



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 09:01 PM BST

PDB ID : 4V95  
Title : Crystal structure of YAEJ bound to the 70S ribosome  
Authors : Gagnon, M.G.; Seetharaman, S.V.; Bulkley, D.P.; Steitz, T.A.  
Deposited on : 2012-01-27  
Resolution : 3.20 Å(reported)

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

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

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

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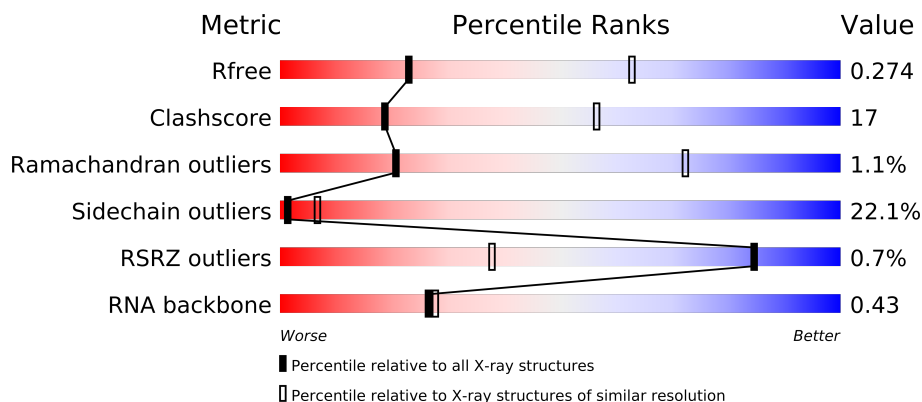
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AY	140	
23	AV	77	
23	CV	77	
24	AX	16	
24	CX	16	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	
28	BE	206	

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Mol	Chain	Length	Quality of chain
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	

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Mol	Chain	Length	Quality of chain
49	D3	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	
55	B9	37	
55	D9	37	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 284877 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	1466	Total	C	N	O	P	0	0	0
			31513	14026	5840	10181	1466			
1	CA	1461	Total	C	N	O	P	0	0	0
			31406	13979	5822	10145	1460			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	233	Total	C	N	O	S	0	0	0
			1809	1157	322	325	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1817	1160	325	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	204	Total	C	N	O	S	0	0	0
			1434	896	277	260	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1453	908	280	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			
4	CD	208	Total	C	N	O	S	0	0	0
			1537	968	287	276	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	149	Total	C	N	O	S	0	0	0
			1115	706	206	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			
6	CF	100	Total	C	N	O	S	0	0	0
			784	496	137	148	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0	0
			1152	716	222	208	6			
7	CG	154	Total	C	N	O	S	0	0	0
			1149	715	222	206	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1049	667	188	192	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O		0	0	0
			863	542	164	157				
9	CI	125	Total	C	N	O		0	0	0
			849	531	161	157				

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O		0	0	0
			659	408	131	120				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			657	407	129	121	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	115	Total	C	N	O	S		
			843	524	160	156	3	0	0
11	CK	114	Total	C	N	O	S		
			828	516	155	154	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			909	570	179	159	1	0	0
12	CL	122	Total	C	N	O	S		
			905	567	178	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S		
			814	503	166	144	1	0	0
13	CM	112	Total	C	N	O	S		
			784	486	159	138	1	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	59	Total	C	N	O	S		
			473	300	98	71	4	0	0
14	CN	59	Total	C	N	O	S		
			469	297	97	71	4	0	0

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			724	453	143	126	2	0	0
15	CO	88	Total	C	N	O	S		
			724	453	143	126	2	0	0



- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	81	Total	C	N	O	S	0	0	0
			646	413	122	110	1			
16	CP	82	Total	C	N	O	S	0	0	0
			661	421	126	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			819	525	150	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	75	Total	C	N	O	S	0	0	0
			529	332	102	93	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			714	438	154	120	2			
20	CT	104	Total	C	N	O	S	0	0	0
			773	476	162	133	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CU	23	Total	C	N	O	0	0	0
			180	112	41	27			

- Molecule 22 is a protein called YAEJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	132	Total	C	N	O	S	0	0	0
			1031	638	204	187	2			

- Molecule 23 is a RNA chain called P-site fMet-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			
24	CX	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2752	Total	C	N	O	P	0	0	0
			59281	26384	11101	19045	2751			
25	DA	2722	Total	C	N	O	P	0	0	0
			58627	26093	10971	18843	2720			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1578	1007	297	272	2			

- 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
			1368	879	242	244	3			
30	DG	180	Total	C	N	O	S	0	0	0
			1361	874	241	243	3			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
31	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	147	Total	C	N	O	S	0	0	0
			1066	687	184	194	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1057	682	182	192	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
34	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	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	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			865	544	172	149				
38	DS	110	Total	C	N	O		0	0	0
			873	550	174	149				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	132	Total	C	N	O	S	0	0	0
			1072	672	215	184	1			
39	DT	130	Total	C	N	O	S	0	0	0
			1058	663	212	182	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	100	Total	C	N	O	S	0	0	0
			766	493	139	133	1			
41	DV	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
42	DW	111	Total	C	N	O	S	0	0	0
			877	552	171	152	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
43	DX	95	Total	C	N	O	S	0	0	0
			732	477	130	124	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			781	502	145	128	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			
45	DZ	189	Total	C	N	O	S	0	0	0
			1451	925	253	270	3			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
46	D0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
47	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	71	Total	C	N	O	S	0	0	0
			584	361	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				
49	D3	58	Total	C	N	O	S	0	0	0
			453	290	86	77				

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
50	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	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
			455	286	90	74	5			
51	D5	59	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			437	272	84	77	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	D7	48	Total	C	N	O	S	0	0	0
			402	248	97	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
55	D9	35	Total	C	N	O	S	0	0	0
			292	180	65	44	3			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	896	Total	Mg	0	0
			896	896		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	2	Total	Mg	0	0
			2	2		
56	DF	3	Total	Mg	0	0
			3	3		
56	CV	10	Total	Mg	0	0
			10	10		
56	B8	2	Total	Mg	0	0
			2	2		
56	BE	5	Total	Mg	0	0
			5	5		
56	DU	1	Total	Mg	0	0
			1	1		
56	B1	3	Total	Mg	0	0
			3	3		
56	CD	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BP	2	Total 2	Mg 2	0	0
56	DR	1	Total 1	Mg 1	0	0
56	CA	219	Total 219	Mg 219	0	0
56	B5	3	Total 3	Mg 3	0	0
56	BB	30	Total 30	Mg 30	0	0
56	BT	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	7	Total 7	Mg 7	0	0
56	AV	18	Total 18	Mg 18	0	0
56	BX	1	Total 1	Mg 1	0	0
56	B2	2	Total 2	Mg 2	0	0
56	AA	348	Total 348	Mg 348	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	D6	2	Total 2	Mg 2	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DV	1	Total 1	Mg 1	0	0
56	B6	1	Total 1	Mg 1	0	0
56	BU	1	Total 1	Mg 1	0	0
56	D7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AD	2	Total 2	Mg 2	0	0
56	DD	4	Total 4	Mg 4	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	4	Total 4	Mg 4	0	0
56	BG	2	Total 2	Mg 2	0	0
56	AI	2	Total 2	Mg 2	0	0
56	BY	2	Total 2	Mg 2	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	2	Total 2	Mg 2	0	0
56	BR	2	Total 2	Mg 2	0	0
56	DA	696	Total 696	Mg 696	0	0
56	B7	1	Total 1	Mg 1	0	0
56	BV	2	Total 2	Mg 2	0	0
56	DO	3	Total 3	Mg 3	0	0
56	BO	2	Total 2	Mg 2	0	0
56	D1	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	BZ	2	Total 2	Mg 2	0	0
56	D5	1	Total 1	Mg 1	0	0
56	BD	5	Total 5	Mg 5	0	0
56	AT	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DT	3	Total 3	Mg 3	0	0
56	B0	5	Total 5	Mg 5	0	0
56	AY	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	16	Total 16	Mg 16	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B5	1	Total 1	Zn 1	0	0
57	B4	1	Total 1	Zn 1	0	0
57	AD	1	Total 1	Zn 1	0	0
57	CD	1	Total 1	Zn 1	0	0
57	B9	1	Total 1	Zn 1	0	0
57	BY	1	Total 1	Zn 1	0	0
57	DY	1	Total 1	Zn 1	0	0
57	D5	1	Total 1	Zn 1	0	0
57	D4	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0
57	CN	1	Total 1	Zn 1	0	0
57	D6	1	Total 1	Zn 1	0	0
57	D9	1	Total 1	Zn 1	0	0
57	B6	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	372	Total 372	O 372	0	0
58	AD	2	Total 2	O 2	0	0
58	AE	3	Total 3	O 3	0	0
58	AI	1	Total 1	O 1	0	0
58	AK	2	Total 2	O 2	0	0
58	AL	2	Total 2	O 2	0	0
58	AN	1	Total 1	O 1	0	0
58	AT	5	Total 5	O 5	0	0
58	AY	2	Total 2	O 2	0	0
58	AV	16	Total 16	O 16	0	0
58	AX	1	Total 1	O 1	0	0
58	BA	1491	Total 1491	O 1491	0	0
58	BB	46	Total 46	O 46	0	0
58	BD	10	Total 10	O 10	0	0
58	BE	5	Total 5	O 5	0	0
58	BF	5	Total 5	O 5	0	0
58	BG	5	Total 5	O 5	0	0
58	BH	1	Total 1	O 1	0	0
58	BN	3	Total 3	O 3	0	0
58	BO	3	Total 3	O 3	0	0
58	BP	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BQ	4	Total 4	O 4	0	0
58	BR	7	Total 7	O 7	0	0
58	BT	1	Total 1	O 1	0	0
58	BU	7	Total 7	O 7	0	0
58	BV	1	Total 1	O 1	0	0
58	BW	2	Total 2	O 2	0	0
58	BX	2	Total 2	O 2	0	0
58	BY	1	Total 1	O 1	0	0
58	B0	4	Total 4	O 4	0	0
58	B1	1	Total 1	O 1	0	0
58	B3	1	Total 1	O 1	0	0
58	B6	4	Total 4	O 4	0	0
58	B7	2	Total 2	O 2	0	0
58	B8	4	Total 4	O 4	0	0
58	B9	1	Total 1	O 1	0	0
58	CA	330	Total 330	O 330	0	0
58	CB	1	Total 1	O 1	0	0
58	CC	1	Total 1	O 1	0	0
58	CD	3	Total 3	O 3	0	0
58	CE	1	Total 1	O 1	0	0
58	CK	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CL	3	Total 3	O 3	0	0
58	CN	2	Total 2	O 2	0	0
58	CO	2	Total 2	O 2	0	0
58	CQ	2	Total 2	O 2	0	0
58	CT	2	Total 2	O 2	0	0
58	CV	13	Total 13	O 13	0	0
58	CX	1	Total 1	O 1	0	0
58	DA	1028	Total 1028	O 1028	0	0
58	DB	40	Total 40	O 40	0	0
58	DD	8	Total 8	O 8	0	0
58	DE	11	Total 11	O 11	0	0
58	DF	4	Total 4	O 4	0	0
58	DG	1	Total 1	O 1	0	0
58	DN	3	Total 3	O 3	0	0
58	DO	5	Total 5	O 5	0	0
58	DP	4	Total 4	O 4	0	0
58	DR	5	Total 5	O 5	0	0
58	DT	3	Total 3	O 3	0	0
58	DV	1	Total 1	O 1	0	0
58	DW	1	Total 1	O 1	0	0
58	DY	2	Total 2	O 2	0	0

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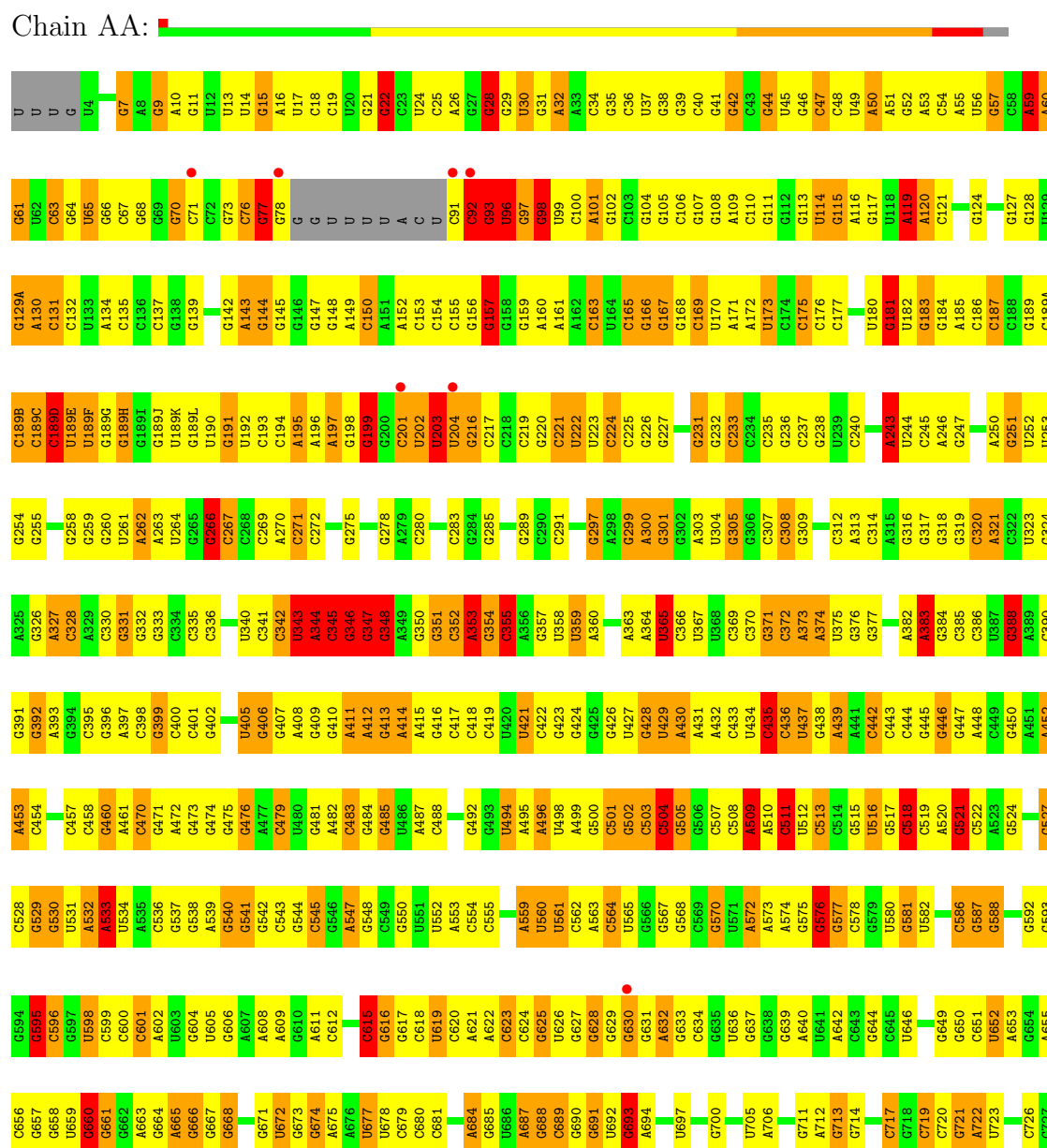
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	D1	3	Total 3	O 3	0	0
58	D3	1	Total 1	O 1	0	0
58	D6	2	Total 2	O 2	0	0
58	D7	2	Total 2	O 2	0	0
58	D8	4	Total 4	O 4	0	0

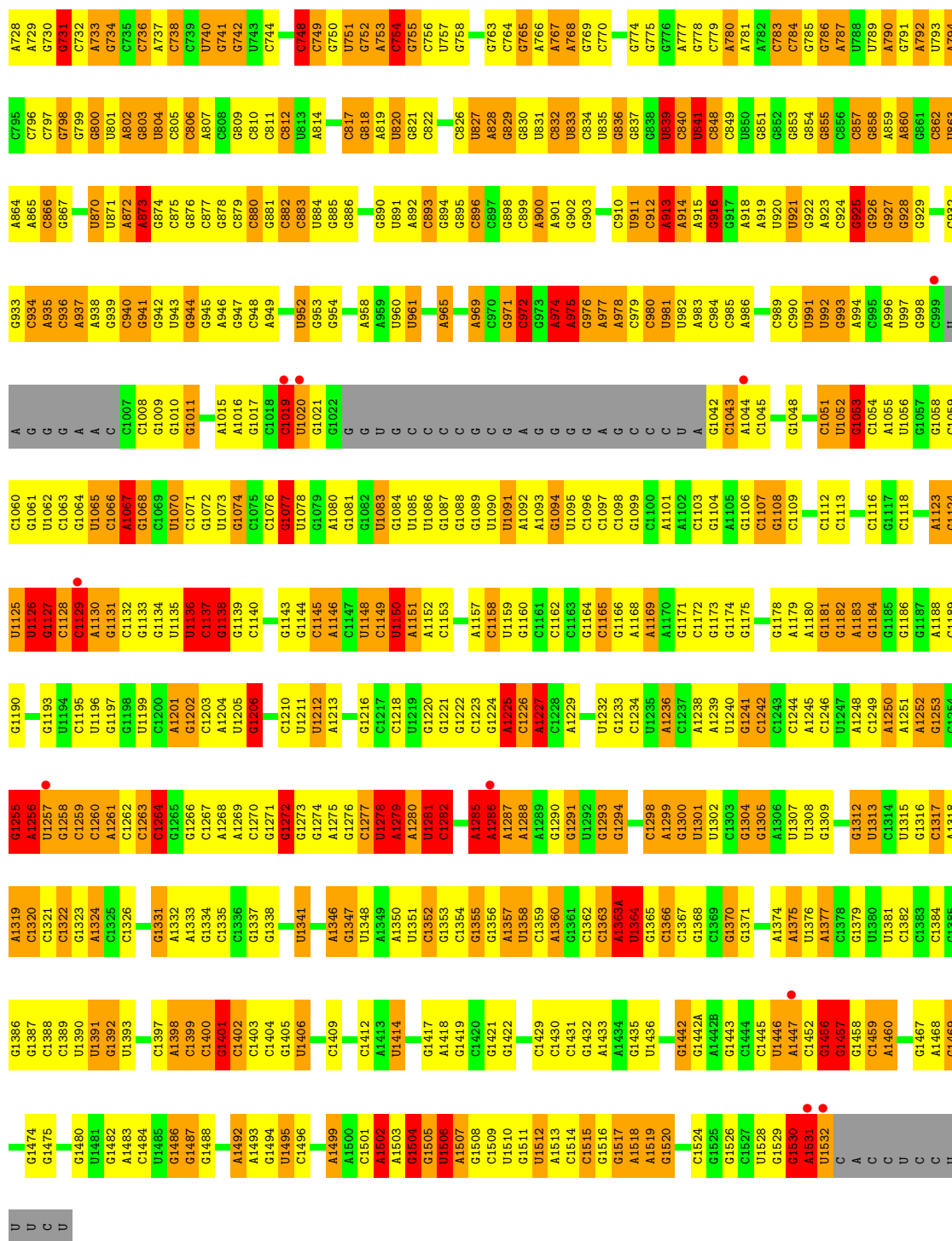
### 3 Residue-property plots

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

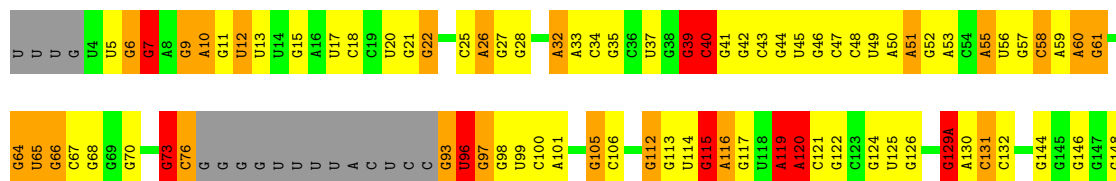




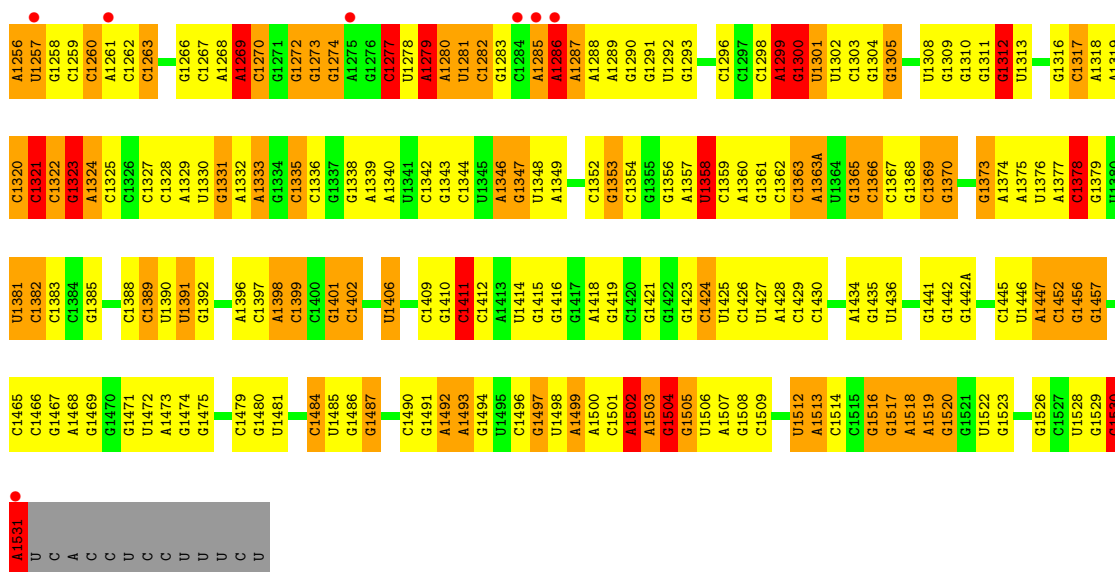


### • Molecule 1: 16S Ribosomal RNA

Chain CA:

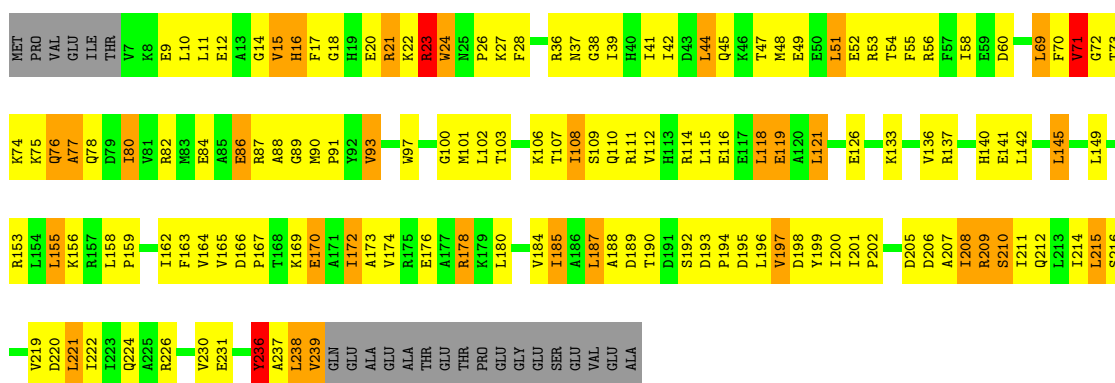






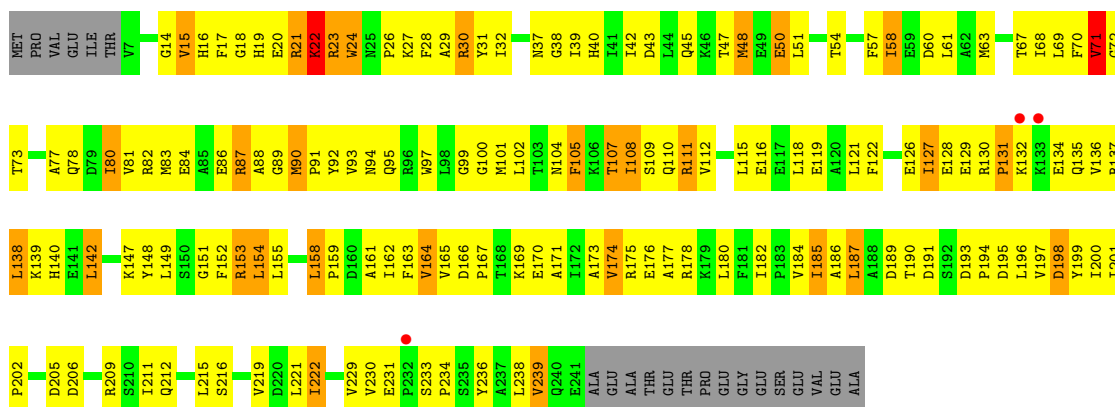
• Molecule 2: 30S Ribosomal Protein S2

Chain AB:



• Molecule 2: 30S Ribosomal Protein S2

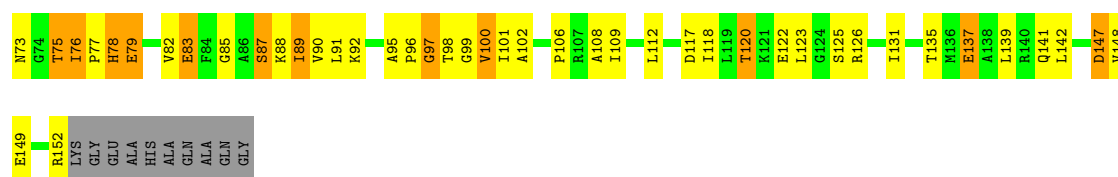
Chain CB:



• Molecule 3: 30S Ribosomal Protein S3

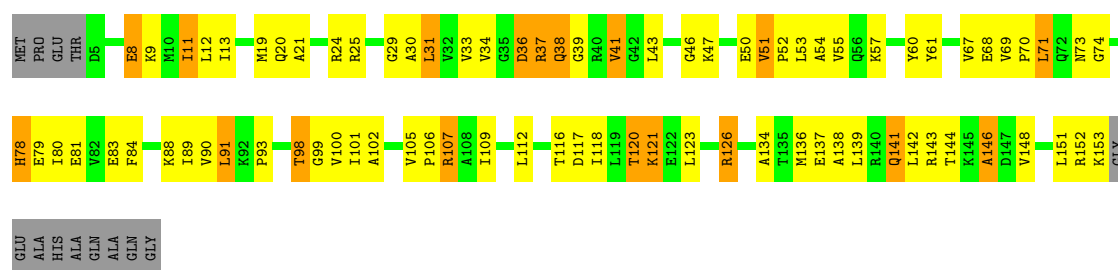
Chain AC:





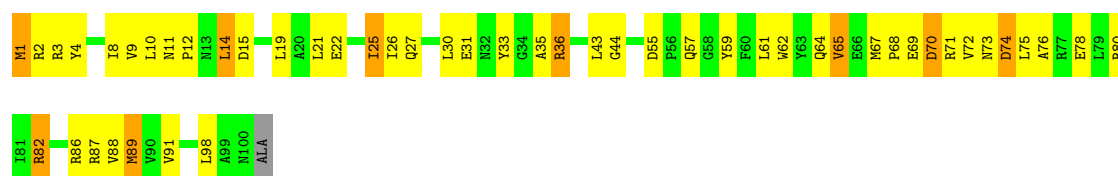
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



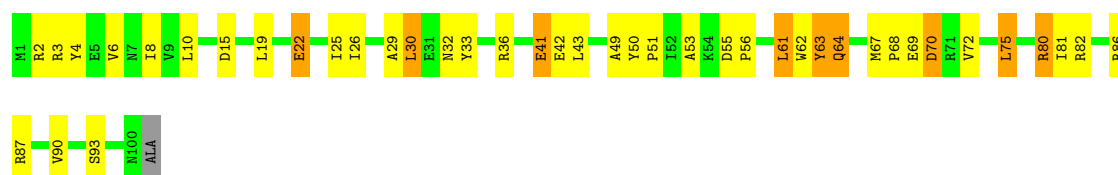
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



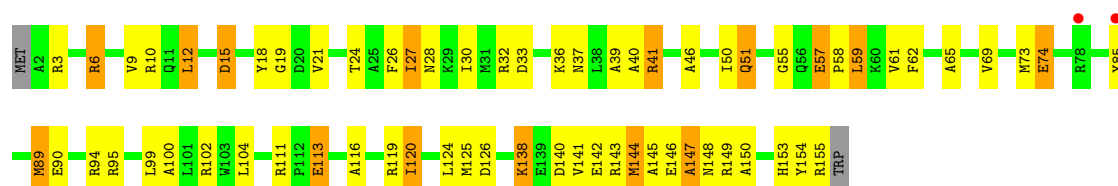
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



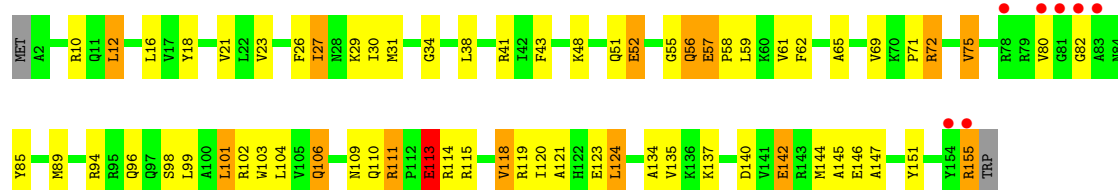
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



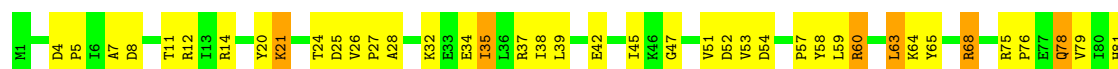
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:



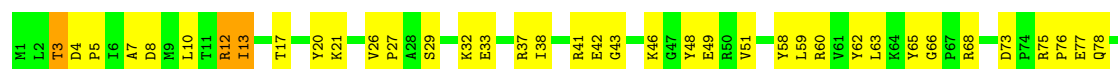
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



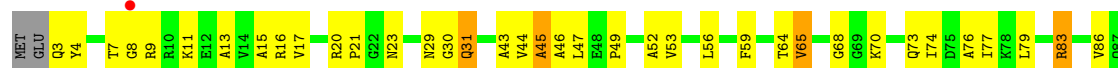
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:



• Molecule 9: 30S Ribosomal Protein S9

Chain AI:



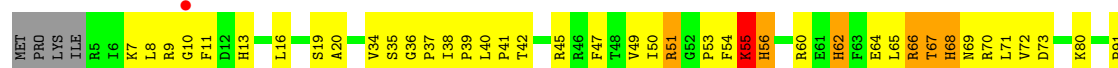
• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:





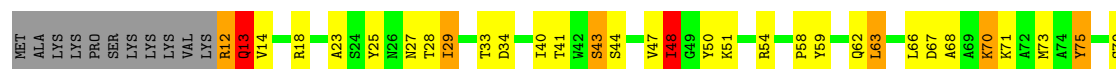
• Molecule 10: 30S Ribosomal Protein S10

Chain CJ:



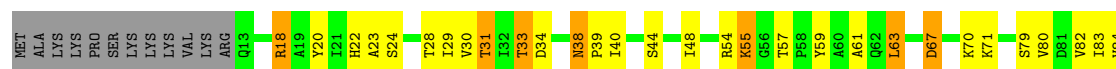
• Molecule 11: 30S Ribosomal Protein S11

Chain AK:



• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



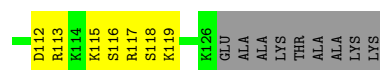
• Molecule 12: 30S Ribosomal Protein S12

Chain AL:



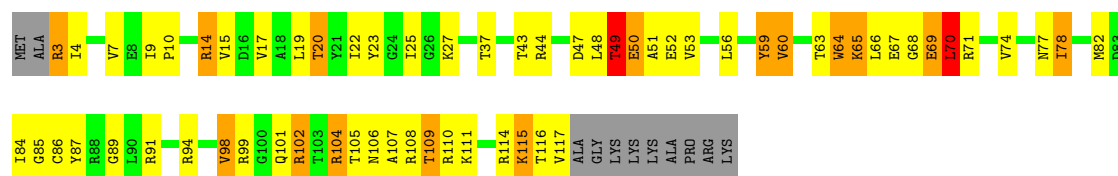
• Molecule 12: 30S Ribosomal Protein S12

Chain CL:



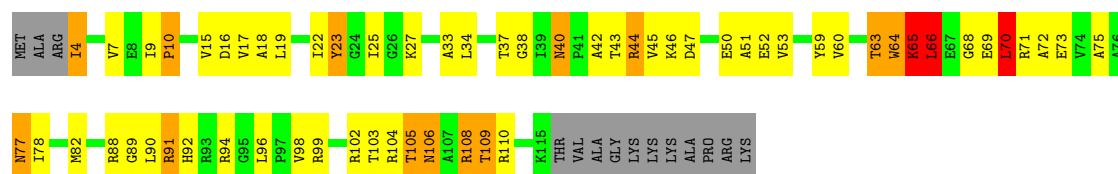
• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



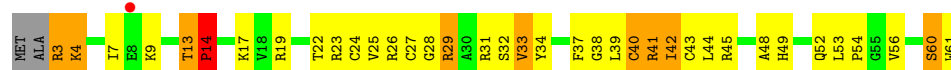
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



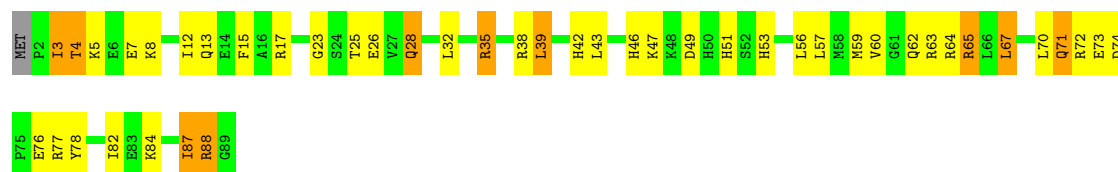
• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



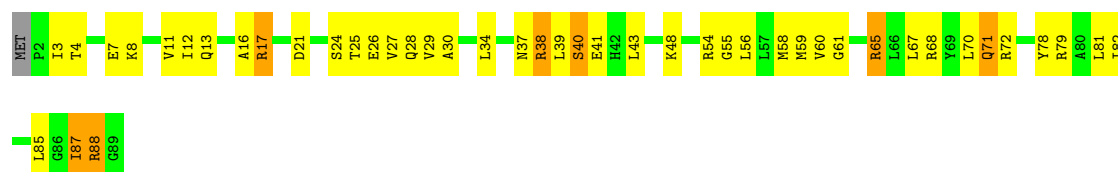
• Molecule 15: 30S Ribosomal Protein S15

Chain AO:



• Molecule 15: 30S Ribosomal Protein S15

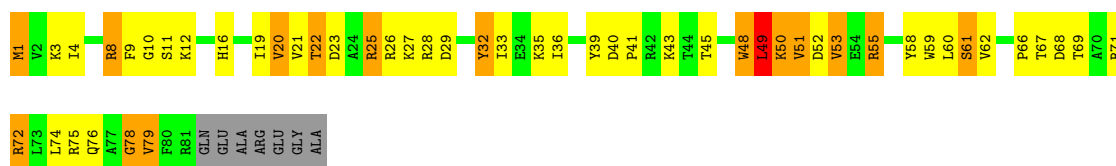
Chain CO:



• Molecule 16: 30S Ribosomal Protein S16

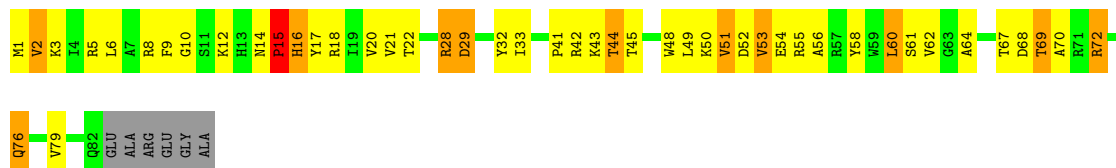
Chain AP:





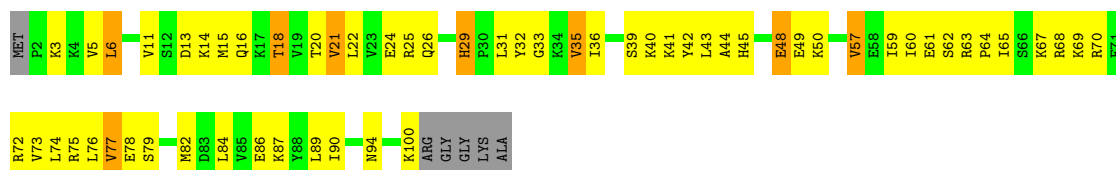
• Molecule 16: 30S Ribosomal Protein S16

Chain CP:



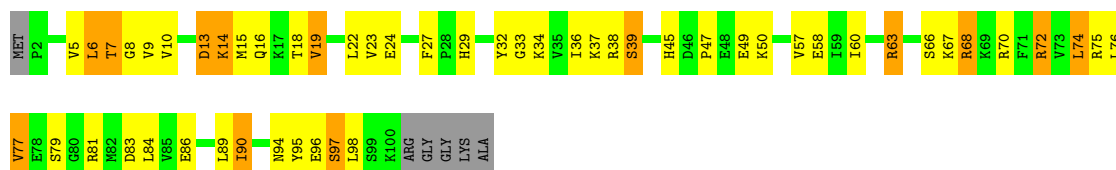
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



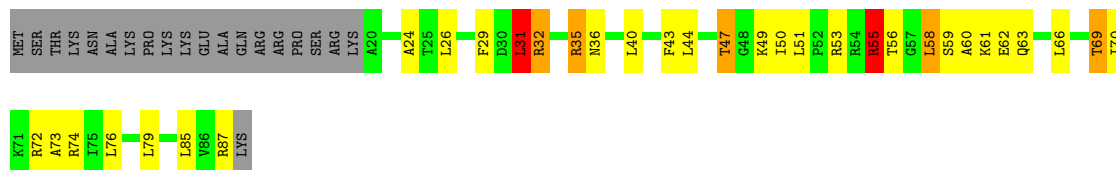
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



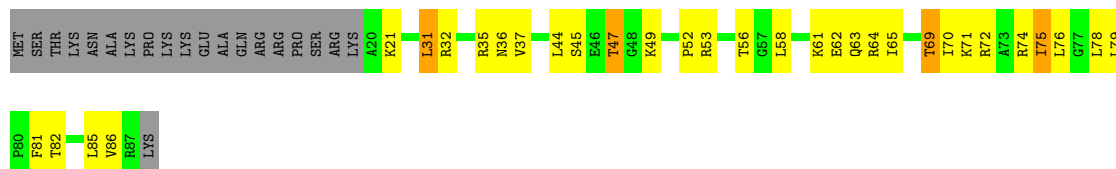
• Molecule 18: 30S Ribosomal Protein S18

Chain AR:



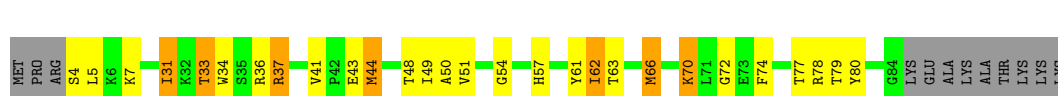
• Molecule 18: 30S Ribosomal Protein S18

Chain CR:



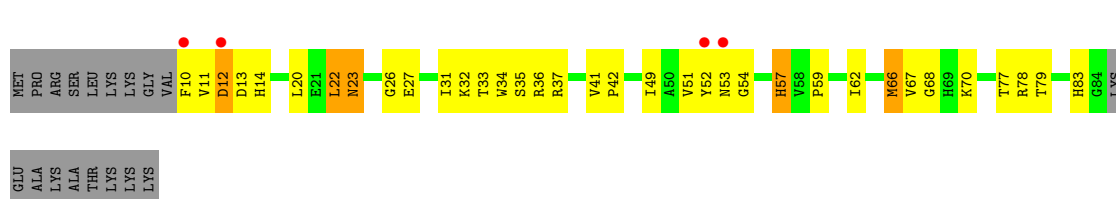
- Molecule 19: 30S Ribosomal Protein S19

Chain AS:



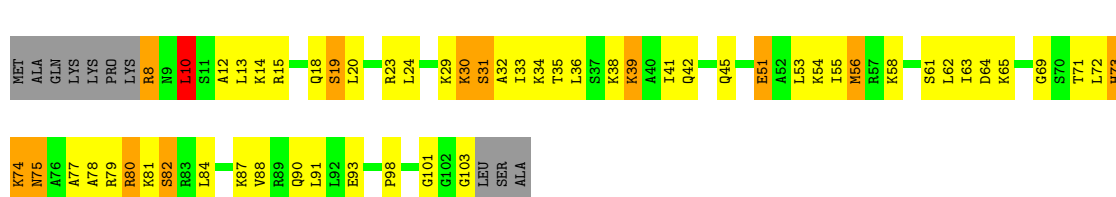
- Molecule 19: 30S Ribosomal Protein S19

Chain CS:



- Molecule 20: 30S Ribosomal Protein S20

Chain AT:



- Molecule 20: 30S Ribosomal Protein S20

Chain CT:



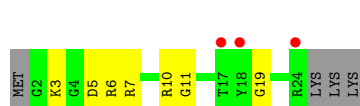
- Molecule 21: 30S Ribosomal Protein THX

Chain AU:



- Molecule 21: 30S Ribosomal Protein THX

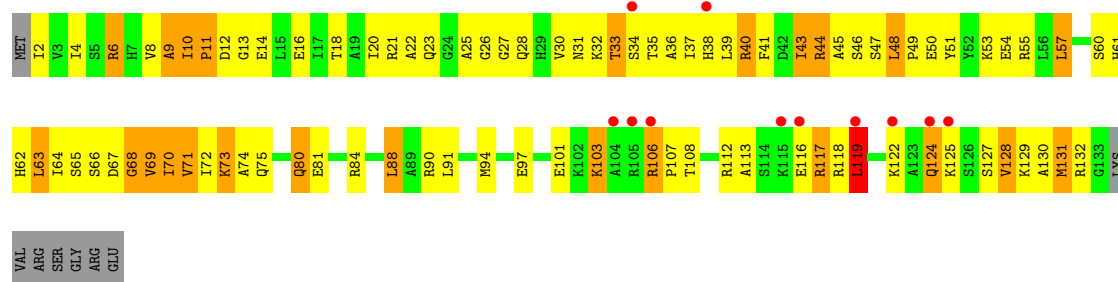
Chain CU:



- Molecule 22: YAEJ

Chain AY:





- Molecule 23: P-site fMet-tRNA

Chain AV:

- Molecule 23: P-site fMet-tRNA

Chain CV:

- Molecule 24: mRNA

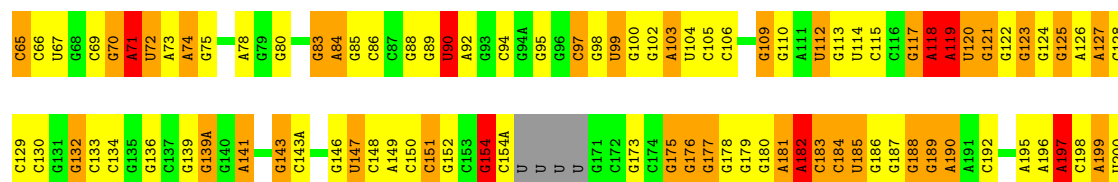
Chain AX:

- Molecule 24: mRNA

Chain CX:

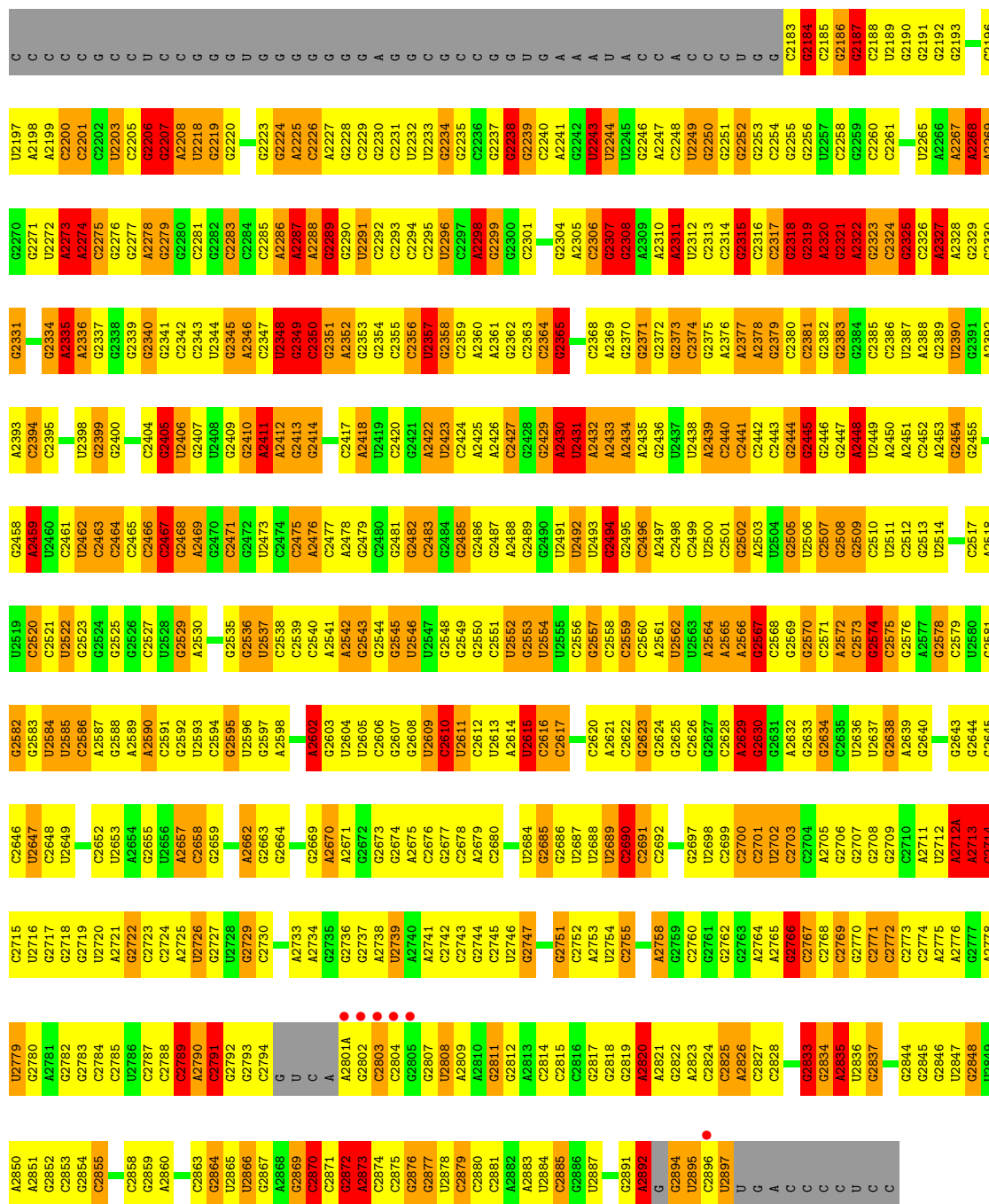
- Molecule 25: 23S Ribosomal RNA

Chain BA:



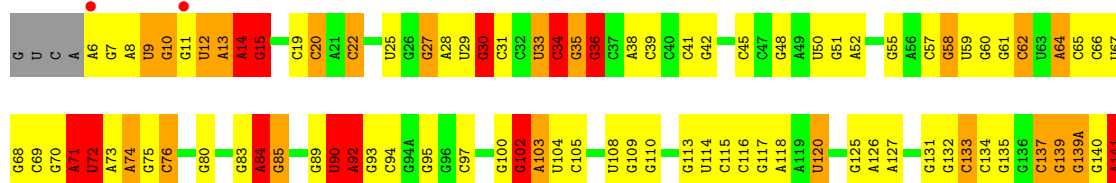
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A	C1038	G375A	C914	C850	A786	A727	G665	G622	U562	G496	A432	A363F	U303	U202
G	G1039	G978	C915	U851	A789	G728	C666	G623	G563	A497	C433	C364	U303	C203
C	C1040	G979	C916	G854	C790	G729	C666	C624	C564	A498	U434	C365	A204	A204
U	G1041	G980	A917	G855	C791	C730	U667	C625	C565	U499	C435	C366	U306	G205
C	C1042	A980	A918	G856	C792	C731	G668	U626	U566	G500	C436	G370	U306	U206
A	C1043	A981	G919	C856	A793	C732	G669	A627	A567	A501	G437	A371	G307	A207
C	G1044	C982	G920	C857	G794	G733	A670	G630	U568	A502	G438	G372	G308	C208
U	A1045	U858	G921	U858	C795	G734	C671	G630	A503	A503	U441	G373	G309	C209
G1106	A1046	A983	G922	U859	A796	A735	C672	A631	G570	U504	G442	A374	G310	C210
G1107	G1047	C985	C923	U860	C797	C736	C673	A632	A505	A505	A443	C375	A311	A211
U1108	G1048	C986	C924	A861	G798	C737	G674	A633	A572	G506	C444	C376	G312	G212
C1109	G1049	G987	C925	G862	G799	G738	A675	C634	G573	G507	C445	C377	C313	A213
G1110	A1050	A988	A926	A863	A800	G739	A676	C635	C574	C509	G446	C378	A314	G214
A1111	G1051	G989	G927	G864	G801	G740	A677	G636	A575	C510	A447	G379	G315	G215
G1112	C1052	A990	G928	C865	A802	G741	C678	G636	U576	U511	U448	U380	C316	G216
U1113	A	A991	U930	A866	U803	G744	C679	G638	G577	G512	A449	G381	G317	G217
G1114	C	C992	G931	C867	A804	G745	G680	U639	A578	A513	G450	G382	G318	A218
G1115	G	G993	G932	U868	G805	G746	G681	C640	G579	A514	C451	U383	C319	G219
G1116	A	C994	A933	C869	C806	A746	G682	C641	C580	A515	A452	U384	A320	G220
G1117	G	C995	G934	A870	U807	U747	G683	G642	C581	C516	G455	C385	G321	A221
C1118	G	A996	C935	A871	G808	G748	G684	A643	G582	C517	C456	U387	A322	A222
G	G	G997	C936	A872	U810	C749	A685	A644	G583	G518	A457	U388	A324	A223
U	U	A1001	G938	G874	U811	A751	C687	A645	C584	U519	G458	G389	A325	G224
G1122	G	G1002	G939	G875	C812	A752	U688	G647	A586	G521	U459	A390	G325	G225
C1123	C	G1003	G940	U876	U813	C753	A699	G648	C587	G522	A460	G391	G329	G226
G1125	G	C1004	A941	C877	C814	C754	G690	G649	C588	G523	C461	C392	A330	A227
A1126	U	C1005	U943	A878	C815	C755	C691	C650	C589	U524	C462	C393	A331	A228
A1127	U	C1006	G944	G879	C815	C756	C692	C650	A590	U525	C463	A394	A332	U230
A1128	A	C1007	A945	G880	G818	U757	C693	A652A	C591	A526	U464	U395	G333	C231
A1129	G	C1008	G946	C881	A819	C758	U694	A652B	G592	C527	C465	G396	C334	G232
U1130	A	A1009	G947	G882	A820	G759	G695	A652C	G593	A528	A466	G397	C335	A233
G1131	G	A1010	C948	G883	U821	G760	U696	C652D	U597	C529	U467	G398	C336	C234
A1132	G	G1011	C949	C884	A822	U761	C697	G652E	G598	G530	G468	C399	C337	U235
U1133	C	U1012	G950	C885	G823	U762	C698	G652F	G599	C531	C469	G400	G338	C236
G1135	A	C1013	C951	C886	A824	G763	A699	G652G	G600	A532	A470	A401	U339	C237
G1136	G	U1014	G952	A887	C825	A764	G700	C652H	G601	G533	A471	C404	A340	C238
G1137	C	G1015	A953	C888	U826	C765	G701	C652I	C801	U534	A472	U405	G341	U239
G1139	C	G1016	G954	C889	U827	C766	G702	G652J	G602	C535	G473	G342	G342	G240
U1140	A	G1017	C955	A890	U828	U767	U703	A	A603	A536	G474	G343	A241	A241
C1141	U	C1018	G956	G892	A829	G768	G704	C	G604	C537	U475	G344	C272J	G242
U1142	C	U1019	A957	G892	G830	G769	A705	G	C605	C540	G476	G411	A345	U243
A1143	U	A1020	U958	U895	C831	G770	A706	G	U606	C540	A477	A412	G348	A244
A1144	U	A1021	A959	A896	G832	G771	G707	C652O	U607	C541	A478	C413	G349	G246
C1145	U	G1022	A960	C897	U833	C772	C708	G652P	A608	C542	A479	C414	U350	C247
A	A	U1023	C961	C898	C834	U773	G	G652Q	A609	C543	A480	A415	G351	G248
A	A	G1024	G962	A899	A835	A774	G713	C652R	G610	G545	G481	C279	G352	C249
A	A	U1025	U963	A900	G836	G775	U714	C652S	C611	C546	A482	G418	G353	G250
A	A	U1026	C964	A901	C837	G776	G715	C652T	C612	A	A483	C419	G354	A251
A	A	A1027	C965	G902	C838	A777	A716	G652U	G613	A548	C484	C420	G355	G252
G1150	G	A1028	G966	C903	G717	G778	G717	A	U614	G549	C485	U421	G356	C253
G1151	G	A1029	C967	C904	A841	U779	A718	A654	U614A	U554	C486	A422	A357	G254
C1152	U	G1030	U905	G904	G842	C780	C719	A655	G614B	U555	C487	A423	A357	G255
G1153	G	G1031	G968	U906	C843	A781	C720	G656	A614C	U556	G488	G424	G363	A256
G1154	C	U907	C970	U907	C844	A782	C721	U657	G615	G556	G489	G425	U362	G257
A1155	G	U1032	C971	U907	C845	A783	A722	C858	G616	U557	G491	G426	G363	A258
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A2077	U2016	G1888	G1813	C1752	G1661	C1599	A	A1471	U1405	G1344	G1285	C1221A	C1161
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U2079	C2018	A1890	A1815	C1754	C1663	G1601	G1537	G1473	C1407	A1472	G1286	G1223	G1163
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A2020	C2020	C1894	G1817	G1756	A1665	A1603	G1539	C1475	C1409	G1348	U1288	G1225	U1165
C2081	U2021	A1896	G1818	U1757	G1666	C1604	U1540	A1477	G1410	A1349	C1289	A1226	C1166
A2082	U2022	G1896	A1819	G1758	G1667	C1605	G1541	G1478	U1415	C1350	C1290	U1167	U1167
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U2085	C2024	U1898	G1821	C1760	A1669	C1607	C1543	G1480	C1417	U1352	U1292	G1228	G1169
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G2090	G2029	G1903	C1827	C1765	G1674	C1612	C1548	A1486	G1421	A1358	G1297	G1234	U1175
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C2100	C2040	U1918	C1838	G1776	G1687	G1624	G1559	U1497	A1434	G1369	A1308	G1245	G1186
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C	C2057	C1930	A1854	C1788	G1699	A1634	A1571	C1509	A1445	G1381	C1320	C1257	U1198
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G	C2060	A1933	G1857	U1791	G1705	A1637	C1574	G1510	G1447	A1384	U1323	G1260	C1201
G	G2061	G1934	G1858	G1792	G1706	C1638	C1574	C1511	G1448	G1385	G1324	G1261	C1202
G	A2062	C1935	U1793	C1793	U1707	U1639	U1577	U1514	A1449	C1386	G1325	U1262	G1203
G	C2063	A1936	A1859	U1794	G1708	C1640	A1578	G1515	G1450	C1387	U1326	U1263	A1204
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G	A2065	A1938	U1796	U1796	U1709	G1642	A1580	U1518	U1453	G1389	U1328	A1265	G1206
G	C2066	G1939	C1797	C1797	U1710	G1643	G1581	G1519	G1455	U1390	G1329	G1266	C1207
G	G2067	U1940	U1798	C1711	C1711	G1644	A1582	G1520	G1456	U1391	U1330	U1267	C1208
A	C2068	G1941	G1800	G1799	G1717	G1649	A1584	U1523	A1457	A1392	A1331	A1268	G1209
G	A2069	C1942	A1801	C1800	G1718	G1650	C1586	G1524	C1458	U1394	G1332	A1269	A1210
G	C2070	G1943	A1802	G1802	G1719	G1651	A1587	G1525	G1459	C1393	C1333	G1270	U1211
C	G2071	U1944	A1803	U1720	U1720	A1652	C1588	G1526	A1460	A1395	G1334	G1271	G1212
C	C2072	C1945	C1804	G1721	G1721	G1653	C1588	G1527	G1461	U1396	U1335	A1272	A1213
U	G2073	U1946	A1722	A1654	U1722	A1654	C1588	G1527	G1461	U1397	A1336	U1273	A1214
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A	A2078	A1951	A1885	A1810	G1746	C1658	C1588	G1527	G1461	C1401	U1340	A1278	G1219
A	A2079	A1952	C1886	G1811	G1750	U1659	A1597	G	G	C1403	A1342	G1280	A1220



### ● Molecule 25: 23S Ribosomal RNA

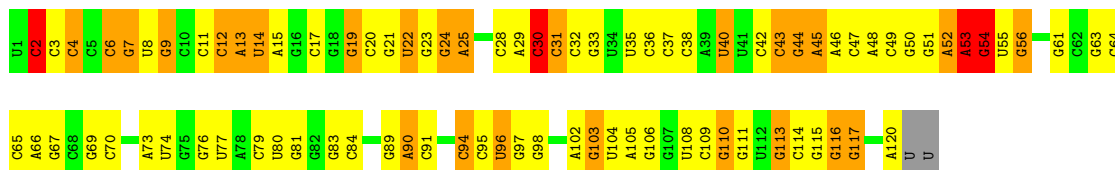
Chain DA:





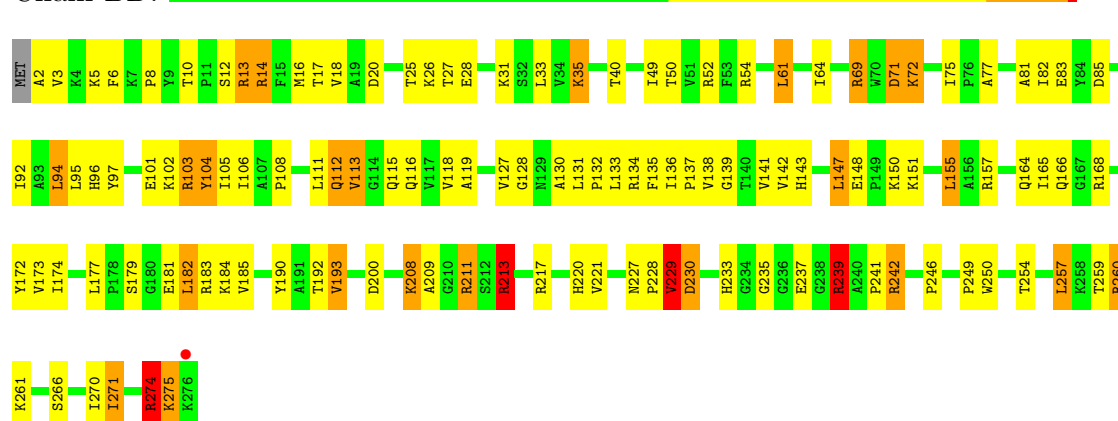






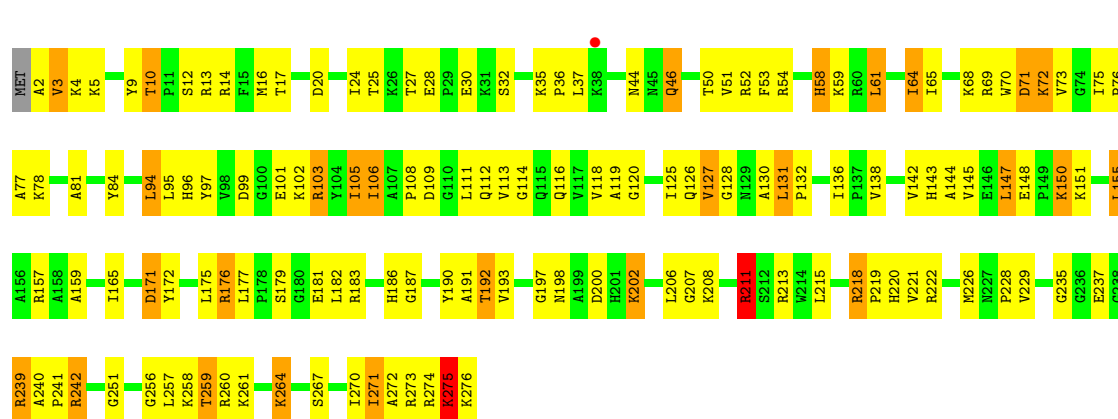
- Molecule 27: 50S Ribosomal Protein L2

Chain BD:



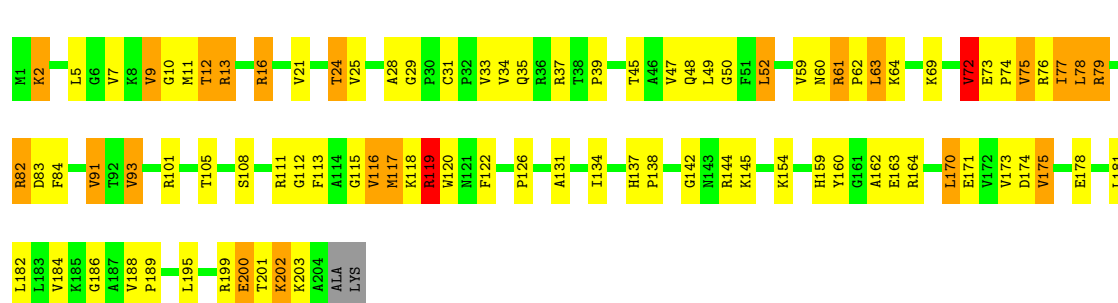
- Molecule 27: 50S Ribosomal Protein L2

Chain DD:



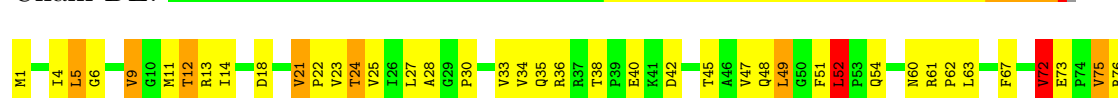
- Molecule 28: 50S Ribosomal Protein L3

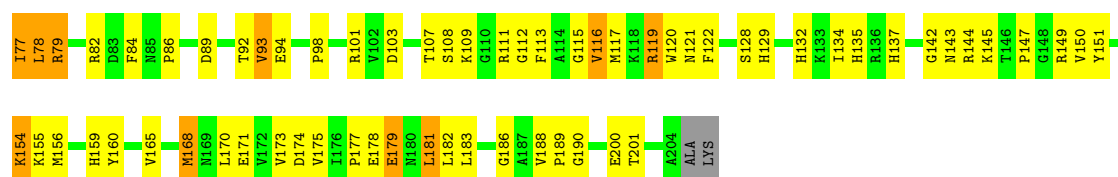
Chain BE:



- Molecule 28: 50S Ribosomal Protein L3

Chain DE:





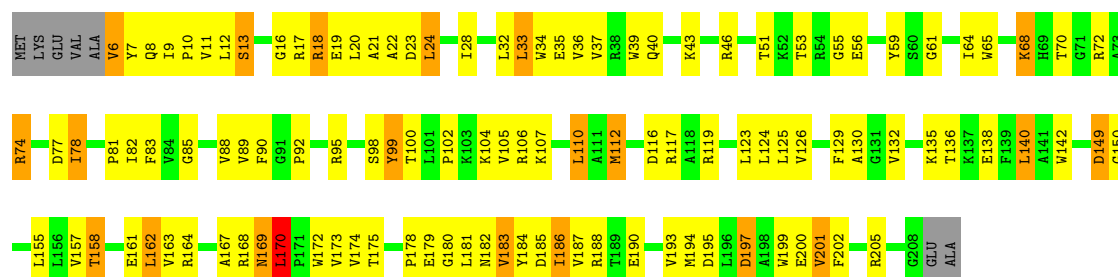
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



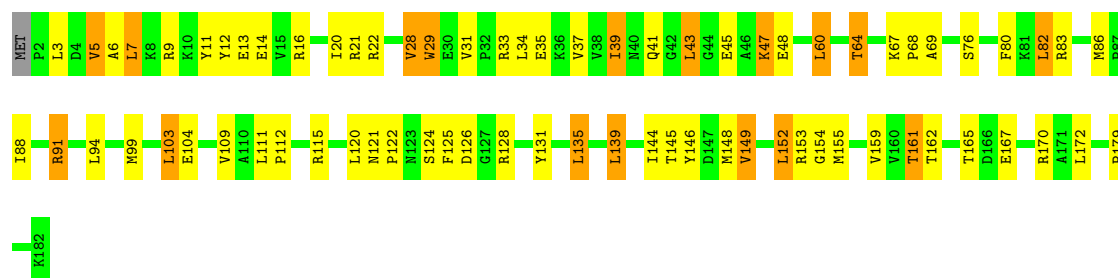
• Molecule 29: 50S Ribosomal Protein L4

Chain DF:



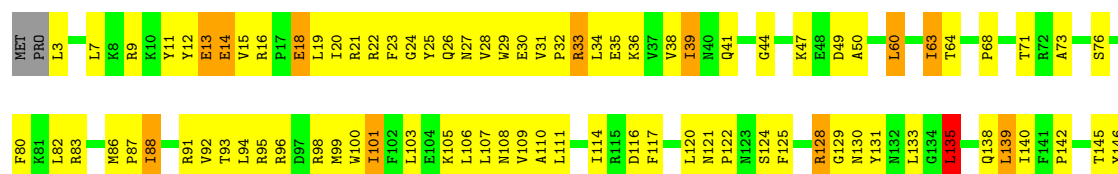
• Molecule 30: 50S Ribosomal Protein L5

Chain BG:



• Molecule 30: 50S Ribosomal Protein L5

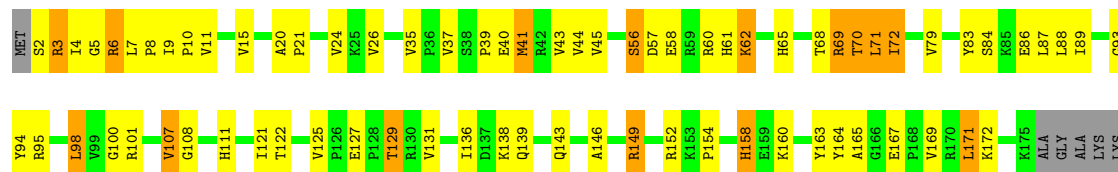
Chain DG:





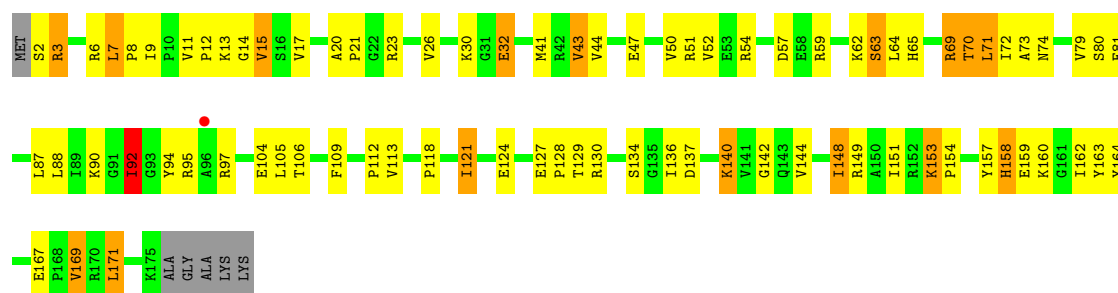
• Molecule 31: 50S Ribosomal Protein L6

Chain BH:



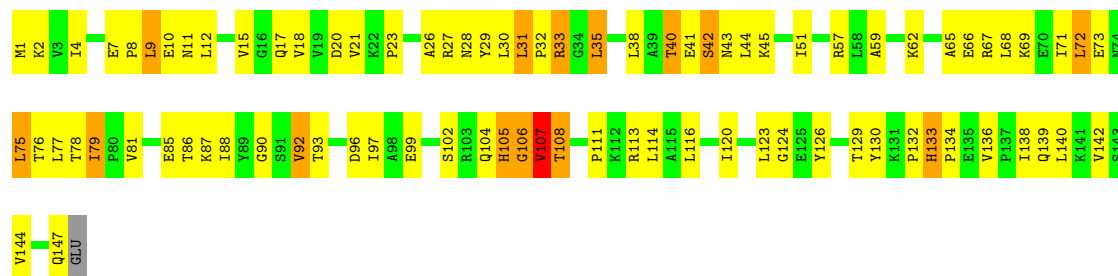
• Molecule 31: 50S Ribosomal Protein L6

Chain DH:



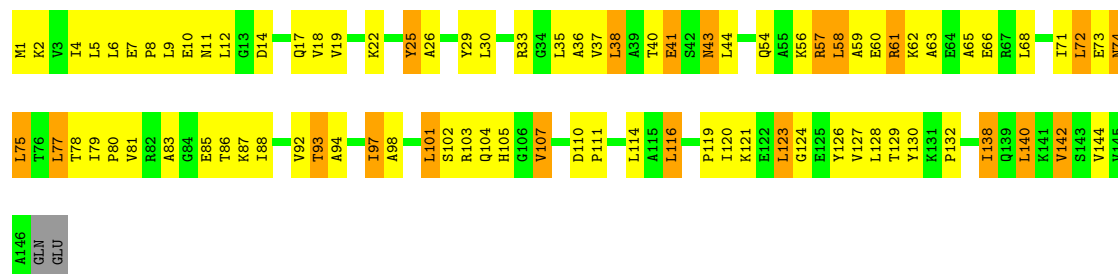
• Molecule 32: 50S Ribosomal Protein L9

Chain BI:



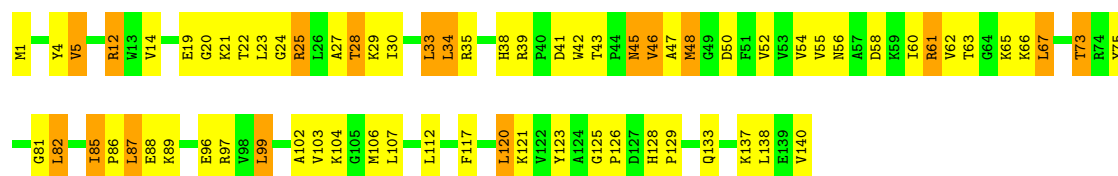
• Molecule 32: 50S Ribosomal Protein L9

Chain DI:



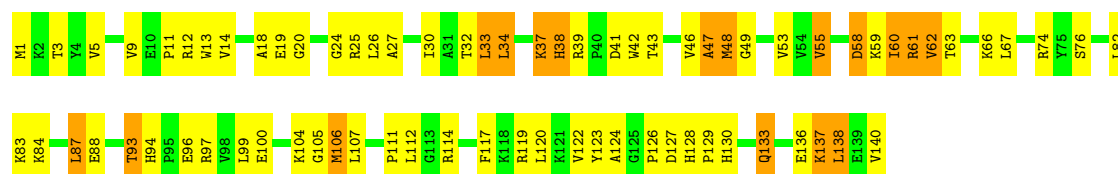
• Molecule 33: 50S Ribosomal Protein L13

Chain BN: 



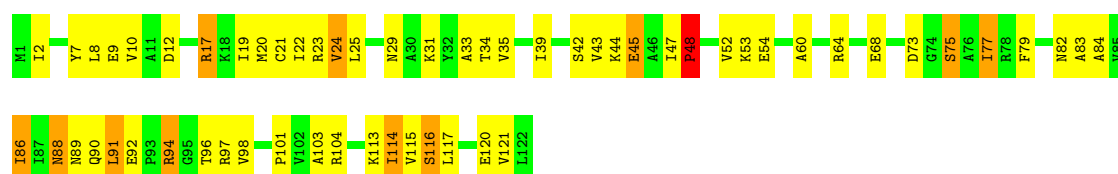
• Molecule 33: 50S Ribosomal Protein L13

Chain DN: 



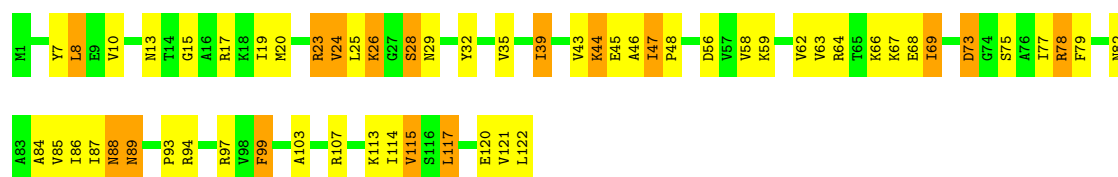
• Molecule 34: 50S Ribosomal Protein L14

Chain BO: 



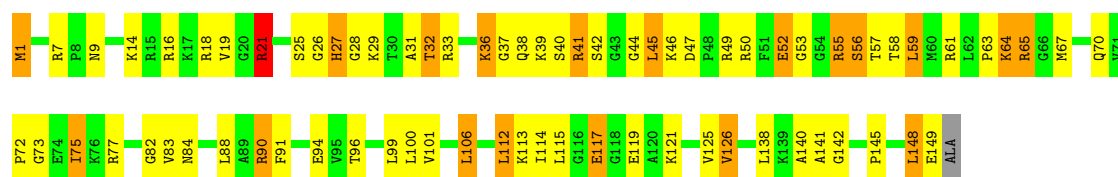
• Molecule 34: 50S Ribosomal Protein L14

Chain DO: 



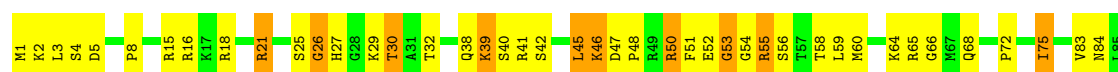
• Molecule 35: 50S Ribosomal Protein L15

Chain BP: 



• Molecule 35: 50S Ribosomal Protein L15

Chain DP: 





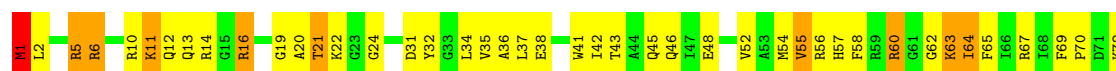
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



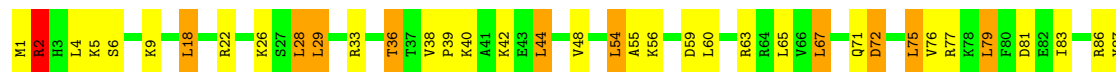
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



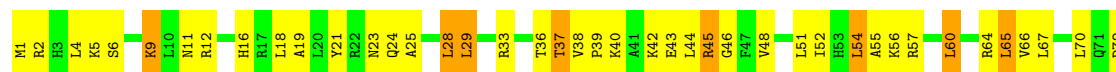
• Molecule 37: 50S Ribosomal Protein L17

Chain BR:



• Molecule 37: 50S Ribosomal Protein L17

Chain DR:



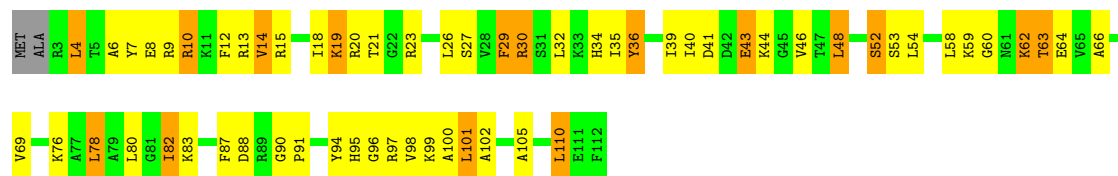
• Molecule 38: 50S Ribosomal Protein L18

Chain BS:



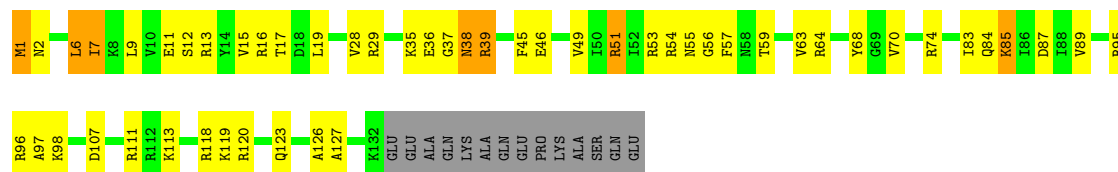
• Molecule 38: 50S Ribosomal Protein L18

Chain DS:



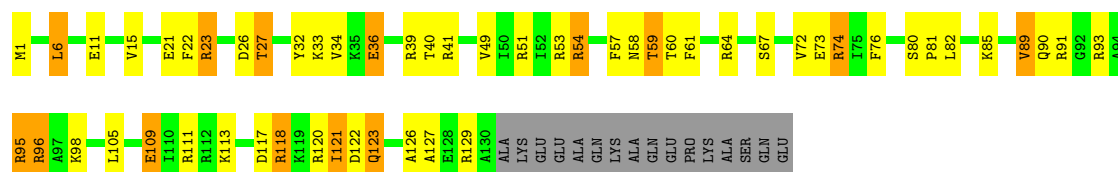
• Molecule 39: 50S Ribosomal Protein L19

Chain BT:



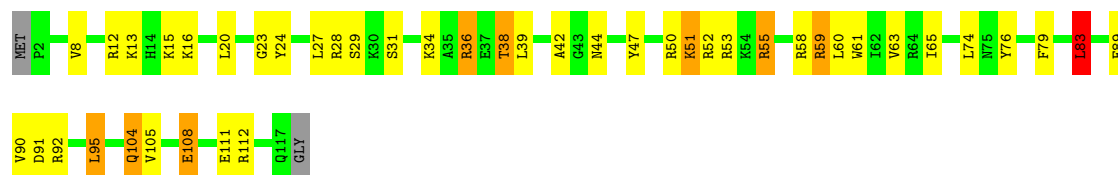
• Molecule 39: 50S Ribosomal Protein L19

Chain DT:



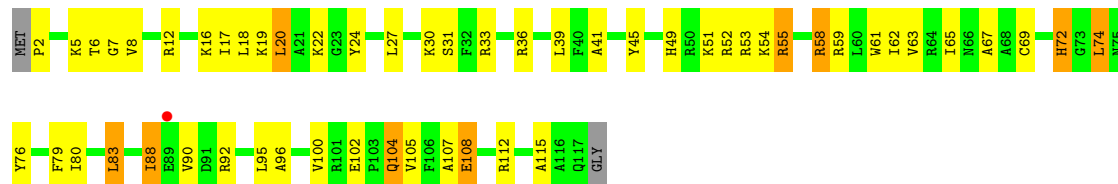
• Molecule 40: 50S Ribosomal Protein L20

Chain BU:



• Molecule 40: 50S Ribosomal Protein L20

Chain DU:



• Molecule 41: 50S Ribosomal Protein L21

Chain BV:





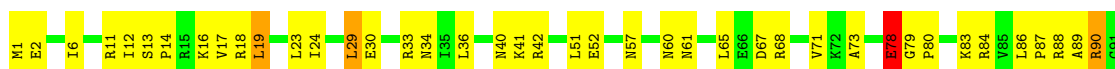
- Molecule 41: 50S Ribosomal Protein L21

Chain DV:



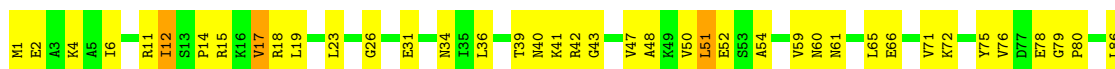
- Molecule 42: 50S Ribosomal Protein L22

Chain BW:



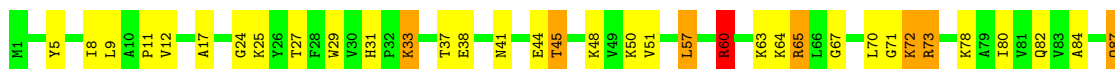
- Molecule 42: 50S Ribosomal Protein L22

Chain DW:



- Molecule 43: 50S Ribosomal Protein L23

Chain BX:



- Molecule 43: 50S Ribosomal Protein L23

Chain DX:



- Molecule 44: 50S Ribosomal Protein L24

Chain BY:

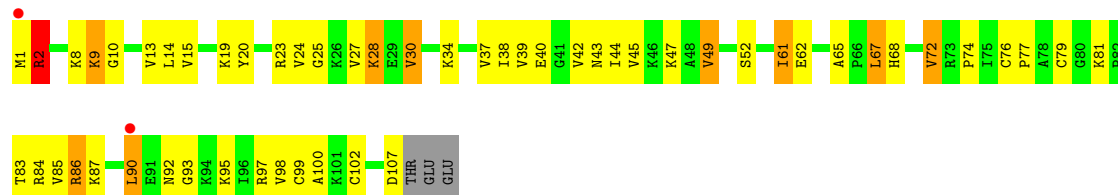






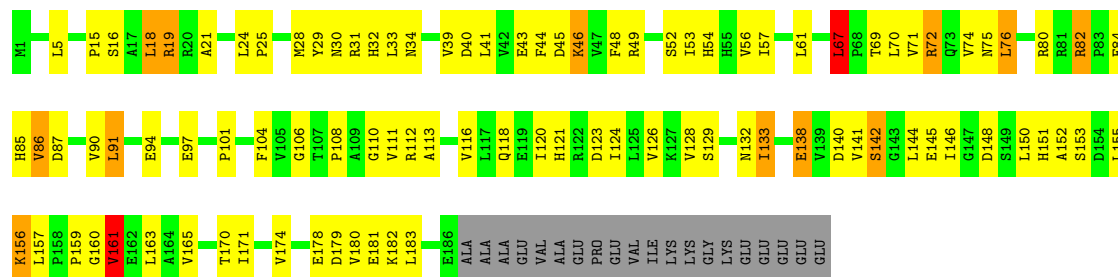
• Molecule 44: 50S Ribosomal Protein L24

Chain DY:



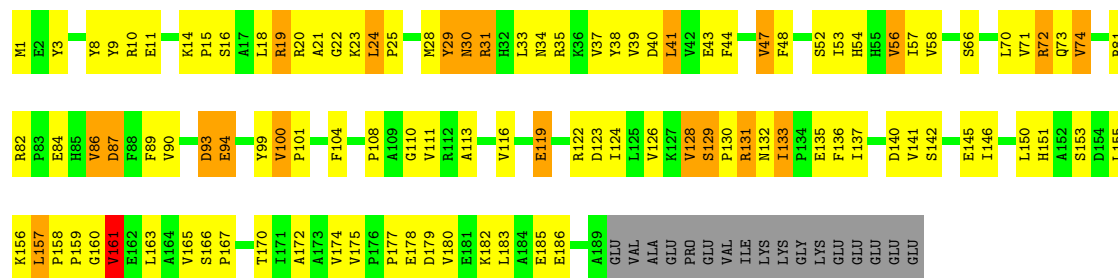
• Molecule 45: 50S Ribosomal Protein L25

Chain BZ:



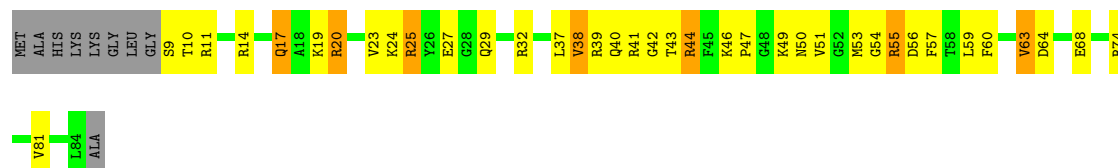
• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:



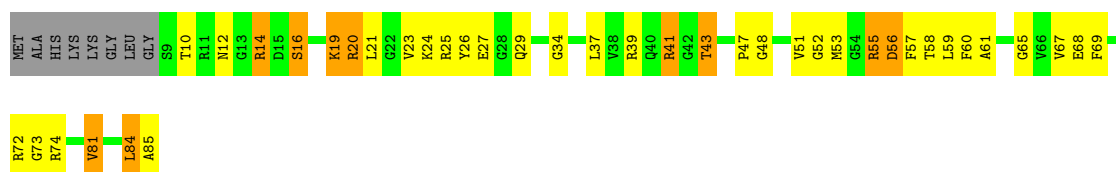
• Molecule 46: 50S Ribosomal Protein L27

Chain B0:



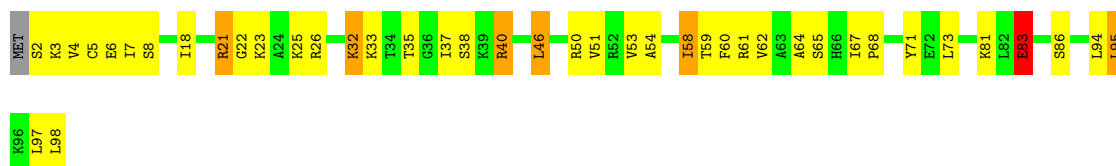
• Molecule 46: 50S Ribosomal Protein L27

Chain D0:



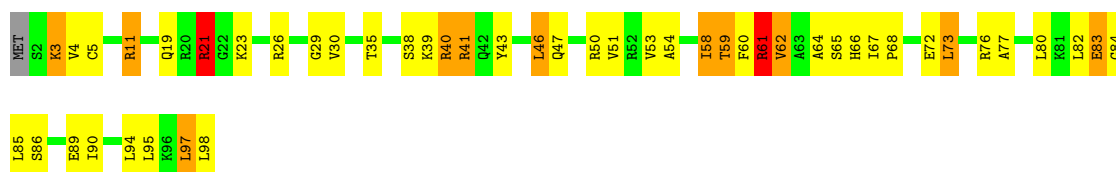
• Molecule 47: 50S Ribosomal Protein L28

Chain B1:



• Molecule 47: 50S Ribosomal Protein L28

Chain D1:



• Molecule 48: 50S Ribosomal Protein L29

Chain B2:



• Molecule 48: 50S Ribosomal Protein L29

Chain D2:



• Molecule 49: 50S Ribosomal Protein L30

Chain B3:



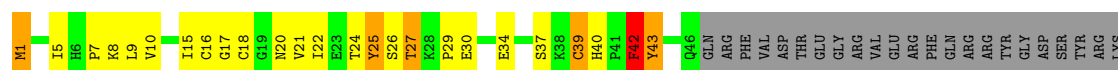
• Molecule 49: 50S Ribosomal Protein L30

Chain D3:



• Molecule 50: 50S Ribosomal Protein L31

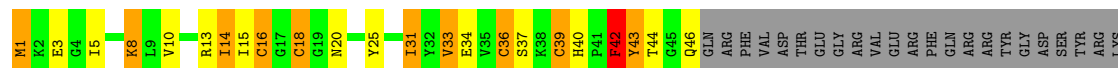
Chain B4: 



GLY  
ARG

- Molecule 50: 50S Ribosomal Protein L31

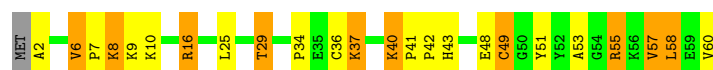
Chain D4: 



GLY  
ARG

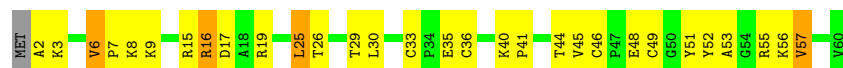
- Molecule 51: 50S Ribosomal Protein L32

Chain B5: 



- Molecule 51: 50S Ribosomal Protein L32

Chain D5: 



- Molecule 52: 50S Ribosomal Protein L33

Chain B6: 



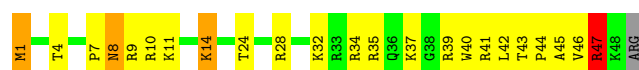
- Molecule 52: 50S Ribosomal Protein L33

Chain D6: 



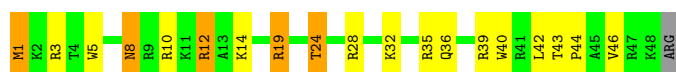
- Molecule 53: 50S Ribosomal Protein L34

Chain B7: 



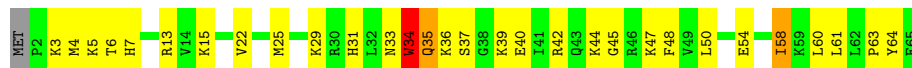
- Molecule 53: 50S Ribosomal Protein L34

Chain D7: 



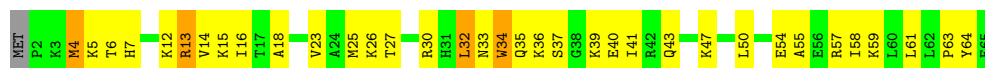
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:



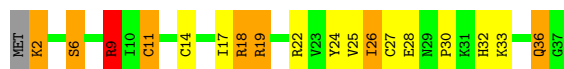
- Molecule 54: 50S Ribosomal Protein L35

Chain D8:



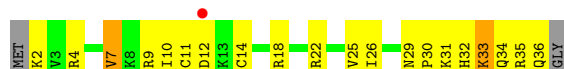
- Molecule 55: 50S Ribosomal Protein L36

Chain B9:



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.96Å 448.86Å 624.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 3.20 34.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.91-3.20) 99.8 (34.91-3.20)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.188 , 0.245 0.222 , 0.274	Depositor DCC
$R_{free}$ test set	39335 reflections (4.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 956750 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	284877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.97	30/35273 (0.1%)	1.68	779/55046 (1.4%)
1	CA	0.89	15/35152 (0.0%)	1.51	525/54858 (1.0%)
2	AB	0.67	3/1844 (0.2%)	0.87	1/2498 (0.0%)
2	CB	0.55	0/1852	0.79	1/2510 (0.0%)
3	AC	0.56	0/1458	0.84	0/1981
3	CC	0.53	0/1477	0.75	0/2006
4	AD	0.66	2/1550 (0.1%)	0.93	4/2106 (0.2%)
4	CD	0.70	3/1567 (0.2%)	0.95	4/2125 (0.2%)
5	AE	0.64	0/1121	0.90	0/1517
5	CE	0.68	0/1131	0.92	0/1529
6	AF	0.62	0/794	0.86	1/1082 (0.1%)
6	CF	0.60	0/797	0.81	0/1085
7	AG	0.53	0/1169	0.73	0/1580
7	CG	0.53	0/1166	0.77	0/1576
8	AH	0.63	0/1065	0.83	0/1445
8	CH	0.57	0/1069	0.80	0/1450
9	AI	0.60	0/879	0.96	1/1195 (0.1%)
9	CI	0.53	0/864	0.80	1/1177 (0.1%)
10	AJ	0.57	0/672	0.81	0/919
10	CJ	0.55	0/670	0.84	0/917
11	AK	0.70	0/858	0.91	1/1163 (0.1%)
11	CK	0.58	0/843	0.77	0/1144
12	AL	0.70	0/925	0.87	0/1251
12	CL	0.64	0/921	0.88	0/1247
13	AM	0.66	1/824 (0.1%)	0.92	1/1120 (0.1%)
13	CM	0.55	0/794	0.81	1/1081 (0.1%)
14	AN	0.59	0/482	0.86	2/642 (0.3%)
14	CN	0.60	0/478	0.86	0/638
15	AO	0.62	0/735	0.87	1/981 (0.1%)
15	CO	0.59	0/735	0.84	0/981
16	AP	0.60	0/662	0.99	3/898 (0.3%)
16	CP	0.60	0/677	0.91	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.70	0/836	0.90	0/1117
17	CQ	0.63	0/832	0.84	1/1113 (0.1%)
18	AR	0.64	0/519	0.96	3/699 (0.4%)
18	CR	0.59	0/519	0.79	0/699
19	AS	0.51	0/574	0.83	0/781
19	CS	0.46	0/543	0.73	1/740 (0.1%)
20	AT	0.57	0/716	0.82	0/947
20	CT	0.62	0/776	0.85	0/1026
21	AU	0.66	0/221	0.84	0/288
21	CU	0.60	0/184	0.78	0/244
22	AY	0.78	1/1043 (0.1%)	1.02	5/1399 (0.4%)
23	AV	1.07	3/1836 (0.2%)	1.55	36/2859 (1.3%)
23	CV	0.78	1/1836 (0.1%)	1.29	11/2859 (0.4%)
24	AX	0.94	0/147	1.18	0/227
24	CX	0.85	0/147	1.11	0/227
25	BA	1.52	551/66391 (0.8%)	2.06	3990/103628 (3.9%)
25	DA	1.06	69/65653 (0.1%)	1.63	1707/102473 (1.7%)
26	BB	1.26	6/2878 (0.2%)	1.93	156/4490 (3.5%)
26	DB	0.88	1/2878 (0.0%)	1.42	35/4490 (0.8%)
27	BD	1.02	3/2181 (0.1%)	1.14	8/2940 (0.3%)
27	DD	0.83	3/2186 (0.1%)	0.98	2/2944 (0.1%)
28	BE	0.96	0/1588	1.09	4/2145 (0.2%)
28	DE	0.72	0/1588	0.90	1/2145 (0.0%)
29	BF	0.93	0/1609	0.97	2/2177 (0.1%)
29	DF	0.64	0/1611	0.87	2/2180 (0.1%)
30	BG	0.70	1/1393 (0.1%)	0.92	0/1892
30	DG	0.53	0/1385	0.83	1/1881 (0.1%)
31	BH	0.84	0/1343	0.94	0/1820
31	DH	0.53	0/1343	0.76	1/1820 (0.1%)
32	BI	0.63	0/1081	0.92	2/1477 (0.1%)
32	DI	0.59	0/1072	0.85	1/1465 (0.1%)
33	BN	1.00	0/1139	1.10	3/1538 (0.2%)
33	DN	0.63	0/1139	0.83	0/1538
34	BO	0.96	0/933	1.03	2/1257 (0.2%)
34	DO	0.74	0/933	0.93	2/1257 (0.2%)
35	BP	0.89	0/1148	1.09	5/1529 (0.3%)
35	DP	0.65	0/1148	0.91	2/1529 (0.1%)
36	BQ	1.01	0/1143	1.04	4/1527 (0.3%)
36	DQ	0.67	0/1143	0.89	1/1527 (0.1%)
37	BR	0.90	0/982	1.08	3/1312 (0.2%)
37	DR	0.65	0/982	0.90	0/1312
38	BS	0.80	0/875	1.06	3/1168 (0.3%)
38	DS	0.55	0/883	0.87	0/1176

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	BT	0.89	0/1086	1.05	1/1455 (0.1%)
39	DT	0.68	0/1072	0.81	0/1437
40	BU	1.10	1/977 (0.1%)	1.09	5/1301 (0.4%)
40	DU	0.70	0/977	0.87	0/1301
41	BV	1.02	0/777	1.10	1/1044 (0.1%)
41	DV	0.67	0/781	0.86	1/1048 (0.1%)
42	BW	1.05	1/901 (0.1%)	1.10	3/1209 (0.2%)
42	DW	0.77	0/887	0.90	2/1192 (0.2%)
43	BX	0.99	0/756	1.06	2/1016 (0.2%)
43	DX	0.75	0/746	0.88	1/1005 (0.1%)
44	BY	0.85	0/798	1.03	2/1073 (0.2%)
44	DY	0.64	0/794	0.87	0/1067
45	BZ	0.80	0/1486	0.94	2/2022 (0.1%)
45	DZ	0.58	0/1483	0.80	0/2023
46	B0	0.95	0/602	1.10	3/804 (0.4%)
46	D0	0.64	0/615	0.89	0/820
47	B1	0.94	0/752	1.07	1/1003 (0.1%)
47	D1	0.70	0/752	0.92	2/1003 (0.2%)
48	B2	0.96	2/590 (0.3%)	1.00	1/781 (0.1%)
48	D2	0.63	0/586	0.79	1/779 (0.1%)
49	B3	1.02	0/463	1.07	0/623
49	D3	0.57	0/458	0.79	0/616
50	B4	0.62	0/358	0.97	2/487 (0.4%)
50	D4	0.66	0/358	0.82	1/487 (0.2%)
51	B5	1.01	1/469 (0.2%)	1.09	2/634 (0.3%)
51	D5	0.69	0/465	0.90	0/630
52	B6	0.96	0/456	1.09	2/609 (0.3%)
52	D6	0.73	0/444	0.87	0/595
53	B7	1.10	0/426	1.21	4/561 (0.7%)
53	D7	0.78	0/410	0.88	0/543
54	B8	0.99	0/516	1.14	2/679 (0.3%)
54	D8	0.75	0/516	0.93	0/679
55	B9	1.07	1/300 (0.3%)	1.25	3/395 (0.8%)
55	D9	0.68	0/295	0.87	0/390
All	All	1.07	699/303213 (0.2%)	1.58	7364/453838 (1.6%)

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
1	AA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	1
2	AB	0	4
2	CB	0	2
3	AC	0	2
4	AD	0	4
4	CD	0	5
5	AE	0	2
5	CE	0	1
7	AG	0	1
7	CG	0	1
9	AI	0	3
10	AJ	0	2
10	CJ	0	2
11	AK	0	1
12	AL	0	1
13	AM	0	3
13	CM	0	2
14	CN	0	1
16	CP	0	1
18	AR	0	1
20	AT	0	2
20	CT	0	2
21	CU	0	1
22	AY	0	1
27	BD	0	2
28	BE	0	2
28	DE	0	1
29	BF	0	2
29	DF	0	1
30	DG	0	3
31	DH	0	1
32	BI	0	3
34	BO	0	1
34	DO	0	1
35	BP	0	1
35	DP	0	1
36	BQ	0	2
36	DQ	0	1
38	BS	0	1
38	DS	0	1
39	BT	0	1
39	DT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	BX	0	1
45	BZ	0	1
47	B1	0	1
47	D1	0	1
48	D2	0	1
50	B4	0	1
50	D4	0	1
51	B5	0	1
52	D6	0	1
All	All	0	82

The worst 5 of 699 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1142(A)	A	N9-C4	-17.94	1.27	1.37
25	BA	528	A	N9-C4	-17.30	1.27	1.37
1	CA	189(D)	C	N3-C4	-15.70	1.23	1.33
25	BA	676	A	N9-C4	-15.14	1.28	1.37
25	BA	1021	A	N9-C4	-14.78	1.28	1.37

The worst 5 of 7364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	189(D)	C	N3-C4-N4	-102.71	46.10	118.00
1	CA	189(D)	C	N1-C2-O2	44.80	145.78	118.90
1	CA	189(D)	C	N3-C4-N4	-44.60	86.78	118.00
1	AA	189(D)	C	C2-N3-C4	43.68	141.74	119.90
1	AA	189(D)	C	C5-C4-N4	42.13	149.69	120.20

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(D)	C	Sidechain
2	AB	14	GLY	Peptide
2	AB	23	ARG	Peptide
2	AB	71	VAL	Peptide
2	AB	76	GLN	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	31513	0	15906	882	0
1	CA	31406	0	15852	823	0
2	AB	1809	0	1781	104	0
2	CB	1817	0	1785	126	0
3	AC	1434	0	1299	59	0
3	CC	1453	0	1320	64	0
4	AD	1520	0	1407	80	0
4	CD	1537	0	1430	81	1
5	AE	1105	0	1130	50	0
5	CE	1115	0	1145	55	0
6	AF	781	0	741	36	1
6	CF	784	0	739	30	0
7	AG	1152	0	1098	58	0
7	CG	1149	0	1096	52	0
8	AH	1045	0	1033	52	0
8	CH	1049	0	1037	52	0
9	AI	863	0	760	54	0
9	CI	849	0	735	54	0
10	AJ	659	0	552	38	0
10	CJ	657	0	547	40	0
11	AK	843	0	841	34	0
11	CK	828	0	822	31	0
12	AL	909	0	927	50	0
12	CL	905	0	916	30	0
13	AM	814	0	765	47	0
13	CM	784	0	730	51	0
14	AN	473	0	491	39	0
14	CN	469	0	482	37	0
15	AO	724	0	749	34	0
15	CO	724	0	749	30	0
16	AP	646	0	636	42	0
16	CP	661	0	653	45	0
17	AQ	823	0	891	52	0
17	CQ	819	0	880	38	0
18	AR	514	0	530	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	514	0	530	21	0
19	AS	560	0	466	24	0
19	CS	529	0	443	22	0
20	AT	714	0	775	41	0
20	CT	773	0	836	32	0
21	AU	217	0	234	7	0
21	CU	180	0	173	4	0
22	AY	1031	0	1087	85	0
23	AV	1644	0	836	23	0
23	CV	1644	0	836	38	0
24	AX	131	0	66	4	0
24	CX	131	0	66	2	0
25	BA	59281	0	29884	1053	0
25	DA	58627	0	29570	1197	0
26	BB	2573	0	1306	47	0
26	DB	2573	0	1306	83	0
27	BD	2131	0	2207	97	0
27	DD	2136	0	2218	104	0
28	BE	1555	0	1607	65	0
28	DE	1555	0	1607	72	0
29	BF	1576	0	1616	71	0
29	DF	1578	0	1623	96	0
30	BG	1368	0	1324	52	0
30	DG	1361	0	1316	76	0
31	BH	1317	0	1376	52	0
31	DH	1317	0	1376	59	0
32	BI	1066	0	1095	47	0
32	DI	1057	0	1087	56	0
33	BN	1112	0	1180	49	0
33	DN	1112	0	1180	64	0
34	BO	923	0	981	37	0
34	DO	923	0	981	38	0
35	BP	1131	0	1201	61	0
35	DP	1131	0	1201	66	0
36	BQ	1122	0	1179	46	0
36	DQ	1122	0	1179	66	0
37	BR	968	0	1033	42	0
37	DR	968	0	1033	56	0
38	BS	865	0	905	53	0
38	DS	873	0	927	64	0
39	BT	1072	0	1116	31	0
39	DT	1058	0	1098	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	BU	959	0	1019	35	0
40	DU	959	0	1019	49	0
41	BV	766	0	827	24	0
41	DV	770	0	838	40	0
42	BW	890	0	951	33	0
42	DW	877	0	932	32	0
43	BX	742	0	799	36	0
43	DX	732	0	777	17	0
44	BY	785	0	828	25	0
44	DY	781	0	829	42	0
45	BZ	1454	0	1452	66	0
45	DZ	1451	0	1421	72	0
46	B0	594	0	604	30	0
46	D0	607	0	622	39	0
47	B1	745	0	804	33	0
47	D1	745	0	804	37	0
48	B2	588	0	643	28	0
48	D2	584	0	623	26	0
49	B3	458	0	503	16	0
49	D3	453	0	501	28	0
50	B4	349	0	336	22	0
50	D4	349	0	336	19	0
51	B5	455	0	472	20	0
51	D5	451	0	461	25	0
52	B6	449	0	462	25	0
52	D6	437	0	440	16	0
53	B7	418	0	467	22	0
53	D7	402	0	434	11	0
54	B8	509	0	565	24	0
54	D8	509	0	565	26	0
55	B9	297	0	316	16	0
55	D9	292	0	313	14	0
56	AA	348	0	0	0	0
56	AD	2	0	0	0	0
56	AE	1	0	0	0	0
56	AF	1	0	0	0	0
56	AI	2	0	0	0	0
56	AK	1	0	0	0	0
56	AT	1	0	0	0	0
56	AV	18	0	0	0	0
56	AY	1	0	0	0	0
56	B0	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B1	3	0	0	0	0
56	B2	2	0	0	0	0
56	B3	2	0	0	0	0
56	B5	3	0	0	0	0
56	B6	1	0	0	0	0
56	B7	1	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0
56	BA	896	0	0	0	0
56	BB	30	0	0	0	0
56	BD	5	0	0	0	0
56	BE	5	0	0	0	0
56	BF	7	0	0	0	0
56	BG	2	0	0	0	0
56	BO	2	0	0	0	0
56	BP	2	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	2	0	0	0	0
56	BT	1	0	0	0	0
56	BU	1	0	0	0	0
56	BV	2	0	0	0	0
56	BX	1	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	2	0	0	0	0
56	CA	219	0	0	0	0
56	CD	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	10	0	0	0	0
56	CX	1	0	0	0	0
56	D0	4	0	0	0	0
56	D1	1	0	0	0	0
56	D5	1	0	0	0	0
56	D6	2	0	0	0	0
56	D7	1	0	0	0	0
56	D8	1	0	0	0	0
56	DA	696	0	0	0	0
56	DB	16	0	0	0	0
56	DD	4	0	0	0	0
56	DE	4	0	0	0	0
56	DF	3	0	0	0	0
56	DO	3	0	0	0	0
56	DQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DR	1	0	0	0	0
56	DT	3	0	0	0	0
56	DU	1	0	0	0	0
56	DV	1	0	0	0	0
56	DX	1	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0
57	B6	1	0	0	0	0
57	B9	1	0	0	0	0
57	BY	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
57	D4	1	0	0	0	0
57	D5	1	0	0	0	0
57	D6	1	0	0	0	0
57	D9	1	0	0	0	0
57	DY	1	0	0	0	0
58	AA	372	0	0	22	0
58	AD	2	0	0	0	0
58	AE	3	0	0	0	0
58	AI	1	0	0	1	0
58	AK	2	0	0	0	0
58	AL	2	0	0	0	0
58	AN	1	0	0	0	0
58	AT	5	0	0	1	0
58	AV	16	0	0	1	0
58	AX	1	0	0	0	0
58	AY	2	0	0	1	0
58	B0	4	0	0	0	0
58	B1	1	0	0	0	0
58	B3	1	0	0	0	0
58	B6	4	0	0	0	0
58	B7	2	0	0	0	0
58	B8	4	0	0	1	0
58	B9	1	0	0	0	0
58	BA	1491	0	0	71	0
58	BB	46	0	0	1	0
58	BD	10	0	0	0	0
58	BE	5	0	0	0	0
58	BF	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BG	5	0	0	1	0
58	BH	1	0	0	0	0
58	BN	3	0	0	0	0
58	BO	3	0	0	0	0
58	BP	9	0	0	2	0
58	BQ	4	0	0	0	0
58	BR	7	0	0	0	0
58	BT	1	0	0	0	0
58	BU	7	0	0	1	0
58	BV	1	0	0	0	0
58	BW	2	0	0	0	0
58	BX	2	0	0	0	0
58	BY	1	0	0	0	0
58	CA	330	0	0	17	0
58	CB	1	0	0	1	0
58	CC	1	0	0	0	0
58	CD	3	0	0	0	0
58	CE	1	0	0	0	0
58	CK	2	0	0	0	0
58	CL	3	0	0	1	0
58	CN	2	0	0	0	0
58	CO	2	0	0	1	0
58	CQ	2	0	0	1	0
58	CT	2	0	0	0	0
58	CV	13	0	0	0	0
58	CX	1	0	0	0	0
58	D1	3	0	0	1	0
58	D3	1	0	0	0	0
58	D6	2	0	0	0	0
58	D7	2	0	0	0	0
58	D8	4	0	0	1	0
58	DA	1028	0	0	63	0
58	DB	40	0	0	2	0
58	DD	8	0	0	0	0
58	DE	11	0	0	1	0
58	DF	4	0	0	0	0
58	DG	1	0	0	0	0
58	DN	3	0	0	0	0
58	DO	5	0	0	1	0
58	DP	4	0	0	0	0
58	DR	5	0	0	1	0
58	DT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DV	1	0	0	0	0
58	DW	1	0	0	0	0
58	DY	2	0	0	0	0
All	All	284877	0	186478	7600	1

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 17.

The worst 5 of 7600 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
55:D9:11:CYS:SG	55:D9:32:HIS:HE1	1.40	1.43
25:DA:885:C:N4	25:DA:890:A:N6	1.81	1.27
25:BA:885:C:N4	25:BA:890:A:N6	1.88	1.22
1:CA:1358:U:H3	1:CA:1363(A):A:N6	1.35	1.22
1:AA:1358:U:H3	1:AA:1363(A):A:N6	1.41	1.16

All (1) 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)
6:AF:14:LEU:O	4:CD:20:TYR:OH[3.654]	2.11	0.09

## 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	AB	231/256 (90%)	179 (78%)	50 (22%)	2 (1%)	25 76
2	CB	233/256 (91%)	182 (78%)	45 (19%)	6 (3%)	8 47
3	AC	202/239 (84%)	165 (82%)	33 (16%)	4 (2%)	11 56
3	CC	204/239 (85%)	168 (82%)	36 (18%)	0	100 100
4	AD	206/209 (99%)	166 (81%)	35 (17%)	5 (2%)	9 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	9	51
5	AE	146/162 (90%)	120 (82%)	26 (18%)	0	100	100
5	CE	147/162 (91%)	129 (88%)	13 (9%)	5 (3%)	6	38
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
7	AG	152/156 (97%)	134 (88%)	17 (11%)	1 (1%)	30	80
7	CG	152/156 (97%)	131 (86%)	20 (13%)	1 (1%)	30	80
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	30	80
8	CH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	AI	123/128 (96%)	105 (85%)	15 (12%)	3 (2%)	9	51
9	CI	123/128 (96%)	106 (86%)	13 (11%)	4 (3%)	6	38
10	AJ	94/105 (90%)	81 (86%)	9 (10%)	4 (4%)	4	30
10	CJ	94/105 (90%)	74 (79%)	17 (18%)	3 (3%)	6	39
11	AK	113/129 (88%)	101 (89%)	11 (10%)	1 (1%)	25	76
11	CK	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
12	AL	120/132 (91%)	108 (90%)	10 (8%)	2 (2%)	14	62
12	CL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	14	62
13	AM	113/126 (90%)	89 (79%)	20 (18%)	4 (4%)	6	37
13	CM	110/126 (87%)	82 (74%)	21 (19%)	7 (6%)	2	17
14	AN	57/61 (93%)	44 (77%)	13 (23%)	0	100	100
14	CN	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	13	60
15	AO	86/89 (97%)	74 (86%)	12 (14%)	0	100	100
15	CO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	AP	79/88 (90%)	62 (78%)	14 (18%)	3 (4%)	5	34
16	CP	80/88 (91%)	66 (82%)	10 (12%)	4 (5%)	3	26
17	AQ	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	22	74
17	CQ	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	22	74
18	AR	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
18	CR	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
19	AS	79/93 (85%)	63 (80%)	15 (19%)	1 (1%)	18	68
19	CS	73/93 (78%)	60 (82%)	13 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	94/106 (89%)	73 (78%)	19 (20%)	2 (2%)	11	55
20	CT	102/106 (96%)	73 (72%)	26 (26%)	3 (3%)	7	43
21	AU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	AY	130/140 (93%)	107 (82%)	21 (16%)	2 (2%)	15	64
27	BD	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	30	80
28	BE	202/206 (98%)	189 (94%)	9 (4%)	4 (2%)	11	56
28	DE	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	15	64
29	BF	198/210 (94%)	183 (92%)	15 (8%)	0	100	100
29	DF	198/210 (94%)	175 (88%)	23 (12%)	0	100	100
30	BG	179/182 (98%)	158 (88%)	17 (10%)	4 (2%)	10	53
30	DG	178/182 (98%)	150 (84%)	28 (16%)	0	100	100
31	BH	172/180 (96%)	160 (93%)	12 (7%)	0	100	100
31	DH	172/180 (96%)	153 (89%)	17 (10%)	2 (1%)	19	70
32	BI	145/148 (98%)	116 (80%)	25 (17%)	4 (3%)	8	44
32	DI	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	16	66
33	BN	138/140 (99%)	124 (90%)	11 (8%)	3 (2%)	10	53
33	DN	138/140 (99%)	117 (85%)	19 (14%)	2 (1%)	16	66
34	BO	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	27	77
34	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	BP	147/150 (98%)	128 (87%)	17 (12%)	2 (1%)	16	66
35	DP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	16	66
36	BQ	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	16	66
36	DQ	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
37	BR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
37	DR	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
38	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	8	44
38	DS	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	12	59
39	BT	130/146 (89%)	124 (95%)	6 (5%)	0	100	100
39	DT	128/146 (88%)	119 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
40	DU	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
41	BV	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
41	DV	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
42	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
42	DW	109/113 (96%)	97 (89%)	12 (11%)	0	100	100
43	BX	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
43	DX	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
44	BY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	74
44	DY	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	22	74
45	BZ	184/206 (89%)	161 (88%)	21 (11%)	2 (1%)	21	72
45	DZ	187/206 (91%)	163 (87%)	21 (11%)	3 (2%)	14	63
46	B0	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
46	D0	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
47	B1	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	21	72
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	B2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	15	64
48	D2	69/72 (96%)	60 (87%)	9 (13%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	13	60
49	D3	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
50	B4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
50	D4	44/71 (62%)	34 (77%)	9 (20%)	1 (2%)	10	52
51	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
51	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
53	B7	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	4	30
53	D7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	10	53
54	B8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
54	D8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	B9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	D9	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
All	All	11478/12268 (94%)	10072 (88%)	1276 (11%)	130 (1%)	21	72

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	77	ALA
3	AC	99	VAL
3	AC	100	ALA
3	AC	157	ILE
4	AD	110	PHE

### 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	AB	180/220 (82%)	127 (71%)	53 (29%)	0	1
2	CB	181/220 (82%)	132 (73%)	49 (27%)	1	2
3	AC	112/188 (60%)	89 (80%)	23 (20%)	2	8
3	CC	114/188 (61%)	96 (84%)	18 (16%)	4	16
4	AD	139/181 (77%)	112 (81%)	27 (19%)	2	10
4	CD	142/181 (78%)	112 (79%)	30 (21%)	1	8
5	AE	108/123 (88%)	77 (71%)	31 (29%)	0	1
5	CE	109/123 (89%)	84 (77%)	25 (23%)	1	5
6	AF	77/90 (86%)	64 (83%)	13 (17%)	3	14
6	CF	76/90 (84%)	61 (80%)	15 (20%)	2	10
7	AG	103/127 (81%)	83 (81%)	20 (19%)	2	10
7	CG	102/127 (80%)	78 (76%)	24 (24%)	1	5
8	AH	103/119 (87%)	85 (82%)	18 (18%)	3	13
8	CH	104/119 (87%)	89 (86%)	15 (14%)	5	22
9	AI	64/99 (65%)	55 (86%)	9 (14%)	5	23
9	CI	62/99 (63%)	52 (84%)	10 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	52/92 (56%)	38 (73%)	14 (27%)	1	2
10	CJ	52/92 (56%)	36 (69%)	16 (31%)	0	1
11	AK	83/99 (84%)	60 (72%)	23 (28%)	0	2
11	CK	81/99 (82%)	61 (75%)	20 (25%)	1	3
12	AL	92/109 (84%)	73 (79%)	19 (21%)	2	8
12	CL	91/109 (84%)	71 (78%)	20 (22%)	1	7
13	AM	66/101 (65%)	44 (67%)	22 (33%)	0	0
13	CM	62/101 (61%)	39 (63%)	23 (37%)	0	0
14	AN	46/50 (92%)	40 (87%)	6 (13%)	6	28
14	CN	45/50 (90%)	30 (67%)	15 (33%)	0	0
15	AO	77/80 (96%)	61 (79%)	16 (21%)	2	8
15	CO	77/80 (96%)	64 (83%)	13 (17%)	3	14
16	AP	63/74 (85%)	44 (70%)	19 (30%)	0	1
16	CP	65/74 (88%)	49 (75%)	16 (25%)	1	3
17	AQ	94/97 (97%)	79 (84%)	15 (16%)	3	16
17	CQ	93/97 (96%)	77 (83%)	16 (17%)	3	14
18	AR	49/77 (64%)	41 (84%)	8 (16%)	3	15
18	CR	49/77 (64%)	36 (74%)	13 (26%)	1	2
19	AS	43/80 (54%)	34 (79%)	9 (21%)	1	8
19	CS	42/80 (52%)	28 (67%)	14 (33%)	0	0
20	AT	66/82 (80%)	47 (71%)	19 (29%)	0	1
20	CT	72/82 (88%)	56 (78%)	16 (22%)	1	6
21	AU	20/22 (91%)	14 (70%)	6 (30%)	0	1
21	CU	14/22 (64%)	13 (93%)	1 (7%)	21	63
22	AY	108/115 (94%)	74 (68%)	34 (32%)	0	1
27	BD	214/218 (98%)	169 (79%)	45 (21%)	1	8
27	DD	215/218 (99%)	167 (78%)	48 (22%)	1	6
28	BE	163/166 (98%)	126 (77%)	37 (23%)	1	6
28	DE	163/166 (98%)	128 (78%)	35 (22%)	1	7
29	BF	158/166 (95%)	123 (78%)	35 (22%)	1	6
29	DF	159/166 (96%)	128 (80%)	31 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BG	128/156 (82%)	103 (80%)	25 (20%)	2	10
30	DG	127/156 (81%)	95 (75%)	32 (25%)	1	3
31	BH	141/148 (95%)	113 (80%)	28 (20%)	2	9
31	DH	141/148 (95%)	111 (79%)	30 (21%)	1	7
32	BI	105/124 (85%)	75 (71%)	30 (29%)	0	1
32	DI	104/124 (84%)	76 (73%)	28 (27%)	1	2
33	BN	117/119 (98%)	93 (80%)	24 (20%)	2	8
33	DN	117/119 (98%)	90 (77%)	27 (23%)	1	5
34	BO	98/100 (98%)	73 (74%)	25 (26%)	1	3
34	DO	98/100 (98%)	70 (71%)	28 (29%)	0	1
35	BP	114/116 (98%)	87 (76%)	27 (24%)	1	4
35	DP	114/116 (98%)	90 (79%)	24 (21%)	1	8
36	BQ	111/111 (100%)	91 (82%)	20 (18%)	2	12
36	DQ	111/111 (100%)	93 (84%)	18 (16%)	3	15
37	BR	101/101 (100%)	79 (78%)	22 (22%)	1	7
37	DR	101/101 (100%)	79 (78%)	22 (22%)	1	7
38	BS	84/88 (96%)	66 (79%)	18 (21%)	1	7
38	DS	86/88 (98%)	68 (79%)	18 (21%)	1	8
39	BT	111/127 (87%)	90 (81%)	21 (19%)	2	11
39	DT	110/127 (87%)	82 (74%)	28 (26%)	1	3
40	BU	93/94 (99%)	77 (83%)	16 (17%)	3	14
40	DU	93/94 (99%)	77 (83%)	16 (17%)	3	14
41	BV	80/82 (98%)	66 (82%)	14 (18%)	3	13
41	DV	81/82 (99%)	56 (69%)	25 (31%)	0	1
42	BW	91/92 (99%)	71 (78%)	20 (22%)	1	7
42	DW	89/92 (97%)	74 (83%)	15 (17%)	3	14
43	BX	75/78 (96%)	63 (84%)	12 (16%)	3	16
43	DX	73/78 (94%)	61 (84%)	12 (16%)	3	15
44	BY	80/91 (88%)	63 (79%)	17 (21%)	1	7
44	DY	79/91 (87%)	59 (75%)	20 (25%)	1	3
45	BZ	156/179 (87%)	128 (82%)	28 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DZ	152/179 (85%)	119 (78%)	33 (22%)	1	7
46	B0	59/67 (88%)	47 (80%)	12 (20%)	2	9
46	D0	61/67 (91%)	47 (77%)	14 (23%)	1	5
47	B1	78/83 (94%)	61 (78%)	17 (22%)	1	7
47	D1	78/83 (94%)	58 (74%)	20 (26%)	1	2
48	B2	65/67 (97%)	49 (75%)	16 (25%)	1	3
48	D2	63/67 (94%)	50 (79%)	13 (21%)	2	8
49	B3	49/52 (94%)	44 (90%)	5 (10%)	11	40
49	D3	49/52 (94%)	40 (82%)	9 (18%)	2	11
50	B4	39/63 (62%)	28 (72%)	11 (28%)	0	2
50	D4	39/63 (62%)	25 (64%)	14 (36%)	0	0
51	B5	50/52 (96%)	41 (82%)	9 (18%)	2	12
51	D5	49/52 (94%)	39 (80%)	10 (20%)	2	8
52	B6	50/52 (96%)	34 (68%)	16 (32%)	0	1
52	D6	48/52 (92%)	38 (79%)	10 (21%)	2	8
53	B7	41/42 (98%)	32 (78%)	9 (22%)	1	7
53	D7	38/42 (90%)	30 (79%)	8 (21%)	1	8
54	B8	52/55 (94%)	45 (86%)	7 (14%)	6	26
54	D8	52/55 (94%)	43 (83%)	9 (17%)	3	13
55	B9	32/34 (94%)	26 (81%)	6 (19%)	2	11
55	D9	32/34 (94%)	25 (78%)	7 (22%)	1	7
All	All	8835/10181 (87%)	6886 (78%)	1949 (22%)	1	7

5 of 1949 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B1	26	ARG
5	CE	112	LEU
44	DY	107	ASP
48	B2	51	ARG
2	CB	80	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:



Mol	Chain	Res	Type
45	BZ	54	HIS
6	CF	73	ASN
46	D0	12	ASN
52	B6	20	ASN
2	CB	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1462/1522 (96%)	386 (26%)	33 (2%)
1	CA	1457/1522 (95%)	367 (25%)	33 (2%)
23	AV	76/77 (98%)	20 (26%)	1 (1%)
23	CV	76/77 (98%)	21 (27%)	0
24	AX	5/16 (31%)	1 (20%)	0
24	CX	5/16 (31%)	0	0
25	BA	2744/2915 (94%)	642 (23%)	64 (2%)
25	DA	2711/2915 (93%)	632 (23%)	55 (2%)
26	BB	119/122 (97%)	24 (20%)	0
26	DB	119/122 (97%)	26 (21%)	2 (1%)
All	All	8774/9304 (94%)	2119 (24%)	188 (2%)

5 of 2119 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	13	U
1	AA	22	G
1	AA	28	G

5 of 188 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2318	G
1	CA	428	G
25	DA	2282	G
25	BA	2335	A
25	BA	2778	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2350 ligands modelled in this entry, 2350 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1466/1522 (96%)	-0.28	17 (1%) 75 26	43, 93, 137, 172	0
1	CA	1461/1522 (95%)	-0.18	18 (1%) 75 26	55, 104, 145, 167	0
2	AB	233/256 (91%)	-0.18	0 100 100	72, 113, 134, 153	0
2	CB	235/256 (91%)	-0.03	3 (1%) 74 24	100, 125, 139, 147	0
3	AC	204/239 (85%)	-0.15	0 100 100	97, 112, 125, 133	0
3	CC	206/239 (86%)	-0.01	1 (0%) 88 46	110, 125, 136, 142	0
4	AD	208/209 (99%)	-0.22	0 100 100	76, 103, 118, 125	0
4	CD	208/209 (99%)	-0.26	0 100 100	85, 98, 114, 120	0
5	AE	148/162 (91%)	-0.31	0 100 100	67, 89, 108, 134	0
5	CE	149/162 (91%)	-0.22	0 100 100	83, 99, 110, 131	0
6	AF	100/101 (99%)	-0.34	0 100 100	68, 88, 104, 110	0
6	CF	100/101 (99%)	-0.33	0 100 100	78, 96, 110, 117	0
7	AG	154/156 (98%)	-0.14	2 (1%) 74 24	87, 102, 120, 133	0
7	CG	154/156 (98%)	0.03	7 (4%) 32 6	107, 119, 133, 144	0
8	AH	138/138 (100%)	-0.31	0 100 100	73, 91, 100, 111	0
8	CH	138/138 (100%)	-0.29	0 100 100	82, 100, 111, 116	0
9	AI	125/128 (97%)	-0.05	1 (0%) 83 35	71, 114, 126, 137	0
9	CI	125/128 (97%)	0.22	3 (2%) 56 13	101, 130, 138, 142	0
10	AJ	96/105 (91%)	0.16	1 (1%) 79 29	88, 119, 136, 140	0
10	CJ	96/105 (91%)	0.54	4 (4%) 35 7	111, 133, 141, 143	0
11	AK	115/129 (89%)	-0.28	0 100 100	53, 87, 104, 113	0
11	CK	114/129 (88%)	-0.17	0 100 100	78, 103, 118, 127	0
12	AL	122/132 (92%)	-0.33	0 100 100	61, 84, 100, 111	0
12	CL	122/132 (92%)	-0.24	0 100 100	72, 90, 105, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	115/126 (91%)	-0.19	0 100 100	66, 100, 113, 118	0
13	CM	112/126 (88%)	0.02	0 100 100	102, 127, 135, 139	0
14	AN	59/61 (96%)	-0.09	1 (1%) 67 19	94, 106, 114, 121	0
14	CN	59/61 (96%)	0.33	1 (1%) 67 19	116, 125, 133, 135	0
15	AO	88/89 (98%)	-0.26	0 100 100	65, 86, 106, 117	0
15	CO	88/89 (98%)	-0.22	0 100 100	74, 96, 114, 118	0
16	AP	81/88 (92%)	-0.21	0 100 100	83, 100, 122, 127	0
16	CP	82/88 (93%)	-0.22	0 100 100	84, 94, 112, 122	0
17	AQ	99/105 (94%)	-0.18	0 100 100	68, 89, 104, 113	0
17	CQ	99/105 (94%)	-0.24	0 100 100	77, 95, 110, 113	0
18	AR	68/88 (77%)	-0.33	0 100 100	69, 84, 102, 106	0
18	CR	68/88 (77%)	-0.22	0 100 100	82, 92, 111, 115	0
19	AS	81/93 (87%)	-0.05	0 100 100	96, 110, 130, 141	0
19	CS	75/93 (80%)	0.30	4 (5%) 25 5	107, 131, 142, 146	0
20	AT	96/106 (90%)	-0.23	0 100 100	77, 97, 113, 118	0
20	CT	104/106 (98%)	-0.14	0 100 100	81, 101, 123, 139	0
21	AU	25/27 (92%)	0.47	0 100 100	80, 98, 105, 107	0
21	CU	23/27 (85%)	1.09	3 (13%) 4 1	115, 126, 132, 134	0
22	AY	132/140 (94%)	0.83	11 (8%) 11 3	69, 110, 138, 152	0
23	AV	77/77 (100%)	-0.20	1 (1%) 74 24	55, 82, 112, 134	0
23	CV	77/77 (100%)	-0.11	2 (2%) 53 11	73, 109, 133, 156	0
24	AX	6/16 (37%)	0.93	1 (16%) 2 1	67, 73, 127, 128	0
24	CX	6/16 (37%)	0.98	2 (33%) 1 0	89, 96, 142, 147	0
25	BA	2752/2915 (94%)	-0.55	21 (0%) 83 35	23, 43, 115, 170	0
25	DA	2722/2915 (93%)	-0.40	35 (1%) 74 24	44, 74, 127, 170	0
26	BB	120/122 (98%)	-0.57	0 100 100	36, 64, 90, 125	0
26	DB	120/122 (98%)	-0.07	0 100 100	73, 114, 129, 146	0
27	BD	275/276 (99%)	-0.44	1 (0%) 90 51	27, 43, 62, 110	0
27	DD	275/276 (99%)	-0.28	1 (0%) 90 51	41, 62, 82, 100	0
28	BE	204/206 (99%)	-0.48	0 100 100	22, 45, 71, 94	0
28	DE	204/206 (99%)	-0.32	0 100 100	43, 74, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	BF	203/210 (96%)	-0.42	0 100 100	26, 49, 87, 115	0
29	DF	203/210 (96%)	-0.29	0 100 100	47, 88, 114, 127	0
30	BG	181/182 (99%)	-0.35	0 100 100	58, 77, 105, 116	0
30	DG	180/182 (98%)	-0.15	0 100 100	101, 117, 127, 136	0
31	BH	174/180 (96%)	-0.36	0 100 100	38, 65, 84, 98	0
31	DH	174/180 (96%)	0.16	1 (0%) 86 41	96, 116, 130, 140	0
32	BI	147/148 (99%)	-0.29	0 100 100	50, 95, 112, 128	0
32	DI	146/148 (98%)	-0.10	0 100 100	68, 108, 126, 131	0
33	BN	140/140 (100%)	-0.49	0 100 100	30, 42, 69, 83	0
33	DN	140/140 (100%)	-0.24	0 100 100	64, 86, 107, 117	0
34	BO	122/122 (100%)	-0.47	0 100 100	33, 52, 71, 82	0
34	DO	122/122 (100%)	-0.42	0 100 100	57, 73, 88, 96	0
35	BP	149/150 (99%)	-0.41	0 100 100	25, 55, 86, 108	0
35	DP	149/150 (99%)	-0.19	0 100 100	52, 91, 116, 127	0
36	BQ	141/141 (100%)	-0.44	0 100 100	33, 50, 70, 90	0
36	DQ	141/141 (100%)	-0.22	1 (0%) 84 38	67, 90, 106, 114	0
37	BR	118/118 (100%)	-0.53	0 100 100	27, 41, 59, 67	0
37	DR	118/118 (100%)	-0.39	0 100 100	49, 65, 86, 95	0
38	BS	110/112 (98%)	-0.43	0 100 100	44, 62, 86, 97	0
38	DS	110/112 (98%)	-0.15	0 100 100	90, 109, 119, 127	0
39	BT	132/146 (90%)	-0.49	0 100 100	41, 55, 94, 127	0
39	DT	130/146 (89%)	-0.35	0 100 100	62, 77, 108, 123	0
40	BU	116/118 (98%)	-0.53	0 100 100	25, 36, 55, 71	0
40	DU	116/118 (98%)	-0.31	1 (0%) 81 32	54, 82, 103, 108	0
41	BV	100/101 (99%)	-0.52	0 100 100	28, 46, 73, 90	0
41	DV	100/101 (99%)	-0.15	0 100 100	56, 98, 119, 123	0
42	BW	112/113 (99%)	-0.45	0 100 100	28, 37, 63, 89	0
42	DW	111/113 (98%)	-0.31	0 100 100	49, 63, 89, 114	0
43	BX	95/96 (98%)	-0.46	0 100 100	34, 46, 77, 92	0
43	DX	95/96 (98%)	-0.30	0 100 100	61, 77, 100, 107	0
44	BY	107/110 (97%)	-0.34	0 100 100	41, 60, 91, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DY	107/110 (97%)	-0.04	2 (1%) 64 18	77, 96, 112, 124	0
45	BZ	186/206 (90%)	-0.32	0 100 100	49, 76, 104, 126	0
45	DZ	189/206 (91%)	0.02	0 100 100	98, 114, 131, 139	0
46	B0	76/85 (89%)	-0.45	0 100 100	32, 42, 59, 83	0
46	D0	77/85 (90%)	-0.08	0 100 100	73, 85, 101, 124	0
47	B1	97/98 (98%)	-0.31	0 100 100	32, 51, 90, 104	0
47	D1	97/98 (98%)	-0.17	0 100 100	50, 72, 105, 115	0
48	B2	70/72 (97%)	-0.39	0 100 100	41, 60, 78, 103	0
48	D2	71/72 (98%)	-0.20	1 (1%) 72 22	78, 94, 106, 110	0
49	B3	59/60 (98%)	-0.50	0 100 100	33, 41, 76, 93	0
49	D3	58/60 (96%)	-0.01	0 100 100	71, 84, 114, 128	0
50	B4	46/71 (64%)	-0.44	0 100 100	78, 96, 112, 114	0
50	D4	46/71 (64%)	-0.19	0 100 100	118, 126, 136, 138	0
51	B5	59/60 (98%)	-0.56	0 100 100	25, 41, 62, 74	0
51	D5	59/60 (98%)	-0.41	0 100 100	47, 66, 85, 106	0
52	B6	53/54 (98%)	-0.48	0 100 100	42, 49, 66, 76	0
52	D6	53/54 (98%)	-0.27	0 100 100	67, 81, 93, 101	0
53	B7	48/49 (97%)	-0.30	0 100 100	25, 33, 68, 89	0
53	D7	48/49 (97%)	-0.21	0 100 100	41, 53, 82, 105	0
54	B8	64/65 (98%)	-0.44	0 100 100	35, 41, 49, 72	0
54	D8	64/65 (98%)	-0.22	0 100 100	60, 71, 83, 94	0
55	B9	36/37 (97%)	-0.21	0 100 100	33, 46, 58, 72	0
55	D9	35/37 (94%)	0.29	1 (2%) 49 10	73, 88, 103, 115	0
All	All	20489/21572 (94%)	-0.29	148 (0%) 84 38	22, 83, 131, 172	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	BA	1509	C	9.5
1	CA	1286	A	6.1
25	BA	1508	A	5.4
25	BA	2801(A)	A	5.0
25	DA	1509	C	5.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3540	1/1	0.25	-	57,57,57,57	0
56	MG	BA	3013	1/1	0.31	-	57,57,57,57	0
56	MG	DB	215	1/1	0.12	-	94,94,94,94	0
56	MG	AA	1838	1/1	0.16	-	72,72,72,72	0
56	MG	BA	3076	1/1	0.53	-	39,39,39,39	0
56	MG	DA	3229	1/1	0.44	-	52,52,52,52	0
56	MG	DA	3461	1/1	0.29	-	50,50,50,50	0
56	MG	BA	3128	1/1	0.32	-	60,60,60,60	0
56	MG	DA	3435	1/1	0.09	-	70,70,70,70	0
56	MG	DA	3486	1/1	0.24	-	42,42,42,42	0
56	MG	BA	3162	1/1	0.18	-	36,36,36,36	0
56	MG	DA	3056	1/1	0.28	-	59,59,59,59	0
56	MG	DA	3314	1/1	0.17	-	52,52,52,52	0
56	MG	DA	3284	1/1	0.52	-	75,75,75,75	0
56	MG	DA	3035	1/1	0.23	-	76,76,76,76	0
56	MG	BA	3594	1/1	0.15	-	44,44,44,44	0
56	MG	DA	3159	1/1	0.25	-	66,66,66,66	0
56	MG	DA	3441	1/1	0.18	-	72,72,72,72	0
56	MG	BA	3873	1/1	0.07	-	74,74,74,74	0
56	MG	AA	1841	1/1	0.08	-	75,75,75,75	0
56	MG	AA	1821	1/1	0.24	-	78,78,78,78	0
56	MG	DO	202	1/1	0.16	-	95,95,95,95	0
56	MG	BA	3721	1/1	0.24	-	23,23,23,23	0
56	MG	BA	3374	1/1	0.37	-	24,24,24,24	0
56	MG	DA	3146	1/1	0.24	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	D5	101	1/1	0.57	-	62,62,62,62	0
56	MG	BA	3338	1/1	0.30	-	63,63,63,63	0
56	MG	DA	3425	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3354	1/1	0.09	-	34,34,34,34	0
56	MG	BA	3795	1/1	0.22	-	84,84,84,84	0
56	MG	BA	3853	1/1	0.25	-	76,76,76,76	0
56	MG	AA	1633	1/1	0.48	-	32,32,32,32	0
56	MG	AA	1751	1/1	0.21	-	74,74,74,74	0
56	MG	DA	3577	1/1	0.17	-	95,95,95,95	0
56	MG	BA	3135	1/1	0.30	-	58,58,58,58	0
56	MG	BA	3344	1/1	0.17	-	62,62,62,62	0
56	MG	DA	3646	1/1	0.18	-	62,62,62,62	0
56	MG	AA	1833	1/1	0.18	-	70,70,70,70	0
56	MG	B2	101	1/1	0.21	-	63,63,63,63	0
56	MG	AA	1805	1/1	0.74	-	89,89,89,89	0
56	MG	DA	3516	1/1	0.16	-	50,50,50,50	0
56	MG	BA	3556	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3507	1/1	0.30	-	53,53,53,53	0
56	MG	DA	3287	1/1	0.38	-	62,62,62,62	0
56	MG	DA	3422	1/1	0.09	-	47,47,47,47	0
57	ZN	D4	101	1/1	0.12	-	178,178,178,178	0
56	MG	BA	3667	1/1	0.10	-	27,27,27,27	0
56	MG	DA	3645	1/1	0.06	-	93,93,93,93	0
56	MG	DA	3281	1/1	0.26	-	70,70,70,70	0
56	MG	DA	3258	1/1	0.44	-	91,91,91,91	0
56	MG	DA	3015	1/1	0.18	-	66,66,66,66	0
56	MG	DA	3315	1/1	0.51	-	47,47,47,47	0
56	MG	DA	3561	1/1	0.20	-	70,70,70,70	0
56	MG	AA	1629	1/1	0.39	-	68,68,68,68	0
56	MG	AA	1649	1/1	0.17	-	60,60,60,60	0
56	MG	CA	1717	1/1	0.50	-	77,77,77,77	0
56	MG	CA	1783	1/1	0.06	-	78,78,78,78	0
56	MG	BA	3393	1/1	0.13	-	28,28,28,28	0
56	MG	DA	3426	1/1	0.14	-	42,42,42,42	0
56	MG	BA	3359	1/1	0.46	-	72,72,72,72	0
56	MG	DA	3613	1/1	0.11	-	60,60,60,60	0
56	MG	DA	3469	1/1	0.09	-	84,84,84,84	0
56	MG	DA	3048	1/1	0.14	-	74,74,74,74	0
56	MG	BA	3236	1/1	0.15	-	50,50,50,50	0
56	MG	AV	107	1/1	0.30	-	87,87,87,87	0
56	MG	BA	3027	1/1	0.16	-	44,44,44,44	0
56	MG	DA	3026	1/1	0.21	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1643	1/1	0.40	-	53,53,53,53	0
56	MG	BA	3539	1/1	0.12	-	22,22,22,22	0
56	MG	AA	1857	1/1	0.23	-	62,62,62,62	0
56	MG	CA	1800	1/1	0.06	-	105,105,105,105	0
56	MG	DA	3543	1/1	0.06	-	74,74,74,74	0
56	MG	BA	3335	1/1	0.29	-	47,47,47,47	0
56	MG	DA	3419	1/1	0.24	-	35,35,35,35	0
56	MG	BA	3254	1/1	0.37	-	21,21,21,21	0
56	MG	AA	1734	1/1	0.24	-	80,80,80,80	0
56	MG	BA	3818	1/1	0.29	-	86,86,86,86	0
56	MG	AV	104	1/1	0.32	-	81,81,81,81	0
56	MG	DA	3311	1/1	0.36	-	68,68,68,68	0
56	MG	BA	3042	1/1	0.25	-	37,37,37,37	0
56	MG	BV	201	1/1	0.45	-	39,39,39,39	0
56	MG	DA	3444	1/1	0.09	-	54,54,54,54	0
56	MG	AA	1609	1/1	0.59	-	61,61,61,61	0
56	MG	BA	3472	1/1	0.62	-	58,58,58,58	0
56	MG	BA	3835	1/1	0.37	-	86,86,86,86	0
56	MG	DA	3438	1/1	0.11	-	66,66,66,66	0
56	MG	DA	3414	1/1	0.15	-	50,50,50,50	0
56	MG	DA	3538	1/1	0.25	-	96,96,96,96	0
56	MG	AA	1822	1/1	0.48	-	77,77,77,77	0
56	MG	CA	1619	1/1	0.35	-	71,71,71,71	0
56	MG	BA	3308	1/1	0.19	-	51,51,51,51	0
56	MG	DA	3181	1/1	0.22	-	59,59,59,59	0
56	MG	CA	1609	1/1	0.12	-	70,70,70,70	0
56	MG	DA	3497	1/1	0.19	-	70,70,70,70	0
56	MG	BA	3170	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3430	1/1	0.21	-	83,83,83,83	0
56	MG	AA	1842	1/1	0.56	-	89,89,89,89	0
56	MG	DA	3629	1/1	0.37	-	104,104,104,104	0
56	MG	BA	3103	1/1	0.35	-	54,54,54,54	0
56	MG	AY	201	1/1	0.17	-	111,111,111,111	0
56	MG	BA	3077	1/1	0.23	-	45,45,45,45	0
56	MG	DA	3025	1/1	0.38	-	76,76,76,76	0
56	MG	DA	3530	1/1	0.29	-	72,72,72,72	0
56	MG	BZ	301	1/1	0.25	-	54,54,54,54	0
56	MG	AA	1654	1/1	0.38	-	80,80,80,80	0
56	MG	DA	3692	1/1	0.24	-	46,46,46,46	0
56	MG	CA	1713	1/1	0.15	-	71,71,71,71	0
56	MG	CA	1691	1/1	0.47	-	53,53,53,53	0
56	MG	BA	3119	1/1	0.15	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BU	201	1/1	0.31	-	38,38,38,38	0
56	MG	BA	3772	1/1	0.10	-	26,26,26,26	0
56	MG	AA	1652	1/1	0.26	-	69,69,69,69	0
56	MG	AA	1631	1/1	0.25	-	59,59,59,59	0
56	MG	DB	210	1/1	0.18	-	91,91,91,91	0
57	ZN	DY	201	1/1	0.06	-	123,123,123,123	0
56	MG	DA	3005	1/1	0.41	-	73,73,73,73	0
56	MG	BA	3621	1/1	0.17	-	30,30,30,30	0
56	MG	DA	3149	1/1	0.15	-	51,51,51,51	0
56	MG	AA	1740	1/1	0.48	-	72,72,72,72	0
56	MG	BA	3187	1/1	0.21	-	47,47,47,47	0
56	MG	BA	3676	1/1	0.15	-	20,20,20,20	0
56	MG	BA	3305	1/1	0.18	-	35,35,35,35	0
56	MG	DA	3021	1/1	0.24	-	58,58,58,58	0
56	MG	DA	3595	1/1	0.16	-	43,43,43,43	0
56	MG	BF	301	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3452	1/1	0.35	-	60,60,60,60	0
56	MG	BB	212	1/1	0.26	-	62,62,62,62	0
56	MG	AV	102	1/1	0.19	-	66,66,66,66	0
56	MG	CA	1676	1/1	0.19	-	83,83,83,83	0
56	MG	BA	3089	1/1	0.42	-	54,54,54,54	0
56	MG	BA	3792	1/1	0.21	-	48,48,48,48	0
56	MG	BA	3708	1/1	0.07	-	85,85,85,85	0
56	MG	DA	3163	1/1	0.56	-	68,68,68,68	0
56	MG	BA	3391	1/1	0.25	-	27,27,27,27	0
56	MG	DA	3409	1/1	0.07	-	64,64,64,64	0
56	MG	BA	3470	1/1	0.24	-	52,52,52,52	0
56	MG	DF	302	1/1	0.29	-	75,75,75,75	0
56	MG	BA	3688	1/1	0.12	-	25,25,25,25	0
56	MG	BA	3848	1/1	0.19	-	43,43,43,43	0
56	MG	BA	3815	1/1	0.10	-	51,51,51,51	0
56	MG	AA	1867	1/1	1.13	-	80,80,80,80	0
56	MG	DA	3622	1/1	0.18	-	74,74,74,74	0
56	MG	BY	203	1/1	0.55	-	65,65,65,65	0
56	MG	CA	1660	1/1	0.18	-	92,92,92,92	0
56	MG	DA	3437	1/1	0.17	-	70,70,70,70	0
56	MG	AA	1815	1/1	0.41	-	69,69,69,69	0
56	MG	DA	3554	1/1	0.28	-	49,49,49,49	0
56	MG	DA	3573	1/1	0.16	-	42,42,42,42	0
56	MG	BA	3768	1/1	0.04	-	90,90,90,90	0
56	MG	B2	102	1/1	0.39	-	66,66,66,66	0
56	MG	CA	1764	1/1	0.11	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3012	1/1	0.11	-	76,76,76,76	0
56	MG	BA	3882	1/1	0.08	-	73,73,73,73	0
56	MG	BQ	201	1/1	0.17	-	18,18,18,18	0
56	MG	BA	3459	1/1	0.19	-	49,49,49,49	0
56	MG	DA	3064	1/1	0.28	-	66,66,66,66	0
56	MG	BA	3411	1/1	0.23	-	55,55,55,55	0
56	MG	BA	3191	1/1	0.40	-	78,78,78,78	0
56	MG	DA	3548	1/1	0.16	-	72,72,72,72	0
56	MG	BA	3640	1/1	0.09	-	33,33,33,33	0
56	MG	DA	3061	1/1	0.80	-	78,78,78,78	0
56	MG	BA	3477	1/1	0.32	-	45,45,45,45	0
56	MG	DA	3693	1/1	0.30	-	103,103,103,103	0
56	MG	DA	3665	1/1	0.09	-	87,87,87,87	0
56	MG	BA	3241	1/1	0.31	-	38,38,38,38	0
56	MG	BA	3123	1/1	0.25	-	58,58,58,58	0
56	MG	DA	3143	1/1	0.20	-	50,50,50,50	0
56	MG	DA	3487	1/1	0.06	-	70,70,70,70	0
56	MG	DA	3135	1/1	0.39	-	66,66,66,66	0
56	MG	DA	3051	1/1	0.25	-	60,60,60,60	0
56	MG	BA	3028	1/1	0.16	-	33,33,33,33	0
56	MG	DA	3367	1/1	0.11	-	75,75,75,75	0
56	MG	BA	3137	1/1	0.28	-	55,55,55,55	0
56	MG	BA	3800	1/1	0.11	-	111,111,111,111	0
56	MG	DA	3075	1/1	0.38	-	84,84,84,84	0
56	MG	BA	3635	1/1	0.13	-	75,75,75,75	0
56	MG	CA	1695	1/1	0.13	-	94,94,94,94	0
56	MG	BA	3166	1/1	0.48	-	30,30,30,30	0
56	MG	DA	3277	1/1	0.27	-	67,67,67,67	0
56	MG	BA	3816	1/1	0.12	-	85,85,85,85	0
56	MG	DA	3416	1/1	0.09	-	53,53,53,53	0
56	MG	BA	3404	1/1	0.17	-	52,52,52,52	0
56	MG	AA	1680	1/1	0.11	-	65,65,65,65	0
56	MG	AA	1687	1/1	0.81	-	105,105,105,105	0
56	MG	AA	1911	1/1	0.25	-	106,106,106,106	0
56	MG	AA	1720	1/1	0.45	-	92,92,92,92	0
56	MG	DA	3465	1/1	0.13	-	104,104,104,104	0
56	MG	BB	230	1/1	0.21	-	56,56,56,56	0
56	MG	DA	3436	1/1	0.27	-	50,50,50,50	0
56	MG	DA	3184	1/1	0.35	-	57,57,57,57	0
56	MG	BA	3316	1/1	0.20	-	48,48,48,48	0
56	MG	BA	3844	1/1	0.18	-	99,99,99,99	0
56	MG	AA	1804	1/1	0.17	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1885	1/1	0.23	-	90,90,90,90	0
56	MG	BA	3080	1/1	0.17	-	44,44,44,44	0
56	MG	DA	3598	1/1	0.32	-	69,69,69,69	0
56	MG	BA	3491	1/1	0.30	-	41,41,41,41	0
56	MG	DA	3655	1/1	0.23	-	75,75,75,75	0
56	MG	BA	3026	1/1	0.33	-	92,92,92,92	0
56	MG	BA	3426	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3529	1/1	0.15	-	82,82,82,82	0
56	MG	AA	1923	1/1	0.13	-	115,115,115,115	0
56	MG	DA	3002	1/1	0.28	-	69,69,69,69	0
56	MG	BA	3789	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3563	1/1	0.13	-	45,45,45,45	0
56	MG	BA	3630	1/1	0.12	-	23,23,23,23	0
56	MG	BA	3620	1/1	0.07	-	49,49,49,49	0
56	MG	BB	225	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3454	1/1	0.18	-	91,91,91,91	0
56	MG	CA	1616	1/1	0.62	-	54,54,54,54	0
56	MG	DA	3524	1/1	0.17	-	99,99,99,99	0
56	MG	BA	3256	1/1	0.23	-	77,77,77,77	0
56	MG	DA	3630	1/1	0.21	-	47,47,47,47	0
56	MG	DA	3515	1/1	0.23	-	51,51,51,51	0
56	MG	AV	116	1/1	0.13	-	84,84,84,84	0
56	MG	DA	3262	1/1	0.64	-	67,67,67,67	0
56	MG	DA	3266	1/1	0.23	-	62,62,62,62	0
56	MG	D0	103	1/1	0.17	-	55,55,55,55	0
56	MG	DB	208	1/1	0.18	-	98,98,98,98	0
56	MG	DA	3349	1/1	0.47	-	72,72,72,72	0
56	MG	BA	3619	1/1	0.05	-	86,86,86,86	0
56	MG	BA	3414	1/1	0.12	-	72,72,72,72	0
56	MG	BA	3698	1/1	0.07	-	44,44,44,44	0
56	MG	DA	3318	1/1	0.14	-	83,83,83,83	0
56	MG	CA	1757	1/1	0.30	-	94,94,94,94	0
56	MG	DA	3128	1/1	0.43	-	59,59,59,59	0
56	MG	BA	3874	1/1	0.27	-	90,90,90,90	0
56	MG	BA	3601	1/1	0.13	-	24,24,24,24	0
56	MG	CA	1645	1/1	0.38	-	74,74,74,74	0
56	MG	BA	3005	1/1	0.12	-	59,59,59,59	0
56	MG	BA	3189	1/1	0.25	-	49,49,49,49	0
56	MG	CA	1708	1/1	0.90	-	91,91,91,91	0
56	MG	BA	3525	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3302	1/1	0.36	-	76,76,76,76	0
56	MG	BA	3603	1/1	0.11	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B0	105	1/1	0.13	-	76,76,76,76	0
56	MG	DA	3526	1/1	0.10	-	64,64,64,64	0
56	MG	BA	3666	1/1	0.06	-	28,28,28,28	0
56	MG	AA	1846	1/1	0.29	-	90,90,90,90	0
56	MG	BA	3807	1/1	0.17	-	64,64,64,64	0
56	MG	AA	1924	1/1	0.10	-	80,80,80,80	0
56	MG	BA	3799	1/1	0.09	-	72,72,72,72	0
56	MG	DA	3042	1/1	0.20	-	47,47,47,47	0
56	MG	AA	1707	1/1	0.19	-	64,64,64,64	0
56	MG	BA	3675	1/1	0.19	-	33,33,33,33	0
56	MG	AA	1749	1/1	0.68	-	69,69,69,69	0
56	MG	AA	1831	1/1	0.17	-	63,63,63,63	0
56	MG	BA	3767	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3218	1/1	0.66	-	71,71,71,71	0
56	MG	DA	3207	1/1	0.15	-	74,74,74,74	0
56	MG	CA	1731	1/1	0.44	-	84,84,84,84	0
56	MG	BA	3573	1/1	0.07	-	54,54,54,54	0
56	MG	DA	3477	1/1	0.09	-	78,78,78,78	0
56	MG	BA	3054	1/1	0.26	-	58,58,58,58	0
56	MG	BA	3731	1/1	0.14	-	53,53,53,53	0
56	MG	CA	1641	1/1	0.25	-	80,80,80,80	0
56	MG	BA	3230	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3197	1/1	0.22	-	41,41,41,41	0
56	MG	BA	3303	1/1	0.51	-	51,51,51,51	0
56	MG	AA	1938	1/1	0.11	-	84,84,84,84	0
56	MG	CA	1613	1/1	0.40	-	75,75,75,75	0
56	MG	DA	3369	1/1	0.22	-	94,94,94,94	0
56	MG	BA	3232	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3013	1/1	0.20	-	97,97,97,97	0
56	MG	BB	220	1/1	0.11	-	44,44,44,44	0
56	MG	AA	1758	1/1	0.25	-	72,72,72,72	0
56	MG	CA	1750	1/1	0.18	-	56,56,56,56	0
56	MG	DA	3110	1/1	0.31	-	60,60,60,60	0
56	MG	CA	1781	1/1	0.21	-	103,103,103,103	0
56	MG	BA	3431	1/1	0.28	-	75,75,75,75	0
56	MG	CA	1680	1/1	0.31	-	70,70,70,70	0
56	MG	BA	3086	1/1	0.32	-	51,51,51,51	0
56	MG	CA	1646	1/1	0.08	-	73,73,73,73	0
56	MG	BA	3145	1/1	0.24	-	26,26,26,26	0
56	MG	DA	3556	1/1	0.06	-	58,58,58,58	0
56	MG	DA	3571	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3589	1/1	0.11	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1657	1/1	0.52	-	67,67,67,67	0
56	MG	DA	3004	1/1	0.35	-	75,75,75,75	0
56	MG	BA	3178	1/1	0.33	-	43,43,43,43	0
56	MG	CA	1689	1/1	0.80	-	84,84,84,84	0
56	MG	CA	1602	1/1	0.23	-	72,72,72,72	0
56	MG	BA	3587	1/1	0.15	-	48,48,48,48	0
56	MG	DA	3296	1/1	0.31	-	80,80,80,80	0
56	MG	DA	3348	1/1	0.33	-	77,77,77,77	0
56	MG	BA	3880	1/1	0.09	-	84,84,84,84	0
56	MG	BA	3362	1/1	0.39	-	51,51,51,51	0
56	MG	BA	3082	1/1	0.27	-	45,45,45,45	0
56	MG	AV	106	1/1	0.22	-	68,68,68,68	0
56	MG	BA	3595	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3693	1/1	0.09	-	38,38,38,38	0
56	MG	D0	104	1/1	0.22	-	86,86,86,86	0
56	MG	DA	3450	1/1	0.32	-	59,59,59,59	0
56	MG	CA	1716	1/1	0.24	-	66,66,66,66	0
56	MG	BA	3416	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3608	1/1	0.14	-	81,81,81,81	0
56	MG	DA	3198	1/1	0.42	-	80,80,80,80	0
56	MG	CA	1618	1/1	0.14	-	78,78,78,78	0
56	MG	DA	3386	1/1	0.28	-	47,47,47,47	0
56	MG	BA	3330	1/1	0.25	-	57,57,57,57	0
56	MG	DA	3392	1/1	0.10	-	42,42,42,42	0
56	MG	CA	1714	1/1	0.16	-	74,74,74,74	0
56	MG	DA	3235	1/1	0.23	-	53,53,53,53	0
56	MG	BB	208	1/1	0.34	-	54,54,54,54	0
56	MG	AA	1777	1/1	0.36	-	61,61,61,61	0
56	MG	CA	1756	1/1	0.78	-	84,84,84,84	0
56	MG	DA	3380	1/1	0.15	-	84,84,84,84	0
56	MG	DA	3031	1/1	0.14	-	49,49,49,49	0
56	MG	DA	3536	1/1	0.30	-	54,54,54,54	0
56	MG	BB	213	1/1	0.34	-	58,58,58,58	0
56	MG	BB	223	1/1	0.17	-	38,38,38,38	0
56	MG	AA	1861	1/1	0.12	-	71,71,71,71	0
56	MG	BG	201	1/1	0.30	-	54,54,54,54	0
56	MG	BA	3210	1/1	0.30	-	36,36,36,36	0
56	MG	CA	1789	1/1	0.21	-	66,66,66,66	0
56	MG	AA	1883	1/1	0.07	-	86,86,86,86	0
56	MG	BB	205	1/1	0.15	-	29,29,29,29	0
56	MG	AA	1682	1/1	0.28	-	118,118,118,118	0
56	MG	DA	3162	1/1	0.73	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3584	1/1	0.14	-	54,54,54,54	0
56	MG	BB	202	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3130	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3674	1/1	0.12	-	27,27,27,27	0
56	MG	BA	3118	1/1	0.56	-	44,44,44,44	0
56	MG	BA	3092	1/1	0.35	-	34,34,34,34	0
56	MG	AA	1617	1/1	0.06	-	58,58,58,58	0
56	MG	BA	3015	1/1	0.51	-	59,59,59,59	0
56	MG	BB	218	1/1	0.11	-	57,57,57,57	0
56	MG	DA	3248	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3386	1/1	0.15	-	54,54,54,54	0
56	MG	BA	3449	1/1	0.48	-	34,34,34,34	0
56	MG	DA	3158	1/1	0.57	-	82,82,82,82	0
56	MG	D1	101	1/1	0.23	-	61,61,61,61	0
56	MG	BA	3409	1/1	0.16	-	45,45,45,45	0
56	MG	BA	3798	1/1	0.19	-	45,45,45,45	0
56	MG	DA	3456	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3150	1/1	0.48	-	54,54,54,54	0
56	MG	AA	1606	1/1	0.30	-	35,35,35,35	0
56	MG	BA	3410	1/1	0.46	-	54,54,54,54	0
56	MG	DA	3093	1/1	0.34	-	77,77,77,77	0
56	MG	BA	3050	1/1	0.24	-	60,60,60,60	0
56	MG	BA	3268	1/1	0.14	-	52,52,52,52	0
56	MG	B7	101	1/1	0.23	-	51,51,51,51	0
56	MG	AA	1709	1/1	0.11	-	86,86,86,86	0
56	MG	DA	3024	1/1	0.42	-	60,60,60,60	0
56	MG	BA	3194	1/1	0.27	-	70,70,70,70	0
56	MG	CA	1679	1/1	0.23	-	65,65,65,65	0
56	MG	AA	1784	1/1	0.34	-	69,69,69,69	0
56	MG	AV	113	1/1	0.43	-	84,84,84,84	0
56	MG	AA	1817	1/1	0.86	-	93,93,93,93	0
56	MG	BA	3492	1/1	0.28	-	61,61,61,61	0
56	MG	DA	3187	1/1	0.26	-	109,109,109,109	0
56	MG	AA	1896	1/1	0.09	-	88,88,88,88	0
56	MG	DA	3043	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3743	1/1	0.33	-	71,71,71,71	0
56	MG	AA	1914	1/1	0.20	-	104,104,104,104	0
56	MG	DA	3676	1/1	0.23	-	94,94,94,94	0
56	MG	BA	3126	1/1	0.45	-	40,40,40,40	0
56	MG	DA	3569	1/1	0.09	-	76,76,76,76	0
56	MG	DA	3237	1/1	0.23	-	61,61,61,61	0
56	MG	BB	214	1/1	0.21	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3002	1/1	0.36	-	65,65,65,65	0
56	MG	DA	3115	1/1	0.63	-	75,75,75,75	0
56	MG	DA	3534	1/1	0.14	-	73,73,73,73	0
56	MG	BA	3012	1/1	0.50	-	69,69,69,69	0
56	MG	BA	3231	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3712	1/1	0.19	-	48,48,48,48	0
56	MG	BA	3380	1/1	0.18	-	44,44,44,44	0
56	MG	BA	3761	1/1	0.19	-	77,77,77,77	0
56	MG	BA	3578	1/1	0.17	-	68,68,68,68	0
56	MG	D6	103	1/1	0.25	-	93,93,93,93	0
56	MG	DA	3028	1/1	0.48	-	56,56,56,56	0
56	MG	CA	1653	1/1	0.37	-	78,78,78,78	0
56	MG	DA	3440	1/1	0.07	-	47,47,47,47	0
56	MG	AA	1905	1/1	0.10	-	130,130,130,130	0
56	MG	DA	3387	1/1	0.16	-	40,40,40,40	0
56	MG	AA	1866	1/1	0.37	-	86,86,86,86	0
56	MG	DA	3491	1/1	0.13	-	101,101,101,101	0
56	MG	CA	1651	1/1	0.37	-	54,54,54,54	0
56	MG	DA	3506	1/1	0.13	-	66,66,66,66	0
56	MG	AA	1671	1/1	0.46	-	94,94,94,94	0
56	MG	BA	3718	1/1	0.11	-	87,87,87,87	0
56	MG	AA	1826	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3429	1/1	0.05	-	73,73,73,73	0
56	MG	DA	3604	1/1	0.15	-	97,97,97,97	0
56	MG	BA	3626	1/1	0.08	-	70,70,70,70	0
56	MG	DA	3079	1/1	0.35	-	57,57,57,57	0
56	MG	CA	1633	1/1	0.39	-	81,81,81,81	0
56	MG	DA	3591	1/1	0.15	-	86,86,86,86	0
56	MG	BA	3716	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3673	1/1	0.18	-	43,43,43,43	0
56	MG	AA	1765	1/1	0.14	-	48,48,48,48	0
56	MG	BA	3396	1/1	0.16	-	95,95,95,95	0
56	MG	DA	3485	1/1	0.12	-	42,42,42,42	0
56	MG	AA	1909	1/1	0.06	-	91,91,91,91	0
56	MG	BA	3046	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3335	1/1	0.49	-	74,74,74,74	0
56	MG	DA	3600	1/1	0.24	-	57,57,57,57	0
56	MG	BA	3142	1/1	0.37	-	44,44,44,44	0
56	MG	AA	1772	1/1	0.43	-	77,77,77,77	0
56	MG	DA	3089	1/1	0.49	-	82,82,82,82	0
56	MG	BA	3272	1/1	0.39	-	72,72,72,72	0
56	MG	CA	1601	1/1	0.75	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B5	101	1/1	0.32	-	50,50,50,50	0
56	MG	BA	3505	1/1	0.42	-	64,64,64,64	0
56	MG	AA	1864	1/1	0.15	-	67,67,67,67	0
56	MG	BA	3317	1/1	0.31	-	61,61,61,61	0
56	MG	BA	3548	1/1	0.22	-	39,39,39,39	0
56	MG	AA	1699	1/1	0.19	-	109,109,109,109	0
56	MG	DA	3433	1/1	0.24	-	46,46,46,46	0
56	MG	BA	3861	1/1	0.09	-	66,66,66,66	0
56	MG	BA	3091	1/1	0.34	-	60,60,60,60	0
56	MG	BA	3747	1/1	0.14	-	20,20,20,20	0
56	MG	DA	3294	1/1	0.24	-	82,82,82,82	0
56	MG	DA	3291	1/1	0.20	-	50,50,50,50	0
56	MG	BA	3055	1/1	0.16	-	37,37,37,37	0
56	MG	AA	1642	1/1	0.33	-	73,73,73,73	0
56	MG	BA	3430	1/1	0.20	-	69,69,69,69	0
56	MG	AA	1710	1/1	0.10	-	76,76,76,76	0
56	MG	DA	3431	1/1	0.18	-	33,33,33,33	0
56	MG	AA	1918	1/1	0.11	-	68,68,68,68	0
56	MG	BA	3749	1/1	0.16	-	76,76,76,76	0
56	MG	AA	1739	1/1	0.49	-	99,99,99,99	0
56	MG	DA	3478	1/1	0.31	-	90,90,90,90	0
56	MG	DA	3268	1/1	0.30	-	64,64,64,64	0
56	MG	CA	1654	1/1	0.37	-	74,74,74,74	0
56	MG	BA	3846	1/1	0.18	-	27,27,27,27	0
56	MG	DA	3572	1/1	0.25	-	45,45,45,45	0
56	MG	DB	216	1/1	0.10	-	109,109,109,109	0
56	MG	DA	3542	1/1	0.10	-	84,84,84,84	0
56	MG	BA	3295	1/1	0.32	-	45,45,45,45	0
56	MG	DA	3500	1/1	0.09	-	68,68,68,68	0
56	MG	BA	3291	1/1	0.27	-	61,61,61,61	0
56	MG	AA	1730	1/1	0.16	-	61,61,61,61	0
56	MG	DA	3374	1/1	0.40	-	75,75,75,75	0
56	MG	BB	207	1/1	0.26	-	44,44,44,44	0
56	MG	DF	301	1/1	0.41	-	71,71,71,71	0
56	MG	BA	3007	1/1	0.09	-	91,91,91,91	0
56	MG	BA	3327	1/1	0.27	-	80,80,80,80	0
56	MG	DA	3010	1/1	0.22	-	78,78,78,78	0
56	MG	BA	3668	1/1	0.13	-	29,29,29,29	0
56	MG	AA	1653	1/1	0.62	-	82,82,82,82	0
56	MG	AA	1693	1/1	0.32	-	103,103,103,103	0
56	MG	BA	3385	1/1	0.15	-	58,58,58,58	0
56	MG	DA	3459	1/1	0.39	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3443	1/1	0.16	-	41,41,41,41	0
56	MG	DD	302	1/1	0.54	-	48,48,48,48	0
56	MG	BA	3408	1/1	0.26	-	44,44,44,44	0
56	MG	DA	3063	1/1	0.39	-	50,50,50,50	0
56	MG	BA	3680	1/1	0.07	-	46,46,46,46	0
56	MG	DA	3510	1/1	0.23	-	77,77,77,77	0
56	MG	BA	3494	1/1	0.30	-	62,62,62,62	0
56	MG	AA	1770	1/1	0.29	-	76,76,76,76	0
56	MG	BA	3803	1/1	0.24	-	71,71,71,71	0
56	MG	BA	3720	1/1	0.16	-	22,22,22,22	0
56	MG	AA	1628	1/1	0.28	-	22,22,22,22	0
56	MG	BA	3456	1/1	0.41	-	73,73,73,73	0
56	MG	DA	3165	1/1	0.64	-	65,65,65,65	0
56	MG	DA	3523	1/1	0.08	-	86,86,86,86	0
56	MG	BA	3547	1/1	0.04	-	49,49,49,49	0
56	MG	BA	3867	1/1	0.17	-	60,60,60,60	0
56	MG	AD	303	1/1	0.22	-	93,93,93,93	0
56	MG	BA	3522	1/1	0.22	-	62,62,62,62	0
56	MG	BA	3025	1/1	0.43	-	68,68,68,68	0
56	MG	BA	3102	1/1	0.19	-	51,51,51,51	0
56	MG	BA	3143	1/1	0.32	-	20,20,20,20	0
56	MG	AA	1852	1/1	0.12	-	93,93,93,93	0
56	MG	BA	3827	1/1	0.18	-	77,77,77,77	0
56	MG	BA	3058	1/1	0.26	-	46,46,46,46	0
56	MG	AA	1812	1/1	0.31	-	122,122,122,122	0
56	MG	AA	1929	1/1	0.14	-	48,48,48,48	0
56	MG	AA	1779	1/1	0.42	-	60,60,60,60	0
56	MG	AA	1745	1/1	0.18	-	64,64,64,64	0
56	MG	BA	3336	1/1	0.27	-	46,46,46,46	0
56	MG	CA	1803	1/1	0.18	-	102,102,102,102	0
56	MG	BA	3193	1/1	0.29	-	45,45,45,45	0
56	MG	BA	3742	1/1	0.22	-	72,72,72,72	0
56	MG	BA	3808	1/1	0.14	-	70,70,70,70	0
56	MG	BA	3250	1/1	0.41	-	27,27,27,27	0
56	MG	DA	3036	1/1	0.19	-	57,57,57,57	0
56	MG	DA	3071	1/1	0.33	-	44,44,44,44	0
56	MG	DA	3312	1/1	0.28	-	52,52,52,52	0
56	MG	DA	3659	1/1	0.22	-	77,77,77,77	0
56	MG	DA	3384	1/1	0.21	-	51,51,51,51	0
56	MG	BA	3518	1/1	0.27	-	33,33,33,33	0
56	MG	DR	201	1/1	0.18	-	44,44,44,44	0
56	MG	BA	3140	1/1	0.22	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3551	1/1	0.03	-	68,68,68,68	0
56	MG	BA	3535	1/1	0.15	-	68,68,68,68	0
56	MG	BA	3425	1/1	0.34	-	46,46,46,46	0
56	MG	BA	3188	1/1	0.34	-	74,74,74,74	0
56	MG	BA	3186	1/1	0.45	-	27,27,27,27	0
56	MG	DA	3494	1/1	0.20	-	70,70,70,70	0
56	MG	DA	3355	1/1	0.30	-	55,55,55,55	0
56	MG	DA	3633	1/1	0.22	-	62,62,62,62	0
56	MG	BA	3837	1/1	0.23	-	33,33,33,33	0
56	MG	BA	3504	1/1	0.20	-	57,57,57,57	0
56	MG	DA	3122	1/1	0.72	-	65,65,65,65	0
56	MG	BA	3814	1/1	0.29	-	86,86,86,86	0
56	MG	BA	3852	1/1	0.24	-	59,59,59,59	0
56	MG	DA	3088	1/1	0.34	-	73,73,73,73	0
56	MG	DA	3590	1/1	0.32	-	89,89,89,89	0
56	MG	BA	3653	1/1	0.17	-	38,38,38,38	0
56	MG	CA	1794	1/1	0.13	-	59,59,59,59	0
56	MG	BA	3201	1/1	0.28	-	54,54,54,54	0
56	MG	BA	3124	1/1	0.20	-	34,34,34,34	0
56	MG	BA	3219	1/1	0.32	-	43,43,43,43	0
56	MG	DA	3505	1/1	0.16	-	81,81,81,81	0
56	MG	CA	1763	1/1	0.09	-	62,62,62,62	0
56	MG	BA	3040	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3423	1/1	0.25	-	45,45,45,45	0
56	MG	DA	3408	1/1	0.05	-	71,71,71,71	0
56	MG	AV	105	1/1	0.18	-	64,64,64,64	0
56	MG	CA	1644	1/1	0.20	-	69,69,69,69	0
56	MG	DA	3066	1/1	0.51	-	68,68,68,68	0
56	MG	BA	3650	1/1	0.08	-	46,46,46,46	0
56	MG	CA	1809	1/1	0.09	-	101,101,101,101	0
56	MG	AA	1794	1/1	0.50	-	68,68,68,68	0
56	MG	BA	3214	1/1	0.14	-	49,49,49,49	0
56	MG	AA	1853	1/1	0.20	-	93,93,93,93	0
56	MG	B3	102	1/1	0.27	-	56,56,56,56	0
56	MG	BA	3280	1/1	0.33	-	58,58,58,58	0
56	MG	DA	3555	1/1	0.07	-	94,94,94,94	0
56	MG	AA	1764	1/1	0.29	-	72,72,72,72	0
56	MG	DA	3668	1/1	0.16	-	100,100,100,100	0
56	MG	AA	1807	1/1	0.33	-	84,84,84,84	0
56	MG	BA	3412	1/1	0.32	-	56,56,56,56	0
56	MG	DA	3382	1/1	0.70	-	72,72,72,72	0
56	MG	BA	3073	1/1	0.69	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3094	1/1	0.17	-	34,34,34,34	0
56	MG	AA	1748	1/1	0.14	-	90,90,90,90	0
56	MG	CA	1813	1/1	0.23	-	113,113,113,113	0
56	MG	DA	3224	1/1	0.44	-	75,75,75,75	0
56	MG	BA	3441	1/1	0.34	-	47,47,47,47	0
56	MG	AA	1683	1/1	0.28	-	106,106,106,106	0
56	MG	BR	202	1/1	0.27	-	30,30,30,30	0
56	MG	CA	1727	1/1	0.25	-	74,74,74,74	0
56	MG	BB	228	1/1	0.10	-	69,69,69,69	0
56	MG	AV	112	1/1	0.34	-	79,79,79,79	0
56	MG	BA	3260	1/1	0.28	-	60,60,60,60	0
56	MG	BA	3279	1/1	0.12	-	50,50,50,50	0
56	MG	CA	1705	1/1	0.49	-	112,112,112,112	0
56	MG	BA	3784	1/1	0.21	-	88,88,88,88	0
56	MG	BA	3405	1/1	0.40	-	62,62,62,62	0
56	MG	CA	1706	1/1	0.71	-	75,75,75,75	0
56	MG	DA	3151	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3021	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3402	1/1	0.11	-	38,38,38,38	0
56	MG	DA	3650	1/1	0.16	-	43,43,43,43	0
56	MG	BA	3099	1/1	0.24	-	32,32,32,32	0
56	MG	AA	1819	1/1	0.56	-	91,91,91,91	0
56	MG	CA	1797	1/1	0.41	-	121,121,121,121	0
56	MG	BA	3222	1/1	0.36	-	28,28,28,28	0
56	MG	BA	3876	1/1	0.07	-	54,54,54,54	0
56	MG	AA	1607	1/1	0.28	-	44,44,44,44	0
56	MG	B1	103	1/1	0.19	-	36,36,36,36	0
56	MG	BA	3671	1/1	0.06	-	41,41,41,41	0
56	MG	BA	3566	1/1	0.05	-	54,54,54,54	0
56	MG	DA	3083	1/1	0.45	-	82,82,82,82	0
56	MG	BA	3683	1/1	0.17	-	31,31,31,31	0
56	MG	DA	3501	1/1	0.11	-	81,81,81,81	0
56	MG	DA	3618	1/1	0.19	-	80,80,80,80	0
56	MG	DA	3095	1/1	0.37	-	41,41,41,41	0
56	MG	BA	3454	1/1	0.23	-	58,58,58,58	0
56	MG	DA	3495	1/1	0.12	-	62,62,62,62	0
56	MG	DA	3214	1/1	0.31	-	64,64,64,64	0
56	MG	DA	3222	1/1	0.59	-	73,73,73,73	0
56	MG	DA	3643	1/1	0.11	-	89,89,89,89	0
56	MG	BA	3709	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3466	1/1	0.08	-	75,75,75,75	0
56	MG	DB	207	1/1	0.12	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CD	302	1/1	0.38	-	53,53,53,53	0
56	MG	CA	1782	1/1	0.37	-	96,96,96,96	0
56	MG	BA	3185	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3618	1/1	0.11	-	46,46,46,46	0
56	MG	DT	203	1/1	0.18	-	73,73,73,73	0
56	MG	DA	3411	1/1	0.39	-	55,55,55,55	0
56	MG	AA	1811	1/1	0.28	-	120,120,120,120	0
56	MG	DA	3326	1/1	0.41	-	62,62,62,62	0
56	MG	BA	3293	1/1	0.30	-	45,45,45,45	0
56	MG	DA	3105	1/1	0.41	-	52,52,52,52	0
56	MG	BA	3806	1/1	0.19	-	57,57,57,57	0
56	MG	BA	3758	1/1	0.09	-	60,60,60,60	0
56	MG	DA	3331	1/1	0.49	-	77,77,77,77	0
57	ZN	D9	101	1/1	0.17	-	117,117,117,117	0
56	MG	DA	3403	1/1	0.41	-	60,60,60,60	0
56	MG	CA	1697	1/1	0.59	-	117,117,117,117	0
56	MG	BR	201	1/1	0.23	-	19,19,19,19	0
56	MG	BA	3764	1/1	0.08	-	85,85,85,85	0
56	MG	CA	1657	1/1	0.15	-	64,64,64,64	0
56	MG	BA	3824	1/1	0.24	-	90,90,90,90	0
56	MG	AA	1778	1/1	0.53	-	83,83,83,83	0
56	MG	BA	3439	1/1	0.33	-	82,82,82,82	0
56	MG	DA	3225	1/1	0.46	-	43,43,43,43	0
56	MG	BA	3627	1/1	0.08	-	56,56,56,56	0
56	MG	CA	1761	1/1	0.28	-	68,68,68,68	0
56	MG	CA	1720	1/1	0.20	-	84,84,84,84	0
56	MG	BA	3258	1/1	0.42	-	71,71,71,71	0
56	MG	BA	3165	1/1	0.45	-	17,17,17,17	0
56	MG	BA	3463	1/1	0.31	-	57,57,57,57	0
56	MG	CA	1652	1/1	0.30	-	75,75,75,75	0
56	MG	BA	3117	1/1	0.32	-	46,46,46,46	0
56	MG	BA	3192	1/1	0.32	-	53,53,53,53	0
56	MG	AA	1796	1/1	0.30	-	77,77,77,77	0
56	MG	BA	3237	1/1	0.35	-	59,59,59,59	0
56	MG	BA	3685	1/1	0.09	-	40,40,40,40	0
57	ZN	B6	101	1/1	0.10	-	48,48,48,48	0
56	MG	DA	3401	1/1	0.28	-	36,36,36,36	0
56	MG	AA	1830	1/1	0.42	-	57,57,57,57	0
56	MG	CA	1683	1/1	0.29	-	71,71,71,71	0
56	MG	BA	3281	1/1	0.45	-	72,72,72,72	0
56	MG	DA	3246	1/1	0.17	-	48,48,48,48	0
56	MG	BA	3832	1/1	0.14	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1753	1/1	0.34	-	86,86,86,86	0
56	MG	AA	1872	1/1	0.19	-	41,41,41,41	0
56	MG	BA	3403	1/1	0.44	-	51,51,51,51	0
56	MG	BA	3885	1/1	0.31	-	91,91,91,91	0
56	MG	BF	303	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3087	1/1	0.09	-	77,77,77,77	0
56	MG	BA	3781	1/1	0.16	-	84,84,84,84	0
56	MG	AA	1904	1/1	0.07	-	118,118,118,118	0
56	MG	DA	3304	1/1	0.42	-	67,67,67,67	0
56	MG	BA	3728	1/1	0.24	-	68,68,68,68	0
56	MG	DA	3608	1/1	0.07	-	82,82,82,82	0
56	MG	CA	1707	1/1	1.35	-	72,72,72,72	0
56	MG	BA	3570	1/1	0.10	-	60,60,60,60	0
56	MG	BA	3840	1/1	0.07	-	41,41,41,41	0
56	MG	BA	3278	1/1	0.10	-	59,59,59,59	0
56	MG	DA	3525	1/1	0.18	-	77,77,77,77	0
56	MG	DA	3077	1/1	0.22	-	74,74,74,74	0
56	MG	BA	3239	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3875	1/1	0.39	-	74,74,74,74	0
56	MG	AA	1941	1/1	0.17	-	94,94,94,94	0
56	MG	BA	3417	1/1	0.37	-	44,44,44,44	0
56	MG	DA	3325	1/1	0.40	-	62,62,62,62	0
56	MG	BF	304	1/1	0.36	-	44,44,44,44	0
56	MG	BA	3111	1/1	0.25	-	66,66,66,66	0
56	MG	BA	3220	1/1	0.35	-	27,27,27,27	0
56	MG	AA	1790	1/1	0.19	-	70,70,70,70	0
56	MG	DA	3627	1/1	0.18	-	81,81,81,81	0
56	MG	AA	1711	1/1	0.41	-	76,76,76,76	0
56	MG	BA	3586	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3226	1/1	0.22	-	36,36,36,36	0
56	MG	AA	1824	1/1	0.28	-	33,33,33,33	0
56	MG	AA	1670	1/1	0.25	-	88,88,88,88	0
56	MG	DA	3511	1/1	0.20	-	77,77,77,77	0
56	MG	DA	3371	1/1	0.19	-	65,65,65,65	0
56	MG	AA	1800	1/1	0.64	-	76,76,76,76	0
56	MG	DA	3156	1/1	0.42	-	57,57,57,57	0
56	MG	BA	3883	1/1	0.27	-	43,43,43,43	0
56	MG	BA	3877	1/1	0.21	-	21,21,21,21	0
56	MG	BA	3090	1/1	0.38	-	46,46,46,46	0
56	MG	CV	109	1/1	0.09	-	102,102,102,102	0
56	MG	DA	3097	1/1	0.47	-	31,31,31,31	0
56	MG	AA	1873	1/1	0.15	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3351	1/1	0.37	-	57,57,57,57	0
56	MG	DA	3172	1/1	0.43	-	51,51,51,51	0
56	MG	BA	3565	1/1	0.13	-	34,34,34,34	0
56	MG	BA	3713	1/1	0.11	-	85,85,85,85	0
56	MG	BA	3442	1/1	0.29	-	45,45,45,45	0
56	MG	DA	3155	1/1	0.28	-	56,56,56,56	0
56	MG	DA	3227	1/1	0.32	-	79,79,79,79	0
56	MG	AA	1879	1/1	0.23	-	71,71,71,71	0
56	MG	BA	3658	1/1	0.27	-	44,44,44,44	0
56	MG	BA	3828	1/1	0.17	-	99,99,99,99	0
56	MG	BA	3691	1/1	0.09	-	31,31,31,31	0
56	MG	CA	1773	1/1	0.16	-	124,124,124,124	0
56	MG	DA	3473	1/1	0.16	-	81,81,81,81	0
56	MG	AA	1632	1/1	0.48	-	51,51,51,51	0
56	MG	BA	3413	1/1	0.22	-	58,58,58,58	0
56	MG	BA	3687	1/1	0.20	-	23,23,23,23	0
56	MG	CA	1751	1/1	0.08	-	86,86,86,86	0
56	MG	BA	3235	1/1	0.06	-	55,55,55,55	0
56	MG	DA	3475	1/1	0.18	-	78,78,78,78	0
56	MG	BB	217	1/1	0.11	-	80,80,80,80	0
56	MG	DA	3270	1/1	0.26	-	70,70,70,70	0
56	MG	DA	3539	1/1	0.28	-	102,102,102,102	0
56	MG	CA	1696	1/1	0.10	-	99,99,99,99	0
57	ZN	B4	101	1/1	0.05	-	137,137,137,137	0
56	MG	DA	3251	1/1	0.27	-	62,62,62,62	0
56	MG	BA	3771	1/1	0.16	-	79,79,79,79	0
56	MG	BA	3179	1/1	0.25	-	45,45,45,45	0
56	MG	BA	3131	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3596	1/1	0.19	-	67,67,67,67	0
56	MG	DA	3257	1/1	0.61	-	51,51,51,51	0
56	MG	DA	3038	1/1	0.13	-	50,50,50,50	0
56	MG	DA	3200	1/1	0.56	-	53,53,53,53	0
56	MG	BA	3155	1/1	0.42	-	58,58,58,58	0
56	MG	AA	1613	1/1	0.50	-	68,68,68,68	0
56	MG	AA	1694	1/1	0.31	-	74,74,74,74	0
56	MG	AA	1875	1/1	0.23	-	59,59,59,59	0
56	MG	B0	101	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3230	1/1	0.14	-	68,68,68,68	0
56	MG	BA	3129	1/1	0.28	-	49,49,49,49	0
56	MG	BA	3453	1/1	0.48	-	63,63,63,63	0
56	MG	BA	3144	1/1	0.11	-	34,34,34,34	0
56	MG	BA	3506	1/1	0.40	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3017	1/1	0.22	-	64,64,64,64	0
56	MG	DA	3588	1/1	0.10	-	109,109,109,109	0
56	MG	DA	3153	1/1	0.81	-	66,66,66,66	0
56	MG	DA	3658	1/1	0.22	-	79,79,79,79	0
56	MG	BA	3113	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3057	1/1	0.23	-	30,30,30,30	0
56	MG	CA	1631	1/1	0.52	-	66,66,66,66	0
56	MG	BA	3011	1/1	0.35	-	54,54,54,54	0
56	MG	B1	102	1/1	0.15	-	45,45,45,45	0
56	MG	BA	3342	1/1	0.42	-	66,66,66,66	0
56	MG	BA	3801	1/1	0.38	-	93,93,93,93	0
56	MG	BA	3591	1/1	0.26	-	64,64,64,64	0
56	MG	CA	1605	1/1	0.55	-	59,59,59,59	0
56	MG	DA	3508	1/1	0.15	-	87,87,87,87	0
56	MG	AA	1795	1/1	0.53	-	70,70,70,70	0
56	MG	CA	1642	1/1	0.54	-	84,84,84,84	0
56	MG	BE	301	1/1	0.39	-	36,36,36,36	0
56	MG	BA	3652	1/1	0.18	-	53,53,53,53	0
56	MG	CA	1704	1/1	0.24	-	93,93,93,93	0
56	MG	BA	3360	1/1	0.18	-	51,51,51,51	0
56	MG	BA	3841	1/1	0.25	-	91,91,91,91	0
56	MG	BA	3163	1/1	0.19	-	40,40,40,40	0
56	MG	CA	1806	1/1	0.07	-	102,102,102,102	0
56	MG	DA	3593	1/1	0.07	-	75,75,75,75	0
56	MG	DA	3058	1/1	0.35	-	83,83,83,83	0
56	MG	DA	3583	1/1	0.18	-	96,96,96,96	0
56	MG	DA	3276	1/1	0.24	-	63,63,63,63	0
56	MG	DA	3502	1/1	0.14	-	68,68,68,68	0
56	MG	DB	211	1/1	0.07	-	83,83,83,83	0
56	MG	DA	3354	1/1	0.23	-	43,43,43,43	0
56	MG	AA	1913	1/1	0.15	-	109,109,109,109	0
56	MG	DA	3687	1/1	0.09	-	64,64,64,64	0
56	MG	CA	1769	1/1	0.20	-	93,93,93,93	0
56	MG	BA	3864	1/1	0.11	-	79,79,79,79	0
56	MG	AA	1762	1/1	0.32	-	74,74,74,74	0
56	MG	BB	227	1/1	0.06	-	81,81,81,81	0
56	MG	AA	1622	1/1	0.76	-	56,56,56,56	0
56	MG	BA	3834	1/1	0.20	-	27,27,27,27	0
56	MG	DA	3197	1/1	0.28	-	82,82,82,82	0
56	MG	BA	3304	1/1	0.22	-	45,45,45,45	0
56	MG	AA	1892	1/1	0.08	-	84,84,84,84	0
56	MG	CA	1712	1/1	0.27	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3757	1/1	0.15	-	28,28,28,28	0
56	MG	DA	3306	1/1	0.06	-	106,106,106,106	0
56	MG	BA	3406	1/1	0.22	-	64,64,64,64	0
56	MG	DA	3340	1/1	0.48	-	55,55,55,55	0
56	MG	AA	1787	1/1	0.32	-	66,66,66,66	0
56	MG	BA	3368	1/1	0.23	-	63,63,63,63	0
56	MG	BA	3122	1/1	0.32	-	56,56,56,56	0
56	MG	DB	205	1/1	0.35	-	79,79,79,79	0
56	MG	BA	3632	1/1	0.11	-	59,59,59,59	0
56	MG	AA	1785	1/1	0.31	-	68,68,68,68	0
56	MG	BA	3461	1/1	0.15	-	58,58,58,58	0
56	MG	CA	1765	1/1	0.35	-	61,61,61,61	0
56	MG	BA	3228	1/1	0.21	-	59,59,59,59	0
56	MG	AV	101	1/1	0.36	-	48,48,48,48	0
56	MG	DA	3231	1/1	0.20	-	74,74,74,74	0
56	MG	BQ	203	1/1	0.22	-	62,62,62,62	0
56	MG	CA	1791	1/1	0.23	-	85,85,85,85	0
56	MG	D0	101	1/1	0.20	-	79,79,79,79	0
56	MG	DA	3675	1/1	0.12	-	75,75,75,75	0
56	MG	AA	1917	1/1	0.16	-	71,71,71,71	0
56	MG	BA	3434	1/1	0.47	-	22,22,22,22	0
56	MG	AA	1755	1/1	0.31	-	70,70,70,70	0
56	MG	BA	3433	1/1	0.26	-	30,30,30,30	0
56	MG	BA	3615	1/1	0.18	-	68,68,68,68	0
56	MG	DA	3568	1/1	0.15	-	82,82,82,82	0
56	MG	AA	1876	1/1	0.07	-	89,89,89,89	0
56	MG	DA	3527	1/1	0.24	-	81,81,81,81	0
56	MG	AA	1637	1/1	0.16	-	73,73,73,73	0
56	MG	AA	1679	1/1	0.27	-	84,84,84,84	0
56	MG	CV	107	1/1	0.33	-	70,70,70,70	0
56	MG	DA	3498	1/1	0.06	-	51,51,51,51	0
56	MG	B0	103	1/1	0.15	-	68,68,68,68	0
56	MG	BA	3067	1/1	0.12	-	40,40,40,40	0
56	MG	BA	3552	1/1	0.06	-	39,39,39,39	0
56	MG	CA	1678	1/1	0.20	-	84,84,84,84	0
56	MG	AA	1808	1/1	0.36	-	75,75,75,75	0
56	MG	CA	1626	1/1	0.29	-	50,50,50,50	0
56	MG	CA	1804	1/1	0.31	-	103,103,103,103	0
56	MG	BA	3704	1/1	0.15	-	44,44,44,44	0
56	MG	DA	3112	1/1	0.29	-	61,61,61,61	0
56	MG	BA	3748	1/1	0.15	-	28,28,28,28	0
56	MG	AA	1690	1/1	0.38	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3368	1/1	0.14	-	80,80,80,80	0
56	MG	BA	3154	1/1	0.32	-	53,53,53,53	0
56	MG	BA	3182	1/1	0.37	-	25,25,25,25	0
56	MG	AA	1763	1/1	0.23	-	54,54,54,54	0
56	MG	BA	3134	1/1	0.24	-	35,35,35,35	0
56	MG	AA	1843	1/1	0.10	-	73,73,73,73	0
56	MG	DA	3637	1/1	0.08	-	57,57,57,57	0
56	MG	DA	3160	1/1	0.32	-	69,69,69,69	0
56	MG	AA	1859	1/1	0.14	-	91,91,91,91	0
56	MG	AA	1834	1/1	0.38	-	76,76,76,76	0
56	MG	BA	3173	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3216	1/1	0.16	-	28,28,28,28	0
56	MG	DA	3390	1/1	0.13	-	55,55,55,55	0
56	MG	CA	1778	1/1	0.40	-	81,81,81,81	0
56	MG	BB	204	1/1	0.32	-	57,57,57,57	0
56	MG	DA	3594	1/1	0.22	-	44,44,44,44	0
56	MG	BA	3229	1/1	0.17	-	41,41,41,41	0
56	MG	DA	3199	1/1	1.24	-	81,81,81,81	0
56	MG	AA	1641	1/1	0.46	-	44,44,44,44	0
56	MG	CA	1686	1/1	0.20	-	72,72,72,72	0
56	MG	DO	203	1/1	0.14	-	79,79,79,79	0
56	MG	BA	3324	1/1	0.54	-	62,62,62,62	0
56	MG	CA	1673	1/1	0.25	-	54,54,54,54	0
56	MG	DA	3470	1/1	0.30	-	73,73,73,73	0
56	MG	CA	1738	1/1	0.20	-	98,98,98,98	0
56	MG	BA	3365	1/1	0.21	-	69,69,69,69	0
56	MG	BA	3270	1/1	0.37	-	53,53,53,53	0
56	MG	BA	3887	1/1	0.25	-	17,17,17,17	0
56	MG	AA	1935	1/1	0.19	-	56,56,56,56	0
56	MG	CA	1650	1/1	0.33	-	61,61,61,61	0
56	MG	BA	3240	1/1	0.19	-	57,57,57,57	0
56	MG	BA	3817	1/1	0.16	-	22,22,22,22	0
56	MG	DA	3661	1/1	0.16	-	61,61,61,61	0
56	MG	BQ	202	1/1	0.18	-	46,46,46,46	0
56	MG	CA	1724	1/1	0.20	-	88,88,88,88	0
56	MG	BA	3850	1/1	0.29	-	82,82,82,82	0
56	MG	BA	3284	1/1	0.21	-	41,41,41,41	0
56	MG	DA	3405	1/1	0.23	-	43,43,43,43	0
56	MG	AA	1713	1/1	0.26	-	60,60,60,60	0
56	MG	DA	3249	1/1	0.30	-	55,55,55,55	0
56	MG	BA	3337	1/1	0.20	-	51,51,51,51	0
56	MG	DA	3482	1/1	0.20	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	1686	1/1	0.49	-	112,112,112,112	0
56	MG	DA	3615	1/1	0.16	-	77,77,77,77	0
56	MG	DA	3377	1/1	0.51	-	89,89,89,89	0
56	MG	CA	1788	1/1	0.29	-	118,118,118,118	0
56	MG	DA	3086	1/1	0.35	-	32,32,32,32	0
56	MG	DA	3288	1/1	0.31	-	83,83,83,83	0
56	MG	DA	3420	1/1	0.09	-	38,38,38,38	0
56	MG	BA	3110	1/1	0.24	-	51,51,51,51	0
56	MG	CA	1647	1/1	0.25	-	71,71,71,71	0
56	MG	DA	3547	1/1	0.10	-	83,83,83,83	0
56	MG	BA	3637	1/1	0.09	-	62,62,62,62	0
56	MG	AF	201	1/1	0.33	-	79,79,79,79	0
56	MG	BA	3064	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3375	1/1	0.15	-	84,84,84,84	0
56	MG	BA	3839	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3038	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3004	1/1	0.29	-	57,57,57,57	0
56	MG	DA	3299	1/1	0.62	-	57,57,57,57	0
56	MG	CA	1732	1/1	0.25	-	81,81,81,81	0
56	MG	BA	3893	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3820	1/1	0.31	-	93,93,93,93	0
56	MG	BA	3531	1/1	0.04	-	59,59,59,59	0
56	MG	D0	102	1/1	0.37	-	99,99,99,99	0
56	MG	DA	3641	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3788	1/1	0.13	-	48,48,48,48	0
56	MG	BA	3078	1/1	0.43	-	49,49,49,49	0
56	MG	AA	1721	1/1	0.23	-	84,84,84,84	0
56	MG	CA	1637	1/1	0.24	-	80,80,80,80	0
56	MG	DA	3550	1/1	0.44	-	42,42,42,42	0
56	MG	BA	3168	1/1	0.15	-	27,27,27,27	0
56	MG	CA	1808	1/1	0.37	-	102,102,102,102	0
56	MG	DA	3513	1/1	0.19	-	59,59,59,59	0
56	MG	AV	111	1/1	0.29	-	85,85,85,85	0
56	MG	DA	3691	1/1	0.10	-	91,91,91,91	0
56	MG	DA	3410	1/1	0.24	-	55,55,55,55	0
56	MG	BA	3352	1/1	0.32	-	68,68,68,68	0
56	MG	DA	3252	1/1	0.12	-	58,58,58,58	0
56	MG	DO	201	1/1	0.30	-	80,80,80,80	0
56	MG	CA	1759	1/1	0.17	-	76,76,76,76	0
56	MG	BA	3161	1/1	0.34	-	49,49,49,49	0
56	MG	DA	3642	1/1	0.10	-	71,71,71,71	0
56	MG	DA	3493	1/1	0.19	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3752	1/1	0.23	-	28,28,28,28	0
56	MG	BA	3265	1/1	0.25	-	67,67,67,67	0
56	MG	CA	1801	1/1	0.16	-	83,83,83,83	0
56	MG	BA	3148	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3448	1/1	0.37	-	60,60,60,60	0
56	MG	DA	3310	1/1	0.95	-	72,72,72,72	0
56	MG	DA	3060	1/1	0.16	-	90,90,90,90	0
56	MG	BA	3501	1/1	0.32	-	80,80,80,80	0
56	MG	BA	3715	1/1	0.14	-	21,21,21,21	0
56	MG	BA	3127	1/1	0.17	-	41,41,41,41	0
56	MG	BA	3520	1/1	0.43	-	38,38,38,38	0
56	MG	BA	3339	1/1	0.34	-	70,70,70,70	0
57	ZN	BY	201	1/1	0.05	-	70,70,70,70	0
56	MG	DA	3157	1/1	0.34	-	82,82,82,82	0
56	MG	BA	3321	1/1	0.32	-	52,52,52,52	0
56	MG	BA	3555	1/1	0.07	-	47,47,47,47	0
56	MG	DA	3059	1/1	0.33	-	67,67,67,67	0
56	MG	BA	3033	1/1	0.26	-	55,55,55,55	0
56	MG	BA	3855	1/1	0.43	-	103,103,103,103	0
56	MG	BA	3290	1/1	0.26	-	63,63,63,63	0
56	MG	DA	3666	1/1	0.44	-	100,100,100,100	0
56	MG	BA	3395	1/1	0.15	-	100,100,100,100	0
56	MG	DA	3081	1/1	0.38	-	65,65,65,65	0
56	MG	AA	1714	1/1	0.22	-	74,74,74,74	0
56	MG	AV	118	1/1	0.08	-	83,83,83,83	0
56	MG	BA	3894	1/1	0.18	-	52,52,52,52	0
56	MG	CA	1718	1/1	0.50	-	88,88,88,88	0
56	MG	DA	3460	1/1	0.31	-	67,67,67,67	0
56	MG	BB	206	1/1	0.18	-	61,61,61,61	0
56	MG	DA	3007	1/1	0.14	-	82,82,82,82	0
56	MG	BA	3209	1/1	0.29	-	25,25,25,25	0
56	MG	BA	3896	1/1	0.17	-	72,72,72,72	0
56	MG	BA	3372	1/1	0.14	-	77,77,77,77	0
56	MG	BA	3823	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3863	1/1	0.08	-	72,72,72,72	0
56	MG	BA	3299	1/1	0.25	-	58,58,58,58	0
56	MG	BA	3180	1/1	0.32	-	41,41,41,41	0
56	MG	CA	1723	1/1	0.07	-	96,96,96,96	0
56	MG	DA	3567	1/1	0.30	-	77,77,77,77	0
56	MG	BA	3283	1/1	0.22	-	47,47,47,47	0
56	MG	BA	3331	1/1	0.24	-	66,66,66,66	0
56	MG	BA	3132	1/1	0.15	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1603	1/1	0.62	-	72,72,72,72	0
56	MG	CA	1656	1/1	0.28	-	77,77,77,77	0
56	MG	DA	3018	1/1	0.29	-	51,51,51,51	0
56	MG	AA	1717	1/1	0.22	-	76,76,76,76	0
56	MG	CA	1796	1/1	0.15	-	102,102,102,102	0
56	MG	DA	3357	1/1	0.24	-	51,51,51,51	0
56	MG	BA	3436	1/1	0.15	-	70,70,70,70	0
56	MG	DA	3490	1/1	0.24	-	45,45,45,45	0
56	MG	DA	3301	1/1	0.11	-	62,62,62,62	0
56	MG	BA	3476	1/1	0.13	-	50,50,50,50	0
56	MG	BA	3732	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3638	1/1	0.24	-	54,54,54,54	0
56	MG	BA	3107	1/1	0.15	-	44,44,44,44	0
56	MG	DA	3336	1/1	0.40	-	71,71,71,71	0
56	MG	DA	3078	1/1	0.49	-	75,75,75,75	0
56	MG	DA	3545	1/1	0.10	-	83,83,83,83	0
56	MG	BT	201	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3847	1/1	0.24	-	82,82,82,82	0
56	MG	DA	3102	1/1	0.26	-	60,60,60,60	0
56	MG	AA	1797	1/1	0.35	-	65,65,65,65	0
56	MG	BA	3243	1/1	0.38	-	35,35,35,35	0
56	MG	AA	1921	1/1	0.09	-	97,97,97,97	0
56	MG	DB	209	1/1	0.34	-	86,86,86,86	0
56	MG	BA	3810	1/1	0.11	-	27,27,27,27	0
56	MG	BA	3639	1/1	0.10	-	63,63,63,63	0
56	MG	AA	1664	1/1	0.16	-	51,51,51,51	0
56	MG	BA	3112	1/1	0.21	-	56,56,56,56	0
56	MG	CA	1636	1/1	0.46	-	50,50,50,50	0
56	MG	CA	1785	1/1	0.11	-	87,87,87,87	0
56	MG	DA	3660	1/1	0.14	-	78,78,78,78	0
56	MG	DA	3678	1/1	0.28	-	89,89,89,89	0
56	MG	DA	3040	1/1	0.15	-	78,78,78,78	0
56	MG	AA	1608	1/1	0.18	-	80,80,80,80	0
56	MG	D7	101	1/1	0.74	-	63,63,63,63	0
56	MG	BA	3812	1/1	0.10	-	87,87,87,87	0
56	MG	AA	1868	1/1	0.29	-	62,62,62,62	0
56	MG	DA	3667	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3465	1/1	0.26	-	40,40,40,40	0
56	MG	BA	3114	1/1	0.40	-	37,37,37,37	0
56	MG	AA	1934	1/1	0.07	-	48,48,48,48	0
56	MG	DA	3541	1/1	0.11	-	106,106,106,106	0
56	MG	DA	3694	1/1	0.14	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	214	1/1	0.34	-	83,83,83,83	0
56	MG	DA	3443	1/1	0.12	-	70,70,70,70	0
56	MG	BA	3419	1/1	0.18	-	62,62,62,62	0
56	MG	BA	3575	1/1	0.12	-	44,44,44,44	0
56	MG	AA	1634	1/1	0.34	-	47,47,47,47	0
56	MG	CA	1640	1/1	0.22	-	72,72,72,72	0
56	MG	AA	1775	1/1	0.10	-	77,77,77,77	0
56	MG	CA	1722	1/1	0.30	-	76,76,76,76	0
56	MG	BA	3351	1/1	0.11	-	51,51,51,51	0
56	MG	BA	3458	1/1	0.29	-	44,44,44,44	0
56	MG	DA	3389	1/1	0.08	-	66,66,66,66	0
56	MG	BE	302	1/1	0.46	-	51,51,51,51	0
56	MG	AA	1733	1/1	0.14	-	94,94,94,94	0
56	MG	BA	3610	1/1	0.09	-	41,41,41,41	0
56	MG	AI	202	1/1	0.35	-	90,90,90,90	0
56	MG	BA	3519	1/1	0.44	-	53,53,53,53	0
56	MG	BA	3651	1/1	0.15	-	49,49,49,49	0
56	MG	BA	3370	1/1	0.16	-	64,64,64,64	0
56	MG	CA	1681	1/1	0.25	-	70,70,70,70	0
56	MG	CA	1733	1/1	0.07	-	90,90,90,90	0
56	MG	DA	3260	1/1	0.18	-	71,71,71,71	0
56	MG	AA	1756	1/1	0.24	-	90,90,90,90	0
56	MG	B0	102	1/1	0.21	-	50,50,50,50	0
56	MG	AA	1850	1/1	0.34	-	85,85,85,85	0
56	MG	DA	3376	1/1	0.30	-	69,69,69,69	0
56	MG	AA	1877	1/1	0.08	-	70,70,70,70	0
56	MG	BA	3779	1/1	0.49	-	80,80,80,80	0
56	MG	AA	1931	1/1	0.40	-	103,103,103,103	0
56	MG	DA	3228	1/1	0.24	-	90,90,90,90	0
56	MG	DA	3576	1/1	0.28	-	75,75,75,75	0
56	MG	BA	3325	1/1	0.20	-	83,83,83,83	0
57	ZN	D6	101	1/1	0.09	-	106,106,106,106	0
56	MG	BA	3689	1/1	0.08	-	25,25,25,25	0
56	MG	BB	229	1/1	0.05	-	67,67,67,67	0
56	MG	BA	3605	1/1	0.19	-	75,75,75,75	0
56	MG	AA	1656	1/1	0.08	-	72,72,72,72	0
56	MG	BA	3599	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3769	1/1	0.12	-	55,55,55,55	0
56	MG	CA	1736	1/1	0.07	-	97,97,97,97	0
56	MG	BA	3521	1/1	0.36	-	68,68,68,68	0
56	MG	DA	3587	1/1	0.17	-	86,86,86,86	0
56	MG	DA	3130	1/1	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BG	202	1/1	0.06	-	82,82,82,82	0
56	MG	DA	3517	1/1	0.16	-	64,64,64,64	0
56	MG	BA	3826	1/1	0.54	-	92,92,92,92	0
56	MG	BA	3654	1/1	0.20	-	59,59,59,59	0
56	MG	CA	1792	1/1	0.10	-	82,82,82,82	0
56	MG	BA	3523	1/1	0.44	-	76,76,76,76	0
56	MG	DA	3589	1/1	0.10	-	81,81,81,81	0
56	MG	BA	3478	1/1	0.27	-	67,67,67,67	0
56	MG	BA	3609	1/1	0.07	-	53,53,53,53	0
56	MG	DA	3211	1/1	0.36	-	83,83,83,83	0
56	MG	BA	3710	1/1	0.14	-	58,58,58,58	0
56	MG	BA	3678	1/1	0.14	-	22,22,22,22	0
56	MG	BA	3438	1/1	0.30	-	62,62,62,62	0
56	MG	CA	1663	1/1	0.48	-	63,63,63,63	0
56	MG	BA	3445	1/1	0.17	-	68,68,68,68	0
56	MG	AA	1731	1/1	0.20	-	70,70,70,70	0
56	MG	CA	1700	1/1	0.62	-	90,90,90,90	0
56	MG	DA	3285	1/1	0.36	-	62,62,62,62	0
56	MG	D6	102	1/1	0.94	-	82,82,82,82	0
56	MG	BA	3212	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3745	1/1	0.11	-	75,75,75,75	0
56	MG	BA	3813	1/1	0.08	-	66,66,66,66	0
56	MG	BA	3851	1/1	0.13	-	35,35,35,35	0
56	MG	BA	3629	1/1	0.10	-	64,64,64,64	0
56	MG	DA	3052	1/1	0.97	-	79,79,79,79	0
56	MG	AA	1605	1/1	0.23	-	81,81,81,81	0
56	MG	CA	1606	1/1	0.20	-	77,77,77,77	0
56	MG	BA	3429	1/1	0.26	-	54,54,54,54	0
56	MG	BA	3829	1/1	0.48	-	82,82,82,82	0
56	MG	BA	3862	1/1	0.12	-	59,59,59,59	0
56	MG	BA	3508	1/1	0.27	-	41,41,41,41	0
56	MG	AA	1933	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3621	1/1	0.06	-	73,73,73,73	0
56	MG	DA	3183	1/1	0.14	-	106,106,106,106	0
56	MG	DA	3544	1/1	0.13	-	79,79,79,79	0
56	MG	DA	3628	1/1	0.12	-	80,80,80,80	0
56	MG	DA	3137	1/1	0.20	-	39,39,39,39	0
56	MG	DA	3345	1/1	0.10	-	67,67,67,67	0
56	MG	DA	3129	1/1	0.19	-	53,53,53,53	0
56	MG	CV	105	1/1	0.23	-	106,106,106,106	0
56	MG	DA	3396	1/1	0.12	-	37,37,37,37	0
56	MG	CA	1710	1/1	0.16	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1912	1/1	0.12	-	106,106,106,106	0
56	MG	DA	3578	1/1	0.16	-	50,50,50,50	0
56	MG	CA	1639	1/1	0.76	-	96,96,96,96	0
56	MG	AA	1823	1/1	0.97	-	77,77,77,77	0
56	MG	CA	1684	1/1	0.18	-	70,70,70,70	0
56	MG	DA	3256	1/1	0.34	-	73,73,73,73	0
56	MG	BA	3423	1/1	0.13	-	85,85,85,85	0
56	MG	AA	1616	1/1	0.11	-	65,65,65,65	0
56	MG	AA	1803	1/1	0.90	-	92,92,92,92	0
56	MG	BA	3298	1/1	0.25	-	50,50,50,50	0
56	MG	DA	3108	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3251	1/1	0.39	-	51,51,51,51	0
56	MG	BA	3760	1/1	0.07	-	68,68,68,68	0
56	MG	AA	1801	1/1	0.39	-	65,65,65,65	0
56	MG	DA	3535	1/1	0.32	-	96,96,96,96	0
56	MG	BA	3030	1/1	0.17	-	36,36,36,36	0
56	MG	DA	3679	1/1	0.25	-	76,76,76,76	0
56	MG	BA	3560	1/1	0.17	-	39,39,39,39	0
56	MG	BA	3473	1/1	0.32	-	22,22,22,22	0
56	MG	BA	3282	1/1	0.15	-	59,59,59,59	0
56	MG	BA	3389	1/1	0.58	-	38,38,38,38	0
56	MG	AA	1894	1/1	0.34	-	83,83,83,83	0
56	MG	AA	1747	1/1	0.26	-	93,93,93,93	0
56	MG	BA	3871	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3334	1/1	0.40	-	51,51,51,51	0
56	MG	BA	3207	1/1	0.33	-	41,41,41,41	0
56	MG	B1	101	1/1	0.26	-	60,60,60,60	0
56	MG	BA	3294	1/1	0.14	-	67,67,67,67	0
56	MG	BA	3679	1/1	0.04	-	34,34,34,34	0
56	MG	AA	1945	1/1	0.09	-	107,107,107,107	0
56	MG	BA	3095	1/1	0.20	-	48,48,48,48	0
56	MG	BA	3450	1/1	0.25	-	42,42,42,42	0
56	MG	AA	1744	1/1	0.19	-	68,68,68,68	0
56	MG	DA	3320	1/1	0.21	-	56,56,56,56	0
56	MG	DA	3243	1/1	0.09	-	78,78,78,78	0
56	MG	DA	3219	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3167	1/1	0.39	-	67,67,67,67	0
56	MG	BA	3341	1/1	0.23	-	53,53,53,53	0
56	MG	DB	213	1/1	0.33	-	115,115,115,115	0
56	MG	AA	1663	1/1	0.20	-	76,76,76,76	0
56	MG	DA	3638	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3533	1/1	0.13	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B0	104	1/1	0.18	-	58,58,58,58	0
56	MG	AA	1839	1/1	0.06	-	69,69,69,69	0
56	MG	CA	1674	1/1	0.40	-	79,79,79,79	0
56	MG	AA	1942	1/1	0.27	-	93,93,93,93	0
56	MG	DA	3091	1/1	0.11	-	47,47,47,47	0
56	MG	BA	3582	1/1	0.19	-	30,30,30,30	0
56	MG	AA	1623	1/1	0.16	-	59,59,59,59	0
56	MG	BA	3010	1/1	0.57	-	56,56,56,56	0
56	MG	BA	3574	1/1	0.20	-	36,36,36,36	0
56	MG	AA	1706	1/1	0.21	-	62,62,62,62	0
56	MG	AA	1910	1/1	0.17	-	87,87,87,87	0
56	MG	DA	3220	1/1	0.17	-	83,83,83,83	0
56	MG	BA	3697	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3865	1/1	0.13	-	97,97,97,97	0
56	MG	BA	3706	1/1	0.21	-	29,29,29,29	0
56	MG	DA	3328	1/1	0.16	-	59,59,59,59	0
56	MG	BA	3633	1/1	0.12	-	52,52,52,52	0
56	MG	DQ	201	1/1	0.45	-	43,43,43,43	0
56	MG	BA	3248	1/1	0.23	-	24,24,24,24	0
56	MG	BA	3717	1/1	0.15	-	21,21,21,21	0
56	MG	DA	3072	1/1	0.40	-	65,65,65,65	0
56	MG	BA	3224	1/1	0.23	-	33,33,33,33	0
56	MG	BB	222	1/1	0.09	-	70,70,70,70	0
56	MG	DA	3065	1/1	1.04	-	59,59,59,59	0
56	MG	BF	305	1/1	0.17	-	52,52,52,52	0
56	MG	AA	1676	1/1	0.58	-	72,72,72,72	0
56	MG	DA	3154	1/1	0.35	-	65,65,65,65	0
56	MG	BA	3796	1/1	0.44	-	83,83,83,83	0
56	MG	BA	3804	1/1	0.09	-	59,59,59,59	0
56	MG	DA	3358	1/1	0.20	-	60,60,60,60	0
56	MG	BA	3094	1/1	0.19	-	45,45,45,45	0
56	MG	BA	3657	1/1	0.25	-	51,51,51,51	0
56	MG	CA	1669	1/1	0.80	-	78,78,78,78	0
56	MG	CA	1775	1/1	0.15	-	99,99,99,99	0
56	MG	DA	3030	1/1	0.34	-	66,66,66,66	0
56	MG	DA	3232	1/1	0.41	-	91,91,91,91	0
56	MG	CA	1799	1/1	0.13	-	94,94,94,94	0
56	MG	CA	1692	1/1	0.79	-	84,84,84,84	0
56	MG	BA	3854	1/1	0.16	-	25,25,25,25	0
56	MG	BA	3878	1/1	0.10	-	81,81,81,81	0
56	MG	BA	3031	1/1	0.21	-	29,29,29,29	0
56	MG	BA	3146	1/1	0.31	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1643	1/1	0.54	-	59,59,59,59	0
56	MG	DA	3179	1/1	0.21	-	67,67,67,67	0
56	MG	BA	3811	1/1	0.17	-	85,85,85,85	0
56	MG	AA	1723	1/1	0.22	-	102,102,102,102	0
56	MG	DA	3271	1/1	0.48	-	68,68,68,68	0
56	MG	BA	3037	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3509	1/1	0.53	-	54,54,54,54	0
56	MG	BA	3437	1/1	0.62	-	63,63,63,63	0
56	MG	DA	3186	1/1	0.38	-	76,76,76,76	0
56	MG	AA	1928	1/1	0.11	-	71,71,71,71	0
56	MG	BA	3139	1/1	0.45	-	56,56,56,56	0
56	MG	BA	3072	1/1	0.67	-	48,48,48,48	0
56	MG	BA	3172	1/1	0.50	-	44,44,44,44	0
56	MG	CA	1658	1/1	0.17	-	91,91,91,91	0
56	MG	BA	3019	1/1	0.21	-	33,33,33,33	0
56	MG	AA	1810	1/1	0.26	-	84,84,84,84	0
56	MG	DA	3674	1/1	0.23	-	105,105,105,105	0
56	MG	BA	3041	1/1	0.11	-	43,43,43,43	0
56	MG	BA	3532	1/1	0.22	-	34,34,34,34	0
56	MG	DA	3322	1/1	0.36	-	52,52,52,52	0
56	MG	AA	1614	1/1	0.15	-	72,72,72,72	0
56	MG	DA	3695	1/1	0.12	-	107,107,107,107	0
56	MG	DA	3564	1/1	0.13	-	88,88,88,88	0
56	MG	DA	3445	1/1	0.15	-	43,43,43,43	0
56	MG	CA	1665	1/1	0.58	-	64,64,64,64	0
56	MG	CA	1622	1/1	0.70	-	80,80,80,80	0
56	MG	BA	3484	1/1	0.27	-	49,49,49,49	0
56	MG	AA	1646	1/1	0.42	-	64,64,64,64	0
56	MG	CA	1635	1/1	0.37	-	72,72,72,72	0
56	MG	BA	3774	1/1	0.28	-	72,72,72,72	0
56	MG	BA	3063	1/1	0.12	-	53,53,53,53	0
56	MG	CV	110	1/1	0.11	-	100,100,100,100	0
56	MG	BA	3756	1/1	0.14	-	56,56,56,56	0
56	MG	AA	1625	1/1	0.18	-	69,69,69,69	0
56	MG	BA	3656	1/1	0.15	-	63,63,63,63	0
56	MG	AA	1816	1/1	0.22	-	107,107,107,107	0
56	MG	BA	3273	1/1	0.37	-	63,63,63,63	0
56	MG	DA	3412	1/1	0.11	-	52,52,52,52	0
56	MG	CA	1810	1/1	0.07	-	92,92,92,92	0
56	MG	AA	1697	1/1	0.25	-	75,75,75,75	0
56	MG	BA	3703	1/1	0.09	-	65,65,65,65	0
56	MG	AA	1665	1/1	0.27	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AT	201	1/1	0.22	-	111,111,111,111	0
56	MG	CA	1784	1/1	0.16	-	96,96,96,96	0
56	MG	BA	3884	1/1	0.08	-	66,66,66,66	0
56	MG	AA	1888	1/1	0.24	-	97,97,97,97	0
56	MG	BA	3257	1/1	0.28	-	48,48,48,48	0
56	MG	AA	1906	1/1	0.24	-	89,89,89,89	0
56	MG	AA	1725	1/1	0.26	-	65,65,65,65	0
56	MG	DA	3032	1/1	0.16	-	51,51,51,51	0
56	MG	BA	3527	1/1	0.08	-	90,90,90,90	0
56	MG	AA	1771	1/1	0.29	-	68,68,68,68	0
56	MG	CA	1802	1/1	0.09	-	115,115,115,115	0
56	MG	DA	3164	1/1	0.32	-	87,87,87,87	0
56	MG	BA	3157	1/1	0.37	-	42,42,42,42	0
56	MG	AA	1915	1/1	0.21	-	121,121,121,121	0
56	MG	BA	3486	1/1	0.32	-	60,60,60,60	0
56	MG	BA	3515	1/1	0.51	-	49,49,49,49	0
56	MG	BA	3398	1/1	0.22	-	62,62,62,62	0
56	MG	DA	3342	1/1	0.27	-	70,70,70,70	0
56	MG	DA	3185	1/1	0.29	-	58,58,58,58	0
56	MG	AA	1621	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3293	1/1	0.15	-	94,94,94,94	0
56	MG	BA	3418	1/1	0.22	-	59,59,59,59	0
56	MG	BA	3694	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3200	1/1	0.46	-	35,35,35,35	0
56	MG	DA	3309	1/1	0.42	-	88,88,88,88	0
56	MG	AA	1766	1/1	0.16	-	53,53,53,53	0
56	MG	AA	1626	1/1	0.41	-	62,62,62,62	0
56	MG	BA	3009	1/1	0.17	-	83,83,83,83	0
56	MG	DA	3085	1/1	0.34	-	64,64,64,64	0
56	MG	CA	1766	1/1	0.10	-	106,106,106,106	0
56	MG	DB	212	1/1	0.14	-	111,111,111,111	0
56	MG	CA	1604	1/1	0.47	-	114,114,114,114	0
56	MG	DA	3606	1/1	0.08	-	76,76,76,76	0
56	MG	DA	3370	1/1	0.47	-	67,67,67,67	0
56	MG	BA	3402	1/1	0.39	-	55,55,55,55	0
56	MG	BE	305	1/1	0.10	-	22,22,22,22	0
56	MG	BA	3888	1/1	0.12	-	99,99,99,99	0
56	MG	BA	3065	1/1	0.12	-	28,28,28,28	0
56	MG	BA	3777	1/1	0.36	-	65,65,65,65	0
56	MG	DB	201	1/1	0.24	-	61,61,61,61	0
56	MG	BA	3670	1/1	0.07	-	57,57,57,57	0
56	MG	BA	3636	1/1	0.06	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3027	1/1	0.45	-	72,72,72,72	0
56	MG	AA	1604	1/1	0.20	-	42,42,42,42	0
56	MG	DA	3190	1/1	0.43	-	70,70,70,70	0
56	MG	BA	3783	1/1	0.22	-	74,74,74,74	0
56	MG	BA	3849	1/1	0.22	-	83,83,83,83	0
56	MG	AA	1862	1/1	0.08	-	45,45,45,45	0
56	MG	BA	3175	1/1	0.36	-	34,34,34,34	0
56	MG	CA	1610	1/1	0.10	-	63,63,63,63	0
56	MG	DA	3672	1/1	0.12	-	87,87,87,87	0
56	MG	CA	1744	1/1	0.06	-	80,80,80,80	0
56	MG	AA	1698	1/1	0.18	-	97,97,97,97	0
56	MG	BA	3604	1/1	0.08	-	80,80,80,80	0
56	MG	B9	102	1/1	0.27	-	43,43,43,43	0
56	MG	AA	1651	1/1	0.27	-	80,80,80,80	0
56	MG	BA	3682	1/1	0.19	-	28,28,28,28	0
56	MG	DA	3062	1/1	0.22	-	65,65,65,65	0
56	MG	BD	303	1/1	0.38	-	29,29,29,29	0
56	MG	CV	103	1/1	0.22	-	88,88,88,88	0
56	MG	BA	3384	1/1	0.66	-	72,72,72,72	0
56	MG	BA	3543	1/1	0.11	-	56,56,56,56	0
56	MG	BA	3259	1/1	0.30	-	66,66,66,66	0
56	MG	BA	3483	1/1	0.28	-	70,70,70,70	0
56	MG	BA	3468	1/1	0.19	-	54,54,54,54	0
56	MG	AA	1869	1/1	0.30	-	81,81,81,81	0
56	MG	DA	3076	1/1	0.18	-	51,51,51,51	0
56	MG	BA	3474	1/1	0.34	-	56,56,56,56	0
56	MG	CT	201	1/1	0.30	-	67,67,67,67	0
56	MG	BA	3034	1/1	0.18	-	23,23,23,23	0
56	MG	CA	1735	1/1	0.07	-	78,78,78,78	0
56	MG	DA	3528	1/1	0.19	-	88,88,88,88	0
56	MG	DA	3557	1/1	0.50	-	93,93,93,93	0
56	MG	BA	3262	1/1	0.28	-	57,57,57,57	0
56	MG	CA	1795	1/1	0.12	-	100,100,100,100	0
56	MG	BA	3665	1/1	0.14	-	44,44,44,44	0
56	MG	BB	219	1/1	0.20	-	85,85,85,85	0
56	MG	AA	1722	1/1	0.42	-	68,68,68,68	0
56	MG	BA	3296	1/1	0.31	-	43,43,43,43	0
56	MG	BA	3534	1/1	0.06	-	44,44,44,44	0
56	MG	DA	3323	1/1	0.12	-	57,57,57,57	0
56	MG	BA	3018	1/1	0.36	-	53,53,53,53	0
56	MG	DA	3492	1/1	0.12	-	63,63,63,63	0
56	MG	BA	3363	1/1	0.45	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3052	1/1	0.30	-	35,35,35,35	0
56	MG	DA	3343	1/1	0.68	-	70,70,70,70	0
56	MG	AA	1602	1/1	0.19	-	104,104,104,104	0
56	MG	DA	3321	1/1	0.63	-	50,50,50,50	0
56	MG	BA	3400	1/1	0.07	-	122,122,122,122	0
56	MG	AA	1799	1/1	0.18	-	95,95,95,95	0
56	MG	BA	3199	1/1	0.34	-	29,29,29,29	0
56	MG	AA	1832	1/1	0.44	-	75,75,75,75	0
56	MG	DA	3664	1/1	0.24	-	97,97,97,97	0
56	MG	CA	1728	1/1	0.17	-	83,83,83,83	0
56	MG	BA	3366	1/1	0.38	-	52,52,52,52	0
56	MG	AA	1674	1/1	0.46	-	74,74,74,74	0
56	MG	DA	3395	1/1	0.14	-	58,58,58,58	0
56	MG	BA	3006	1/1	0.22	-	55,55,55,55	0
56	MG	AA	1692	1/1	0.29	-	67,67,67,67	0
56	MG	BA	3516	1/1	0.32	-	56,56,56,56	0
56	MG	AA	1783	1/1	0.24	-	61,61,61,61	0
56	MG	CA	1817	1/1	0.29	-	111,111,111,111	0
56	MG	BA	3726	1/1	0.36	-	48,48,48,48	0
56	MG	CA	1611	1/1	0.18	-	74,74,74,74	0
56	MG	BA	3264	1/1	0.23	-	59,59,59,59	0
56	MG	DA	3169	1/1	0.23	-	51,51,51,51	0
56	MG	DA	3037	1/1	0.18	-	83,83,83,83	0
56	MG	DA	3109	1/1	0.25	-	74,74,74,74	0
56	MG	BA	3045	1/1	0.28	-	35,35,35,35	0
56	MG	AA	1865	1/1	0.18	-	81,81,81,81	0
56	MG	AV	103	1/1	0.31	-	53,53,53,53	0
56	MG	DA	3082	1/1	0.12	-	89,89,89,89	0
56	MG	BA	3723	1/1	0.09	-	51,51,51,51	0
56	MG	BA	3500	1/1	0.16	-	93,93,93,93	0
56	MG	BA	3269	1/1	0.19	-	55,55,55,55	0
56	MG	BA	3032	1/1	0.14	-	45,45,45,45	0
56	MG	DB	202	1/1	0.40	-	73,73,73,73	0
56	MG	BA	3079	1/1	0.46	-	54,54,54,54	0
56	MG	BA	3205	1/1	0.39	-	43,43,43,43	0
56	MG	DA	3372	1/1	0.28	-	78,78,78,78	0
56	MG	CA	1815	1/1	0.12	-	119,119,119,119	0
56	MG	DA	3121	1/1	0.31	-	37,37,37,37	0
56	MG	DA	3584	1/1	0.11	-	76,76,76,76	0
56	MG	DA	3657	1/1	0.06	-	89,89,89,89	0
56	MG	CA	1667	1/1	0.34	-	66,66,66,66	0
56	MG	CA	1758	1/1	0.20	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3300	1/1	0.29	-	55,55,55,55	0
56	MG	BA	3238	1/1	0.27	-	55,55,55,55	0
56	MG	AA	1738	1/1	0.16	-	84,84,84,84	0
56	MG	AA	1681	1/1	0.24	-	91,91,91,91	0
56	MG	DA	3045	1/1	0.10	-	62,62,62,62	0
56	MG	BA	3700	1/1	0.27	-	26,26,26,26	0
56	MG	AA	1647	1/1	0.30	-	77,77,77,77	0
56	MG	BA	3075	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3023	1/1	0.13	-	46,46,46,46	0
56	MG	BA	3348	1/1	0.29	-	62,62,62,62	0
56	MG	BA	3460	1/1	0.36	-	52,52,52,52	0
56	MG	DA	3406	1/1	0.10	-	48,48,48,48	0
56	MG	CA	1701	1/1	0.18	-	109,109,109,109	0
56	MG	DA	3226	1/1	0.72	-	62,62,62,62	0
56	MG	CA	1819	1/1	0.23	-	96,96,96,96	0
56	MG	BA	3424	1/1	0.20	-	42,42,42,42	0
56	MG	CA	1617	1/1	0.46	-	61,61,61,61	0
56	MG	DA	3464	1/1	0.20	-	82,82,82,82	0
56	MG	BA	3274	1/1	0.20	-	35,35,35,35	0
56	MG	DA	3681	1/1	0.12	-	71,71,71,71	0
56	MG	DA	3388	1/1	0.11	-	74,74,74,74	0
56	MG	BA	3051	1/1	0.38	-	41,41,41,41	0
56	MG	BA	3377	1/1	0.38	-	50,50,50,50	0
56	MG	DA	3484	1/1	0.11	-	45,45,45,45	0
56	MG	AA	1700	1/1	0.20	-	116,116,116,116	0
56	MG	BA	3664	1/1	0.13	-	31,31,31,31	0
56	MG	BA	3227	1/1	0.32	-	41,41,41,41	0
56	MG	BA	3724	1/1	0.16	-	88,88,88,88	0
56	MG	DA	3424	1/1	0.13	-	72,72,72,72	0
56	MG	BA	3356	1/1	0.16	-	66,66,66,66	0
56	MG	DA	3599	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3891	1/1	0.21	-	74,74,74,74	0
56	MG	BA	3043	1/1	1.02	-	42,42,42,42	0
56	MG	CA	1675	1/1	0.36	-	77,77,77,77	0
56	MG	AA	1878	1/1	0.14	-	46,46,46,46	0
56	MG	BA	3550	1/1	0.25	-	27,27,27,27	0
56	MG	DA	3341	1/1	0.47	-	60,60,60,60	0
56	MG	AA	1930	1/1	0.13	-	58,58,58,58	0
56	MG	BA	3315	1/1	0.39	-	54,54,54,54	0
56	MG	DA	3008	1/1	0.39	-	108,108,108,108	0
56	MG	BA	3579	1/1	0.15	-	64,64,64,64	0
56	MG	DA	3068	1/1	0.33	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3181	1/1	0.34	-	69,69,69,69	0
56	MG	DA	3023	1/1	0.20	-	56,56,56,56	0
56	MG	DA	3472	1/1	0.15	-	78,78,78,78	0
56	MG	BA	3202	1/1	0.16	-	42,42,42,42	0
56	MG	BA	3696	1/1	0.06	-	30,30,30,30	0
56	MG	AA	1940	1/1	0.14	-	92,92,92,92	0
56	MG	BA	3790	1/1	0.23	-	75,75,75,75	0
56	MG	AA	1818	1/1	0.19	-	73,73,73,73	0
56	MG	BA	3645	1/1	0.13	-	46,46,46,46	0
56	MG	BA	3481	1/1	0.14	-	87,87,87,87	0
56	MG	DA	3119	1/1	0.44	-	39,39,39,39	0
56	MG	DA	3399	1/1	0.38	-	47,47,47,47	0
56	MG	DA	3101	1/1	0.31	-	53,53,53,53	0
56	MG	CV	102	1/1	0.19	-	85,85,85,85	0
56	MG	CA	1760	1/1	0.74	-	103,103,103,103	0
56	MG	BA	3510	1/1	0.24	-	60,60,60,60	0
56	MG	BA	3892	1/1	0.24	-	94,94,94,94	0
56	MG	BA	3822	1/1	0.14	-	66,66,66,66	0
56	MG	BA	3497	1/1	0.20	-	61,61,61,61	0
56	MG	BA	3838	1/1	0.20	-	28,28,28,28	0
56	MG	BA	3836	1/1	0.20	-	23,23,23,23	0
56	MG	BA	3617	1/1	0.07	-	58,58,58,58	0
56	MG	DA	3313	1/1	0.22	-	74,74,74,74	0
56	MG	AA	1870	1/1	0.15	-	85,85,85,85	0
56	MG	BA	3001	1/1	0.18	-	35,35,35,35	0
56	MG	CA	1812	1/1	0.31	-	114,114,114,114	0
56	MG	BA	3568	1/1	0.15	-	70,70,70,70	0
56	MG	DA	3208	1/1	0.30	-	91,91,91,91	0
56	MG	DA	3236	1/1	0.38	-	68,68,68,68	0
56	MG	BA	3136	1/1	0.25	-	32,32,32,32	0
56	MG	DA	3194	1/1	0.45	-	65,65,65,65	0
56	MG	DA	3601	1/1	0.31	-	53,53,53,53	0
56	MG	DA	3619	1/1	0.12	-	39,39,39,39	0
56	MG	BA	3381	1/1	0.33	-	19,19,19,19	0
56	MG	BA	3184	1/1	0.32	-	31,31,31,31	0
56	MG	BA	3174	1/1	0.21	-	62,62,62,62	0
56	MG	DD	304	1/1	0.46	-	65,65,65,65	0
56	MG	DA	3677	1/1	0.27	-	51,51,51,51	0
56	MG	AA	1926	1/1	0.10	-	90,90,90,90	0
56	MG	DA	3148	1/1	0.50	-	80,80,80,80	0
56	MG	DA	3111	1/1	0.21	-	51,51,51,51	0
56	MG	BD	304	1/1	0.42	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3365	1/1	0.13	-	71,71,71,71	0
56	MG	BA	3869	1/1	0.09	-	64,64,64,64	0
56	MG	BA	3577	1/1	0.12	-	78,78,78,78	0
56	MG	BA	3275	1/1	0.29	-	55,55,55,55	0
56	MG	BA	3376	1/1	0.34	-	43,43,43,43	0
56	MG	BA	3843	1/1	0.09	-	78,78,78,78	0
56	MG	AA	1719	1/1	0.26	-	70,70,70,70	0
56	MG	BA	3588	1/1	0.16	-	78,78,78,78	0
56	MG	AI	201	1/1	0.28	-	66,66,66,66	0
56	MG	BA	3613	1/1	0.23	-	40,40,40,40	0
56	MG	CA	1742	1/1	0.31	-	89,89,89,89	0
56	MG	BA	3785	1/1	0.17	-	69,69,69,69	0
56	MG	AA	1884	1/1	0.18	-	82,82,82,82	0
56	MG	CA	1780	1/1	0.15	-	90,90,90,90	0
56	MG	AA	1937	1/1	0.12	-	79,79,79,79	0
56	MG	BA	3061	1/1	0.27	-	45,45,45,45	0
56	MG	CA	1614	1/1	0.12	-	81,81,81,81	0
56	MG	BA	3203	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3180	1/1	0.10	-	75,75,75,75	0
56	MG	DA	3116	1/1	0.27	-	79,79,79,79	0
56	MG	BA	3276	1/1	0.21	-	57,57,57,57	0
56	MG	DA	3210	1/1	0.30	-	74,74,74,74	0
56	MG	BA	3809	1/1	0.17	-	40,40,40,40	0
56	MG	DA	3582	1/1	0.11	-	85,85,85,85	0
56	MG	DA	3280	1/1	0.37	-	80,80,80,80	0
56	MG	AA	1742	1/1	0.16	-	93,93,93,93	0
56	MG	AA	1655	1/1	0.26	-	77,77,77,77	0
56	MG	BA	3707	1/1	0.13	-	25,25,25,25	0
56	MG	BA	3420	1/1	0.21	-	65,65,65,65	0
56	MG	BA	3765	1/1	0.07	-	59,59,59,59	0
56	MG	BA	3263	1/1	0.15	-	41,41,41,41	0
56	MG	DA	3044	1/1	0.29	-	62,62,62,62	0
56	MG	AA	1752	1/1	0.39	-	88,88,88,88	0
56	MG	BA	3312	1/1	0.23	-	54,54,54,54	0
56	MG	DA	3209	1/1	0.18	-	89,89,89,89	0
56	MG	DA	3305	1/1	0.20	-	76,76,76,76	0
56	MG	CA	1725	1/1	0.18	-	79,79,79,79	0
56	MG	DA	3688	1/1	0.17	-	80,80,80,80	0
56	MG	DA	3346	1/1	0.30	-	70,70,70,70	0
56	MG	BA	3737	1/1	0.07	-	60,60,60,60	0
56	MG	BA	3567	1/1	0.13	-	55,55,55,55	0
56	MG	BA	3559	1/1	0.08	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3057	1/1	0.34	-	66,66,66,66	0
56	MG	BA	3116	1/1	0.26	-	37,37,37,37	0
56	MG	BA	3695	1/1	0.06	-	29,29,29,29	0
56	MG	DA	3690	1/1	0.08	-	107,107,107,107	0
56	MG	CA	1752	1/1	0.19	-	58,58,58,58	0
56	MG	AA	1702	1/1	0.18	-	71,71,71,71	0
56	MG	DA	3653	1/1	0.17	-	59,59,59,59	0
56	MG	BA	3791	1/1	0.24	-	29,29,29,29	0
56	MG	AA	1669	1/1	0.37	-	84,84,84,84	0
56	MG	BA	3845	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3684	1/1	0.21	-	42,42,42,42	0
56	MG	AA	1828	1/1	0.35	-	70,70,70,70	0
56	MG	BA	3750	1/1	0.13	-	65,65,65,65	0
56	MG	DA	3269	1/1	0.17	-	85,85,85,85	0
56	MG	DA	3421	1/1	0.13	-	52,52,52,52	0
56	MG	AA	1718	1/1	0.25	-	70,70,70,70	0
56	MG	DA	3644	1/1	0.07	-	80,80,80,80	0
56	MG	CA	1787	1/1	0.24	-	98,98,98,98	0
56	MG	DA	3518	1/1	0.21	-	46,46,46,46	0
56	MG	DA	3096	1/1	0.17	-	41,41,41,41	0
56	MG	BA	3349	1/1	0.19	-	52,52,52,52	0
56	MG	DA	3682	1/1	0.14	-	90,90,90,90	0
56	MG	DA	3247	1/1	0.48	-	58,58,58,58	0
56	MG	CA	1715	1/1	0.12	-	66,66,66,66	0
56	MG	BA	3447	1/1	0.13	-	45,45,45,45	0
56	MG	AA	1886	1/1	0.10	-	79,79,79,79	0
56	MG	BA	3735	1/1	0.06	-	58,58,58,58	0
56	MG	DA	3234	1/1	0.32	-	62,62,62,62	0
56	MG	DA	3279	1/1	0.25	-	74,74,74,74	0
56	MG	AA	1760	1/1	0.75	-	64,64,64,64	0
56	MG	DA	3632	1/1	0.25	-	69,69,69,69	0
56	MG	BA	3390	1/1	0.19	-	28,28,28,28	0
56	MG	CA	1677	1/1	0.12	-	88,88,88,88	0
56	MG	BA	3345	1/1	0.21	-	74,74,74,74	0
56	MG	BA	3842	1/1	0.16	-	85,85,85,85	0
56	MG	CA	1777	1/1	0.10	-	82,82,82,82	0
56	MG	BA	3513	1/1	0.13	-	60,60,60,60	0
56	MG	DA	3337	1/1	0.20	-	65,65,65,65	0
56	MG	BP	202	1/1	0.16	-	62,62,62,62	0
56	MG	BA	3432	1/1	0.16	-	29,29,29,29	0
56	MG	CA	1638	1/1	0.54	-	99,99,99,99	0
56	MG	BA	3060	1/1	0.14	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1678	1/1	0.28	-	90,90,90,90	0
56	MG	AA	1735	1/1	0.70	-	84,84,84,84	0
56	MG	DA	3522	1/1	0.21	-	76,76,76,76	0
56	MG	BF	306	1/1	0.20	-	48,48,48,48	0
56	MG	DA	3133	1/1	0.41	-	51,51,51,51	0
56	MG	DE	302	1/1	0.65	-	55,55,55,55	0
56	MG	CA	1687	1/1	0.29	-	81,81,81,81	0
56	MG	AA	1848	1/1	0.39	-	71,71,71,71	0
56	MG	DA	3398	1/1	0.11	-	58,58,58,58	0
56	MG	DA	3616	1/1	0.53	-	115,115,115,115	0
56	MG	DA	3113	1/1	0.25	-	59,59,59,59	0
56	MG	CA	1779	1/1	0.17	-	95,95,95,95	0
56	MG	AA	1691	1/1	0.30	-	121,121,121,121	0
56	MG	CA	1699	1/1	0.22	-	97,97,97,97	0
56	MG	DA	3204	1/1	0.41	-	76,76,76,76	0
56	MG	CA	1620	1/1	0.13	-	70,70,70,70	0
56	MG	BA	3805	1/1	0.24	-	63,63,63,63	0
56	MG	AA	1900	1/1	0.12	-	110,110,110,110	0
56	MG	DA	3212	1/1	0.28	-	66,66,66,66	0
56	MG	DA	3327	1/1	0.39	-	64,64,64,64	0
56	MG	DA	3259	1/1	0.46	-	78,78,78,78	0
56	MG	DA	3239	1/1	0.34	-	62,62,62,62	0
56	MG	DA	3603	1/1	0.37	-	100,100,100,100	0
56	MG	BA	3125	1/1	0.47	-	48,48,48,48	0
56	MG	AA	1840	1/1	0.16	-	83,83,83,83	0
56	MG	BA	3701	1/1	0.12	-	26,26,26,26	0
56	MG	CA	1798	1/1	0.17	-	94,94,94,94	0
56	MG	BA	3071	1/1	0.31	-	41,41,41,41	0
56	MG	CA	1762	1/1	0.18	-	76,76,76,76	0
56	MG	AA	1836	1/1	0.15	-	59,59,59,59	0
56	MG	AA	1916	1/1	0.06	-	82,82,82,82	0
56	MG	BB	209	1/1	0.31	-	79,79,79,79	0
56	MG	BA	3120	1/1	0.22	-	51,51,51,51	0
56	MG	BA	3672	1/1	0.14	-	41,41,41,41	0
56	MG	DA	3103	1/1	0.42	-	45,45,45,45	0
56	MG	BA	3830	1/1	0.12	-	31,31,31,31	0
56	MG	AA	1612	1/1	0.25	-	60,60,60,60	0
56	MG	AA	1798	1/1	0.38	-	54,54,54,54	0
56	MG	BA	3218	1/1	0.22	-	20,20,20,20	0
56	MG	CA	1734	1/1	0.22	-	80,80,80,80	0
56	MG	BA	3085	1/1	0.29	-	35,35,35,35	0
56	MG	DV	201	1/1	0.31	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3166	1/1	0.68	-	66,66,66,66	0
56	MG	DA	3499	1/1	0.16	-	68,68,68,68	0
56	MG	BA	3297	1/1	0.26	-	53,53,53,53	0
56	MG	BA	3225	1/1	0.24	-	46,46,46,46	0
56	MG	DA	3242	1/1	0.31	-	77,77,77,77	0
56	MG	DQ	202	1/1	0.34	-	77,77,77,77	0
56	MG	DA	3624	1/1	0.15	-	82,82,82,82	0
57	ZN	CD	301	1/1	0.28	-	90,90,90,90	0
56	MG	AA	1645	1/1	0.31	-	54,54,54,54	0
56	MG	BA	3234	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3050	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3442	1/1	0.18	-	56,56,56,56	0
56	MG	DD	301	1/1	0.20	-	84,84,84,84	0
56	MG	AA	1786	1/1	0.30	-	69,69,69,69	0
56	MG	DA	3019	1/1	0.12	-	65,65,65,65	0
56	MG	DA	3333	1/1	0.42	-	50,50,50,50	0
56	MG	DA	3029	1/1	0.66	-	68,68,68,68	0
56	MG	AA	1673	1/1	0.21	-	74,74,74,74	0
56	MG	BA	3648	1/1	0.19	-	49,49,49,49	0
56	MG	DA	3611	1/1	0.27	-	80,80,80,80	0
56	MG	AA	1624	1/1	0.46	-	57,57,57,57	0
56	MG	CA	1814	1/1	0.08	-	114,114,114,114	0
56	MG	DA	3126	1/1	0.22	-	69,69,69,69	0
56	MG	AA	1922	1/1	0.19	-	106,106,106,106	0
56	MG	AA	1757	1/1	0.18	-	58,58,58,58	0
56	MG	AA	1769	1/1	0.17	-	84,84,84,84	0
56	MG	DA	3009	1/1	0.11	-	90,90,90,90	0
56	MG	AA	1946	1/1	0.10	-	81,81,81,81	0
56	MG	CA	1671	1/1	0.22	-	82,82,82,82	0
56	MG	BA	3746	1/1	0.24	-	77,77,77,77	0
56	MG	BA	3100	1/1	0.19	-	48,48,48,48	0
56	MG	DA	3073	1/1	0.47	-	63,63,63,63	0
56	MG	AA	1802	1/1	0.37	-	67,67,67,67	0
56	MG	BA	3733	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3546	1/1	0.09	-	73,73,73,73	0
56	MG	DA	3138	1/1	0.42	-	58,58,58,58	0
56	MG	CV	104	1/1	0.20	-	92,92,92,92	0
56	MG	BA	3068	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3217	1/1	0.16	-	38,38,38,38	0
56	MG	DA	3016	1/1	0.27	-	42,42,42,42	0
56	MG	BO	202	1/1	0.34	-	42,42,42,42	0
56	MG	CA	1655	1/1	0.37	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3507	1/1	0.21	-	109,109,109,109	0
56	MG	BA	3223	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3597	1/1	0.07	-	66,66,66,66	0
56	MG	AA	1847	1/1	0.33	-	98,98,98,98	0
56	MG	BA	3164	1/1	0.12	-	26,26,26,26	0
56	MG	BA	3066	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3551	1/1	0.25	-	42,42,42,42	0
56	MG	DA	3415	1/1	0.42	-	33,33,33,33	0
56	MG	BA	3213	1/1	0.24	-	37,37,37,37	0
56	MG	BA	3856	1/1	0.14	-	68,68,68,68	0
56	MG	BA	3053	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3607	1/1	0.15	-	90,90,90,90	0
56	MG	DA	3366	1/1	0.17	-	81,81,81,81	0
56	MG	DA	3417	1/1	0.36	-	46,46,46,46	0
56	MG	BA	3108	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3332	1/1	0.34	-	74,74,74,74	0
56	MG	AA	1672	1/1	0.28	-	78,78,78,78	0
56	MG	BA	3719	1/1	0.11	-	71,71,71,71	0
56	MG	CA	1630	1/1	0.54	-	70,70,70,70	0
56	MG	BA	3379	1/1	0.27	-	39,39,39,39	0
56	MG	BA	3793	1/1	0.42	-	69,69,69,69	0
56	MG	DA	3217	1/1	0.24	-	68,68,68,68	0
56	MG	DA	3189	1/1	0.22	-	63,63,63,63	0
56	MG	BA	3361	1/1	0.28	-	60,60,60,60	0
56	MG	AA	1907	1/1	0.15	-	78,78,78,78	0
56	MG	DA	3531	1/1	0.21	-	66,66,66,66	0
56	MG	BA	3859	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3156	1/1	0.73	-	54,54,54,54	0
56	MG	DF	303	1/1	0.14	-	77,77,77,77	0
56	MG	BA	3868	1/1	0.19	-	34,34,34,34	0
56	MG	BA	3655	1/1	0.11	-	46,46,46,46	0
56	MG	DE	301	1/1	0.21	-	64,64,64,64	0
56	MG	BA	3253	1/1	0.36	-	20,20,20,20	0
56	MG	DA	3240	1/1	0.13	-	74,74,74,74	0
56	MG	AA	1927	1/1	0.08	-	85,85,85,85	0
56	MG	AA	1887	1/1	0.26	-	90,90,90,90	0
56	MG	CA	1774	1/1	0.17	-	111,111,111,111	0
56	MG	BA	3169	1/1	0.43	-	14,14,14,14	0
56	MG	DA	3617	1/1	0.09	-	86,86,86,86	0
56	MG	BA	3786	1/1	0.16	-	44,44,44,44	0
56	MG	BA	3277	1/1	0.13	-	65,65,65,65	0
56	MG	BA	3399	1/1	0.12	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3097	1/1	0.14	-	34,34,34,34	0
56	MG	DA	3193	1/1	0.21	-	67,67,67,67	0
56	MG	CA	1615	1/1	0.28	-	74,74,74,74	0
56	MG	BA	3499	1/1	0.29	-	73,73,73,73	0
56	MG	BA	3029	1/1	0.22	-	33,33,33,33	0
56	MG	BA	3488	1/1	0.60	-	35,35,35,35	0
56	MG	BA	3471	1/1	0.24	-	49,49,49,49	0
56	MG	AA	1603	1/1	0.09	-	78,78,78,78	0
56	MG	DA	3381	1/1	0.17	-	88,88,88,88	0
56	MG	BA	3069	1/1	0.27	-	42,42,42,42	0
56	MG	DA	3144	1/1	0.42	-	71,71,71,71	0
56	MG	DD	303	1/1	0.26	-	59,59,59,59	0
56	MG	BA	3138	1/1	0.17	-	33,33,33,33	0
56	MG	DA	3253	1/1	0.35	-	67,67,67,67	0
56	MG	CA	1737	1/1	0.28	-	90,90,90,90	0
56	MG	BA	3493	1/1	0.45	-	62,62,62,62	0
56	MG	DB	206	1/1	0.27	-	77,77,77,77	0
56	MG	BX	101	1/1	0.49	-	78,78,78,78	0
56	MG	BA	3301	1/1	0.13	-	70,70,70,70	0
56	MG	BA	3690	1/1	0.11	-	27,27,27,27	0
56	MG	DA	3123	1/1	0.43	-	61,61,61,61	0
56	MG	AA	1932	1/1	0.23	-	116,116,116,116	0
56	MG	BA	3825	1/1	0.06	-	37,37,37,37	0
56	MG	BA	3526	1/1	0.08	-	40,40,40,40	0
56	MG	BA	3106	1/1	0.15	-	28,28,28,28	0
56	MG	DA	3125	1/1	0.16	-	65,65,65,65	0
56	MG	DA	3170	1/1	0.24	-	96,96,96,96	0
56	MG	BA	3242	1/1	0.22	-	47,47,47,47	0
56	MG	BA	3267	1/1	0.35	-	53,53,53,53	0
56	MG	AA	1895	1/1	0.18	-	87,87,87,87	0
56	MG	AA	1849	1/1	0.22	-	59,59,59,59	0
56	MG	CA	1745	1/1	0.21	-	99,99,99,99	0
56	MG	DA	3087	1/1	0.35	-	40,40,40,40	0
56	MG	B6	102	1/1	0.07	-	73,73,73,73	0
56	MG	BA	3576	1/1	0.13	-	66,66,66,66	0
56	MG	DA	3648	1/1	0.26	-	53,53,53,53	0
56	MG	DA	3191	1/1	0.18	-	77,77,77,77	0
56	MG	AA	1640	1/1	0.20	-	43,43,43,43	0
56	MG	BA	3775	1/1	0.24	-	74,74,74,74	0
56	MG	AA	1809	1/1	0.20	-	83,83,83,83	0
56	MG	DA	3174	1/1	0.49	-	68,68,68,68	0
56	MG	AA	1767	1/1	0.18	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1623	1/1	0.24	-	68,68,68,68	0
56	MG	AA	1675	1/1	0.90	-	78,78,78,78	0
56	MG	DA	3614	1/1	0.51	-	98,98,98,98	0
56	MG	BA	3554	1/1	0.16	-	55,55,55,55	0
56	MG	BA	3115	1/1	0.22	-	52,52,52,52	0
56	MG	DA	3533	1/1	0.18	-	95,95,95,95	0
56	MG	BA	3211	1/1	0.33	-	46,46,46,46	0
56	MG	DA	3283	1/1	0.59	-	76,76,76,76	0
56	MG	BA	3105	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3711	1/1	0.16	-	24,24,24,24	0
56	MG	DA	3640	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3221	1/1	0.33	-	17,17,17,17	0
56	MG	AA	1750	1/1	0.14	-	79,79,79,79	0
56	MG	BA	3314	1/1	0.33	-	65,65,65,65	0
56	MG	BA	3503	1/1	0.28	-	51,51,51,51	0
56	MG	BA	3206	1/1	0.32	-	31,31,31,31	0
56	MG	BB	203	1/1	0.38	-	63,63,63,63	0
56	MG	BA	3382	1/1	0.12	-	68,68,68,68	0
56	MG	AA	1729	1/1	0.16	-	79,79,79,79	0
56	MG	DA	3350	1/1	0.28	-	72,72,72,72	0
56	MG	DA	3205	1/1	0.22	-	68,68,68,68	0
56	MG	BA	3204	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3662	1/1	0.14	-	30,30,30,30	0
56	MG	AA	1630	1/1	0.24	-	98,98,98,98	0
56	MG	AA	1677	1/1	0.47	-	84,84,84,84	0
56	MG	BB	216	1/1	0.18	-	38,38,38,38	0
56	MG	DA	3652	1/1	0.08	-	85,85,85,85	0
56	MG	DA	3391	1/1	0.16	-	48,48,48,48	0
56	MG	BA	3306	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3415	1/1	0.31	-	50,50,50,50	0
56	MG	BA	3517	1/1	0.49	-	58,58,58,58	0
56	MG	AA	1947	1/1	0.07	-	63,63,63,63	0
56	MG	BA	3616	1/1	0.24	-	40,40,40,40	0
56	MG	BA	3367	1/1	0.80	-	50,50,50,50	0
56	MG	AA	1639	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3623	1/1	0.05	-	75,75,75,75	0
56	MG	BA	3776	1/1	0.56	-	68,68,68,68	0
56	MG	AA	1791	1/1	0.27	-	99,99,99,99	0
56	MG	AA	1920	1/1	0.12	-	86,86,86,86	0
56	MG	D8	201	1/1	0.24	-	67,67,67,67	0
56	MG	BA	3530	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3485	1/1	0.23	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AE	201	1/1	0.46	-	83,83,83,83	0
56	MG	BA	3762	1/1	0.13	-	48,48,48,48	0
56	MG	CA	1807	1/1	0.14	-	100,100,100,100	0
56	MG	AA	1902	1/1	0.26	-	121,121,121,121	0
56	MG	BA	3036	1/1	0.30	-	54,54,54,54	0
56	MG	BA	3056	1/1	0.28	-	50,50,50,50	0
56	MG	DA	3684	1/1	0.20	-	98,98,98,98	0
56	MG	DA	3683	1/1	0.29	-	94,94,94,94	0
56	MG	BA	3857	1/1	0.21	-	78,78,78,78	0
56	MG	CA	1662	1/1	0.51	-	92,92,92,92	0
56	MG	CA	1627	1/1	0.59	-	50,50,50,50	0
56	MG	BA	3545	1/1	0.12	-	53,53,53,53	0
56	MG	BV	202	1/1	0.22	-	67,67,67,67	0
56	MG	BA	3754	1/1	0.16	-	68,68,68,68	0
56	MG	DA	3223	1/1	0.56	-	70,70,70,70	0
56	MG	BA	3890	1/1	0.08	-	70,70,70,70	0
56	MG	BA	3730	1/1	0.05	-	63,63,63,63	0
56	MG	AV	110	1/1	0.30	-	80,80,80,80	0
56	MG	AA	1708	1/1	0.28	-	79,79,79,79	0
56	MG	DA	3512	1/1	0.36	-	49,49,49,49	0
56	MG	DA	3455	1/1	0.15	-	61,61,61,61	0
56	MG	BA	3401	1/1	0.23	-	57,57,57,57	0
56	MG	DA	3363	1/1	0.29	-	64,64,64,64	0
56	MG	BA	3353	1/1	0.22	-	57,57,57,57	0
56	MG	BA	3661	1/1	0.24	-	53,53,53,53	0
56	MG	BA	3159	1/1	0.21	-	43,43,43,43	0
56	MG	AA	1780	1/1	0.24	-	55,55,55,55	0
56	MG	DA	3131	1/1	0.33	-	46,46,46,46	0
56	MG	BA	3538	1/1	0.12	-	33,33,33,33	0
56	MG	CA	1746	1/1	0.07	-	65,65,65,65	0
56	MG	DA	3011	1/1	0.16	-	66,66,66,66	0
56	MG	DA	3552	1/1	0.29	-	39,39,39,39	0
56	MG	AA	1845	1/1	0.55	-	59,59,59,59	0
56	MG	CA	1747	1/1	0.19	-	96,96,96,96	0
56	MG	BA	3271	1/1	0.19	-	44,44,44,44	0
56	MG	DA	3178	1/1	0.39	-	77,77,77,77	0
56	MG	BA	3451	1/1	0.19	-	47,47,47,47	0
56	MG	BZ	302	1/1	0.48	-	62,62,62,62	0
56	MG	DA	3496	1/1	0.20	-	47,47,47,47	0
56	MG	DA	3196	1/1	0.13	-	77,77,77,77	0
56	MG	BA	3614	1/1	0.48	-	58,58,58,58	0
56	MG	CA	1672	1/1	0.45	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3319	1/1	0.54	-	69,69,69,69	0
56	MG	DA	3489	1/1	0.10	-	68,68,68,68	0
56	MG	BA	3151	1/1	0.20	-	38,38,38,38	0
56	MG	BA	3266	1/1	0.41	-	59,59,59,59	0
56	MG	BA	3860	1/1	0.05	-	57,57,57,57	0
56	MG	DA	3685	1/1	0.24	-	96,96,96,96	0
56	MG	DA	3560	1/1	0.20	-	64,64,64,64	0
56	MG	AA	1726	1/1	0.27	-	55,55,55,55	0
56	MG	DA	3663	1/1	0.09	-	81,81,81,81	0
56	MG	AA	1741	1/1	0.53	-	85,85,85,85	0
56	MG	BA	3319	1/1	0.16	-	59,59,59,59	0
56	MG	DA	3434	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3581	1/1	0.09	-	46,46,46,46	0
56	MG	BD	301	1/1	0.26	-	65,65,65,65	0
56	MG	BA	3692	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3039	1/1	0.16	-	34,34,34,34	0
56	MG	AA	1712	1/1	0.17	-	72,72,72,72	0
56	MG	BA	3133	1/1	0.53	-	27,27,27,27	0
56	MG	AA	1773	1/1	0.45	-	58,58,58,58	0
56	MG	AA	1854	1/1	0.20	-	73,73,73,73	0
56	MG	BA	3285	1/1	0.12	-	55,55,55,55	0
56	MG	BA	3870	1/1	0.24	-	100,100,100,100	0
56	MG	CA	1688	1/1	0.35	-	68,68,68,68	0
56	MG	BA	3329	1/1	0.12	-	85,85,85,85	0
56	MG	BA	3044	1/1	0.16	-	46,46,46,46	0
56	MG	BY	202	1/1	0.33	-	54,54,54,54	0
56	MG	BA	3208	1/1	0.11	-	57,57,57,57	0
56	MG	BA	3444	1/1	0.20	-	74,74,74,74	0
56	MG	BA	3322	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3624	1/1	0.14	-	57,57,57,57	0
56	MG	DA	3362	1/1	0.34	-	75,75,75,75	0
56	MG	BA	3529	1/1	0.14	-	49,49,49,49	0
56	MG	CA	1811	1/1	0.08	-	102,102,102,102	0
56	MG	BA	3482	1/1	0.15	-	73,73,73,73	0
56	MG	BA	3375	1/1	0.25	-	47,47,47,47	0
56	MG	BA	3512	1/1	0.31	-	56,56,56,56	0
56	MG	BA	3183	1/1	0.36	-	22,22,22,22	0
56	MG	DA	3636	1/1	0.15	-	78,78,78,78	0
56	MG	BA	3641	1/1	0.11	-	62,62,62,62	0
56	MG	BA	3725	1/1	0.13	-	69,69,69,69	0
56	MG	BA	3753	1/1	0.26	-	31,31,31,31	0
56	MG	AA	1768	1/1	0.25	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1635	1/1	0.21	-	65,65,65,65	0
56	MG	BA	3643	1/1	0.06	-	54,54,54,54	0
56	MG	CA	1693	1/1	0.35	-	83,83,83,83	0
56	MG	CA	1753	1/1	0.21	-	61,61,61,61	0
56	MG	AA	1666	1/1	0.17	-	70,70,70,70	0
56	MG	BA	3364	1/1	0.24	-	69,69,69,69	0
56	MG	DA	3069	1/1	0.50	-	83,83,83,83	0
56	MG	CA	1659	1/1	0.09	-	85,85,85,85	0
56	MG	BA	3340	1/1	0.31	-	55,55,55,55	0
56	MG	BA	3388	1/1	0.29	-	77,77,77,77	0
56	MG	DA	3245	1/1	0.18	-	39,39,39,39	0
56	MG	AA	1899	1/1	0.18	-	115,115,115,115	0
56	MG	DU	201	1/1	0.29	-	72,72,72,72	0
56	MG	DA	3136	1/1	0.99	-	67,67,67,67	0
56	MG	AA	1650	1/1	0.48	-	65,65,65,65	0
56	MG	DA	3563	1/1	0.10	-	73,73,73,73	0
56	MG	AA	1851	1/1	0.12	-	80,80,80,80	0
56	MG	DA	3457	1/1	0.32	-	102,102,102,102	0
56	MG	CA	1664	1/1	0.35	-	76,76,76,76	0
56	MG	BA	3536	1/1	0.14	-	42,42,42,42	0
56	MG	AA	1732	1/1	0.14	-	65,65,65,65	0
56	MG	CV	108	1/1	0.27	-	79,79,79,79	0
56	MG	BA	3705	1/1	0.21	-	79,79,79,79	0
56	MG	DA	3221	1/1	0.42	-	82,82,82,82	0
56	MG	BA	3287	1/1	0.28	-	82,82,82,82	0
56	MG	BA	3457	1/1	0.21	-	59,59,59,59	0
56	MG	DA	3553	1/1	0.19	-	46,46,46,46	0
56	MG	BA	3343	1/1	0.28	-	37,37,37,37	0
56	MG	AA	1827	1/1	0.18	-	69,69,69,69	0
56	MG	BA	3751	1/1	0.08	-	56,56,56,56	0
56	MG	BA	3427	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3364	1/1	0.15	-	94,94,94,94	0
56	MG	DA	3017	1/1	0.30	-	69,69,69,69	0
57	ZN	B5	104	1/1	0.09	-	75,75,75,75	0
56	MG	BA	3606	1/1	0.07	-	63,63,63,63	0
56	MG	CA	1709	1/1	0.69	-	82,82,82,82	0
56	MG	DA	3120	1/1	0.13	-	42,42,42,42	0
57	ZN	B9	101	1/1	0.07	-	51,51,51,51	0
56	MG	DT	201	1/1	0.22	-	73,73,73,73	0
56	MG	AA	1601	1/1	0.17	-	65,65,65,65	0
56	MG	BA	3886	1/1	0.28	-	94,94,94,94	0
56	MG	CA	1771	1/1	0.26	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3564	1/1	0.11	-	63,63,63,63	0
56	MG	DA	3047	1/1	0.24	-	65,65,65,65	0
56	MG	BA	3611	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3195	1/1	0.33	-	19,19,19,19	0
56	MG	BA	3255	1/1	0.34	-	16,16,16,16	0
56	MG	AA	1636	1/1	0.44	-	65,65,65,65	0
56	MG	DA	3140	1/1	0.49	-	44,44,44,44	0
56	MG	DA	3625	1/1	0.26	-	80,80,80,80	0
56	MG	BA	3244	1/1	0.23	-	60,60,60,60	0
56	MG	BA	3557	1/1	0.07	-	62,62,62,62	0
56	MG	AA	1615	1/1	0.09	-	75,75,75,75	0
56	MG	BA	3098	1/1	0.27	-	51,51,51,51	0
56	MG	DA	3145	1/1	0.17	-	41,41,41,41	0
56	MG	AV	108	1/1	0.21	-	98,98,98,98	0
56	MG	CA	1818	1/1	0.24	-	87,87,87,87	0
56	MG	DA	3474	1/1	0.11	-	76,76,76,76	0
56	MG	DA	3673	1/1	0.34	-	111,111,111,111	0
56	MG	BA	3794	1/1	0.20	-	80,80,80,80	0
56	MG	DA	3339	1/1	0.33	-	74,74,74,74	0
56	MG	BA	3440	1/1	0.77	-	56,56,56,56	0
56	MG	CA	1770	1/1	0.15	-	93,93,93,93	0
56	MG	CA	1768	1/1	0.21	-	94,94,94,94	0
56	MG	BA	3528	1/1	0.08	-	71,71,71,71	0
56	MG	DA	3462	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3646	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3233	1/1	0.32	-	80,80,80,80	0
56	MG	DA	3039	1/1	0.21	-	50,50,50,50	0
56	MG	DA	3192	1/1	0.53	-	71,71,71,71	0
56	MG	CA	1754	1/1	0.21	-	70,70,70,70	0
56	MG	DA	3106	1/1	0.33	-	48,48,48,48	0
56	MG	BB	210	1/1	0.37	-	53,53,53,53	0
56	MG	BE	304	1/1	0.42	-	14,14,14,14	0
56	MG	BA	3047	1/1	0.31	-	32,32,32,32	0
56	MG	BA	3428	1/1	0.23	-	63,63,63,63	0
56	MG	CA	1628	1/1	0.40	-	51,51,51,51	0
56	MG	BB	224	1/1	0.08	-	57,57,57,57	0
56	MG	DA	3254	1/1	0.43	-	71,71,71,71	0
56	MG	AA	1889	1/1	0.18	-	71,71,71,71	0
56	MG	BA	3479	1/1	0.45	-	63,63,63,63	0
56	MG	DA	3290	1/1	0.34	-	79,79,79,79	0
56	MG	AA	1618	1/1	0.35	-	61,61,61,61	0
56	MG	BA	3313	1/1	0.28	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3590	1/1	0.09	-	56,56,56,56	0
56	MG	DA	3379	1/1	0.40	-	80,80,80,80	0
56	MG	BA	3736	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3308	1/1	0.14	-	60,60,60,60	0
56	MG	BA	3596	1/1	0.08	-	39,39,39,39	0
56	MG	CA	1608	1/1	0.52	-	80,80,80,80	0
56	MG	AA	1704	1/1	0.29	-	79,79,79,79	0
56	MG	CA	1772	1/1	0.12	-	77,77,77,77	0
56	MG	DA	3504	1/1	0.08	-	94,94,94,94	0
56	MG	BA	3049	1/1	0.46	-	49,49,49,49	0
56	MG	CA	1726	1/1	0.27	-	70,70,70,70	0
56	MG	DA	3274	1/1	0.79	-	70,70,70,70	0
56	MG	AA	1667	1/1	0.34	-	71,71,71,71	0
56	MG	DA	3195	1/1	0.19	-	58,58,58,58	0
56	MG	BA	3549	1/1	0.23	-	19,19,19,19	0
56	MG	BA	3326	1/1	0.13	-	100,100,100,100	0
56	MG	CA	1721	1/1	0.11	-	75,75,75,75	0
56	MG	DA	3098	1/1	0.22	-	39,39,39,39	0
56	MG	DA	3453	1/1	0.14	-	77,77,77,77	0
56	MG	DB	204	1/1	0.24	-	107,107,107,107	0
56	MG	CA	1711	1/1	0.30	-	70,70,70,70	0
56	MG	AA	1898	1/1	0.14	-	98,98,98,98	0
56	MG	DA	3651	1/1	0.04	-	61,61,61,61	0
56	MG	BA	3544	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3158	1/1	0.36	-	48,48,48,48	0
56	MG	DA	3671	1/1	0.10	-	92,92,92,92	0
56	MG	BA	3261	1/1	0.22	-	69,69,69,69	0
56	MG	DA	3100	1/1	0.29	-	45,45,45,45	0
56	MG	CA	1685	1/1	0.32	-	64,64,64,64	0
56	MG	BA	3422	1/1	0.07	-	82,82,82,82	0
56	MG	B8	101	1/1	0.52	-	49,49,49,49	0
56	MG	AA	1746	1/1	0.32	-	81,81,81,81	0
56	MG	DA	3117	1/1	0.31	-	70,70,70,70	0
56	MG	BA	3498	1/1	0.23	-	54,54,54,54	0
56	MG	BA	3121	1/1	0.17	-	40,40,40,40	0
56	MG	CA	1607	1/1	0.18	-	73,73,73,73	0
56	MG	DA	3519	1/1	0.09	-	93,93,93,93	0
56	MG	BA	3452	1/1	0.29	-	55,55,55,55	0
56	MG	DA	3152	1/1	0.34	-	69,69,69,69	0
56	MG	BA	3141	1/1	0.15	-	38,38,38,38	0
56	MG	DA	3080	1/1	0.38	-	36,36,36,36	0
56	MG	CA	1624	1/1	0.22	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3649	1/1	0.11	-	73,73,73,73	0
56	MG	BA	3383	1/1	0.18	-	45,45,45,45	0
56	MG	AA	1701	1/1	0.21	-	57,57,57,57	0
56	MG	DA	3428	1/1	0.12	-	53,53,53,53	0
56	MG	DA	3634	1/1	0.13	-	70,70,70,70	0
56	MG	DA	3139	1/1	0.45	-	64,64,64,64	0
56	MG	DA	3272	1/1	0.17	-	68,68,68,68	0
56	MG	BA	3583	1/1	0.10	-	22,22,22,22	0
56	MG	CA	1698	1/1	0.85	-	114,114,114,114	0
56	MG	AK	201	1/1	0.40	-	107,107,107,107	0
56	MG	DA	3168	1/1	0.32	-	53,53,53,53	0
56	MG	DA	3448	1/1	0.18	-	73,73,73,73	0
56	MG	BA	3490	1/1	0.29	-	49,49,49,49	0
56	MG	AA	1789	1/1	0.37	-	77,77,77,77	0
56	MG	BA	3553	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3092	1/1	0.21	-	92,92,92,92	0
56	MG	BA	3070	1/1	0.61	-	51,51,51,51	0
56	MG	DA	3360	1/1	0.25	-	61,61,61,61	0
56	MG	BA	3778	1/1	0.17	-	92,92,92,92	0
56	MG	DA	3558	1/1	0.29	-	59,59,59,59	0
56	MG	DA	3286	1/1	0.36	-	69,69,69,69	0
56	MG	DA	3182	1/1	0.29	-	68,68,68,68	0
56	MG	BA	3035	1/1	0.25	-	82,82,82,82	0
56	MG	BA	3190	1/1	0.24	-	42,42,42,42	0
56	MG	AA	1882	1/1	0.10	-	55,55,55,55	0
56	MG	BA	3435	1/1	0.13	-	84,84,84,84	0
56	MG	CA	1694	1/1	0.46	-	80,80,80,80	0
56	MG	DA	3330	1/1	0.56	-	78,78,78,78	0
56	MG	AV	114	1/1	0.18	-	67,67,67,67	0
56	MG	BA	3677	1/1	0.18	-	29,29,29,29	0
56	MG	BA	3024	1/1	0.24	-	36,36,36,36	0
56	MG	BA	3872	1/1	0.18	-	24,24,24,24	0
56	MG	DA	3407	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3738	1/1	0.37	-	42,42,42,42	0
56	MG	DA	3134	1/1	0.15	-	61,61,61,61	0
56	MG	AA	1835	1/1	0.08	-	88,88,88,88	0
56	MG	AA	1627	1/1	0.52	-	83,83,83,83	0
56	MG	DA	3173	1/1	0.29	-	62,62,62,62	0
56	MG	DA	3427	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3819	1/1	0.13	-	71,71,71,71	0
56	MG	BF	302	1/1	0.39	-	41,41,41,41	0
56	MG	BA	3469	1/1	0.33	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3048	1/1	0.35	-	54,54,54,54	0
56	MG	BB	215	1/1	0.17	-	62,62,62,62	0
56	MG	AA	1897	1/1	0.21	-	74,74,74,74	0
56	MG	BA	3634	1/1	0.08	-	46,46,46,46	0
56	MG	BE	303	1/1	0.17	-	32,32,32,32	0
56	MG	DA	3282	1/1	0.59	-	75,75,75,75	0
56	MG	BA	3355	1/1	0.30	-	62,62,62,62	0
56	MG	BA	3797	1/1	0.23	-	91,91,91,91	0
56	MG	BA	3323	1/1	0.31	-	45,45,45,45	0
56	MG	CA	1729	1/1	0.15	-	80,80,80,80	0
56	MG	DA	3575	1/1	0.10	-	65,65,65,65	0
56	MG	BA	3895	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3167	1/1	0.25	-	31,31,31,31	0
56	MG	AA	1660	1/1	0.21	-	59,59,59,59	0
56	MG	BA	3008	1/1	0.24	-	84,84,84,84	0
56	MG	DA	3446	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3383	1/1	0.45	-	76,76,76,76	0
56	MG	DA	3353	1/1	0.65	-	80,80,80,80	0
56	MG	DA	3124	1/1	0.50	-	50,50,50,50	0
56	MG	BA	3062	1/1	0.14	-	34,34,34,34	0
56	MG	DA	3216	1/1	0.23	-	46,46,46,46	0
56	MG	AA	1620	1/1	0.53	-	74,74,74,74	0
56	MG	CA	1612	1/1	0.23	-	84,84,84,84	0
56	MG	CA	1682	1/1	0.49	-	73,73,73,73	0
56	MG	BA	3879	1/1	0.20	-	53,53,53,53	0
56	MG	AA	1689	1/1	0.19	-	77,77,77,77	0
56	MG	BA	3371	1/1	0.18	-	66,66,66,66	0
56	MG	DA	3307	1/1	0.26	-	65,65,65,65	0
56	MG	BA	3686	1/1	0.12	-	26,26,26,26	0
56	MG	DA	3175	1/1	0.22	-	75,75,75,75	0
56	MG	DA	3099	1/1	0.41	-	42,42,42,42	0
56	MG	AA	1948	1/1	0.09	-	88,88,88,88	0
56	MG	BA	3722	1/1	0.06	-	61,61,61,61	0
56	MG	CA	1634	1/1	0.39	-	63,63,63,63	0
56	MG	BA	3247	1/1	0.17	-	20,20,20,20	0
56	MG	DA	3275	1/1	0.34	-	42,42,42,42	0
56	MG	DE	304	1/1	0.20	-	70,70,70,70	0
56	MG	CA	1755	1/1	0.17	-	93,93,93,93	0
56	MG	DA	3439	1/1	0.07	-	42,42,42,42	0
56	MG	BA	3572	1/1	0.07	-	66,66,66,66	0
56	MG	AA	1837	1/1	0.18	-	66,66,66,66	0
56	MG	AA	1737	1/1	0.47	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3537	1/1	0.52	-	68,68,68,68	0
56	MG	BB	226	1/1	0.06	-	61,61,61,61	0
56	MG	DA	3297	1/1	0.23	-	81,81,81,81	0
56	MG	DA	3303	1/1	0.27	-	54,54,54,54	0
56	MG	AA	1825	1/1	0.23	-	64,64,64,64	0
56	MG	BA	3333	1/1	0.25	-	58,58,58,58	0
56	MG	AA	1814	1/1	0.28	-	81,81,81,81	0
56	MG	BA	3074	1/1	0.22	-	52,52,52,52	0
56	MG	DA	3397	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3541	1/1	0.08	-	35,35,35,35	0
56	MG	BA	3773	1/1	0.07	-	44,44,44,44	0
56	MG	DA	3565	1/1	0.13	-	50,50,50,50	0
56	MG	DA	3570	1/1	0.24	-	79,79,79,79	0
56	MG	CA	1666	1/1	0.28	-	73,73,73,73	0
56	MG	DA	3201	1/1	0.59	-	80,80,80,80	0
56	MG	DA	3034	1/1	0.43	-	77,77,77,77	0
56	MG	DA	3206	1/1	0.18	-	92,92,92,92	0
56	MG	DA	3503	1/1	0.18	-	80,80,80,80	0
56	MG	BA	3487	1/1	0.15	-	53,53,53,53	0
56	MG	CA	1749	1/1	0.20	-	92,92,92,92	0
56	MG	BA	3147	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3241	1/1	0.15	-	76,76,76,76	0
56	MG	BA	3734	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3476	1/1	0.16	-	71,71,71,71	0
56	MG	BQ	204	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3622	1/1	0.15	-	65,65,65,65	0
56	MG	BA	3502	1/1	0.27	-	33,33,33,33	0
56	MG	DA	3585	1/1	0.21	-	104,104,104,104	0
56	MG	AA	1806	1/1	0.42	-	59,59,59,59	0
56	MG	AA	1696	1/1	0.56	-	95,95,95,95	0
56	MG	BA	3496	1/1	0.21	-	61,61,61,61	0
56	MG	DA	3001	1/1	0.13	-	58,58,58,58	0
56	MG	BA	3763	1/1	0.10	-	84,84,84,84	0
56	MG	BA	3016	1/1	0.41	-	52,52,52,52	0
56	MG	BA	3310	1/1	0.25	-	54,54,54,54	0
56	MG	DA	3250	1/1	0.41	-	62,62,62,62	0
56	MG	BA	3663	1/1	0.14	-	21,21,21,21	0
56	MG	AA	1759	1/1	0.37	-	60,60,60,60	0
56	MG	AA	1610	1/1	0.36	-	48,48,48,48	0
56	MG	BA	3782	1/1	0.32	-	75,75,75,75	0
56	MG	BA	3866	1/1	0.08	-	82,82,82,82	0
56	MG	AA	1688	1/1	0.11	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1625	1/1	0.41	-	71,71,71,71	0
56	MG	DA	3656	1/1	0.09	-	90,90,90,90	0
56	MG	BA	3714	1/1	0.29	-	62,62,62,62	0
56	MG	B5	102	1/1	0.22	-	58,58,58,58	0
56	MG	AA	1874	1/1	0.29	-	95,95,95,95	0
56	MG	BA	3741	1/1	0.14	-	63,63,63,63	0
56	MG	BA	3593	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3292	1/1	0.14	-	47,47,47,47	0
56	MG	DA	3022	1/1	0.12	-	46,46,46,46	0
56	MG	DA	3669	1/1	0.09	-	93,93,93,93	0
56	MG	CV	106	1/1	0.37	-	78,78,78,78	0
56	MG	BA	3475	1/1	0.19	-	42,42,42,42	0
56	MG	BA	3740	1/1	0.17	-	48,48,48,48	0
56	MG	BF	307	1/1	0.18	-	42,42,42,42	0
56	MG	BA	3540	1/1	0.15	-	19,19,19,19	0
56	MG	AA	1813	1/1	0.13	-	121,121,121,121	0
56	MG	BA	3176	1/1	0.15	-	63,63,63,63	0
56	MG	AA	1901	1/1	0.13	-	119,119,119,119	0
56	MG	AA	1792	1/1	0.18	-	44,44,44,44	0
56	MG	DA	3033	1/1	0.12	-	74,74,74,74	0
56	MG	DA	3579	1/1	0.20	-	104,104,104,104	0
56	MG	AA	1903	1/1	0.19	-	117,117,117,117	0
56	MG	BA	3246	1/1	0.39	-	53,53,53,53	0
56	MG	DA	3549	1/1	0.16	-	87,87,87,87	0
56	MG	CA	1776	1/1	0.41	-	90,90,90,90	0
56	MG	AA	1936	1/1	0.19	-	84,84,84,84	0
56	MG	BA	3659	1/1	0.14	-	60,60,60,60	0
56	MG	BA	3373	1/1	0.35	-	69,69,69,69	0
56	MG	DA	3532	1/1	0.21	-	90,90,90,90	0
56	MG	DA	3104	1/1	0.43	-	60,60,60,60	0
56	MG	DA	3147	1/1	0.30	-	70,70,70,70	0
56	MG	BA	3569	1/1	0.26	-	49,49,49,49	0
56	MG	CV	101	1/1	0.20	-	59,59,59,59	0
56	MG	BA	3524	1/1	0.12	-	81,81,81,81	0
56	MG	BA	3152	1/1	0.09	-	42,42,42,42	0
56	MG	DA	3404	1/1	0.12	-	56,56,56,56	0
56	MG	BA	3088	1/1	0.23	-	45,45,45,45	0
56	MG	BA	3464	1/1	0.37	-	53,53,53,53	0
56	MG	B3	101	1/1	0.52	-	57,57,57,57	0
56	MG	DA	3481	1/1	0.37	-	85,85,85,85	0
56	MG	DA	3488	1/1	0.68	-	73,73,73,73	0
56	MG	AA	1781	1/1	0.54	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3263	1/1	0.28	-	67,67,67,67	0
56	MG	BA	3462	1/1	0.28	-	47,47,47,47	0
56	MG	CA	1748	1/1	0.13	-	75,75,75,75	0
56	MG	BA	3101	1/1	0.32	-	26,26,26,26	0
56	MG	AA	1715	1/1	0.49	-	72,72,72,72	0
56	MG	DA	3244	1/1	0.28	-	64,64,64,64	0
56	MG	CA	1661	1/1	0.15	-	101,101,101,101	0
56	MG	DA	3127	1/1	0.30	-	37,37,37,37	0
56	MG	DA	3132	1/1	0.15	-	66,66,66,66	0
56	MG	BA	3699	1/1	0.12	-	38,38,38,38	0
56	MG	AA	1871	1/1	0.06	-	71,71,71,71	0
56	MG	BA	3302	1/1	0.25	-	53,53,53,53	0
56	MG	DA	3689	1/1	0.22	-	104,104,104,104	0
56	MG	DA	3332	1/1	0.33	-	63,63,63,63	0
56	MG	AA	1661	1/1	0.40	-	56,56,56,56	0
56	MG	BA	3421	1/1	0.32	-	75,75,75,75	0
56	MG	BA	3802	1/1	0.20	-	71,71,71,71	0
56	MG	BA	3171	1/1	0.38	-	38,38,38,38	0
56	MG	BA	3369	1/1	0.33	-	65,65,65,65	0
56	MG	DA	3295	1/1	0.10	-	75,75,75,75	0
56	MG	AA	1685	1/1	0.65	-	91,91,91,91	0
56	MG	AA	1891	1/1	0.04	-	75,75,75,75	0
56	MG	BA	3003	1/1	0.13	-	59,59,59,59	0
56	MG	BA	3198	1/1	0.21	-	17,17,17,17	0
56	MG	DA	3324	1/1	0.17	-	55,55,55,55	0
56	MG	BA	3600	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3546	1/1	0.07	-	48,48,48,48	0
57	ZN	D5	102	1/1	0.08	-	88,88,88,88	0
56	MG	DA	3289	1/1	0.18	-	86,86,86,86	0
56	MG	CA	1816	1/1	0.23	-	110,110,110,110	0
56	MG	BA	3357	1/1	0.19	-	82,82,82,82	0
56	MG	BA	3059	1/1	0.35	-	25,25,25,25	0
56	MG	BA	3598	1/1	0.04	-	54,54,54,54	0
56	MG	CA	1690	1/1	0.23	-	74,74,74,74	0
56	MG	AA	1860	1/1	0.11	-	85,85,85,85	0
56	MG	BA	3612	1/1	0.08	-	61,61,61,61	0
56	MG	BD	305	1/1	0.40	-	54,54,54,54	0
56	MG	DA	3467	1/1	0.16	-	91,91,91,91	0
56	MG	DA	3418	1/1	0.31	-	52,52,52,52	0
57	ZN	AD	301	1/1	0.29	-	93,93,93,93	0
56	MG	BA	3289	1/1	0.20	-	61,61,61,61	0
56	MG	DA	3161	1/1	0.18	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3770	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3356	1/1	0.15	-	85,85,85,85	0
56	MG	DA	3347	1/1	0.57	-	77,77,77,77	0
56	MG	DA	3352	1/1	0.36	-	68,68,68,68	0
56	MG	DA	3680	1/1	0.09	-	79,79,79,79	0
56	MG	DA	3610	1/1	0.35	-	97,97,97,97	0
56	MG	CA	1702	1/1	0.36	-	114,114,114,114	0
56	MG	DA	3597	1/1	0.11	-	57,57,57,57	0
56	MG	DA	3273	1/1	0.42	-	62,62,62,62	0
56	MG	DA	3373	1/1	0.38	-	75,75,75,75	0
56	MG	AA	1908	1/1	0.10	-	97,97,97,97	0
56	MG	DA	3635	1/1	0.14	-	88,88,88,88	0
56	MG	BA	3702	1/1	0.23	-	49,49,49,49	0
56	MG	BA	3109	1/1	0.24	-	58,58,58,58	0
56	MG	AA	1724	1/1	0.38	-	92,92,92,92	0
56	MG	BA	3537	1/1	0.15	-	47,47,47,47	0
57	ZN	CN	101	1/1	0.10	-	165,165,165,165	0
56	MG	BA	3177	1/1	0.21	-	46,46,46,46	0
56	MG	BA	3766	1/1	0.22	-	38,38,38,38	0
56	MG	BA	3446	1/1	0.21	-	87,87,87,87	0
56	MG	CA	1648	1/1	0.21	-	73,73,73,73	0
56	MG	CA	1793	1/1	0.21	-	73,73,73,73	0
56	MG	AV	115	1/1	0.21	-	65,65,65,65	0
56	MG	DA	3238	1/1	0.29	-	65,65,65,65	0
56	MG	DA	3141	1/1	0.27	-	60,60,60,60	0
56	MG	DA	3393	1/1	0.34	-	63,63,63,63	0
56	MG	DA	3605	1/1	0.18	-	101,101,101,101	0
56	MG	AA	1880	1/1	0.37	-	79,79,79,79	0
56	MG	DA	3602	1/1	0.20	-	47,47,47,47	0
56	MG	DA	3562	1/1	0.25	-	69,69,69,69	0
56	MG	DA	3520	1/1	0.07	-	67,67,67,67	0
56	MG	BA	3787	1/1	0.06	-	35,35,35,35	0
56	MG	DA	3203	1/1	0.35	-	91,91,91,91	0
56	MG	AA	1774	1/1	0.28	-	69,69,69,69	0
56	MG	DA	3142	1/1	0.26	-	50,50,50,50	0
56	MG	DA	3483	1/1	0.17	-	84,84,84,84	0
56	MG	BA	3022	1/1	0.14	-	85,85,85,85	0
56	MG	DA	3468	1/1	0.09	-	80,80,80,80	0
56	MG	BB	221	1/1	0.09	-	44,44,44,44	0
56	MG	BO	201	1/1	0.29	-	62,62,62,62	0
56	MG	DA	3620	1/1	0.27	-	95,95,95,95	0
56	MG	DA	3361	1/1	0.17	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1855	1/1	0.16	-	80,80,80,80	0
56	MG	DA	3521	1/1	0.51	-	60,60,60,60	0
56	MG	DA	3626	1/1	0.29	-	103,103,103,103	0
56	MG	DA	3171	1/1	0.26	-	66,66,66,66	0
56	MG	BA	3309	1/1	0.47	-	56,56,56,56	0
56	MG	CA	1740	1/1	0.15	-	73,73,73,73	0
56	MG	BA	3881	1/1	0.10	-	75,75,75,75	0
56	MG	AV	109	1/1	0.20	-	81,81,81,81	0
56	MG	DA	3413	1/1	0.28	-	40,40,40,40	0
56	MG	BA	3669	1/1	0.09	-	34,34,34,34	0
56	MG	AA	1829	1/1	0.18	-	63,63,63,63	0
56	MG	CA	1668	1/1	0.11	-	59,59,59,59	0
56	MG	DA	3177	1/1	0.42	-	75,75,75,75	0
56	MG	AA	1890	1/1	0.23	-	89,89,89,89	0
56	MG	DA	3329	1/1	0.46	-	63,63,63,63	0
56	MG	B5	103	1/1	0.13	-	61,61,61,61	0
56	MG	CA	1767	1/1	0.23	-	62,62,62,62	0
56	MG	BA	3514	1/1	0.26	-	58,58,58,58	0
56	MG	AA	1716	1/1	0.12	-	70,70,70,70	0
56	MG	DA	3654	1/1	0.36	-	118,118,118,118	0
56	MG	CA	1629	1/1	0.74	-	74,74,74,74	0
56	MG	DA	3264	1/1	0.23	-	74,74,74,74	0
56	MG	DA	3586	1/1	0.27	-	50,50,50,50	0
56	MG	BA	3153	1/1	0.23	-	56,56,56,56	0
56	MG	CA	1649	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3511	1/1	0.35	-	48,48,48,48	0
56	MG	CA	1743	1/1	0.58	-	86,86,86,86	0
56	MG	DA	3020	1/1	0.47	-	75,75,75,75	0
56	MG	BA	3759	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3118	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3407	1/1	0.21	-	44,44,44,44	0
56	MG	BA	3607	1/1	0.31	-	59,59,59,59	0
56	MG	DA	3046	1/1	0.12	-	79,79,79,79	0
56	MG	AA	1743	1/1	0.51	-	80,80,80,80	0
56	MG	BA	3358	1/1	0.72	-	63,63,63,63	0
56	MG	DA	3090	1/1	0.52	-	76,76,76,76	0
56	MG	DA	3267	1/1	0.49	-	66,66,66,66	0
56	MG	AA	1619	1/1	0.43	-	68,68,68,68	0
56	MG	AA	1703	1/1	0.38	-	74,74,74,74	0
56	MG	DA	3054	1/1	0.32	-	78,78,78,78	0
56	MG	DA	3317	1/1	0.19	-	84,84,84,84	0
56	MG	BA	3681	1/1	0.17	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3245	1/1	0.27	-	42,42,42,42	0
56	MG	CA	1741	1/1	0.07	-	92,92,92,92	0
56	MG	AA	1793	1/1	0.27	-	72,72,72,72	0
56	MG	BA	3286	1/1	0.15	-	61,61,61,61	0
56	MG	DA	3084	1/1	0.30	-	76,76,76,76	0
56	MG	BA	3642	1/1	0.07	-	78,78,78,78	0
56	MG	AA	1727	1/1	0.51	-	73,73,73,73	0
56	MG	BA	3585	1/1	0.06	-	35,35,35,35	0
56	MG	BA	3480	1/1	0.32	-	59,59,59,59	0
56	MG	BA	3288	1/1	0.09	-	77,77,77,77	0
56	MG	BA	3727	1/1	0.08	-	66,66,66,66	0
56	MG	BA	3318	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3542	1/1	0.12	-	79,79,79,79	0
56	MG	DA	3566	1/1	0.15	-	84,84,84,84	0
56	MG	AA	1736	1/1	0.52	-	82,82,82,82	0
56	MG	DA	3609	1/1	0.23	-	75,75,75,75	0
56	MG	BA	3347	1/1	0.46	-	20,20,20,20	0
56	MG	BA	3571	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3149	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3334	1/1	0.39	-	83,83,83,83	0
56	MG	DA	3114	1/1	0.19	-	70,70,70,70	0
56	MG	CA	1719	1/1	0.20	-	85,85,85,85	0
56	MG	DA	3055	1/1	0.25	-	57,57,57,57	0
56	MG	AA	1638	1/1	0.26	-	78,78,78,78	0
56	MG	BA	3625	1/1	0.09	-	41,41,41,41	0
56	MG	BA	3084	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3574	1/1	0.13	-	53,53,53,53	0
56	MG	BB	201	1/1	0.31	-	57,57,57,57	0
56	MG	DT	202	1/1	0.19	-	38,38,38,38	0
56	MG	AA	1863	1/1	0.24	-	54,54,54,54	0
56	MG	BA	3014	1/1	0.46	-	49,49,49,49	0
56	MG	DA	3359	1/1	0.16	-	59,59,59,59	0
56	MG	DA	3261	1/1	0.24	-	69,69,69,69	0
56	MG	CA	1739	1/1	0.24	-	79,79,79,79	0
56	MG	BA	3780	1/1	0.23	-	86,86,86,86	0
56	MG	AD	302	1/1	0.43	-	79,79,79,79	0
56	MG	DA	3394	1/1	0.11	-	36,36,36,36	0
56	MG	DA	3631	1/1	0.28	-	94,94,94,94	0
56	MG	AA	1856	1/1	0.12	-	66,66,66,66	0
56	MG	BD	302	1/1	0.58	-	51,51,51,51	0
56	MG	BA	3467	1/1	0.37	-	56,56,56,56	0
56	MG	AA	1684	1/1	0.20	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3067	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3755	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3592	1/1	0.09	-	52,52,52,52	0
56	MG	AA	1668	1/1	0.28	-	65,65,65,65	0
56	MG	CA	1786	1/1	0.16	-	80,80,80,80	0
56	MG	AA	1611	1/1	0.16	-	97,97,97,97	0
56	MG	BA	3196	1/1	0.16	-	66,66,66,66	0
56	MG	BA	3350	1/1	0.21	-	69,69,69,69	0
56	MG	DA	3463	1/1	0.11	-	68,68,68,68	0
56	MG	DA	3480	1/1	0.19	-	70,70,70,70	0
56	MG	BA	3378	1/1	0.21	-	40,40,40,40	0
56	MG	BA	3233	1/1	0.24	-	22,22,22,22	0
56	MG	DA	3471	1/1	0.07	-	87,87,87,87	0
56	MG	CA	1730	1/1	0.36	-	69,69,69,69	0
56	MG	DB	203	1/1	0.26	-	105,105,105,105	0
56	MG	AA	1662	1/1	0.51	-	71,71,71,71	0
56	MG	DA	3559	1/1	0.15	-	76,76,76,76	0
56	MG	BA	3083	1/1	0.17	-	48,48,48,48	0
56	MG	AA	1761	1/1	0.30	-	58,58,58,58	0
56	MG	BA	3602	1/1	0.22	-	22,22,22,22	0
56	MG	BA	3631	1/1	0.08	-	25,25,25,25	0
56	MG	BA	3081	1/1	0.28	-	53,53,53,53	0
56	MG	BA	3489	1/1	0.12	-	55,55,55,55	0
56	MG	BA	3739	1/1	0.07	-	42,42,42,42	0
56	MG	CA	1703	1/1	0.35	-	100,100,100,100	0
56	MG	AA	1939	1/1	0.31	-	105,105,105,105	0
56	MG	BA	3249	1/1	0.29	-	24,24,24,24	0
56	MG	DA	3580	1/1	0.07	-	76,76,76,76	0
56	MG	BA	3020	1/1	0.13	-	44,44,44,44	0
56	MG	CA	1632	1/1	0.45	-	77,77,77,77	0
56	MG	AA	1782	1/1	0.27	-	51,51,51,51	0
56	MG	DA	3432	1/1	0.16	-	85,85,85,85	0
56	MG	AA	1919	1/1	0.23	-	63,63,63,63	0
56	MG	BA	3644	1/1	0.12	-	72,72,72,72	0
56	MG	BA	3320	1/1	0.32	-	58,58,58,58	0
56	MG	DA	3670	1/1	0.11	-	83,83,83,83	0
56	MG	CX	101	1/1	0.23	-	99,99,99,99	0
56	MG	BA	3397	1/1	0.37	-	66,66,66,66	0
56	MG	DA	3449	1/1	0.26	-	45,45,45,45	0
56	MG	BP	201	1/1	0.34	-	33,33,33,33	0
56	MG	DA	3049	1/1	0.21	-	76,76,76,76	0
56	MG	BA	3300	1/1	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3346	1/1	0.27	-	43,43,43,43	0
56	MG	AA	1658	1/1	0.78	-	73,73,73,73	0
56	MG	CA	1805	1/1	0.09	-	88,88,88,88	0
56	MG	DA	3344	1/1	0.38	-	88,88,88,88	0
57	ZN	AN	101	1/1	0.15	-	164,164,164,164	0
56	MG	BA	3744	1/1	0.39	-	44,44,44,44	0
56	MG	DA	3592	1/1	0.15	-	69,69,69,69	0
56	MG	BA	3628	1/1	0.14	-	66,66,66,66	0
56	MG	BA	3647	1/1	0.13	-	61,61,61,61	0
56	MG	AA	1695	1/1	0.27	-	102,102,102,102	0
56	MG	BA	3580	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3213	1/1	0.45	-	89,89,89,89	0
56	MG	CA	1621	1/1	0.21	-	100,100,100,100	0
56	MG	DA	3176	1/1	0.34	-	67,67,67,67	0
56	MG	DA	3298	1/1	0.21	-	55,55,55,55	0
56	MG	AV	117	1/1	0.10	-	69,69,69,69	0
56	MG	BA	3455	1/1	0.47	-	22,22,22,22	0
56	MG	AA	1820	1/1	0.26	-	86,86,86,86	0
56	MG	DA	3215	1/1	0.60	-	46,46,46,46	0
56	MG	BA	3831	1/1	0.13	-	22,22,22,22	0
56	MG	DA	3003	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3041	1/1	0.50	-	54,54,54,54	0
56	MG	DX	101	1/1	0.22	-	55,55,55,55	0
56	MG	CA	1670	1/1	0.22	-	69,69,69,69	0
56	MG	BA	3561	1/1	0.13	-	64,64,64,64	0
56	MG	BA	3495	1/1	0.44	-	56,56,56,56	0
56	MG	DA	3292	1/1	0.26	-	69,69,69,69	0
56	MG	DE	303	1/1	0.47	-	63,63,63,63	0
56	MG	DA	3451	1/1	0.27	-	39,39,39,39	0
56	MG	DA	3278	1/1	0.63	-	66,66,66,66	0
56	MG	DA	3623	1/1	0.20	-	85,85,85,85	0
56	MG	BA	3649	1/1	0.12	-	60,60,60,60	0
56	MG	DA	3514	1/1	0.19	-	76,76,76,76	0
56	MG	BA	3093	1/1	0.12	-	42,42,42,42	0
56	MG	DA	3696	1/1	0.38	-	96,96,96,96	0
56	MG	BA	3160	1/1	0.37	-	41,41,41,41	0
56	MG	AA	1881	1/1	0.13	-	50,50,50,50	0
56	MG	DA	3338	1/1	0.40	-	69,69,69,69	0
56	MG	DA	3150	1/1	0.11	-	65,65,65,65	0
56	MG	DA	3479	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3458	1/1	0.12	-	49,49,49,49	0
56	MG	DA	3509	1/1	0.34	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1943	1/1	0.15	-	92,92,92,92	0
56	MG	BA	3387	1/1	0.18	-	48,48,48,48	0
56	MG	AA	1705	1/1	0.21	-	55,55,55,55	0
56	MG	DA	3053	1/1	0.15	-	55,55,55,55	0
56	MG	BA	3858	1/1	0.28	-	70,70,70,70	0
56	MG	DA	3265	1/1	0.39	-	68,68,68,68	0
56	MG	BA	3311	1/1	0.19	-	59,59,59,59	0
56	MG	AA	1728	1/1	0.42	-	81,81,81,81	0
56	MG	DA	3070	1/1	0.11	-	74,74,74,74	0
56	MG	DA	3316	1/1	0.13	-	80,80,80,80	0
56	MG	BA	3889	1/1	0.18	-	80,80,80,80	0
56	MG	B8	102	1/1	0.15	-	49,49,49,49	0
56	MG	DA	3686	1/1	0.21	-	74,74,74,74	0
56	MG	AA	1648	1/1	0.23	-	65,65,65,65	0
56	MG	AA	1788	1/1	0.43	-	62,62,62,62	0
56	MG	BA	3466	1/1	0.33	-	50,50,50,50	0
56	MG	DA	3202	1/1	0.23	-	73,73,73,73	0
56	MG	BA	3660	1/1	0.09	-	28,28,28,28	0
56	MG	AA	1944	1/1	0.23	-	97,97,97,97	0
56	MG	BA	3562	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3662	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3014	1/1	0.19	-	38,38,38,38	0
56	MG	AA	1776	1/1	0.21	-	89,89,89,89	0
56	MG	BA	3392	1/1	0.24	-	54,54,54,54	0
56	MG	BA	3833	1/1	0.12	-	41,41,41,41	0
56	MG	AA	1858	1/1	0.04	-	90,90,90,90	0
56	MG	AA	1754	1/1	0.32	-	59,59,59,59	0
56	MG	BA	3328	1/1	0.10	-	68,68,68,68	0
56	MG	BA	3394	1/1	0.28	-	58,58,58,58	0
56	MG	DA	3385	1/1	0.17	-	48,48,48,48	0
56	MG	DA	3378	1/1	0.29	-	64,64,64,64	0
56	MG	DA	3612	1/1	0.20	-	87,87,87,87	0
56	MG	BA	3729	1/1	0.10	-	59,59,59,59	0
56	MG	DA	3074	1/1	0.33	-	69,69,69,69	0
56	MG	CA	1790	1/1	0.29	-	64,64,64,64	0
56	MG	BA	3307	1/1	0.30	-	48,48,48,48	0
56	MG	DA	3255	1/1	0.26	-	72,72,72,72	0
56	MG	BA	3821	1/1	0.08	-	76,76,76,76	0
56	MG	BA	3096	1/1	0.11	-	37,37,37,37	0
56	MG	BA	3215	1/1	0.40	-	16,16,16,16	0
56	MG	DA	3647	1/1	0.20	-	70,70,70,70	0
56	MG	AA	1925	1/1	0.09	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3447	1/1	0.13	-	62,62,62,62	0
56	MG	DA	3188	1/1	0.57	-	77,77,77,77	0
56	MG	DA	3400	1/1	0.26	-	53,53,53,53	0
56	MG	AA	1893	1/1	0.33	-	95,95,95,95	0
56	MG	BA	3581	1/1	0.17	-	29,29,29,29	0
56	MG	AA	1659	1/1	0.43	-	97,97,97,97	0
56	MG	AA	1644	1/1	0.31	-	48,48,48,48	0
56	MG	AA	1844	1/1	0.33	-	86,86,86,86	0
56	MG	DA	3006	1/1	0.19	-	56,56,56,56	0
56	MG	DA	3107	1/1	0.20	-	58,58,58,58	0
56	MG	BA	3558	1/1	0.13	-	61,61,61,61	0
56	MG	BA	3104	1/1	0.25	-	50,50,50,50	0
56	MG	BB	211	1/1	0.21	-	66,66,66,66	0
56	MG	DA	3639	1/1	0.12	-	82,82,82,82	0
56	MG	BA	3252	1/1	0.49	-	20,20,20,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.