1328	U1406	G1473	C1551	G1651	C1754	C1832	U1946
G2036	C903	G974	C1040	U1105	G1169	G1252	U1329	C1408	C1474	G1552	A1652	G1755	G1833	G1950
A2042	C904	C974A	C1041	G1109	G1170	A1253	C1330	C1409	C1475	C1556	G1653	G1756	C1843	U1951
C2043	U905	C974B	C1042	C1112	G1171	G1254	A1331	A1412	A1477	C1557	A1654	U1757	G1844	U1952
G2049	G906	G975	C1043	U1111	G1172	U1255	G1336	G1413	G1478	C1558	C1657	U1758	A1847	U1955
C2050	U907	G976	C1044	A1111	A1174	G1256	U1337	G1414	G1479	G1559	C1658	A1759	A1848	U1956
A2055	U907	G977	G1044	G1112	U1175	G1256	U1338	G1416	U1482	G1560	A1684	C1761	U1851	U1963
G2056	C908	G978	A1045	U1113	G1176	G1259	G1339	G1417	G1483	G1568	A1685	G1762	C1852	G2056
A2059	A909	C979	A1046	U1116	G1178	G1260	U1340	G1418	G1484	G1569	G1686	G1763	A1853	C2055
G2061	C914	A981	A1048	C1117	C1180	C1261	U1341	A1419	G1485	A1570	G1687	G1764	U1854	U1964
A2062	C915	A982	C1049	C1118	C1181	A1268	U1342	U1420	A1486	A1571	A1688	C1771	G1858	A2059
C2065	G916	A983	G1051	C1119	C1182	G1269	G1343	G1422	A1490	C1577	C1670	G1772	A1859	C2061
G2066	G917	C985	A1054	G1120	G1187	G1266	G1344	G1426	C1493	U1578	U1671	U1778	G1860	A1969
G2067	A918	C986	G1055	G1121	U1188	U1267	C1345	A1427	A1494	C1579	C1672	U1779	A1864	A1970
U2068	G919	A988	G1056	G1122	A1189	A1268	G1346	C1428	A1495	C1582	G1673	U1780	U1865	A1971
G2069	G920	A989	A1057	G1125	G1191	G1270	G1347	G1429	A1496	C1583	C1674	A1781	A1872	G1972
A2071	G921	C991	U1065	A1126	G1192	A1271	U1348	C1430	U1503	A1586	C1675	G1782	G1878	G1989
C2077	C924	C992	U1066	G1127	G1193	A1272	U1352	C1432	C1504	A1587	G1678	A1783	C1882	C1990
G2078	G925	G993	U1067	A1128	A1194	U1273	U1356	U1433	C1505	C1588	G1681	A1785	G1883	U1991
U2079	C926	C994	G1063	A1129	G1196	G1278	U1357	U1434	A1508	C1589	C1686	A1786	A1884	U1993
G2080	A926	C995	G1064	G1130	U1197	G1279	G1358	G1436	C1509	U1590	G1687	C1790	G1888	C1996
C2081	G928	A996	C1064	A1132	U1198	G1279	G1359	U1437	A1510	C1591	U1688	C1791	A1889	G1997
G2086	G929	G997	U1065	U1133	U1199	G1285	A1359	U1438	A1511	G1593	A1689	G1792	A1890	G1998
U2087	U930	C998	U1066	G1135	C1200	G1285	A1360	A1439	G1512	G1595	U1693	C1793	G1899	C2000
C2082	G931	U999	A1067	G1136	C1201	U1288	A1365	G1442	C1514	C1598	G1696	U1794	A1900	A2001
G2087	G932	A1000	G1068	G1137	G1202	U1288	A1366	G1443	C1515	C1599	G1697	C1795	A1901	G2002
U2092	A933	A1001	A1069	G1138	G1203	C1291	A1367	G1444	U1516	C1598	G1698	U1796	C1902	C2007
G2093	G934	G1002	A1070	G1139	U1204	C1291	A1368	U1444A	U1516	U1602	A1698	C1797	G1903	C2008
C2094	G938	C1005	G1071	U1141	U1205	C1297	G1369	C1445	U1520	G1606	G1699	C1800	G1906	C2009
U2097	A941	C1006	A1073	U1142	A1210	C1298	C1370	C1446	G1521	G1607	G1699	G1801	G1907	G2010
G2098	G942	C1007	G1074	A1142A	U1211	G1299	A1379	G1447	G1522	A1608	A1701	A1802	C1914	U2011
U2099	U943	G1011	C1075	G1144	G1212	U1300	G1380	G1448	U1523	A1609	G1710	U1805	U1915	G2012
C2097	A945	U1012	C1076	G1145	G1217	A1301	A1384	A1449	G1524	A1610	C1711	G1810	A1916	A2013
G2098	G946	C1013	A1077	C1146	G1218	A1302	G1385	G1450	G1525	G1526	C1712	A1811	U1923	A2014
U2099	G947	U1014	U1078	C1147	G1219	G1303	G1386	C1451	G1527	A1528	U1716	G1812	U1923	A2015
G2101	G948	G1015	U1081	A1148	A1220	A1308	C1387	A1454	G1527	U1621	G1717			U2016
	G948	G1016	A1085	C1150	C1222	G1309	G1388	U1454						





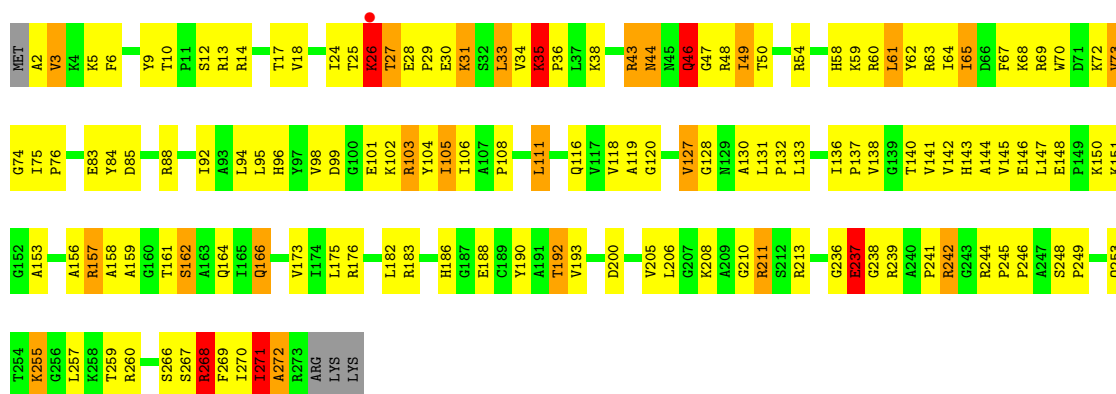
• Molecule 27: 50S ribosomal protein L2

Chain BD:



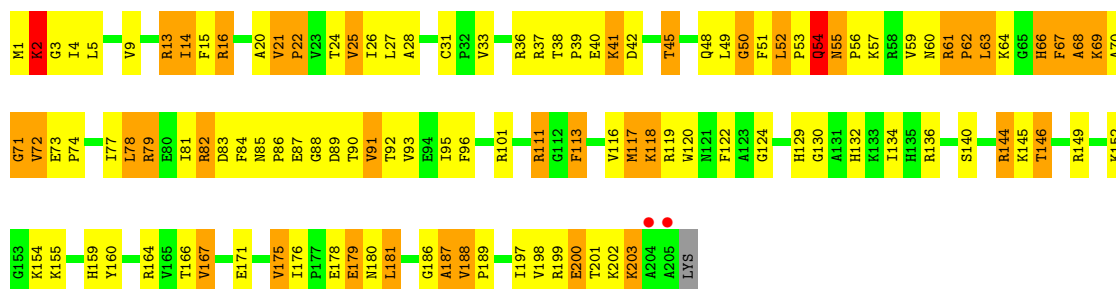
• Molecule 27: 50S ribosomal protein L2

Chain DD:



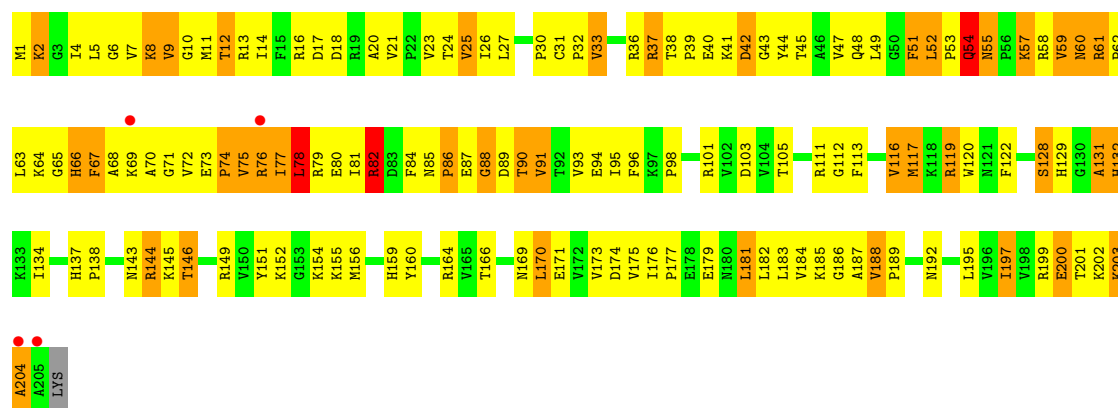
• Molecule 28: 50S ribosomal protein L3

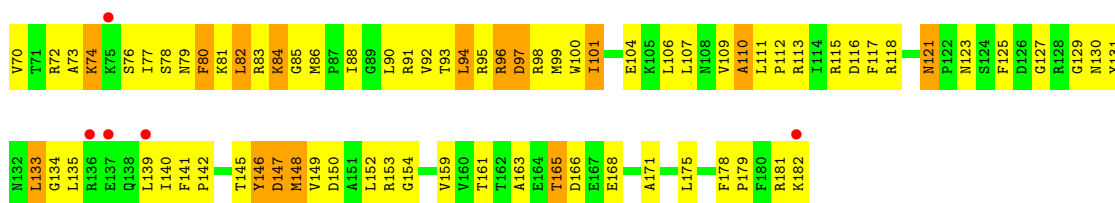
Chain BE:



• Molecule 28: 50S ribosomal protein L3

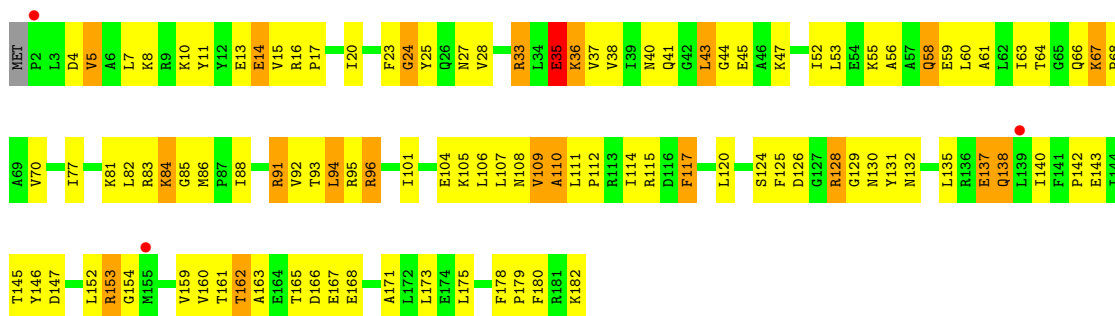
Chain DE:





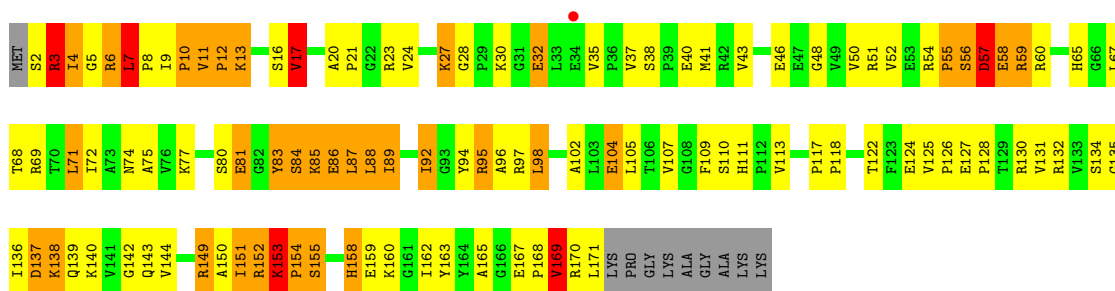
• Molecule 30: 50S ribosomal protein L5

Chain DG:



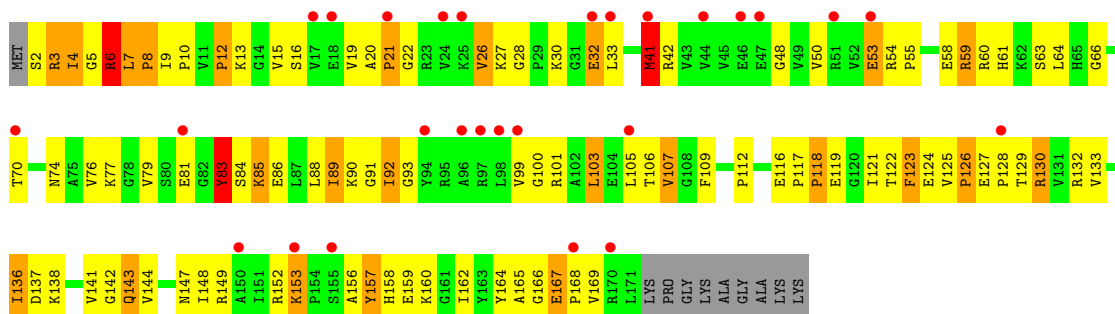
• Molecule 31: 50S ribosomal protein L6

Chain BH:



• Molecule 31: 50S ribosomal protein L6

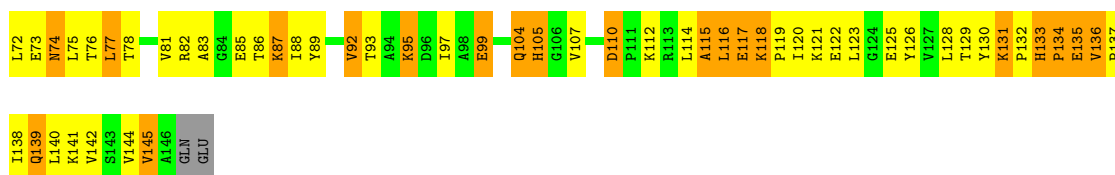
Chain DH:



• Molecule 32: 50S ribosomal protein L9

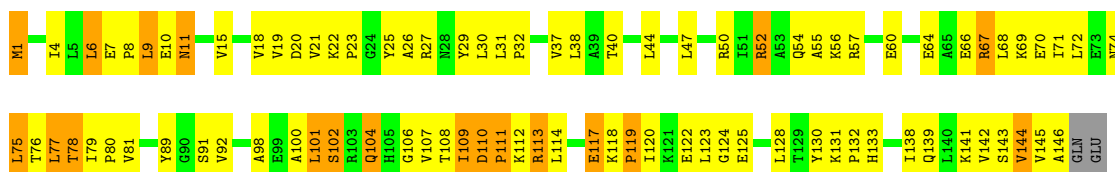
Chain BK:





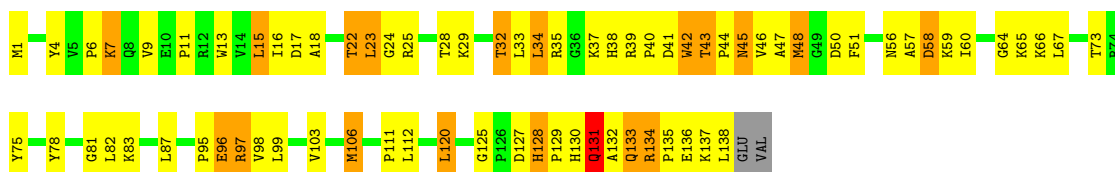
• Molecule 32: 50S ribosomal protein L9

Chain DK:



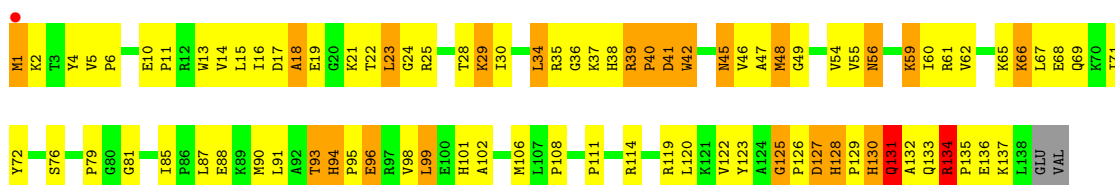
• Molecule 33: 50S ribosomal protein L13

Chain BM:



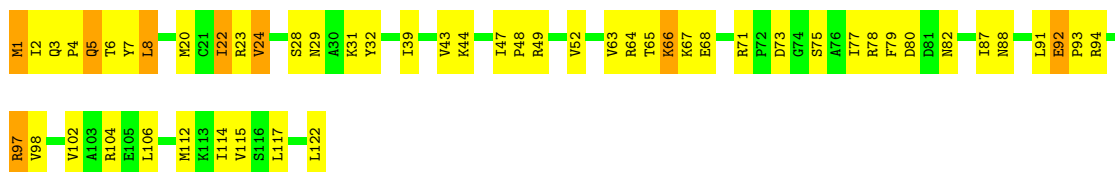
• Molecule 33: 50S ribosomal protein L13

Chain DM:



• Molecule 34: 50S ribosomal protein L14

Chain BN:



• Molecule 34: 50S ribosomal protein L14

Chain DN:





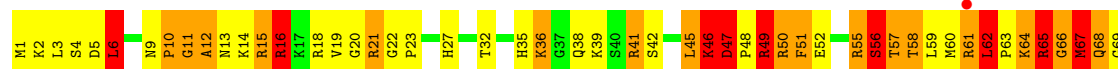
- Molecule 35: 50S ribosomal protein L15

Chain BO:



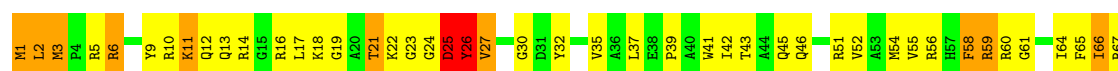
- Molecule 35: 50S ribosomal protein L15

Chain DO:



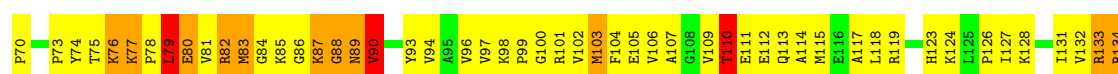
- Molecule 36: 50S ribosomal protein L16

Chain BP:



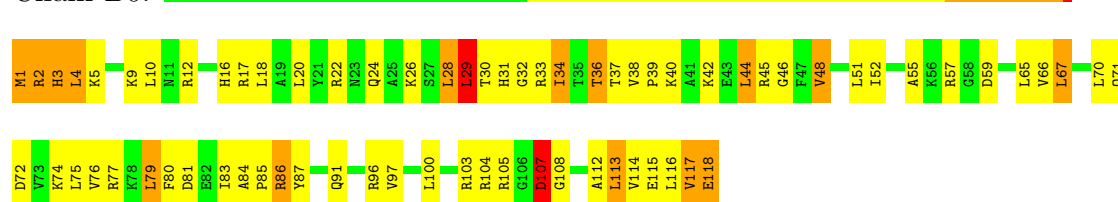
- Molecule 36: 50S ribosomal protein L16

Chain DP:



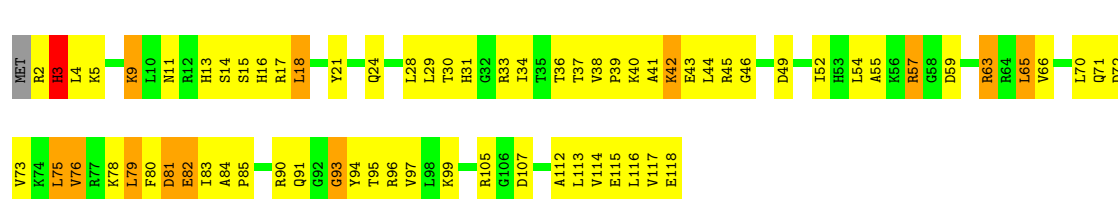
- Molecule 37: 50S ribosomal protein L17

Chain B0:



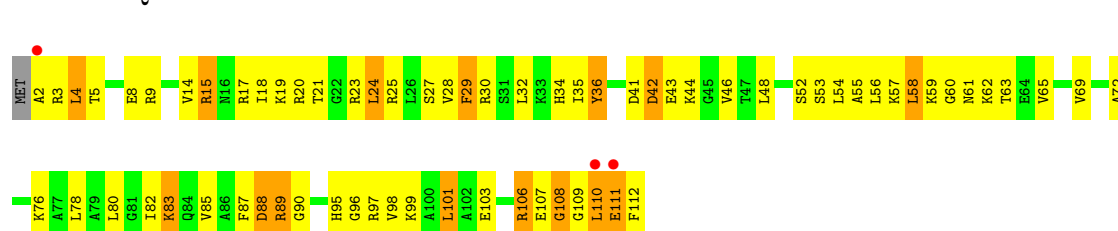
- Molecule 37: 50S ribosomal protein L17

Chain D0:



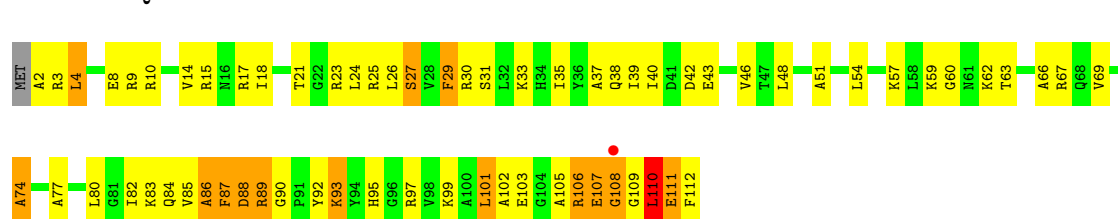
- Molecule 38: 50S ribosomal protein L18

Chain BQ:



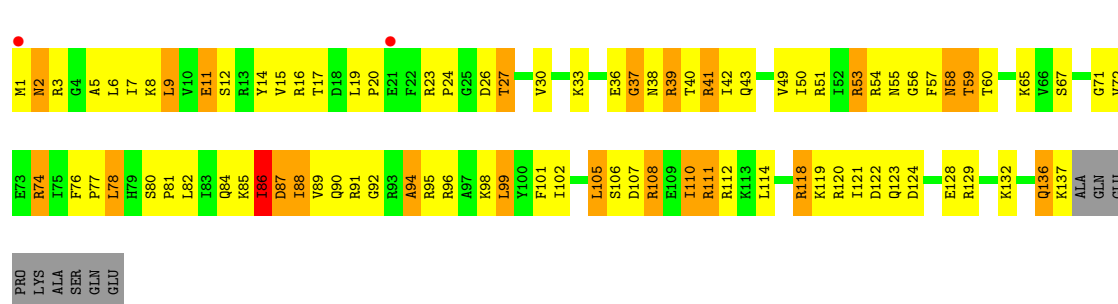
- Molecule 38: 50S ribosomal protein L18

Chain DQ:



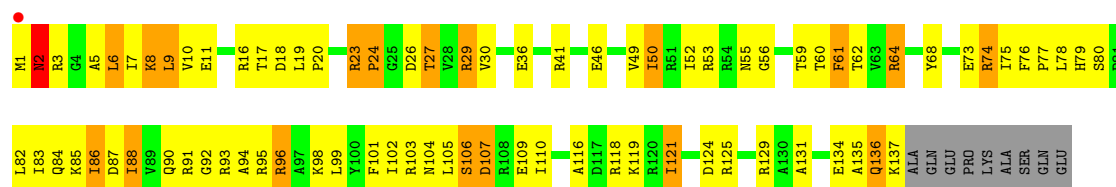
- Molecule 39: 50S ribosomal protein L19

Chain BR:



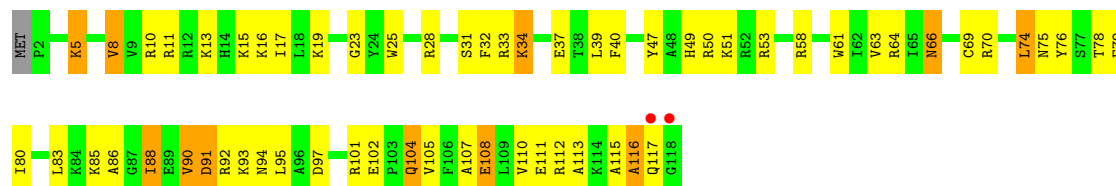
- Molecule 39: 50S ribosomal protein L19

Chain DR:



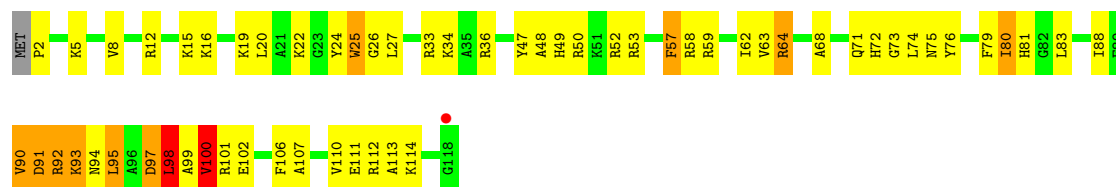
- Molecule 40: 50S ribosomal protein L20

Chain B1:



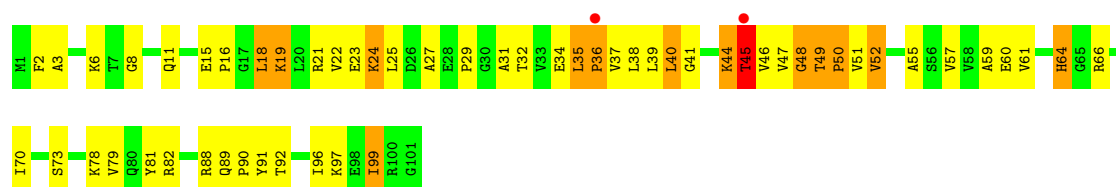
- Molecule 40: 50S ribosomal protein L20

Chain D1:



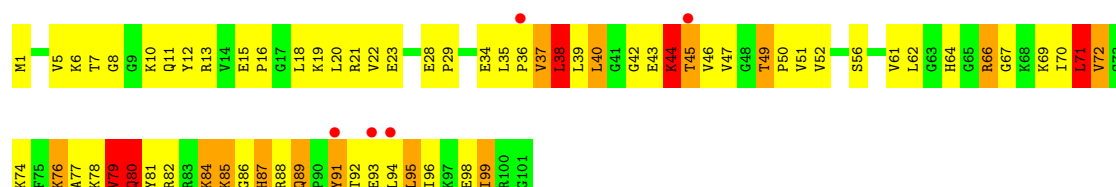
- Molecule 41: 50S ribosomal protein L21

Chain B2:



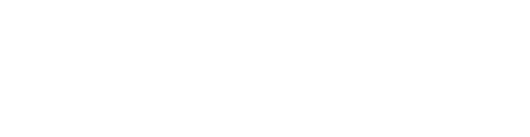
- Molecule 41: 50S ribosomal protein L21

Chain D2:



- Molecule 42: 50S ribosomal protein L22

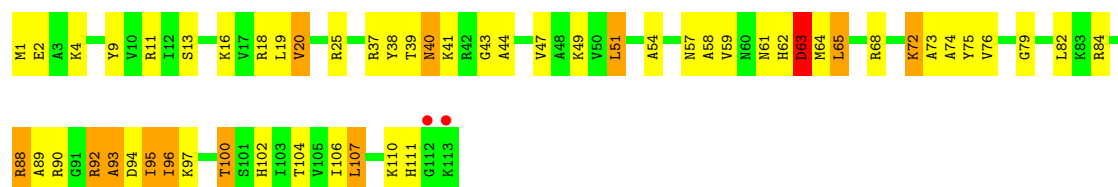
Chain BS:





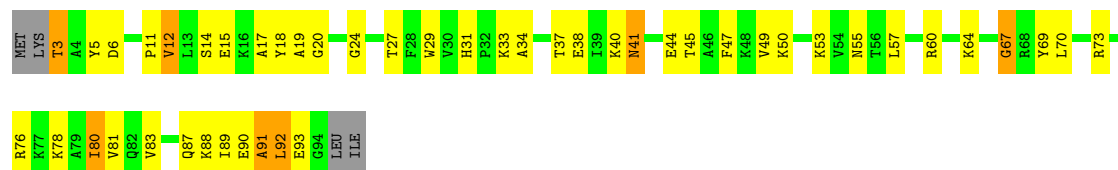
• Molecule 42: 50S ribosomal protein L22

Chain DS:



• Molecule 43: 50S ribosomal protein L23

Chain BT:



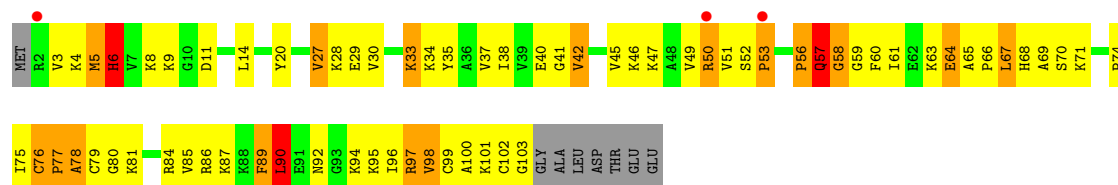
• Molecule 43: 50S ribosomal protein L23

Chain DT:



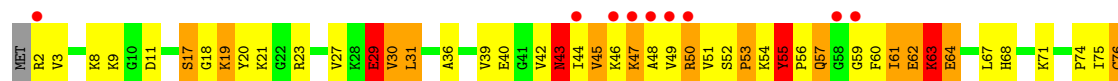
• Molecule 44: 50S ribosomal protein L24

Chain BU:



• Molecule 44: 50S ribosomal protein L24

Chain DU:

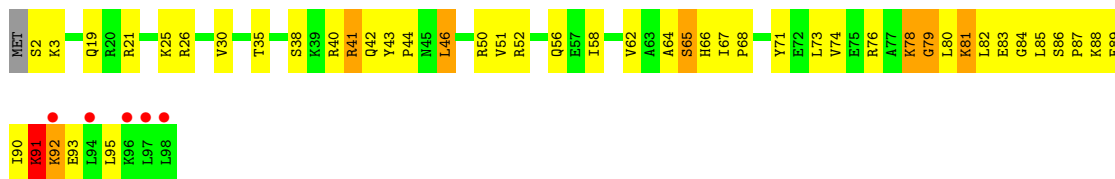






- Molecule 47: 50S ribosomal protein L28

Chain BZ:



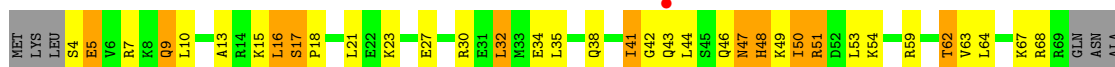
- Molecule 47: 50S ribosomal protein L28

Chain DZ:



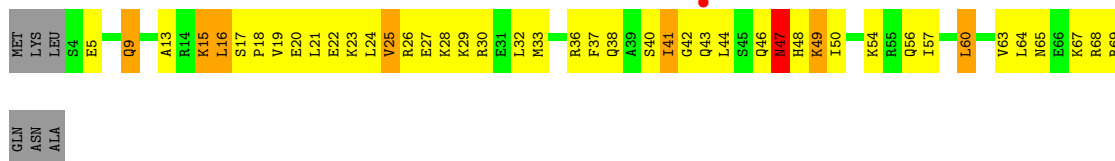
- Molecule 48: 50S ribosomal protein L29

Chain BW:



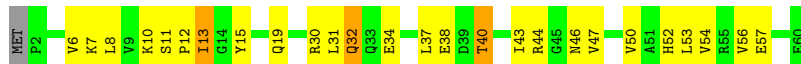
- Molecule 48: 50S ribosomal protein L29

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:

Chain D7: 



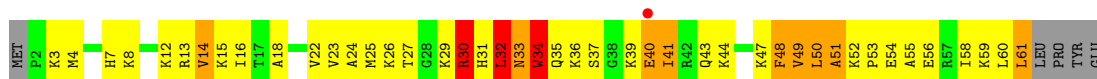
- Molecule 54: 50S ribosomal protein L35

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, α , β , γ	210.67Å 451.75Å 625.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.06 – 3.00 257.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.06-3.00) 93.5 (257.02-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.203 , 0.235 0.242 , 0.262	Depositor DCC
R_{free} test set	930 reflections (0.08%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.6	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	1 of 1175691 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299676	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 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	0.28	0/36139	0.67	20/56406 (0.0%)
1	CA	0.28	0/36142	0.66	20/56410 (0.0%)
2	AE	0.22	0/1959	0.42	0/2642
2	CE	0.22	0/1959	0.42	0/2642
3	AF	0.22	0/1629	0.42	0/2195
3	CF	0.21	0/1636	0.40	0/2205
4	AG	0.29	1/1733 (0.1%)	0.44	0/2318
4	CG	0.27	0/1733	0.47	0/2318
5	AH	0.24	0/1171	0.44	0/1576
5	CH	0.24	0/1171	0.44	0/1576
6	AI	0.24	0/856	0.42	0/1154
6	CI	0.24	0/856	0.42	0/1154
7	AJ	0.22	0/1276	0.40	0/1709
7	CJ	0.22	0/1276	0.38	0/1709
8	AK	0.23	0/1136	0.44	0/1527
8	CK	0.22	0/1136	0.42	0/1527
9	AL	0.23	0/1029	0.41	0/1379
9	CL	0.22	0/1029	0.42	0/1379
10	AM	0.22	0/814	0.42	0/1095
10	CM	0.21	0/814	0.43	0/1095
11	AN	0.24	0/900	0.44	0/1213
11	CN	0.24	0/900	0.43	0/1213
12	AO	0.26	0/991	0.49	0/1327
12	CO	0.25	0/991	0.49	0/1327
13	AP	0.22	0/938	0.45	0/1258
13	CP	0.20	0/943	0.41	0/1265
14	AQ	0.27	0/485	0.47	0/643
14	CQ	0.23	0/485	0.43	0/643
15	AR	0.24	0/745	0.43	0/992
15	CR	0.23	0/745	0.39	0/992
16	AS	0.22	0/721	0.44	0/970
16	CS	0.23	0/721	0.42	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/847	0.43	0/1131
17	CT	0.24	0/847	0.42	0/1131
18	AU	0.25	0/596	0.45	0/790
18	CU	0.24	0/596	0.44	0/790
19	AV	0.23	0/638	0.45	0/860
19	CV	0.22	0/638	0.43	0/860
20	AW	0.22	0/765	0.42	0/1007
20	CW	0.23	0/765	0.45	0/1007
21	AX	0.22	0/221	0.41	0/288
21	CX	0.21	0/221	0.40	0/288
22	AB	0.28	0/1992	0.60	0/3099
22	AD	0.21	0/1992	0.50	0/3099
22	CB	0.26	0/1992	0.57	0/3099
22	CD	0.20	0/1992	0.49	0/3099
23	AC	0.25	0/1835	0.59	1/2859 (0.0%)
23	CC	0.24	0/1835	0.57	0/2859
24	A1	0.33	0/389	0.64	0/604
24	C1	0.38	0/389	0.65	0/604
25	BA	0.37	0/70233	0.75	52/109643 (0.0%)
25	DA	0.33	1/70122 (0.0%)	0.70	54/109469 (0.0%)
26	BB	0.33	0/2928	0.80	11/4568 (0.2%)
26	DB	0.29	0/2928	0.74	4/4568 (0.1%)
27	BD	0.32	0/2165	0.58	1/2919 (0.0%)
27	DD	0.29	0/2165	0.52	0/2919
28	BE	0.29	0/1601	0.55	0/2160
28	DE	0.27	0/1601	0.52	0/2160
29	BF	0.28	0/1620	0.50	0/2194
29	DF	0.26	0/1662	0.52	0/2249
30	BG	0.24	0/1499	0.43	0/2016
30	DG	0.21	0/1499	0.42	0/2016
31	BH	0.25	0/1332	0.50	0/1802
31	DH	0.21	0/1332	0.44	0/1802
32	BK	0.24	0/1151	0.49	0/1558
32	DK	0.23	0/1151	0.51	0/1558
33	BM	0.26	0/1131	0.49	0/1525
33	DM	0.23	0/1131	0.44	0/1525
34	BN	0.27	0/943	0.46	0/1269
34	DN	0.26	0/943	0.46	0/1269
35	BO	0.28	0/1162	0.58	0/1544
35	DO	0.24	0/1162	0.45	0/1544
36	BP	0.27	0/1143	0.46	0/1527
36	DP	0.24	0/1143	0.41	0/1527
37	B0	0.26	0/982	0.48	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	D0	0.25	0/974	0.45	0/1302
38	BQ	0.26	0/892	0.50	0/1187
38	DQ	0.23	0/892	0.46	0/1187
39	BR	0.28	0/1155	0.49	0/1542
39	DR	0.25	0/1155	0.44	0/1542
40	B1	0.28	0/982	0.49	0/1306
40	D1	0.24	0/982	0.44	0/1306
41	B2	0.26	0/790	0.48	0/1057
41	D2	0.27	0/790	0.51	0/1057
42	BS	0.27	0/911	0.47	0/1220
42	DS	0.26	0/911	0.44	0/1220
43	BT	0.31	0/739	0.49	0/993
43	DT	0.28	0/739	0.46	0/993
44	BU	0.29	0/798	0.52	0/1064
44	DU	0.26	0/798	0.48	0/1064
45	BV	0.23	0/1427	0.48	1/1935 (0.1%)
45	DV	0.22	0/1460	0.43	0/1982
46	B3	0.28	0/615	0.46	0/819
46	D3	0.26	0/621	0.44	0/827
47	BZ	0.27	0/770	0.50	0/1022
47	DZ	0.26	0/770	0.50	0/1022
48	BW	0.28	0/560	0.52	0/741
48	DW	0.25	0/560	0.45	0/741
49	BX	0.25	0/474	0.42	0/635
49	DX	0.22	0/474	0.41	0/635
50	B4	0.22	0/545	0.49	0/733
50	D4	0.23	0/527	0.51	0/709
51	B5	0.25	0/473	0.51	0/639
51	D5	0.24	0/473	0.54	0/639
52	B6	0.26	0/396	0.46	0/529
52	D6	0.23	0/396	0.51	0/529
53	B7	0.31	0/399	0.44	0/526
53	D7	0.26	0/399	0.44	0/526
54	B8	0.33	0/486	0.55	0/638
54	D8	0.33	0/486	0.67	0/638
All	All	0.30	2/324157 (0.0%)	0.65	164/485451 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	BH	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	2873	A	N7-C5	-5.99	1.35	1.39
4	AG	12	CYS	CB-SG	5.09	1.90	1.82

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	2311	A	N1-C2-N3	12.09	135.35	129.30
25	DA	2311	A	N1-C6-N6	10.02	124.61	118.60
25	BA	673	C	C2-N3-C4	-10.01	114.89	119.90
26	BB	95	U	C5-C4-O4	9.25	131.45	125.90
25	DA	673	C	C2-N3-C4	-9.13	115.33	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	BH	153	LYS	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32284	0	16296	1132	1
1	CA	32287	0	16295	1151	1
2	AE	1924	0	1975	160	0
2	CE	1924	0	1975	155	0
3	AF	1605	0	1668	115	0
3	CF	1612	0	1677	117	0
4	AG	1703	0	1763	116	0
4	CG	1703	0	1763	116	0
5	AH	1155	0	1213	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CH	1155	0	1213	63	0
6	AI	843	0	857	52	0
6	CI	843	0	857	41	0
7	AJ	1257	0	1296	66	0
7	CJ	1257	0	1296	73	0
8	AK	1116	0	1177	76	0
8	CK	1116	0	1177	48	0
9	AL	1010	0	1037	80	0
9	CL	1010	0	1037	112	0
10	AM	801	0	849	76	0
10	CM	801	0	849	83	0
11	AN	885	0	904	58	0
11	CN	885	0	904	38	0
12	AO	975	0	1062	96	0
12	CO	975	0	1062	66	0
13	AP	928	0	987	76	0
13	CP	933	0	992	81	0
14	AQ	476	0	511	42	0
14	CQ	476	0	511	39	0
15	AR	734	0	771	33	0
15	CR	734	0	771	32	0
16	AS	705	0	725	57	0
16	CS	705	0	725	23	0
17	AT	834	0	904	43	0
17	CT	834	0	904	39	0
18	AU	591	0	662	27	0
18	CU	591	0	662	37	0
19	AV	624	0	636	52	0
19	CV	624	0	636	67	0
20	AW	763	0	861	63	0
20	CW	763	0	861	58	0
21	AX	217	0	234	18	0
21	CX	217	0	234	20	0
22	AB	1814	0	932	112	0
22	AD	1814	0	932	110	0
22	CB	1814	0	932	111	0
22	CD	1814	0	932	99	0
23	AC	1643	0	837	41	0
23	CC	1643	0	837	38	0
24	A1	346	0	174	19	0
24	C1	346	0	174	17	0
25	BA	62707	0	31614	1935	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DA	62607	0	31565	2087	1
26	BB	2617	0	1328	89	0
26	DB	2617	0	1328	108	0
27	BD	2115	0	2195	197	0
27	DD	2115	0	2195	189	0
28	BE	1568	0	1634	146	0
28	DE	1568	0	1634	183	0
29	BF	1585	0	1632	111	0
29	DF	1627	0	1680	162	0
30	BG	1474	0	1535	129	0
30	DG	1474	0	1535	101	0
31	BH	1307	0	1382	147	0
31	DH	1307	0	1382	101	1
32	BK	1136	0	1223	102	0
32	DK	1136	0	1223	79	0
33	BM	1104	0	1180	75	0
33	DM	1104	0	1180	82	0
34	BN	933	0	996	51	0
34	DN	933	0	996	55	0
35	BO	1145	0	1228	176	0
35	DO	1145	0	1228	299	0
36	BP	1122	0	1179	140	0
36	DP	1122	0	1179	166	0
37	B0	968	0	1033	75	0
37	D0	960	0	1021	66	0
38	BQ	882	0	943	84	0
38	DQ	882	0	943	79	0
39	BR	1141	0	1202	98	0
39	DR	1141	0	1202	94	0
40	B1	964	0	1022	74	0
40	D1	964	0	1022	84	0
41	B2	779	0	852	72	0
41	D2	779	0	852	114	0
42	BS	900	0	964	41	0
42	DS	900	0	964	52	0
43	BT	725	0	778	48	0
43	DT	725	0	778	50	0
44	BU	785	0	878	99	0
44	DU	785	0	878	91	0
45	BV	1397	0	1430	138	0
45	DV	1428	0	1454	125	0
46	B3	607	0	628	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	D3	613	0	633	45	0
47	BZ	763	0	848	50	0
47	DZ	763	0	848	48	0
48	BW	558	0	610	38	0
48	DW	558	0	610	43	0
49	BX	469	0	518	21	0
49	DX	469	0	518	24	0
50	B4	533	0	522	128	0
50	D4	515	0	510	71	0
51	B5	459	0	480	92	0
51	D5	459	0	476	39	0
52	B6	389	0	404	80	0
52	D6	389	0	404	51	0
53	B7	391	0	432	17	0
53	D7	391	0	432	25	0
54	B8	480	0	549	116	0
54	D8	480	0	549	81	0
55	A1	1	0	0	0	0
55	AA	220	0	0	0	0
55	AB	4	0	0	0	0
55	AC	8	0	0	0	0
55	AD	3	0	0	0	0
55	AG	2	0	0	0	0
55	AN	1	0	0	0	0
55	AR	1	0	0	0	0
55	AS	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	2	0	0	0	0
55	B2	1	0	0	0	0
55	B3	3	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B7	1	0	0	0	0
55	BA	568	0	0	0	0
55	BB	18	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BW	1	0	0	0	0
55	CA	219	0	0	0	0
55	CB	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CC	9	0	0	0	0
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CK	1	0	0	0	0
55	CR	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	1	0	0	0	0
55	D3	1	0	0	0	0
55	D5	2	0	0	0	0
55	D7	1	0	0	0	0
55	D8	1	0	0	0	0
55	DA	488	0	0	0	0
55	DB	20	0	0	0	0
55	DD	3	0	0	0	0
55	DE	1	0	0	0	0
55	DO	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	299676	0	200977	13379	2

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 27.

The worst 5 of 13379 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
35:DO:46:LYS:HD3	35:DO:51:PHE:CD1	1.38	1.55
54:B8:34:TRP:CB	54:B8:35:GLN:HB2	1.34	1.55
50:B4:37:SER:HB3	50:B4:42:PHE:CD1	1.40	1.52
35:DO:71:VAL:HG13	35:DO:72:PRO:CD	1.44	1.47
35:BO:19:VAL:HG23	35:BO:27:HIS:CB	1.45	1.46

All (2) 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]	1.97	0.23
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	170 (72%)	44 (19%)	21 (9%)	1	5
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	1	3
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	3	20
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	2	11
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	5	26
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	2	8
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	6	31
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	18	62
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	7	34
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	6	32
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	5	26
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	2	14
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	10	45
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	2	8
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	2	8
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	7	34
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	3	18
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	4	23
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	6	31
12	AO	123/132 (93%)	104 (85%)	7 (6%)	12 (10%)	1	4
12	CO	123/132 (93%)	96 (78%)	21 (17%)	6 (5%)	3	20
13	AP	114/126 (90%)	76 (67%)	26 (23%)	12 (10%)	1	3
13	CP	115/126 (91%)	83 (72%)	18 (16%)	14 (12%)	1	2
14	AQ	56/61 (92%)	37 (66%)	7 (12%)	12 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CQ	56/61 (92%)	39 (70%)	9 (16%)	8 (14%)	0	1
15	AR	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	4	21
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	10	43
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	2	14
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	2	14
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	7	34
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	3	16
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	4	23
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	1	3
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	5
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	6
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	1	5
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	5
21	CX	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	2
27	BD	270/276 (98%)	227 (84%)	30 (11%)	13 (5%)	4	20
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	4	22
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	1	3
28	DE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	BF	200/210 (95%)	177 (88%)	14 (7%)	9 (4%)	4	22
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	1	3
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	2	8
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	2	14
31	BH	168/180 (93%)	113 (67%)	20 (12%)	35 (21%)	0	0
31	DH	168/180 (93%)	108 (64%)	36 (21%)	24 (14%)	0	1
32	BK	144/148 (97%)	90 (62%)	39 (27%)	15 (10%)	1	4
32	DK	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	2	9
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	2	14
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	1	4
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	14	54
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BO	148/150 (99%)	99 (67%)	29 (20%)	20 (14%)	0	2
35	DO	148/150 (99%)	92 (62%)	25 (17%)	31 (21%)	0	0
36	BP	139/141 (99%)	102 (73%)	19 (14%)	18 (13%)	0	2
36	DP	139/141 (99%)	92 (66%)	31 (22%)	16 (12%)	1	3
37	B0	116/118 (98%)	97 (84%)	11 (10%)	8 (7%)	2	9
37	D0	115/118 (98%)	95 (83%)	15 (13%)	5 (4%)	4	23
38	BQ	109/112 (97%)	85 (78%)	17 (16%)	7 (6%)	2	11
38	DQ	109/112 (97%)	73 (67%)	26 (24%)	10 (9%)	1	5
39	BR	135/146 (92%)	105 (78%)	21 (16%)	9 (7%)	2	10
39	DR	135/146 (92%)	108 (80%)	18 (13%)	9 (7%)	2	10
40	B1	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	4	23
40	D1	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	3	18
41	B2	99/101 (98%)	81 (82%)	12 (12%)	6 (6%)	2	14
41	D2	99/101 (98%)	68 (69%)	17 (17%)	14 (14%)	0	2
42	BS	111/113 (98%)	92 (83%)	13 (12%)	6 (5%)	3	17
42	DS	111/113 (98%)	92 (83%)	15 (14%)	4 (4%)	5	29
43	BT	90/96 (94%)	81 (90%)	5 (6%)	4 (4%)	4	22
43	DT	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	3	16
44	BU	100/110 (91%)	65 (65%)	21 (21%)	14 (14%)	0	2
44	DU	100/110 (91%)	62 (62%)	19 (19%)	19 (19%)	0	0
45	BV	173/206 (84%)	112 (65%)	32 (18%)	29 (17%)	0	1
45	DV	177/206 (86%)	109 (62%)	39 (22%)	29 (16%)	0	1
46	B3	74/85 (87%)	65 (88%)	6 (8%)	3 (4%)	4	24
46	D3	75/85 (88%)	64 (85%)	8 (11%)	3 (4%)	5	25
47	BZ	95/98 (97%)	79 (83%)	12 (13%)	4 (4%)	4	24
47	DZ	95/98 (97%)	76 (80%)	11 (12%)	8 (8%)	1	6
48	BW	64/72 (89%)	53 (83%)	6 (9%)	5 (8%)	1	7
48	DW	64/72 (89%)	54 (84%)	6 (9%)	4 (6%)	2	12
49	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	13	53
49	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	3	18
50	B4	64/71 (90%)	36 (56%)	12 (19%)	16 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	61/71 (86%)	22 (36%)	22 (36%)	17 (28%)	0	0
51	B5	57/60 (95%)	44 (77%)	6 (10%)	7 (12%)	1	2
51	D5	57/60 (95%)	46 (81%)	8 (14%)	3 (5%)	3	18
52	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
52	D6	43/54 (80%)	26 (60%)	8 (19%)	9 (21%)	0	0
53	B7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	D7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
54	B8	58/65 (89%)	42 (72%)	8 (14%)	8 (14%)	0	2
54	D8	58/65 (89%)	37 (64%)	13 (22%)	8 (14%)	0	2
All	All	11319/12052 (94%)	8735 (77%)	1671 (15%)	913 (8%)	1	7

5 of 913 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	195	ASP
2	AE	236	TYR
2	AE	237	ALA
3	AF	4	LYS
3	AF	12	LEU

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%)	165 (80%)	40 (20%)	2	11
2	CE	205/220 (93%)	180 (88%)	25 (12%)	7	29
3	AF	159/188 (85%)	141 (89%)	18 (11%)	9	33
3	CF	160/188 (85%)	143 (89%)	17 (11%)	10	36
4	AG	180/180 (100%)	160 (89%)	20 (11%)	9	34
4	CG	180/180 (100%)	160 (89%)	20 (11%)	9	34
5	AH	116/123 (94%)	97 (84%)	19 (16%)	3	16
5	CH	116/123 (94%)	102 (88%)	14 (12%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AI	90/90 (100%)	80 (89%)	10 (11%)	9	34
6	CI	90/90 (100%)	81 (90%)	9 (10%)	11	39
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	4	17
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	3	16
8	AK	119/119 (100%)	106 (89%)	13 (11%)	9	35
8	CK	119/119 (100%)	111 (93%)	8 (7%)	23	64
9	AL	98/99 (99%)	86 (88%)	12 (12%)	7	29
9	CL	98/99 (99%)	81 (83%)	17 (17%)	3	14
10	AM	89/92 (97%)	79 (89%)	10 (11%)	9	33
10	CM	89/92 (97%)	78 (88%)	11 (12%)	7	28
11	AN	90/99 (91%)	79 (88%)	11 (12%)	7	29
11	CN	90/99 (91%)	85 (94%)	5 (6%)	30	72
12	AO	104/109 (95%)	95 (91%)	9 (9%)	15	49
12	CO	104/109 (95%)	94 (90%)	10 (10%)	12	43
13	AP	94/101 (93%)	87 (93%)	7 (7%)	20	58
13	CP	94/101 (93%)	83 (88%)	11 (12%)	8	31
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	7	28
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	16	52
15	AR	79/80 (99%)	73 (92%)	6 (8%)	19	57
15	CR	79/80 (99%)	67 (85%)	12 (15%)	4	20
16	AS	72/74 (97%)	68 (94%)	4 (6%)	30	72
16	CS	72/74 (97%)	64 (89%)	8 (11%)	9	34
17	AT	95/97 (98%)	85 (90%)	10 (10%)	10	37
17	CT	95/97 (98%)	92 (97%)	3 (3%)	51	89
18	AU	63/77 (82%)	57 (90%)	6 (10%)	12	44
18	CU	63/77 (82%)	51 (81%)	12 (19%)	2	12
19	AV	67/80 (84%)	55 (82%)	12 (18%)	2	13
19	CV	67/80 (84%)	58 (87%)	9 (13%)	6	24
20	AW	76/82 (93%)	68 (90%)	8 (10%)	10	37
20	CW	76/82 (93%)	66 (87%)	10 (13%)	6	25
21	AX	20/22 (91%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	178 (83%)	36 (17%)	3	15
27	DD	214/218 (98%)	181 (85%)	33 (15%)	4	19
28	BE	165/166 (99%)	135 (82%)	30 (18%)	2	13
28	DE	165/166 (99%)	139 (84%)	26 (16%)	4	18
29	BF	161/166 (97%)	141 (88%)	20 (12%)	7	28
29	DF	165/166 (99%)	140 (85%)	25 (15%)	4	20
30	BG	155/156 (99%)	135 (87%)	20 (13%)	6	26
30	DG	155/156 (99%)	139 (90%)	16 (10%)	10	38
31	BH	142/148 (96%)	122 (86%)	20 (14%)	5	23
31	DH	142/148 (96%)	124 (87%)	18 (13%)	6	27
32	BK	122/124 (98%)	101 (83%)	21 (17%)	3	14
32	DK	122/124 (98%)	106 (87%)	16 (13%)	6	25
33	BM	117/119 (98%)	98 (84%)	19 (16%)	3	17
33	DM	117/119 (98%)	97 (83%)	20 (17%)	3	15
34	BN	100/100 (100%)	92 (92%)	8 (8%)	17	53
34	DN	100/100 (100%)	87 (87%)	13 (13%)	6	26
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	3
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	2
36	BP	111/111 (100%)	94 (85%)	17 (15%)	4	19
36	DP	111/111 (100%)	89 (80%)	22 (20%)	2	11
37	B0	101/101 (100%)	85 (84%)	16 (16%)	4	18
37	D0	100/101 (99%)	82 (82%)	18 (18%)	2	13
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	3	17
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	13	46
39	BR	120/127 (94%)	99 (82%)	21 (18%)	3	14
39	DR	120/127 (94%)	102 (85%)	18 (15%)	4	20
40	B1	93/94 (99%)	85 (91%)	8 (9%)	15	50
40	D1	93/94 (99%)	82 (88%)	11 (12%)	8	30
41	B2	82/82 (100%)	70 (85%)	12 (15%)	5	21
41	D2	82/82 (100%)	69 (84%)	13 (16%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BS	92/92 (100%)	79 (86%)	13 (14%)	5	23
42	DS	92/92 (100%)	76 (83%)	16 (17%)	3	14
43	BT	74/78 (95%)	65 (88%)	9 (12%)	7	29
43	DT	74/78 (95%)	63 (85%)	11 (15%)	4	20
44	BU	85/91 (93%)	72 (85%)	13 (15%)	4	19
44	DU	85/91 (93%)	67 (79%)	18 (21%)	1	8
45	BV	154/179 (86%)	126 (82%)	28 (18%)	2	13
45	DV	158/179 (88%)	138 (87%)	20 (13%)	6	27
46	B3	61/67 (91%)	57 (93%)	4 (7%)	24	64
46	D3	62/67 (92%)	55 (89%)	7 (11%)	9	33
47	BZ	82/83 (99%)	69 (84%)	13 (16%)	4	17
47	DZ	82/83 (99%)	68 (83%)	14 (17%)	3	15
48	BW	62/67 (92%)	51 (82%)	11 (18%)	3	14
48	DW	62/67 (92%)	51 (82%)	11 (18%)	3	14
49	BX	51/52 (98%)	46 (90%)	5 (10%)	12	41
49	DX	51/52 (98%)	48 (94%)	3 (6%)	28	70
50	B4	59/63 (94%)	49 (83%)	10 (17%)	3	15
50	D4	57/63 (90%)	46 (81%)	11 (19%)	2	12
51	B5	51/52 (98%)	42 (82%)	9 (18%)	3	14
51	D5	51/52 (98%)	41 (80%)	10 (20%)	2	11
52	B6	44/52 (85%)	34 (77%)	10 (23%)	1	6
52	D6	44/52 (85%)	40 (91%)	4 (9%)	14	46
53	B7	38/42 (90%)	33 (87%)	5 (13%)	6	25
53	D7	38/42 (90%)	33 (87%)	5 (13%)	6	25
54	B8	50/55 (91%)	37 (74%)	13 (26%)	1	4
54	D8	50/55 (91%)	41 (82%)	9 (18%)	2	13
All	All	9565/9996 (96%)	8229 (86%)	1336 (14%)	5	23

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BZ	26	ARG
5	CH	75	THR

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Mol	Chain	Res	Type
44	DU	64	GLU
48	BW	50	ILE
2	CE	5	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
47	BZ	56	GLN
5	CH	141	GLN
45	DV	75	ASN
49	BX	19	GLN
54	B8	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1501/1506 (99%)	295 (19%)	43 (2%)
1	CA	1501/1506 (99%)	296 (19%)	49 (3%)
22	AB	83/85 (97%)	38 (45%)	8 (9%)
22	AD	83/85 (97%)	26 (31%)	5 (6%)
22	CB	83/85 (97%)	38 (45%)	9 (10%)
22	CD	83/85 (97%)	25 (30%)	4 (4%)
23	AC	76/77 (98%)	11 (14%)	1 (1%)
23	CC	76/77 (98%)	13 (17%)	3 (3%)
24	A1	15/16 (93%)	6 (40%)	2 (13%)
24	C1	15/16 (93%)	6 (40%)	3 (20%)
25	BA	2911/2912 (99%)	542 (18%)	51 (1%)
25	DA	2905/2912 (99%)	569 (19%)	53 (1%)
26	BB	121/122 (99%)	17 (14%)	0
26	DB	121/122 (99%)	27 (22%)	1 (0%)
All	All	9574/9606 (99%)	1909 (19%)	232 (2%)

5 of 1909 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	32	A

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2566	A
1	CA	509	A
25	DA	2211	G
25	BA	2689	U
1	CA	201	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	MIA	AB	38	22	29,31,32	1.68	3 (10%)	41,44,47	1.97	9 (21%)
22	MIA	AD	38	22	29,31,32	1.69	3 (10%)	41,44,47	2.36	9 (21%)
22	MIA	CB	38	22	29,31,32	1.69	3 (10%)	41,44,47	2.12	11 (26%)
22	MIA	CD	38	22	29,31,32	1.71	3 (10%)	41,44,47	2.37	10 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	AB	38	22	-	0/16/33/34	0/3/3/3
22	MIA	AD	38	22	-	1/16/33/34	0/3/3/3
22	MIA	CB	38	22	-	2/16/33/34	0/3/3/3
22	MIA	CD	38	22	-	1/16/33/34	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CB	38	MIA	C6-N6	6.74	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CD	38	MIA	C6-N6	6.45	1.46	1.34
22	AD	38	MIA	C6-N6	6.35	1.45	1.34
22	AB	38	MIA	C6-N6	6.23	1.45	1.34
22	CB	38	MIA	P-OP1	4.47	1.51	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	38	MIA	C11-S10-C2	10.52	109.88	102.23
22	AD	38	MIA	C11-S10-C2	10.02	109.51	102.23
22	CB	38	MIA	C11-S10-C2	7.83	107.92	102.23
22	AB	38	MIA	C11-S10-C2	6.18	106.72	102.23
22	AB	38	MIA	C5-C4-N3	-5.91	119.27	126.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CB	38	MIA	N3-C2-S10-C11
22	CB	38	MIA	N1-C2-S10-C11
22	CD	38	MIA	OP2-P-O5'-C5'
22	AD	38	MIA	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1608 ligands modelled in this entry, 1608 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1502/1506 (99%)	-0.46	4 (0%) 91 48	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.41	11 (0%) 84 28	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.06	1 (0%) 90 41	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.24	3 (1%) 74 19	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.15	1 (0%) 88 36	88, 113, 149, 158	0
3	CF	206/239 (86%)	0.60	5 (2%) 56 11	101, 135, 165, 180	0
4	AG	208/208 (100%)	-0.26	0 100 100	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.04	0 100 100	75, 95, 123, 135	0
5	AH	151/162 (93%)	-0.10	0 100 100	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.04	1 (0%) 84 28	84, 106, 131, 167	0
6	AI	101/101 (100%)	0.13	0 100 100	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.12	0 100 100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.39	6 (3%) 37 7	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.01	3 (1%) 64 13	100, 119, 147, 158	0
8	AK	138/138 (100%)	-0.21	0 100 100	81, 103, 117, 132	0
8	CK	138/138 (100%)	-0.08	0 100 100	81, 109, 125, 136	0
9	AL	127/128 (99%)	0.15	1 (0%) 83 26	83, 138, 159, 166	0
9	CL	127/128 (99%)	-0.03	0 100 100	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.36	4 (4%) 36 7	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.40	3 (3%) 48 9	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.49	3 (2%) 54 11	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.12	1 (0%) 83 26	74, 99, 133, 164	0
12	AO	125/132 (94%)	-0.09	1 (0%) 83 26	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.41	3 (2%) 56 11	63, 91, 126, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.15	1 (0%) 81 24	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.04	2 (1%) 67 15	91, 145, 161, 169	0
14	AQ	58/61 (95%)	-0.13	0 100 100	87, 103, 120, 127	0
14	CQ	58/61 (95%)	0.76	4 (6%) 17 4	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.10	0 100 100	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.05	0 100 100	67, 96, 124, 136	0
16	AS	84/88 (95%)	-0.19	0 100 100	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.21	0 100 100	76, 91, 118, 157	0
17	AT	100/105 (95%)	-0.20	1 (1%) 79 22	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.04	2 (2%) 62 12	75, 100, 126, 144	0
18	AU	72/88 (81%)	0.23	2 (2%) 50 10	77, 97, 135, 164	0
18	CU	72/88 (81%)	0.03	1 (1%) 72 18	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.02	0 100 100	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.20	1 (1%) 74 19	128, 152, 178, 186	0
20	AW	99/106 (93%)	-0.14	0 100 100	97, 121, 148, 153	0
20	CW	99/106 (93%)	0.15	0 100 100	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.20	0 100 100	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.52	1 (4%) 36 7	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.47	8 (9%) 8 2	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.12	8 (9%) 8 2	70, 147, 206, 218	0
22	CB	84/85 (98%)	1.29	25 (29%) 1 0	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.71	0 100 100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.49	0 100 100	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.62	0 100 100	79, 104, 143, 165	0
24	A1	16/16 (100%)	-0.14	0 100 100	66, 97, 168, 177	0
24	C1	16/16 (100%)	-0.14	0 100 100	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.21	33 (1%) 77 21	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.32	43 (1%) 70 16	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.46	1 (0%) 83 26	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.58	2 (1%) 68 16	78, 110, 139, 198	0
27	BD	272/276 (98%)	-0.01	0 100 100	39, 59, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	-0.03	1 (0%) 90 41	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.02	2 (0%) 79 22	44, 77, 125, 150	0
28	DE	205/206 (99%)	-0.02	4 (1%) 62 12	56, 93, 144, 157	0
29	BF	202/210 (96%)	-0.05	1 (0%) 88 36	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.48	12 (5%) 22 5	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.46	6 (3%) 44 8	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.15	3 (1%) 67 15	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.02	1 (0%) 86 32	71, 105, 126, 151	0
31	DH	170/180 (94%)	0.94	27 (15%) 3 1	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.17	0 100 100	72, 120, 141, 153	0
32	DK	146/148 (98%)	-0.15	0 100 100	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.02	0 100 100	58, 79, 115, 136	0
33	DM	138/140 (98%)	-0.00	1 (0%) 84 28	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.07	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	-0.02	0 100 100	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.22	1 (0%) 84 28	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.55	9 (6%) 21 5	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.08	1 (0%) 84 28	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.30	3 (2%) 60 12	58, 100, 130, 154	0
37	B0	118/118 (100%)	-0.04	0 100 100	53, 74, 96, 106	0
37	D0	117/118 (99%)	-0.03	0 100 100	62, 81, 100, 117	0
38	BQ	111/112 (99%)	0.31	3 (2%) 52 10	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.06	1 (0%) 81 24	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.06	2 (1%) 70 16	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.01	1 (0%) 84 28	73, 94, 154, 184	0
40	B1	117/118 (99%)	-0.04	2 (1%) 67 15	50, 70, 98, 140	0
40	D1	117/118 (99%)	0.22	1 (0%) 81 24	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.03	2 (1%) 62 12	46, 91, 116, 128	0
41	D2	101/101 (100%)	0.46	5 (4%) 28 6	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.07	1 (0%) 81 24	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.15	2 (1%) 65 14	61, 75, 109, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.20	0	100	100	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.15	0	100	100	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.32	3 (2%)	49	9	70, 94, 144, 165	0
44	DU	102/110 (92%)	0.94	15 (14%)	3	1	78, 111, 162, 172	0
45	BV	175/206 (84%)	0.73	13 (7%)	14	3	79, 120, 189, 194	0
45	DV	179/206 (86%)	1.02	26 (14%)	3	1	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.05	1 (1%)	74	19	51, 72, 92, 125	0
46	D3	77/85 (90%)	0.04	0	100	100	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.28	5 (5%)	26	6	48, 71, 115, 155	0
47	DZ	97/98 (98%)	0.05	2 (2%)	60	12	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.17	1 (1%)	70	16	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.15	1 (1%)	70	16	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.11	0	100	100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.26	0	100	100	76, 103, 136, 159	0
50	B4	66/71 (92%)	1.38	15 (22%)	1	1	112, 153, 176, 181	0
50	D4	63/71 (88%)	0.95	5 (7%)	13	3	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.21	4 (6%)	17	4	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.50	7 (11%)	5	1	61, 84, 169, 188	0
52	B6	45/54 (83%)	2.99	33 (73%)	0	0	117, 148, 164, 173	0
52	D6	45/54 (83%)	1.63	14 (31%)	1	0	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.01	0	100	100	38, 48, 68, 85	0
53	D7	45/49 (91%)	0.07	0	100	100	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.19	0	100	100	51, 68, 88, 115	0
54	D8	60/65 (92%)	0.36	1 (1%)	67	15	64, 80, 106, 132	0
All	All	21100/21658 (97%)	-0.04	424 (2%)	62	12	38, 95, 177, 247	0

The worst 5 of 424 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	654(J)	A	14.6
25	BA	654(K)	C	13.9
25	DA	654(L)	G	13.2
25	DA	654(K)	C	12.3
29	DF	1	MET	12.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	MIA	CB	38	29/30	0.19	-	63,95,112,126	0
22	MIA	AB	38	29/30	0.19	-	65,78,90,93	0
22	MIA	AD	38	29/30	0.18	-	98,122,141,145	0
22	MIA	CD	38	29/30	0.20	-	101,121,146,154	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3410	1/1	0.23	-	84,84,84,84	0
55	MG	DA	3274	1/1	0.25	-	85,85,85,85	0
55	MG	BA	3366	1/1	0.23	-	91,91,91,91	0
56	ZN	AQ	101	1/1	0.14	-	142,142,142,142	0
55	MG	BA	3312	1/1	-	-	62,62,62,62	1
55	MG	BA	3531	1/1	0.21	-	31,31,31,31	0
55	MG	AA	1717	1/1	0.38	-	73,73,73,73	0
55	MG	CB	103	1/1	1.52	-	147,147,147,147	0
55	MG	BA	3341	1/1	0.36	-	89,89,89,89	0
55	MG	CA	1791	1/1	0.20	-	80,80,80,80	0
55	MG	DA	3056	1/1	0.43	-	52,52,52,52	0
55	MG	AA	1692	1/1	0.24	-	73,73,73,73	0
55	MG	DA	3365	1/1	0.36	-	112,112,112,112	0
55	MG	CA	1616	1/1	0.25	-	87,87,87,87	0
55	MG	DA	3420	1/1	0.18	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1758	1/1	0.23	-	107,107,107,107	0
55	MG	DA	3096	1/1	0.43	-	47,47,47,47	0
55	MG	AA	1621	1/1	0.28	-	102,102,102,102	0
55	MG	DA	3388	1/1	0.20	-	138,138,138,138	0
55	MG	DA	3010	1/1	0.29	-	53,53,53,53	0
55	MG	DA	3242	1/1	0.11	-	81,81,81,81	0
55	MG	D7	101	1/1	0.33	-	86,86,86,86	0
55	MG	BA	3237	1/1	0.34	-	102,102,102,102	0
55	MG	DA	3070	1/1	0.30	-	49,49,49,49	0
55	MG	BA	3495	1/1	0.38	-	75,75,75,75	0
55	MG	BA	3056	1/1	0.27	-	57,57,57,57	0
55	MG	BA	3416	1/1	0.37	-	98,98,98,98	0
55	MG	BA	3250	1/1	0.17	-	90,90,90,90	0
55	MG	CA	1638	1/1	0.29	-	68,68,68,68	0
55	MG	AA	1716	1/1	0.26	-	82,82,82,82	0
55	MG	BA	3095	1/1	0.25	-	79,79,79,79	0
55	MG	AA	1617	1/1	0.36	-	76,76,76,76	0
55	MG	DA	3108	1/1	0.38	-	54,54,54,54	0
55	MG	BA	3157	1/1	0.49	-	50,50,50,50	0
55	MG	BA	3435	1/1	0.47	-	49,49,49,49	0
55	MG	BA	3480	1/1	0.33	-	76,76,76,76	0
55	MG	CA	1725	1/1	0.37	-	86,86,86,86	0
55	MG	AA	1748	1/1	0.30	-	116,116,116,116	0
55	MG	DA	3090	1/1	0.26	-	71,71,71,71	0
55	MG	CA	1647	1/1	0.35	-	96,96,96,96	0
55	MG	DA	3066	1/1	0.28	-	76,76,76,76	0
55	MG	DA	3411	1/1	0.38	-	144,144,144,144	0
55	MG	DA	3395	1/1	0.29	-	87,87,87,87	0
55	MG	DA	3285	1/1	0.36	-	79,79,79,79	0
55	MG	AA	1712	1/1	0.17	-	73,73,73,73	0
55	MG	CA	1634	1/1	0.44	-	58,58,58,58	0
55	MG	DA	3205	1/1	0.21	-	110,110,110,110	0
55	MG	BA	3460	1/1	0.36	-	97,97,97,97	0
55	MG	DA	3051	1/1	0.13	-	87,87,87,87	0
55	MG	DA	3255	1/1	0.14	-	82,82,82,82	0
55	MG	DA	3129	1/1	0.35	-	65,65,65,65	0
55	MG	BB	213	1/1	0.24	-	101,101,101,101	0
55	MG	CA	1718	1/1	0.13	-	64,64,64,64	0
55	MG	AA	1780	1/1	0.20	-	103,103,103,103	0
55	MG	BA	3054	1/1	0.27	-	52,52,52,52	0
55	MG	BA	3215	1/1	0.23	-	44,44,44,44	0
55	MG	DA	3288	1/1	0.09	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	207	1/1	0.33	-	69,69,69,69	0
55	MG	DA	3210	1/1	0.35	-	77,77,77,77	0
55	MG	CA	1779	1/1	0.33	-	109,109,109,109	0
55	MG	DA	3102	1/1	0.31	-	72,72,72,72	0
55	MG	BA	3374	1/1	0.26	-	93,93,93,93	0
55	MG	DA	3031	1/1	0.15	-	70,70,70,70	0
55	MG	AA	1795	1/1	0.35	-	113,113,113,113	0
55	MG	AA	1642	1/1	0.33	-	70,70,70,70	0
55	MG	AA	1718	1/1	0.22	-	82,82,82,82	0
55	MG	DA	3012	1/1	0.32	-	50,50,50,50	0
55	MG	BA	3471	1/1	0.43	-	126,126,126,126	0
55	MG	BA	3514	1/1	0.38	-	113,113,113,113	0
55	MG	DA	3256	1/1	0.24	-	91,91,91,91	0
55	MG	DA	3082	1/1	0.20	-	91,91,91,91	0
55	MG	DA	3207	1/1	0.44	-	83,83,83,83	0
55	MG	DA	3360	1/1	0.14	-	97,97,97,97	0
55	MG	BA	3391	1/1	0.61	-	112,112,112,112	0
55	MG	BA	3061	1/1	0.32	-	73,73,73,73	0
55	MG	BA	3200	1/1	0.29	-	81,81,81,81	0
55	MG	DA	3335	1/1	0.09	-	80,80,80,80	0
55	MG	BA	3145	1/1	0.27	-	54,54,54,54	0
55	MG	CD	101	1/1	0.14	-	145,145,145,145	0
55	MG	BA	3018	1/1	0.38	-	44,44,44,44	0
55	MG	BA	3504	1/1	0.50	-	88,88,88,88	0
55	MG	DA	3405	1/1	0.24	-	135,135,135,135	0
55	MG	BA	3110	1/1	0.28	-	69,69,69,69	0
55	MG	AA	1767	1/1	0.18	-	116,116,116,116	0
55	MG	BA	3371	1/1	0.20	-	83,83,83,83	0
55	MG	BA	3234	1/1	0.23	-	107,107,107,107	0
55	MG	CA	1612	1/1	0.27	-	75,75,75,75	0
55	MG	BA	3150	1/1	0.47	-	49,49,49,49	0
55	MG	AA	1805	1/1	0.74	-	152,152,152,152	0
55	MG	DA	3362	1/1	0.31	-	150,150,150,150	0
55	MG	DA	3306	1/1	0.38	-	96,96,96,96	0
55	MG	CA	1601	1/1	0.26	-	67,67,67,67	0
55	MG	BA	3100	1/1	0.43	-	93,93,93,93	0
55	MG	BA	3369	1/1	0.21	-	92,92,92,92	0
55	MG	DA	3169	1/1	0.28	-	92,92,92,92	0
55	MG	BA	3171	1/1	0.43	-	96,96,96,96	0
55	MG	DA	3467	1/1	0.11	-	103,103,103,103	0
55	MG	BA	3470	1/1	0.47	-	83,83,83,83	0
55	MG	AA	1722	1/1	-	-	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3207	1/1	0.54	-	70,70,70,70	0
55	MG	DA	3029	1/1	0.30	-	82,82,82,82	0
55	MG	BA	3313	1/1	0.22	-	74,74,74,74	0
55	MG	DA	3109	1/1	0.34	-	55,55,55,55	0
55	MG	DA	3261	1/1	0.20	-	78,78,78,78	0
55	MG	DA	3226	1/1	0.29	-	85,85,85,85	0
55	MG	BA	3131	1/1	0.38	-	41,41,41,41	0
55	MG	CA	1735	1/1	0.42	-	119,119,119,119	0
55	MG	BA	3219	1/1	0.28	-	68,68,68,68	0
55	MG	DA	3314	1/1	0.16	-	95,95,95,95	0
55	MG	BA	3073	1/1	0.27	-	65,65,65,65	0
55	MG	DA	3384	1/1	0.39	-	97,97,97,97	0
55	MG	DA	3326	1/1	0.31	-	109,109,109,109	0
55	MG	AA	1685	1/1	0.30	-	85,85,85,85	0
55	MG	CA	1653	1/1	0.29	-	97,97,97,97	0
55	MG	BA	3051	1/1	0.32	-	103,103,103,103	0
55	MG	DA	3296	1/1	0.17	-	93,93,93,93	0
55	MG	DA	3284	1/1	0.24	-	90,90,90,90	0
55	MG	AA	1737	1/1	0.26	-	81,81,81,81	0
55	MG	DA	3050	1/1	0.24	-	90,90,90,90	0
55	MG	AA	1736	1/1	0.79	-	108,108,108,108	0
55	MG	BA	3210	1/1	0.38	-	99,99,99,99	0
55	MG	BA	3121	1/1	0.34	-	72,72,72,72	0
55	MG	DB	220	1/1	0.14	-	121,121,121,121	0
55	MG	CC	107	1/1	0.26	-	123,123,123,123	0
55	MG	BA	3498	1/1	0.24	-	40,40,40,40	0
55	MG	BA	3427	1/1	0.45	-	97,97,97,97	0
55	MG	BA	3173	1/1	0.38	-	58,58,58,58	0
55	MG	BA	3472	1/1	0.59	-	133,133,133,133	0
55	MG	B1	201	1/1	0.27	-	71,71,71,71	0
55	MG	DA	3481	1/1	0.13	-	79,79,79,79	0
55	MG	BA	3356	1/1	0.31	-	60,60,60,60	0
55	MG	AA	1647	1/1	0.31	-	81,81,81,81	0
55	MG	DA	3224	1/1	0.20	-	75,75,75,75	0
55	MG	AA	1652	1/1	0.40	-	72,72,72,72	0
56	ZN	AG	303	1/1	0.35	-	100,100,100,100	0
55	MG	AA	1814	1/1	0.38	-	107,107,107,107	0
55	MG	DA	3445	1/1	0.15	-	118,118,118,118	0
55	MG	DA	3424	1/1	0.26	-	83,83,83,83	0
55	MG	CA	1686	1/1	0.25	-	77,77,77,77	0
55	MG	DA	3194	1/1	0.35	-	104,104,104,104	0
55	MG	DA	3321	1/1	0.17	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1662	1/1	0.20	-	41,41,41,41	0
55	MG	BA	3288	1/1	0.27	-	75,75,75,75	0
55	MG	DB	218	1/1	0.12	-	107,107,107,107	0
55	MG	BA	3024	1/1	0.36	-	44,44,44,44	0
55	MG	BA	3007	1/1	0.28	-	36,36,36,36	0
55	MG	BA	3290	1/1	0.29	-	75,75,75,75	0
55	MG	DA	3060	1/1	0.31	-	67,67,67,67	0
55	MG	BA	3292	1/1	0.27	-	63,63,63,63	0
55	MG	BB	216	1/1	0.41	-	63,63,63,63	0
55	MG	DA	3094	1/1	0.26	-	48,48,48,48	0
55	MG	BA	3074	1/1	0.18	-	91,91,91,91	0
55	MG	BA	3411	1/1	0.28	-	102,102,102,102	0
55	MG	CA	1754	1/1	0.39	-	92,92,92,92	0
55	MG	DA	3230	1/1	0.32	-	74,74,74,74	0
55	MG	CA	1708	1/1	0.17	-	124,124,124,124	0
55	MG	BA	3105	1/1	0.16	-	71,71,71,71	0
55	MG	BA	3390	1/1	0.40	-	98,98,98,98	0
55	MG	DA	3139	1/1	0.27	-	53,53,53,53	0
55	MG	DA	3064	1/1	0.29	-	70,70,70,70	0
55	MG	DA	3465	1/1	0.22	-	112,112,112,112	0
55	MG	BA	3550	1/1	1.25	-	131,131,131,131	0
55	MG	DA	3454	1/1	0.32	-	52,52,52,52	0
55	MG	DA	3063	1/1	0.23	-	45,45,45,45	0
55	MG	DA	3484	1/1	0.21	-	84,84,84,84	0
55	MG	BA	3022	1/1	0.30	-	46,46,46,46	0
55	MG	BA	3098	1/1	0.37	-	88,88,88,88	0
55	MG	AA	1699	1/1	0.16	-	99,99,99,99	0
55	MG	BA	3518	1/1	0.47	-	36,36,36,36	0
55	MG	BA	3176	1/1	0.27	-	78,78,78,78	0
55	MG	DA	3034	1/1	0.30	-	76,76,76,76	0
55	MG	CA	1699	1/1	0.32	-	87,87,87,87	0
55	MG	DA	3039	1/1	0.21	-	101,101,101,101	0
55	MG	DA	3359	1/1	0.12	-	111,111,111,111	0
55	MG	BA	3084	1/1	0.37	-	37,37,37,37	0
55	MG	AA	1693	1/1	0.31	-	72,72,72,72	0
55	MG	BA	3511	1/1	0.17	-	83,83,83,83	0
55	MG	BA	3198	1/1	0.18	-	74,74,74,74	0
55	MG	DA	3004	1/1	0.20	-	39,39,39,39	0
55	MG	BB	215	1/1	0.23	-	91,91,91,91	0
55	MG	DA	3235	1/1	0.33	-	69,69,69,69	0
55	MG	DA	3249	1/1	0.06	-	81,81,81,81	0
55	MG	AA	1616	1/1	0.12	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3127	1/1	0.34	-	73,73,73,73	0
55	MG	BA	3299	1/1	0.24	-	66,66,66,66	0
55	MG	AA	1813	1/1	0.37	-	85,85,85,85	0
55	MG	BB	212	1/1	0.47	-	74,74,74,74	0
55	MG	BA	3418	1/1	0.29	-	82,82,82,82	0
55	MG	AA	1635	1/1	0.16	-	81,81,81,81	0
55	MG	BA	3058	1/1	0.30	-	88,88,88,88	0
55	MG	CA	1766	1/1	0.13	-	114,114,114,114	0
55	MG	DD	303	1/1	0.16	-	69,69,69,69	0
55	MG	CA	1795	1/1	0.39	-	73,73,73,73	0
55	MG	BA	3111	1/1	0.19	-	55,55,55,55	0
55	MG	AA	1641	1/1	0.27	-	56,56,56,56	0
55	MG	BA	3240	1/1	0.27	-	73,73,73,73	0
55	MG	DA	3084	1/1	0.35	-	57,57,57,57	0
55	MG	DA	3244	1/1	0.36	-	80,80,80,80	0
55	MG	DA	3271	1/1	0.22	-	71,71,71,71	0
55	MG	DA	3414	1/1	0.29	-	111,111,111,111	0
55	MG	DA	3277	1/1	0.16	-	78,78,78,78	0
55	MG	BA	3287	1/1	0.28	-	60,60,60,60	0
55	MG	BE	301	1/1	0.11	-	57,57,57,57	0
55	MG	CA	1661	1/1	0.19	-	92,92,92,92	0
55	MG	CA	1810	1/1	0.26	-	101,101,101,101	0
55	MG	DA	3252	1/1	0.18	-	99,99,99,99	0
55	MG	BA	3274	1/1	0.45	-	108,108,108,108	0
55	MG	DA	3347	1/1	0.17	-	91,91,91,91	0
55	MG	DA	3415	1/1	0.36	-	85,85,85,85	0
55	MG	CA	1632	1/1	0.17	-	53,53,53,53	0
55	MG	DA	3250	1/1	0.22	-	62,62,62,62	0
55	MG	BA	3567	1/1	0.24	-	99,99,99,99	0
55	MG	DA	3140	1/1	0.30	-	76,76,76,76	0
55	MG	B5	101	1/1	0.16	-	49,49,49,49	0
55	MG	DA	3446	1/1	0.41	-	166,166,166,166	0
55	MG	DA	3352	1/1	0.25	-	122,122,122,122	0
55	MG	BA	3032	1/1	0.30	-	41,41,41,41	0
55	MG	BA	3265	1/1	0.14	-	89,89,89,89	0
55	MG	DA	3138	1/1	0.34	-	54,54,54,54	0
55	MG	CA	1672	1/1	0.19	-	119,119,119,119	0
55	MG	BA	3117	1/1	0.38	-	52,52,52,52	0
55	MG	DD	302	1/1	0.22	-	82,82,82,82	0
55	MG	DA	3299	1/1	0.18	-	84,84,84,84	0
55	MG	BA	3213	1/1	0.40	-	41,41,41,41	0
55	MG	AC	106	1/1	0.37	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	3196	1/1	0.20	-	45,45,45,45	0
55	MG	CA	1760	1/1	0.23	-	105,105,105,105	0
55	MG	BA	3552	1/1	0.37	-	45,45,45,45	0
55	MG	AA	1761	1/1	0.33	-	77,77,77,77	0
55	MG	AA	1706	1/1	0.20	-	91,91,91,91	0
55	MG	DA	3327	1/1	0.21	-	93,93,93,93	0
55	MG	DA	3100	1/1	0.67	-	116,116,116,116	0
55	MG	DA	3173	1/1	0.23	-	90,90,90,90	0
55	MG	BA	3236	1/1	0.37	-	67,67,67,67	0
55	MG	DA	3219	1/1	0.27	-	128,128,128,128	0
55	MG	DA	3155	1/1	0.15	-	90,90,90,90	0
55	MG	BA	3089	1/1	0.36	-	61,61,61,61	0
55	MG	BA	3260	1/1	0.43	-	65,65,65,65	0
55	MG	AA	1769	1/1	0.17	-	95,95,95,95	0
55	MG	DA	3416	1/1	0.49	-	77,77,77,77	0
55	MG	BA	3208	1/1	0.52	-	55,55,55,55	0
55	MG	CA	1696	1/1	0.17	-	104,104,104,104	0
55	MG	BO	202	1/1	0.20	-	98,98,98,98	0
55	MG	AD	102	1/1	0.23	-	125,125,125,125	0
55	MG	BA	3135	1/1	0.41	-	69,69,69,69	0
55	MG	AA	1806	1/1	0.38	-	85,85,85,85	0
55	MG	CA	1698	1/1	0.20	-	79,79,79,79	0
55	MG	BA	3038	1/1	0.20	-	33,33,33,33	0
55	MG	DB	216	1/1	0.15	-	100,100,100,100	0
55	MG	BB	208	1/1	0.33	-	117,117,117,117	0
55	MG	BA	3494	1/1	0.31	-	76,76,76,76	0
55	MG	BA	3218	1/1	0.24	-	64,64,64,64	0
55	MG	BA	3194	1/1	0.27	-	74,74,74,74	0
55	MG	BA	3065	1/1	0.32	-	82,82,82,82	0
55	MG	BA	3311	1/1	0.38	-	68,68,68,68	0
55	MG	CA	1817	1/1	0.36	-	106,106,106,106	0
55	MG	BA	3508	1/1	0.32	-	77,77,77,77	0
55	MG	DA	3022	1/1	0.26	-	74,74,74,74	0
55	MG	BA	3273	1/1	0.35	-	73,73,73,73	0
55	MG	DA	3212	1/1	0.29	-	121,121,121,121	0
55	MG	DA	3231	1/1	0.26	-	101,101,101,101	0
55	MG	BA	3443	1/1	0.17	-	125,125,125,125	0
55	MG	AA	1749	1/1	0.35	-	110,110,110,110	0
55	MG	DA	3474	1/1	0.29	-	60,60,60,60	0
55	MG	DA	3047	1/1	0.35	-	67,67,67,67	0
55	MG	DA	3260	1/1	0.36	-	73,73,73,73	0
55	MG	BA	3262	1/1	0.41	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3375	1/1	0.14	-	86,86,86,86	0
55	MG	CA	1802	1/1	0.27	-	73,73,73,73	0
55	MG	DA	3220	1/1	0.28	-	64,64,64,64	0
55	MG	DA	3398	1/1	0.32	-	101,101,101,101	0
55	MG	DB	211	1/1	0.23	-	111,111,111,111	0
55	MG	BA	3123	1/1	0.36	-	81,81,81,81	0
55	MG	BA	3457	1/1	0.16	-	85,85,85,85	0
55	MG	DA	3391	1/1	0.31	-	102,102,102,102	0
55	MG	BB	201	1/1	0.29	-	97,97,97,97	0
55	MG	DA	3025	1/1	0.14	-	70,70,70,70	0
55	MG	BA	3019	1/1	0.29	-	45,45,45,45	0
55	MG	CA	1767	1/1	0.18	-	87,87,87,87	0
55	MG	AA	1628	1/1	0.47	-	77,77,77,77	0
55	MG	DA	3027	1/1	0.12	-	47,47,47,47	0
55	MG	DA	3217	1/1	0.15	-	125,125,125,125	0
55	MG	DA	3005	1/1	0.28	-	48,48,48,48	0
55	MG	BA	3033	1/1	0.32	-	77,77,77,77	0
55	MG	DA	3132	1/1	0.18	-	77,77,77,77	0
55	MG	DA	3202	1/1	0.35	-	67,67,67,67	0
55	MG	BA	3041	1/1	0.49	-	80,80,80,80	0
55	MG	DA	3086	1/1	0.46	-	75,75,75,75	0
55	MG	BA	3070	1/1	0.28	-	68,68,68,68	0
55	MG	BA	3452	1/1	0.35	-	103,103,103,103	0
55	MG	DA	3041	1/1	0.40	-	47,47,47,47	0
55	MG	BA	3381	1/1	0.53	-	87,87,87,87	0
55	MG	DA	3413	1/1	0.38	-	86,86,86,86	0
55	MG	DA	3172	1/1	0.40	-	122,122,122,122	0
55	MG	BA	3128	1/1	0.22	-	71,71,71,71	0
55	MG	BA	3254	1/1	0.46	-	89,89,89,89	0
55	MG	AA	1709	1/1	0.20	-	56,56,56,56	0
55	MG	BA	3308	1/1	0.15	-	63,63,63,63	0
55	MG	CA	1668	1/1	0.44	-	72,72,72,72	0
55	MG	DA	3309	1/1	0.48	-	116,116,116,116	0
55	MG	BA	3195	1/1	0.61	-	97,97,97,97	0
55	MG	B6	101	1/1	0.34	-	102,102,102,102	0
55	MG	AA	1738	1/1	0.27	-	91,91,91,91	0
55	MG	CA	1792	1/1	0.17	-	104,104,104,104	0
55	MG	AA	1764	1/1	0.33	-	146,146,146,146	0
55	MG	DA	3429	1/1	0.31	-	54,54,54,54	0
55	MG	BA	3087	1/1	0.33	-	38,38,38,38	0
55	MG	BA	3486	1/1	0.27	-	42,42,42,42	0
55	MG	BA	3253	1/1	0.48	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1770	1/1	0.36	-	82,82,82,82	0
55	MG	CA	1741	1/1	0.18	-	85,85,85,85	0
55	MG	DA	3336	1/1	0.39	-	115,115,115,115	0
55	MG	CC	104	1/1	0.17	-	98,98,98,98	0
55	MG	DA	3437	1/1	0.18	-	66,66,66,66	0
55	MG	BA	3468	1/1	0.39	-	78,78,78,78	0
55	MG	AA	1797	1/1	0.25	-	79,79,79,79	0
55	MG	BA	3133	1/1	0.26	-	42,42,42,42	0
55	MG	BA	3064	1/1	0.32	-	87,87,87,87	0
55	MG	AA	1701	1/1	0.57	-	87,87,87,87	0
55	MG	BA	3485	1/1	0.26	-	98,98,98,98	0
55	MG	DA	3036	1/1	0.20	-	100,100,100,100	0
55	MG	CA	1640	1/1	0.31	-	89,89,89,89	0
55	MG	DA	3158	1/1	0.38	-	80,80,80,80	0
55	MG	DA	3272	1/1	0.43	-	68,68,68,68	0
55	MG	BA	3168	1/1	0.34	-	47,47,47,47	0
55	MG	DA	3061	1/1	0.34	-	53,53,53,53	0
55	MG	DA	3303	1/1	0.22	-	76,76,76,76	0
55	MG	DA	3206	1/1	0.27	-	109,109,109,109	0
55	MG	DA	3311	1/1	0.29	-	109,109,109,109	0
55	MG	CA	1720	1/1	0.34	-	68,68,68,68	0
55	MG	CA	1688	1/1	0.26	-	95,95,95,95	0
55	MG	BA	3318	1/1	0.40	-	102,102,102,102	0
55	MG	BA	3560	1/1	0.38	-	69,69,69,69	0
55	MG	DA	3234	1/1	0.45	-	73,73,73,73	0
55	MG	DA	3267	1/1	0.46	-	80,80,80,80	0
55	MG	AA	1648	1/1	0.36	-	115,115,115,115	0
55	MG	DA	3456	1/1	0.29	-	57,57,57,57	0
55	MG	BA	3010	1/1	0.38	-	45,45,45,45	0
55	MG	BA	3401	1/1	0.28	-	86,86,86,86	0
55	MG	DA	3053	1/1	0.29	-	72,72,72,72	0
55	MG	BA	3330	1/1	0.26	-	61,61,61,61	0
55	MG	AA	1601	1/1	0.31	-	60,60,60,60	0
55	MG	DA	3184	1/1	0.31	-	78,78,78,78	0
55	MG	AA	1804	1/1	0.45	-	113,113,113,113	0
55	MG	CA	1636	1/1	0.29	-	53,53,53,53	0
55	MG	AA	1739	1/1	0.35	-	82,82,82,82	0
55	MG	BA	3519	1/1	0.35	-	24,24,24,24	0
55	MG	BA	3050	1/1	0.32	-	65,65,65,65	0
55	MG	BA	3466	1/1	0.60	-	92,92,92,92	0
55	MG	AA	1688	1/1	0.14	-	93,93,93,93	0
55	MG	BA	3338	1/1	0.34	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3005	1/1	0.37	-	40,40,40,40	0
55	MG	DA	3044	1/1	0.34	-	66,66,66,66	0
55	MG	CA	1664	1/1	0.30	-	64,64,64,64	0
55	MG	DA	3018	1/1	0.24	-	46,46,46,46	0
55	MG	BA	3367	1/1	0.54	-	72,72,72,72	0
55	MG	DA	3265	1/1	0.37	-	76,76,76,76	0
55	MG	BA	3268	1/1	0.26	-	90,90,90,90	0
55	MG	BA	3561	1/1	0.32	-	84,84,84,84	0
55	MG	CA	1777	1/1	0.16	-	112,112,112,112	0
55	MG	BA	3180	1/1	0.23	-	91,91,91,91	0
55	MG	CA	1723	1/1	0.16	-	90,90,90,90	0
55	MG	BA	3439	1/1	0.44	-	115,115,115,115	0
55	MG	BA	3289	1/1	0.40	-	95,95,95,95	0
55	MG	BA	3163	1/1	0.33	-	86,86,86,86	0
55	MG	BA	3209	1/1	0.45	-	78,78,78,78	0
55	MG	DA	3097	1/1	0.34	-	53,53,53,53	0
55	MG	DA	3200	1/1	0.35	-	55,55,55,55	0
55	MG	CA	1775	1/1	0.46	-	69,69,69,69	0
55	MG	DA	3450	1/1	0.31	-	54,54,54,54	0
55	MG	BA	3386	1/1	0.39	-	115,115,115,115	0
55	MG	AC	102	1/1	0.38	-	106,106,106,106	0
55	MG	BA	3175	1/1	0.32	-	62,62,62,62	0
55	MG	BA	3307	1/1	0.51	-	79,79,79,79	0
55	MG	BA	3075	1/1	0.41	-	75,75,75,75	0
55	MG	BA	3529	1/1	0.46	-	42,42,42,42	0
55	MG	BA	3103	1/1	0.51	-	76,76,76,76	0
55	MG	AA	1711	1/1	0.15	-	97,97,97,97	0
55	MG	CC	103	1/1	0.22	-	114,114,114,114	0
55	MG	AA	1713	1/1	0.39	-	98,98,98,98	0
55	MG	CA	1633	1/1	0.36	-	61,61,61,61	0
55	MG	DA	3478	1/1	0.13	-	89,89,89,89	0
55	MG	BA	3406	1/1	1.15	-	182,182,182,182	0
55	MG	DA	3170	1/1	0.39	-	59,59,59,59	0
55	MG	DA	3443	1/1	0.21	-	94,94,94,94	0
55	MG	BA	3322	1/1	0.37	-	81,81,81,81	0
55	MG	DA	3353	1/1	0.26	-	102,102,102,102	0
55	MG	AA	1683	1/1	0.43	-	87,87,87,87	0
55	MG	CA	1625	1/1	0.25	-	104,104,104,104	0
55	MG	DA	3351	1/1	0.21	-	151,151,151,151	0
55	MG	DA	3257	1/1	0.41	-	77,77,77,77	0
55	MG	BA	3421	1/1	0.92	-	97,97,97,97	0
55	MG	BA	3337	1/1	0.44	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1752	1/1	0.35	-	67,67,67,67	0
55	MG	AA	1606	1/1	0.06	-	77,77,77,77	0
55	MG	BA	3497	1/1	0.25	-	30,30,30,30	0
55	MG	CA	1658	1/1	0.30	-	90,90,90,90	0
55	MG	AD	103	1/1	0.22	-	89,89,89,89	0
55	MG	BA	3197	1/1	0.41	-	57,57,57,57	0
55	MG	CA	1665	1/1	0.31	-	70,70,70,70	0
55	MG	DA	3204	1/1	0.13	-	48,48,48,48	0
55	MG	DA	3033	1/1	0.27	-	83,83,83,83	0
55	MG	BA	3304	1/1	0.34	-	80,80,80,80	0
55	MG	BA	3125	1/1	0.33	-	107,107,107,107	0
55	MG	BA	3146	1/1	0.33	-	62,62,62,62	0
55	MG	DA	3147	1/1	0.19	-	87,87,87,87	0
55	MG	AA	1759	1/1	0.20	-	66,66,66,66	0
55	MG	DA	3163	1/1	0.34	-	75,75,75,75	0
55	MG	BA	3006	1/1	0.40	-	58,58,58,58	0
55	MG	AA	1638	1/1	0.34	-	105,105,105,105	0
55	MG	DA	3120	1/1	0.40	-	73,73,73,73	0
55	MG	DA	3323	1/1	0.88	-	104,104,104,104	0
55	MG	CA	1666	1/1	0.15	-	90,90,90,90	0
55	MG	DA	3068	1/1	0.28	-	54,54,54,54	0
55	MG	DA	3185	1/1	0.17	-	78,78,78,78	0
55	MG	DA	3122	1/1	0.41	-	69,69,69,69	0
55	MG	CA	1604	1/1	0.19	-	60,60,60,60	0
55	MG	DA	3457	1/1	0.27	-	48,48,48,48	0
55	MG	CA	1769	1/1	0.30	-	67,67,67,67	0
55	MG	DA	3374	1/1	0.21	-	92,92,92,92	0
55	MG	BA	3245	1/1	0.46	-	107,107,107,107	0
55	MG	AA	1675	1/1	0.18	-	81,81,81,81	0
55	MG	CA	1627	1/1	0.19	-	140,140,140,140	0
55	MG	AA	1708	1/1	0.18	-	77,77,77,77	0
55	MG	DA	3081	1/1	0.29	-	84,84,84,84	0
55	MG	BA	3011	1/1	0.38	-	40,40,40,40	0
55	MG	DA	3190	1/1	0.31	-	66,66,66,66	0
55	MG	AA	1655	1/1	0.40	-	78,78,78,78	0
55	MG	CA	1737	1/1	0.24	-	122,122,122,122	0
55	MG	DA	3422	1/1	0.20	-	75,75,75,75	0
55	MG	BA	3004	1/1	0.35	-	36,36,36,36	0
55	MG	D8	101	1/1	0.16	-	88,88,88,88	0
55	MG	DA	3464	1/1	0.29	-	90,90,90,90	0
55	MG	CA	1655	1/1	0.12	-	85,85,85,85	0
55	MG	DA	3110	1/1	0.15	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3164	1/1	0.37	-	47,47,47,47	0
55	MG	BA	3563	1/1	0.21	-	100,100,100,100	0
55	MG	AA	1819	1/1	0.34	-	126,126,126,126	0
55	MG	AA	1719	1/1	0.22	-	80,80,80,80	0
55	MG	BA	3144	1/1	0.40	-	39,39,39,39	0
55	MG	AA	1755	1/1	0.30	-	88,88,88,88	0
55	MG	CA	1764	1/1	0.24	-	117,117,117,117	0
55	MG	AA	1742	1/1	0.25	-	88,88,88,88	0
55	MG	DA	3245	1/1	0.18	-	91,91,91,91	0
55	MG	BA	3325	1/1	0.21	-	81,81,81,81	0
55	MG	AA	1793	1/1	0.17	-	87,87,87,87	0
55	MG	CA	1660	1/1	0.12	-	85,85,85,85	0
55	MG	DA	3049	1/1	0.40	-	55,55,55,55	0
55	MG	AA	1730	1/1	0.17	-	113,113,113,113	0
55	MG	DA	3011	1/1	0.33	-	50,50,50,50	0
55	MG	DA	3009	1/1	0.34	-	53,53,53,53	0
55	MG	BA	3166	1/1	0.22	-	28,28,28,28	0
55	MG	DA	3278	1/1	0.23	-	100,100,100,100	0
55	MG	DA	3071	1/1	0.38	-	57,57,57,57	0
55	MG	AC	108	1/1	0.13	-	82,82,82,82	0
55	MG	DA	3193	1/1	0.47	-	48,48,48,48	0
55	MG	AA	1654	1/1	0.25	-	77,77,77,77	0
55	MG	CA	1782	1/1	0.11	-	113,113,113,113	0
55	MG	BA	3151	1/1	0.55	-	97,97,97,97	0
55	MG	BA	3062	1/1	0.35	-	79,79,79,79	0
55	MG	CA	1784	1/1	0.10	-	92,92,92,92	0
55	MG	BA	3423	1/1	0.49	-	90,90,90,90	0
55	MG	CA	1734	1/1	0.12	-	80,80,80,80	0
55	MG	CA	1717	1/1	0.39	-	73,73,73,73	0
55	MG	DA	3197	1/1	0.26	-	48,48,48,48	0
55	MG	DA	3466	1/1	0.12	-	81,81,81,81	0
55	MG	AA	1785	1/1	2.37	-	125,125,125,125	0
55	MG	B0	201	1/1	0.31	-	46,46,46,46	0
55	MG	DA	3431	1/1	0.22	-	69,69,69,69	0
55	MG	BA	3188	1/1	0.34	-	64,64,64,64	0
55	MG	DA	3030	1/1	0.21	-	85,85,85,85	0
55	MG	AA	1687	1/1	0.28	-	108,108,108,108	0
55	MG	BA	3261	1/1	0.47	-	57,57,57,57	0
55	MG	AA	1672	1/1	0.51	-	67,67,67,67	0
55	MG	BA	3012	1/1	0.36	-	45,45,45,45	0
55	MG	BF	301	1/1	0.13	-	79,79,79,79	0
55	MG	BA	3080	1/1	0.26	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3072	1/1	0.34	-	67,67,67,67	0
55	MG	DA	3112	1/1	0.32	-	63,63,63,63	0
55	MG	AA	1697	1/1	0.36	-	101,101,101,101	0
55	MG	BA	3149	1/1	0.35	-	41,41,41,41	0
55	MG	DA	3273	1/1	0.14	-	77,77,77,77	0
55	MG	BA	3048	1/1	0.26	-	60,60,60,60	0
55	MG	AA	1766	1/1	0.32	-	98,98,98,98	0
55	MG	BA	3251	1/1	0.43	-	80,80,80,80	0
55	MG	DA	3067	1/1	0.17	-	50,50,50,50	0
55	MG	BA	3437	1/1	0.33	-	97,97,97,97	0
55	MG	DA	3182	1/1	0.24	-	47,47,47,47	0
55	MG	BA	3124	1/1	0.34	-	66,66,66,66	0
55	MG	BA	3067	1/1	0.25	-	79,79,79,79	0
55	MG	BA	3143	1/1	0.17	-	43,43,43,43	0
55	MG	CA	1809	1/1	0.35	-	93,93,93,93	0
55	MG	BA	3161	1/1	0.45	-	45,45,45,45	0
55	MG	DA	3042	1/1	0.36	-	51,51,51,51	0
55	MG	AA	1645	1/1	0.14	-	65,65,65,65	0
55	MG	CC	108	1/1	0.22	-	95,95,95,95	0
56	ZN	CQ	101	1/1	0.17	-	118,118,118,118	0
55	MG	BA	3244	1/1	0.16	-	34,34,34,34	0
55	MG	CA	1622	1/1	0.78	-	110,110,110,110	0
55	MG	B3	101	1/1	0.43	-	81,81,81,81	0
55	MG	AA	1607	1/1	0.17	-	86,86,86,86	0
55	MG	BA	3227	1/1	0.43	-	64,64,64,64	0
55	MG	DA	3134	1/1	0.25	-	93,93,93,93	0
55	MG	BA	3526	1/1	0.36	-	41,41,41,41	0
55	MG	AA	1791	1/1	0.45	-	90,90,90,90	0
55	MG	BA	3052	1/1	0.23	-	66,66,66,66	0
55	MG	DA	3149	1/1	0.25	-	93,93,93,93	0
55	MG	BB	204	1/1	0.33	-	91,91,91,91	0
55	MG	BA	3388	1/1	0.35	-	76,76,76,76	0
55	MG	CA	1748	1/1	0.31	-	76,76,76,76	0
55	MG	BA	3324	1/1	0.43	-	105,105,105,105	0
55	MG	BA	3119	1/1	0.41	-	61,61,61,61	0
55	MG	BA	3284	1/1	0.42	-	75,75,75,75	0
55	MG	CA	1749	1/1	0.37	-	117,117,117,117	0
55	MG	BA	3266	1/1	0.40	-	71,71,71,71	0
55	MG	DA	3014	1/1	0.36	-	76,76,76,76	0
55	MG	DA	3287	1/1	0.39	-	120,120,120,120	0
55	MG	DA	3076	1/1	0.29	-	107,107,107,107	0
55	MG	DA	3026	1/1	0.30	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3080	1/1	0.29	-	73,73,73,73	0
55	MG	DA	3074	1/1	0.37	-	65,65,65,65	0
55	MG	BA	3481	1/1	0.24	-	97,97,97,97	0
55	MG	DA	3345	1/1	0.23	-	85,85,85,85	0
55	MG	BE	303	1/1	0.27	-	105,105,105,105	0
55	MG	BA	3568	1/1	0.21	-	106,106,106,106	0
55	MG	DA	3160	1/1	0.34	-	59,59,59,59	0
55	MG	DA	3329	1/1	0.26	-	71,71,71,71	0
55	MG	BA	3229	1/1	0.39	-	65,65,65,65	0
55	MG	BA	3488	1/1	0.32	-	137,137,137,137	0
55	MG	BA	3139	1/1	0.46	-	43,43,43,43	0
55	MG	BA	3130	1/1	0.41	-	50,50,50,50	0
55	MG	BA	3478	1/1	0.31	-	61,61,61,61	0
55	MG	DA	3144	1/1	0.49	-	66,66,66,66	0
55	MG	BB	217	1/1	0.32	-	104,104,104,104	0
55	MG	DB	204	1/1	0.34	-	94,94,94,94	0
55	MG	DA	3433	1/1	0.35	-	50,50,50,50	0
55	MG	AA	1613	1/1	0.47	-	116,116,116,116	0
55	MG	BA	3362	1/1	0.21	-	84,84,84,84	0
55	MG	BA	3055	1/1	0.32	-	78,78,78,78	0
55	MG	BA	3060	1/1	0.18	-	51,51,51,51	0
55	MG	DA	3298	1/1	0.29	-	80,80,80,80	0
55	MG	CA	1755	1/1	0.34	-	104,104,104,104	0
55	MG	DA	3363	1/1	0.21	-	78,78,78,78	0
55	MG	DA	3228	1/1	0.59	-	103,103,103,103	0
55	MG	CA	1729	1/1	0.41	-	102,102,102,102	0
55	MG	BA	3402	1/1	0.26	-	76,76,76,76	0
55	MG	AA	1702	1/1	0.34	-	89,89,89,89	0
55	MG	DA	3376	1/1	0.38	-	107,107,107,107	0
55	MG	BA	3316	1/1	0.37	-	87,87,87,87	0
55	MG	DA	3297	1/1	0.42	-	82,82,82,82	0
55	MG	DA	3412	1/1	0.32	-	92,92,92,92	0
55	MG	DA	3401	1/1	0.13	-	75,75,75,75	0
55	MG	AB	103	1/1	0.31	-	104,104,104,104	0
55	MG	AA	1784	1/1	0.23	-	112,112,112,112	0
55	MG	CA	1631	1/1	0.27	-	65,65,65,65	0
55	MG	BA	3461	1/1	0.30	-	98,98,98,98	0
55	MG	DA	3062	1/1	0.16	-	39,39,39,39	0
55	MG	BA	3112	1/1	0.47	-	73,73,73,73	0
55	MG	DB	215	1/1	0.29	-	129,129,129,129	0
55	MG	DA	3482	1/1	0.38	-	83,83,83,83	0
55	MG	BA	3459	1/1	0.35	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3366	1/1	0.34	-	105,105,105,105	0
55	MG	DA	3183	1/1	0.28	-	75,75,75,75	0
55	MG	BA	3378	1/1	0.32	-	140,140,140,140	0
55	MG	CA	1745	1/1	0.20	-	159,159,159,159	0
55	MG	DA	3075	1/1	0.31	-	57,57,57,57	0
55	MG	BA	3178	1/1	0.33	-	96,96,96,96	0
55	MG	DA	3364	1/1	0.13	-	93,93,93,93	0
55	MG	DA	3020	1/1	0.21	-	45,45,45,45	0
55	MG	DA	3302	1/1	0.32	-	69,69,69,69	0
55	MG	BA	3049	1/1	0.23	-	75,75,75,75	0
55	MG	DA	3382	1/1	0.41	-	121,121,121,121	0
55	MG	DA	3331	1/1	0.27	-	91,91,91,91	0
55	MG	BA	3447	1/1	0.41	-	72,72,72,72	0
55	MG	CA	1620	1/1	0.15	-	64,64,64,64	0
55	MG	DA	3282	1/1	0.29	-	64,64,64,64	0
55	MG	AA	1627	1/1	0.32	-	62,62,62,62	0
55	MG	CA	1781	1/1	0.26	-	172,172,172,172	0
55	MG	BA	3114	1/1	0.21	-	37,37,37,37	0
55	MG	BA	3474	1/1	0.34	-	72,72,72,72	0
55	MG	DA	3426	1/1	0.34	-	103,103,103,103	0
55	MG	BA	3523	1/1	0.41	-	36,36,36,36	0
55	MG	BA	3484	1/1	0.34	-	87,87,87,87	0
55	MG	DA	3024	1/1	0.33	-	104,104,104,104	0
55	MG	CA	1712	1/1	0.43	-	76,76,76,76	0
55	MG	BB	207	1/1	0.20	-	109,109,109,109	0
55	MG	BA	3104	1/1	0.32	-	82,82,82,82	0
55	MG	CA	1768	1/1	0.46	-	138,138,138,138	0
55	MG	DA	3371	1/1	0.20	-	122,122,122,122	0
55	MG	BA	3414	1/1	0.35	-	100,100,100,100	0
55	MG	CA	1650	1/1	0.19	-	78,78,78,78	0
55	MG	DA	3045	1/1	0.42	-	71,71,71,71	0
55	MG	DA	3334	1/1	0.30	-	87,87,87,87	0
55	MG	BA	3499	1/1	0.45	-	38,38,38,38	0
55	MG	BA	3405	1/1	0.18	-	82,82,82,82	0
55	MG	BA	3093	1/1	0.33	-	57,57,57,57	0
55	MG	DA	3400	1/1	0.13	-	115,115,115,115	0
55	MG	AA	1698	1/1	0.47	-	76,76,76,76	0
55	MG	BA	3445	1/1	0.26	-	82,82,82,82	0
55	MG	DA	3372	1/1	0.61	-	125,125,125,125	0
55	MG	BA	3167	1/1	0.38	-	45,45,45,45	0
55	MG	BA	3490	1/1	0.35	-	36,36,36,36	0
55	MG	BA	3231	1/1	0.34	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3277	1/1	0.31	-	79,79,79,79	0
55	MG	BA	3109	1/1	0.34	-	81,81,81,81	0
55	MG	BA	3257	1/1	0.25	-	87,87,87,87	0
55	MG	BA	3270	1/1	0.34	-	96,96,96,96	0
55	MG	AA	1728	1/1	0.47	-	99,99,99,99	0
55	MG	BA	3238	1/1	0.31	-	75,75,75,75	0
55	MG	CA	1714	1/1	0.25	-	87,87,87,87	0
55	MG	BA	3017	1/1	0.41	-	58,58,58,58	0
55	MG	CA	1700	1/1	0.30	-	96,96,96,96	0
55	MG	DA	3310	1/1	0.26	-	105,105,105,105	0
55	MG	BA	3122	1/1	0.51	-	106,106,106,106	0
55	MG	BA	3368	1/1	0.31	-	59,59,59,59	0
55	MG	AA	1744	1/1	0.37	-	79,79,79,79	0
55	MG	CA	1728	1/1	0.43	-	58,58,58,58	0
55	MG	BA	3221	1/1	0.36	-	59,59,59,59	0
55	MG	DA	3385	1/1	0.10	-	86,86,86,86	0
55	MG	DA	3103	1/1	0.35	-	60,60,60,60	0
55	MG	DA	3369	1/1	0.36	-	108,108,108,108	0
55	MG	CB	102	1/1	0.18	-	102,102,102,102	0
55	MG	BA	3044	1/1	0.27	-	68,68,68,68	0
55	MG	DA	3236	1/1	0.36	-	62,62,62,62	0
55	MG	DA	3192	1/1	0.17	-	90,90,90,90	0
55	MG	DA	3354	1/1	0.20	-	83,83,83,83	0
55	MG	CA	1624	1/1	0.17	-	93,93,93,93	0
55	MG	CA	1630	1/1	0.16	-	149,149,149,149	0
55	MG	DA	3128	1/1	0.28	-	47,47,47,47	0
55	MG	DA	3017	1/1	0.20	-	90,90,90,90	0
55	MG	DA	3065	1/1	0.36	-	75,75,75,75	0
55	MG	AA	1703	1/1	0.31	-	106,106,106,106	0
55	MG	BA	3404	1/1	0.39	-	100,100,100,100	0
55	MG	AA	1624	1/1	0.17	-	94,94,94,94	0
55	MG	AA	1794	1/1	0.47	-	112,112,112,112	0
55	MG	DA	3392	1/1	0.21	-	126,126,126,126	0
55	MG	BA	3281	1/1	0.25	-	78,78,78,78	0
55	MG	BA	3389	1/1	0.27	-	56,56,56,56	0
55	MG	DA	3239	1/1	0.29	-	92,92,92,92	0
55	MG	BA	3053	1/1	0.12	-	106,106,106,106	0
55	MG	AA	1792	1/1	0.26	-	97,97,97,97	0
55	MG	BA	3272	1/1	0.23	-	59,59,59,59	0
55	MG	CA	1772	1/1	0.15	-	107,107,107,107	0
55	MG	BA	3372	1/1	0.46	-	76,76,76,76	0
55	MG	BA	3027	1/1	0.24	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3032	1/1	0.31	-	77,77,77,77	0
55	MG	BA	3396	1/1	0.57	-	87,87,87,87	0
55	MG	CA	1615	1/1	0.29	-	106,106,106,106	0
55	MG	AA	1817	1/1	0.17	-	61,61,61,61	0
55	MG	DA	3123	1/1	0.42	-	50,50,50,50	0
55	MG	CA	1617	1/1	0.38	-	83,83,83,83	0
55	MG	CA	1701	1/1	1.49	-	108,108,108,108	0
55	MG	CG	302	1/1	0.11	-	89,89,89,89	0
55	MG	BA	3487	1/1	0.49	-	100,100,100,100	0
55	MG	BA	3506	1/1	0.22	-	73,73,73,73	0
55	MG	BA	3294	1/1	0.33	-	61,61,61,61	0
55	MG	DA	3348	1/1	0.18	-	56,56,56,56	0
55	MG	BA	3557	1/1	0.32	-	94,94,94,94	0
55	MG	AR	101	1/1	0.17	-	114,114,114,114	0
55	MG	BA	3263	1/1	0.47	-	80,80,80,80	0
55	MG	BA	3329	1/1	0.61	-	67,67,67,67	0
55	MG	BA	3385	1/1	0.18	-	86,86,86,86	0
55	MG	BA	3156	1/1	0.34	-	61,61,61,61	0
55	MG	DA	3338	1/1	0.28	-	69,69,69,69	0
55	MG	BA	3383	1/1	0.22	-	94,94,94,94	0
55	MG	BA	3363	1/1	0.36	-	57,57,57,57	0
55	MG	DA	3367	1/1	0.37	-	82,82,82,82	0
55	MG	BA	3102	1/1	0.25	-	68,68,68,68	0
55	MG	BA	3298	1/1	0.39	-	66,66,66,66	0
55	MG	BA	3185	1/1	0.16	-	46,46,46,46	0
55	MG	BA	3426	1/1	0.42	-	86,86,86,86	0
55	MG	AA	1816	1/1	0.24	-	95,95,95,95	0
55	MG	DA	3390	1/1	0.20	-	92,92,92,92	0
55	MG	BW	101	1/1	0.18	-	64,64,64,64	0
55	MG	AA	1772	1/1	0.53	-	131,131,131,131	0
55	MG	DA	3154	1/1	0.21	-	77,77,77,77	0
55	MG	CC	106	1/1	0.34	-	94,94,94,94	0
55	MG	CA	1736	1/1	0.95	-	143,143,143,143	0
55	MG	BA	3351	1/1	0.26	-	88,88,88,88	0
55	MG	BA	3556	1/1	0.20	-	98,98,98,98	0
55	MG	AA	1665	1/1	0.16	-	52,52,52,52	0
55	MG	BA	3500	1/1	0.47	-	64,64,64,64	0
55	MG	B3	102	1/1	0.51	-	107,107,107,107	0
55	MG	BA	3420	1/1	0.22	-	114,114,114,114	0
55	MG	CA	1602	1/1	0.33	-	64,64,64,64	0
55	MG	BA	3217	1/1	0.34	-	40,40,40,40	0
55	MG	DA	3145	1/1	0.28	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3417	1/1	0.58	-	86,86,86,86	0
55	MG	BA	3489	1/1	0.40	-	95,95,95,95	0
55	MG	CA	1681	1/1	0.37	-	89,89,89,89	0
55	MG	BA	3256	1/1	0.44	-	80,80,80,80	0
55	MG	CA	1685	1/1	0.36	-	91,91,91,91	0
55	MG	CA	1808	1/1	0.50	-	153,153,153,153	0
55	MG	BA	3535	1/1	0.32	-	82,82,82,82	0
55	MG	DA	3180	1/1	0.26	-	48,48,48,48	0
55	MG	BA	3275	1/1	0.36	-	60,60,60,60	0
55	MG	CA	1785	1/1	0.38	-	155,155,155,155	0
55	MG	BA	3170	1/1	0.30	-	54,54,54,54	0
55	MG	AA	1762	1/1	0.21	-	121,121,121,121	0
55	MG	BA	3493	1/1	0.33	-	51,51,51,51	0
55	MG	DA	3472	1/1	0.23	-	53,53,53,53	0
55	MG	BA	3398	1/1	0.19	-	57,57,57,57	0
55	MG	DA	3237	1/1	0.28	-	79,79,79,79	0
55	MG	DA	3319	1/1	0.21	-	95,95,95,95	0
55	MG	BA	3088	1/1	0.44	-	57,57,57,57	0
55	MG	BA	3002	1/1	0.37	-	40,40,40,40	0
55	MG	BA	3492	1/1	0.39	-	54,54,54,54	0
55	MG	DA	3439	1/1	0.41	-	107,107,107,107	0
55	MG	BA	3357	1/1	0.39	-	78,78,78,78	0
55	MG	DA	3046	1/1	0.06	-	100,100,100,100	0
55	MG	CA	1752	1/1	0.43	-	80,80,80,80	0
55	MG	DA	3083	1/1	0.08	-	65,65,65,65	0
55	MG	CA	1773	1/1	0.55	-	139,139,139,139	0
55	MG	DA	3117	1/1	0.24	-	61,61,61,61	0
55	MG	AA	1668	1/1	0.40	-	68,68,68,68	0
55	MG	DA	3175	1/1	0.36	-	60,60,60,60	0
55	MG	CA	1656	1/1	0.33	-	72,72,72,72	0
55	MG	DB	217	1/1	0.32	-	97,97,97,97	0
55	MG	AA	1733	1/1	0.33	-	101,101,101,101	0
55	MG	DA	3203	1/1	0.30	-	74,74,74,74	0
55	MG	BF	302	1/1	0.62	-	88,88,88,88	0
55	MG	BA	3412	1/1	0.33	-	89,89,89,89	0
55	MG	CA	1747	1/1	0.33	-	109,109,109,109	0
55	MG	D3	101	1/1	0.11	-	91,91,91,91	0
55	MG	DA	3078	1/1	0.37	-	76,76,76,76	0
55	MG	BA	3565	1/1	0.38	-	105,105,105,105	0
55	MG	AA	1637	1/1	0.24	-	112,112,112,112	0
55	MG	BA	3444	1/1	0.20	-	87,87,87,87	0
55	MG	BA	3148	1/1	0.14	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1703	1/1	0.44	-	72,72,72,72	0
55	MG	BA	3029	1/1	0.23	-	57,57,57,57	0
55	MG	DA	3043	1/1	0.28	-	69,69,69,69	0
55	MG	B1	202	1/1	0.35	-	86,86,86,86	0
55	MG	BD	301	1/1	0.22	-	80,80,80,80	0
55	MG	DA	3453	1/1	0.41	-	65,65,65,65	0
55	MG	BA	3538	1/1	0.23	-	79,79,79,79	0
55	MG	BA	3129	1/1	0.41	-	50,50,50,50	0
55	MG	CA	1618	1/1	0.20	-	95,95,95,95	0
55	MG	BA	3365	1/1	0.23	-	81,81,81,81	0
55	MG	AA	1640	1/1	0.34	-	71,71,71,71	0
55	MG	DA	3153	1/1	0.08	-	88,88,88,88	0
55	MG	DA	3448	1/1	0.20	-	129,129,129,129	0
55	MG	DA	3341	1/1	0.34	-	56,56,56,56	0
55	MG	DA	3028	1/1	0.30	-	73,73,73,73	0
55	MG	BA	3077	1/1	0.20	-	83,83,83,83	0
55	MG	AA	1810	1/1	0.31	-	148,148,148,148	0
55	MG	BA	3532	1/1	0.39	-	54,54,54,54	0
55	MG	CA	1690	1/1	0.16	-	90,90,90,90	0
55	MG	BA	3162	1/1	0.27	-	67,67,67,67	0
55	MG	CA	1794	1/1	0.10	-	67,67,67,67	0
55	MG	AA	1609	1/1	0.36	-	88,88,88,88	0
55	MG	DA	3104	1/1	0.35	-	62,62,62,62	0
55	MG	DA	3318	1/1	0.28	-	77,77,77,77	0
55	MG	BA	3453	1/1	0.21	-	75,75,75,75	0
55	MG	BA	3155	1/1	1.17	-	114,114,114,114	0
55	MG	DA	3151	1/1	0.33	-	78,78,78,78	0
55	MG	DA	3214	1/1	0.31	-	76,76,76,76	0
55	MG	DA	3253	1/1	0.25	-	77,77,77,77	0
55	MG	BA	3327	1/1	0.30	-	69,69,69,69	0
55	MG	CA	1641	1/1	0.15	-	64,64,64,64	0
55	MG	BA	3243	1/1	0.27	-	79,79,79,79	0
55	MG	DB	205	1/1	0.35	-	73,73,73,73	0
55	MG	BA	3483	1/1	0.37	-	120,120,120,120	0
55	MG	AA	1779	1/1	0.28	-	119,119,119,119	0
55	MG	DA	3475	1/1	0.25	-	62,62,62,62	0
55	MG	DA	3003	1/1	0.23	-	58,58,58,58	0
55	MG	AA	1740	1/1	0.44	-	76,76,76,76	0
55	MG	DA	3087	1/1	0.26	-	85,85,85,85	0
55	MG	CA	1746	1/1	0.33	-	87,87,87,87	0
55	MG	DA	3333	1/1	0.38	-	95,95,95,95	0
55	MG	AA	1801	1/1	0.18	-	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3090	1/1	0.24	-	40,40,40,40	0
55	MG	DB	210	1/1	0.75	-	128,128,128,128	0
55	MG	AA	1679	1/1	0.44	-	83,83,83,83	0
55	MG	DA	3218	1/1	0.28	-	86,86,86,86	0
55	MG	CA	1649	1/1	0.41	-	77,77,77,77	0
55	MG	BA	3220	1/1	0.25	-	70,70,70,70	0
55	MG	BA	3352	1/1	0.41	-	75,75,75,75	0
55	MG	AB	104	1/1	0.45	-	97,97,97,97	0
55	MG	CA	1762	1/1	0.40	-	108,108,108,108	0
55	MG	CA	1635	1/1	0.29	-	72,72,72,72	0
55	MG	DA	3105	1/1	0.31	-	37,37,37,37	0
55	MG	BA	3527	1/1	0.10	-	40,40,40,40	0
55	MG	CA	1730	1/1	0.14	-	79,79,79,79	0
55	MG	CA	1765	1/1	0.23	-	115,115,115,115	0
55	MG	BA	3339	1/1	0.34	-	74,74,74,74	0
55	MG	CA	1818	1/1	0.41	-	81,81,81,81	0
55	MG	DA	3164	1/1	0.25	-	67,67,67,67	0
55	MG	CA	1796	1/1	0.23	-	146,146,146,146	0
55	MG	CA	1687	1/1	0.28	-	99,99,99,99	0
55	MG	DA	3259	1/1	0.30	-	92,92,92,92	0
55	MG	DA	3095	1/1	0.30	-	89,89,89,89	0
55	MG	DA	3308	1/1	0.32	-	99,99,99,99	0
55	MG	DA	3243	1/1	0.22	-	97,97,97,97	0
55	MG	BA	3346	1/1	0.50	-	69,69,69,69	0
55	MG	AA	1659	1/1	0.38	-	46,46,46,46	0
55	MG	DB	208	1/1	0.20	-	99,99,99,99	0
55	MG	BA	3211	1/1	0.35	-	55,55,55,55	0
55	MG	DA	3488	1/1	0.20	-	100,100,100,100	0
55	MG	AA	1745	1/1	0.23	-	83,83,83,83	0
55	MG	DA	3339	1/1	0.38	-	104,104,104,104	0
55	MG	BA	3246	1/1	0.19	-	89,89,89,89	0
55	MG	AA	1815	1/1	0.43	-	114,114,114,114	0
55	MG	CA	1771	1/1	0.21	-	117,117,117,117	0
55	MG	BA	3543	1/1	0.36	-	101,101,101,101	0
55	MG	BA	3045	1/1	0.38	-	105,105,105,105	0
55	MG	DA	3143	1/1	0.33	-	74,74,74,74	0
55	MG	DA	3485	1/1	0.34	-	84,84,84,84	0
55	MG	BA	3373	1/1	0.47	-	92,92,92,92	0
55	MG	BA	3047	1/1	0.19	-	46,46,46,46	0
55	MG	CA	1691	1/1	0.20	-	90,90,90,90	0
55	MG	AA	1809	1/1	0.53	-	204,204,204,204	0
55	MG	CA	1646	1/1	0.24	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3332	1/1	0.15	-	84,84,84,84	0
55	MG	DB	202	1/1	0.14	-	91,91,91,91	0
55	MG	DA	3021	1/1	0.21	-	77,77,77,77	0
55	MG	BA	3037	1/1	0.38	-	105,105,105,105	0
55	MG	BA	3295	1/1	0.19	-	92,92,92,92	0
55	MG	DA	3001	1/1	0.28	-	46,46,46,46	0
55	MG	DA	3179	1/1	0.35	-	88,88,88,88	0
55	MG	AA	1778	1/1	0.16	-	143,143,143,143	0
55	MG	BA	3505	1/1	0.23	-	61,61,61,61	0
55	MG	BA	3456	1/1	0.45	-	168,168,168,168	0
55	MG	DA	3227	1/1	2.12	-	118,118,118,118	0
55	MG	BA	3142	1/1	0.12	-	49,49,49,49	0
55	MG	DA	3435	1/1	0.18	-	51,51,51,51	0
55	MG	BA	3057	1/1	0.20	-	46,46,46,46	0
55	MG	DB	219	1/1	0.14	-	94,94,94,94	0
55	MG	CA	1731	1/1	0.35	-	97,97,97,97	0
55	MG	BA	3039	1/1	0.28	-	55,55,55,55	0
55	MG	DA	3276	1/1	0.13	-	81,81,81,81	0
55	MG	CA	1740	1/1	0.48	-	122,122,122,122	0
55	MG	DA	3215	1/1	0.29	-	83,83,83,83	0
55	MG	BA	3137	1/1	0.34	-	88,88,88,88	0
55	MG	DA	3136	1/1	0.39	-	73,73,73,73	0
55	MG	AA	1799	1/1	0.18	-	101,101,101,101	0
55	MG	DA	3107	1/1	0.34	-	55,55,55,55	0
55	MG	CA	1793	1/1	0.21	-	110,110,110,110	0
55	MG	BA	3440	1/1	0.52	-	96,96,96,96	0
55	MG	BA	3108	1/1	0.38	-	58,58,58,58	0
55	MG	BB	211	1/1	0.22	-	109,109,109,109	0
55	MG	BA	3152	1/1	0.42	-	58,58,58,58	0
55	MG	B3	103	1/1	0.32	-	83,83,83,83	0
55	MG	DA	3430	1/1	0.41	-	52,52,52,52	0
55	MG	BE	302	1/1	0.40	-	40,40,40,40	0
55	MG	D5	102	1/1	0.32	-	104,104,104,104	0
55	MG	BA	3305	1/1	0.53	-	94,94,94,94	0
55	MG	DB	209	1/1	0.30	-	130,130,130,130	0
55	MG	BA	3136	1/1	0.16	-	53,53,53,53	0
55	MG	DA	3115	1/1	0.44	-	64,64,64,64	0
55	MG	AA	1673	1/1	0.29	-	75,75,75,75	0
55	MG	BA	3477	1/1	0.56	-	77,77,77,77	0
55	MG	BA	3264	1/1	0.42	-	61,61,61,61	0
55	MG	AA	1729	1/1	0.28	-	84,84,84,84	0
55	MG	BB	205	1/1	0.29	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3399	1/1	0.54	-	117,117,117,117	0
55	MG	BA	3343	1/1	0.37	-	114,114,114,114	0
55	MG	DA	3208	1/1	0.30	-	91,91,91,91	0
55	MG	DA	3135	1/1	0.16	-	87,87,87,87	0
55	MG	AA	1734	1/1	0.43	-	93,93,93,93	0
55	MG	BA	3138	1/1	0.48	-	86,86,86,86	0
55	MG	DA	3057	1/1	0.32	-	56,56,56,56	0
55	MG	BA	3364	1/1	0.29	-	72,72,72,72	0
55	MG	DB	212	1/1	0.36	-	120,120,120,120	0
55	MG	DA	3425	1/1	0.44	-	88,88,88,88	0
55	MG	CC	102	1/1	0.25	-	85,85,85,85	0
55	MG	DA	3409	1/1	0.52	-	124,124,124,124	0
55	MG	DA	3479	1/1	0.16	-	97,97,97,97	0
55	MG	BA	3310	1/1	0.30	-	76,76,76,76	0
55	MG	DA	3317	1/1	0.31	-	58,58,58,58	0
55	MG	AA	1623	1/1	0.33	-	63,63,63,63	0
55	MG	BA	3393	1/1	0.36	-	118,118,118,118	0
55	MG	BA	3242	1/1	0.27	-	116,116,116,116	0
55	MG	BA	3541	1/1	0.21	-	66,66,66,66	0
55	MG	BA	3233	1/1	0.36	-	66,66,66,66	0
55	MG	CA	1608	1/1	0.20	-	74,74,74,74	0
55	MG	B7	101	1/1	0.29	-	72,72,72,72	0
55	MG	BA	3554	1/1	0.26	-	48,48,48,48	0
55	MG	DA	3418	1/1	0.18	-	85,85,85,85	0
55	MG	CA	1679	1/1	0.21	-	80,80,80,80	0
55	MG	DA	3216	1/1	0.36	-	90,90,90,90	0
55	MG	BA	3191	1/1	0.52	-	89,89,89,89	0
55	MG	DA	3447	1/1	0.23	-	92,92,92,92	0
55	MG	D0	201	1/1	0.21	-	63,63,63,63	0
55	MG	CA	1671	1/1	0.20	-	100,100,100,100	0
55	MG	DA	3055	1/1	0.39	-	52,52,52,52	0
55	MG	CA	1788	1/1	0.23	-	132,132,132,132	0
55	MG	DA	3355	1/1	0.39	-	83,83,83,83	0
55	MG	AA	1727	1/1	0.20	-	95,95,95,95	0
55	MG	DA	3002	1/1	0.36	-	48,48,48,48	0
55	MG	CB	101	1/1	0.20	-	106,106,106,106	0
55	MG	BA	3078	1/1	0.54	-	101,101,101,101	0
55	MG	BA	3379	1/1	0.44	-	78,78,78,78	0
55	MG	CA	1637	1/1	0.11	-	70,70,70,70	0
55	MG	DA	3209	1/1	0.34	-	96,96,96,96	0
55	MG	AA	1649	1/1	0.21	-	95,95,95,95	0
55	MG	BA	3107	1/1	0.17	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AG	301	1/1	0.25	-	98,98,98,98	0
55	MG	BA	3286	1/1	0.49	-	46,46,46,46	0
55	MG	AA	1710	1/1	0.21	-	56,56,56,56	0
55	MG	BA	3354	1/1	0.45	-	73,73,73,73	0
55	MG	CA	1719	1/1	0.24	-	91,91,91,91	0
55	MG	BA	3205	1/1	0.20	-	59,59,59,59	0
55	MG	DA	3380	1/1	0.18	-	80,80,80,80	0
55	MG	BA	3501	1/1	0.32	-	86,86,86,86	0
55	MG	BA	3259	1/1	0.24	-	109,109,109,109	0
55	MG	AA	1812	1/1	0.46	-	69,69,69,69	0
55	MG	DB	203	1/1	0.09	-	111,111,111,111	0
55	MG	DA	3427	1/1	0.28	-	56,56,56,56	0
55	MG	CA	1800	1/1	0.28	-	99,99,99,99	0
55	MG	AB	101	1/1	0.15	-	92,92,92,92	0
55	MG	BA	3083	1/1	0.50	-	47,47,47,47	0
55	MG	CC	109	1/1	0.28	-	114,114,114,114	0
55	MG	DA	3150	1/1	0.54	-	77,77,77,77	0
55	MG	BA	3126	1/1	0.64	-	95,95,95,95	0
55	MG	BA	3545	1/1	0.17	-	82,82,82,82	0
55	MG	BA	3282	1/1	0.43	-	103,103,103,103	0
55	MG	BA	3432	1/1	0.23	-	106,106,106,106	0
55	MG	DA	3126	1/1	0.17	-	63,63,63,63	0
55	MG	DA	3268	1/1	0.21	-	77,77,77,77	0
55	MG	BA	3302	1/1	0.22	-	83,83,83,83	0
55	MG	BA	3534	1/1	0.25	-	69,69,69,69	0
55	MG	DA	3404	1/1	0.23	-	119,119,119,119	0
55	MG	BA	3184	1/1	0.43	-	46,46,46,46	0
55	MG	BA	3429	1/1	0.61	-	146,146,146,146	0
55	MG	BA	3300	1/1	0.42	-	80,80,80,80	0
55	MG	BA	3015	1/1	0.38	-	35,35,35,35	0
55	MG	BA	3387	1/1	0.16	-	88,88,88,88	0
55	MG	AA	1790	1/1	0.24	-	79,79,79,79	0
55	MG	DA	3241	1/1	0.32	-	75,75,75,75	0
55	MG	BA	3403	1/1	0.35	-	71,71,71,71	0
55	MG	BA	3455	1/1	0.64	-	89,89,89,89	0
55	MG	BA	3512	1/1	0.29	-	90,90,90,90	0
55	MG	BA	3496	1/1	0.27	-	45,45,45,45	0
55	MG	CA	1815	1/1	0.23	-	95,95,95,95	0
55	MG	BA	3120	1/1	0.38	-	42,42,42,42	0
55	MG	DA	3281	1/1	0.24	-	90,90,90,90	0
55	MG	DA	3048	1/1	0.36	-	76,76,76,76	0
55	MG	BA	3276	1/1	0.19	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3521	1/1	0.23	-	45,45,45,45	0
55	MG	AA	1605	1/1	0.24	-	75,75,75,75	0
55	MG	BA	3562	1/1	0.38	-	91,91,91,91	0
55	MG	BA	3408	1/1	0.15	-	82,82,82,82	0
55	MG	BA	3419	1/1	0.51	-	80,80,80,80	0
55	MG	BA	3247	1/1	0.30	-	97,97,97,97	0
55	MG	BA	3422	1/1	0.74	-	110,110,110,110	0
55	MG	AA	1770	1/1	0.23	-	80,80,80,80	0
55	MG	BA	3267	1/1	0.33	-	62,62,62,62	0
55	MG	BA	3333	1/1	0.47	-	80,80,80,80	0
55	MG	BA	3127	1/1	0.36	-	73,73,73,73	0
55	MG	CA	1694	1/1	0.16	-	80,80,80,80	0
55	MG	DA	3387	1/1	0.28	-	102,102,102,102	0
55	MG	DA	3166	1/1	0.23	-	90,90,90,90	0
55	MG	CA	1702	1/1	0.28	-	106,106,106,106	0
55	MG	CA	1657	1/1	0.34	-	68,68,68,68	0
55	MG	CA	1673	1/1	0.65	-	136,136,136,136	0
55	MG	DA	3394	1/1	0.30	-	101,101,101,101	0
55	MG	AA	1747	1/1	0.18	-	98,98,98,98	0
55	MG	DB	214	1/1	0.11	-	95,95,95,95	0
55	MG	BB	202	1/1	0.25	-	74,74,74,74	0
55	MG	CA	1799	1/1	0.17	-	81,81,81,81	0
55	MG	CA	1813	1/1	0.24	-	108,108,108,108	0
55	MG	BA	3553	1/1	0.27	-	49,49,49,49	0
55	MG	CA	1732	1/1	0.41	-	105,105,105,105	0
55	MG	AA	1633	1/1	0.37	-	102,102,102,102	0
55	MG	CA	1662	1/1	0.41	-	84,84,84,84	0
55	MG	BA	3301	1/1	0.23	-	84,84,84,84	0
55	MG	AS	101	1/1	0.21	-	96,96,96,96	0
55	MG	DA	3305	1/1	0.14	-	93,93,93,93	0
55	MG	AA	1602	1/1	0.25	-	71,71,71,71	0
55	MG	DA	3141	1/1	0.28	-	101,101,101,101	0
55	MG	BA	3424	1/1	0.46	-	84,84,84,84	0
55	MG	BA	3076	1/1	0.38	-	81,81,81,81	0
55	MG	BA	3186	1/1	0.29	-	45,45,45,45	0
55	MG	BA	3165	1/1	0.28	-	60,60,60,60	0
55	MG	CA	1707	1/1	0.35	-	109,109,109,109	0
55	MG	DA	3167	1/1	0.18	-	95,95,95,95	0
55	MG	DA	3148	1/1	0.10	-	111,111,111,111	0
55	MG	BA	3451	1/1	0.48	-	101,101,101,101	0
55	MG	CA	1805	1/1	0.18	-	102,102,102,102	0
55	MG	BA	3434	1/1	0.40	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1750	1/1	0.25	-	86,86,86,86	0
55	MG	DA	3468	1/1	0.13	-	101,101,101,101	0
55	MG	CA	1659	1/1	0.38	-	75,75,75,75	0
55	MG	DA	3052	1/1	0.17	-	78,78,78,78	0
55	MG	DA	3142	1/1	0.33	-	81,81,81,81	0
55	MG	BA	3458	1/1	0.35	-	91,91,91,91	0
55	MG	CA	1684	1/1	0.25	-	101,101,101,101	0
55	MG	BA	3334	1/1	0.26	-	67,67,67,67	0
55	MG	CC	101	1/1	0.31	-	77,77,77,77	0
55	MG	DA	3286	1/1	0.30	-	78,78,78,78	0
55	MG	BA	3433	1/1	0.35	-	99,99,99,99	0
55	MG	CA	1607	1/1	0.15	-	70,70,70,70	0
55	MG	BA	3441	1/1	0.27	-	84,84,84,84	0
55	MG	DA	3451	1/1	0.23	-	92,92,92,92	0
55	MG	BA	3159	1/1	0.37	-	57,57,57,57	0
55	MG	BA	3353	1/1	0.45	-	77,77,77,77	0
55	MG	AA	1604	1/1	0.35	-	52,52,52,52	0
55	MG	DA	3221	1/1	1.39	-	154,154,154,154	0
55	MG	BA	3361	1/1	0.21	-	70,70,70,70	0
55	MG	CA	1693	1/1	0.22	-	103,103,103,103	0
55	MG	AA	1760	1/1	0.36	-	77,77,77,77	0
55	MG	CA	1651	1/1	0.35	-	77,77,77,77	0
55	MG	DA	3188	1/1	0.28	-	113,113,113,113	0
55	MG	BA	3189	1/1	0.62	-	108,108,108,108	0
55	MG	CA	1626	1/1	0.34	-	69,69,69,69	0
55	MG	DA	3035	1/1	0.33	-	124,124,124,124	0
55	MG	CA	1621	1/1	0.17	-	97,97,97,97	0
55	MG	AC	107	1/1	0.42	-	124,124,124,124	0
55	MG	BA	3026	1/1	0.30	-	43,43,43,43	0
55	MG	CA	1709	1/1	0.36	-	110,110,110,110	0
55	MG	BA	3559	1/1	0.23	-	86,86,86,86	0
55	MG	DA	3449	1/1	0.26	-	66,66,66,66	0
55	MG	DA	3054	1/1	0.57	-	108,108,108,108	0
55	MG	DA	3213	1/1	0.19	-	103,103,103,103	0
55	MG	DA	3291	1/1	0.33	-	149,149,149,149	0
55	MG	DA	3092	1/1	0.16	-	87,87,87,87	0
55	MG	AA	1660	1/1	0.41	-	77,77,77,77	0
55	MG	BA	3332	1/1	0.39	-	76,76,76,76	0
55	MG	AA	1700	1/1	0.14	-	136,136,136,136	0
55	MG	AA	1691	1/1	0.30	-	88,88,88,88	0
55	MG	BA	3335	1/1	0.32	-	102,102,102,102	0
55	MG	DA	3059	1/1	0.30	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3072	1/1	0.38	-	65,65,65,65	0
55	MG	BA	3042	1/1	0.39	-	75,75,75,75	0
55	MG	CK	201	1/1	1.33	-	124,124,124,124	0
55	MG	AA	1746	1/1	0.30	-	93,93,93,93	0
55	MG	CA	1726	1/1	0.10	-	73,73,73,73	0
55	MG	CA	1812	1/1	0.50	-	176,176,176,176	0
55	MG	BA	3183	1/1	0.44	-	84,84,84,84	0
55	MG	CA	1819	1/1	0.49	-	134,134,134,134	0
55	MG	DA	3432	1/1	0.27	-	64,64,64,64	0
55	MG	DA	3269	1/1	0.29	-	78,78,78,78	0
55	MG	AA	1782	1/1	0.12	-	118,118,118,118	0
55	MG	AA	1680	1/1	0.46	-	97,97,97,97	0
55	MG	DA	3342	1/1	0.77	-	122,122,122,122	0
55	MG	AA	1682	1/1	0.22	-	93,93,93,93	0
55	MG	DA	3471	1/1	0.21	-	60,60,60,60	0
55	MG	DA	3290	1/1	0.15	-	99,99,99,99	0
55	MG	DA	3077	1/1	0.41	-	72,72,72,72	0
55	MG	BA	3081	1/1	0.46	-	91,91,91,91	0
55	MG	DA	3452	1/1	0.28	-	52,52,52,52	0
55	MG	CA	1780	1/1	0.19	-	88,88,88,88	0
55	MG	CA	1751	1/1	0.26	-	90,90,90,90	0
55	MG	DD	301	1/1	0.37	-	51,51,51,51	0
55	MG	CC	105	1/1	0.14	-	94,94,94,94	0
55	MG	BA	3446	1/1	0.44	-	121,121,121,121	0
55	MG	DA	3356	1/1	0.37	-	76,76,76,76	0
55	MG	AA	1674	1/1	0.31	-	56,56,56,56	0
55	MG	BA	3431	1/1	0.18	-	66,66,66,66	0
55	MG	DA	3487	1/1	0.21	-	85,85,85,85	0
55	MG	CA	1753	1/1	0.31	-	103,103,103,103	0
55	MG	DA	3159	1/1	0.30	-	68,68,68,68	0
55	MG	BA	3513	1/1	0.31	-	92,92,92,92	0
55	MG	B2	201	1/1	0.40	-	91,91,91,91	0
55	MG	BA	3467	1/1	0.24	-	69,69,69,69	0
55	MG	BA	3533	1/1	0.35	-	91,91,91,91	0
55	MG	DA	3006	1/1	0.30	-	50,50,50,50	0
55	MG	AA	1667	1/1	0.53	-	78,78,78,78	0
55	MG	AA	1753	1/1	0.27	-	97,97,97,97	0
55	MG	BA	3465	1/1	0.49	-	61,61,61,61	0
55	MG	AA	1789	1/1	0.32	-	63,63,63,63	0
55	MG	DA	3337	1/1	0.31	-	86,86,86,86	0
55	MG	BA	3448	1/1	0.23	-	104,104,104,104	0
55	MG	BA	3222	1/1	0.46	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3240	1/1	0.20	-	55,55,55,55	0
55	MG	CA	1614	1/1	0.28	-	79,79,79,79	0
55	MG	CA	1678	1/1	0.50	-	83,83,83,83	0
55	MG	DA	3137	1/1	0.21	-	53,53,53,53	0
55	MG	DA	3247	1/1	0.32	-	58,58,58,58	0
55	MG	BA	3153	1/1	0.48	-	78,78,78,78	0
55	MG	AA	1818	1/1	0.48	-	124,124,124,124	0
55	MG	DA	3270	1/1	0.34	-	76,76,76,76	0
55	MG	DA	3013	1/1	0.25	-	51,51,51,51	0
55	MG	DA	3279	1/1	0.56	-	135,135,135,135	0
55	MG	BA	3086	1/1	0.29	-	56,56,56,56	0
55	MG	BA	3348	1/1	0.21	-	96,96,96,96	0
55	MG	BA	3345	1/1	0.26	-	46,46,46,46	0
55	MG	AA	1614	1/1	0.30	-	92,92,92,92	0
55	MG	AA	1610	1/1	0.33	-	58,58,58,58	0
55	MG	DA	3223	1/1	0.15	-	81,81,81,81	0
55	MG	AA	1650	1/1	0.28	-	80,80,80,80	0
55	MG	CA	1744	1/1	0.26	-	73,73,73,73	0
55	MG	BA	3239	1/1	0.17	-	69,69,69,69	0
55	MG	BA	3392	1/1	0.34	-	78,78,78,78	0
55	MG	DA	3098	1/1	0.29	-	48,48,48,48	0
55	MG	DA	3114	1/1	0.39	-	91,91,91,91	0
55	MG	CA	1692	1/1	0.10	-	157,157,157,157	0
55	MG	BA	3328	1/1	0.21	-	52,52,52,52	0
55	MG	BA	3115	1/1	0.42	-	41,41,41,41	0
55	MG	BA	3179	1/1	0.38	-	72,72,72,72	0
55	MG	DA	3460	1/1	0.27	-	116,116,116,116	0
55	MG	AA	1808	1/1	0.33	-	88,88,88,88	0
55	MG	CA	1654	1/1	0.25	-	78,78,78,78	0
55	MG	BA	3525	1/1	0.33	-	51,51,51,51	0
55	MG	DA	3328	1/1	0.27	-	84,84,84,84	0
55	MG	BA	3028	1/1	0.32	-	52,52,52,52	0
55	MG	BA	3350	1/1	0.44	-	92,92,92,92	0
55	MG	CA	1680	1/1	0.19	-	99,99,99,99	0
55	MG	AA	1626	1/1	0.27	-	91,91,91,91	0
55	MG	DA	3121	1/1	0.19	-	104,104,104,104	0
55	MG	CA	1774	1/1	0.18	-	75,75,75,75	0
55	MG	BA	3192	1/1	0.45	-	92,92,92,92	0
55	MG	BA	3172	1/1	0.42	-	74,74,74,74	0
55	MG	BA	3154	1/1	0.49	-	87,87,87,87	0
55	MG	AA	1631	1/1	0.23	-	84,84,84,84	0
55	MG	DA	3469	1/1	0.28	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3101	1/1	0.30	-	76,76,76,76	0
55	MG	DA	3289	1/1	0.38	-	62,62,62,62	0
55	MG	BA	3204	1/1	0.15	-	56,56,56,56	0
55	MG	AA	1656	1/1	0.40	-	87,87,87,87	0
55	MG	BA	3285	1/1	0.33	-	102,102,102,102	0
55	MG	BA	3507	1/1	0.30	-	79,79,79,79	0
55	MG	BA	3475	1/1	0.20	-	212,212,212,212	0
55	MG	BB	214	1/1	0.27	-	76,76,76,76	0
55	MG	DA	3480	1/1	0.19	-	109,109,109,109	0
55	MG	BA	3036	1/1	0.35	-	58,58,58,58	0
55	MG	DA	3292	1/1	0.40	-	98,98,98,98	0
55	MG	BA	3355	1/1	0.24	-	95,95,95,95	0
55	MG	BA	3491	1/1	0.33	-	41,41,41,41	0
55	MG	BA	3094	1/1	0.34	-	68,68,68,68	0
55	MG	CA	1675	1/1	0.38	-	111,111,111,111	0
55	MG	DA	3116	1/1	0.34	-	61,61,61,61	0
55	MG	DA	3377	1/1	0.28	-	87,87,87,87	0
55	MG	BA	3023	1/1	0.48	-	64,64,64,64	0
55	MG	DA	3156	1/1	0.25	-	78,78,78,78	0
55	MG	CA	1613	1/1	0.24	-	84,84,84,84	0
55	MG	BA	3003	1/1	0.32	-	50,50,50,50	0
55	MG	BA	3409	1/1	0.37	-	98,98,98,98	0
55	MG	BA	3252	1/1	0.41	-	107,107,107,107	0
55	MG	DA	3088	1/1	0.25	-	62,62,62,62	0
55	MG	DA	3177	1/1	0.13	-	129,129,129,129	0
55	MG	DA	3434	1/1	0.18	-	73,73,73,73	0
55	MG	CA	1789	1/1	0.13	-	71,71,71,71	0
55	MG	DA	3238	1/1	0.42	-	105,105,105,105	0
55	MG	DA	3361	1/1	0.10	-	89,89,89,89	0
55	MG	CA	1763	1/1	0.19	-	100,100,100,100	0
55	MG	DA	3350	1/1	0.37	-	120,120,120,120	0
55	MG	BA	3249	1/1	0.19	-	82,82,82,82	0
55	MG	BA	3370	1/1	0.27	-	78,78,78,78	0
55	MG	AA	1677	1/1	0.43	-	73,73,73,73	0
55	MG	AA	1723	1/1	0.19	-	93,93,93,93	0
55	MG	CA	1611	1/1	0.33	-	82,82,82,82	0
55	MG	DA	3251	1/1	0.34	-	79,79,79,79	0
55	MG	BA	3522	1/1	0.41	-	45,45,45,45	0
55	MG	DA	3016	1/1	0.29	-	78,78,78,78	0
55	MG	AA	1669	1/1	0.25	-	77,77,77,77	0
55	MG	DA	3069	1/1	0.40	-	76,76,76,76	0
55	MG	BA	3255	1/1	0.39	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1721	1/1	0.29	-	60,60,60,60	0
55	MG	DA	3358	1/1	0.44	-	90,90,90,90	0
55	MG	AA	1608	1/1	0.28	-	65,65,65,65	0
55	MG	AA	1803	1/1	0.27	-	89,89,89,89	0
55	MG	AC	105	1/1	0.29	-	102,102,102,102	0
55	MG	CA	1705	1/1	0.25	-	101,101,101,101	0
55	MG	DA	3444	1/1	0.23	-	109,109,109,109	0
55	MG	BF	303	1/1	0.47	-	78,78,78,78	0
55	MG	AA	1630	1/1	0.32	-	112,112,112,112	0
55	MG	BA	3450	1/1	0.24	-	82,82,82,82	0
55	MG	BA	3360	1/1	0.39	-	81,81,81,81	0
55	MG	DA	3442	1/1	0.34	-	98,98,98,98	0
55	MG	BA	3509	1/1	0.43	-	97,97,97,97	0
55	MG	CA	1724	1/1	0.24	-	87,87,87,87	0
55	MG	AA	1798	1/1	0.30	-	84,84,84,84	0
55	MG	BA	3097	1/1	0.21	-	59,59,59,59	0
55	MG	AA	1763	1/1	0.23	-	92,92,92,92	0
55	MG	BA	3397	1/1	0.30	-	131,131,131,131	0
55	MG	CA	1742	1/1	1.06	-	108,108,108,108	0
55	MG	DA	3393	1/1	0.18	-	116,116,116,116	0
55	MG	DA	3111	1/1	0.23	-	45,45,45,45	0
55	MG	DA	3458	1/1	0.31	-	75,75,75,75	0
55	MG	AA	1743	1/1	0.22	-	107,107,107,107	0
55	MG	BA	3248	1/1	0.20	-	34,34,34,34	0
55	MG	AA	1750	1/1	0.42	-	134,134,134,134	0
55	MG	CA	1801	1/1	0.19	-	81,81,81,81	0
55	MG	BA	3542	1/1	0.36	-	85,85,85,85	0
55	MG	DA	3131	1/1	0.33	-	48,48,48,48	0
55	MG	BA	3202	1/1	0.37	-	97,97,97,97	0
55	MG	CA	1648	1/1	0.26	-	113,113,113,113	0
55	MG	BA	3520	1/1	0.37	-	40,40,40,40	0
55	MG	AA	1773	1/1	0.38	-	130,130,130,130	0
55	MG	BA	3008	1/1	0.38	-	44,44,44,44	0
55	MG	DA	3470	1/1	0.33	-	54,54,54,54	0
55	MG	DA	3403	1/1	0.31	-	107,107,107,107	0
55	MG	BA	3375	1/1	0.30	-	87,87,87,87	0
55	MG	BA	3297	1/1	0.18	-	86,86,86,86	0
55	MG	BA	3479	1/1	0.58	-	146,146,146,146	0
55	MG	AA	1676	1/1	0.37	-	89,89,89,89	0
55	MG	BA	3309	1/1	0.44	-	77,77,77,77	0
55	MG	CA	1704	1/1	0.35	-	88,88,88,88	0
55	MG	DA	3486	1/1	0.21	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1757	1/1	0.30	-	95,95,95,95	0
55	MG	BA	3395	1/1	0.32	-	90,90,90,90	0
55	MG	AA	1612	1/1	0.23	-	88,88,88,88	0
55	MG	BA	3280	1/1	0.38	-	80,80,80,80	0
55	MG	DA	3428	1/1	0.32	-	59,59,59,59	0
55	MG	DA	3015	1/1	0.34	-	64,64,64,64	0
55	MG	BA	3206	1/1	0.27	-	68,68,68,68	0
55	MG	CA	1606	1/1	0.18	-	65,65,65,65	0
55	MG	BA	3201	1/1	0.43	-	64,64,64,64	0
55	MG	CB	104	1/1	0.32	-	147,147,147,147	0
55	MG	DA	3079	1/1	0.25	-	103,103,103,103	0
55	MG	CA	1716	1/1	0.34	-	103,103,103,103	0
55	MG	DA	3058	1/1	0.32	-	53,53,53,53	0
55	MG	AA	1768	1/1	0.48	-	71,71,71,71	0
55	MG	BA	3228	1/1	0.52	-	82,82,82,82	0
55	MG	DA	3406	1/1	0.28	-	129,129,129,129	0
55	MG	AA	1724	1/1	0.20	-	78,78,78,78	0
55	MG	DA	3191	1/1	0.44	-	55,55,55,55	0
55	MG	BA	3223	1/1	0.49	-	56,56,56,56	0
55	MG	DA	3113	1/1	0.24	-	80,80,80,80	0
55	MG	BA	3516	1/1	0.33	-	88,88,88,88	0
55	MG	BA	3377	1/1	0.40	-	64,64,64,64	0
55	MG	DA	3233	1/1	0.32	-	90,90,90,90	0
55	MG	BA	3214	1/1	0.42	-	58,58,58,58	0
55	MG	DA	3440	1/1	0.09	-	81,81,81,81	0
55	MG	CA	1628	1/1	0.26	-	123,123,123,123	0
55	MG	AA	1646	1/1	0.40	-	60,60,60,60	0
55	MG	CA	1787	1/1	0.44	-	84,84,84,84	0
55	MG	AA	1800	1/1	0.44	-	131,131,131,131	0
55	MG	CA	1798	1/1	0.36	-	74,74,74,74	0
55	MG	BA	3141	1/1	0.25	-	78,78,78,78	0
55	MG	DA	3423	1/1	1.02	-	118,118,118,118	0
55	MG	CA	1778	1/1	0.21	-	133,133,133,133	0
55	MG	AA	1696	1/1	0.40	-	112,112,112,112	0
55	MG	DA	3322	1/1	0.29	-	99,99,99,99	0
55	MG	BA	3106	1/1	0.21	-	89,89,89,89	0
55	MG	AA	1690	1/1	0.15	-	98,98,98,98	0
55	MG	DA	3008	1/1	0.29	-	57,57,57,57	0
55	MG	AA	1731	1/1	0.10	-	90,90,90,90	0
55	MG	AN	201	1/1	0.07	-	67,67,67,67	0
55	MG	DA	3130	1/1	0.22	-	49,49,49,49	0
55	MG	BA	3400	1/1	0.57	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3113	1/1	0.30	-	47,47,47,47	0
55	MG	DA	3477	1/1	0.35	-	88,88,88,88	0
55	MG	BA	3278	1/1	0.55	-	92,92,92,92	0
55	MG	CG	301	1/1	0.39	-	107,107,107,107	0
55	MG	CA	1682	1/1	0.12	-	100,100,100,100	0
55	MG	BA	3407	1/1	0.25	-	73,73,73,73	0
55	MG	AA	1636	1/1	0.29	-	95,95,95,95	0
55	MG	DA	3441	1/1	0.23	-	89,89,89,89	0
55	MG	CA	1677	1/1	0.17	-	107,107,107,107	0
55	MG	BA	3225	1/1	0.39	-	68,68,68,68	0
55	MG	BA	3336	1/1	0.23	-	78,78,78,78	0
55	MG	AA	1732	1/1	0.35	-	95,95,95,95	0
55	MG	BA	3384	1/1	0.66	-	85,85,85,85	0
55	MG	BA	3177	1/1	0.21	-	34,34,34,34	0
55	MG	AB	102	1/1	0.24	-	96,96,96,96	0
56	ZN	CG	303	1/1	0.30	-	109,109,109,109	0
55	MG	DA	3099	1/1	0.49	-	83,83,83,83	0
55	MG	DA	3340	1/1	0.24	-	75,75,75,75	0
55	MG	AA	1765	1/1	0.30	-	149,149,149,149	0
55	MG	BA	3547	1/1	0.26	-	77,77,77,77	0
55	MG	CA	1711	1/1	0.21	-	101,101,101,101	0
55	MG	AA	1670	1/1	0.37	-	75,75,75,75	0
55	MG	BA	3116	1/1	0.46	-	50,50,50,50	0
55	MG	BA	3394	1/1	0.42	-	80,80,80,80	0
55	MG	DA	3320	1/1	0.29	-	87,87,87,87	0
55	MG	DA	3383	1/1	0.19	-	107,107,107,107	0
55	MG	AA	1639	1/1	0.30	-	84,84,84,84	0
55	MG	DA	3162	1/1	0.31	-	58,58,58,58	0
55	MG	AA	1603	1/1	0.24	-	65,65,65,65	0
55	MG	BA	3014	1/1	0.39	-	43,43,43,43	0
55	MG	DA	3178	1/1	0.26	-	88,88,88,88	0
55	MG	DA	3316	1/1	0.17	-	102,102,102,102	0
55	MG	BA	3566	1/1	0.32	-	83,83,83,83	0
55	MG	DA	3264	1/1	0.38	-	88,88,88,88	0
55	MG	BA	3235	1/1	0.37	-	39,39,39,39	0
55	MG	BB	206	1/1	0.23	-	79,79,79,79	0
55	MG	BA	3216	1/1	0.26	-	53,53,53,53	0
55	MG	DA	3461	1/1	0.21	-	97,97,97,97	0
55	MG	AA	1705	1/1	0.27	-	81,81,81,81	0
55	MG	DA	3459	1/1	0.26	-	76,76,76,76	0
55	MG	BA	3537	1/1	0.46	-	73,73,73,73	0
55	MG	DA	3085	1/1	0.42	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3038	1/1	0.22	-	73,73,73,73	0
55	MG	DA	3007	1/1	0.21	-	55,55,55,55	0
55	MG	BA	3001	1/1	0.49	-	55,55,55,55	0
55	MG	AA	1774	1/1	0.48	-	69,69,69,69	0
55	MG	BA	3199	1/1	0.27	-	65,65,65,65	0
55	MG	BA	3323	1/1	0.68	-	73,73,73,73	0
55	MG	BA	3279	1/1	0.42	-	75,75,75,75	0
55	MG	AA	1787	1/1	0.30	-	101,101,101,101	0
55	MG	DA	3037	1/1	0.13	-	71,71,71,71	0
55	MG	BB	210	1/1	0.32	-	81,81,81,81	0
55	MG	AA	1629	1/1	0.11	-	95,95,95,95	0
55	MG	DA	3386	1/1	0.21	-	130,130,130,130	0
55	MG	BA	3082	1/1	0.26	-	100,100,100,100	0
55	MG	DA	3152	1/1	0.28	-	63,63,63,63	0
55	MG	DA	3378	1/1	0.29	-	88,88,88,88	0
55	MG	BA	3147	1/1	0.32	-	47,47,47,47	0
55	MG	BA	3399	1/1	0.29	-	99,99,99,99	0
55	MG	DA	3146	1/1	0.12	-	89,89,89,89	0
55	MG	AA	1620	1/1	0.28	-	69,69,69,69	0
55	MG	DA	3195	1/1	0.30	-	82,82,82,82	0
55	MG	AA	1757	1/1	0.36	-	101,101,101,101	0
55	MG	BA	3321	1/1	0.45	-	88,88,88,88	0
55	MG	D5	101	1/1	0.24	-	58,58,58,58	0
55	MG	BA	3043	1/1	0.38	-	78,78,78,78	0
55	MG	DA	3091	1/1	0.14	-	74,74,74,74	0
55	MG	BA	3158	1/1	0.39	-	66,66,66,66	0
55	MG	AA	1741	1/1	0.23	-	98,98,98,98	0
55	MG	CA	1761	1/1	0.38	-	143,143,143,143	0
55	MG	BA	3342	1/1	0.21	-	66,66,66,66	0
55	MG	BA	3182	1/1	0.48	-	45,45,45,45	0
55	MG	BA	3464	1/1	0.15	-	91,91,91,91	0
55	MG	BB	218	1/1	0.21	-	98,98,98,98	0
55	MG	BA	3551	1/1	0.31	-	64,64,64,64	0
55	MG	DB	213	1/1	0.16	-	99,99,99,99	0
55	MG	DA	3258	1/1	0.15	-	87,87,87,87	0
55	MG	AA	1653	1/1	0.29	-	95,95,95,95	0
55	MG	DA	3396	1/1	0.27	-	76,76,76,76	0
55	MG	CA	1814	1/1	0.15	-	83,83,83,83	0
55	MG	AA	1644	1/1	0.34	-	94,94,94,94	0
55	MG	DA	3307	1/1	0.36	-	99,99,99,99	0
55	MG	BA	3449	1/1	0.38	-	100,100,100,100	0
55	MG	BA	3473	1/1	0.31	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3359	1/1	0.46	-	78,78,78,78	0
55	MG	CA	1610	1/1	0.25	-	118,118,118,118	0
55	MG	DA	3419	1/1	0.24	-	87,87,87,87	0
55	MG	DA	3325	1/1	0.17	-	97,97,97,97	0
55	MG	AA	1775	1/1	0.49	-	129,129,129,129	0
55	MG	DA	3225	1/1	0.44	-	102,102,102,102	0
55	MG	DA	3119	1/1	0.40	-	65,65,65,65	0
55	MG	BA	3091	1/1	0.41	-	73,73,73,73	0
55	MG	DA	3283	1/1	0.21	-	88,88,88,88	0
55	MG	CA	1790	1/1	0.59	-	142,142,142,142	0
55	MG	BA	3021	1/1	0.26	-	42,42,42,42	0
55	MG	CA	1710	1/1	0.18	-	118,118,118,118	0
55	MG	DA	3455	1/1	0.13	-	44,44,44,44	0
55	MG	AA	1776	1/1	0.34	-	67,67,67,67	0
55	MG	CA	1776	1/1	0.32	-	118,118,118,118	0
55	MG	BA	3376	1/1	0.27	-	83,83,83,83	0
55	MG	DA	3211	1/1	0.32	-	79,79,79,79	0
55	MG	CA	1783	1/1	0.13	-	87,87,87,87	0
55	MG	BA	3241	1/1	0.30	-	62,62,62,62	0
55	MG	A1	101	1/1	0.15	-	102,102,102,102	0
55	MG	BA	3536	1/1	0.12	-	37,37,37,37	0
55	MG	AA	1704	1/1	0.23	-	110,110,110,110	0
55	MG	DA	3040	1/1	0.32	-	118,118,118,118	0
55	MG	BA	3540	1/1	0.44	-	83,83,83,83	0
55	MG	DA	3402	1/1	0.18	-	124,124,124,124	0
55	MG	DA	3266	1/1	0.44	-	82,82,82,82	0
55	MG	BA	3085	1/1	0.39	-	38,38,38,38	0
55	MG	DA	3201	1/1	0.34	-	76,76,76,76	0
55	MG	AA	1695	1/1	0.20	-	128,128,128,128	0
55	MG	DA	3315	1/1	0.15	-	91,91,91,91	0
55	MG	CA	1629	1/1	0.26	-	115,115,115,115	0
55	MG	CA	1721	1/1	0.15	-	82,82,82,82	0
55	MG	DA	3346	1/1	0.20	-	102,102,102,102	0
55	MG	DA	3473	1/1	0.15	-	56,56,56,56	0
55	MG	CA	1807	1/1	0.35	-	95,95,95,95	0
55	MG	DA	3408	1/1	0.23	-	66,66,66,66	0
55	MG	CA	1667	1/1	0.17	-	98,98,98,98	0
55	MG	DB	201	1/1	0.17	-	92,92,92,92	0
55	MG	DA	3106	1/1	0.32	-	57,57,57,57	0
55	MG	DA	3165	1/1	0.45	-	73,73,73,73	0
55	MG	CA	1797	1/1	0.38	-	85,85,85,85	0
55	MG	BA	3442	1/1	0.29	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3368	1/1	0.17	-	97,97,97,97	0
55	MG	DA	3263	1/1	0.28	-	96,96,96,96	0
55	MG	BA	3502	1/1	0.28	-	78,78,78,78	0
55	MG	DA	3300	1/1	0.37	-	75,75,75,75	0
55	MG	BA	3196	1/1	0.20	-	103,103,103,103	0
55	MG	CA	1642	1/1	0.21	-	83,83,83,83	0
55	MG	DA	3118	1/1	0.34	-	55,55,55,55	0
55	MG	BA	3034	1/1	0.29	-	40,40,40,40	0
55	MG	DA	3436	1/1	0.14	-	66,66,66,66	0
55	MG	DA	3421	1/1	0.45	-	84,84,84,84	0
55	MG	BA	3315	1/1	0.41	-	93,93,93,93	0
55	MG	DA	3293	1/1	0.46	-	89,89,89,89	0
55	MG	BA	3517	1/1	0.34	-	69,69,69,69	0
55	MG	DA	3248	1/1	0.19	-	95,95,95,95	0
55	MG	DA	3370	1/1	0.31	-	81,81,81,81	0
55	MG	BA	3069	1/1	0.41	-	93,93,93,93	0
55	MG	CA	1738	1/1	0.44	-	113,113,113,113	0
55	MG	BA	3344	1/1	0.82	-	84,84,84,84	0
55	MG	BA	3269	1/1	0.30	-	79,79,79,79	0
55	MG	DA	3313	1/1	0.19	-	84,84,84,84	0
55	MG	BA	3510	1/1	0.52	-	108,108,108,108	0
55	MG	DA	3133	1/1	0.14	-	91,91,91,91	0
55	MG	AA	1678	1/1	0.39	-	115,115,115,115	0
55	MG	DA	3280	1/1	0.44	-	91,91,91,91	0
55	MG	BA	3071	1/1	0.22	-	63,63,63,63	0
55	MG	DB	206	1/1	0.30	-	89,89,89,89	0
55	MG	DA	3389	1/1	0.33	-	97,97,97,97	0
55	MG	BA	3291	1/1	-	-	56,56,56,56	1
55	MG	AA	1788	1/1	0.25	-	98,98,98,98	0
55	MG	BA	3539	1/1	0.25	-	35,35,35,35	0
55	MG	BA	3319	1/1	0.52	-	64,64,64,64	0
55	MG	AA	1622	1/1	0.22	-	87,87,87,87	0
55	MG	AA	1715	1/1	0.38	-	101,101,101,101	0
55	MG	BA	3463	1/1	0.58	-	101,101,101,101	0
55	MG	AA	1796	1/1	0.43	-	102,102,102,102	0
55	MG	BA	3283	1/1	0.26	-	56,56,56,56	0
55	MG	AG	302	1/1	0.35	-	109,109,109,109	0
55	MG	CA	1715	1/1	0.27	-	89,89,89,89	0
55	MG	DA	3093	1/1	0.31	-	52,52,52,52	0
55	MG	BA	3230	1/1	0.40	-	48,48,48,48	0
55	MG	BA	3326	1/1	0.31	-	67,67,67,67	0
55	MG	DA	3023	1/1	0.11	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3063	1/1	0.18	-	80,80,80,80	0
55	MG	BA	3031	1/1	0.40	-	54,54,54,54	0
55	MG	AA	1611	1/1	0.30	-	94,94,94,94	0
55	MG	CA	1645	1/1	0.23	-	84,84,84,84	0
55	MG	CA	1683	1/1	0.27	-	121,121,121,121	0
55	MG	BA	3544	1/1	0.32	-	82,82,82,82	0
55	MG	BA	3118	1/1	0.39	-	49,49,49,49	0
55	MG	DA	3275	1/1	0.19	-	85,85,85,85	0
55	MG	CA	1816	1/1	0.28	-	102,102,102,102	0
55	MG	DA	3199	1/1	0.17	-	85,85,85,85	0
55	MG	DA	3189	1/1	0.17	-	86,86,86,86	0
55	MG	BA	3212	1/1	0.33	-	68,68,68,68	0
55	MG	CA	1743	1/1	0.27	-	106,106,106,106	0
55	MG	DA	3125	1/1	0.38	-	74,74,74,74	0
55	MG	AC	104	1/1	0.37	-	64,64,64,64	0
55	MG	AA	1618	1/1	0.20	-	91,91,91,91	0
55	MG	BA	3068	1/1	0.41	-	56,56,56,56	0
55	MG	AA	1751	1/1	0.27	-	105,105,105,105	0
55	MG	BA	3203	1/1	0.25	-	106,106,106,106	0
55	MG	AA	1735	1/1	0.19	-	102,102,102,102	0
55	MG	BA	3096	1/1	0.45	-	63,63,63,63	0
55	MG	AA	1663	1/1	0.33	-	72,72,72,72	0
55	MG	BA	3317	1/1	0.43	-	70,70,70,70	0
55	MG	BA	3558	1/1	0.33	-	85,85,85,85	0
55	MG	AA	1664	1/1	0.19	-	53,53,53,53	0
55	MG	AA	1643	1/1	0.65	-	127,127,127,127	0
55	MG	CA	1603	1/1	0.31	-	60,60,60,60	0
55	MG	DO	201	1/1	0.19	-	98,98,98,98	0
55	MG	BA	3546	1/1	0.47	-	101,101,101,101	0
55	MG	CA	1605	1/1	0.17	-	90,90,90,90	0
55	MG	BA	3320	1/1	0.40	-	85,85,85,85	0
55	MG	DA	3089	1/1	0.40	-	60,60,60,60	0
55	MG	DA	3186	1/1	0.24	-	60,60,60,60	0
55	MG	CA	1643	1/1	0.38	-	80,80,80,80	0
55	MG	BA	3548	1/1	0.31	-	95,95,95,95	0
55	MG	AA	1758	1/1	0.34	-	165,165,165,165	0
55	MG	CA	1644	1/1	0.17	-	101,101,101,101	0
55	MG	BA	3306	1/1	0.31	-	84,84,84,84	0
55	MG	DA	3438	1/1	0.31	-	79,79,79,79	0
55	MG	DA	3373	1/1	0.47	-	88,88,88,88	0
55	MG	BA	3347	1/1	0.74	-	79,79,79,79	0
55	MG	CA	1739	1/1	0.22	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1652	1/1	0.15	-	94,94,94,94	0
55	MG	BA	3503	1/1	0.46	-	111,111,111,111	0
55	MG	BA	3438	1/1	0.47	-	84,84,84,84	0
55	MG	DE	301	1/1	0.27	-	59,59,59,59	0
55	MG	DA	3312	1/1	0.36	-	75,75,75,75	0
55	MG	BA	3476	1/1	0.39	-	47,47,47,47	0
55	MG	DA	3379	1/1	0.21	-	87,87,87,87	0
55	MG	DA	3019	1/1	0.28	-	79,79,79,79	0
55	MG	BA	3528	1/1	0.36	-	32,32,32,32	0
55	MG	BA	3296	1/1	0.34	-	60,60,60,60	0
55	MG	BA	3020	1/1	0.28	-	29,29,29,29	0
55	MG	BA	3358	1/1	0.34	-	98,98,98,98	0
55	MG	DA	3463	1/1	0.19	-	84,84,84,84	0
55	MG	AA	1666	1/1	0.54	-	103,103,103,103	0
55	MG	BA	3564	1/1	0.22	-	112,112,112,112	0
55	MG	CA	1609	1/1	0.33	-	71,71,71,71	0
55	MG	AA	1777	1/1	0.39	-	115,115,115,115	0
55	MG	BA	3413	1/1	0.44	-	83,83,83,83	0
55	MG	AA	1714	1/1	0.22	-	89,89,89,89	0
55	MG	AA	1807	1/1	0.26	-	88,88,88,88	0
55	MG	BA	3224	1/1	0.33	-	78,78,78,78	0
55	MG	BA	3462	1/1	0.23	-	116,116,116,116	0
55	MG	BA	3303	1/1	0.42	-	73,73,73,73	0
55	MG	BA	3469	1/1	0.36	-	124,124,124,124	0
55	MG	AA	1720	1/1	0.33	-	83,83,83,83	0
55	MG	DA	3198	1/1	0.33	-	48,48,48,48	0
55	MG	AA	1756	1/1	0.26	-	85,85,85,85	0
55	MG	BA	3454	1/1	0.54	-	80,80,80,80	0
55	MG	AA	1657	1/1	0.34	-	76,76,76,76	0
55	MG	CA	1674	1/1	0.38	-	88,88,88,88	0
55	MG	CA	1669	1/1	0.26	-	85,85,85,85	0
55	MG	BA	3258	1/1	0.46	-	76,76,76,76	0
55	MG	DA	3246	1/1	0.25	-	89,89,89,89	0
55	MG	BA	3040	1/1	0.39	-	74,74,74,74	0
55	MG	CA	1756	1/1	0.28	-	83,83,83,83	0
55	MG	BA	3530	1/1	0.30	-	71,71,71,71	0
55	MG	BA	3092	1/1	0.25	-	67,67,67,67	0
55	MG	DA	3397	1/1	0.19	-	105,105,105,105	0
55	MG	BA	3436	1/1	0.20	-	107,107,107,107	0
55	MG	BA	3025	1/1	0.44	-	46,46,46,46	0
55	MG	CA	1619	1/1	0.12	-	68,68,68,68	0
55	MG	CA	1623	1/1	0.36	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3415	1/1	0.21	-	65,65,65,65	0
55	MG	AC	101	1/1	0.28	-	55,55,55,55	0
55	MG	DA	3407	1/1	0.24	-	103,103,103,103	0
55	MG	DA	3343	1/1	0.33	-	91,91,91,91	0
55	MG	BA	3016	1/1	0.35	-	48,48,48,48	0
55	MG	BA	3035	1/1	0.43	-	61,61,61,61	0
55	MG	AA	1811	1/1	0.46	-	65,65,65,65	0
55	MG	AA	1754	1/1	0.41	-	95,95,95,95	0
55	MG	CA	1663	1/1	0.44	-	80,80,80,80	0
55	MG	AA	1681	1/1	0.39	-	72,72,72,72	0
55	MG	AA	1671	1/1	0.21	-	95,95,95,95	0
55	MG	BA	3271	1/1	0.19	-	92,92,92,92	0
55	MG	BB	209	1/1	0.19	-	96,96,96,96	0
55	MG	BA	3524	1/1	0.35	-	43,43,43,43	0
55	MG	AA	1694	1/1	0.18	-	142,142,142,142	0
55	MG	CA	1727	1/1	0.11	-	84,84,84,84	0
55	MG	AA	1802	1/1	0.23	-	75,75,75,75	0
55	MG	D1	201	1/1	0.26	-	89,89,89,89	0
55	MG	AA	1625	1/1	0.27	-	68,68,68,68	0
55	MG	BA	3314	1/1	0.24	-	83,83,83,83	0
55	MG	DA	3229	1/1	0.40	-	118,118,118,118	0
55	MG	BA	3132	1/1	0.20	-	76,76,76,76	0
55	MG	AA	1661	1/1	0.32	-	56,56,56,56	0
55	MG	BA	3430	1/1	0.21	-	105,105,105,105	0
55	MG	AA	1632	1/1	0.23	-	55,55,55,55	0
55	MG	BA	3382	1/1	0.51	-	93,93,93,93	0
55	MG	BA	3079	1/1	0.25	-	103,103,103,103	0
55	MG	AA	1786	1/1	0.29	-	89,89,89,89	0
55	MG	AA	1689	1/1	0.31	-	107,107,107,107	0
55	MG	AA	1619	1/1	0.39	-	58,58,58,58	0
55	MG	BA	3293	1/1	0.37	-	96,96,96,96	0
55	MG	BA	3013	1/1	0.30	-	52,52,52,52	0
55	MG	DA	3222	1/1	0.17	-	75,75,75,75	0
55	MG	CA	1733	1/1	0.34	-	103,103,103,103	0
55	MG	BA	3425	1/1	0.26	-	87,87,87,87	0
55	MG	DA	3357	1/1	0.18	-	87,87,87,87	0
55	MG	AC	103	1/1	0.34	-	66,66,66,66	0
55	MG	DA	3304	1/1	0.12	-	77,77,77,77	0
55	MG	BA	3169	1/1	0.36	-	45,45,45,45	0
55	MG	CA	1803	1/1	0.24	-	103,103,103,103	0
55	MG	DA	3476	1/1	0.20	-	104,104,104,104	0
55	MG	AA	1726	1/1	0.46	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3410	1/1	0.27	-	103,103,103,103	0
55	MG	DA	3262	1/1	0.71	-	99,99,99,99	0
55	MG	BA	3349	1/1	0.35	-	80,80,80,80	0
55	MG	AA	1615	1/1	0.35	-	90,90,90,90	0
55	MG	BA	3174	1/1	0.39	-	46,46,46,46	0
55	MG	BA	3340	1/1	0.32	-	69,69,69,69	0
55	MG	DA	3181	1/1	0.15	-	50,50,50,50	0
55	MG	DA	3254	1/1	0.14	-	80,80,80,80	0
55	MG	CR	101	1/1	0.90	-	135,135,135,135	0
55	MG	AA	1771	1/1	0.46	-	108,108,108,108	0
55	MG	DA	3171	1/1	0.15	-	73,73,73,73	0
55	MG	BA	3066	1/1	0.19	-	99,99,99,99	0
55	MG	BA	3134	1/1	0.33	-	59,59,59,59	0
55	MG	AA	1725	1/1	0.29	-	100,100,100,100	0
55	MG	CA	1676	1/1	0.36	-	76,76,76,76	0
55	MG	BA	3187	1/1	0.49	-	73,73,73,73	0
55	MG	AA	1651	1/1	0.44	-	79,79,79,79	0
55	MG	DA	3483	1/1	0.41	-	82,82,82,82	0
55	MG	BA	3181	1/1	0.30	-	69,69,69,69	0
55	MG	DA	3232	1/1	0.12	-	56,56,56,56	0
55	MG	BA	3380	1/1	0.43	-	98,98,98,98	0
55	MG	BA	3101	1/1	0.32	-	66,66,66,66	0
55	MG	DA	3124	1/1	0.27	-	47,47,47,47	0
55	MG	BA	3232	1/1	0.20	-	57,57,57,57	0
55	MG	BA	3331	1/1	0.29	-	106,106,106,106	0
55	MG	DA	3330	1/1	0.85	-	100,100,100,100	0
55	MG	AA	1658	1/1	0.32	-	56,56,56,56	0
55	MG	AA	1686	1/1	0.19	-	91,91,91,91	0
55	MG	CA	1695	1/1	0.28	-	69,69,69,69	0
55	MG	CA	1670	1/1	0.40	-	67,67,67,67	0
55	MG	BA	3515	1/1	0.17	-	81,81,81,81	0
55	MG	BA	3555	1/1	0.23	-	47,47,47,47	0
55	MG	DA	3417	1/1	0.35	-	135,135,135,135	0
55	MG	BA	3140	1/1	0.27	-	67,67,67,67	0
55	MG	DA	3381	1/1	0.24	-	90,90,90,90	0
55	MG	CA	1759	1/1	0.75	-	99,99,99,99	0
55	MG	CA	1811	1/1	0.35	-	69,69,69,69	0
55	MG	BA	3009	1/1	0.33	-	58,58,58,58	0
55	MG	BA	3428	1/1	0.39	-	91,91,91,91	0
55	MG	BA	3046	1/1	0.38	-	56,56,56,56	0
55	MG	CA	1706	1/1	0.41	-	79,79,79,79	0
55	MG	BA	3099	1/1	0.23	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3030	1/1	0.33	-	41,41,41,41	0
55	MG	BA	3160	1/1	0.29	-	44,44,44,44	0
55	MG	AD	101	1/1	0.26	-	154,154,154,154	0
55	MG	BA	3482	1/1	0.16	-	82,82,82,82	0
55	MG	AA	1684	1/1	0.34	-	83,83,83,83	0
55	MG	CA	1804	1/1	0.42	-	108,108,108,108	0
55	MG	CA	1713	1/1	0.20	-	82,82,82,82	0
55	MG	DA	3344	1/1	0.25	-	89,89,89,89	0
55	MG	DA	3294	1/1	0.38	-	91,91,91,91	0
55	MG	DA	3168	1/1	0.41	-	87,87,87,87	0
55	MG	DA	3161	1/1	0.22	-	55,55,55,55	0
55	MG	BA	3193	1/1	0.13	-	46,46,46,46	0
55	MG	DA	3324	1/1	0.12	-	91,91,91,91	0
55	MG	DA	3462	1/1	0.30	-	98,98,98,98	0
55	MG	CA	1786	1/1	0.26	-	111,111,111,111	0
55	MG	BO	201	1/1	0.13	-	78,78,78,78	0
55	MG	AA	1783	1/1	0.37	-	167,167,167,167	0
55	MG	CA	1722	1/1	0.69	-	106,106,106,106	0
55	MG	BA	3549	1/1	0.43	-	55,55,55,55	0
55	MG	BA	3059	1/1	0.33	-	63,63,63,63	0
55	MG	AA	1634	1/1	0.33	-	67,67,67,67	0
55	MG	CA	1689	1/1	0.28	-	73,73,73,73	0
55	MG	DA	3157	1/1	0.28	-	51,51,51,51	0
55	MG	BB	203	1/1	0.43	-	71,71,71,71	0
55	MG	DA	3176	1/1	0.41	-	105,105,105,105	0
55	MG	CA	1697	1/1	0.17	-	84,84,84,84	0
55	MG	BA	3190	1/1	0.37	-	86,86,86,86	0
55	MG	DA	3349	1/1	0.21	-	78,78,78,78	0
55	MG	CA	1639	1/1	0.38	-	59,59,59,59	0
55	MG	CA	1806	1/1	0.27	-	103,103,103,103	0
55	MG	AA	1820	1/1	0.12	-	82,82,82,82	0
55	MG	DA	3187	1/1	0.30	-	101,101,101,101	0
55	MG	DA	3174	1/1	0.35	-	63,63,63,63	0
55	MG	DA	3295	1/1	0.33	-	76,76,76,76	0
55	MG	AA	1781	1/1	0.34	-	87,87,87,87	0
55	MG	BA	3226	1/1	0.18	-	69,69,69,69	0
55	MG	DA	3073	1/1	0.30	-	84,84,84,84	0
55	MG	DA	3301	1/1	0.29	-	90,90,90,90	0
55	MG	AA	1707	1/1	0.17	-	81,81,81,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.