



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 03:27 AM UTC

PDB ID : 4V95 / pdb_00004v95
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

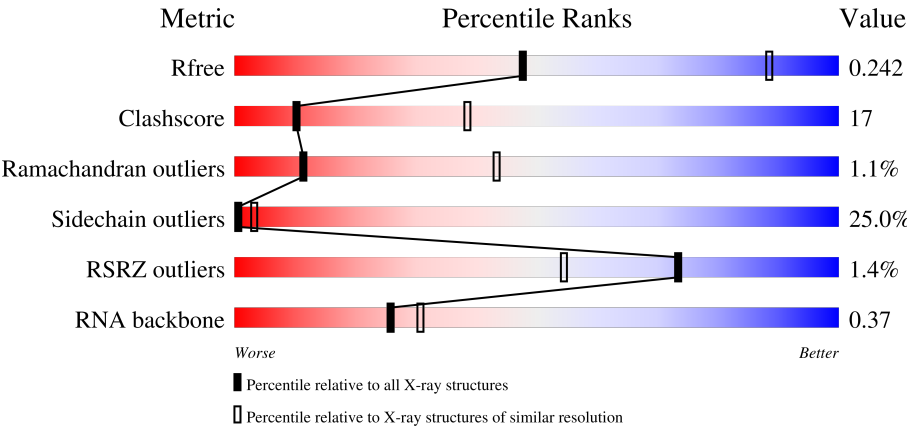
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	33% 47% 17% •
1	CA	1522	35% 45% 16% •
2	AB	256	3% 34% 38% 16% • 9%
2	CB	256	3% 29% 47% 14% • 8%

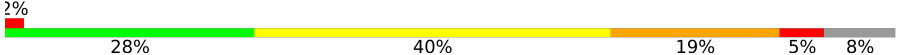
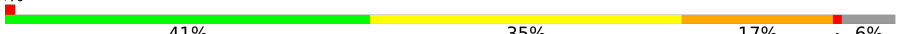
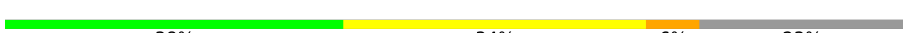
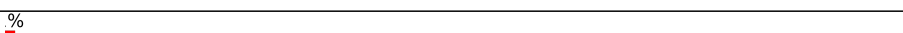
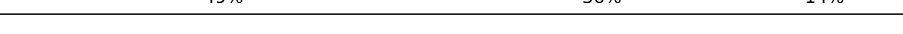
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

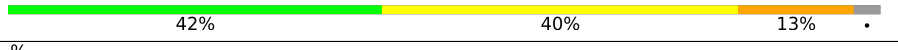
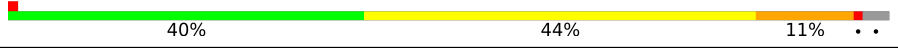
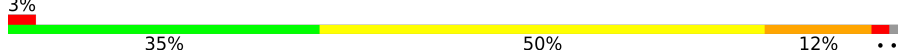
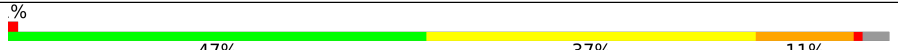
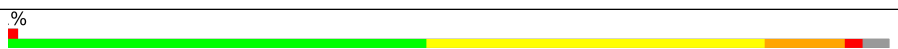
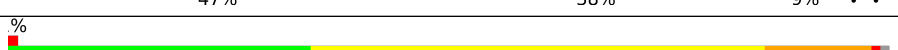
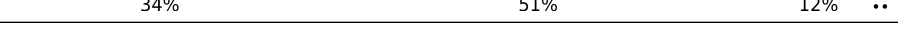
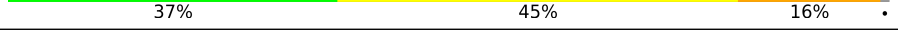
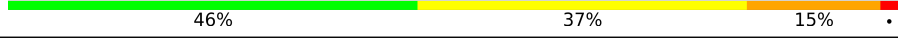
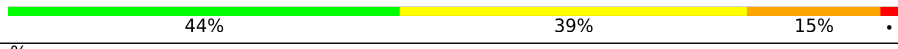
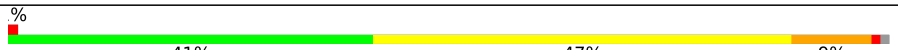
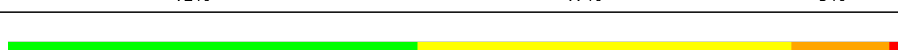
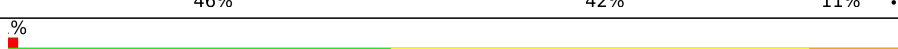
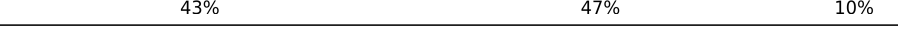
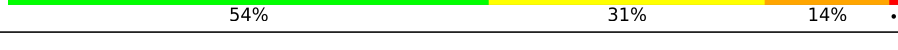
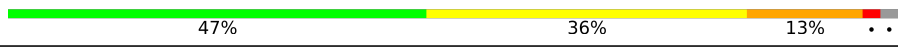
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AY	140	
23	AV	77	
23	CV	77	
24	AX	16	
24	CX	16	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	
28	BE	206	

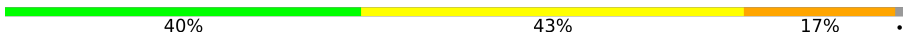
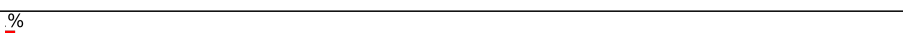
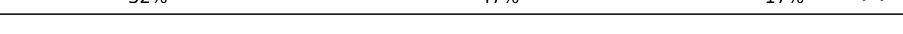
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Mol	Chain	Length	Quality of chain
28	DE	206	% 
29	BF	210	
29	DF	210	% 
30	BG	182	% 
30	DG	182	3% 
31	BH	180	% 
31	DH	180	% 
32	BI	148	% 
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	% 
34	DO	122	
35	BP	150	
35	DP	150	% 
36	BQ	141	
36	DQ	141	% 
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	% 
39	DT	146	% 
40	BU	118	
40	DU	118	% 

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Mol	Chain	Length	Quality of chain
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	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	
53	B7	49	

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Mol	Chain	Length	Quality of chain
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1803	-	-	-	X
56	MG	AA	1805	-	-	-	X
56	MG	AA	1819	-	-	-	X
56	MG	CA	1635	-	-	-	X
56	MG	CA	1669	-	-	-	X
56	MG	CA	1708	-	-	-	X
56	MG	DA	3052	-	-	-	X
56	MG	DA	3065	-	-	-	X
56	MG	DA	3199	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 284877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0	0
			657	407	129	121			

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

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

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

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

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

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

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

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

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

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

- 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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	348	Total	Mg	0	0
			348	348		
56	AD	2	Total	Mg	0	0
			2	2		
56	AE	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AI	2	Total	Mg	0	0
			2	2		
56	AK	1	Total	Mg	0	0
			1	1		
56	AT	1	Total	Mg	0	0
			1	1		
56	AY	1	Total	Mg	0	0
			1	1		
56	AV	18	Total	Mg	0	0
			18	18		
56	BA	896	Total	Mg	0	0
			896	896		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	30	Total 30	Mg 30	0	0
56	BD	5	Total 5	Mg 5	0	0
56	BE	5	Total 5	Mg 5	0	0
56	BF	7	Total 7	Mg 7	0	0
56	BG	2	Total 2	Mg 2	0	0
56	BO	2	Total 2	Mg 2	0	0
56	BP	2	Total 2	Mg 2	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	BR	2	Total 2	Mg 2	0	0
56	BT	1	Total 1	Mg 1	0	0
56	BU	1	Total 1	Mg 1	0	0
56	BV	2	Total 2	Mg 2	0	0
56	BX	1	Total 1	Mg 1	0	0
56	BY	2	Total 2	Mg 2	0	0
56	BZ	2	Total 2	Mg 2	0	0
56	B0	5	Total 5	Mg 5	0	0
56	B1	3	Total 3	Mg 3	0	0
56	B2	2	Total 2	Mg 2	0	0
56	B3	2	Total 2	Mg 2	0	0
56	B5	3	Total 3	Mg 3	0	0
56	B6	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B7	1	Total 1	Mg 1	0	0
56	B8	2	Total 2	Mg 2	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	219	Total 219	Mg 219	0	0
56	CD	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CV	10	Total 10	Mg 10	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DA	696	Total 696	Mg 696	0	0
56	DB	16	Total 16	Mg 16	0	0
56	DD	4	Total 4	Mg 4	0	0
56	DE	4	Total 4	Mg 4	0	0
56	DF	3	Total 3	Mg 3	0	0
56	DO	3	Total 3	Mg 3	0	0
56	DQ	2	Total 2	Mg 2	0	0
56	DR	1	Total 1	Mg 1	0	0
56	DT	3	Total 3	Mg 3	0	0
56	DU	1	Total 1	Mg 1	0	0
56	DV	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	D0	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	D1	1	Total 1	Mg 1	0	0
56	D5	1	Total 1	Mg 1	0	0
56	D6	2	Total 2	Mg 2	0	0
56	D7	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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	O	0	0
			4	4		
58	BR	7	Total	O	0	0
			7	7		
58	BT	1	Total	O	0	0
			1	1		
58	BU	7	Total	O	0	0
			7	7		
58	BV	1	Total	O	0	0
			1	1		
58	BW	2	Total	O	0	0
			2	2		
58	BX	2	Total	O	0	0
			2	2		
58	BY	1	Total	O	0	0
			1	1		
58	B0	4	Total	O	0	0
			4	4		
58	B1	1	Total	O	0	0
			1	1		
58	B3	1	Total	O	0	0
			1	1		
58	B6	4	Total	O	0	0
			4	4		
58	B7	2	Total	O	0	0
			2	2		
58	B8	4	Total	O	0	0
			4	4		
58	B9	1	Total	O	0	0
			1	1		
58	CA	330	Total	O	0	0
			330	330		
58	CB	1	Total	O	0	0
			1	1		
58	CC	1	Total	O	0	0
			1	1		
58	CD	3	Total	O	0	0
			3	3		
58	CE	1	Total	O	0	0
			1	1		
58	CK	2	Total	O	0	0
			2	2		

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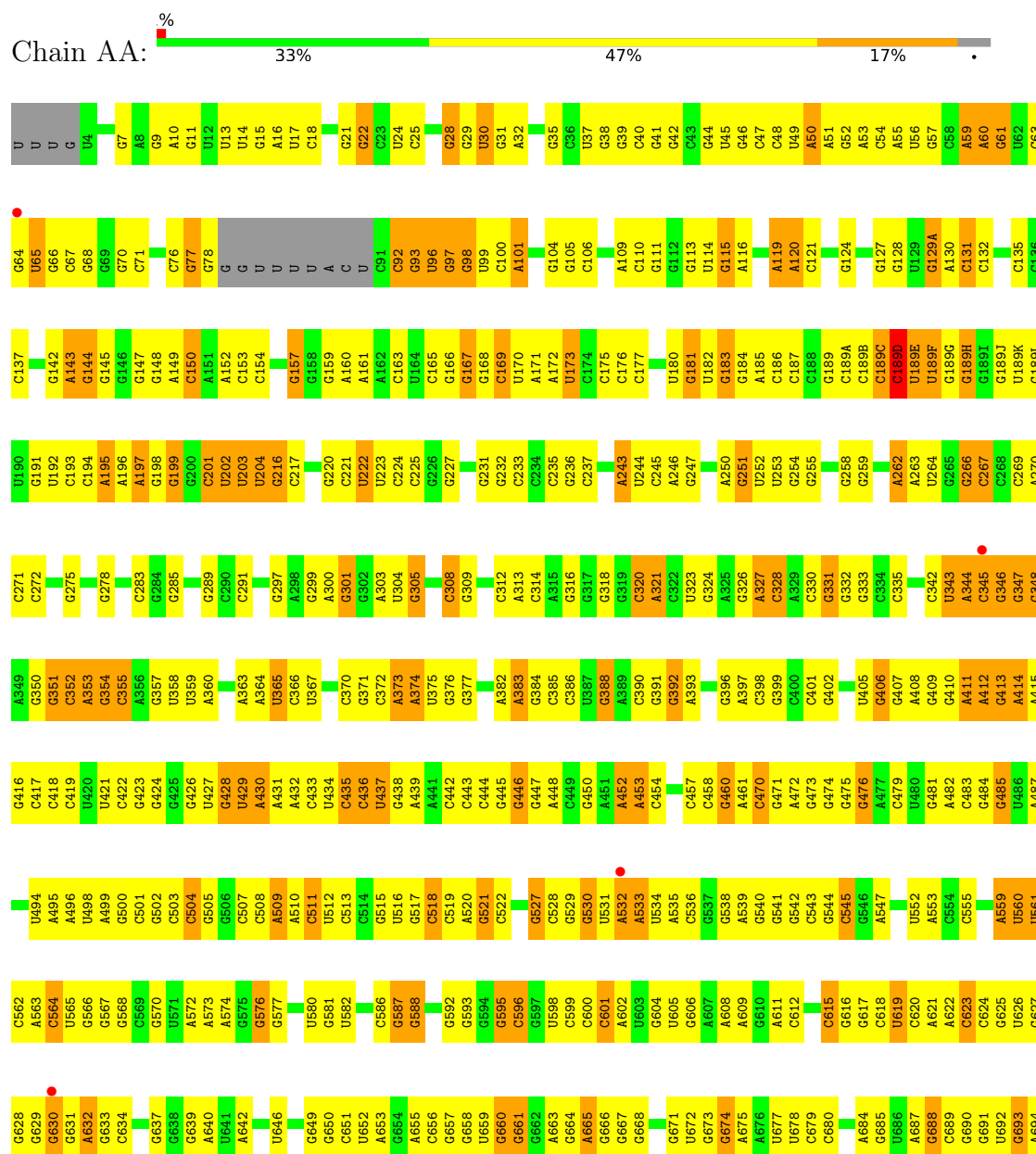
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	D1	3	Total 3	O 3	0	0
58	D3	1	Total 1	O 1	0	0
58	D6	2	Total 2	O 2	0	0
58	D7	2	Total 2	O 2	0	0
58	D8	4	Total 4	O 4	0	0

3 Residue-property plots

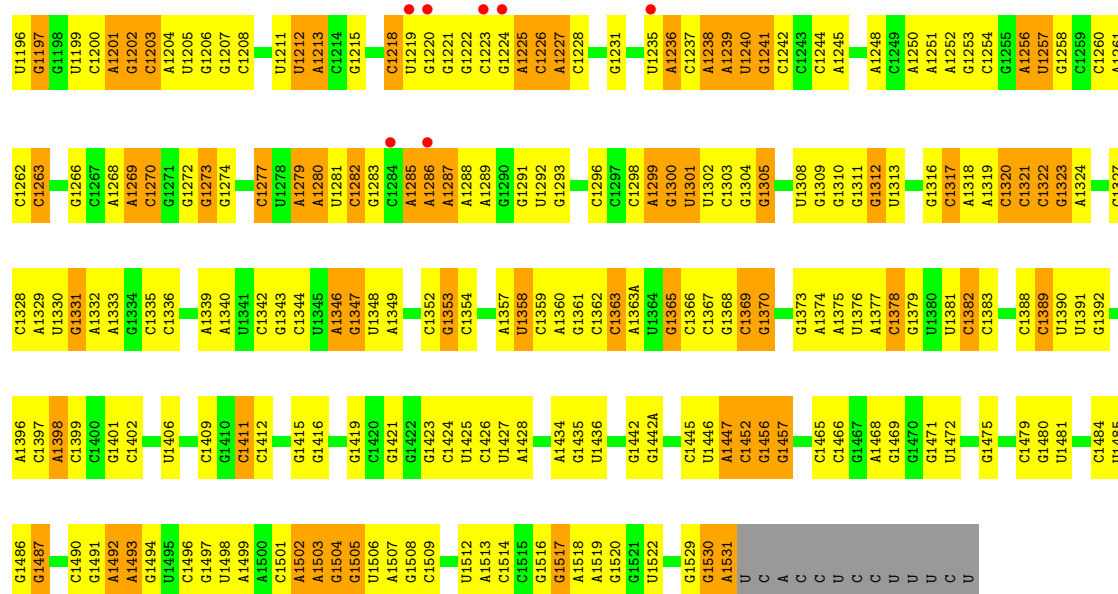
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

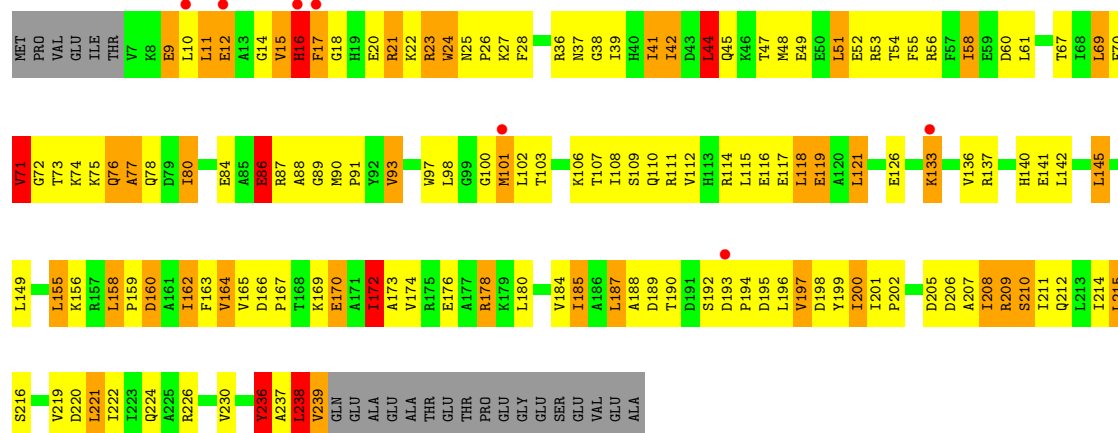


[illegible]

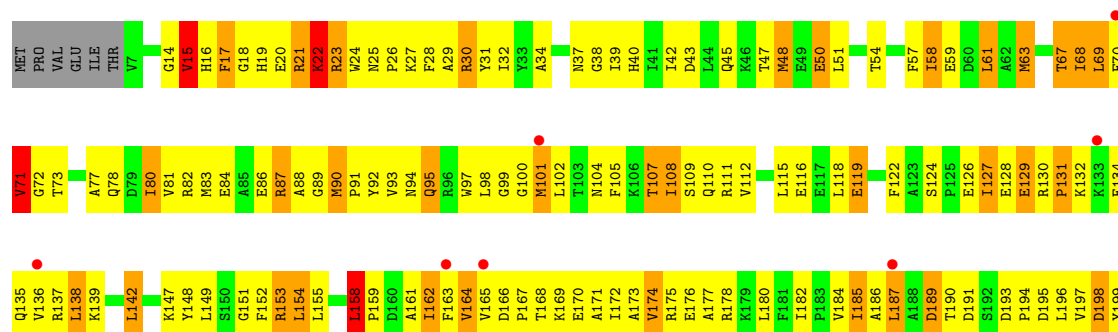
G1064	A	A937	G861	C783	A712	G616	G546	G460	C390	C314	C233	C154	G68
U1065	C	G938	C862	C784	G713	G617	A547	A461	G391	A315	C234	C154	G68
A1067	C1007	G939	C862	C785	G714	C618	A548	C470	G392	G316	C235	A160	G70
G1068	C1008		C866	G786	A715	U619	C549		G393	G319	G236		
C1069	G1009	G942	G867	U788	A716	C620	G550	G473	G394	G320	C237	G163	G73
U1070	G1010	U943	C868	U789	C717	A621	U551	G474		C321	C240	U164	C76
C1137	G1011	G944	C869	A790	G718	A622	U552	G475	A397	A321	C241	G165	G
G1138	U1012	G945	U870	G791	C719	C623	C555	G476	G398		C242	G171	G
G1139	G1013	A946	U871	A792	G720	C624	C556	A477	G399	G324	C243	A172	G
U1072	A1014	G947	A872	U793	C721	G625	C557	C479	C400	A325	C244	U173	U
C1140	A1015	C948	A873	A794	A722		G557	U480	C401	U173	G245	C174	U
G1075	A1016		G874	C795	U723	G630	G558	G481	G402	A327	C245	C175	U
C1076	G1017	G953	C875	C796	G724	G631	A559		C403	C328	A246	C176	U
G1143		G954	G876		G725	A632	U560	G484	U404	A329	G247	C177	A
U1078	G1022		C877	G799	G726	G633	U561	G485	U405	C330			U
G1079	A1080	A959	G878	G800	G727	C634	C562	G491	G406	G331	A250	C	C
A1081	U	U961	C879	U804	A728	G635	A563	G491	G407	G332	G251	U180	U
G1082	G	C962	C881	C805	G730	G636	U565	U494	A408		U252	G181	C
U1083	C	G963	C882	C810	G731		G566	A495	G410	A338	U253	U182	C
G1084	C	A964	C883	C811	A732	U646	G567	A496	G419	C339	G254		G93
U1085	A1151	G1084	U884	C810	C733	C647	G568	A498	A411		G255	C186	U96
U1086	C	G966	G885	C812	G734	A648	C569	A499	A412	A344	U256	C187	G97
	C	C967		U813	G735	G649	G570	G500	G413	C345	G257	C188	G98
	C	A968	A889	A814	C736	G650	U571	C501	A414	G346	G258	G189	U99
U1091	A	A969	G890	A815	A737	G651	A572	G502	C418	G347		C189A	C100
A1092	G	C970	C899	A816	C738	A653	A573	C503	C419	G348	A262	C189B	A101
G1093	G	G971	C899	C817			A574	G504	U420	A349	A263	C189C	
U1094	C	C972	A900	C818	G741	C656	G575		U421	G350	G266	U189D	G105
U1095	U1159	G973	A901	A819	G742	G657	C576		C422	C352	C267	U189E	C106
C1096	G	A974	G902	G820			G577	A509	G423	A353		U189F	
U1097	A	A975	G903	G821	C748	A663	C578	A510	G424	G354	A270	G189G	G112
G1098	C	G976			C749	G664	U579	C511	G425	C355	C271	G189H	G113
C1100	G	A977	C906	C826	G750	A665	U580	C512	G426		C272	U114	
A1101	C	A978	A907	U827	U751	G666	G581	C513	U427	G362	A273	A116	G115
A1169	C	C979	A908	A828			U582		U428	A363	A274	G189I	A116
A1102	U	C980	A909	G829				C518	G429	A364	G275	U190	G117
G1104	A	U981	C910		C754	G671	C586	C519	U429	U365		G191	U118
		U982	U911	C832	G755	U672	G587	A520	A430	U366	G281	U192	A119
G1107	G1042	A983	C912	U833	C756	G673	C588	A520	A431	C366	G281	C193	A120
A1108	C1043	G984	A913	U834	U757	G674	G589	G524	A432	U367	A282	G194	C121
C1109	C1045	C985	A914	U835	G758	A675	C589		C433	U368	C283	C195	G122
	A1046	G986		U836	A759	A676	C590	G527	U434	C369	G284	A196	G123
U1178	G1047	A987	A919	G837	G760	U677	U591		C435		G285	A197	G124
A1179	U1046	G987	U920	G837		U678	G595	G530	C436	C372	G286	G198	U125
C1113	G1048	G988	U921	G838	C763	C679	C596	U531	U437	A373	U287	G199	G126
G1181	U1049	C989	U920	U839	G764		C596	G531	G438	A374	A288	G200	
G1182	C1050	G990	G922	C840	G765	G683	G597	A532	A439	U375	G289	C201	G129A
A1183	G1051	U991	A923	U841	A766	A684	U598	A533	A441	G376	U296	U202	A130
C1118	U1052	C924	C843	C848	A767	G685		U534	C442	G377		U203	C131
C1119	G1053	G992	G925	C849	A768	G686	C601	A535	C443	G378	U296	U204	C132
G1185	C1054	A994		U850	G769	A687	A602	C536	C444	C379	A300	G216	
U1121	U1055	C995	G927	G851	C770	G688	U603	G537	G445		A300	C217	G144
A1123	A1056		G928	G851		C689	G604	G538	G446	C381	A303	C217	G145
C1188	U1057	C999	G929	G854	G776	G690	U605	A539	G447	A382	U304	C221	G146
G1124	U	A	C930	G855	A777	G691		G540		A383	G305	U222	G147
U1125	G1058	C931	C931	C856	G778	U692	A608	G541	G450	G384	G306	U223	G148
A1191	C1059			C857	C779	G693		G542	A451	C385	C307	A149	
G1127	G1060	G		C857	C779	A694	C612	G543	A452	C386	G308	G227	C150
C1128	U1061	G	C934	G858	A780	G694	C613	G544	A453		G309		
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A1129	C1062		C936	A860	A782	G711							

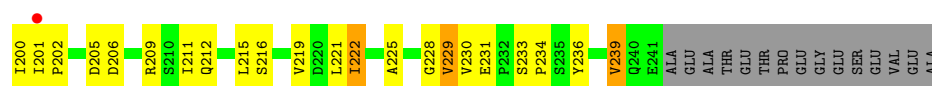


• Molecule 2: 30S Ribosomal Protein S2

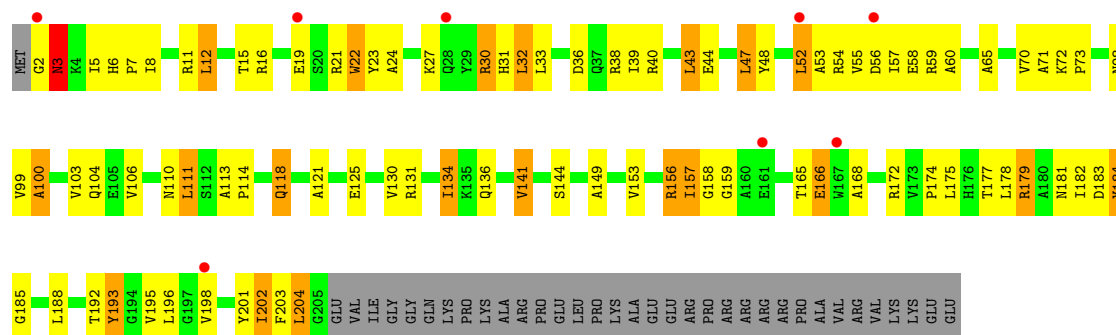


• Molecule 2: 30S Ribosomal Protein S2

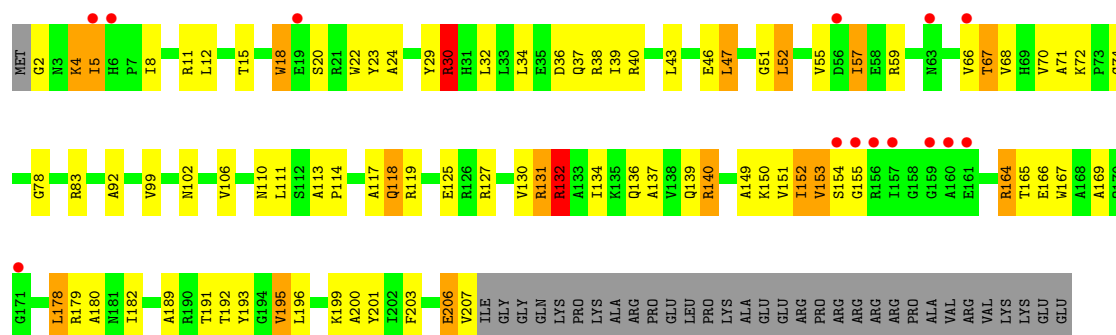




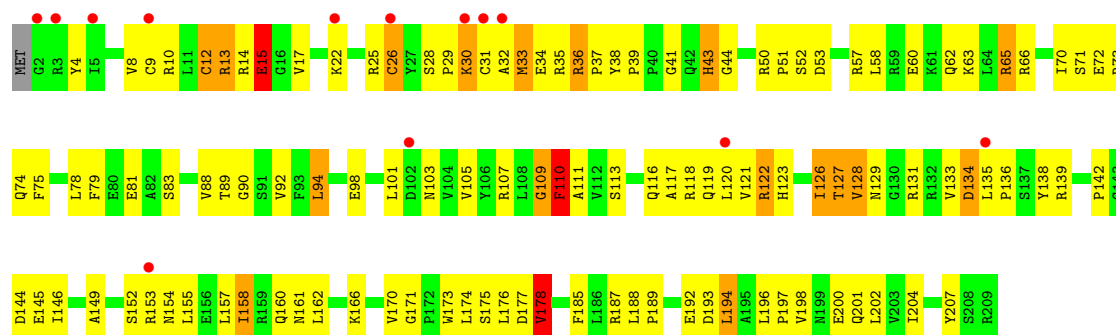
• Molecule 3: 30S Ribosomal Protein S3



• Molecule 3: 30S Ribosomal Protein S3

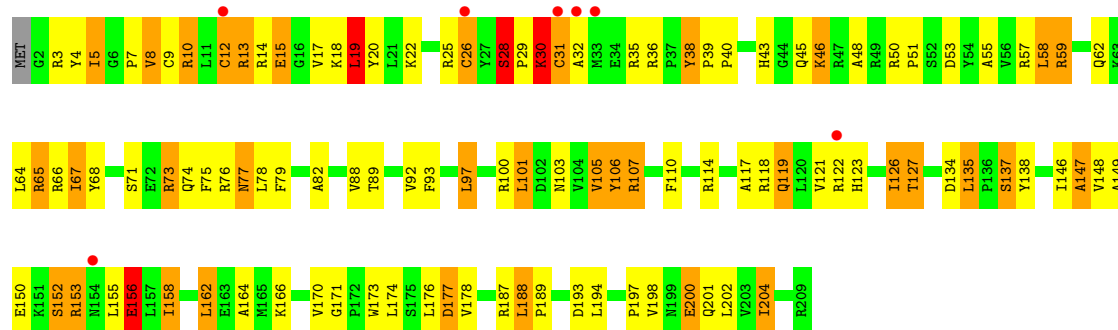


• Molecule 4: 30S Ribosomal Protein S4

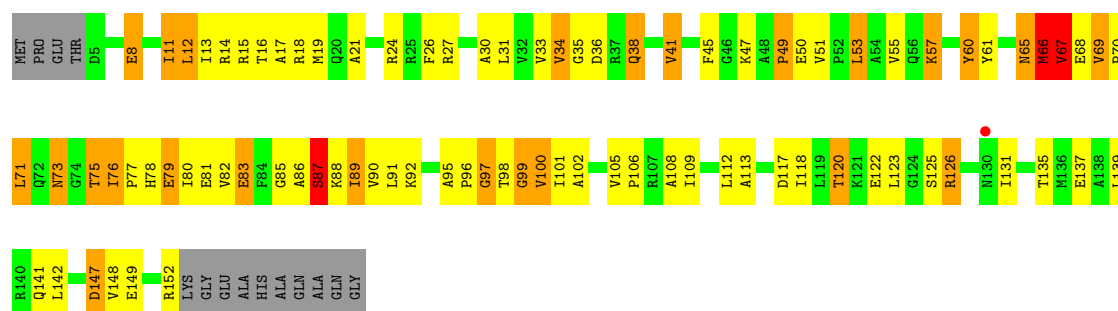


• Molecule 4: 30S Ribosomal Protein S4

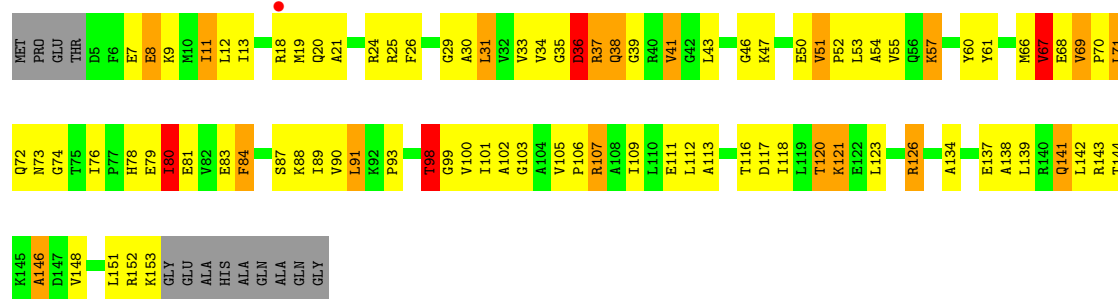




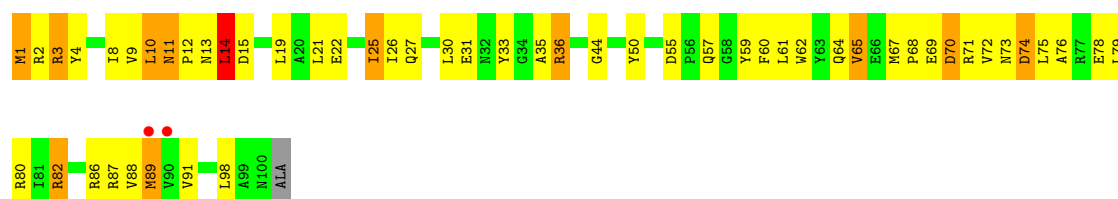
• Molecule 5: 30S Ribosomal Protein S5



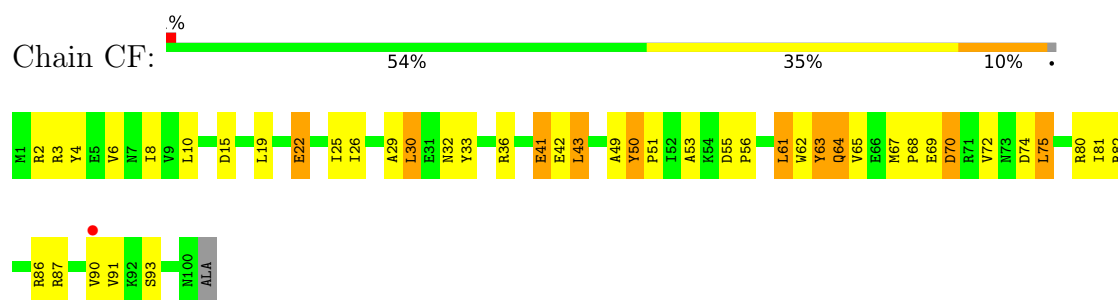
• Molecule 5: 30S Ribosomal Protein S5



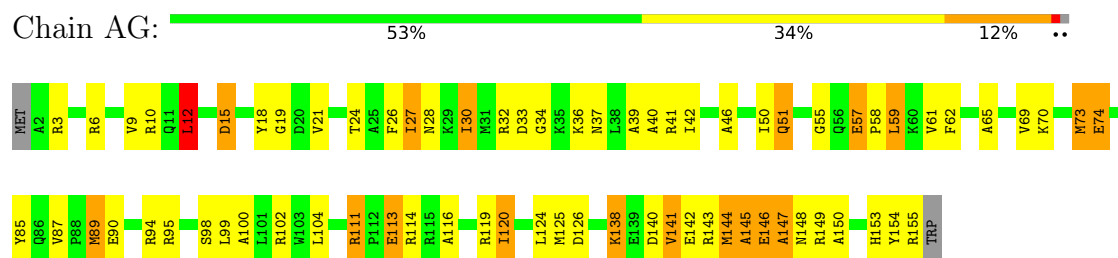
• Molecule 6: 30S Ribosomal Protein S6



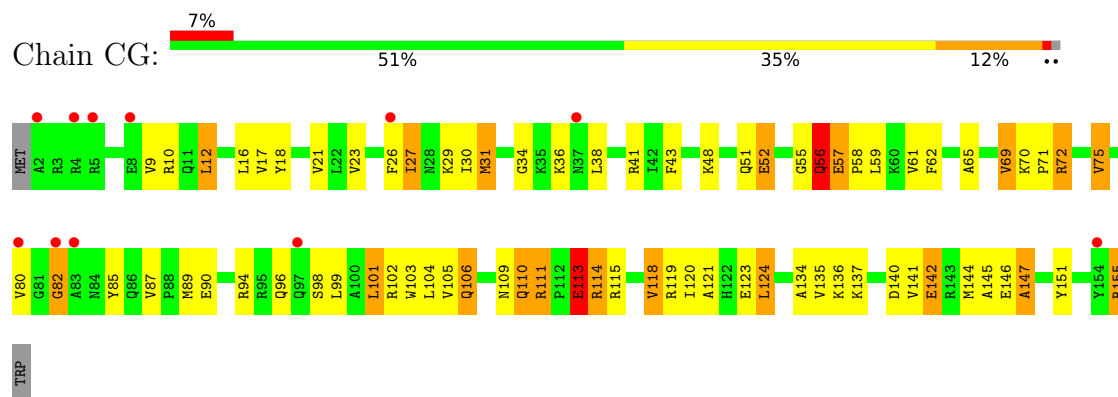
• Molecule 6: 30S Ribosomal Protein S6



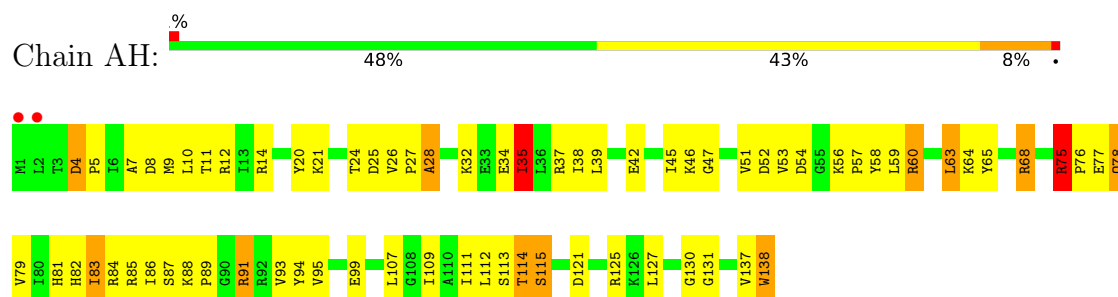
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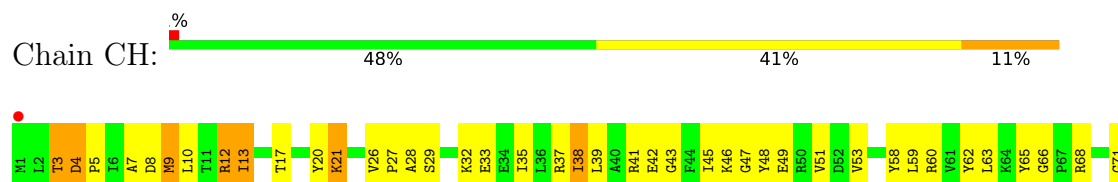
• Molecule 7: 30S Ribosomal Protein S7



• Molecule 8: 30S Ribosomal Protein S8

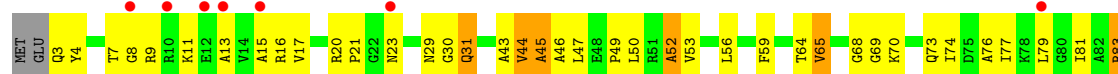


• Molecule 8: 30S Ribosomal Protein S8





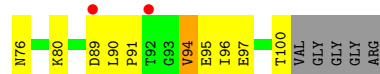
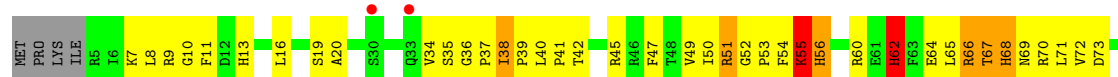
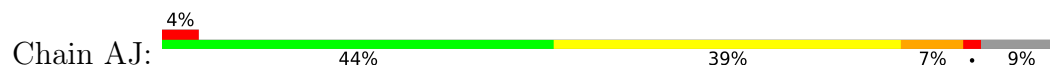
• Molecule 9: 30S Ribosomal Protein S9



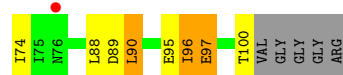
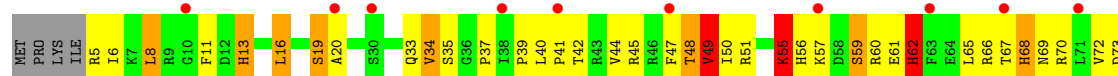
• Molecule 9: 30S Ribosomal Protein S9



• Molecule 10: 30S Ribosomal Protein S10

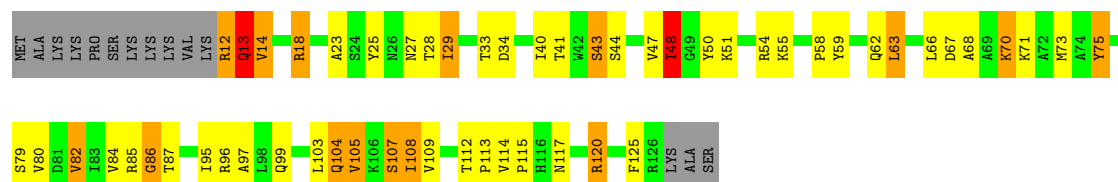


• Molecule 10: 30S Ribosomal Protein S10

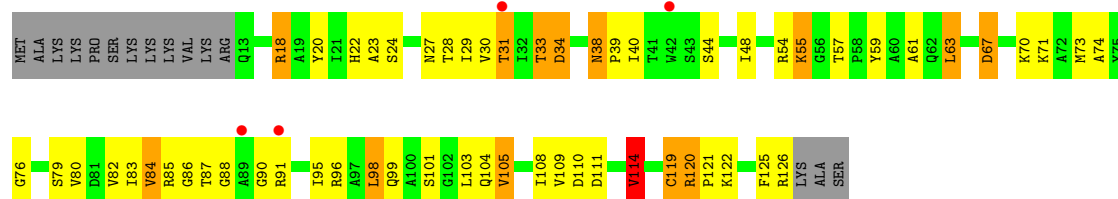


• Molecule 11: 30S Ribosomal Protein S11

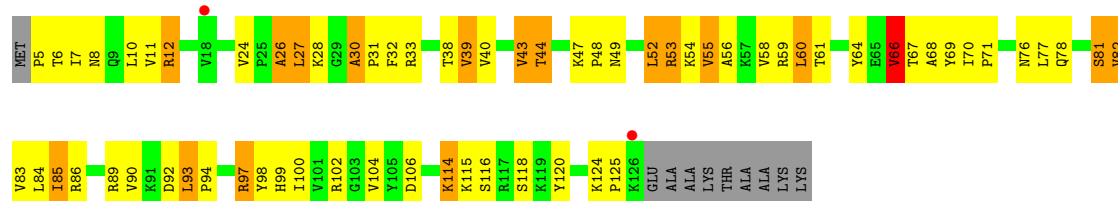
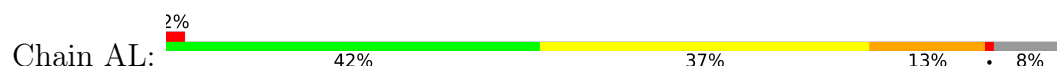




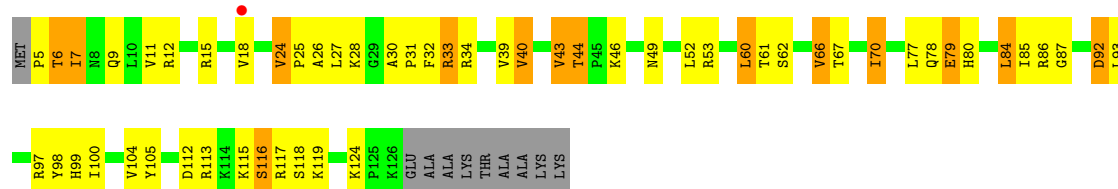
• Molecule 11: 30S Ribosomal Protein S11



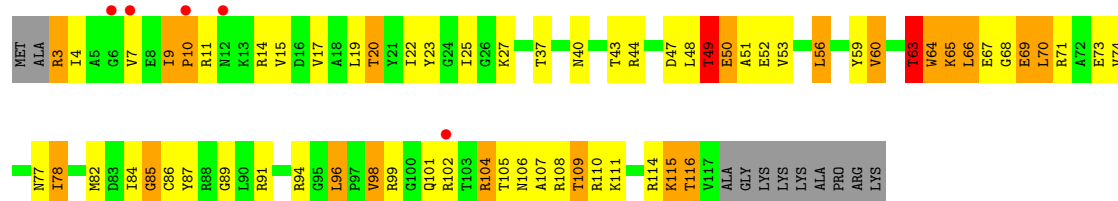
• Molecule 12: 30S Ribosomal Protein S12



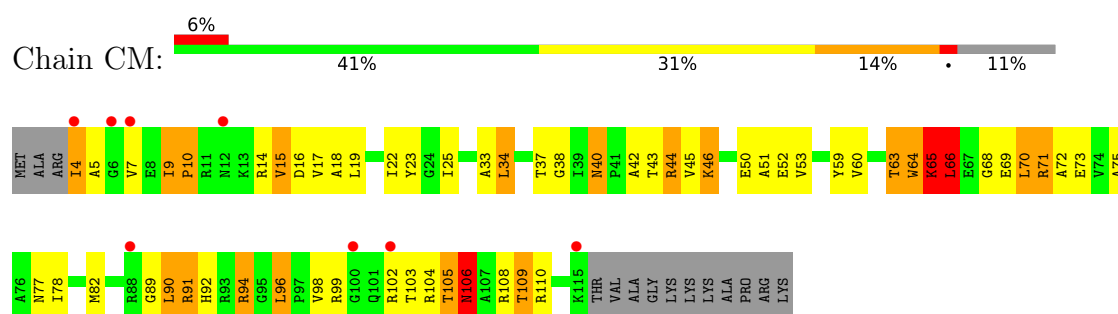
• Molecule 12: 30S Ribosomal Protein S12



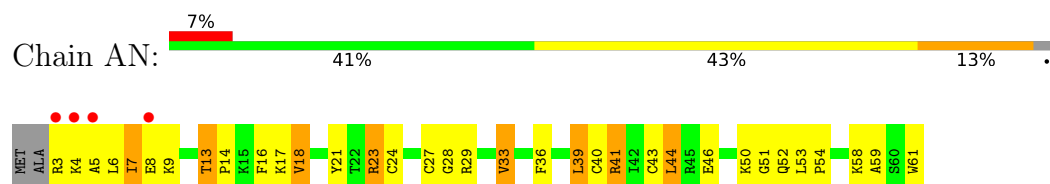
• Molecule 13: 30S Ribosomal Protein S13



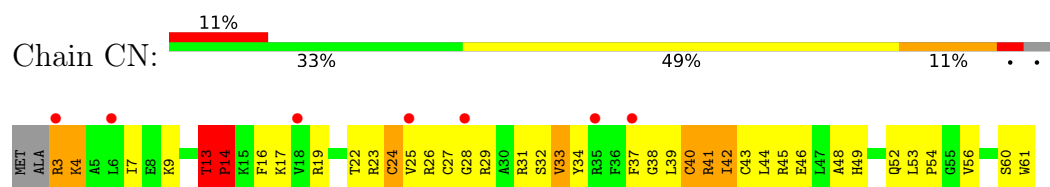
• Molecule 13: 30S Ribosomal Protein S13



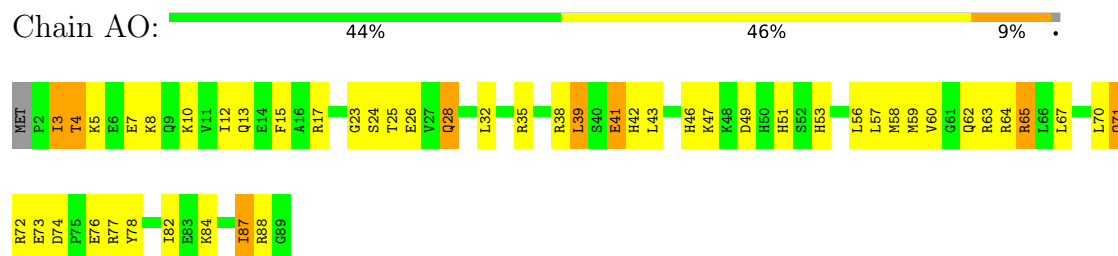
- Molecule 14: 30S Ribosomal Protein S14



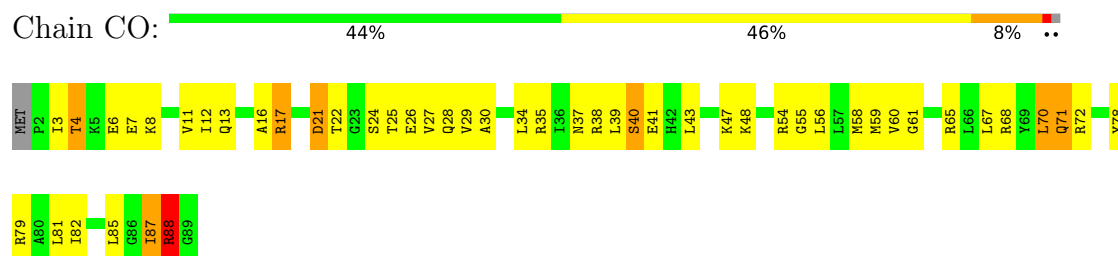
- Molecule 14: 30S Ribosomal Protein S14



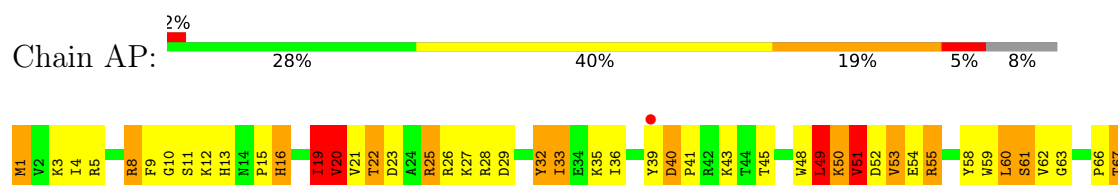
- Molecule 15: 30S Ribosomal Protein S15



- Molecule 15: 30S Ribosomal Protein S15



- Molecule 16: 30S Ribosomal Protein S16





• Molecule 16: 30S Ribosomal Protein S16

Chain CP: 35% 38% 18% 7%



• Molecule 17: 30S Ribosomal Protein S17

Chain AQ: 3% 35% 43% 14% 6%



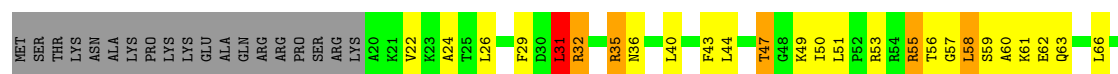
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ: % 41% 35% 17% 6%



• Molecule 18: 30S Ribosomal Protein S18

Chain AR: 38% 31% 8% 23%

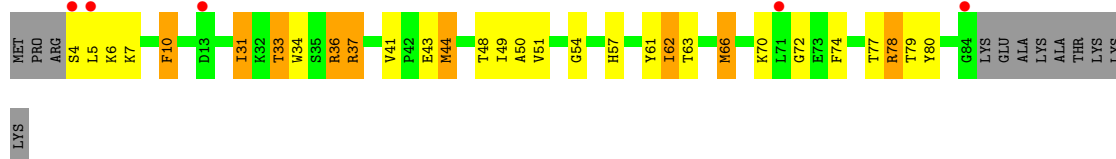


• Molecule 18: 30S Ribosomal Protein S18

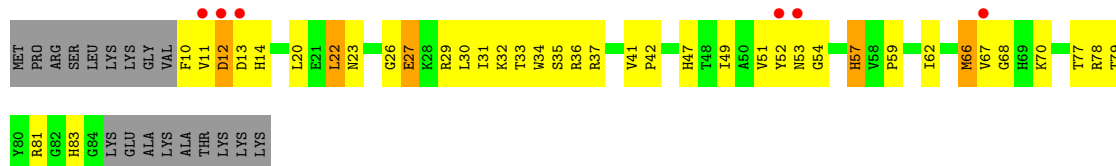
Chain CR: 38% 34% 6% 23%



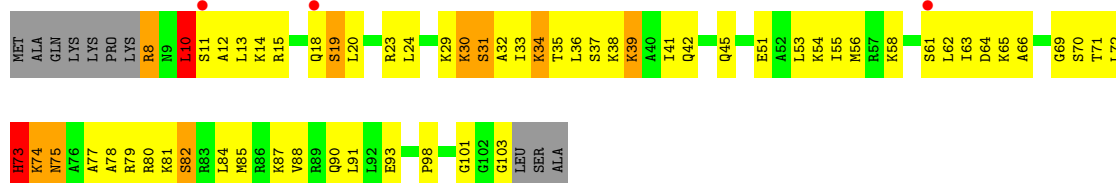
• Molecule 19: 30S Ribosomal Protein S19



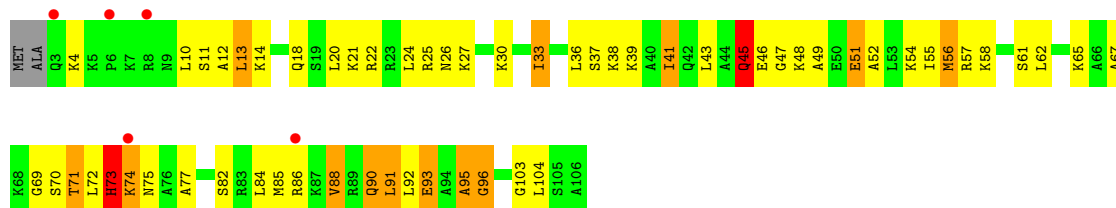
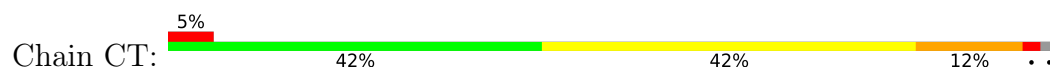
• Molecule 19: 30S Ribosomal Protein S19



• Molecule 20: 30S Ribosomal Protein S20



• Molecule 20: 30S Ribosomal Protein S20

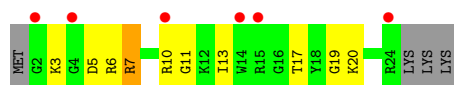


• Molecule 21: 30S Ribosomal Protein THX

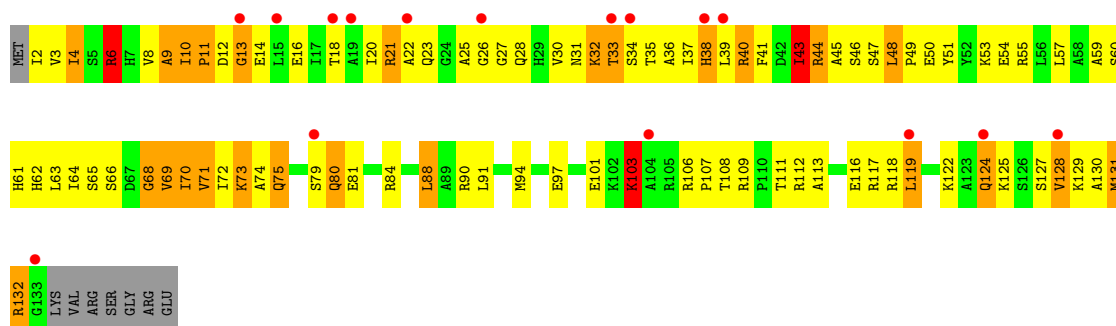




• Molecule 21: 30S Ribosomal Protein THX



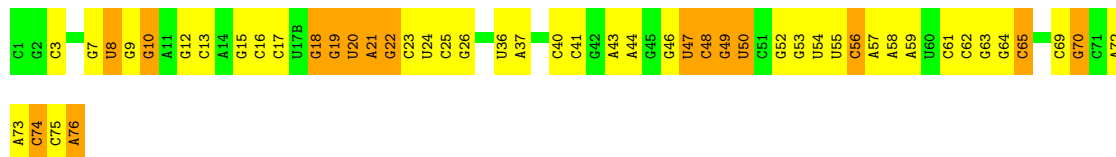
• Molecule 22: YAEJ



• Molecule 23: P-site fMet-tRNA



• Molecule 23: P-site fMet-tRNA



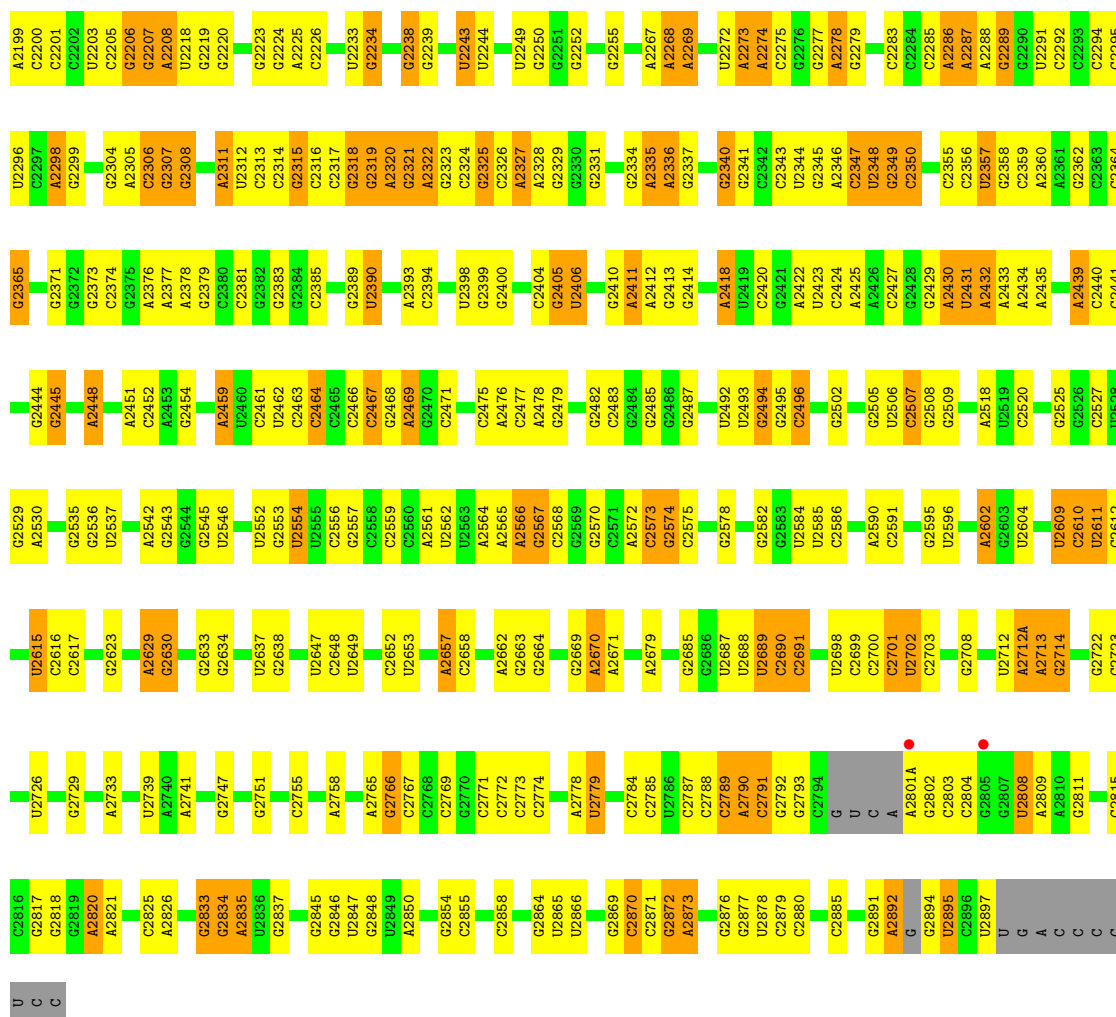
• Molecule 24: mRNA



• Molecule 24: mRNA

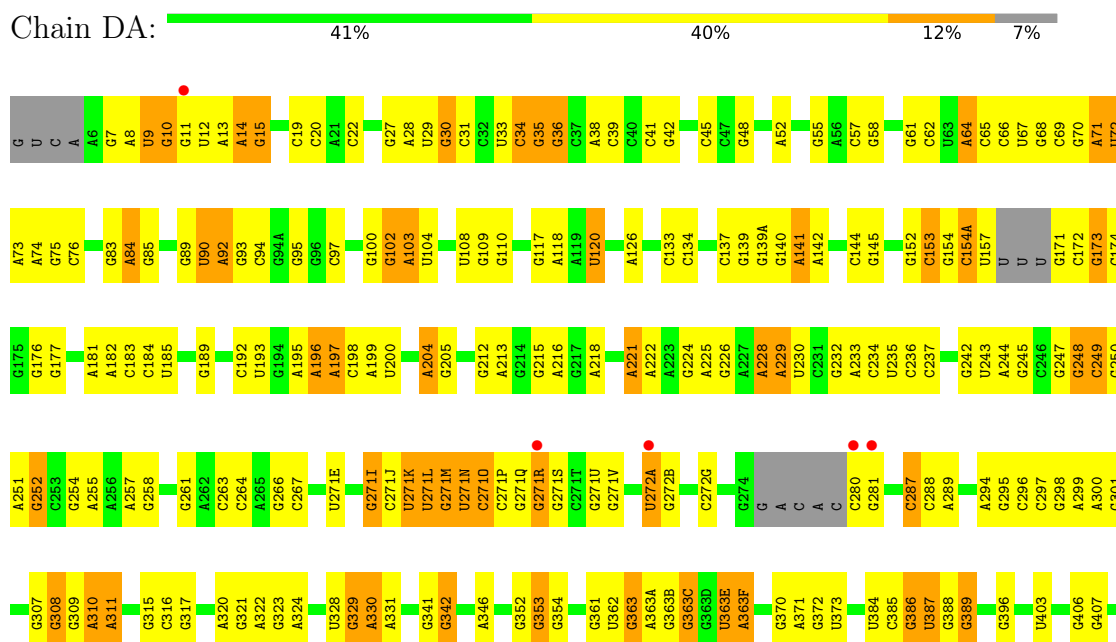


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G	C2032	G1933	G1835	G1758	U1639	C1550	G1478	C1386	A1204	A1126	●	U
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C	A2054	A1952	G1855	A1776	C1660	A1570	A1493	C1408	G1239	U1141	●	C
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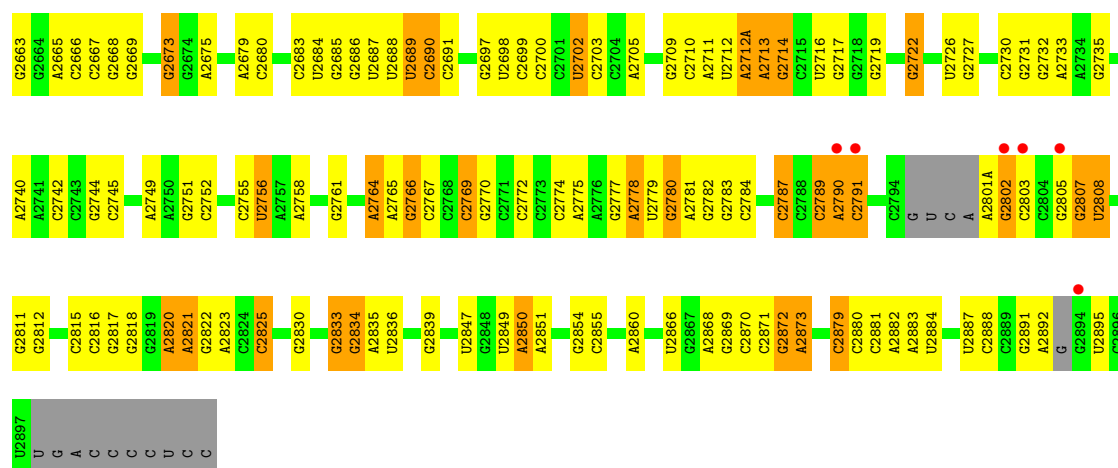
• Molecule 25: 23S Ribosomal RNA

Chain DA:

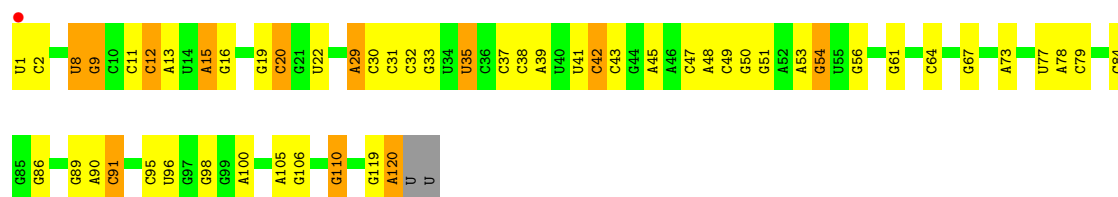




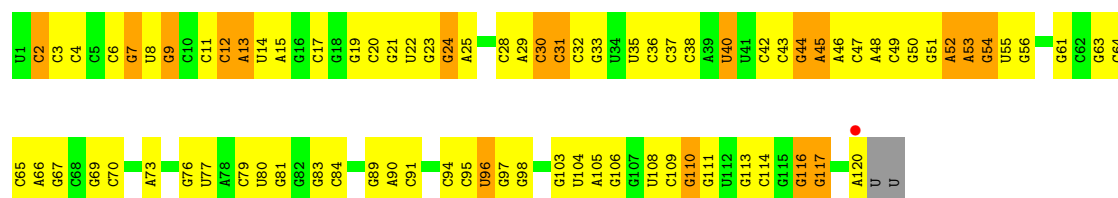
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G2586	A2430	C2430	C2363	A2199	C2065	C1982	A1900	G1801	A1700	G1619	C1531
A2587	U2510	U2431	C2364	C2200	C2065	C1982	A1900	G1801	A1700	G1620	C1532
G2582	U2511	A2432	G2365	C2201	C2066	C1983	A1901	G1802	G1702	U1621	G1533
G2582	G2517	A2435	A2366	G2206	G2069	G1984	G1906	A1803	G1703	G1622	U
G2582	A2518	G2436	G2371	G2207	G2070	U1991	G1907	A1810	U1709	G1625	A
G2593	U2519	G2439	G2372	A2208	A2071	G1992	C1908	G1811	U1710	G1636	C1536
G2601	G2520	A2439	C2374	U2218	G2072	U1993	G1908	A1812	U1629	U1537	G1537
A2602	U2521	C2440	G2375	G2219	C2073	A1913	A1913	G1813	G1630	G1538	G1538
G2603	U2522	A2441	A2376	G2219	C2073	C1996	A1914	G1814	A1722	G1539	G1539
U2604	G2523	C2442	A2377	A2225	U2074	G1997	U1915	A1815	U1739	U1540	U1540
G2608	G2524	G2443	A2378	U2225	U2075	G2006	A1916	G1816	G1740	G1632	G1641
G2609	G2525	G2444	G2379	G2228	C2078	G2006	A1919	G1817	A1741	G1635	A1541
G2610	U2526	G2445	C2380	C2229	U2079	G2009	A1919	U1818	G1742	G1638	A1542
U2611	U2527	A2448	C2381	G2234	G2080	G2010	A1920	A1819	G1746	C1638	A1545
C2612	G2528	G2448	G2382	G2235	C2081	U2011	U1923	U1820	G1747	U1639	G1546
G2615	A2530	G2456	C2383	G2236	A2082	G2012	C1984	A1821	G1747A	C1640	C1547
G2616	A2531	G2459	G2384	C2237	U2091	A2013	U1925	G1822	G1643	G1643	C1557
G2617	G2532	U2460	C2385	G2237	G2097	A2014	U1926	C1827	C1644	C1644	C1557
G2618	A2533	C2461	U2387	G2238	C2097	A2015	U1927	G1828	G1645	A1558	G1559
G2619	A2534	U2462	A2388	C2240	U2098	U2016	A1928	A1829	G1752	G1646	G1559
G2623	G2535	U2463	G2389	U2244	U2099	U2017	G1929	G1834	G1754	G1647	G1560
A2629	G2536	C2463	C2390	G2244	G2100	G2018	G1930	U1835	A1755	G1648	A1567
G2630	U2537	C2464	G2391	G2256	G2101	A2019	A1938	G1835	G1756	G1651	G1568
G2631	C2538	G2465	A2392	G2257	U2102	A2020	G1935	C1836	U1757	G1652	A1569
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G2634	G2543	C2467	C2394	C2261	G2104	U2022	A1937	G1838	A1762	A1654	C1577
G2636	U2546	U2398	C2395	U2262	C2105	G2023	U1939	G1842	G1763	A1655	U1578
G2639	G2550	G2399	G2400	C2263	C	U2028	U1940	G1842	G1764	A1656	A1579
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G2646	U2552	U2402	A2396	A2273	A	A2030	C1941	G1849	U1773	G1658	G1581
G2648	G2553	C2403	G2397	A2274	C	A2031	C1942	G1849	U1774	U1659	C1584
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G2652	U2555	G2405	A2399	G2276	A	A2033	G1945	A1854	U1775	C1668	C1589
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A2657	G2557	G2407	C2400	G2278	G	G2037	G1950	G1856	U1777	A1669	C1599
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G2661	U2570	U2411	G2403	C2281	A	U2041	A1953	A1859	C1781	C1675	C1598
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A2662	G2572	G2413	U2344	G2283	G	C2043	U1955	G1861	A1784	G1678	C1600
G2663	G2573	G2414	G2345	C2284	U	G2049	U1963	A1876	A1785	U1679	A1603
G2667	U2574	A2415	A2346	C2285	G	C2050	G1964	A1877	A1786	C1686	C1607
G2668	G2575	C2416	U2347	G2286	G	A2051	G1967	G1878	A1787	G1687	A1608
G2669	G2576	U2417	G2348	A2287	G	G2052	C1967	C1879	G1788	U1789	A1609
G2670	G2577	A2418	C2349	A2288	A	G2053	C1967	G1883	C1790	C1688	
G2671	U2491	U2419	G2350	G2289	C	A2054	C1967				
G2672	G2578	U2420	U2351	G2290	A						
G2673	G2579	G2421	A2352	U2291	C						



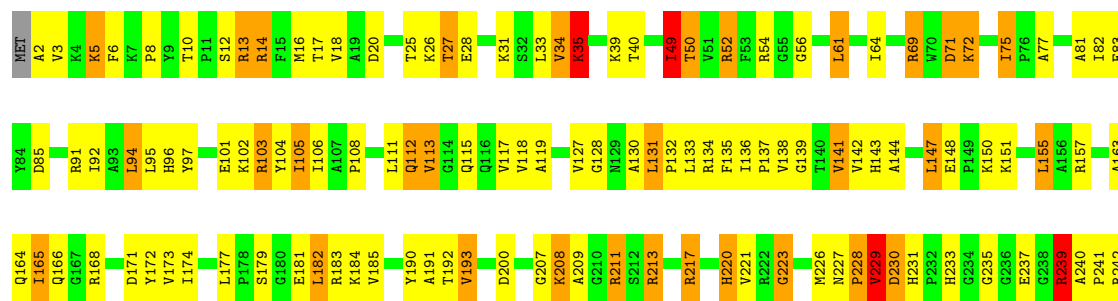
• Molecule 26: 5S Ribosomal RNA

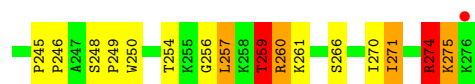


• Molecule 26: 5S Ribosomal RNA



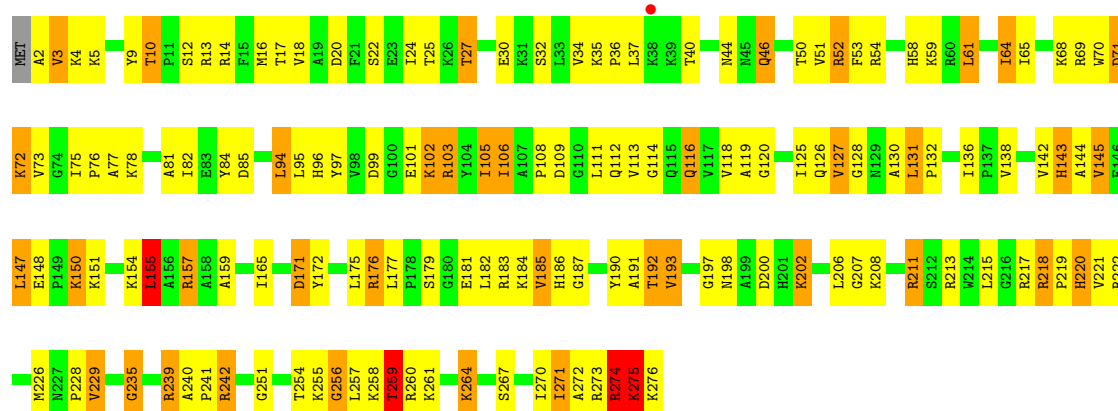
• Molecule 27: 50S Ribosomal Protein L2





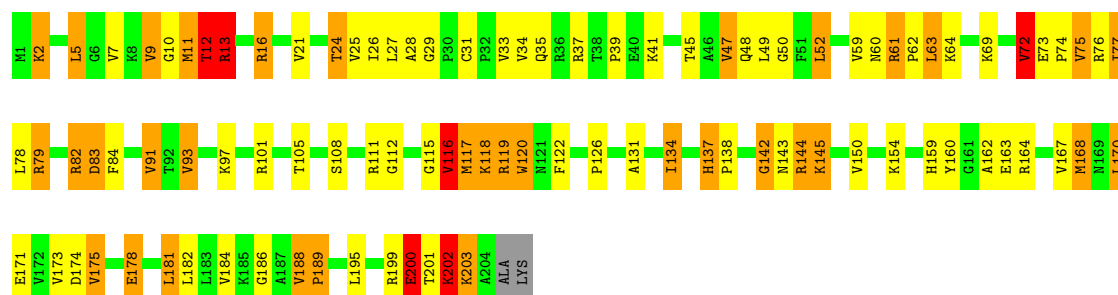
• Molecule 27: 50S Ribosomal Protein L2

Chain DD: 45% 39% 14%



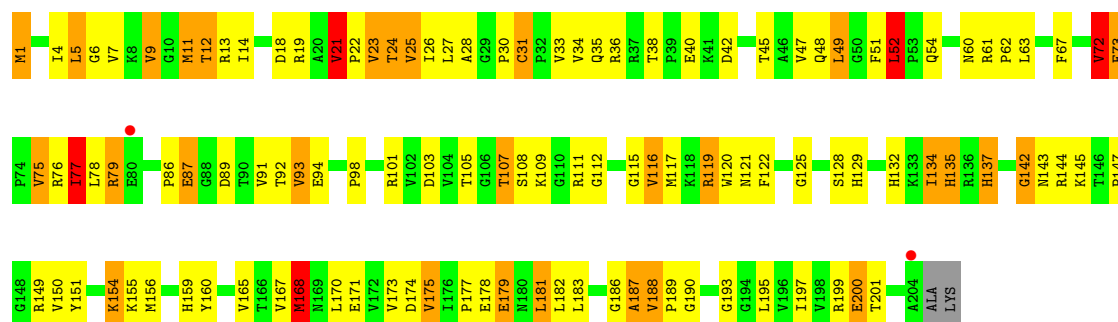
• Molecule 28: 50S Ribosomal Protein L3

Chain BE: 51% 28% 17%



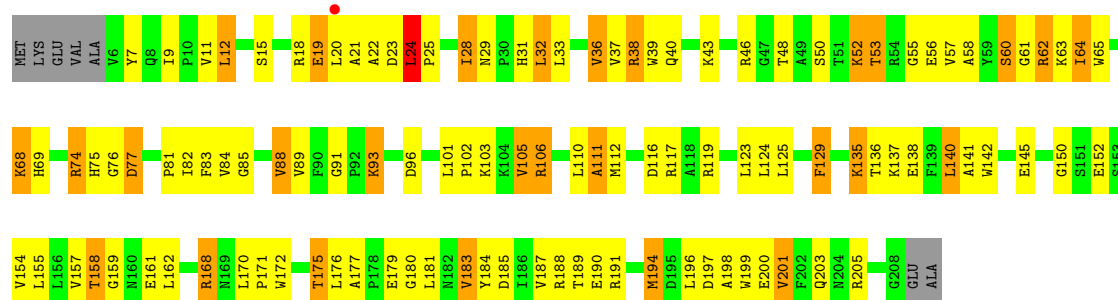
• Molecule 28: 50S Ribosomal Protein L3

Chain DE: 43% 40% 14%

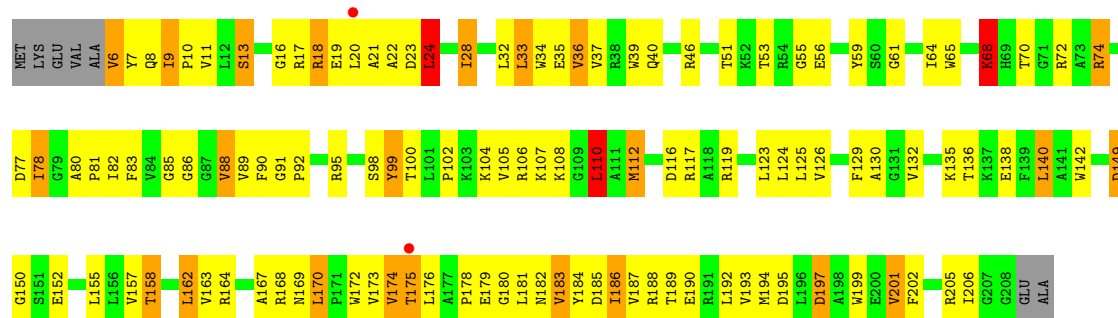


• Molecule 29: 50S Ribosomal Protein L4

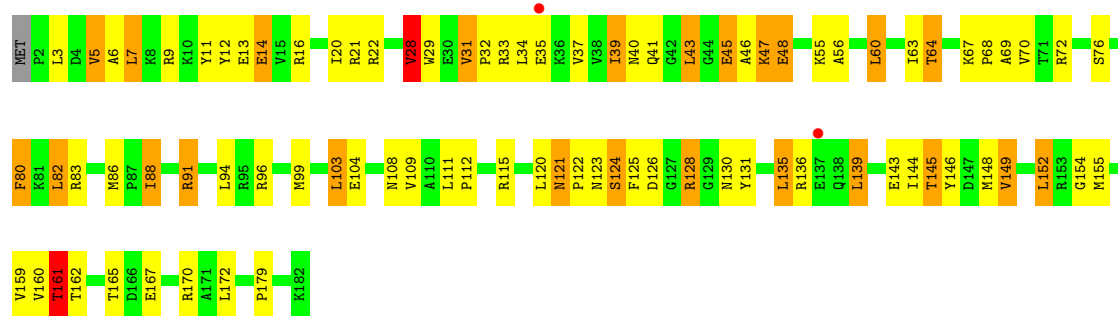
Chain BF: 42% 40% 13%



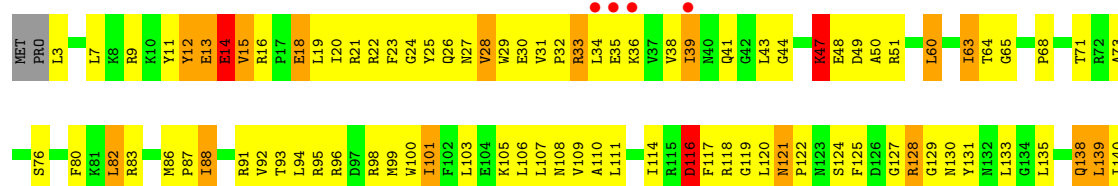
• Molecule 29: 50S Ribosomal Protein L4



• Molecule 30: 50S Ribosomal Protein L5

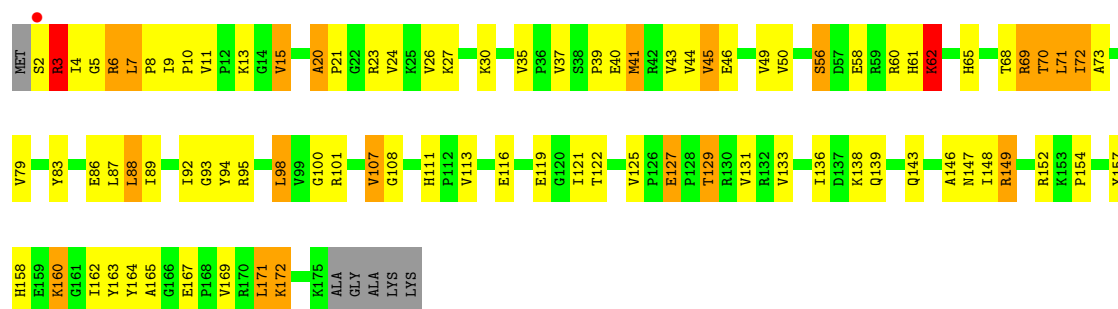


• Molecule 30: 50S Ribosomal Protein L5

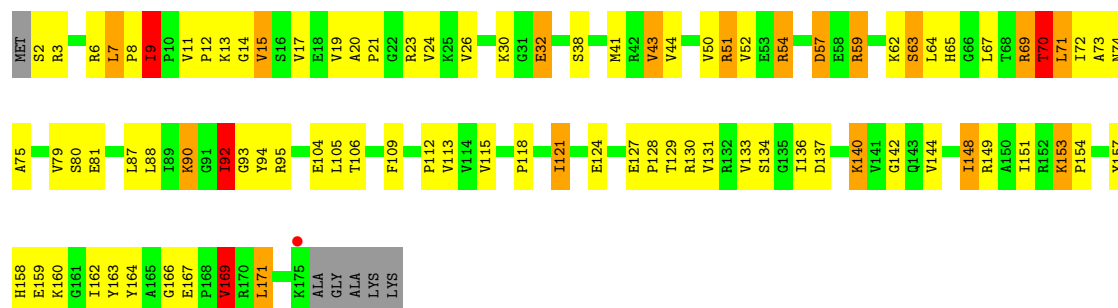




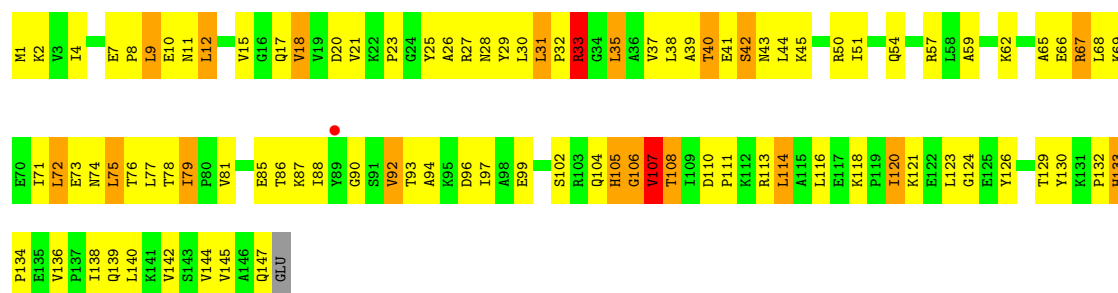
• Molecule 31: 50S Ribosomal Protein L6



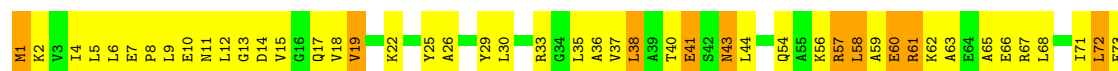
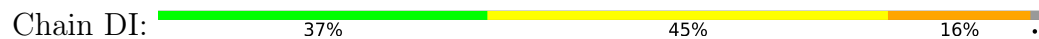
• Molecule 31: 50S Ribosomal Protein L6

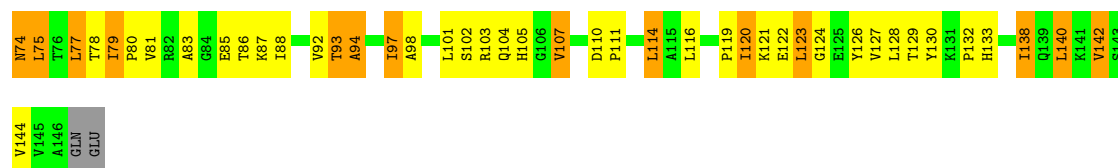


• Molecule 32: 50S Ribosomal Protein L9

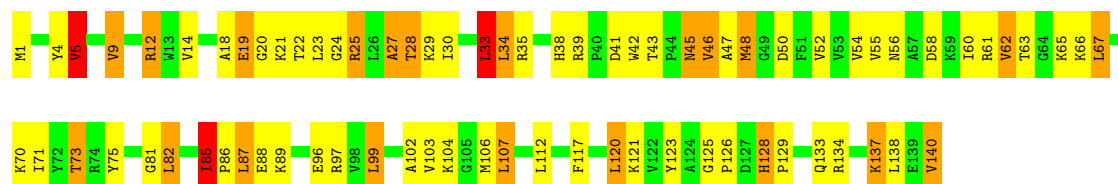


• Molecule 32: 50S Ribosomal Protein L9

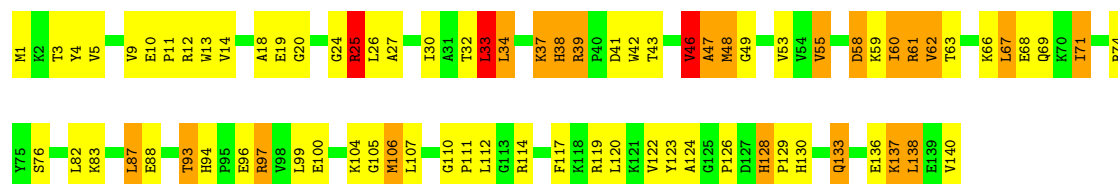




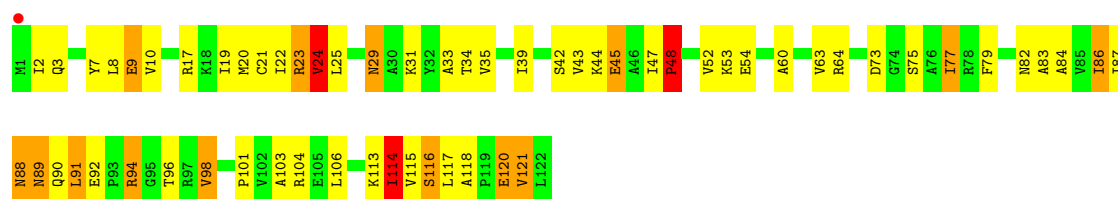
• Molecule 33: 50S Ribosomal Protein L13



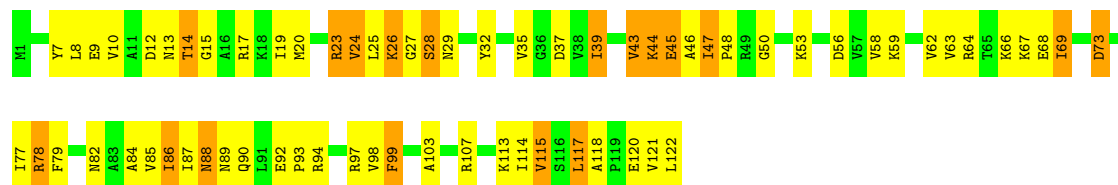
• Molecule 33: 50S Ribosomal Protein L13



• Molecule 34: 50S Ribosomal Protein L14

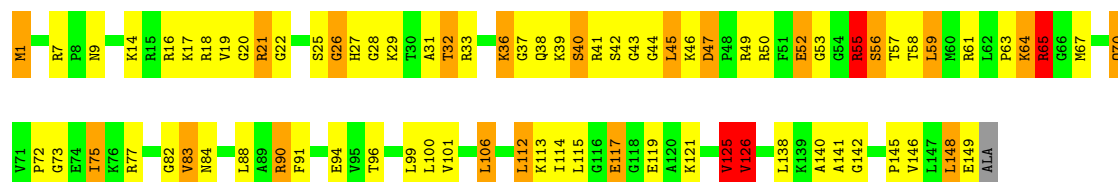


• Molecule 34: 50S Ribosomal Protein L14

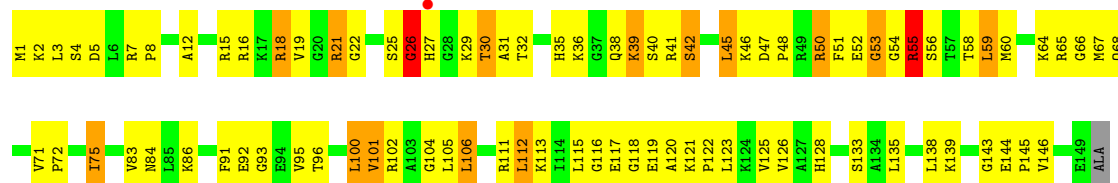
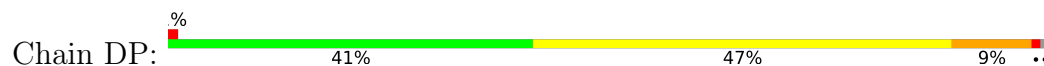


• Molecule 35: 50S Ribosomal Protein L15

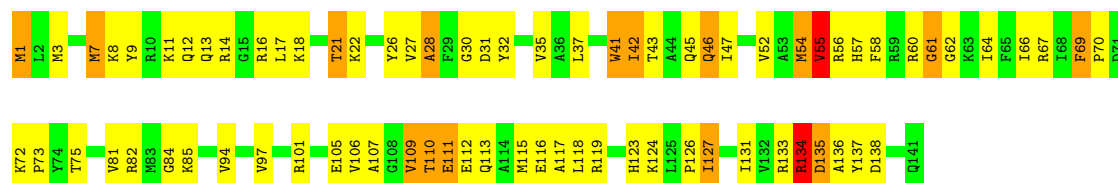




• Molecule 35: 50S Ribosomal Protein L15



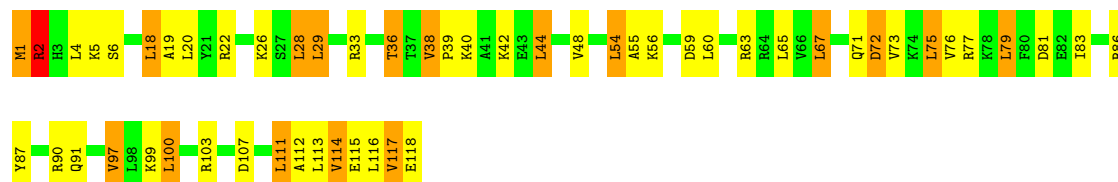
• Molecule 36: 50S Ribosomal Protein L16



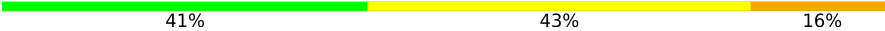
• Molecule 36: 50S Ribosomal Protein L16

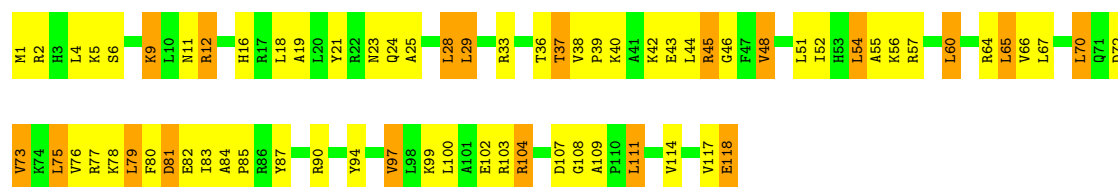


• Molecule 37: 50S Ribosomal Protein L17



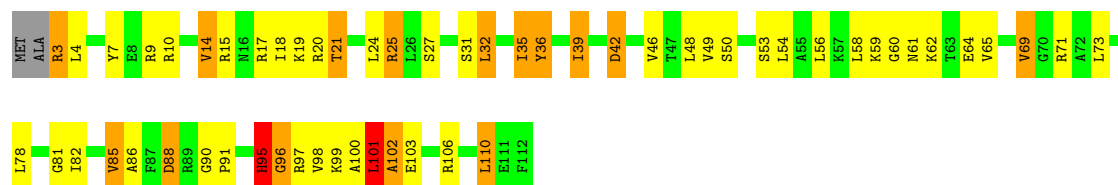
• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 

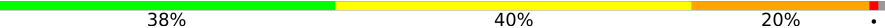


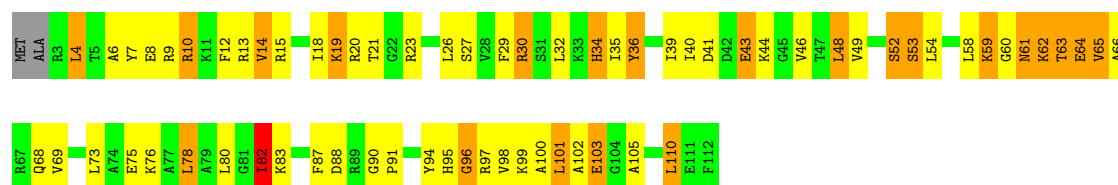
• Molecule 38: 50S Ribosomal Protein L18

Chain BS: 



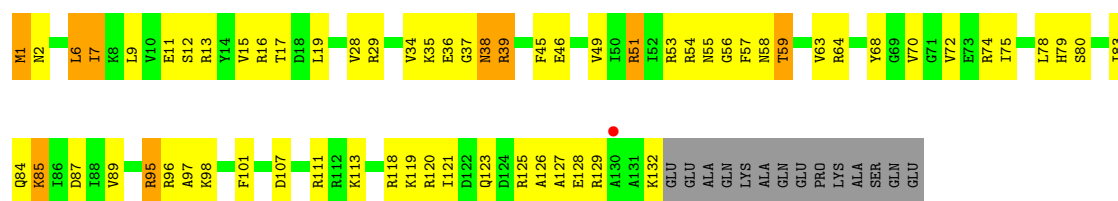
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 



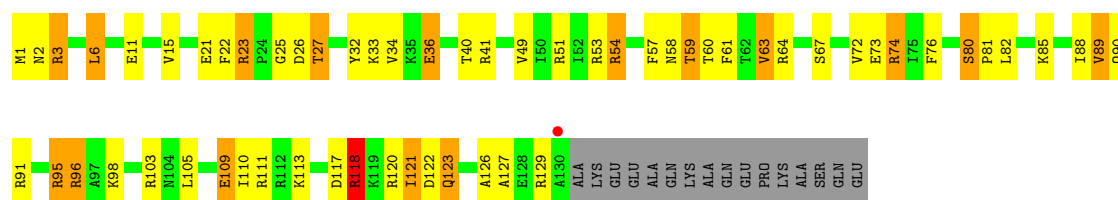
• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 



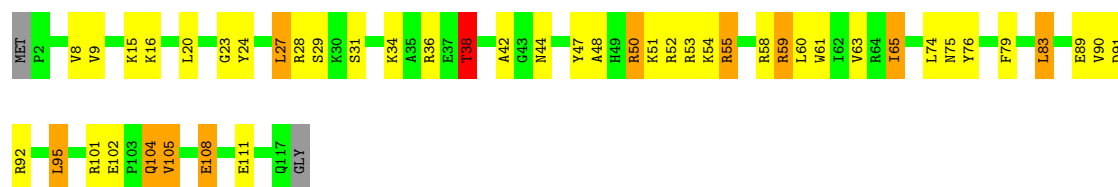
• Molecule 39: 50S Ribosomal Protein L19

Chain DT: 



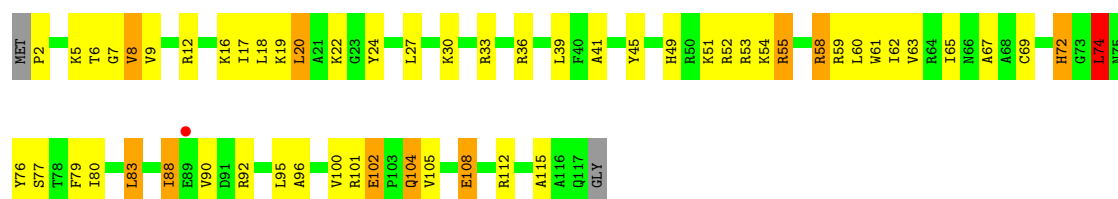
• Molecule 40: 50S Ribosomal Protein L20

Chain BU:  59% 30% 8% ..



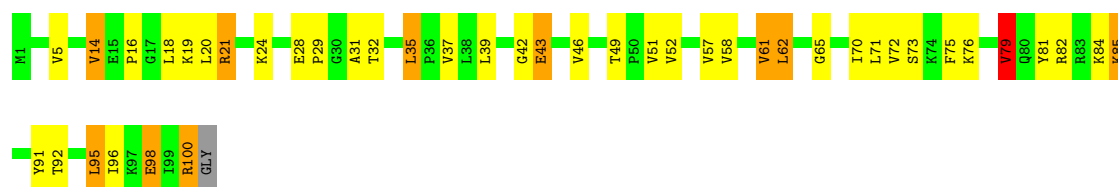
• Molecule 40: 50S Ribosomal Protein L20

Chain DU:  51% 38% 8% ..

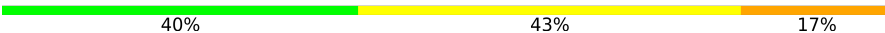


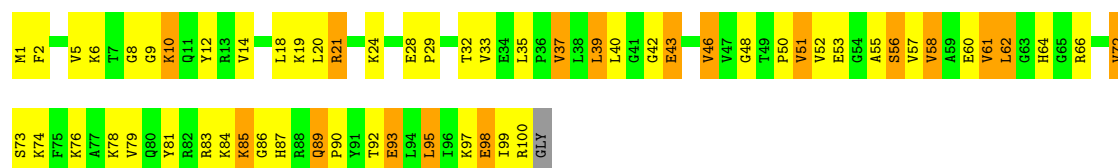
• Molecule 41: 50S Ribosomal Protein L21

Chain BV:  56% 32% 10% ..



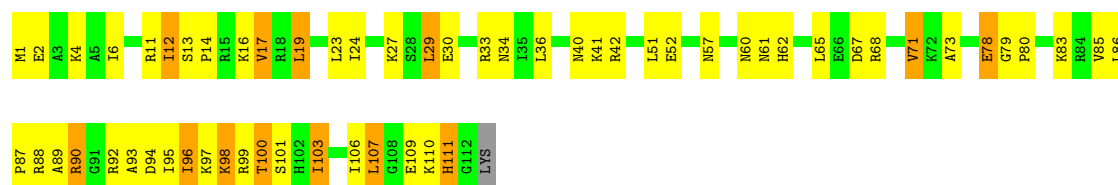
• Molecule 41: 50S Ribosomal Protein L21

Chain DV:  40% 43% 17% .

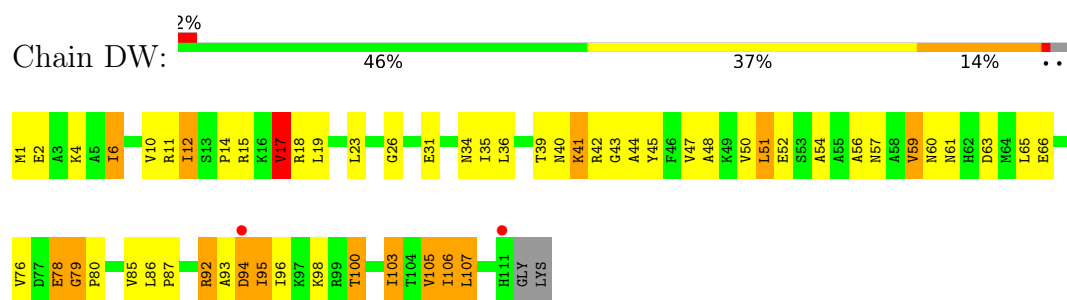


• Molecule 42: 50S Ribosomal Protein L22

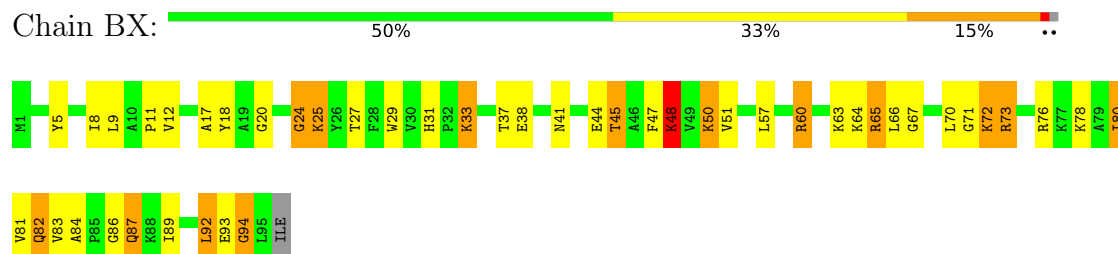
Chain BW:  47% 41% 12% .



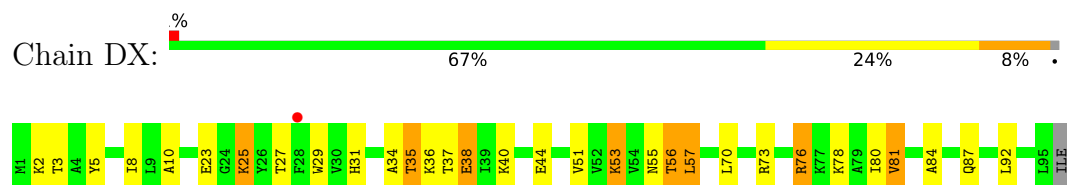
• Molecule 42: 50S Ribosomal Protein L22



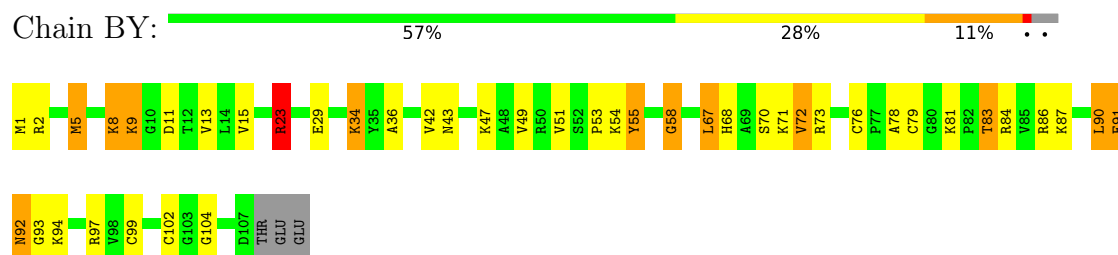
• Molecule 43: 50S Ribosomal Protein L23



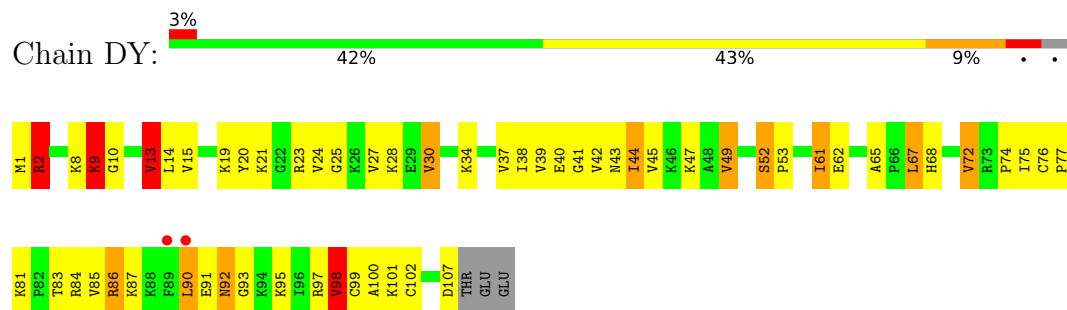
• Molecule 43: 50S Ribosomal Protein L23



• Molecule 44: 50S Ribosomal Protein L24

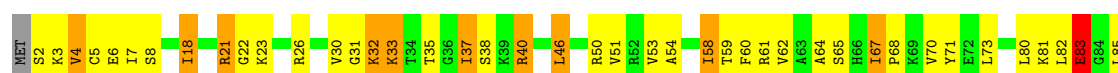


• Molecule 44: 50S Ribosomal Protein L24



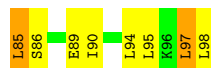
• Molecule 45: 50S Ribosomal Protein L25



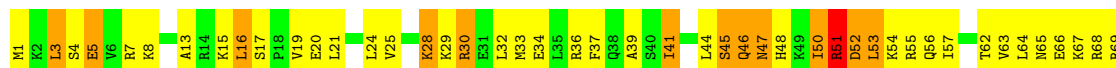




• Molecule 47: 50S Ribosomal Protein L28



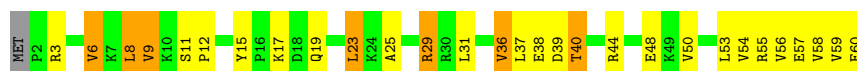
• Molecule 48: 50S Ribosomal Protein L29



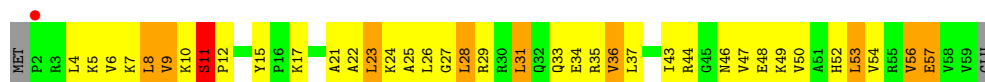
• Molecule 48: 50S Ribosomal Protein L29



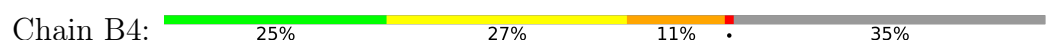
• Molecule 49: 50S Ribosomal Protein L30

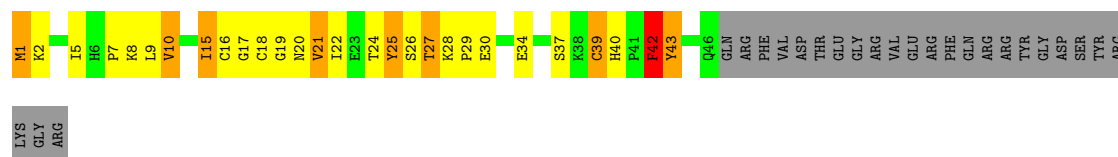


• Molecule 49: 50S Ribosomal Protein L30

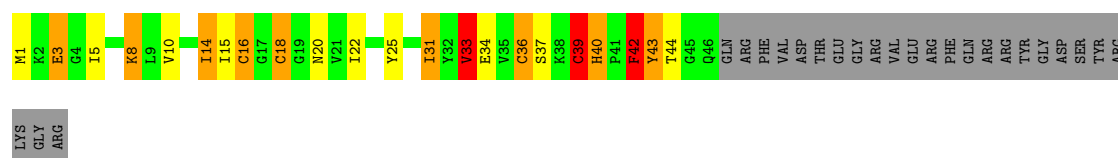
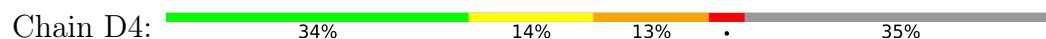


• Molecule 50: 50S Ribosomal Protein L31





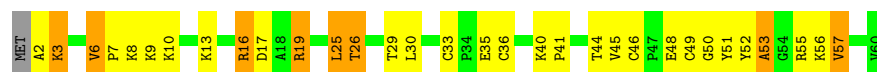
• Molecule 50: 50S Ribosomal Protein L31



• Molecule 51: 50S Ribosomal Protein L32



• Molecule 51: 50S Ribosomal Protein L32



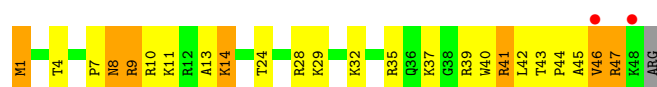
• Molecule 52: 50S Ribosomal Protein L33



• Molecule 52: 50S Ribosomal Protein L33



• Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34

Chain D7:  4% 49% 39% 10%

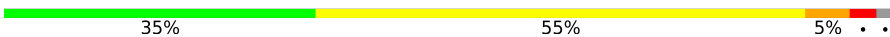


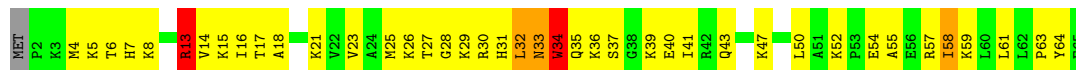
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:  42% 46% 9%



- Molecule 54: 50S Ribosomal Protein L35

Chain D8:  35% 55% 5%



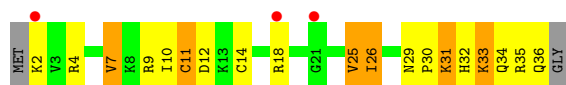
- Molecule 55: 50S Ribosomal Protein L36

Chain B9:  41% 38% 19%



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:  8% 43% 35% 16% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.7 (34.91-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.188 , 0.245 0.186 , 0.242	Depositor DCC
R_{free} test set	48002 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	284877	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.54	0/35273	0.59	10/55046 (0.0%)
1	CA	0.50	3/35152 (0.0%)	0.55	8/54858 (0.0%)
2	AB	0.81	0/1844	1.29	18/2498 (0.7%)
2	CB	0.73	1/1852 (0.1%)	1.21	15/2510 (0.6%)
3	AC	0.76	0/1458	1.24	13/1981 (0.7%)
3	CC	0.72	0/1477	1.16	9/2006 (0.4%)
4	AD	0.81	0/1550	1.36	15/2106 (0.7%)
4	CD	0.86	3/1567 (0.2%)	1.39	23/2125 (1.1%)
5	AE	0.84	1/1121 (0.1%)	1.36	15/1517 (1.0%)
5	CE	0.83	0/1131	1.35	16/1529 (1.0%)
6	AF	0.81	0/794	1.26	6/1082 (0.6%)
6	CF	0.75	0/797	1.12	4/1085 (0.4%)
7	AG	0.71	0/1169	1.16	8/1580 (0.5%)
7	CG	0.67	0/1166	1.21	13/1576 (0.8%)
8	AH	0.78	0/1065	1.31	10/1445 (0.7%)
8	CH	0.73	0/1069	1.19	7/1450 (0.5%)
9	AI	0.85	2/879 (0.2%)	1.38	8/1195 (0.7%)
9	CI	0.76	0/864	1.26	8/1177 (0.7%)
10	AJ	0.85	1/672 (0.1%)	1.28	7/919 (0.8%)
10	CJ	0.83	0/670	1.35	7/917 (0.8%)
11	AK	0.92	2/858 (0.2%)	1.30	7/1163 (0.6%)
11	CK	0.74	0/843	1.25	7/1144 (0.6%)
12	AL	0.91	0/925	1.32	8/1251 (0.6%)
12	CL	0.81	0/921	1.38	14/1247 (1.1%)
13	AM	0.88	1/824 (0.1%)	1.46	10/1120 (0.9%)
13	CM	0.77	0/794	1.32	12/1081 (1.1%)
14	AN	0.76	0/482	1.19	3/642 (0.5%)
14	CN	0.69	0/478	1.22	3/638 (0.5%)
15	AO	0.82	0/735	1.19	0/981
15	CO	0.75	0/735	1.15	4/981 (0.4%)
16	AP	0.79	0/662	1.48	13/898 (1.4%)
16	CP	0.82	0/677	1.30	5/917 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.83	0/836	1.26	7/1117 (0.6%)
17	CQ	0.76	0/832	1.20	6/1113 (0.5%)
18	AR	0.85	0/519	1.27	4/699 (0.6%)
18	CR	0.75	0/519	1.08	1/699 (0.1%)
19	AS	0.75	0/574	1.32	4/781 (0.5%)
19	CS	0.66	0/543	1.21	5/740 (0.7%)
20	AT	0.76	0/716	1.25	5/947 (0.5%)
20	CT	0.83	0/776	1.26	6/1026 (0.6%)
21	AU	0.81	0/221	1.21	1/288 (0.3%)
21	CU	0.74	0/184	1.35	3/244 (1.2%)
22	AY	0.96	2/1043 (0.2%)	1.45	16/1399 (1.1%)
23	AV	0.57	0/1836	0.57	0/2859
23	CV	0.44	0/1836	0.50	0/2859
24	AX	0.47	0/147	0.47	0/227
24	CX	0.49	0/147	0.51	0/227
25	BA	0.81	4/66391 (0.0%)	0.68	12/103628 (0.0%)
25	DA	0.59	0/65653	0.58	3/102473 (0.0%)
26	BB	0.70	0/2878	0.65	0/4490
26	DB	0.50	0/2878	0.54	0/4490
27	BD	1.20	6/2181 (0.3%)	1.58	37/2940 (1.3%)
27	DD	0.97	0/2186	1.37	20/2944 (0.7%)
28	BE	1.22	5/1588 (0.3%)	1.55	24/2145 (1.1%)
28	DE	0.89	0/1588	1.41	21/2145 (1.0%)
29	BF	1.16	4/1609 (0.2%)	1.38	21/2177 (1.0%)
29	DF	0.81	0/1611	1.33	15/2180 (0.7%)
30	BG	0.87	0/1393	1.39	22/1892 (1.2%)
30	DG	0.67	0/1385	1.32	16/1881 (0.9%)
31	BH	1.10	4/1343 (0.3%)	1.50	16/1820 (0.9%)
31	DH	0.68	0/1343	1.25	18/1820 (1.0%)
32	BI	0.86	1/1081 (0.1%)	1.34	10/1477 (0.7%)
32	DI	0.78	0/1072	1.23	10/1465 (0.7%)
33	BN	1.22	2/1139 (0.2%)	1.63	17/1538 (1.1%)
33	DN	0.82	0/1139	1.39	14/1538 (0.9%)
34	BO	1.17	2/933 (0.2%)	1.44	9/1257 (0.7%)
34	DO	0.96	0/933	1.34	9/1257 (0.7%)
35	BP	1.08	0/1148	1.48	19/1529 (1.2%)
35	DP	0.79	0/1148	1.32	15/1529 (1.0%)
36	BQ	1.18	1/1143 (0.1%)	1.43	15/1527 (1.0%)
36	DQ	0.81	0/1143	1.21	7/1527 (0.5%)
37	BR	1.26	2/982 (0.2%)	1.40	7/1312 (0.5%)
37	DR	0.87	0/982	1.23	6/1312 (0.5%)
38	BS	0.99	0/875	1.37	8/1168 (0.7%)
38	DS	0.66	0/883	1.23	7/1176 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BT	1.12	1/1086 (0.1%)	1.42	10/1455 (0.7%)
39	DT	0.82	0/1072	1.20	6/1437 (0.4%)
40	BU	1.31	3/977 (0.3%)	1.36	8/1301 (0.6%)
40	DU	0.86	0/977	1.26	6/1301 (0.5%)
41	BV	1.22	3/777 (0.4%)	1.56	9/1044 (0.9%)
41	DV	0.76	0/781	1.18	3/1048 (0.3%)
42	BW	1.29	2/901 (0.2%)	1.50	10/1209 (0.8%)
42	DW	1.00	0/887	1.31	9/1192 (0.8%)
43	BX	1.21	0/756	1.48	10/1016 (1.0%)
43	DX	0.90	0/746	1.27	6/1005 (0.6%)
44	BY	1.05	1/798 (0.1%)	1.46	11/1073 (1.0%)
44	DY	0.76	0/794	1.30	11/1067 (1.0%)
45	BZ	1.02	3/1486 (0.2%)	1.48	27/2022 (1.3%)
45	DZ	0.72	1/1483 (0.1%)	1.25	15/2023 (0.7%)
46	B0	1.15	0/602	1.45	7/804 (0.9%)
46	D0	0.80	0/615	1.21	4/820 (0.5%)
47	B1	1.25	3/752 (0.4%)	1.43	5/1003 (0.5%)
47	D1	0.89	0/752	1.27	5/1003 (0.5%)
48	B2	1.07	0/590	1.37	7/781 (0.9%)
48	D2	0.77	0/586	1.21	3/779 (0.4%)
49	B3	1.26	1/463 (0.2%)	1.49	10/623 (1.6%)
49	D3	0.69	0/458	1.23	4/616 (0.6%)
50	B4	0.77	0/358	1.59	6/487 (1.2%)
50	D4	0.77	0/358	1.25	5/487 (1.0%)
51	B5	1.24	0/469	1.60	13/634 (2.1%)
51	D5	0.84	0/465	1.32	5/630 (0.8%)
52	B6	1.15	1/456 (0.2%)	1.57	5/609 (0.8%)
52	D6	0.89	0/444	1.29	6/595 (1.0%)
53	B7	1.32	2/426 (0.5%)	1.47	0/561
53	D7	1.06	1/410 (0.2%)	1.24	5/543 (0.9%)
54	B8	1.27	1/516 (0.2%)	1.64	12/679 (1.8%)
54	D8	0.95	1/516 (0.2%)	1.45	9/679 (1.3%)
55	B9	1.24	1/300 (0.3%)	1.55	3/395 (0.8%)
55	D9	0.84	0/295	1.24	2/390 (0.5%)
All	All	0.74	72/303213 (0.0%)	0.87	999/453838 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BR	38	VAL	CA-CB	-14.64	1.46	1.54
45	BZ	92	SER	CA-C	10.02	1.57	1.52
47	B1	67	ILE	CA-CB	-9.90	1.49	1.54
13	AM	116	THR	CA-C	8.12	1.62	1.53
28	BE	203	LYS	CA-C	8.02	1.61	1.53

The worst 5 of 999 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	189(D)	C	N3-C4-N4	-23.96	46.10	118.00
33	BN	46	VAL	N-CA-C	17.05	125.09	111.62
27	BD	239	ARG	N-CA-C	-13.99	86.88	108.42
31	BH	127	GLU	CA-C-N	-13.41	103.07	119.84
31	BH	127	GLU	C-N-CA	-13.41	103.07	119.84

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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	31513	0	15906	885	0
1	CA	31406	0	15852	832	0
2	AB	1809	0	1781	107	0
2	CB	1817	0	1785	132	0
3	AC	1434	0	1299	61	0
3	CC	1453	0	1320	65	0
4	AD	1520	0	1407	85	0
4	CD	1537	0	1430	83	1
5	AE	1105	0	1130	52	0
5	CE	1115	0	1145	55	0
6	AF	781	0	741	36	1
6	CF	784	0	739	32	0
7	AG	1152	0	1098	59	0
7	CG	1149	0	1096	53	0
8	AH	1045	0	1033	56	0
8	CH	1049	0	1037	55	0
9	AI	863	0	760	57	0
9	CI	849	0	735	57	0
10	AJ	659	0	552	39	0
10	CJ	657	0	547	40	0
11	AK	843	0	841	35	0
11	CK	828	0	822	34	0
12	AL	909	0	927	51	0
12	CL	905	0	916	30	0
13	AM	814	0	765	49	0
13	CM	784	0	730	52	0
14	AN	473	0	491	40	0
14	CN	469	0	482	37	0
15	AO	724	0	749	38	0
15	CO	724	0	749	30	0
16	AP	646	0	636	44	0
16	CP	661	0	653	49	0
17	AQ	823	0	891	54	0
17	CQ	819	0	880	40	0
18	AR	514	0	530	31	0
18	CR	514	0	530	23	0
19	AS	560	0	466	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	529	0	443	22	0
20	AT	714	0	775	42	0
20	CT	773	0	836	36	0
21	AU	217	0	234	7	0
21	CU	180	0	173	4	0
22	AY	1031	0	1087	87	0
23	AV	1644	0	836	24	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	1060	0
25	DA	58627	0	29570	1211	0
26	BB	2573	0	1306	47	0
26	DB	2573	0	1306	82	0
27	BD	2131	0	2207	99	0
27	DD	2136	0	2218	107	0
28	BE	1555	0	1607	68	0
28	DE	1555	0	1607	78	0
29	BF	1576	0	1616	75	0
29	DF	1578	0	1623	97	0
30	BG	1368	0	1324	53	0
30	DG	1361	0	1316	78	0
31	BH	1317	0	1376	53	0
31	DH	1317	0	1376	61	0
32	BI	1066	0	1095	51	0
32	DI	1057	0	1087	60	0
33	BN	1112	0	1180	50	0
33	DN	1112	0	1180	65	0
34	BO	923	0	981	37	0
34	DO	923	0	981	40	0
35	BP	1131	0	1201	63	0
35	DP	1131	0	1201	69	0
36	BQ	1122	0	1179	48	0
36	DQ	1122	0	1179	70	0
37	BR	968	0	1033	46	0
37	DR	968	0	1033	58	0
38	BS	865	0	905	53	0
38	DS	873	0	927	67	0
39	BT	1072	0	1116	35	0
39	DT	1058	0	1098	38	0
40	BU	959	0	1019	36	0
40	DU	959	0	1019	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	BV	766	0	827	27	0
41	DV	770	0	838	41	0
42	BW	890	0	951	33	0
42	DW	877	0	932	33	0
43	BX	742	0	799	39	0
43	DX	732	0	777	18	0
44	BY	785	0	828	27	0
44	DY	781	0	829	43	0
45	BZ	1454	0	1452	68	0
45	DZ	1451	0	1421	74	0
46	B0	594	0	604	33	0
46	D0	607	0	622	42	0
47	B1	745	0	804	35	0
47	D1	745	0	804	36	0
48	B2	588	0	643	29	0
48	D2	584	0	623	28	0
49	B3	458	0	503	15	0
49	D3	453	0	501	28	0
50	B4	349	0	336	23	0
50	D4	349	0	336	19	0
51	B5	455	0	472	21	0
51	D5	451	0	461	25	0
52	B6	449	0	462	26	0
52	D6	437	0	440	18	0
53	B7	418	0	467	22	0
53	D7	402	0	434	11	0
54	B8	509	0	565	25	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
56	B1	3	0	0	0	0
56	B2	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
56	DR	1	0	0	0	0
56	DT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
58	BG	5	0	0	1	0
58	BH	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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
58	DV	1	0	0	0	0
58	DW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DY	2	0	0	0	0
All	All	284877	0	186478	7790	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 7790 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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	Interatomic distance (Å)	Clash overlap (Å)
6:AF:14:LEU:O	4:CD:20:TYR:OH[3_654]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	14	47
2	CB	233/256 (91%)	182 (78%)	45 (19%)	6 (3%)	4	26
3	AC	202/239 (84%)	165 (82%)	33 (16%)	4 (2%)	6	31
3	CC	204/239 (85%)	168 (82%)	36 (18%)	0	100	100
4	AD	206/209 (99%)	166 (81%)	35 (17%)	5 (2%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	4	28
5	AE	146/162 (90%)	120 (82%)	26 (18%)	0	100	100
5	CE	147/162 (91%)	129 (88%)	13 (9%)	5 (3%)	3	20
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%)	18	52
7	CG	152/156 (97%)	131 (86%)	20 (13%)	1 (1%)	18	52
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	18	52
8	CH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	AI	123/128 (96%)	105 (85%)	15 (12%)	3 (2%)	4	28
9	CI	123/128 (96%)	106 (86%)	13 (11%)	4 (3%)	3	21
10	AJ	94/105 (90%)	81 (86%)	9 (10%)	4 (4%)	2	16
10	CJ	94/105 (90%)	74 (79%)	17 (18%)	3 (3%)	3	21
11	AK	113/129 (88%)	101 (89%)	11 (10%)	1 (1%)	14	47
11	CK	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
12	AL	120/132 (91%)	108 (90%)	10 (8%)	2 (2%)	7	35
12	CL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	7	35
13	AM	113/126 (90%)	89 (79%)	20 (18%)	4 (4%)	3	20
13	CM	110/126 (87%)	82 (74%)	21 (19%)	7 (6%)	1	8
14	AN	57/61 (93%)	44 (77%)	13 (23%)	0	100	100
14	CN	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6	34
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%)	2	18
16	CP	80/88 (91%)	66 (82%)	10 (12%)	4 (5%)	1	13
17	AQ	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	12	45
17	CQ	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	12	45
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%)	9	40
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%)	5	31
20	CT	102/106 (96%)	73 (72%)	26 (26%)	3 (3%)	3	24
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%)	8	37
27	BD	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	18	52
28	BE	202/206 (98%)	189 (94%)	9 (4%)	4 (2%)	6	31
28	DE	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	8	37
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%)	5	29
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%)	10	42
32	BI	145/148 (98%)	116 (80%)	25 (17%)	4 (3%)	4	25
32	DI	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	9	39
33	BN	138/140 (99%)	124 (90%)	11 (8%)	3 (2%)	5	29
33	DN	138/140 (99%)	117 (85%)	19 (14%)	2 (1%)	9	39
34	BO	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	50
34	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	BP	147/150 (98%)	128 (87%)	17 (12%)	2 (1%)	9	39
35	DP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	39
36	BQ	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	9	39
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%)	4	25
38	DS	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	6	33
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%)	12	45
44	DY	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	12	45
45	BZ	184/206 (89%)	161 (88%)	21 (11%)	2 (1%)	11	43
45	DZ	187/206 (91%)	163 (87%)	21 (11%)	3 (2%)	7	36
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%)	11	43
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	B2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	8	37
48	D2	69/72 (96%)	60 (87%)	9 (13%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	34
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%)	5	29
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%)	2	16
53	D7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	5	29
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%)	11	43

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%)	122 (68%)	58 (32%)	0	1
2	CB	181/220 (82%)	132 (73%)	49 (27%)	0	2
3	AC	112/188 (60%)	87 (78%)	25 (22%)	1	5
3	CC	114/188 (61%)	92 (81%)	22 (19%)	1	8
4	AD	139/181 (77%)	108 (78%)	31 (22%)	1	5
4	CD	142/181 (78%)	107 (75%)	35 (25%)	1	3
5	AE	108/123 (88%)	70 (65%)	38 (35%)	0	0
5	CE	109/123 (89%)	80 (73%)	29 (27%)	0	3
6	AF	77/90 (86%)	62 (80%)	15 (20%)	1	8
6	CF	76/90 (84%)	60 (79%)	16 (21%)	1	6
7	AG	103/127 (81%)	79 (77%)	24 (23%)	1	5
7	CG	102/127 (80%)	72 (71%)	30 (29%)	0	1
8	AH	103/119 (87%)	84 (82%)	19 (18%)	1	9
8	CH	104/119 (87%)	81 (78%)	23 (22%)	1	5
9	AI	64/99 (65%)	54 (84%)	10 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CI	62/99 (63%)	52 (84%)	10 (16%)	2	13
10	AJ	52/92 (56%)	38 (73%)	14 (27%)	0	2
10	CJ	52/92 (56%)	36 (69%)	16 (31%)	0	1
11	AK	83/99 (84%)	58 (70%)	25 (30%)	0	1
11	CK	81/99 (82%)	59 (73%)	22 (27%)	0	2
12	AL	92/109 (84%)	70 (76%)	22 (24%)	1	4
12	CL	91/109 (84%)	69 (76%)	22 (24%)	1	4
13	AM	66/101 (65%)	43 (65%)	23 (35%)	0	0
13	CM	62/101 (61%)	43 (69%)	19 (31%)	0	1
14	AN	46/50 (92%)	39 (85%)	7 (15%)	3	14
14	CN	45/50 (90%)	31 (69%)	14 (31%)	0	1
15	AO	77/80 (96%)	61 (79%)	16 (21%)	1	7
15	CO	77/80 (96%)	63 (82%)	14 (18%)	2	9
16	AP	63/74 (85%)	41 (65%)	22 (35%)	0	0
16	CP	65/74 (88%)	45 (69%)	20 (31%)	0	1
17	AQ	94/97 (97%)	73 (78%)	21 (22%)	1	5
17	CQ	93/97 (96%)	73 (78%)	20 (22%)	1	6
18	AR	49/77 (64%)	40 (82%)	9 (18%)	1	9
18	CR	49/77 (64%)	35 (71%)	14 (29%)	0	2
19	AS	43/80 (54%)	35 (81%)	8 (19%)	1	9
19	CS	42/80 (52%)	28 (67%)	14 (33%)	0	1
20	AT	66/82 (80%)	48 (73%)	18 (27%)	0	2
20	CT	72/82 (88%)	53 (74%)	19 (26%)	0	3
21	AU	20/22 (91%)	13 (65%)	7 (35%)	0	0
21	CU	14/22 (64%)	12 (86%)	2 (14%)	3	16
22	AY	108/115 (94%)	75 (69%)	33 (31%)	0	1
27	BD	214/218 (98%)	163 (76%)	51 (24%)	1	4
27	DD	215/218 (99%)	156 (73%)	59 (27%)	0	2
28	BE	163/166 (98%)	119 (73%)	44 (27%)	0	2
28	DE	163/166 (98%)	117 (72%)	46 (28%)	0	2
29	BF	158/166 (95%)	115 (73%)	43 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DF	159/166 (96%)	124 (78%)	35 (22%)	1	6
30	BG	128/156 (82%)	97 (76%)	31 (24%)	1	4
30	DG	127/156 (81%)	92 (72%)	35 (28%)	0	2
31	BH	141/148 (95%)	105 (74%)	36 (26%)	0	3
31	DH	141/148 (95%)	109 (77%)	32 (23%)	1	5
32	BI	105/124 (85%)	67 (64%)	38 (36%)	0	0
32	DI	104/124 (84%)	76 (73%)	28 (27%)	0	2
33	BN	117/119 (98%)	90 (77%)	27 (23%)	1	5
33	DN	117/119 (98%)	85 (73%)	32 (27%)	0	2
34	BO	98/100 (98%)	73 (74%)	25 (26%)	0	3
34	DO	98/100 (98%)	67 (68%)	31 (32%)	0	1
35	BP	114/116 (98%)	84 (74%)	30 (26%)	0	3
35	DP	114/116 (98%)	87 (76%)	27 (24%)	1	4
36	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	6
36	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	12
37	BR	101/101 (100%)	77 (76%)	24 (24%)	1	4
37	DR	101/101 (100%)	79 (78%)	22 (22%)	1	6
38	BS	84/88 (96%)	63 (75%)	21 (25%)	0	3
38	DS	86/88 (98%)	63 (73%)	23 (27%)	0	3
39	BT	111/127 (87%)	86 (78%)	25 (22%)	1	5
39	DT	110/127 (87%)	81 (74%)	29 (26%)	0	3
40	BU	93/94 (99%)	78 (84%)	15 (16%)	2	13
40	DU	93/94 (99%)	77 (83%)	16 (17%)	2	10
41	BV	80/82 (98%)	61 (76%)	19 (24%)	1	4
41	DV	81/82 (99%)	56 (69%)	25 (31%)	0	1
42	BW	91/92 (99%)	67 (74%)	24 (26%)	0	3
42	DW	89/92 (97%)	66 (74%)	23 (26%)	0	3
43	BX	75/78 (96%)	58 (77%)	17 (23%)	1	5
43	DX	73/78 (94%)	60 (82%)	13 (18%)	2	10
44	BY	80/91 (88%)	63 (79%)	17 (21%)	1	6
44	DY	79/91 (87%)	56 (71%)	23 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BZ	156/179 (87%)	121 (78%)	35 (22%)	1	5
45	DZ	152/179 (85%)	114 (75%)	38 (25%)	0	3
46	B0	59/67 (88%)	46 (78%)	13 (22%)	1	6
46	D0	61/67 (91%)	47 (77%)	14 (23%)	1	5
47	B1	78/83 (94%)	57 (73%)	21 (27%)	0	2
47	D1	78/83 (94%)	56 (72%)	22 (28%)	0	2
48	B2	65/67 (97%)	46 (71%)	19 (29%)	0	1
48	D2	63/67 (94%)	45 (71%)	18 (29%)	0	2
49	B3	49/52 (94%)	39 (80%)	10 (20%)	1	7
49	D3	49/52 (94%)	37 (76%)	12 (24%)	1	3
50	B4	39/63 (62%)	25 (64%)	14 (36%)	0	0
50	D4	39/63 (62%)	25 (64%)	14 (36%)	0	0
51	B5	50/52 (96%)	41 (82%)	9 (18%)	2	9
51	D5	49/52 (94%)	37 (76%)	12 (24%)	1	3
52	B6	50/52 (96%)	37 (74%)	13 (26%)	0	3
52	D6	48/52 (92%)	39 (81%)	9 (19%)	1	9
53	B7	41/42 (98%)	28 (68%)	13 (32%)	0	1
53	D7	38/42 (90%)	30 (79%)	8 (21%)	1	6
54	B8	52/55 (94%)	43 (83%)	9 (17%)	2	10
54	D8	52/55 (94%)	43 (83%)	9 (17%)	2	10
55	B9	32/34 (94%)	25 (78%)	7 (22%)	1	5
55	D9	32/34 (94%)	24 (75%)	8 (25%)	0	3
All	All	8835/10181 (87%)	6625 (75%)	2210 (25%)	0	3

5 of 2210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	DP	144	GLU
38	DS	61	ASN
35	DP	135	LEU
45	DZ	170	THR
36	BQ	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
11	CK	104	GLN
29	DF	40	GLN
15	CO	28	GLN
20	CT	45	GLN
33	DN	133	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1462/1522 (96%)	387 (26%)	33 (2%)
1	CA	1457/1522 (95%)	369 (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%)	648 (23%)	64 (2%)
25	DA	2711/2915 (93%)	638 (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%)	2134 (24%)	188 (2%)

5 of 2134 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
1	CA	913	A
25	DA	587	C
1	CA	1061	G
1	CA	1530	G
25	DA	856	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1466/1522 (96%)	-0.22	10 (0%) 84 69	43, 93, 137, 172	0
1	CA	1461/1522 (95%)	-0.08	16 (1%) 78 61	55, 104, 145, 167	0
2	AB	233/256 (91%)	0.36	7 (3%) 52 33	72, 113, 134, 153	0
2	CB	235/256 (91%)	0.41	8 (3%) 48 30	100, 125, 139, 147	0
3	AC	204/239 (85%)	0.36	8 (3%) 43 27	97, 112, 125, 133	0
3	CC	206/239 (86%)	0.57	14 (6%) 23 15	110, 125, 136, 142	0
4	AD	208/209 (99%)	0.54	13 (6%) 26 17	76, 103, 118, 125	0
4	CD	208/209 (99%)	0.42	7 (3%) 48 30	85, 98, 114, 120	0
5	AE	148/162 (91%)	-0.02	1 (0%) 84 69	67, 89, 108, 134	0
5	CE	149/162 (91%)	0.16	1 (0%) 84 69	83, 99, 110, 131	0
6	AF	100/101 (99%)	-0.03	2 (2%) 65 45	68, 88, 104, 110	0
6	CF	100/101 (99%)	0.03	1 (1%) 79 63	78, 96, 110, 117	0
7	AG	154/156 (98%)	0.15	0 100 100	87, 102, 120, 133	0
7	CG	154/156 (98%)	0.33	11 (7%) 22 14	107, 119, 133, 144	0
8	AH	138/138 (100%)	-0.10	2 (1%) 73 54	73, 91, 100, 111	0
8	CH	138/138 (100%)	0.08	1 (0%) 84 69	82, 100, 111, 116	0
9	AI	125/128 (97%)	0.61	8 (6%) 25 16	71, 114, 126, 137	0
9	CI	125/128 (97%)	0.80	13 (10%) 11 8	101, 130, 138, 142	0
10	AJ	96/105 (91%)	0.77	4 (4%) 40 25	88, 119, 136, 140	0
10	CJ	96/105 (91%)	1.16	11 (11%) 9 7	111, 133, 141, 143	0
11	AK	115/129 (89%)	-0.02	0 100 100	53, 87, 104, 113	0
11	CK	114/129 (88%)	0.29	4 (3%) 47 29	78, 103, 118, 127	0
12	AL	122/132 (92%)	-0.05	2 (1%) 70 51	61, 84, 100, 111	0
12	CL	122/132 (92%)	0.09	1 (0%) 82 67	72, 90, 105, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	0.32	5 (4%)	40	24	66, 100, 113, 118	0
13	CM	112/126 (88%)	0.57	8 (7%)	22	14	102, 127, 135, 139	0
14	AN	59/61 (96%)	0.53	4 (6%)	23	15	94, 106, 114, 121	0
14	CN	59/61 (96%)	1.08	7 (11%)	9	6	116, 125, 133, 135	0
15	AO	88/89 (98%)	-0.02	0	100	100	65, 86, 106, 117	0
15	CO	88/89 (98%)	0.08	0	100	100	74, 96, 114, 118	0
16	AP	81/88 (92%)	0.35	2 (2%)	58	39	83, 100, 122, 127	0
16	CP	82/88 (93%)	0.29	0	100	100	84, 94, 112, 122	0
17	AQ	99/105 (94%)	0.03	3 (3%)	52	33	68, 89, 104, 113	0
17	CQ	99/105 (94%)	0.03	1 (1%)	79	63	77, 95, 110, 113	0
18	AR	68/88 (77%)	-0.16	0	100	100	69, 84, 102, 106	0
18	CR	68/88 (77%)	-0.07	0	100	100	82, 92, 111, 115	0
19	AS	81/93 (87%)	0.37	5 (6%)	26	17	96, 110, 130, 141	0
19	CS	75/93 (80%)	0.62	6 (8%)	18	12	107, 131, 142, 146	0
20	AT	96/106 (90%)	0.28	3 (3%)	51	32	77, 97, 113, 118	0
20	CT	104/106 (98%)	0.21	5 (4%)	35	22	81, 101, 123, 139	0
21	AU	25/27 (92%)	1.04	2 (8%)	18	12	80, 98, 105, 107	0
21	CU	23/27 (85%)	1.68	6 (26%)	1	2	115, 126, 132, 134	0
22	AY	132/140 (94%)	0.83	16 (12%)	8	6	69, 110, 138, 152	0
23	AV	77/77 (100%)	-0.38	1 (1%)	75	55	55, 82, 112, 132	0
23	CV	77/77 (100%)	-0.21	0	100	100	73, 109, 133, 150	0
24	AX	6/16 (37%)	0.17	0	100	100	67, 73, 127, 128	0
24	CX	6/16 (37%)	0.60	0	100	100	89, 96, 142, 147	0
25	BA	2752/2915 (94%)	-0.96	10 (0%)	88	79	23, 43, 115, 170	0
25	DA	2722/2915 (93%)	-0.57	13 (0%)	87	76	44, 74, 127, 170	0
26	BB	120/122 (98%)	-0.71	1 (0%)	82	67	36, 64, 90, 125	0
26	DB	120/122 (98%)	0.12	1 (0%)	82	67	73, 114, 129, 146	0
27	BD	275/276 (99%)	-0.66	1 (0%)	88	79	27, 43, 62, 110	0
27	DD	275/276 (99%)	-0.34	1 (0%)	88	79	41, 62, 82, 100	0
28	BE	204/206 (99%)	-0.69	0	100	100	22, 45, 71, 94	0
28	DE	204/206 (99%)	-0.27	2 (0%)	79	63	43, 74, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BF	203/210 (96%)	-0.57	1 (0%) 87 76	26, 49, 87, 115	0
29	DF	203/210 (96%)	-0.09	2 (0%) 79 63	47, 88, 114, 127	0
30	BG	181/182 (99%)	-0.14	2 (1%) 78 61	58, 77, 105, 116	0
30	DG	180/182 (98%)	0.41	6 (3%) 49 30	101, 117, 127, 136	0
31	BH	174/180 (96%)	-0.45	1 (0%) 85 73	38, 65, 84, 98	0
31	DH	174/180 (96%)	0.23	1 (0%) 85 73	96, 116, 130, 140	0
32	BI	147/148 (99%)	-0.17	1 (0%) 84 69	50, 95, 112, 128	0
32	DI	146/148 (98%)	0.15	0 100 100	68, 108, 126, 131	0
33	BN	140/140 (100%)	-0.69	0 100 100	30, 42, 69, 83	0
33	DN	140/140 (100%)	-0.10	0 100 100	64, 86, 107, 117	0
34	BO	122/122 (100%)	-0.72	1 (0%) 82 67	33, 52, 71, 82	0
34	DO	122/122 (100%)	-0.35	0 100 100	57, 73, 88, 96	0
35	BP	149/150 (99%)	-0.37	0 100 100	25, 55, 86, 108	0
35	DP	149/150 (99%)	0.01	1 (0%) 84 69	52, 91, 116, 127	0
36	BQ	141/141 (100%)	-0.55	0 100 100	33, 50, 70, 90	0
36	DQ	141/141 (100%)	0.11	2 (1%) 73 54	67, 90, 106, 114	0
37	BR	118/118 (100%)	-0.75	0 100 100	27, 41, 59, 67	0
37	DR	118/118 (100%)	-0.36	0 100 100	49, 65, 86, 95	0
38	BS	110/112 (98%)	-0.40	0 100 100	44, 62, 86, 97	0
38	DS	110/112 (98%)	0.18	0 100 100	90, 109, 119, 127	0
39	BT	132/146 (90%)	-0.47	1 (0%) 82 67	41, 55, 94, 127	0
39	DT	130/146 (89%)	-0.23	1 (0%) 82 67	62, 77, 108, 123	0
40	BU	116/118 (98%)	-0.76	0 100 100	25, 36, 55, 71	0
40	DU	116/118 (98%)	-0.12	1 (0%) 81 64	54, 82, 103, 108	0
41	BV	100/101 (99%)	-0.80	0 100 100	28, 46, 73, 90	0
41	DV	100/101 (99%)	-0.06	0 100 100	56, 98, 119, 123	0
42	BW	112/113 (99%)	-0.80	0 100 100	28, 37, 63, 89	0
42	DW	111/113 (98%)	-0.40	2 (1%) 67 48	49, 63, 89, 114	0
43	BX	95/96 (98%)	-0.55	0 100 100	34, 46, 77, 92	0
43	DX	95/96 (98%)	-0.15	1 (1%) 78 61	61, 77, 100, 107	0
44	BY	107/110 (97%)	-0.51	0 100 100	41, 60, 91, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/110 (97%)	0.19	3 (2%) 55 35	77, 96, 112, 124	0
45	BZ	186/206 (90%)	-0.18	0 100 100	49, 76, 104, 126	0
45	DZ	189/206 (91%)	0.28	4 (2%) 63 43	98, 114, 131, 139	0
46	B0	76/85 (89%)	-0.59	0 100 100	32, 42, 59, 83	0
46	D0	77/85 (90%)	0.18	2 (2%) 57 37	73, 85, 101, 124	0
47	B1	97/98 (98%)	-0.43	0 100 100	32, 51, 90, 104	0
47	D1	97/98 (98%)	-0.16	1 (1%) 79 63	50, 72, 105, 115	0
48	B2	70/72 (97%)	-0.38	1 (1%) 73 54	41, 60, 78, 103	0
48	D2	71/72 (98%)	-0.02	0 100 100	78, 94, 106, 110	0
49	B3	59/60 (98%)	-0.78	0 100 100	33, 41, 76, 93	0
49	D3	58/60 (96%)	0.00	1 (1%) 69 49	71, 84, 114, 128	0
50	B4	46/71 (64%)	-0.32	0 100 100	78, 96, 112, 114	0
50	D4	46/71 (64%)	0.18	0 100 100	118, 126, 136, 138	0
51	B5	59/60 (98%)	-0.79	0 100 100	25, 41, 62, 74	0
51	D5	59/60 (98%)	-0.22	0 100 100	47, 66, 85, 106	0
52	B6	53/54 (98%)	-0.69	0 100 100	42, 49, 66, 76	0
52	D6	53/54 (98%)	-0.12	0 100 100	67, 81, 93, 101	0
53	B7	48/49 (97%)	-0.41	2 (4%) 40 25	25, 33, 68, 88	0
53	D7	48/49 (97%)	-0.21	2 (4%) 40 25	41, 53, 82, 105	0
54	B8	64/65 (98%)	-0.68	0 100 100	35, 41, 49, 72	0
54	D8	64/65 (98%)	-0.03	0 100 100	60, 71, 83, 94	0
55	B9	36/37 (97%)	-0.52	0 100 100	33, 46, 58, 72	0
55	D9	35/37 (94%)	0.64	3 (8%) 16 11	73, 88, 103, 115	0
All	All	20489/21572 (94%)	-0.25	291 (1%) 73 54	22, 83, 131, 172	0

The worst 5 of 291 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DG	35	GLU	6.7
8	CH	1	MET	6.6
9	CI	126	SER	5.2
53	D7	48	LYS	4.9
13	AM	6	GLY	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1686	1/1	0.26	0.33	112,112,112,112	0
56	MG	CA	1796	1/1	0.32	0.22	102,102,102,102	0
56	MG	CA	1701	1/1	0.49	0.24	109,109,109,109	0
56	MG	AA	1816	1/1	0.53	0.19	107,107,107,107	0
56	MG	BA	3742	1/1	0.54	0.23	72,72,72,72	0
56	MG	CA	1604	1/1	0.55	0.33	114,114,114,114	0
56	MG	AA	1683	1/1	0.55	0.30	106,106,106,106	0
56	MG	AA	1811	1/1	0.55	0.23	120,120,120,120	0
56	MG	AA	1695	1/1	0.56	0.32	102,102,102,102	0
56	MG	AA	1689	1/1	0.57	0.20	77,77,77,77	0
56	MG	DA	3432	1/1	0.57	0.13	85,85,85,85	0
56	MG	CA	1747	1/1	0.58	0.22	96,96,96,96	0
56	MG	CA	1708	1/1	0.59	0.47	91,91,91,91	0
56	MG	DA	3616	1/1	0.59	0.17	115,115,115,115	0
56	MG	CA	1782	1/1	0.60	0.16	96,96,96,96	0
56	MG	AA	1699	1/1	0.60	0.16	109,109,109,109	0
56	MG	AA	1742	1/1	0.60	0.23	93,93,93,93	0
56	MG	CA	1671	1/1	0.60	0.13	82,82,82,82	0
56	MG	DA	3570	1/1	0.61	0.24	79,79,79,79	0
56	MG	DA	3232	1/1	0.61	0.26	91,91,91,91	0
56	MG	AA	1932	1/1	0.62	0.12	116,116,116,116	0
56	MG	CA	1704	1/1	0.62	0.23	93,93,93,93	0
56	MG	CA	1775	1/1	0.62	0.24	99,99,99,99	0
56	MG	DA	3309	1/1	0.63	0.20	88,88,88,88	0
56	MG	CA	1797	1/1	0.64	0.17	121,121,121,121	0
56	MG	BA	3736	1/1	0.65	0.18	59,59,59,59	0
56	MG	AA	1711	1/1	0.65	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3335	1/1	0.65	0.17	74,74,74,74	0
56	MG	AA	1813	1/1	0.65	0.16	121,121,121,121	0
56	MG	CA	1815	1/1	0.65	0.21	119,119,119,119	0
56	MG	CV	105	1/1	0.65	0.27	106,106,106,106	0
56	MG	AA	1915	1/1	0.66	0.13	121,121,121,121	0
56	MG	DA	3369	1/1	0.66	0.29	94,94,94,94	0
56	MG	AA	1709	1/1	0.66	0.22	86,86,86,86	0
56	MG	DA	3259	1/1	0.66	0.30	78,78,78,78	0
56	MG	AA	1612	1/1	0.66	0.25	60,60,60,60	0
56	MG	CA	1723	1/1	0.67	0.20	96,96,96,96	0
56	MG	BA	3799	1/1	0.68	0.11	72,72,72,72	0
56	MG	DA	3148	1/1	0.68	0.28	80,80,80,80	0
56	MG	AA	1685	1/1	0.68	0.26	91,91,91,91	0
56	MG	AA	1844	1/1	0.68	0.21	86,86,86,86	0
56	MG	CA	1780	1/1	0.68	0.14	90,90,90,90	0
56	MG	AV	108	1/1	0.69	0.12	98,98,98,98	0
56	MG	AA	1796	1/1	0.69	0.32	77,77,77,77	0
56	MG	BA	3853	1/1	0.69	0.14	76,76,76,76	0
56	MG	CA	1703	1/1	0.69	0.26	100,100,100,100	0
56	MG	AA	1884	1/1	0.70	0.12	82,82,82,82	0
56	MG	CA	1702	1/1	0.70	0.21	114,114,114,114	0
56	MG	DA	3472	1/1	0.70	0.21	78,78,78,78	0
56	MG	DA	3017	1/1	0.70	0.31	69,69,69,69	0
56	MG	AA	1743	1/1	0.70	0.19	80,80,80,80	0
56	MG	DB	208	1/1	0.70	0.27	98,98,98,98	0
56	MG	CA	1659	1/1	0.71	0.18	85,85,85,85	0
56	MG	DA	3318	1/1	0.71	0.17	83,83,83,83	0
56	MG	BA	3430	1/1	0.71	0.17	69,69,69,69	0
56	MG	CA	1700	1/1	0.71	0.35	90,90,90,90	0
56	MG	DA	3025	1/1	0.71	0.19	76,76,76,76	0
56	MG	CA	1793	1/1	0.71	0.17	73,73,73,73	0
56	MG	DA	3152	1/1	0.71	0.26	69,69,69,69	0
56	MG	AA	1653	1/1	0.71	0.38	82,82,82,82	0
56	MG	CA	1614	1/1	0.71	0.20	81,81,81,81	0
56	MG	AA	1620	1/1	0.72	0.22	74,74,74,74	0
56	MG	AA	1838	1/1	0.72	0.15	72,72,72,72	0
56	MG	CA	1788	1/1	0.72	0.11	118,118,118,118	0
56	MG	CA	1722	1/1	0.72	0.24	76,76,76,76	0
56	MG	DA	3158	1/1	0.72	0.21	82,82,82,82	0
56	MG	CX	101	1/1	0.72	0.20	99,99,99,99	0
56	MG	DA	3519	1/1	0.72	0.14	93,93,93,93	0
56	MG	DA	3255	1/1	0.72	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3013	1/1	0.72	0.19	97,97,97,97	0
56	MG	DA	3654	1/1	0.72	0.13	118,118,118,118	0
56	MG	DA	3265	1/1	0.72	0.19	68,68,68,68	0
56	MG	DA	3284	1/1	0.73	0.32	75,75,75,75	0
56	MG	DA	3296	1/1	0.73	0.23	80,80,80,80	0
56	MG	BA	3885	1/1	0.73	0.13	91,91,91,91	0
56	MG	BA	3102	1/1	0.73	0.15	51,51,51,51	0
56	MG	DA	3065	1/1	0.73	0.50	59,59,59,59	0
56	MG	BA	3395	1/1	0.73	0.25	100,100,100,100	0
56	MG	AA	1698	1/1	0.73	0.28	97,97,97,97	0
56	MG	AA	1812	1/1	0.73	0.14	122,122,122,122	0
56	MG	DA	3509	1/1	0.73	0.10	122,122,122,122	0
56	MG	AA	1718	1/1	0.73	0.10	70,70,70,70	0
56	MG	DA	3541	1/1	0.73	0.22	106,106,106,106	0
56	MG	CA	1770	1/1	0.73	0.17	93,93,93,93	0
56	MG	DA	3590	1/1	0.73	0.19	89,89,89,89	0
56	MG	DA	3258	1/1	0.73	0.40	91,91,91,91	0
56	MG	AA	1795	1/1	0.73	0.39	70,70,70,70	0
56	MG	DA	3657	1/1	0.73	0.14	89,89,89,89	0
56	MG	DB	204	1/1	0.73	0.20	107,107,107,107	0
56	MG	AA	1736	1/1	0.73	0.16	82,82,82,82	0
56	MG	DB	212	1/1	0.73	0.10	111,111,111,111	0
56	MG	D0	102	1/1	0.73	0.13	99,99,99,99	0
56	MG	CA	1813	1/1	0.74	0.19	113,113,113,113	0
56	MG	BA	3778	1/1	0.74	0.12	92,92,92,92	0
56	MG	AA	1799	1/1	0.74	0.18	95,95,95,95	0
56	MG	BA	3826	1/1	0.74	0.19	92,92,92,92	0
56	MG	DA	3364	1/1	0.74	0.18	94,94,94,94	0
56	MG	CA	1705	1/1	0.74	0.23	112,112,112,112	0
56	MG	AA	1823	1/1	0.74	0.34	77,77,77,77	0
56	MG	AA	1803	1/1	0.74	0.54	92,92,92,92	0
56	MG	BA	3237	1/1	0.74	0.16	59,59,59,59	0
56	MG	AA	1756	1/1	0.74	0.21	90,90,90,90	0
56	MG	CA	1621	1/1	0.74	0.22	100,100,100,100	0
56	MG	DA	3157	1/1	0.74	0.29	82,82,82,82	0
56	MG	CA	1639	1/1	0.74	0.34	96,96,96,96	0
56	MG	DA	3199	1/1	0.74	0.56	81,81,81,81	0
56	MG	CA	1649	1/1	0.74	0.13	78,78,78,78	0
56	MG	AA	1659	1/1	0.74	0.27	97,97,97,97	0
56	MG	DA	3666	1/1	0.74	0.17	100,100,100,100	0
56	MG	CA	1664	1/1	0.74	0.35	76,76,76,76	0
56	MG	BA	3542	1/1	0.74	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1741	1/1	0.74	0.30	85,85,85,85	0
56	MG	AA	1923	1/1	0.74	0.13	115,115,115,115	0
56	MG	DA	3009	1/1	0.75	0.20	90,90,90,90	0
56	MG	AA	1819	1/1	0.75	0.45	91,91,91,91	0
56	MG	CA	1692	1/1	0.75	0.38	84,84,84,84	0
56	MG	CA	1697	1/1	0.75	0.28	117,117,117,117	0
56	MG	DA	3564	1/1	0.75	0.20	88,88,88,88	0
56	MG	DA	3052	1/1	0.75	0.41	79,79,79,79	0
56	MG	CA	1795	1/1	0.75	0.16	100,100,100,100	0
56	MG	BA	3500	1/1	0.75	0.25	93,93,93,93	0
56	MG	DA	3620	1/1	0.75	0.14	95,95,95,95	0
56	MG	CA	1736	1/1	0.75	0.17	97,97,97,97	0
56	MG	AA	1901	1/1	0.75	0.09	119,119,119,119	0
56	MG	BA	3591	1/1	0.75	0.19	64,64,64,64	0
56	MG	DB	203	1/1	0.75	0.23	105,105,105,105	0
56	MG	AA	1800	1/1	0.75	0.24	76,76,76,76	0
56	MG	DA	3381	1/1	0.75	0.21	88,88,88,88	0
56	MG	DA	3430	1/1	0.75	0.22	83,83,83,83	0
56	MG	BA	3399	1/1	0.75	0.21	95,95,95,95	0
56	MG	DA	3040	1/1	0.76	0.16	78,78,78,78	0
56	MG	DA	3306	1/1	0.76	0.13	106,106,106,106	0
56	MG	DA	3213	1/1	0.76	0.17	89,89,89,89	0
56	MG	DA	3664	1/1	0.76	0.11	97,97,97,97	0
56	MG	CA	1669	1/1	0.76	0.45	78,78,78,78	0
56	MG	AA	1687	1/1	0.76	0.33	105,105,105,105	0
56	MG	CA	1745	1/1	0.76	0.13	99,99,99,99	0
56	MG	CA	1799	1/1	0.76	0.11	94,94,94,94	0
56	MG	BA	3397	1/1	0.76	0.14	66,66,66,66	0
56	MG	AA	1675	1/1	0.76	0.36	78,78,78,78	0
56	MG	BA	3035	1/1	0.77	0.15	82,82,82,82	0
56	MG	AA	1727	1/1	0.77	0.30	73,73,73,73	0
56	MG	DA	3557	1/1	0.77	0.28	93,93,93,93	0
56	MG	AA	1821	1/1	0.77	0.24	78,78,78,78	0
56	MG	BA	3760	1/1	0.77	0.12	68,68,68,68	0
56	MG	AA	1657	1/1	0.77	0.33	67,67,67,67	0
56	MG	CA	1718	1/1	0.77	0.29	88,88,88,88	0
56	MG	AA	1737	1/1	0.77	0.29	88,88,88,88	0
56	MG	DA	3634	1/1	0.77	0.13	70,70,70,70	0
56	MG	DA	3348	1/1	0.77	0.23	77,77,77,77	0
56	MG	DA	3360	1/1	0.77	0.19	61,61,61,61	0
56	MG	BA	3820	1/1	0.77	0.18	93,93,93,93	0
56	MG	AA	1723	1/1	0.77	0.25	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3678	1/1	0.77	0.13	89,89,89,89	0
56	MG	AI	202	1/1	0.77	0.17	90,90,90,90	0
56	MG	CA	1695	1/1	0.77	0.14	94,94,94,94	0
56	MG	AA	1859	1/1	0.77	0.14	91,91,91,91	0
56	MG	BB	203	1/1	0.77	0.17	63,63,63,63	0
56	MG	BA	3012	1/1	0.77	0.36	69,69,69,69	0
56	MG	DA	3510	1/1	0.78	0.26	77,77,77,77	0
56	MG	BA	3294	1/1	0.78	0.20	67,67,67,67	0
56	MG	CA	1662	1/1	0.78	0.19	92,92,92,92	0
56	MG	BA	3588	1/1	0.78	0.22	78,78,78,78	0
56	MG	BA	3855	1/1	0.78	0.24	103,103,103,103	0
56	MG	AV	112	1/1	0.78	0.19	79,79,79,79	0
56	MG	BA	3396	1/1	0.78	0.28	95,95,95,95	0
56	MG	AA	1746	1/1	0.78	0.28	81,81,81,81	0
56	MG	CA	1733	1/1	0.78	0.17	90,90,90,90	0
56	MG	AA	1937	1/1	0.78	0.14	79,79,79,79	0
56	MG	CA	1812	1/1	0.78	0.11	114,114,114,114	0
56	MG	DA	3182	1/1	0.78	0.13	68,68,68,68	0
56	MG	AA	1720	1/1	0.78	0.28	92,92,92,92	0
56	MG	DA	3372	1/1	0.78	0.19	78,78,78,78	0
56	MG	BA	3446	1/1	0.78	0.20	87,87,87,87	0
56	MG	DA	3228	1/1	0.78	0.35	90,90,90,90	0
56	MG	CA	1748	1/1	0.78	0.18	75,75,75,75	0
56	MG	AA	1611	1/1	0.78	0.20	97,97,97,97	0
56	MG	DA	3497	1/1	0.78	0.11	70,70,70,70	0
56	MG	CA	1771	1/1	0.78	0.24	78,78,78,78	0
56	MG	DA	3206	1/1	0.79	0.21	92,92,92,92	0
56	MG	BA	3743	1/1	0.79	0.22	71,71,71,71	0
56	MG	AE	201	1/1	0.79	0.37	83,83,83,83	0
56	MG	AA	1747	1/1	0.79	0.10	93,93,93,93	0
56	MG	DA	3082	1/1	0.79	0.30	89,89,89,89	0
56	MG	DA	3631	1/1	0.79	0.18	94,94,94,94	0
56	MG	AK	201	1/1	0.79	0.20	107,107,107,107	0
56	MG	AA	1733	1/1	0.79	0.13	94,94,94,94	0
56	MG	AA	1794	1/1	0.79	0.35	68,68,68,68	0
56	MG	CA	1684	1/1	0.79	0.19	70,70,70,70	0
56	MG	DA	3294	1/1	0.79	0.20	82,82,82,82	0
56	MG	CA	1635	1/1	0.79	0.53	72,72,72,72	0
56	MG	DA	3185	1/1	0.79	0.14	58,58,58,58	0
56	MG	DA	3191	1/1	0.79	0.21	77,77,77,77	0
56	MG	DB	207	1/1	0.79	0.23	79,79,79,79	0
56	MG	DA	3532	1/1	0.79	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3331	1/1	0.79	0.21	66,66,66,66	0
56	MG	DU	201	1/1	0.79	0.19	72,72,72,72	0
56	MG	DA	3201	1/1	0.79	0.13	80,80,80,80	0
56	MG	CA	1760	1/1	0.80	0.27	103,103,103,103	0
56	MG	AA	1693	1/1	0.80	0.18	103,103,103,103	0
56	MG	DA	3373	1/1	0.80	0.40	75,75,75,75	0
56	MG	DA	3380	1/1	0.80	0.21	84,84,84,84	0
56	MG	DA	3005	1/1	0.80	0.09	73,73,73,73	0
56	MG	BA	3558	1/1	0.80	0.17	61,61,61,61	0
56	MG	DA	3207	1/1	0.80	0.23	74,74,74,74	0
56	MG	DA	3208	1/1	0.80	0.34	91,91,91,91	0
56	MG	BA	3388	1/1	0.80	0.14	77,77,77,77	0
56	MG	AA	1602	1/1	0.80	0.16	104,104,104,104	0
56	MG	AA	1805	1/1	0.80	0.41	89,89,89,89	0
56	MG	DA	3254	1/1	0.80	0.12	71,71,71,71	0
56	MG	CA	1784	1/1	0.80	0.14	96,96,96,96	0
56	MG	DA	3539	1/1	0.80	0.12	102,102,102,102	0
56	MG	DA	3049	1/1	0.80	0.23	76,76,76,76	0
56	MG	AA	1880	1/1	0.80	0.26	79,79,79,79	0
56	MG	CA	1675	1/1	0.80	0.15	77,77,77,77	0
56	MG	DA	3268	1/1	0.80	0.18	64,64,64,64	0
56	MG	DA	3272	1/1	0.80	0.20	68,68,68,68	0
56	MG	DA	3614	1/1	0.80	0.14	98,98,98,98	0
56	MG	DA	3279	1/1	0.80	0.19	74,74,74,74	0
56	MG	DA	3282	1/1	0.80	0.40	75,75,75,75	0
56	MG	AA	1715	1/1	0.80	0.19	72,72,72,72	0
56	MG	DA	3288	1/1	0.80	0.13	83,83,83,83	0
56	MG	CA	1612	1/1	0.80	0.28	84,84,84,84	0
56	MG	BA	3236	1/1	0.80	0.09	50,50,50,50	0
56	MG	CA	1737	1/1	0.80	0.30	90,90,90,90	0
56	MG	AA	1704	1/1	0.80	0.23	79,79,79,79	0
56	MG	DA	3674	1/1	0.80	0.10	105,105,105,105	0
56	MG	DA	3170	1/1	0.80	0.09	96,96,96,96	0
56	MG	DA	3177	1/1	0.80	0.28	75,75,75,75	0
56	MG	DA	3343	1/1	0.80	0.34	70,70,70,70	0
56	MG	AA	1903	1/1	0.80	0.12	117,117,117,117	0
56	MG	DA	3356	1/1	0.80	0.28	85,85,85,85	0
56	MG	BA	3808	1/1	0.80	0.11	70,70,70,70	0
56	MG	DA	3362	1/1	0.80	0.21	75,75,75,75	0
56	MG	DA	3186	1/1	0.80	0.37	76,76,76,76	0
56	MG	DA	3533	1/1	0.81	0.12	95,95,95,95	0
56	MG	CA	1699	1/1	0.81	0.16	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1601	1/1	0.81	0.19	65,65,65,65	0
56	MG	AD	303	1/1	0.81	0.25	93,93,93,93	0
56	MG	BA	3026	1/1	0.81	0.20	92,92,92,92	0
56	MG	DA	3171	1/1	0.81	0.11	66,66,66,66	0
56	MG	BA	3708	1/1	0.81	0.10	85,85,85,85	0
56	MG	DA	3363	1/1	0.81	0.21	64,64,64,64	0
56	MG	AA	1913	1/1	0.81	0.08	109,109,109,109	0
56	MG	DA	3366	1/1	0.81	0.09	81,81,81,81	0
56	MG	AA	1629	1/1	0.81	0.28	68,68,68,68	0
56	MG	CA	1706	1/1	0.81	0.46	75,75,75,75	0
56	MG	DA	3280	1/1	0.81	0.13	80,80,80,80	0
56	MG	BB	228	1/1	0.81	0.10	69,69,69,69	0
56	MG	CA	1717	1/1	0.81	0.23	77,77,77,77	0
56	MG	DA	3400	1/1	0.81	0.22	53,53,53,53	0
56	MG	AA	1618	1/1	0.81	0.26	61,61,61,61	0
56	MG	DA	3289	1/1	0.81	0.18	86,86,86,86	0
56	MG	DB	202	1/1	0.81	0.42	73,73,73,73	0
56	MG	AA	1851	1/1	0.81	0.09	80,80,80,80	0
56	MG	DA	3478	1/1	0.81	0.16	90,90,90,90	0
56	MG	CA	1687	1/1	0.81	0.21	81,81,81,81	0
56	MG	BA	3256	1/1	0.81	0.25	77,77,77,77	0
56	MG	AV	111	1/1	0.81	0.30	85,85,85,85	0
56	MG	BA	3300	1/1	0.81	0.26	70,70,70,70	0
56	MG	DA	3331	1/1	0.81	0.29	77,77,77,77	0
56	MG	AA	1922	1/1	0.82	0.11	106,106,106,106	0
56	MG	AA	1669	1/1	0.82	0.28	84,84,84,84	0
56	MG	CA	1688	1/1	0.82	0.24	68,68,68,68	0
56	MG	CA	1803	1/1	0.82	0.09	102,102,102,102	0
56	MG	DA	3178	1/1	0.82	0.23	77,77,77,77	0
56	MG	BA	3414	1/1	0.82	0.15	72,72,72,72	0
56	MG	CA	1694	1/1	0.82	0.30	80,80,80,80	0
56	MG	AA	1759	1/1	0.82	0.17	60,60,60,60	0
56	MG	BA	3435	1/1	0.82	0.14	84,84,84,84	0
56	MG	BA	3339	1/1	0.82	0.22	70,70,70,70	0
56	MG	CA	1752	1/1	0.82	0.18	58,58,58,58	0
56	MG	DA	3202	1/1	0.82	0.18	73,73,73,73	0
56	MG	DA	3607	1/1	0.82	0.11	90,90,90,90	0
56	MG	DA	3203	1/1	0.82	0.29	91,91,91,91	0
56	MG	CA	1757	1/1	0.82	0.13	94,94,94,94	0
56	MG	BA	3476	1/1	0.82	0.12	50,50,50,50	0
56	MG	DA	3625	1/1	0.82	0.12	80,80,80,80	0
56	MG	DA	3629	1/1	0.82	0.22	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3481	1/1	0.82	0.10	87,87,87,87	0
56	MG	CA	1658	1/1	0.82	0.39	91,91,91,91	0
56	MG	DA	3227	1/1	0.82	0.27	79,79,79,79	0
56	MG	BA	3353	1/1	0.82	0.20	57,57,57,57	0
56	MG	BA	3363	1/1	0.82	0.29	63,63,63,63	0
56	MG	AA	1820	1/1	0.82	0.22	86,86,86,86	0
56	MG	AA	1655	1/1	0.82	0.24	77,77,77,77	0
56	MG	DA	3379	1/1	0.82	0.28	80,80,80,80	0
56	MG	DA	3072	1/1	0.82	0.18	65,65,65,65	0
56	MG	CA	1785	1/1	0.82	0.15	87,87,87,87	0
56	MG	DA	3092	1/1	0.82	0.27	92,92,92,92	0
56	MG	DA	3109	1/1	0.82	0.27	74,74,74,74	0
56	MG	AA	1688	1/1	0.82	0.16	96,96,96,96	0
56	MG	DB	209	1/1	0.82	0.26	86,86,86,86	0
56	MG	DA	3465	1/1	0.82	0.11	104,104,104,104	0
56	MG	BA	3605	1/1	0.82	0.11	75,75,75,75	0
56	MG	CA	1683	1/1	0.82	0.42	71,71,71,71	0
56	MG	AV	113	1/1	0.83	0.19	84,84,84,84	0
56	MG	BA	3523	1/1	0.83	0.17	76,76,76,76	0
56	MG	BA	3287	1/1	0.83	0.25	82,82,82,82	0
56	MG	CA	1798	1/1	0.83	0.14	94,94,94,94	0
56	MG	BA	3844	1/1	0.83	0.08	99,99,99,99	0
56	MG	AA	1703	1/1	0.83	0.12	74,74,74,74	0
56	MG	DA	3522	1/1	0.83	0.17	76,76,76,76	0
56	MG	CA	1806	1/1	0.83	0.09	102,102,102,102	0
56	MG	DA	3295	1/1	0.83	0.21	75,75,75,75	0
56	MG	AY	201	1/1	0.83	0.12	111,111,111,111	0
56	MG	DA	3297	1/1	0.83	0.23	81,81,81,81	0
56	MG	AV	107	1/1	0.83	0.28	87,87,87,87	0
56	MG	BA	3892	1/1	0.83	0.20	94,94,94,94	0
56	MG	CV	104	1/1	0.83	0.24	92,92,92,92	0
56	MG	DA	3588	1/1	0.83	0.11	109,109,109,109	0
56	MG	BA	3420	1/1	0.83	0.16	65,65,65,65	0
56	MG	DA	3197	1/1	0.83	0.31	82,82,82,82	0
56	MG	BB	209	1/1	0.83	0.24	79,79,79,79	0
56	MG	DA	3004	1/1	0.83	0.42	75,75,75,75	0
56	MG	BA	3628	1/1	0.83	0.14	66,66,66,66	0
56	MG	AA	1731	1/1	0.83	0.24	70,70,70,70	0
56	MG	BA	3193	1/1	0.83	0.21	45,45,45,45	0
56	MG	BA	3439	1/1	0.83	0.26	82,82,82,82	0
56	MG	CA	1618	1/1	0.83	0.25	78,78,78,78	0
56	MG	DA	3365	1/1	0.83	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3444	1/1	0.83	0.28	74,74,74,74	0
56	MG	AA	1724	1/1	0.83	0.20	92,92,92,92	0
56	MG	CA	1638	1/1	0.83	0.28	99,99,99,99	0
56	MG	BA	3372	1/1	0.83	0.16	77,77,77,77	0
56	MG	DA	3374	1/1	0.83	0.21	75,75,75,75	0
56	MG	DA	3682	1/1	0.83	0.09	90,90,90,90	0
56	MG	DA	3696	1/1	0.83	0.18	96,96,96,96	0
56	MG	CA	1645	1/1	0.83	0.32	74,74,74,74	0
56	MG	DA	3081	1/1	0.83	0.23	65,65,65,65	0
56	MG	BA	3792	1/1	0.83	0.15	48,48,48,48	0
56	MG	DB	206	1/1	0.83	0.21	77,77,77,77	0
56	MG	DA	3398	1/1	0.83	0.09	58,58,58,58	0
56	MG	AA	1775	1/1	0.83	0.07	77,77,77,77	0
56	MG	CA	1707	1/1	0.83	0.23	72,72,72,72	0
56	MG	DA	3114	1/1	0.83	0.28	70,70,70,70	0
56	MG	DB	213	1/1	0.83	0.15	115,115,115,115	0
56	MG	DE	304	1/1	0.83	0.19	70,70,70,70	0
56	MG	DO	201	1/1	0.83	0.15	80,80,80,80	0
56	MG	DA	3448	1/1	0.83	0.10	73,73,73,73	0
56	MG	DA	3119	1/1	0.83	0.19	39,39,39,39	0
56	MG	BA	3188	1/1	0.84	0.26	74,74,74,74	0
56	MG	DA	3585	1/1	0.84	0.17	104,104,104,104	0
56	MG	CA	1808	1/1	0.84	0.09	102,102,102,102	0
56	MG	DA	3116	1/1	0.84	0.24	79,79,79,79	0
56	MG	DA	3117	1/1	0.84	0.27	70,70,70,70	0
56	MG	AA	1784	1/1	0.84	0.28	69,69,69,69	0
56	MG	CA	1661	1/1	0.84	0.24	101,101,101,101	0
56	MG	DA	3618	1/1	0.84	0.15	80,80,80,80	0
56	MG	DA	3150	1/1	0.84	0.09	65,65,65,65	0
56	MG	BA	3230	1/1	0.84	0.15	57,57,57,57	0
56	MG	CA	1762	1/1	0.84	0.16	76,76,76,76	0
56	MG	DA	3269	1/1	0.84	0.29	85,85,85,85	0
56	MG	CA	1765	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3278	1/1	0.84	0.09	66,66,66,66	0
56	MG	DA	3165	1/1	0.84	0.31	65,65,65,65	0
56	MG	AA	1726	1/1	0.84	0.22	55,55,55,55	0
56	MG	AA	1808	1/1	0.84	0.23	75,75,75,75	0
56	MG	BA	3499	1/1	0.84	0.29	73,73,73,73	0
56	MG	BA	3790	1/1	0.84	0.08	75,75,75,75	0
56	MG	DA	3180	1/1	0.84	0.19	75,75,75,75	0
56	MG	CA	1678	1/1	0.84	0.22	84,84,84,84	0
56	MG	AA	1898	1/1	0.84	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3286	1/1	0.84	0.17	61,61,61,61	0
56	MG	AA	1900	1/1	0.84	0.12	110,110,110,110	0
56	MG	DB	205	1/1	0.84	0.09	79,79,79,79	0
56	MG	CA	1633	1/1	0.84	0.28	81,81,81,81	0
56	MG	AA	1810	1/1	0.84	0.22	84,84,84,84	0
56	MG	AA	1678	1/1	0.84	0.23	90,90,90,90	0
56	MG	DA	3069	1/1	0.84	0.29	83,83,83,83	0
56	MG	BA	3423	1/1	0.84	0.14	85,85,85,85	0
56	MG	CA	1742	1/1	0.84	0.18	89,89,89,89	0
56	MG	AA	1853	1/1	0.84	0.20	93,93,93,93	0
56	MG	DA	3549	1/1	0.84	0.13	87,87,87,87	0
56	MG	AA	1856	1/1	0.84	0.16	66,66,66,66	0
56	MG	D0	101	1/1	0.84	0.37	79,79,79,79	0
56	MG	DA	3093	1/1	0.84	0.29	77,77,77,77	0
57	ZN	AN	101	1/1	0.84	0.15	164,164,164,164	0
56	MG	DA	3122	1/1	0.85	0.29	65,65,65,65	0
56	MG	DA	3126	1/1	0.85	0.12	69,69,69,69	0
56	MG	AA	1642	1/1	0.85	0.30	73,73,73,73	0
56	MG	AA	1846	1/1	0.85	0.17	90,90,90,90	0
56	MG	AA	1755	1/1	0.85	0.12	70,70,70,70	0
56	MG	AA	1697	1/1	0.85	0.10	75,75,75,75	0
56	MG	AA	1666	1/1	0.85	0.22	70,70,70,70	0
56	MG	CA	1814	1/1	0.85	0.10	114,114,114,114	0
56	MG	DA	3293	1/1	0.85	0.29	94,94,94,94	0
56	MG	DA	3167	1/1	0.85	0.18	67,67,67,67	0
56	MG	BB	208	1/1	0.85	0.12	54,54,54,54	0
56	MG	CA	1682	1/1	0.85	0.30	73,73,73,73	0
56	MG	AA	1714	1/1	0.85	0.20	74,74,74,74	0
56	MG	CV	108	1/1	0.85	0.18	79,79,79,79	0
56	MG	BB	219	1/1	0.85	0.27	85,85,85,85	0
56	MG	DA	3002	1/1	0.85	0.21	69,69,69,69	0
56	MG	DA	3598	1/1	0.85	0.21	69,69,69,69	0
56	MG	AA	1879	1/1	0.85	0.26	71,71,71,71	0
56	MG	BF	305	1/1	0.85	0.18	52,52,52,52	0
56	MG	CA	1601	1/1	0.85	0.34	79,79,79,79	0
56	MG	DA	3347	1/1	0.85	0.34	77,77,77,77	0
56	MG	AA	1690	1/1	0.85	0.09	65,65,65,65	0
56	MG	DA	3354	1/1	0.85	0.18	43,43,43,43	0
56	MG	DA	3628	1/1	0.85	0.19	80,80,80,80	0
56	MG	AD	302	1/1	0.85	0.31	79,79,79,79	0
56	MG	AA	1729	1/1	0.85	0.22	79,79,79,79	0
56	MG	BA	3120	1/1	0.85	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3764	1/1	0.85	0.09	85,85,85,85	0
56	MG	DA	3656	1/1	0.85	0.09	90,90,90,90	0
56	MG	CA	1776	1/1	0.85	0.27	90,90,90,90	0
56	MG	DA	3056	1/1	0.85	0.15	59,59,59,59	0
56	MG	CA	1622	1/1	0.85	0.41	80,80,80,80	0
56	MG	DA	3673	1/1	0.85	0.13	111,111,111,111	0
56	MG	DA	3367	1/1	0.85	0.14	75,75,75,75	0
56	MG	DA	3368	1/1	0.85	0.21	80,80,80,80	0
56	MG	BA	3777	1/1	0.85	0.19	65,65,65,65	0
56	MG	DA	3685	1/1	0.85	0.11	96,96,96,96	0
56	MG	DA	3690	1/1	0.85	0.09	107,107,107,107	0
56	MG	DA	3224	1/1	0.85	0.21	75,75,75,75	0
56	MG	BA	3364	1/1	0.85	0.08	69,69,69,69	0
56	MG	AA	1893	1/1	0.85	0.10	95,95,95,95	0
56	MG	CA	1787	1/1	0.85	0.11	98,98,98,98	0
56	MG	DA	3233	1/1	0.85	0.20	80,80,80,80	0
56	MG	DA	3236	1/1	0.85	0.23	68,68,68,68	0
56	MG	DA	3241	1/1	0.85	0.27	76,76,76,76	0
56	MG	BA	3483	1/1	0.85	0.17	70,70,70,70	0
56	MG	BA	3486	1/1	0.85	0.08	60,60,60,60	0
56	MG	BA	3491	1/1	0.85	0.13	41,41,41,41	0
56	MG	BA	3384	1/1	0.85	0.12	72,72,72,72	0
56	MG	DB	214	1/1	0.85	0.14	83,83,83,83	0
56	MG	CA	1716	1/1	0.85	0.10	66,66,66,66	0
56	MG	AA	1827	1/1	0.85	0.13	69,69,69,69	0
56	MG	DA	3473	1/1	0.85	0.24	81,81,81,81	0
56	MG	AA	1622	1/1	0.85	0.31	56,56,56,56	0
56	MG	DA	3481	1/1	0.85	0.34	85,85,85,85	0
56	MG	DA	3488	1/1	0.85	0.24	73,73,73,73	0
56	MG	CA	1710	1/1	0.86	0.14	95,95,95,95	0
56	MG	DA	3525	1/1	0.86	0.20	77,77,77,77	0
56	MG	AA	1930	1/1	0.86	0.12	58,58,58,58	0
56	MG	AA	1716	1/1	0.86	0.14	70,70,70,70	0
56	MG	BA	3355	1/1	0.86	0.16	62,62,62,62	0
56	MG	AA	1651	1/1	0.86	0.17	80,80,80,80	0
56	MG	AA	1942	1/1	0.86	0.16	93,93,93,93	0
56	MG	DA	3299	1/1	0.86	0.27	57,57,57,57	0
56	MG	DA	3303	1/1	0.86	0.24	54,54,54,54	0
56	MG	DA	3304	1/1	0.86	0.08	67,67,67,67	0
56	MG	DA	3579	1/1	0.86	0.14	104,104,104,104	0
56	MG	CA	1816	1/1	0.86	0.09	110,110,110,110	0
56	MG	DA	3176	1/1	0.86	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3311	1/1	0.86	0.27	68,68,68,68	0
56	MG	DA	3317	1/1	0.86	0.09	84,84,84,84	0
56	MG	BA	3866	1/1	0.86	0.09	82,82,82,82	0
56	MG	BA	3875	1/1	0.86	0.17	74,74,74,74	0
56	MG	CA	1666	1/1	0.86	0.25	73,73,73,73	0
56	MG	BA	3107	1/1	0.86	0.10	44,44,44,44	0
56	MG	AA	1834	1/1	0.86	0.14	76,76,76,76	0
56	MG	BA	3896	1/1	0.86	0.11	72,72,72,72	0
56	MG	DA	3626	1/1	0.86	0.13	103,103,103,103	0
56	MG	CA	1676	1/1	0.86	0.23	83,83,83,83	0
56	MG	DA	3008	1/1	0.86	0.09	108,108,108,108	0
56	MG	CA	1677	1/1	0.86	0.10	88,88,88,88	0
56	MG	AA	1694	1/1	0.86	0.22	74,74,74,74	0
56	MG	DA	3016	1/1	0.86	0.14	42,42,42,42	0
56	MG	AA	1722	1/1	0.86	0.15	68,68,68,68	0
56	MG	AA	1680	1/1	0.86	0.13	65,65,65,65	0
56	MG	BA	3235	1/1	0.86	0.10	55,55,55,55	0
56	MG	AA	1603	1/1	0.86	0.11	78,78,78,78	0
56	MG	AA	1902	1/1	0.86	0.06	121,121,121,121	0
56	MG	CA	1689	1/1	0.86	0.36	84,84,84,84	0
56	MG	BA	3741	1/1	0.86	0.08	63,63,63,63	0
56	MG	CA	1603	1/1	0.86	0.31	72,72,72,72	0
56	MG	BA	3244	1/1	0.86	0.14	60,60,60,60	0
56	MG	DA	3375	1/1	0.86	0.13	84,84,84,84	0
56	MG	DA	3073	1/1	0.86	0.18	63,63,63,63	0
56	MG	DA	3074	1/1	0.86	0.16	69,69,69,69	0
56	MG	DA	3240	1/1	0.86	0.21	74,74,74,74	0
56	MG	AA	1725	1/1	0.86	0.28	65,65,65,65	0
56	MG	BA	3258	1/1	0.86	0.11	71,71,71,71	0
56	MG	DA	3084	1/1	0.86	0.12	76,76,76,76	0
56	MG	CA	1786	1/1	0.86	0.14	80,80,80,80	0
56	MG	BA	3281	1/1	0.86	0.18	72,72,72,72	0
56	MG	DA	3098	1/1	0.86	0.17	39,39,39,39	0
56	MG	AA	1739	1/1	0.86	0.21	99,99,99,99	0
56	MG	CA	1790	1/1	0.86	0.17	64,64,64,64	0
56	MG	AV	109	1/1	0.86	0.18	81,81,81,81	0
56	MG	CA	1629	1/1	0.86	0.44	74,74,74,74	0
56	MG	AA	1764	1/1	0.86	0.11	72,72,72,72	0
56	MG	AA	1863	1/1	0.86	0.19	54,54,54,54	0
56	MG	BA	3326	1/1	0.86	0.16	100,100,100,100	0
56	MG	AA	1865	1/1	0.86	0.28	81,81,81,81	0
56	MG	CA	1642	1/1	0.86	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3467	1/1	0.87	0.12	91,91,91,91	0
56	MG	BA	3714	1/1	0.87	0.10	62,62,62,62	0
56	MG	AA	1679	1/1	0.87	0.21	84,84,84,84	0
56	MG	DA	3475	1/1	0.87	0.18	78,78,78,78	0
56	MG	DA	3253	1/1	0.87	0.28	67,67,67,67	0
56	MG	AT	201	1/1	0.87	0.05	111,111,111,111	0
56	MG	BA	3312	1/1	0.87	0.20	54,54,54,54	0
56	MG	DA	3256	1/1	0.87	0.18	73,73,73,73	0
56	MG	AA	1702	1/1	0.87	0.21	71,71,71,71	0
56	MG	BA	3135	1/1	0.87	0.25	58,58,58,58	0
56	MG	DA	3511	1/1	0.87	0.12	77,77,77,77	0
56	MG	DA	3264	1/1	0.87	0.17	74,74,74,74	0
56	MG	BA	3463	1/1	0.87	0.09	57,57,57,57	0
56	MG	DA	3083	1/1	0.87	0.20	82,82,82,82	0
56	MG	DA	3529	1/1	0.87	0.23	82,82,82,82	0
56	MG	BA	3182	1/1	0.87	0.25	25,25,25,25	0
56	MG	DA	3086	1/1	0.87	0.22	32,32,32,32	0
56	MG	CA	1605	1/1	0.87	0.21	59,59,59,59	0
56	MG	CA	1693	1/1	0.87	0.17	83,83,83,83	0
56	MG	DA	3544	1/1	0.87	0.10	79,79,79,79	0
56	MG	CA	1606	1/1	0.87	0.27	77,77,77,77	0
56	MG	DA	3550	1/1	0.87	0.26	42,42,42,42	0
56	MG	AA	1674	1/1	0.87	0.28	74,74,74,74	0
56	MG	AA	1617	1/1	0.87	0.12	58,58,58,58	0
56	MG	AA	1807	1/1	0.87	0.16	84,84,84,84	0
56	MG	CA	1619	1/1	0.87	0.17	71,71,71,71	0
56	MG	BA	3796	1/1	0.87	0.24	83,83,83,83	0
56	MG	BA	3797	1/1	0.87	0.12	91,91,91,91	0
56	MG	AA	1939	1/1	0.87	0.14	105,105,105,105	0
56	MG	DA	3139	1/1	0.87	0.39	64,64,64,64	0
56	MG	CA	1630	1/1	0.87	0.35	70,70,70,70	0
56	MG	CA	1804	1/1	0.87	0.12	103,103,103,103	0
56	MG	BA	3807	1/1	0.87	0.16	64,64,64,64	0
56	MG	CA	1634	1/1	0.87	0.28	63,63,63,63	0
56	MG	CA	1811	1/1	0.87	0.07	102,102,102,102	0
56	MG	DA	3163	1/1	0.87	0.37	68,68,68,68	0
56	MG	AA	1858	1/1	0.87	0.10	90,90,90,90	0
56	MG	AA	1788	1/1	0.87	0.26	62,62,62,62	0
56	MG	BA	3501	1/1	0.87	0.11	80,80,80,80	0
56	MG	CA	1711	1/1	0.87	0.31	70,70,70,70	0
56	MG	DA	3175	1/1	0.87	0.25	75,75,75,75	0
56	MG	CA	1641	1/1	0.87	0.20	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1752	1/1	0.87	0.13	88,88,88,88	0
56	MG	BA	3848	1/1	0.87	0.14	43,43,43,43	0
56	MG	DA	3659	1/1	0.87	0.17	77,77,77,77	0
56	MG	DA	3179	1/1	0.87	0.12	67,67,67,67	0
56	MG	DA	3355	1/1	0.87	0.24	55,55,55,55	0
56	MG	CA	1719	1/1	0.87	0.14	85,85,85,85	0
56	MG	BA	3248	1/1	0.87	0.25	24,24,24,24	0
56	MG	CA	1651	1/1	0.87	0.15	54,54,54,54	0
56	MG	AA	1684	1/1	0.87	0.20	102,102,102,102	0
56	MG	DA	3187	1/1	0.87	0.25	109,109,109,109	0
56	MG	BA	3857	1/1	0.87	0.10	78,78,78,78	0
56	MG	DA	3693	1/1	0.87	0.14	103,103,103,103	0
56	MG	CA	1660	1/1	0.87	0.16	92,92,92,92	0
56	MG	BA	3863	1/1	0.87	0.08	72,72,72,72	0
56	MG	DA	3010	1/1	0.87	0.15	78,78,78,78	0
56	MG	AA	1670	1/1	0.87	0.24	88,88,88,88	0
56	MG	DA	3371	1/1	0.87	0.09	65,65,65,65	0
56	MG	BA	3271	1/1	0.87	0.07	44,44,44,44	0
56	MG	BA	3044	1/1	0.87	0.08	46,46,46,46	0
56	MG	DA	3023	1/1	0.87	0.18	56,56,56,56	0
56	MG	BA	3886	1/1	0.87	0.12	94,94,94,94	0
56	MG	DA	3210	1/1	0.87	0.23	74,74,74,74	0
56	MG	DA	3035	1/1	0.87	0.18	76,76,76,76	0
56	MG	DA	3216	1/1	0.87	0.10	46,46,46,46	0
56	MG	BA	3048	1/1	0.87	0.13	54,54,54,54	0
56	MG	CA	1674	1/1	0.87	0.22	79,79,79,79	0
56	MG	BA	3652	1/1	0.87	0.07	53,53,53,53	0
56	MG	BA	3054	1/1	0.87	0.21	58,58,58,58	0
56	MG	DA	3058	1/1	0.87	0.18	83,83,83,83	0
56	MG	DA	3060	1/1	0.87	0.20	90,90,90,90	0
57	ZN	D9	101	1/1	0.87	0.13	117,117,117,117	0
56	MG	DA	3271	1/1	0.88	0.15	68,68,68,68	0
56	MG	DA	3144	1/1	0.88	0.23	71,71,71,71	0
56	MG	DA	3491	1/1	0.88	0.10	101,101,101,101	0
56	MG	DA	3494	1/1	0.88	0.18	70,70,70,70	0
56	MG	DA	3274	1/1	0.88	0.31	70,70,70,70	0
56	MG	BA	3111	1/1	0.88	0.31	66,66,66,66	0
56	MG	DA	3149	1/1	0.88	0.15	51,51,51,51	0
56	MG	BA	3475	1/1	0.88	0.07	42,42,42,42	0
56	MG	BA	3319	1/1	0.88	0.10	59,59,59,59	0
56	MG	DA	3521	1/1	0.88	0.20	60,60,60,60	0
56	MG	CA	1617	1/1	0.88	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3287	1/1	0.88	0.22	62,62,62,62	0
56	MG	DA	3007	1/1	0.88	0.09	82,82,82,82	0
56	MG	DA	3162	1/1	0.88	0.26	54,54,54,54	0
56	MG	DA	3290	1/1	0.88	0.18	79,79,79,79	0
56	MG	DA	3535	1/1	0.88	0.14	96,96,96,96	0
56	MG	AA	1637	1/1	0.88	0.18	73,73,73,73	0
56	MG	DA	3164	1/1	0.88	0.16	87,87,87,87	0
56	MG	AA	1626	1/1	0.88	0.25	62,62,62,62	0
56	MG	AA	1789	1/1	0.88	0.12	77,77,77,77	0
56	MG	CA	1773	1/1	0.88	0.11	124,124,124,124	0
56	MG	DA	3554	1/1	0.88	0.19	49,49,49,49	0
56	MG	DA	3555	1/1	0.88	0.15	94,94,94,94	0
56	MG	AA	1848	1/1	0.88	0.21	71,71,71,71	0
56	MG	AA	1911	1/1	0.88	0.06	106,106,106,106	0
56	MG	CA	1778	1/1	0.88	0.27	81,81,81,81	0
56	MG	BA	3356	1/1	0.88	0.20	66,66,66,66	0
56	MG	DA	3583	1/1	0.88	0.08	96,96,96,96	0
56	MG	DA	3028	1/1	0.88	0.27	56,56,56,56	0
56	MG	DA	3310	1/1	0.88	0.29	72,72,72,72	0
56	MG	DA	3029	1/1	0.88	0.24	68,68,68,68	0
56	MG	DA	3033	1/1	0.88	0.20	74,74,74,74	0
56	MG	BA	3357	1/1	0.88	0.16	82,82,82,82	0
56	MG	DA	3611	1/1	0.88	0.11	80,80,80,80	0
56	MG	DA	3319	1/1	0.88	0.35	69,69,69,69	0
56	MG	DA	3325	1/1	0.88	0.29	62,62,62,62	0
56	MG	DA	3617	1/1	0.88	0.10	86,86,86,86	0
56	MG	BA	3217	1/1	0.88	0.14	38,38,38,38	0
56	MG	DA	3044	1/1	0.88	0.24	62,62,62,62	0
56	MG	DA	3338	1/1	0.88	0.24	69,69,69,69	0
56	MG	DA	3339	1/1	0.88	0.17	74,74,74,74	0
56	MG	BA	3533	1/1	0.88	0.12	61,61,61,61	0
56	MG	DA	3346	1/1	0.88	0.21	70,70,70,70	0
56	MG	DA	3051	1/1	0.88	0.09	60,60,60,60	0
56	MG	BA	3229	1/1	0.88	0.08	41,41,41,41	0
56	MG	DA	3647	1/1	0.88	0.20	70,70,70,70	0
56	MG	AA	1647	1/1	0.88	0.24	77,77,77,77	0
56	MG	AA	1658	1/1	0.88	0.34	73,73,73,73	0
56	MG	AA	1921	1/1	0.88	0.09	97,97,97,97	0
56	MG	DA	3062	1/1	0.88	0.15	65,65,65,65	0
56	MG	AA	1696	1/1	0.88	0.26	95,95,95,95	0
56	MG	DA	3066	1/1	0.88	0.36	68,68,68,68	0
56	MG	AA	1817	1/1	0.88	0.31	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3010	1/1	0.88	0.21	56,56,56,56	0
56	MG	BA	3888	1/1	0.88	0.07	99,99,99,99	0
56	MG	AA	1758	1/1	0.88	0.14	72,72,72,72	0
56	MG	DA	3219	1/1	0.88	0.17	67,67,67,67	0
56	MG	DA	3689	1/1	0.88	0.10	104,104,104,104	0
56	MG	DA	3220	1/1	0.88	0.11	83,83,83,83	0
56	MG	CA	1713	1/1	0.88	0.22	71,71,71,71	0
56	MG	CA	1802	1/1	0.88	0.08	115,115,115,115	0
56	MG	DB	201	1/1	0.88	0.25	61,61,61,61	0
56	MG	BA	3713	1/1	0.88	0.17	85,85,85,85	0
56	MG	AA	1719	1/1	0.88	0.11	70,70,70,70	0
56	MG	AA	1802	1/1	0.88	0.17	67,67,67,67	0
56	MG	BA	3737	1/1	0.88	0.10	60,60,60,60	0
56	MG	AA	1728	1/1	0.88	0.28	81,81,81,81	0
56	MG	BA	3283	1/1	0.88	0.08	47,47,47,47	0
56	MG	DA	3247	1/1	0.88	0.08	58,58,58,58	0
56	MG	AA	1615	1/1	0.88	0.15	75,75,75,75	0
56	MG	BX	101	1/1	0.88	0.65	78,78,78,78	0
56	MG	B2	101	1/1	0.88	0.25	63,63,63,63	0
56	MG	AA	1831	1/1	0.88	0.14	63,63,63,63	0
56	MG	CA	1818	1/1	0.88	0.10	87,87,87,87	0
56	MG	BA	3441	1/1	0.88	0.13	47,47,47,47	0
56	MG	DO	202	1/1	0.88	0.06	95,95,95,95	0
56	MG	DA	3471	1/1	0.88	0.14	87,87,87,87	0
56	MG	DV	201	1/1	0.88	0.11	62,62,62,62	0
56	MG	DA	3123	1/1	0.88	0.21	61,61,61,61	0
56	MG	DA	3125	1/1	0.88	0.15	65,65,65,65	0
56	MG	D5	101	1/1	0.88	0.23	62,62,62,62	0
56	MG	AA	1782	1/1	0.88	0.15	51,51,51,51	0
56	MG	AA	1835	1/1	0.88	0.14	88,88,88,88	0
56	MG	AA	1661	1/1	0.89	0.26	56,56,56,56	0
56	MG	DA	3499	1/1	0.89	0.12	68,68,68,68	0
56	MG	DA	3507	1/1	0.89	0.12	109,109,109,109	0
56	MG	DA	3099	1/1	0.89	0.20	42,42,42,42	0
56	MG	AA	1663	1/1	0.89	0.14	76,76,76,76	0
56	MG	DA	3113	1/1	0.89	0.17	59,59,59,59	0
56	MG	DA	3514	1/1	0.89	0.15	76,76,76,76	0
56	MG	BA	3365	1/1	0.89	0.14	69,69,69,69	0
56	MG	BB	206	1/1	0.89	0.23	61,61,61,61	0
56	MG	DA	3277	1/1	0.89	0.13	67,67,67,67	0
56	MG	AA	1908	1/1	0.89	0.14	97,97,97,97	0
56	MG	DA	3527	1/1	0.89	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1638	1/1	0.89	0.12	78,78,78,78	0
56	MG	CA	1686	1/1	0.89	0.08	72,72,72,72	0
56	MG	BB	217	1/1	0.89	0.17	80,80,80,80	0
56	MG	DA	3283	1/1	0.89	0.30	76,76,76,76	0
56	MG	BA	3387	1/1	0.89	0.20	48,48,48,48	0
56	MG	BB	222	1/1	0.89	0.16	70,70,70,70	0
56	MG	BA	3608	1/1	0.89	0.11	81,81,81,81	0
56	MG	AA	1874	1/1	0.89	0.20	95,95,95,95	0
56	MG	DA	3146	1/1	0.89	0.14	66,66,66,66	0
56	MG	BO	201	1/1	0.89	0.18	62,62,62,62	0
56	MG	BA	3072	1/1	0.89	0.33	48,48,48,48	0
56	MG	BA	3656	1/1	0.89	0.08	63,63,63,63	0
56	MG	DA	3560	1/1	0.89	0.13	64,64,64,64	0
56	MG	BA	3098	1/1	0.89	0.11	51,51,51,51	0
56	MG	DA	3567	1/1	0.89	0.19	77,77,77,77	0
56	MG	CA	1602	1/1	0.89	0.24	72,72,72,72	0
56	MG	BA	3262	1/1	0.89	0.18	57,57,57,57	0
56	MG	BA	3264	1/1	0.89	0.13	59,59,59,59	0
56	MG	BA	3716	1/1	0.89	0.16	40,40,40,40	0
56	MG	BA	3400	1/1	0.89	0.20	122,122,122,122	0
56	MG	CA	1608	1/1	0.89	0.35	80,80,80,80	0
56	MG	CV	102	1/1	0.89	0.19	85,85,85,85	0
56	MG	DA	3606	1/1	0.89	0.06	76,76,76,76	0
56	MG	CA	1610	1/1	0.89	0.22	63,63,63,63	0
56	MG	BA	3408	1/1	0.89	0.19	44,44,44,44	0
56	MG	DA	3174	1/1	0.89	0.27	68,68,68,68	0
56	MG	BA	3099	1/1	0.89	0.15	32,32,32,32	0
56	MG	BA	3419	1/1	0.89	0.25	62,62,62,62	0
56	MG	BA	3280	1/1	0.89	0.09	58,58,58,58	0
56	MG	AA	1769	1/1	0.89	0.15	84,84,84,84	0
56	MG	DA	3622	1/1	0.89	0.13	74,74,74,74	0
56	MG	CA	1714	1/1	0.89	0.11	74,74,74,74	0
56	MG	BA	3427	1/1	0.89	0.17	48,48,48,48	0
56	MG	BA	3776	1/1	0.89	0.30	68,68,68,68	0
56	MG	DA	3183	1/1	0.89	0.08	106,106,106,106	0
56	MG	AA	1636	1/1	0.89	0.36	65,65,65,65	0
56	MG	AA	1809	1/1	0.89	0.19	83,83,83,83	0
56	MG	BA	3436	1/1	0.89	0.19	70,70,70,70	0
56	MG	AA	1887	1/1	0.89	0.06	90,90,90,90	0
56	MG	DA	3655	1/1	0.89	0.10	75,75,75,75	0
56	MG	CA	1728	1/1	0.89	0.20	83,83,83,83	0
56	MG	DA	3198	1/1	0.89	0.31	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1731	1/1	0.89	0.21	84,84,84,84	0
56	MG	AA	1798	1/1	0.89	0.20	54,54,54,54	0
56	MG	CA	1636	1/1	0.89	0.34	50,50,50,50	0
56	MG	BA	3149	1/1	0.89	0.09	35,35,35,35	0
56	MG	DA	3204	1/1	0.89	0.08	76,76,76,76	0
56	MG	DA	3205	1/1	0.89	0.14	68,68,68,68	0
56	MG	CA	1738	1/1	0.89	0.10	98,98,98,98	0
56	MG	CA	1740	1/1	0.89	0.12	73,73,73,73	0
56	MG	BA	3153	1/1	0.89	0.13	56,56,56,56	0
56	MG	BA	3806	1/1	0.89	0.19	57,57,57,57	0
56	MG	BA	3448	1/1	0.89	0.08	60,60,60,60	0
56	MG	CA	1644	1/1	0.89	0.23	69,69,69,69	0
56	MG	BA	3158	1/1	0.89	0.14	48,48,48,48	0
56	MG	BA	3474	1/1	0.89	0.13	56,56,56,56	0
56	MG	BA	3322	1/1	0.89	0.28	54,54,54,54	0
56	MG	CA	1654	1/1	0.89	0.18	74,74,74,74	0
56	MG	DA	3382	1/1	0.89	0.26	72,72,72,72	0
56	MG	DA	3388	1/1	0.89	0.09	74,74,74,74	0
56	MG	AA	1931	1/1	0.89	0.07	103,103,103,103	0
56	MG	CA	1768	1/1	0.89	0.12	94,94,94,94	0
56	MG	BA	3327	1/1	0.89	0.20	80,80,80,80	0
56	MG	DA	3234	1/1	0.89	0.18	62,62,62,62	0
56	MG	BA	3329	1/1	0.89	0.24	85,85,85,85	0
56	MG	AA	1894	1/1	0.89	0.19	83,83,83,83	0
56	MG	DE	301	1/1	0.89	0.08	64,64,64,64	0
56	MG	BA	3488	1/1	0.89	0.18	35,35,35,35	0
56	MG	DF	301	1/1	0.89	0.13	71,71,71,71	0
56	MG	DA	3242	1/1	0.89	0.17	77,77,77,77	0
56	MG	AA	1825	1/1	0.89	0.27	64,64,64,64	0
56	MG	CA	1777	1/1	0.89	0.12	82,82,82,82	0
56	MG	BA	3002	1/1	0.89	0.13	65,65,65,65	0
56	MG	CA	1779	1/1	0.89	0.22	95,95,95,95	0
56	MG	BA	3228	1/1	0.89	0.29	59,59,59,59	0
56	MG	AA	1627	1/1	0.89	0.44	83,83,83,83	0
56	MG	BA	3511	1/1	0.89	0.22	48,48,48,48	0
56	MG	AA	1732	1/1	0.89	0.17	65,65,65,65	0
56	MG	AV	114	1/1	0.90	0.11	67,67,67,67	0
56	MG	DA	3034	1/1	0.90	0.19	77,77,77,77	0
56	MG	AA	1905	1/1	0.90	0.06	130,130,130,130	0
56	MG	BA	3746	1/1	0.90	0.18	77,77,77,77	0
56	MG	CA	1631	1/1	0.90	0.32	66,66,66,66	0
56	MG	CA	1632	1/1	0.90	0.20	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1843	1/1	0.90	0.08	73,73,73,73	0
56	MG	BA	3422	1/1	0.90	0.17	82,82,82,82	0
56	MG	CA	1741	1/1	0.90	0.12	92,92,92,92	0
56	MG	AA	1767	1/1	0.90	0.14	59,59,59,59	0
56	MG	BA	3017	1/1	0.90	0.11	64,64,64,64	0
56	MG	AA	1768	1/1	0.90	0.12	88,88,88,88	0
56	MG	BA	3433	1/1	0.90	0.15	30,30,30,30	0
56	MG	AA	1635	1/1	0.90	0.16	65,65,65,65	0
56	MG	DA	3244	1/1	0.90	0.13	64,64,64,64	0
56	MG	AA	1850	1/1	0.90	0.15	85,85,85,85	0
56	MG	AA	1744	1/1	0.90	0.15	68,68,68,68	0
56	MG	BA	3440	1/1	0.90	0.24	56,56,56,56	0
56	MG	CA	1646	1/1	0.90	0.13	73,73,73,73	0
56	MG	DA	3078	1/1	0.90	0.39	75,75,75,75	0
56	MG	CA	1766	1/1	0.90	0.08	106,106,106,106	0
56	MG	DA	3524	1/1	0.90	0.09	99,99,99,99	0
56	MG	BA	3284	1/1	0.90	0.10	41,41,41,41	0
56	MG	AA	1745	1/1	0.90	0.22	64,64,64,64	0
56	MG	CA	1652	1/1	0.90	0.23	75,75,75,75	0
56	MG	DA	3530	1/1	0.90	0.09	72,72,72,72	0
56	MG	AA	1855	1/1	0.90	0.17	80,80,80,80	0
56	MG	CA	1655	1/1	0.90	0.17	66,66,66,66	0
56	MG	DA	3270	1/1	0.90	0.14	70,70,70,70	0
56	MG	BA	3076	1/1	0.90	0.35	39,39,39,39	0
56	MG	BA	3457	1/1	0.90	0.08	59,59,59,59	0
56	MG	BA	3078	1/1	0.90	0.20	49,49,49,49	0
56	MG	DA	3276	1/1	0.90	0.17	63,63,63,63	0
56	MG	DA	3101	1/1	0.90	0.23	53,53,53,53	0
56	MG	DA	3107	1/1	0.90	0.11	58,58,58,58	0
56	MG	BA	3081	1/1	0.90	0.09	53,53,53,53	0
56	MG	DA	3112	1/1	0.90	0.20	61,61,61,61	0
56	MG	DA	3559	1/1	0.90	0.18	76,76,76,76	0
56	MG	DA	3281	1/1	0.90	0.16	70,70,70,70	0
56	MG	BA	3314	1/1	0.90	0.23	65,65,65,65	0
56	MG	DA	3566	1/1	0.90	0.10	84,84,84,84	0
56	MG	CA	1663	1/1	0.90	0.30	63,63,63,63	0
56	MG	AA	1643	1/1	0.90	0.28	59,59,59,59	0
56	MG	DA	3574	1/1	0.90	0.14	53,53,53,53	0
56	MG	AA	1785	1/1	0.90	0.18	68,68,68,68	0
56	MG	BA	3482	1/1	0.90	0.07	73,73,73,73	0
56	MG	BA	3100	1/1	0.90	0.13	48,48,48,48	0
56	MG	CA	1672	1/1	0.90	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1710	1/1	0.90	0.23	76,76,76,76	0
56	MG	BA	3328	1/1	0.90	0.14	68,68,68,68	0
56	MG	DA	3603	1/1	0.90	0.12	100,100,100,100	0
56	MG	DA	3132	1/1	0.90	0.19	66,66,66,66	0
56	MG	DA	3136	1/1	0.90	0.40	67,67,67,67	0
56	MG	AA	1749	1/1	0.90	0.23	69,69,69,69	0
56	MG	DA	3142	1/1	0.90	0.19	50,50,50,50	0
56	MG	AA	1790	1/1	0.90	0.13	70,70,70,70	0
56	MG	AA	1948	1/1	0.90	0.07	88,88,88,88	0
56	MG	BA	3342	1/1	0.90	0.27	66,66,66,66	0
56	MG	BA	3121	1/1	0.90	0.13	40,40,40,40	0
56	MG	BA	3515	1/1	0.90	0.26	49,49,49,49	0
56	MG	BB	207	1/1	0.90	0.24	44,44,44,44	0
56	MG	BA	3522	1/1	0.90	0.09	62,62,62,62	0
56	MG	AA	1751	1/1	0.90	0.12	74,74,74,74	0
56	MG	DA	3160	1/1	0.90	0.22	69,69,69,69	0
56	MG	DA	3320	1/1	0.90	0.16	56,56,56,56	0
56	MG	DA	3633	1/1	0.90	0.18	62,62,62,62	0
56	MG	BB	210	1/1	0.90	0.10	53,53,53,53	0
56	MG	BA	3524	1/1	0.90	0.08	81,81,81,81	0
56	MG	DA	3334	1/1	0.90	0.20	83,83,83,83	0
56	MG	AA	1672	1/1	0.90	0.11	78,78,78,78	0
56	MG	AA	1822	1/1	0.90	0.19	77,77,77,77	0
56	MG	DA	3166	1/1	0.90	0.29	66,66,66,66	0
56	MG	AF	201	1/1	0.90	0.23	79,79,79,79	0
56	MG	DA	3345	1/1	0.90	0.09	67,67,67,67	0
56	MG	BB	230	1/1	0.90	0.13	56,56,56,56	0
56	MG	DA	3671	1/1	0.90	0.08	92,92,92,92	0
56	MG	AA	1681	1/1	0.90	0.13	91,91,91,91	0
56	MG	CA	1817	1/1	0.90	0.11	111,111,111,111	0
56	MG	DA	3349	1/1	0.90	0.17	72,72,72,72	0
56	MG	BG	201	1/1	0.90	0.18	54,54,54,54	0
56	MG	CT	201	1/1	0.90	0.13	67,67,67,67	0
56	MG	AA	1608	1/1	0.90	0.21	80,80,80,80	0
56	MG	BP	202	1/1	0.90	0.07	62,62,62,62	0
56	MG	DA	3361	1/1	0.90	0.14	60,60,60,60	0
56	MG	BA	3600	1/1	0.90	0.15	36,36,36,36	0
56	MG	AA	1667	1/1	0.90	0.08	71,71,71,71	0
56	MG	DA	3181	1/1	0.90	0.23	59,59,59,59	0
56	MG	BA	3211	1/1	0.90	0.17	46,46,46,46	0
56	MG	DA	3001	1/1	0.90	0.15	58,58,58,58	0
56	MG	AA	1717	1/1	0.90	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3648	1/1	0.90	0.10	49,49,49,49	0
56	MG	BA	3651	1/1	0.90	0.08	49,49,49,49	0
56	MG	DA	3188	1/1	0.90	0.17	77,77,77,77	0
56	MG	AV	105	1/1	0.90	0.24	64,64,64,64	0
56	MG	DA	3196	1/1	0.90	0.15	77,77,77,77	0
56	MG	BA	3392	1/1	0.90	0.26	54,54,54,54	0
56	MG	AA	1833	1/1	0.90	0.14	70,70,70,70	0
56	MG	DD	304	1/1	0.90	0.22	65,65,65,65	0
56	MG	AA	1899	1/1	0.90	0.08	115,115,115,115	0
56	MG	DE	303	1/1	0.90	0.23	63,63,63,63	0
56	MG	AA	1761	1/1	0.90	0.15	58,58,58,58	0
56	MG	AA	1762	1/1	0.90	0.09	74,74,74,74	0
56	MG	BA	3719	1/1	0.90	0.12	71,71,71,71	0
56	MG	DA	3383	1/1	0.90	0.21	76,76,76,76	0
56	MG	DT	203	1/1	0.90	0.28	73,73,73,73	0
56	MG	DA	3018	1/1	0.90	0.22	51,51,51,51	0
56	MG	DA	3019	1/1	0.90	0.20	65,65,65,65	0
56	MG	AA	1676	1/1	0.90	0.45	72,72,72,72	0
56	MG	AA	1842	1/1	0.90	0.18	89,89,89,89	0
56	MG	BA	3411	1/1	0.90	0.17	55,55,55,55	0
56	MG	D6	102	1/1	0.90	0.15	82,82,82,82	0
56	MG	CA	1727	1/1	0.90	0.12	74,74,74,74	0
57	ZN	CN	101	1/1	0.90	0.10	165,165,165,165	0
56	MG	DA	3460	1/1	0.90	0.15	67,67,67,67	0
56	MG	DA	3454	1/1	0.91	0.17	91,91,91,91	0
56	MG	BA	3095	1/1	0.91	0.17	48,48,48,48	0
56	MG	AA	1888	1/1	0.91	0.08	97,97,97,97	0
56	MG	AA	1892	1/1	0.91	0.07	84,84,84,84	0
56	MG	DA	3032	1/1	0.91	0.14	51,51,51,51	0
56	MG	DA	3211	1/1	0.91	0.23	83,83,83,83	0
56	MG	AA	1640	1/1	0.91	0.20	43,43,43,43	0
56	MG	DA	3474	1/1	0.91	0.11	76,76,76,76	0
56	MG	AA	1630	1/1	0.91	0.28	98,98,98,98	0
56	MG	BA	3728	1/1	0.91	0.14	68,68,68,68	0
56	MG	AA	1797	1/1	0.91	0.22	65,65,65,65	0
56	MG	DA	3222	1/1	0.91	0.23	73,73,73,73	0
56	MG	CA	1725	1/1	0.91	0.14	79,79,79,79	0
56	MG	AA	1845	1/1	0.91	0.19	59,59,59,59	0
56	MG	CA	1613	1/1	0.91	0.20	75,75,75,75	0
56	MG	DA	3230	1/1	0.91	0.10	68,68,68,68	0
56	MG	BA	3313	1/1	0.91	0.17	66,66,66,66	0
56	MG	DA	3053	1/1	0.91	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1818	1/1	0.91	0.17	73,73,73,73	0
56	MG	CA	1734	1/1	0.91	0.14	80,80,80,80	0
56	MG	AV	103	1/1	0.91	0.20	53,53,53,53	0
56	MG	BA	3445	1/1	0.91	0.19	68,68,68,68	0
56	MG	DA	3064	1/1	0.91	0.09	66,66,66,66	0
56	MG	DA	3243	1/1	0.91	0.25	78,78,78,78	0
56	MG	AA	1625	1/1	0.91	0.18	69,69,69,69	0
56	MG	BA	3144	1/1	0.91	0.12	34,34,34,34	0
56	MG	DA	3249	1/1	0.91	0.20	55,55,55,55	0
56	MG	BA	3775	1/1	0.91	0.11	74,74,74,74	0
56	MG	BA	3454	1/1	0.91	0.13	58,58,58,58	0
56	MG	CA	1743	1/1	0.91	0.29	86,86,86,86	0
56	MG	BA	3455	1/1	0.91	0.20	22,22,22,22	0
56	MG	AV	106	1/1	0.91	0.25	68,68,68,68	0
56	MG	BA	3779	1/1	0.91	0.14	80,80,80,80	0
56	MG	DA	3260	1/1	0.91	0.15	71,71,71,71	0
56	MG	DA	3261	1/1	0.91	0.19	69,69,69,69	0
56	MG	DA	3547	1/1	0.91	0.10	83,83,83,83	0
56	MG	AA	1772	1/1	0.91	0.11	77,77,77,77	0
56	MG	CA	1756	1/1	0.91	0.26	84,84,84,84	0
56	MG	DA	3266	1/1	0.91	0.14	62,62,62,62	0
56	MG	BA	3469	1/1	0.91	0.23	77,77,77,77	0
56	MG	BA	3793	1/1	0.91	0.16	69,69,69,69	0
56	MG	DA	3088	1/1	0.91	0.07	73,73,73,73	0
56	MG	CA	1637	1/1	0.91	0.21	80,80,80,80	0
56	MG	BA	3154	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3155	1/1	0.91	0.24	58,58,58,58	0
56	MG	AA	1754	1/1	0.91	0.21	59,59,59,59	0
56	MG	DA	3100	1/1	0.91	0.20	45,45,45,45	0
56	MG	BA	3801	1/1	0.91	0.21	93,93,93,93	0
56	MG	DA	3578	1/1	0.91	0.14	50,50,50,50	0
56	MG	DA	3102	1/1	0.91	0.14	60,60,60,60	0
56	MG	DA	3580	1/1	0.91	0.09	76,76,76,76	0
56	MG	DA	3582	1/1	0.91	0.11	85,85,85,85	0
56	MG	BA	3477	1/1	0.91	0.23	45,45,45,45	0
56	MG	BA	3479	1/1	0.91	0.20	63,63,63,63	0
56	MG	DA	3587	1/1	0.91	0.09	86,86,86,86	0
56	MG	AA	1776	1/1	0.91	0.17	89,89,89,89	0
56	MG	BA	3812	1/1	0.91	0.08	87,87,87,87	0
56	MG	DA	3596	1/1	0.91	0.12	67,67,67,67	0
56	MG	BA	3352	1/1	0.91	0.27	68,68,68,68	0
56	MG	BA	3187	1/1	0.91	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1653	1/1	0.91	0.15	78,78,78,78	0
56	MG	DA	3118	1/1	0.91	0.21	50,50,50,50	0
56	MG	DA	3609	1/1	0.91	0.08	75,75,75,75	0
56	MG	BA	3828	1/1	0.91	0.05	99,99,99,99	0
56	MG	AA	1646	1/1	0.91	0.28	64,64,64,64	0
56	MG	CA	1656	1/1	0.91	0.45	77,77,77,77	0
56	MG	DA	3124	1/1	0.91	0.29	50,50,50,50	0
56	MG	CA	1657	1/1	0.91	0.12	64,64,64,64	0
56	MG	AA	1706	1/1	0.91	0.18	62,62,62,62	0
56	MG	DA	3129	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3849	1/1	0.91	0.07	83,83,83,83	0
56	MG	DA	3135	1/1	0.91	0.20	66,66,66,66	0
56	MG	AA	1826	1/1	0.91	0.20	63,63,63,63	0
56	MG	DA	3138	1/1	0.91	0.27	58,58,58,58	0
56	MG	BA	3492	1/1	0.91	0.23	61,61,61,61	0
56	MG	CA	1791	1/1	0.91	0.17	85,85,85,85	0
56	MG	DA	3312	1/1	0.91	0.10	52,52,52,52	0
56	MG	AA	1914	1/1	0.91	0.06	104,104,104,104	0
56	MG	BA	3001	1/1	0.91	0.08	35,35,35,35	0
56	MG	AA	1619	1/1	0.91	0.33	68,68,68,68	0
56	MG	BA	3874	1/1	0.91	0.09	90,90,90,90	0
56	MG	AA	1828	1/1	0.91	0.09	70,70,70,70	0
56	MG	BA	3373	1/1	0.91	0.23	69,69,69,69	0
56	MG	DA	3153	1/1	0.91	0.45	66,66,66,66	0
56	MG	BA	3234	1/1	0.91	0.21	43,43,43,43	0
56	MG	AA	1786	1/1	0.91	0.28	69,69,69,69	0
56	MG	DA	3159	1/1	0.91	0.13	66,66,66,66	0
56	MG	BA	3889	1/1	0.91	0.08	80,80,80,80	0
56	MG	AA	1866	1/1	0.91	0.22	86,86,86,86	0
56	MG	BA	3895	1/1	0.91	0.08	78,78,78,78	0
56	MG	BA	3389	1/1	0.91	0.33	38,38,38,38	0
56	MG	CA	1679	1/1	0.91	0.16	65,65,65,65	0
56	MG	AA	1868	1/1	0.91	0.21	62,62,62,62	0
56	MG	DA	3691	1/1	0.91	0.09	91,91,91,91	0
56	MG	DA	3352	1/1	0.91	0.21	68,68,68,68	0
56	MG	BB	204	1/1	0.91	0.16	57,57,57,57	0
56	MG	BA	3032	1/1	0.91	0.10	45,45,45,45	0
56	MG	BA	3568	1/1	0.91	0.12	70,70,70,70	0
56	MG	BA	3578	1/1	0.91	0.15	68,68,68,68	0
56	MG	AA	1873	1/1	0.91	0.16	60,60,60,60	0
56	MG	AA	1607	1/1	0.91	0.18	44,44,44,44	0
56	MG	BA	3592	1/1	0.91	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1875	1/1	0.91	0.17	59,59,59,59	0
56	MG	BA	3260	1/1	0.91	0.25	60,60,60,60	0
56	MG	BA	3607	1/1	0.91	0.24	59,59,59,59	0
56	MG	CV	110	1/1	0.91	0.06	100,100,100,100	0
56	MG	AA	1616	1/1	0.91	0.18	65,65,65,65	0
56	MG	CA	1698	1/1	0.91	0.40	114,114,114,114	0
56	MG	DA	3370	1/1	0.91	0.27	67,67,67,67	0
56	MG	BD	302	1/1	0.91	0.15	51,51,51,51	0
56	MG	BF	304	1/1	0.91	0.13	44,44,44,44	0
56	MG	BA	3614	1/1	0.91	0.21	58,58,58,58	0
56	MG	AA	1654	1/1	0.91	0.19	80,80,80,80	0
56	MG	DF	303	1/1	0.91	0.11	77,77,77,77	0
56	MG	DA	3189	1/1	0.91	0.21	63,63,63,63	0
56	MG	BA	3629	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3193	1/1	0.91	0.20	67,67,67,67	0
56	MG	BP	201	1/1	0.91	0.20	33,33,33,33	0
56	MG	AA	1943	1/1	0.91	0.14	92,92,92,92	0
56	MG	DX	101	1/1	0.91	0.10	55,55,55,55	0
56	MG	BQ	203	1/1	0.91	0.10	62,62,62,62	0
56	MG	BU	201	1/1	0.91	0.14	38,38,38,38	0
56	MG	D1	101	1/1	0.91	0.24	61,61,61,61	0
56	MG	BA	3274	1/1	0.91	0.07	35,35,35,35	0
56	MG	AA	1837	1/1	0.91	0.09	66,66,66,66	0
56	MG	D7	101	1/1	0.91	0.24	63,63,63,63	0
56	MG	B2	102	1/1	0.91	0.12	66,66,66,66	0
56	MG	DA	3020	1/1	0.91	0.29	75,75,75,75	0
56	MG	AA	1748	1/1	0.91	0.12	90,90,90,90	0
56	MG	DA	3079	1/1	0.92	0.12	57,57,57,57	0
56	MG	AA	1882	1/1	0.92	0.06	55,55,55,55	0
56	MG	AA	1849	1/1	0.92	0.13	59,59,59,59	0
56	MG	AA	1641	1/1	0.92	0.18	44,44,44,44	0
56	MG	AA	1668	1/1	0.92	0.16	65,65,65,65	0
56	MG	DA	3483	1/1	0.92	0.07	84,84,84,84	0
56	MG	BA	3529	1/1	0.92	0.12	49,49,49,49	0
56	MG	DA	3489	1/1	0.92	0.07	68,68,68,68	0
56	MG	AA	1682	1/1	0.92	0.11	118,118,118,118	0
56	MG	AA	1614	1/1	0.92	0.20	72,72,72,72	0
56	MG	BA	3272	1/1	0.92	0.05	72,72,72,72	0
56	MG	DA	3252	1/1	0.92	0.14	58,58,58,58	0
56	MG	AA	1936	1/1	0.92	0.09	84,84,84,84	0
56	MG	BA	3571	1/1	0.92	0.07	31,31,31,31	0
56	MG	BA	3576	1/1	0.92	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1791	1/1	0.92	0.16	99,99,99,99	0
56	MG	BA	3413	1/1	0.92	0.19	58,58,58,58	0
56	MG	DA	3104	1/1	0.92	0.26	60,60,60,60	0
56	MG	BA	3589	1/1	0.92	0.08	38,38,38,38	0
56	MG	AV	118	1/1	0.92	0.06	83,83,83,83	0
56	MG	DA	3262	1/1	0.92	0.24	67,67,67,67	0
56	MG	DA	3111	1/1	0.92	0.15	51,51,51,51	0
56	MG	CA	1665	1/1	0.92	0.11	64,64,64,64	0
56	MG	BA	3417	1/1	0.92	0.31	44,44,44,44	0
56	MG	DA	3267	1/1	0.92	0.17	66,66,66,66	0
56	MG	BA	3593	1/1	0.92	0.09	54,54,54,54	0
56	MG	CA	1670	1/1	0.92	0.15	69,69,69,69	0
56	MG	BA	3122	1/1	0.92	0.23	56,56,56,56	0
56	MG	BA	3125	1/1	0.92	0.19	48,48,48,48	0
56	MG	AA	1665	1/1	0.92	0.31	73,73,73,73	0
56	MG	DA	3273	1/1	0.92	0.25	62,62,62,62	0
56	MG	DA	3545	1/1	0.92	0.08	83,83,83,83	0
56	MG	AA	1691	1/1	0.92	0.29	121,121,121,121	0
56	MG	BA	3613	1/1	0.92	0.11	40,40,40,40	0
56	MG	BB	214	1/1	0.92	0.11	51,51,51,51	0
56	MG	AA	1692	1/1	0.92	0.20	67,67,67,67	0
56	MG	BA	3428	1/1	0.92	0.11	63,63,63,63	0
56	MG	CA	1681	1/1	0.92	0.23	70,70,70,70	0
56	MG	AA	1777	1/1	0.92	0.18	61,61,61,61	0
56	MG	DA	3133	1/1	0.92	0.25	51,51,51,51	0
56	MG	DA	3563	1/1	0.92	0.09	73,73,73,73	0
56	MG	DA	3134	1/1	0.92	0.20	61,61,61,61	0
56	MG	BA	3301	1/1	0.92	0.20	70,70,70,70	0
56	MG	DA	3285	1/1	0.92	0.22	62,62,62,62	0
56	MG	DA	3568	1/1	0.92	0.09	82,82,82,82	0
56	MG	AA	1778	1/1	0.92	0.26	83,83,83,83	0
56	MG	BA	3020	1/1	0.92	0.08	44,44,44,44	0
56	MG	DA	3575	1/1	0.92	0.13	65,65,65,65	0
56	MG	DA	3576	1/1	0.92	0.13	75,75,75,75	0
56	MG	AA	1779	1/1	0.92	0.15	60,60,60,60	0
56	MG	BA	3680	1/1	0.92	0.07	46,46,46,46	0
56	MG	DA	3291	1/1	0.92	0.16	50,50,50,50	0
56	MG	DA	3292	1/1	0.92	0.17	69,69,69,69	0
56	MG	BA	3693	1/1	0.92	0.06	38,38,38,38	0
56	MG	BA	3171	1/1	0.92	0.21	38,38,38,38	0
56	MG	BA	3172	1/1	0.92	0.21	44,44,44,44	0
56	MG	AA	1734	1/1	0.92	0.08	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1801	1/1	0.92	0.23	65,65,65,65	0
56	MG	AA	1735	1/1	0.92	0.41	84,84,84,84	0
56	MG	DA	3302	1/1	0.92	0.17	76,76,76,76	0
56	MG	DA	3601	1/1	0.92	0.10	53,53,53,53	0
56	MG	CV	101	1/1	0.92	0.23	59,59,59,59	0
56	MG	DA	3154	1/1	0.92	0.17	65,65,65,65	0
56	MG	AA	1613	1/1	0.92	0.37	68,68,68,68	0
56	MG	DA	3308	1/1	0.92	0.11	60,60,60,60	0
56	MG	B0	102	1/1	0.92	0.05	50,50,50,50	0
56	MG	BA	3453	1/1	0.92	0.31	63,63,63,63	0
56	MG	DA	3615	1/1	0.92	0.07	77,77,77,77	0
56	MG	CV	107	1/1	0.92	0.18	70,70,70,70	0
56	MG	BA	3194	1/1	0.92	0.31	70,70,70,70	0
56	MG	B3	101	1/1	0.92	0.17	57,57,57,57	0
56	MG	B5	102	1/1	0.92	0.10	58,58,58,58	0
56	MG	BA	3333	1/1	0.92	0.25	58,58,58,58	0
56	MG	BA	3199	1/1	0.92	0.18	29,29,29,29	0
56	MG	BA	3461	1/1	0.92	0.14	58,58,58,58	0
56	MG	BA	3744	1/1	0.92	0.21	44,44,44,44	0
56	MG	BA	3209	1/1	0.92	0.15	25,25,25,25	0
56	MG	CA	1709	1/1	0.92	0.32	82,82,82,82	0
56	MG	DA	3336	1/1	0.92	0.32	71,71,71,71	0
56	MG	BA	3344	1/1	0.92	0.16	62,62,62,62	0
56	MG	DA	3639	1/1	0.92	0.14	82,82,82,82	0
56	MG	DA	3645	1/1	0.92	0.13	93,93,93,93	0
56	MG	BA	3470	1/1	0.92	0.15	52,52,52,52	0
56	MG	DA	3341	1/1	0.92	0.15	60,60,60,60	0
56	MG	DA	3342	1/1	0.92	0.19	70,70,70,70	0
56	MG	BA	3770	1/1	0.92	0.11	49,49,49,49	0
56	MG	BA	3772	1/1	0.92	0.07	26,26,26,26	0
56	MG	BA	3472	1/1	0.92	0.18	58,58,58,58	0
56	MG	BA	3345	1/1	0.92	0.20	74,74,74,74	0
56	MG	BA	3050	1/1	0.92	0.13	60,60,60,60	0
56	MG	AA	1804	1/1	0.92	0.13	115,115,115,115	0
56	MG	BA	3222	1/1	0.92	0.21	28,28,28,28	0
56	MG	DA	3353	1/1	0.92	0.11	80,80,80,80	0
56	MG	DA	3676	1/1	0.92	0.16	94,94,94,94	0
56	MG	DA	3024	1/1	0.92	0.17	60,60,60,60	0
56	MG	DA	3681	1/1	0.92	0.08	71,71,71,71	0
56	MG	BA	3780	1/1	0.92	0.12	86,86,86,86	0
56	MG	BA	3223	1/1	0.92	0.10	59,59,59,59	0
56	MG	DA	3357	1/1	0.92	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3358	1/1	0.92	0.08	60,60,60,60	0
56	MG	CA	1624	1/1	0.92	0.24	64,64,64,64	0
56	MG	DA	3692	1/1	0.92	0.11	46,46,46,46	0
56	MG	CA	1625	1/1	0.92	0.24	71,71,71,71	0
56	MG	DA	3694	1/1	0.92	0.06	95,95,95,95	0
56	MG	CA	1628	1/1	0.92	0.28	51,51,51,51	0
56	MG	CA	1732	1/1	0.92	0.12	81,81,81,81	0
56	MG	DA	3194	1/1	0.92	0.32	65,65,65,65	0
56	MG	BA	3058	1/1	0.92	0.09	46,46,46,46	0
56	MG	DA	3036	1/1	0.92	0.19	57,57,57,57	0
56	MG	BA	3359	1/1	0.92	0.14	72,72,72,72	0
56	MG	AA	1881	1/1	0.92	0.15	50,50,50,50	0
56	MG	AA	1918	1/1	0.92	0.07	68,68,68,68	0
56	MG	AV	104	1/1	0.92	0.30	81,81,81,81	0
56	MG	BA	3369	1/1	0.92	0.12	65,65,65,65	0
56	MG	AA	1919	1/1	0.92	0.15	63,63,63,63	0
56	MG	DA	3055	1/1	0.92	0.16	57,57,57,57	0
56	MG	BA	3496	1/1	0.92	0.18	61,61,61,61	0
56	MG	BA	3498	1/1	0.92	0.10	54,54,54,54	0
56	MG	DA	3059	1/1	0.92	0.11	67,67,67,67	0
56	MG	DA	3209	1/1	0.92	0.19	89,89,89,89	0
56	MG	BA	3082	1/1	0.92	0.10	45,45,45,45	0
56	MG	BA	3819	1/1	0.92	0.08	71,71,71,71	0
56	MG	BA	3083	1/1	0.92	0.11	48,48,48,48	0
56	MG	DA	3386	1/1	0.92	0.14	47,47,47,47	0
56	MG	BA	3087	1/1	0.92	0.12	77,77,77,77	0
56	MG	CA	1754	1/1	0.92	0.20	70,70,70,70	0
56	MG	DA	3067	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3221	1/1	0.92	0.10	82,82,82,82	0
56	MG	CA	1755	1/1	0.92	0.07	93,93,93,93	0
56	MG	DA	3070	1/1	0.92	0.17	74,74,74,74	0
56	MG	BA	3505	1/1	0.92	0.08	64,64,64,64	0
56	MG	BA	3509	1/1	0.92	0.20	54,54,54,54	0
56	MG	DA	3461	1/1	0.92	0.17	50,50,50,50	0
56	MG	DA	3229	1/1	0.92	0.19	52,52,52,52	0
56	MG	BA	3090	1/1	0.92	0.19	46,46,46,46	0
56	MG	DA	3469	1/1	0.92	0.11	84,84,84,84	0
56	MG	DA	3077	1/1	0.92	0.25	74,74,74,74	0
56	MG	CA	1648	1/1	0.92	0.30	73,73,73,73	0
56	MG	DA	3021	1/1	0.93	0.17	58,58,58,58	0
56	MG	DA	3441	1/1	0.93	0.09	72,72,72,72	0
56	MG	DA	3443	1/1	0.93	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BB	211	1/1	0.93	0.23	66,66,66,66	0
56	MG	DA	3453	1/1	0.93	0.07	77,77,77,77	0
56	MG	BA	3416	1/1	0.93	0.15	58,58,58,58	0
56	MG	DA	3456	1/1	0.93	0.11	56,56,56,56	0
56	MG	BA	3132	1/1	0.93	0.16	44,44,44,44	0
56	MG	DA	3027	1/1	0.93	0.28	72,72,72,72	0
56	MG	BA	3418	1/1	0.93	0.24	59,59,59,59	0
56	MG	DA	3215	1/1	0.93	0.23	46,46,46,46	0
56	MG	AA	1660	1/1	0.93	0.19	59,59,59,59	0
56	MG	DA	3470	1/1	0.93	0.11	73,73,73,73	0
56	MG	BA	3137	1/1	0.93	0.23	55,55,55,55	0
56	MG	BA	3421	1/1	0.93	0.30	75,75,75,75	0
56	MG	BA	3142	1/1	0.93	0.24	44,44,44,44	0
56	MG	BE	303	1/1	0.93	0.08	32,32,32,32	0
56	MG	BF	301	1/1	0.93	0.09	40,40,40,40	0
56	MG	AA	1793	1/1	0.93	0.17	72,72,72,72	0
56	MG	DA	3041	1/1	0.93	0.32	54,54,54,54	0
56	MG	BA	3148	1/1	0.93	0.15	50,50,50,50	0
56	MG	AA	1707	1/1	0.93	0.26	64,64,64,64	0
56	MG	DA	3231	1/1	0.93	0.12	74,74,74,74	0
56	MG	DA	3490	1/1	0.93	0.17	45,45,45,45	0
56	MG	BA	3045	1/1	0.93	0.08	35,35,35,35	0
56	MG	BA	3431	1/1	0.93	0.23	75,75,75,75	0
56	MG	CA	1712	1/1	0.93	0.21	83,83,83,83	0
56	MG	BA	3293	1/1	0.93	0.06	45,45,45,45	0
56	MG	BA	3658	1/1	0.93	0.16	44,44,44,44	0
56	MG	DA	3057	1/1	0.93	0.25	66,66,66,66	0
56	MG	CA	1715	1/1	0.93	0.08	66,66,66,66	0
56	MG	BA	3659	1/1	0.93	0.09	60,60,60,60	0
56	MG	AA	1852	1/1	0.93	0.10	93,93,93,93	0
56	MG	DA	3061	1/1	0.93	0.34	78,78,78,78	0
56	MG	BA	3297	1/1	0.93	0.13	53,53,53,53	0
56	MG	B1	103	1/1	0.93	0.13	36,36,36,36	0
56	MG	CA	1721	1/1	0.93	0.11	75,75,75,75	0
56	MG	AA	1708	1/1	0.93	0.21	79,79,79,79	0
56	MG	BA	3157	1/1	0.93	0.20	42,42,42,42	0
56	MG	CA	1724	1/1	0.93	0.09	88,88,88,88	0
56	MG	BA	3302	1/1	0.93	0.07	53,53,53,53	0
56	MG	BA	3051	1/1	0.93	0.21	41,41,41,41	0
56	MG	B8	101	1/1	0.93	0.14	49,49,49,49	0
56	MG	BA	3162	1/1	0.93	0.16	36,36,36,36	0
56	MG	BA	3724	1/1	0.93	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3166	1/1	0.93	0.18	30,30,30,30	0
56	MG	BA	3053	1/1	0.93	0.11	44,44,44,44	0
56	MG	BA	3450	1/1	0.93	0.11	42,42,42,42	0
56	MG	BA	3452	1/1	0.93	0.09	55,55,55,55	0
56	MG	CA	1607	1/1	0.93	0.11	73,73,73,73	0
56	MG	CA	1739	1/1	0.93	0.13	79,79,79,79	0
56	MG	DA	3085	1/1	0.93	0.18	64,64,64,64	0
56	MG	AA	1920	1/1	0.93	0.10	86,86,86,86	0
56	MG	CA	1609	1/1	0.93	0.15	70,70,70,70	0
56	MG	DA	3558	1/1	0.93	0.22	59,59,59,59	0
56	MG	DA	3090	1/1	0.93	0.33	76,76,76,76	0
56	MG	BA	3174	1/1	0.93	0.24	62,62,62,62	0
56	MG	DA	3275	1/1	0.93	0.23	42,42,42,42	0
56	MG	BA	3181	1/1	0.93	0.28	69,69,69,69	0
56	MG	BA	3456	1/1	0.93	0.13	73,73,73,73	0
56	MG	BA	3753	1/1	0.93	0.18	31,31,31,31	0
56	MG	CA	1615	1/1	0.93	0.19	74,74,74,74	0
56	MG	CA	1616	1/1	0.93	0.30	54,54,54,54	0
56	MG	AA	1832	1/1	0.93	0.20	75,75,75,75	0
56	MG	BA	3458	1/1	0.93	0.24	44,44,44,44	0
56	MG	DA	3106	1/1	0.93	0.24	48,48,48,48	0
56	MG	DA	3577	1/1	0.93	0.07	95,95,95,95	0
56	MG	BA	3063	1/1	0.93	0.11	53,53,53,53	0
56	MG	AA	1757	1/1	0.93	0.13	58,58,58,58	0
56	MG	BA	3192	1/1	0.93	0.15	53,53,53,53	0
56	MG	CA	1761	1/1	0.93	0.18	68,68,68,68	0
56	MG	BA	3335	1/1	0.93	0.24	47,47,47,47	0
56	MG	BA	3471	1/1	0.93	0.12	49,49,49,49	0
56	MG	CA	1627	1/1	0.93	0.21	50,50,50,50	0
56	MG	AA	1609	1/1	0.93	0.27	61,61,61,61	0
56	MG	AA	1926	1/1	0.93	0.07	90,90,90,90	0
56	MG	BA	3195	1/1	0.93	0.17	19,19,19,19	0
56	MG	BA	3781	1/1	0.93	0.07	84,84,84,84	0
56	MG	CA	1774	1/1	0.93	0.12	111,111,111,111	0
56	MG	BA	3782	1/1	0.93	0.15	75,75,75,75	0
56	MG	BA	3784	1/1	0.93	0.12	88,88,88,88	0
56	MG	DA	3300	1/1	0.93	0.25	55,55,55,55	0
56	MG	DA	3301	1/1	0.93	0.23	62,62,62,62	0
56	MG	BA	3788	1/1	0.93	0.08	48,48,48,48	0
56	MG	BA	3196	1/1	0.93	0.25	66,66,66,66	0
56	MG	BA	3347	1/1	0.93	0.22	20,20,20,20	0
56	MG	AA	1662	1/1	0.93	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3307	1/1	0.93	0.09	65,65,65,65	0
56	MG	BA	3203	1/1	0.93	0.22	44,44,44,44	0
56	MG	CA	1783	1/1	0.93	0.07	78,78,78,78	0
56	MG	AA	1860	1/1	0.93	0.10	85,85,85,85	0
56	MG	DA	3623	1/1	0.93	0.08	85,85,85,85	0
56	MG	DA	3624	1/1	0.93	0.07	82,82,82,82	0
56	MG	CA	1640	1/1	0.93	0.16	72,72,72,72	0
56	MG	AA	1780	1/1	0.93	0.19	55,55,55,55	0
56	MG	DA	3627	1/1	0.93	0.06	81,81,81,81	0
56	MG	DA	3140	1/1	0.93	0.32	44,44,44,44	0
56	MG	AA	1639	1/1	0.93	0.27	74,74,74,74	0
56	MG	AA	1713	1/1	0.93	0.07	60,60,60,60	0
56	MG	BA	3362	1/1	0.93	0.18	51,51,51,51	0
56	MG	DA	3321	1/1	0.93	0.20	50,50,50,50	0
56	MG	DA	3636	1/1	0.93	0.10	78,78,78,78	0
56	MG	BA	3094	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3327	1/1	0.93	0.14	64,64,64,64	0
56	MG	DA	3329	1/1	0.93	0.24	63,63,63,63	0
56	MG	DA	3648	1/1	0.93	0.19	53,53,53,53	0
56	MG	DA	3649	1/1	0.93	0.08	73,73,73,73	0
56	MG	DA	3330	1/1	0.93	0.18	78,78,78,78	0
56	MG	CA	1792	1/1	0.93	0.08	82,82,82,82	0
56	MG	BA	3811	1/1	0.93	0.07	85,85,85,85	0
56	MG	BA	3494	1/1	0.93	0.10	62,62,62,62	0
56	MG	BA	3225	1/1	0.93	0.14	46,46,46,46	0
56	MG	DA	3337	1/1	0.93	0.08	65,65,65,65	0
56	MG	AA	1664	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3823	1/1	0.93	0.09	78,78,78,78	0
56	MG	AA	1941	1/1	0.93	0.07	94,94,94,94	0
56	MG	BA	3827	1/1	0.93	0.06	77,77,77,77	0
56	MG	AA	1671	1/1	0.93	0.09	94,94,94,94	0
56	MG	DA	3161	1/1	0.93	0.15	45,45,45,45	0
56	MG	BA	3833	1/1	0.93	0.08	41,41,41,41	0
56	MG	BA	3835	1/1	0.93	0.16	86,86,86,86	0
56	MG	BA	3837	1/1	0.93	0.09	33,33,33,33	0
56	MG	DA	3688	1/1	0.93	0.07	80,80,80,80	0
56	MG	BA	3841	1/1	0.93	0.15	91,91,91,91	0
56	MG	DA	3351	1/1	0.93	0.11	57,57,57,57	0
56	MG	AA	1904	1/1	0.93	0.05	118,118,118,118	0
56	MG	BA	3376	1/1	0.93	0.12	43,43,43,43	0
56	MG	DA	3168	1/1	0.93	0.30	53,53,53,53	0
56	MG	BA	3003	1/1	0.93	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3104	1/1	0.93	0.15	50,50,50,50	0
56	MG	BA	3512	1/1	0.93	0.20	56,56,56,56	0
56	MG	BA	3514	1/1	0.93	0.17	58,58,58,58	0
56	MG	CA	1668	1/1	0.93	0.14	59,59,59,59	0
56	MG	CD	302	1/1	0.93	0.15	53,53,53,53	0
56	MG	AA	1944	1/1	0.93	0.11	97,97,97,97	0
56	MG	BA	3516	1/1	0.93	0.20	56,56,56,56	0
56	MG	BA	3867	1/1	0.93	0.09	60,60,60,60	0
56	MG	BA	3870	1/1	0.93	0.08	100,100,100,100	0
56	MG	BA	3871	1/1	0.93	0.09	46,46,46,46	0
56	MG	BA	3517	1/1	0.93	0.16	58,58,58,58	0
56	MG	AA	1623	1/1	0.93	0.11	59,59,59,59	0
56	MG	CV	109	1/1	0.93	0.06	102,102,102,102	0
56	MG	DD	303	1/1	0.93	0.09	59,59,59,59	0
56	MG	BA	3879	1/1	0.93	0.11	53,53,53,53	0
56	MG	BA	3118	1/1	0.93	0.36	44,44,44,44	0
56	MG	BA	3251	1/1	0.93	0.16	51,51,51,51	0
56	MG	AA	1740	1/1	0.93	0.28	72,72,72,72	0
56	MG	AA	1770	1/1	0.93	0.10	76,76,76,76	0
56	MG	BA	3259	1/1	0.93	0.19	66,66,66,66	0
56	MG	AA	1912	1/1	0.93	0.06	106,106,106,106	0
56	MG	BA	3402	1/1	0.93	0.11	55,55,55,55	0
56	MG	BA	3405	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3406	1/1	0.93	0.12	64,64,64,64	0
56	MG	BA	3407	1/1	0.93	0.09	44,44,44,44	0
56	MG	CA	1690	1/1	0.93	0.27	74,74,74,74	0
56	MG	BA	3123	1/1	0.93	0.20	58,58,58,58	0
56	MG	DA	3392	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3393	1/1	0.93	0.15	63,63,63,63	0
56	MG	BA	3029	1/1	0.93	0.21	33,33,33,33	0
56	MG	BA	3265	1/1	0.93	0.07	67,67,67,67	0
56	MG	DA	3410	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3423	1/1	0.93	0.11	45,45,45,45	0
56	MG	DA	3424	1/1	0.93	0.11	72,72,72,72	0
56	MG	BA	3129	1/1	0.93	0.06	49,49,49,49	0
56	MG	BA	3273	1/1	0.94	0.09	63,63,63,63	0
56	MG	DA	3413	1/1	0.94	0.12	40,40,40,40	0
56	MG	DA	3414	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3415	1/1	0.94	0.28	33,33,33,33	0
56	MG	DA	3417	1/1	0.94	0.14	46,46,46,46	0
56	MG	CA	1685	1/1	0.94	0.21	64,64,64,64	0
56	MG	BA	3150	1/1	0.94	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3275	1/1	0.94	0.08	55,55,55,55	0
56	MG	AA	1907	1/1	0.94	0.09	78,78,78,78	0
56	MG	AA	1644	1/1	0.94	0.17	48,48,48,48	0
56	MG	DA	3442	1/1	0.94	0.10	56,56,56,56	0
56	MG	BA	3073	1/1	0.94	0.22	39,39,39,39	0
56	MG	AA	1910	1/1	0.94	0.08	87,87,87,87	0
56	MG	BA	3077	1/1	0.94	0.11	45,45,45,45	0
56	MG	BA	3159	1/1	0.94	0.12	43,43,43,43	0
56	MG	BA	3288	1/1	0.94	0.10	77,77,77,77	0
56	MG	CA	1696	1/1	0.94	0.12	99,99,99,99	0
56	MG	DA	3026	1/1	0.94	0.09	64,64,64,64	0
56	MG	DA	3464	1/1	0.94	0.10	82,82,82,82	0
56	MG	BA	3290	1/1	0.94	0.12	63,63,63,63	0
56	MG	DA	3218	1/1	0.94	0.13	71,71,71,71	0
56	MG	BB	213	1/1	0.94	0.09	58,58,58,58	0
56	MG	BA	3615	1/1	0.94	0.11	68,68,68,68	0
56	MG	DA	3031	1/1	0.94	0.15	49,49,49,49	0
56	MG	BA	3616	1/1	0.94	0.18	40,40,40,40	0
56	MG	DA	3223	1/1	0.94	0.23	70,70,70,70	0
56	MG	BB	218	1/1	0.94	0.14	57,57,57,57	0
56	MG	DA	3226	1/1	0.94	0.28	62,62,62,62	0
56	MG	DA	3476	1/1	0.94	0.11	71,71,71,71	0
56	MG	BA	3161	1/1	0.94	0.14	49,49,49,49	0
56	MG	AA	1763	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3635	1/1	0.94	0.16	75,75,75,75	0
56	MG	DA	3037	1/1	0.94	0.24	83,83,83,83	0
56	MG	BA	3642	1/1	0.94	0.13	78,78,78,78	0
56	MG	BD	301	1/1	0.94	0.07	65,65,65,65	0
56	MG	DA	3042	1/1	0.94	0.09	47,47,47,47	0
56	MG	BA	3647	1/1	0.94	0.09	61,61,61,61	0
56	MG	DA	3046	1/1	0.94	0.18	79,79,79,79	0
56	MG	DA	3237	1/1	0.94	0.16	61,61,61,61	0
56	MG	DA	3502	1/1	0.94	0.07	68,68,68,68	0
56	MG	DA	3504	1/1	0.94	0.07	94,94,94,94	0
56	MG	DA	3047	1/1	0.94	0.14	65,65,65,65	0
56	MG	BA	3296	1/1	0.94	0.06	43,43,43,43	0
56	MG	BA	3424	1/1	0.94	0.06	42,42,42,42	0
56	MG	BA	3426	1/1	0.94	0.07	46,46,46,46	0
56	MG	AA	1750	1/1	0.94	0.07	79,79,79,79	0
56	MG	DA	3246	1/1	0.94	0.18	48,48,48,48	0
56	MG	BA	3657	1/1	0.94	0.17	51,51,51,51	0
56	MG	AA	1945	1/1	0.94	0.08	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3251	1/1	0.94	0.14	62,62,62,62	0
56	MG	AA	1814	1/1	0.94	0.17	81,81,81,81	0
56	MG	BA	3661	1/1	0.94	0.16	53,53,53,53	0
56	MG	BQ	202	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3084	1/1	0.94	0.10	43,43,43,43	0
56	MG	BT	201	1/1	0.94	0.09	53,53,53,53	0
56	MG	BA	3683	1/1	0.94	0.06	31,31,31,31	0
56	MG	CA	1720	1/1	0.94	0.10	84,84,84,84	0
56	MG	DA	3536	1/1	0.94	0.20	54,54,54,54	0
56	MG	DA	3537	1/1	0.94	0.19	68,68,68,68	0
56	MG	BA	3303	1/1	0.94	0.11	51,51,51,51	0
56	MG	BA	3697	1/1	0.94	0.07	51,51,51,51	0
56	MG	B1	102	1/1	0.94	0.07	45,45,45,45	0
56	MG	DA	3263	1/1	0.94	0.32	67,67,67,67	0
56	MG	BA	3704	1/1	0.94	0.07	44,44,44,44	0
56	MG	DA	3548	1/1	0.94	0.08	72,72,72,72	0
56	MG	BA	3304	1/1	0.94	0.09	45,45,45,45	0
56	MG	AA	1815	1/1	0.94	0.11	69,69,69,69	0
56	MG	BA	3088	1/1	0.94	0.27	45,45,45,45	0
56	MG	CA	1729	1/1	0.94	0.10	80,80,80,80	0
56	MG	B5	101	1/1	0.94	0.09	50,50,50,50	0
56	MG	BA	3185	1/1	0.94	0.16	57,57,57,57	0
56	MG	B5	103	1/1	0.94	0.10	61,61,61,61	0
56	MG	B7	101	1/1	0.94	0.09	51,51,51,51	0
56	MG	BA	3316	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3089	1/1	0.94	0.29	54,54,54,54	0
56	MG	BA	3726	1/1	0.94	0.19	48,48,48,48	0
56	MG	AA	1700	1/1	0.94	0.10	116,116,116,116	0
56	MG	BA	3733	1/1	0.94	0.08	49,49,49,49	0
56	MG	DA	3087	1/1	0.94	0.13	40,40,40,40	0
56	MG	BA	3734	1/1	0.94	0.14	40,40,40,40	0
56	MG	DA	3089	1/1	0.94	0.10	82,82,82,82	0
56	MG	BA	3325	1/1	0.94	0.22	83,83,83,83	0
56	MG	AA	1730	1/1	0.94	0.15	61,61,61,61	0
56	MG	BA	3738	1/1	0.94	0.26	42,42,42,42	0
56	MG	DA	3095	1/1	0.94	0.20	41,41,41,41	0
56	MG	BA	3740	1/1	0.94	0.10	48,48,48,48	0
56	MG	BA	3449	1/1	0.94	0.21	34,34,34,34	0
56	MG	CA	1751	1/1	0.94	0.08	86,86,86,86	0
56	MG	CA	1611	1/1	0.94	0.13	74,74,74,74	0
56	MG	BA	3013	1/1	0.94	0.13	57,57,57,57	0
56	MG	BA	3097	1/1	0.94	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1836	1/1	0.94	0.14	59,59,59,59	0
56	MG	DA	3591	1/1	0.94	0.10	86,86,86,86	0
56	MG	DA	3592	1/1	0.94	0.06	69,69,69,69	0
56	MG	AI	201	1/1	0.94	0.34	66,66,66,66	0
56	MG	BA	3332	1/1	0.94	0.20	74,74,74,74	0
56	MG	DA	3110	1/1	0.94	0.26	60,60,60,60	0
56	MG	BA	3023	1/1	0.94	0.07	46,46,46,46	0
56	MG	DA	3605	1/1	0.94	0.07	101,101,101,101	0
56	MG	BA	3334	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3298	1/1	0.94	0.20	55,55,55,55	0
56	MG	CA	1764	1/1	0.94	0.07	75,75,75,75	0
56	MG	DA	3610	1/1	0.94	0.15	97,97,97,97	0
56	MG	BA	3765	1/1	0.94	0.08	59,59,59,59	0
56	MG	BA	3025	1/1	0.94	0.07	68,68,68,68	0
56	MG	BA	3460	1/1	0.94	0.14	52,52,52,52	0
56	MG	CA	1769	1/1	0.94	0.09	93,93,93,93	0
56	MG	BA	3337	1/1	0.94	0.09	51,51,51,51	0
56	MG	DA	3121	1/1	0.94	0.19	37,37,37,37	0
56	MG	BA	3204	1/1	0.94	0.27	52,52,52,52	0
56	MG	BA	3340	1/1	0.94	0.21	55,55,55,55	0
56	MG	BA	3205	1/1	0.94	0.23	43,43,43,43	0
56	MG	BA	3343	1/1	0.94	0.24	37,37,37,37	0
56	MG	BA	3206	1/1	0.94	0.18	31,31,31,31	0
56	MG	AA	1753	1/1	0.94	0.26	86,86,86,86	0
56	MG	DA	3316	1/1	0.94	0.15	80,80,80,80	0
56	MG	AA	1652	1/1	0.94	0.28	69,69,69,69	0
56	MG	BA	3350	1/1	0.94	0.07	69,69,69,69	0
56	MG	BA	3109	1/1	0.94	0.12	58,58,58,58	0
56	MG	AA	1712	1/1	0.94	0.13	72,72,72,72	0
56	MG	BA	3115	1/1	0.94	0.19	52,52,52,52	0
56	MG	DA	3322	1/1	0.94	0.21	52,52,52,52	0
56	MG	DA	3324	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3117	1/1	0.94	0.28	46,46,46,46	0
56	MG	DA	3326	1/1	0.94	0.13	62,62,62,62	0
56	MG	BA	3033	1/1	0.94	0.11	55,55,55,55	0
56	MG	AA	1631	1/1	0.94	0.20	59,59,59,59	0
56	MG	DA	3652	1/1	0.94	0.10	85,85,85,85	0
56	MG	DA	3653	1/1	0.94	0.13	59,59,59,59	0
56	MG	BA	3361	1/1	0.94	0.26	60,60,60,60	0
56	MG	DA	3143	1/1	0.94	0.18	50,50,50,50	0
56	MG	BA	3800	1/1	0.94	0.05	111,111,111,111	0
56	MG	BA	3037	1/1	0.94	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1643	1/1	0.94	0.20	53,53,53,53	0
56	MG	BA	3039	1/1	0.94	0.07	34,34,34,34	0
56	MG	BA	3041	1/1	0.94	0.07	43,43,43,43	0
56	MG	DA	3669	1/1	0.94	0.05	93,93,93,93	0
56	MG	BA	3495	1/1	0.94	0.12	56,56,56,56	0
56	MG	AV	101	1/1	0.94	0.22	48,48,48,48	0
56	MG	AA	1925	1/1	0.94	0.05	86,86,86,86	0
56	MG	DA	3155	1/1	0.94	0.16	56,56,56,56	0
56	MG	DA	3156	1/1	0.94	0.15	57,57,57,57	0
56	MG	CA	1650	1/1	0.94	0.24	61,61,61,61	0
56	MG	BA	3370	1/1	0.94	0.10	64,64,64,64	0
56	MG	CA	1801	1/1	0.94	0.09	83,83,83,83	0
56	MG	BA	3371	1/1	0.94	0.17	66,66,66,66	0
56	MG	DA	3350	1/1	0.94	0.12	72,72,72,72	0
56	MG	BA	3239	1/1	0.94	0.13	49,49,49,49	0
56	MG	AA	1673	1/1	0.94	0.20	74,74,74,74	0
56	MG	BA	3507	1/1	0.94	0.14	53,53,53,53	0
56	MG	CA	1807	1/1	0.94	0.05	100,100,100,100	0
56	MG	BA	3133	1/1	0.94	0.14	27,27,27,27	0
56	MG	BA	3379	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3381	1/1	0.94	0.26	19,19,19,19	0
56	MG	BA	3513	1/1	0.94	0.10	60,60,60,60	0
56	MG	DA	3359	1/1	0.94	0.08	59,59,59,59	0
56	MG	DA	3169	1/1	0.94	0.15	51,51,51,51	0
56	MG	BA	3249	1/1	0.94	0.20	24,24,24,24	0
56	MG	BA	3385	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3049	1/1	0.94	0.29	49,49,49,49	0
56	MG	AA	1621	1/1	0.94	0.07	54,54,54,54	0
56	MG	BA	3138	1/1	0.94	0.13	33,33,33,33	0
56	MG	BA	3139	1/1	0.94	0.10	56,56,56,56	0
56	MG	AA	1871	1/1	0.94	0.10	71,71,71,71	0
56	MG	BA	3859	1/1	0.94	0.10	31,31,31,31	0
56	MG	DD	301	1/1	0.94	0.10	84,84,84,84	0
56	MG	AA	1648	1/1	0.94	0.16	65,65,65,65	0
56	MG	CV	103	1/1	0.94	0.16	88,88,88,88	0
56	MG	BA	3531	1/1	0.94	0.06	59,59,59,59	0
56	MG	DE	302	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3145	1/1	0.94	0.17	26,26,26,26	0
56	MG	DA	3184	1/1	0.94	0.20	57,57,57,57	0
56	MG	CV	106	1/1	0.94	0.20	78,78,78,78	0
56	MG	DF	302	1/1	0.94	0.15	75,75,75,75	0
56	MG	BA	3398	1/1	0.94	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3378	1/1	0.94	0.07	64,64,64,64	0
56	MG	CA	1673	1/1	0.94	0.14	54,54,54,54	0
56	MG	DQ	202	1/1	0.94	0.21	77,77,77,77	0
56	MG	DR	201	1/1	0.94	0.12	44,44,44,44	0
56	MG	BA	3544	1/1	0.94	0.09	45,45,45,45	0
56	MG	BA	3147	1/1	0.94	0.23	54,54,54,54	0
56	MG	BA	3266	1/1	0.94	0.16	59,59,59,59	0
56	MG	DA	3192	1/1	0.94	0.29	71,71,71,71	0
56	MG	AA	1847	1/1	0.94	0.14	98,98,98,98	0
56	MG	BA	3881	1/1	0.94	0.05	75,75,75,75	0
56	MG	DA	3390	1/1	0.94	0.09	55,55,55,55	0
56	MG	DA	3391	1/1	0.94	0.12	48,48,48,48	0
56	MG	BA	3403	1/1	0.94	0.09	51,51,51,51	0
56	MG	AA	1650	1/1	0.94	0.28	65,65,65,65	0
56	MG	D8	201	1/1	0.94	0.12	67,67,67,67	0
56	MG	BA	3579	1/1	0.94	0.17	64,64,64,64	0
56	MG	BA	3585	1/1	0.94	0.06	35,35,35,35	0
57	ZN	D6	101	1/1	0.94	0.08	106,106,106,106	0
56	MG	DA	3403	1/1	0.94	0.27	60,60,60,60	0
56	MG	BA	3510	1/1	0.95	0.08	60,60,60,60	0
56	MG	BA	3401	1/1	0.95	0.06	57,57,57,57	0
56	MG	BA	3200	1/1	0.95	0.16	35,35,35,35	0
56	MG	BA	3004	1/1	0.95	0.08	57,57,57,57	0
56	MG	BA	3008	1/1	0.95	0.11	84,84,84,84	0
56	MG	CA	1750	1/1	0.95	0.10	56,56,56,56	0
56	MG	DA	3257	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3065	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3482	1/1	0.95	0.12	63,63,63,63	0
56	MG	BA	3128	1/1	0.95	0.24	60,60,60,60	0
56	MG	DA	3485	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3785	1/1	0.95	0.09	69,69,69,69	0
56	MG	BA	3786	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3308	1/1	0.95	0.06	51,51,51,51	0
56	MG	BA	3521	1/1	0.95	0.07	68,68,68,68	0
56	MG	DA	3493	1/1	0.95	0.08	80,80,80,80	0
56	MG	BA	3791	1/1	0.95	0.14	29,29,29,29	0
56	MG	BA	3410	1/1	0.95	0.27	54,54,54,54	0
56	MG	BA	3311	1/1	0.95	0.09	59,59,59,59	0
56	MG	BA	3067	1/1	0.95	0.11	40,40,40,40	0
56	MG	DA	3096	1/1	0.95	0.16	41,41,41,41	0
56	MG	DA	3505	1/1	0.95	0.08	81,81,81,81	0
56	MG	DA	3506	1/1	0.95	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1623	1/1	0.95	0.21	68,68,68,68	0
56	MG	DA	3508	1/1	0.95	0.07	87,87,87,87	0
56	MG	BA	3130	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3213	1/1	0.95	0.11	37,37,37,37	0
56	MG	CA	1626	1/1	0.95	0.21	50,50,50,50	0
56	MG	DA	3512	1/1	0.95	0.15	49,49,49,49	0
56	MG	BA	3068	1/1	0.95	0.08	56,56,56,56	0
56	MG	DA	3515	1/1	0.95	0.23	51,51,51,51	0
56	MG	DA	3103	1/1	0.95	0.18	45,45,45,45	0
56	MG	BA	3535	1/1	0.95	0.14	68,68,68,68	0
56	MG	DA	3105	1/1	0.95	0.17	52,52,52,52	0
56	MG	CA	1772	1/1	0.95	0.08	77,77,77,77	0
56	MG	BA	3802	1/1	0.95	0.10	71,71,71,71	0
56	MG	BA	3805	1/1	0.95	0.11	63,63,63,63	0
56	MG	BA	3221	1/1	0.95	0.19	17,17,17,17	0
56	MG	BA	3543	1/1	0.95	0.06	56,56,56,56	0
56	MG	DA	3531	1/1	0.95	0.19	66,66,66,66	0
56	MG	BA	3321	1/1	0.95	0.10	52,52,52,52	0
56	MG	BA	3071	1/1	0.95	0.12	41,41,41,41	0
56	MG	DA	3534	1/1	0.95	0.11	73,73,73,73	0
56	MG	BA	3560	1/1	0.95	0.19	39,39,39,39	0
56	MG	DA	3115	1/1	0.95	0.30	75,75,75,75	0
56	MG	DA	3286	1/1	0.95	0.32	69,69,69,69	0
56	MG	BA	3814	1/1	0.95	0.13	86,86,86,86	0
56	MG	CA	1781	1/1	0.95	0.11	103,103,103,103	0
56	MG	BA	3818	1/1	0.95	0.15	86,86,86,86	0
56	MG	BA	3562	1/1	0.95	0.12	53,53,53,53	0
56	MG	DA	3546	1/1	0.95	0.08	73,73,73,73	0
56	MG	BA	3567	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3323	1/1	0.95	0.06	45,45,45,45	0
56	MG	BA	3824	1/1	0.95	0.08	90,90,90,90	0
56	MG	BA	3569	1/1	0.95	0.21	49,49,49,49	0
56	MG	BA	3570	1/1	0.95	0.10	60,60,60,60	0
56	MG	AA	1829	1/1	0.95	0.08	63,63,63,63	0
56	MG	DA	3556	1/1	0.95	0.06	58,58,58,58	0
56	MG	AA	1869	1/1	0.95	0.18	81,81,81,81	0
56	MG	BA	3577	1/1	0.95	0.09	78,78,78,78	0
56	MG	CA	1647	1/1	0.95	0.18	71,71,71,71	0
56	MG	BA	3075	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3561	1/1	0.95	0.17	70,70,70,70	0
56	MG	DA	3562	1/1	0.95	0.17	69,69,69,69	0
56	MG	AA	1830	1/1	0.95	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3842	1/1	0.95	0.08	85,85,85,85	0
56	MG	BA	3843	1/1	0.95	0.08	78,78,78,78	0
56	MG	BA	3584	1/1	0.95	0.09	54,54,54,54	0
56	MG	DA	3305	1/1	0.95	0.23	76,76,76,76	0
56	MG	DA	3569	1/1	0.95	0.06	76,76,76,76	0
56	MG	BA	3140	1/1	0.95	0.30	53,53,53,53	0
56	MG	BA	3015	1/1	0.95	0.24	59,59,59,59	0
56	MG	BA	3850	1/1	0.95	0.11	82,82,82,82	0
56	MG	BA	3851	1/1	0.95	0.06	35,35,35,35	0
56	MG	AA	1645	1/1	0.95	0.21	54,54,54,54	0
56	MG	AA	1928	1/1	0.95	0.06	71,71,71,71	0
56	MG	BA	3022	1/1	0.95	0.08	85,85,85,85	0
56	MG	DA	3313	1/1	0.95	0.09	74,74,74,74	0
56	MG	CA	1810	1/1	0.95	0.07	92,92,92,92	0
56	MG	DA	3151	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3238	1/1	0.95	0.19	55,55,55,55	0
56	MG	DA	3586	1/1	0.95	0.17	50,50,50,50	0
56	MG	BA	3594	1/1	0.95	0.08	44,44,44,44	0
56	MG	AA	1605	1/1	0.95	0.22	81,81,81,81	0
56	MG	BA	3437	1/1	0.95	0.11	63,63,63,63	0
56	MG	BA	3240	1/1	0.95	0.14	57,57,57,57	0
56	MG	AV	102	1/1	0.95	0.21	66,66,66,66	0
56	MG	DA	3593	1/1	0.95	0.07	75,75,75,75	0
56	MG	BA	3612	1/1	0.95	0.06	61,61,61,61	0
56	MG	CA	1667	1/1	0.95	0.22	66,66,66,66	0
56	MG	DA	3600	1/1	0.95	0.14	57,57,57,57	0
56	MG	CA	1819	1/1	0.95	0.08	96,96,96,96	0
56	MG	DA	3328	1/1	0.95	0.10	59,59,59,59	0
56	MG	DA	3604	1/1	0.95	0.06	97,97,97,97	0
56	MG	BA	3341	1/1	0.95	0.07	53,53,53,53	0
56	MG	BA	3246	1/1	0.95	0.21	53,53,53,53	0
56	MG	BA	3086	1/1	0.95	0.14	51,51,51,51	0
56	MG	DA	3332	1/1	0.95	0.37	63,63,63,63	0
56	MG	DA	3333	1/1	0.95	0.23	50,50,50,50	0
56	MG	BA	3151	1/1	0.95	0.10	38,38,38,38	0
56	MG	DA	3612	1/1	0.95	0.10	87,87,87,87	0
56	MG	DA	3613	1/1	0.95	0.15	60,60,60,60	0
56	MG	BA	3619	1/1	0.95	0.07	86,86,86,86	0
56	MG	AA	1792	1/1	0.95	0.18	44,44,44,44	0
56	MG	BA	3346	1/1	0.95	0.07	43,43,43,43	0
56	MG	BA	3254	1/1	0.95	0.22	21,21,21,21	0
56	MG	BA	3893	1/1	0.95	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3255	1/1	0.95	0.18	16,16,16,16	0
56	MG	DA	3621	1/1	0.95	0.09	73,73,73,73	0
56	MG	BA	3646	1/1	0.95	0.12	44,44,44,44	0
56	MG	BA	3351	1/1	0.95	0.15	51,51,51,51	0
56	MG	DA	3344	1/1	0.95	0.20	88,88,88,88	0
56	MG	BA	3027	1/1	0.95	0.11	44,44,44,44	0
56	MG	AA	1738	1/1	0.95	0.07	84,84,84,84	0
56	MG	BA	3030	1/1	0.95	0.12	36,36,36,36	0
56	MG	AA	1806	1/1	0.95	0.20	59,59,59,59	0
56	MG	AA	1760	1/1	0.95	0.17	64,64,64,64	0
56	MG	BA	3358	1/1	0.95	0.27	63,63,63,63	0
56	MG	BA	3096	1/1	0.95	0.15	37,37,37,37	0
56	MG	AA	1783	1/1	0.95	0.19	61,61,61,61	0
56	MG	BA	3672	1/1	0.95	0.06	41,41,41,41	0
56	MG	DA	3011	1/1	0.95	0.05	66,66,66,66	0
56	MG	DA	3640	1/1	0.95	0.07	63,63,63,63	0
56	MG	AA	1883	1/1	0.95	0.06	86,86,86,86	0
56	MG	BA	3269	1/1	0.95	0.09	55,55,55,55	0
56	MG	BA	3270	1/1	0.95	0.28	53,53,53,53	0
56	MG	BA	3169	1/1	0.95	0.26	14,14,14,14	0
56	MG	BB	224	1/1	0.95	0.12	57,57,57,57	0
56	MG	DA	3190	1/1	0.95	0.15	70,70,70,70	0
56	MG	BB	226	1/1	0.95	0.06	61,61,61,61	0
56	MG	BA	3702	1/1	0.95	0.18	49,49,49,49	0
56	MG	BA	3703	1/1	0.95	0.05	65,65,65,65	0
56	MG	AA	1610	1/1	0.95	0.13	48,48,48,48	0
56	MG	AA	1774	1/1	0.95	0.28	69,69,69,69	0
56	MG	BD	304	1/1	0.95	0.21	20,20,20,20	0
56	MG	BE	302	1/1	0.95	0.19	51,51,51,51	0
56	MG	BA	3101	1/1	0.95	0.13	26,26,26,26	0
56	MG	DA	3200	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3179	1/1	0.95	0.25	45,45,45,45	0
56	MG	BF	302	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3478	1/1	0.95	0.26	67,67,67,67	0
56	MG	BA	3718	1/1	0.95	0.06	87,87,87,87	0
56	MG	DA	3679	1/1	0.95	0.07	76,76,76,76	0
56	MG	BA	3277	1/1	0.95	0.15	65,65,65,65	0
56	MG	BA	3480	1/1	0.95	0.26	59,59,59,59	0
56	MG	DA	3683	1/1	0.95	0.12	94,94,94,94	0
56	MG	DA	3684	1/1	0.95	0.08	98,98,98,98	0
56	MG	BO	202	1/1	0.95	0.12	42,42,42,42	0
56	MG	BA	3043	1/1	0.95	0.34	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3038	1/1	0.95	0.07	50,50,50,50	0
56	MG	AA	1701	1/1	0.95	0.11	57,57,57,57	0
56	MG	AA	1890	1/1	0.95	0.09	89,89,89,89	0
56	MG	DA	3212	1/1	0.95	0.28	66,66,66,66	0
56	MG	BA	3484	1/1	0.95	0.17	49,49,49,49	0
56	MG	DA	3214	1/1	0.95	0.12	64,64,64,64	0
56	MG	DA	3043	1/1	0.95	0.11	61,61,61,61	0
56	MG	BA	3485	1/1	0.95	0.17	52,52,52,52	0
56	MG	DA	3217	1/1	0.95	0.21	68,68,68,68	0
56	MG	BA	3383	1/1	0.95	0.17	45,45,45,45	0
56	MG	BA	3186	1/1	0.95	0.20	27,27,27,27	0
56	MG	DA	3048	1/1	0.95	0.14	74,74,74,74	0
56	MG	DA	3401	1/1	0.95	0.22	36,36,36,36	0
56	MG	BZ	301	1/1	0.95	0.10	54,54,54,54	0
56	MG	DA	3050	1/1	0.95	0.23	67,67,67,67	0
56	MG	AA	1917	1/1	0.95	0.07	71,71,71,71	0
56	MG	B0	103	1/1	0.95	0.09	68,68,68,68	0
56	MG	B0	105	1/1	0.95	0.16	76,76,76,76	0
56	MG	B1	101	1/1	0.95	0.07	60,60,60,60	0
56	MG	DA	3418	1/1	0.95	0.12	52,52,52,52	0
56	MG	AV	117	1/1	0.95	0.06	69,69,69,69	0
56	MG	BA	3493	1/1	0.95	0.08	62,62,62,62	0
56	MG	DA	3425	1/1	0.95	0.14	50,50,50,50	0
56	MG	DA	3427	1/1	0.95	0.13	45,45,45,45	0
56	MG	DA	3429	1/1	0.95	0.05	73,73,73,73	0
56	MG	BA	3112	1/1	0.95	0.12	56,56,56,56	0
56	MG	BA	3289	1/1	0.95	0.13	61,61,61,61	0
56	MG	DA	3434	1/1	0.95	0.08	48,48,48,48	0
56	MG	DA	3435	1/1	0.95	0.08	70,70,70,70	0
56	MG	DA	3438	1/1	0.95	0.13	66,66,66,66	0
56	MG	DA	3439	1/1	0.95	0.07	42,42,42,42	0
56	MG	DQ	201	1/1	0.95	0.08	43,43,43,43	0
56	MG	BA	3391	1/1	0.95	0.13	27,27,27,27	0
56	MG	BA	3752	1/1	0.95	0.10	28,28,28,28	0
56	MG	DT	202	1/1	0.95	0.06	38,38,38,38	0
56	MG	BA	3497	1/1	0.95	0.10	61,61,61,61	0
56	MG	BA	3754	1/1	0.95	0.13	68,68,68,68	0
56	MG	DA	3449	1/1	0.95	0.10	45,45,45,45	0
56	MG	AA	1787	1/1	0.95	0.15	66,66,66,66	0
56	MG	DA	3239	1/1	0.95	0.23	62,62,62,62	0
56	MG	BA	3761	1/1	0.95	0.07	77,77,77,77	0
56	MG	D0	104	1/1	0.95	0.18	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3459	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3291	1/1	0.95	0.11	61,61,61,61	0
56	MG	DA	3068	1/1	0.95	0.32	44,44,44,44	0
56	MG	AA	1606	1/1	0.95	0.15	35,35,35,35	0
56	MG	AA	1624	1/1	0.95	0.24	57,57,57,57	0
56	MG	DA	3466	1/1	0.95	0.09	75,75,75,75	0
56	MG	AA	1867	1/1	0.95	0.39	80,80,80,80	0
56	MG	BA	3057	1/1	0.95	0.07	30,30,30,30	0
56	MG	BA	3299	1/1	0.95	0.05	58,58,58,58	0
56	MG	BA	3739	1/1	0.96	0.09	42,42,42,42	0
56	MG	AA	1947	1/1	0.96	0.06	63,63,63,63	0
56	MG	BV	201	1/1	0.96	0.28	39,39,39,39	0
56	MG	CA	1735	1/1	0.96	0.08	78,78,78,78	0
56	MG	BA	3503	1/1	0.96	0.08	51,51,51,51	0
56	MG	BY	202	1/1	0.96	0.08	54,54,54,54	0
56	MG	BY	203	1/1	0.96	0.13	65,65,65,65	0
56	MG	BA	3504	1/1	0.96	0.14	57,57,57,57	0
56	MG	BZ	302	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3031	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3298	1/1	0.96	0.22	50,50,50,50	0
56	MG	BA	3745	1/1	0.96	0.08	75,75,75,75	0
56	MG	CA	1744	1/1	0.96	0.13	80,80,80,80	0
56	MG	BA	3508	1/1	0.96	0.20	41,41,41,41	0
56	MG	BA	3750	1/1	0.96	0.08	65,65,65,65	0
56	MG	DA	3516	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3518	1/1	0.96	0.14	46,46,46,46	0
56	MG	AA	1677	1/1	0.96	0.16	84,84,84,84	0
56	MG	CA	1749	1/1	0.96	0.16	92,92,92,92	0
56	MG	BA	3207	1/1	0.96	0.15	41,41,41,41	0
56	MG	AA	1773	1/1	0.96	0.09	58,58,58,58	0
56	MG	BA	3210	1/1	0.96	0.15	36,36,36,36	0
56	MG	CA	1753	1/1	0.96	0.21	61,61,61,61	0
56	MG	DA	3528	1/1	0.96	0.05	88,88,88,88	0
56	MG	AV	115	1/1	0.96	0.08	65,65,65,65	0
56	MG	BA	3404	1/1	0.96	0.09	52,52,52,52	0
56	MG	DA	3108	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3085	1/1	0.96	0.12	35,35,35,35	0
56	MG	BA	3768	1/1	0.96	0.07	90,90,90,90	0
56	MG	BA	3305	1/1	0.96	0.06	35,35,35,35	0
56	MG	B9	102	1/1	0.96	0.15	43,43,43,43	0
56	MG	BA	3771	1/1	0.96	0.08	79,79,79,79	0
56	MG	CA	1763	1/1	0.96	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3538	1/1	0.96	0.08	96,96,96,96	0
56	MG	BA	3214	1/1	0.96	0.06	49,49,49,49	0
56	MG	AA	1824	1/1	0.96	0.22	33,33,33,33	0
56	MG	BA	3141	1/1	0.96	0.10	38,38,38,38	0
56	MG	CA	1767	1/1	0.96	0.11	62,62,62,62	0
56	MG	BA	3038	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3412	1/1	0.96	0.06	56,56,56,56	0
56	MG	BA	3526	1/1	0.96	0.07	40,40,40,40	0
56	MG	AA	1885	1/1	0.96	0.10	90,90,90,90	0
56	MG	BA	3224	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3317	1/1	0.96	0.11	61,61,61,61	0
56	MG	BA	3318	1/1	0.96	0.13	63,63,63,63	0
56	MG	DA	3128	1/1	0.96	0.29	59,59,59,59	0
56	MG	BA	3040	1/1	0.96	0.09	46,46,46,46	0
56	MG	DA	3130	1/1	0.96	0.07	52,52,52,52	0
56	MG	BA	3227	1/1	0.96	0.25	41,41,41,41	0
56	MG	BA	3146	1/1	0.96	0.16	49,49,49,49	0
56	MG	DA	3314	1/1	0.96	0.11	52,52,52,52	0
56	MG	BA	3547	1/1	0.96	0.07	49,49,49,49	0
56	MG	BA	3548	1/1	0.96	0.13	39,39,39,39	0
56	MG	BA	3556	1/1	0.96	0.12	52,52,52,52	0
56	MG	AA	1906	1/1	0.96	0.10	89,89,89,89	0
56	MG	BA	3093	1/1	0.96	0.13	42,42,42,42	0
56	MG	BA	3231	1/1	0.96	0.19	31,31,31,31	0
56	MG	BA	3564	1/1	0.96	0.07	63,63,63,63	0
56	MG	DA	3323	1/1	0.96	0.07	57,57,57,57	0
56	MG	DA	3572	1/1	0.96	0.19	45,45,45,45	0
56	MG	BA	3233	1/1	0.96	0.11	22,22,22,22	0
56	MG	BA	3425	1/1	0.96	0.09	46,46,46,46	0
56	MG	AA	1927	1/1	0.96	0.05	85,85,85,85	0
56	MG	BA	3803	1/1	0.96	0.16	71,71,71,71	0
56	MG	CA	1789	1/1	0.96	0.07	66,66,66,66	0
56	MG	BA	3804	1/1	0.96	0.07	59,59,59,59	0
56	MG	AA	1886	1/1	0.96	0.05	79,79,79,79	0
56	MG	AA	1721	1/1	0.96	0.20	84,84,84,84	0
56	MG	BA	3572	1/1	0.96	0.07	66,66,66,66	0
56	MG	BA	3429	1/1	0.96	0.17	54,54,54,54	0
56	MG	BA	3046	1/1	0.96	0.10	49,49,49,49	0
56	MG	BA	3006	1/1	0.96	0.12	55,55,55,55	0
56	MG	AA	1632	1/1	0.96	0.32	51,51,51,51	0
56	MG	BA	3815	1/1	0.96	0.04	51,51,51,51	0
56	MG	BA	3009	1/1	0.96	0.08	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3242	1/1	0.96	0.18	47,47,47,47	0
56	MG	DA	3340	1/1	0.96	0.27	55,55,55,55	0
56	MG	AA	1766	1/1	0.96	0.14	53,53,53,53	0
56	MG	AA	1841	1/1	0.96	0.15	75,75,75,75	0
56	MG	BA	3160	1/1	0.96	0.11	41,41,41,41	0
56	MG	BA	3103	1/1	0.96	0.37	54,54,54,54	0
56	MG	BA	3250	1/1	0.96	0.20	27,27,27,27	0
56	MG	CA	1809	1/1	0.96	0.05	101,101,101,101	0
56	MG	AA	1634	1/1	0.96	0.25	47,47,47,47	0
56	MG	BA	3832	1/1	0.96	0.07	40,40,40,40	0
56	MG	BA	3597	1/1	0.96	0.06	66,66,66,66	0
56	MG	BA	3165	1/1	0.96	0.27	17,17,17,17	0
56	MG	BA	3836	1/1	0.96	0.09	23,23,23,23	0
56	MG	DA	3173	1/1	0.96	0.19	62,62,62,62	0
56	MG	BA	3603	1/1	0.96	0.09	32,32,32,32	0
56	MG	BA	3447	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3106	1/1	0.96	0.06	28,28,28,28	0
56	MG	BA	3167	1/1	0.96	0.09	31,31,31,31	0
56	MG	BA	3611	1/1	0.96	0.13	43,43,43,43	0
56	MG	BA	3348	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3056	1/1	0.96	0.05	50,50,50,50	0
56	MG	BA	3014	1/1	0.96	0.17	49,49,49,49	0
56	MG	AA	1938	1/1	0.96	0.07	84,84,84,84	0
56	MG	BA	3852	1/1	0.96	0.17	59,59,59,59	0
56	MG	BA	3061	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3617	1/1	0.96	0.07	58,58,58,58	0
56	MG	BA	3856	1/1	0.96	0.09	68,68,68,68	0
56	MG	BA	3176	1/1	0.96	0.13	63,63,63,63	0
56	MG	BA	3622	1/1	0.96	0.07	65,65,65,65	0
56	MG	BA	3177	1/1	0.96	0.17	46,46,46,46	0
56	MG	BA	3178	1/1	0.96	0.16	43,43,43,43	0
56	MG	DA	3630	1/1	0.96	0.11	47,47,47,47	0
56	MG	BA	3633	1/1	0.96	0.05	52,52,52,52	0
56	MG	BA	3869	1/1	0.96	0.06	64,64,64,64	0
56	MG	BA	3459	1/1	0.96	0.09	49,49,49,49	0
56	MG	DA	3635	1/1	0.96	0.04	88,88,88,88	0
56	MG	BA	3636	1/1	0.96	0.08	63,63,63,63	0
56	MG	DA	3637	1/1	0.96	0.05	57,57,57,57	0
56	MG	BA	3637	1/1	0.96	0.05	62,62,62,62	0
56	MG	BA	3638	1/1	0.96	0.15	54,54,54,54	0
56	MG	DA	3643	1/1	0.96	0.08	89,89,89,89	0
56	MG	DA	3376	1/1	0.96	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3377	1/1	0.96	0.18	89,89,89,89	0
56	MG	BA	3877	1/1	0.96	0.15	21,21,21,21	0
56	MG	BA	3878	1/1	0.96	0.11	81,81,81,81	0
56	MG	DA	3651	1/1	0.96	0.11	61,61,61,61	0
56	MG	BA	3639	1/1	0.96	0.06	63,63,63,63	0
56	MG	BA	3880	1/1	0.96	0.09	84,84,84,84	0
56	MG	BA	3641	1/1	0.96	0.07	62,62,62,62	0
56	MG	BA	3882	1/1	0.96	0.05	73,73,73,73	0
56	MG	DA	3384	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3883	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3658	1/1	0.96	0.15	79,79,79,79	0
56	MG	BA	3114	1/1	0.96	0.21	37,37,37,37	0
56	MG	DA	3662	1/1	0.96	0.07	53,53,53,53	0
56	MG	BA	3644	1/1	0.96	0.06	72,72,72,72	0
56	MG	CA	1680	1/1	0.96	0.25	70,70,70,70	0
56	MG	AA	1705	1/1	0.96	0.04	55,55,55,55	0
56	MG	DA	3670	1/1	0.96	0.05	83,83,83,83	0
56	MG	BA	3018	1/1	0.96	0.25	53,53,53,53	0
56	MG	DA	3672	1/1	0.96	0.11	87,87,87,87	0
56	MG	DA	3395	1/1	0.96	0.07	58,58,58,58	0
56	MG	BA	3464	1/1	0.96	0.07	53,53,53,53	0
56	MG	DA	3399	1/1	0.96	0.23	47,47,47,47	0
56	MG	BA	3649	1/1	0.96	0.12	60,60,60,60	0
56	MG	BA	3894	1/1	0.96	0.11	52,52,52,52	0
56	MG	DA	3680	1/1	0.96	0.08	79,79,79,79	0
56	MG	BA	3466	1/1	0.96	0.14	50,50,50,50	0
56	MG	DA	3405	1/1	0.96	0.14	43,43,43,43	0
56	MG	BA	3183	1/1	0.96	0.28	22,22,22,22	0
56	MG	BB	201	1/1	0.96	0.05	57,57,57,57	0
56	MG	BB	202	1/1	0.96	0.05	57,57,57,57	0
56	MG	DA	3686	1/1	0.96	0.07	74,74,74,74	0
56	MG	BA	3653	1/1	0.96	0.20	38,38,38,38	0
56	MG	CA	1691	1/1	0.96	0.37	53,53,53,53	0
56	MG	BA	3654	1/1	0.96	0.08	59,59,59,59	0
56	MG	DA	3421	1/1	0.96	0.06	52,52,52,52	0
56	MG	AA	1896	1/1	0.96	0.05	88,88,88,88	0
56	MG	BA	3119	1/1	0.96	0.08	50,50,50,50	0
56	MG	AA	1857	1/1	0.96	0.12	62,62,62,62	0
56	MG	DA	3695	1/1	0.96	0.07	107,107,107,107	0
56	MG	BA	3366	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3069	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3668	1/1	0.96	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3278	1/1	0.96	0.21	59,59,59,59	0
56	MG	BA	3190	1/1	0.96	0.21	42,42,42,42	0
56	MG	BB	215	1/1	0.96	0.15	62,62,62,62	0
56	MG	DA	3045	1/1	0.96	0.15	62,62,62,62	0
56	MG	AA	1649	1/1	0.96	0.09	60,60,60,60	0
56	MG	BA	3282	1/1	0.96	0.08	59,59,59,59	0
56	MG	BA	3375	1/1	0.96	0.11	47,47,47,47	0
56	MG	DB	211	1/1	0.96	0.09	83,83,83,83	0
56	MG	BA	3024	1/1	0.96	0.14	36,36,36,36	0
56	MG	BB	223	1/1	0.96	0.09	38,38,38,38	0
56	MG	AA	1656	1/1	0.96	0.12	72,72,72,72	0
56	MG	DB	215	1/1	0.96	0.06	94,94,94,94	0
56	MG	DB	216	1/1	0.96	0.05	109,109,109,109	0
56	MG	DA	3450	1/1	0.96	0.11	59,59,59,59	0
56	MG	DA	3238	1/1	0.96	0.13	65,65,65,65	0
56	MG	BA	3380	1/1	0.96	0.10	44,44,44,44	0
56	MG	BA	3706	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3285	1/1	0.96	0.09	55,55,55,55	0
56	MG	BA	3712	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3382	1/1	0.96	0.09	68,68,68,68	0
56	MG	DA	3462	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3126	1/1	0.96	0.24	40,40,40,40	0
56	MG	AA	1781	1/1	0.96	0.35	68,68,68,68	0
56	MG	BA	3717	1/1	0.96	0.08	21,21,21,21	0
56	MG	BE	304	1/1	0.96	0.26	14,14,14,14	0
56	MG	DO	203	1/1	0.96	0.14	79,79,79,79	0
56	MG	DA	3250	1/1	0.96	0.30	62,62,62,62	0
56	MG	BA	3197	1/1	0.96	0.15	41,41,41,41	0
56	MG	DA	3063	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3386	1/1	0.96	0.17	54,54,54,54	0
56	MG	BA	3198	1/1	0.96	0.12	17,17,17,17	0
56	MG	AV	110	1/1	0.96	0.26	80,80,80,80	0
56	MG	BF	306	1/1	0.96	0.13	48,48,48,48	0
56	MG	AA	1946	1/1	0.96	0.11	81,81,81,81	0
56	MG	BG	202	1/1	0.96	0.04	82,82,82,82	0
56	MG	DA	3480	1/1	0.96	0.13	70,70,70,70	0
56	MG	BA	3731	1/1	0.96	0.09	53,53,53,53	0
56	MG	BA	3292	1/1	0.96	0.13	47,47,47,47	0
56	MG	CA	1726	1/1	0.96	0.17	70,70,70,70	0
56	MG	BA	3202	1/1	0.96	0.13	42,42,42,42	0
56	MG	D6	103	1/1	0.96	0.05	93,93,93,93	0
56	MG	DA	3487	1/1	0.96	0.06	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3075	1/1	0.96	0.07	84,84,84,84	0
56	MG	BA	3393	1/1	0.96	0.10	28,28,28,28	0
57	ZN	B4	101	1/1	0.96	0.08	137,137,137,137	0
57	ZN	CD	301	1/1	0.96	0.18	90,90,90,90	0
56	MG	BA	3394	1/1	0.96	0.14	58,58,58,58	0
57	ZN	D4	101	1/1	0.96	0.11	178,178,178,178	0
56	MG	CA	1730	1/1	0.96	0.24	69,69,69,69	0
56	MG	BA	3131	1/1	0.96	0.05	34,34,34,34	0
56	MG	BA	3774	1/1	0.97	0.17	72,72,72,72	0
56	MG	DA	3172	1/1	0.97	0.17	51,51,51,51	0
56	MG	DA	3012	1/1	0.97	0.04	76,76,76,76	0
56	MG	AA	1765	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3015	1/1	0.97	0.15	66,66,66,66	0
56	MG	BA	3127	1/1	0.97	0.07	41,41,41,41	0
56	MG	BF	307	1/1	0.97	0.05	42,42,42,42	0
56	MG	DA	3551	1/1	0.97	0.13	42,42,42,42	0
56	MG	BA	3215	1/1	0.97	0.21	16,16,16,16	0
56	MG	BA	3596	1/1	0.97	0.04	39,39,39,39	0
56	MG	AA	1839	1/1	0.97	0.05	69,69,69,69	0
56	MG	BA	3599	1/1	0.97	0.05	52,52,52,52	0
56	MG	BA	3279	1/1	0.97	0.08	50,50,50,50	0
56	MG	BA	3602	1/1	0.97	0.07	22,22,22,22	0
56	MG	BA	3409	1/1	0.97	0.06	45,45,45,45	0
56	MG	BA	3604	1/1	0.97	0.08	80,80,80,80	0
56	MG	BQ	204	1/1	0.97	0.06	41,41,41,41	0
56	MG	BR	201	1/1	0.97	0.20	19,19,19,19	0
56	MG	BR	202	1/1	0.97	0.10	30,30,30,30	0
56	MG	DA	3565	1/1	0.97	0.07	50,50,50,50	0
56	MG	DA	3030	1/1	0.97	0.08	66,66,66,66	0
56	MG	BA	3219	1/1	0.97	0.22	43,43,43,43	0
56	MG	BA	3019	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3170	1/1	0.97	0.23	43,43,43,43	0
56	MG	BA	3487	1/1	0.97	0.13	53,53,53,53	0
56	MG	AA	1870	1/1	0.97	0.09	85,85,85,85	0
56	MG	DA	3573	1/1	0.97	0.11	42,42,42,42	0
56	MG	AA	1916	1/1	0.97	0.05	82,82,82,82	0
56	MG	BA	3795	1/1	0.97	0.19	84,84,84,84	0
56	MG	BA	3415	1/1	0.97	0.07	50,50,50,50	0
56	MG	DA	3039	1/1	0.97	0.06	50,50,50,50	0
56	MG	BA	3173	1/1	0.97	0.11	31,31,31,31	0
56	MG	BA	3226	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3070	1/1	0.97	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1864	1/1	0.97	0.10	67,67,67,67	0
56	MG	BA	3620	1/1	0.97	0.05	49,49,49,49	0
56	MG	AA	1872	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3625	1/1	0.97	0.05	41,41,41,41	0
56	MG	BA	3626	1/1	0.97	0.05	70,70,70,70	0
56	MG	BA	3136	1/1	0.97	0.17	32,32,32,32	0
56	MG	BA	3005	1/1	0.97	0.06	59,59,59,59	0
56	MG	AA	1895	1/1	0.97	0.05	87,87,87,87	0
56	MG	BA	3634	1/1	0.97	0.06	46,46,46,46	0
56	MG	BA	3047	1/1	0.97	0.14	32,32,32,32	0
56	MG	BA	3502	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3105	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3295	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3360	1/1	0.97	0.07	51,51,51,51	0
56	MG	DA	3602	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3506	1/1	0.97	0.10	61,61,61,61	0
56	MG	BA	3184	1/1	0.97	0.18	31,31,31,31	0
56	MG	AA	1840	1/1	0.97	0.09	83,83,83,83	0
56	MG	BA	3028	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3143	1/1	0.97	0.21	20,20,20,20	0
56	MG	BA	3432	1/1	0.97	0.10	29,29,29,29	0
56	MG	AA	1897	1/1	0.97	0.11	74,74,74,74	0
56	MG	BA	3110	1/1	0.97	0.20	51,51,51,51	0
56	MG	DA	3225	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3367	1/1	0.97	0.25	50,50,50,50	0
56	MG	BA	3191	1/1	0.97	0.15	78,78,78,78	0
56	MG	BA	3438	1/1	0.97	0.11	62,62,62,62	0
56	MG	BA	3839	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3840	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3071	1/1	0.97	0.25	44,44,44,44	0
56	MG	DA	3619	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3655	1/1	0.97	0.07	46,46,46,46	0
56	MG	BA	3245	1/1	0.97	0.16	42,42,42,42	0
56	MG	BA	3520	1/1	0.97	0.17	38,38,38,38	0
56	MG	DA	3235	1/1	0.97	0.13	53,53,53,53	0
56	MG	AA	1940	1/1	0.97	0.06	92,92,92,92	0
56	MG	DA	3076	1/1	0.97	0.06	51,51,51,51	0
56	MG	CA	1620	1/1	0.97	0.12	70,70,70,70	0
56	MG	CA	1758	1/1	0.97	0.17	56,56,56,56	0
56	MG	DA	3412	1/1	0.97	0.06	52,52,52,52	0
56	MG	CA	1759	1/1	0.97	0.09	76,76,76,76	0
56	MG	BA	3847	1/1	0.97	0.19	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1909	1/1	0.97	0.07	91,91,91,91	0
56	MG	DA	3632	1/1	0.97	0.25	69,69,69,69	0
56	MG	DA	3416	1/1	0.97	0.05	53,53,53,53	0
56	MG	BA	3306	1/1	0.97	0.08	45,45,45,45	0
56	MG	BA	3307	1/1	0.97	0.06	48,48,48,48	0
56	MG	DA	3419	1/1	0.97	0.10	35,35,35,35	0
56	MG	DA	3245	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3113	1/1	0.97	0.07	46,46,46,46	0
56	MG	BA	3527	1/1	0.97	0.09	90,90,90,90	0
56	MG	BA	3378	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3426	1/1	0.97	0.05	42,42,42,42	0
56	MG	DA	3646	1/1	0.97	0.13	62,62,62,62	0
56	MG	BA	3685	1/1	0.97	0.07	40,40,40,40	0
56	MG	BA	3687	1/1	0.97	0.12	23,23,23,23	0
56	MG	BA	3309	1/1	0.97	0.14	56,56,56,56	0
56	MG	DA	3431	1/1	0.97	0.08	33,33,33,33	0
56	MG	DA	3091	1/1	0.97	0.05	47,47,47,47	0
56	MG	BA	3858	1/1	0.97	0.12	70,70,70,70	0
56	MG	BA	3532	1/1	0.97	0.10	34,34,34,34	0
56	MG	DA	3437	1/1	0.97	0.12	70,70,70,70	0
56	MG	DA	3094	1/1	0.97	0.10	34,34,34,34	0
56	MG	BA	3310	1/1	0.97	0.10	54,54,54,54	0
56	MG	BA	3865	1/1	0.97	0.05	97,97,97,97	0
56	MG	DA	3097	1/1	0.97	0.28	31,31,31,31	0
56	MG	AA	1771	1/1	0.97	0.10	68,68,68,68	0
56	MG	DA	3663	1/1	0.97	0.05	81,81,81,81	0
56	MG	BA	3536	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3665	1/1	0.97	0.04	87,87,87,87	0
56	MG	BA	3868	1/1	0.97	0.10	34,34,34,34	0
56	MG	DA	3667	1/1	0.97	0.06	74,74,74,74	0
56	MG	BA	3705	1/1	0.97	0.17	79,79,79,79	0
56	MG	DA	3452	1/1	0.97	0.13	60,60,60,60	0
56	MG	BA	3537	1/1	0.97	0.15	47,47,47,47	0
56	MG	BA	3055	1/1	0.97	0.07	37,37,37,37	0
56	MG	BA	3873	1/1	0.97	0.05	74,74,74,74	0
56	MG	DA	3457	1/1	0.97	0.10	102,102,102,102	0
56	MG	BA	3709	1/1	0.97	0.09	49,49,49,49	0
56	MG	BA	3710	1/1	0.97	0.08	58,58,58,58	0
56	MG	BA	3252	1/1	0.97	0.24	20,20,20,20	0
56	MG	BA	3116	1/1	0.97	0.18	37,37,37,37	0
56	MG	BA	3545	1/1	0.97	0.06	53,53,53,53	0
56	MG	BA	3546	1/1	0.97	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3152	1/1	0.97	0.05	42,42,42,42	0
56	MG	AA	1854	1/1	0.97	0.08	73,73,73,73	0
56	MG	BA	3549	1/1	0.97	0.10	19,19,19,19	0
56	MG	BA	3884	1/1	0.97	0.04	66,66,66,66	0
56	MG	BA	3550	1/1	0.97	0.13	27,27,27,27	0
56	MG	BA	3725	1/1	0.97	0.09	69,69,69,69	0
56	MG	BA	3887	1/1	0.97	0.14	17,17,17,17	0
56	MG	CA	1794	1/1	0.97	0.09	59,59,59,59	0
56	MG	BA	3552	1/1	0.97	0.10	39,39,39,39	0
56	MG	BA	3554	1/1	0.97	0.06	55,55,55,55	0
56	MG	BA	3891	1/1	0.97	0.08	74,74,74,74	0
56	MG	BA	3729	1/1	0.97	0.06	59,59,59,59	0
56	MG	BA	3555	1/1	0.97	0.06	47,47,47,47	0
56	MG	BA	3732	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3257	1/1	0.97	0.18	48,48,48,48	0
56	MG	DA	3127	1/1	0.97	0.20	37,37,37,37	0
56	MG	BA	3557	1/1	0.97	0.05	62,62,62,62	0
56	MG	BA	3735	1/1	0.97	0.06	58,58,58,58	0
56	MG	BA	3034	1/1	0.97	0.08	23,23,23,23	0
56	MG	AA	1876	1/1	0.97	0.05	89,89,89,89	0
56	MG	BA	3156	1/1	0.97	0.27	54,54,54,54	0
56	MG	BB	205	1/1	0.97	0.20	29,29,29,29	0
56	MG	DB	210	1/1	0.97	0.15	91,91,91,91	0
56	MG	BA	3060	1/1	0.97	0.05	52,52,52,52	0
56	MG	DA	3495	1/1	0.97	0.04	62,62,62,62	0
56	MG	BA	3462	1/1	0.97	0.14	47,47,47,47	0
56	MG	DA	3137	1/1	0.97	0.13	39,39,39,39	0
56	MG	DA	3500	1/1	0.97	0.09	68,68,68,68	0
56	MG	BA	3324	1/1	0.97	0.21	62,62,62,62	0
56	MG	DA	3503	1/1	0.97	0.15	80,80,80,80	0
56	MG	DD	302	1/1	0.97	0.26	48,48,48,48	0
56	MG	BA	3036	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3465	1/1	0.97	0.11	40,40,40,40	0
56	MG	BA	3091	1/1	0.97	0.12	60,60,60,60	0
56	MG	BB	212	1/1	0.97	0.07	62,62,62,62	0
56	MG	BA	3468	1/1	0.97	0.10	54,54,54,54	0
56	MG	DA	3145	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3575	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3147	1/1	0.97	0.06	70,70,70,70	0
56	MG	BA	3748	1/1	0.97	0.05	28,28,28,28	0
56	MG	BA	3749	1/1	0.97	0.11	76,76,76,76	0
56	MG	BA	3092	1/1	0.97	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3268	1/1	0.97	0.09	52,52,52,52	0
56	MG	DA	3517	1/1	0.97	0.10	64,64,64,64	0
56	MG	BB	220	1/1	0.97	0.08	44,44,44,44	0
56	MG	BA	3208	1/1	0.97	0.13	57,57,57,57	0
56	MG	DT	201	1/1	0.97	0.11	73,73,73,73	0
56	MG	DA	3520	1/1	0.97	0.05	67,67,67,67	0
56	MG	BA	3330	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	3756	1/1	0.97	0.08	56,56,56,56	0
56	MG	DA	3523	1/1	0.97	0.05	86,86,86,86	0
56	MG	DA	3315	1/1	0.97	0.24	47,47,47,47	0
56	MG	BB	225	1/1	0.97	0.14	56,56,56,56	0
56	MG	BA	3580	1/1	0.97	0.04	68,68,68,68	0
56	MG	BB	227	1/1	0.97	0.07	81,81,81,81	0
56	MG	BA	3581	1/1	0.97	0.06	29,29,29,29	0
56	MG	BA	3763	1/1	0.97	0.05	84,84,84,84	0
56	MG	BA	3582	1/1	0.97	0.08	30,30,30,30	0
56	MG	BA	3473	1/1	0.97	0.20	22,22,22,22	0
56	MG	BA	3767	1/1	0.97	0.05	51,51,51,51	0
56	MG	DA	3003	1/1	0.97	0.05	43,43,43,43	0
57	ZN	AD	301	1/1	0.97	0.16	93,93,93,93	0
56	MG	BE	301	1/1	0.97	0.17	36,36,36,36	0
56	MG	BA	3124	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3769	1/1	0.97	0.06	55,55,55,55	0
56	MG	BA	3062	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3163	1/1	0.97	0.16	40,40,40,40	0
56	MG	BA	3212	1/1	0.97	0.03	35,35,35,35	0
56	MG	DA	3542	1/1	0.97	0.07	84,84,84,84	0
56	MG	BA	3829	1/1	0.98	0.20	82,82,82,82	0
56	MG	BA	3830	1/1	0.98	0.06	31,31,31,31	0
56	MG	DA	3436	1/1	0.98	0.13	50,50,50,50	0
56	MG	DA	3594	1/1	0.98	0.15	44,44,44,44	0
56	MG	DA	3595	1/1	0.98	0.10	43,43,43,43	0
56	MG	BA	3831	1/1	0.98	0.10	22,22,22,22	0
56	MG	DA	3597	1/1	0.98	0.05	57,57,57,57	0
56	MG	BA	3727	1/1	0.98	0.05	66,66,66,66	0
56	MG	BA	3247	1/1	0.98	0.11	20,20,20,20	0
56	MG	DA	3440	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3834	1/1	0.98	0.10	27,27,27,27	0
56	MG	BA	3374	1/1	0.98	0.20	24,24,24,24	0
56	MG	BA	3730	1/1	0.98	0.05	63,63,63,63	0
56	MG	DA	3444	1/1	0.98	0.04	54,54,54,54	0
56	MG	DA	3445	1/1	0.98	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3108	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3608	1/1	0.98	0.05	82,82,82,82	0
56	MG	BA	3042	1/1	0.98	0.08	37,37,37,37	0
56	MG	BQ	201	1/1	0.98	0.03	18,18,18,18	0
56	MG	DA	3451	1/1	0.98	0.12	39,39,39,39	0
56	MG	BA	3377	1/1	0.98	0.11	50,50,50,50	0
56	MG	BA	3538	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3539	1/1	0.98	0.07	22,22,22,22	0
56	MG	DA	3455	1/1	0.98	0.04	61,61,61,61	0
56	MG	BA	3540	1/1	0.98	0.05	19,19,19,19	0
56	MG	AA	1628	1/1	0.98	0.19	22,22,22,22	0
56	MG	BA	3845	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3621	1/1	0.98	0.09	30,30,30,30	0
56	MG	DA	3195	1/1	0.98	0.17	58,58,58,58	0
56	MG	BA	3216	1/1	0.98	0.12	28,28,28,28	0
56	MG	DA	3463	1/1	0.98	0.07	68,68,68,68	0
56	MG	BV	202	1/1	0.98	0.20	67,67,67,67	0
56	MG	BA	3623	1/1	0.98	0.06	75,75,75,75	0
56	MG	BA	3624	1/1	0.98	0.05	57,57,57,57	0
56	MG	BA	3011	1/1	0.98	0.15	54,54,54,54	0
56	MG	DA	3468	1/1	0.98	0.04	80,80,80,80	0
56	MG	BA	3253	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3218	1/1	0.98	0.12	20,20,20,20	0
56	MG	CA	1800	1/1	0.98	0.04	105,105,105,105	0
56	MG	B0	101	1/1	0.98	0.05	43,43,43,43	0
56	MG	BA	3189	1/1	0.98	0.21	49,49,49,49	0
56	MG	BA	3632	1/1	0.98	0.07	59,59,59,59	0
56	MG	B0	104	1/1	0.98	0.07	58,58,58,58	0
56	MG	CA	1805	1/1	0.98	0.04	88,88,88,88	0
56	MG	BA	3336	1/1	0.98	0.07	46,46,46,46	0
56	MG	DA	3479	1/1	0.98	0.04	68,68,68,68	0
56	MG	BA	3220	1/1	0.98	0.19	27,27,27,27	0
56	MG	BA	3338	1/1	0.98	0.23	63,63,63,63	0
56	MG	BA	3861	1/1	0.98	0.04	66,66,66,66	0
56	MG	DA	3644	1/1	0.98	0.05	80,80,80,80	0
56	MG	BA	3489	1/1	0.98	0.10	55,55,55,55	0
56	MG	DA	3484	1/1	0.98	0.05	45,45,45,45	0
56	MG	BA	3864	1/1	0.98	0.04	79,79,79,79	0
56	MG	BA	3553	1/1	0.98	0.04	29,29,29,29	0
56	MG	B3	102	1/1	0.98	0.17	56,56,56,56	0
56	MG	DA	3650	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3490	1/1	0.98	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AV	116	1/1	0.98	0.04	84,84,84,84	0
56	MG	BA	3757	1/1	0.98	0.07	28,28,28,28	0
56	MG	DA	3492	1/1	0.98	0.08	63,63,63,63	0
56	MG	BA	3759	1/1	0.98	0.15	40,40,40,40	0
56	MG	BA	3066	1/1	0.98	0.07	35,35,35,35	0
56	MG	AA	1862	1/1	0.98	0.04	45,45,45,45	0
56	MG	AA	1633	1/1	0.98	0.23	32,32,32,32	0
56	MG	BA	3261	1/1	0.98	0.09	69,69,69,69	0
56	MG	DA	3660	1/1	0.98	0.07	78,78,78,78	0
56	MG	DA	3661	1/1	0.98	0.10	61,61,61,61	0
56	MG	BA	3561	1/1	0.98	0.09	64,64,64,64	0
56	MG	BA	3766	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3442	1/1	0.98	0.16	45,45,45,45	0
56	MG	BA	3563	1/1	0.98	0.11	45,45,45,45	0
56	MG	AA	1604	1/1	0.98	0.06	42,42,42,42	0
56	MG	BA	3263	1/1	0.98	0.06	41,41,41,41	0
56	MG	DA	3668	1/1	0.98	0.09	100,100,100,100	0
56	MG	BA	3016	1/1	0.98	0.28	52,52,52,52	0
56	MG	AA	1889	1/1	0.98	0.04	71,71,71,71	0
56	MG	AA	1877	1/1	0.98	0.05	70,70,70,70	0
56	MG	BA	3349	1/1	0.98	0.08	52,52,52,52	0
56	MG	BA	3267	1/1	0.98	0.06	53,53,53,53	0
56	MG	BA	3573	1/1	0.98	0.08	54,54,54,54	0
56	MG	DA	3675	1/1	0.98	0.08	75,75,75,75	0
56	MG	BA	3052	1/1	0.98	0.10	35,35,35,35	0
56	MG	BA	3074	1/1	0.98	0.08	52,52,52,52	0
56	MG	DA	3120	1/1	0.98	0.08	42,42,42,42	0
56	MG	BA	3890	1/1	0.98	0.04	70,70,70,70	0
56	MG	BA	3663	1/1	0.98	0.05	21,21,21,21	0
56	MG	DA	3006	1/1	0.98	0.06	56,56,56,56	0
56	MG	BA	3665	1/1	0.98	0.04	44,44,44,44	0
56	MG	AA	1933	1/1	0.98	0.06	54,54,54,54	0
56	MG	BA	3783	1/1	0.98	0.08	74,74,74,74	0
56	MG	BA	3354	1/1	0.98	0.14	34,34,34,34	0
56	MG	DA	3687	1/1	0.98	0.03	64,64,64,64	0
56	MG	BA	3673	1/1	0.98	0.10	43,43,43,43	0
56	MG	DA	3248	1/1	0.98	0.13	53,53,53,53	0
56	MG	BA	3232	1/1	0.98	0.21	40,40,40,40	0
56	MG	BA	3201	1/1	0.98	0.22	54,54,54,54	0
56	MG	DA	3131	1/1	0.98	0.18	46,46,46,46	0
56	MG	DA	3014	1/1	0.98	0.15	38,38,38,38	0
56	MG	BA	3684	1/1	0.98	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1934	1/1	0.98	0.04	48,48,48,48	0
56	MG	BA	3175	1/1	0.98	0.21	34,34,34,34	0
56	MG	BA	3688	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3794	1/1	0.98	0.10	80,80,80,80	0
56	MG	BA	3021	1/1	0.98	0.04	35,35,35,35	0
56	MG	BA	3696	1/1	0.98	0.07	30,30,30,30	0
56	MG	DA	3022	1/1	0.98	0.15	46,46,46,46	0
56	MG	DA	3141	1/1	0.98	0.21	60,60,60,60	0
56	MG	DA	3540	1/1	0.98	0.18	57,57,57,57	0
56	MG	BA	3315	1/1	0.98	0.19	54,54,54,54	0
56	MG	BA	3700	1/1	0.98	0.10	26,26,26,26	0
56	MG	DA	3543	1/1	0.98	0.04	74,74,74,74	0
56	MG	BA	3276	1/1	0.98	0.13	57,57,57,57	0
56	MG	AA	1891	1/1	0.98	0.04	75,75,75,75	0
56	MG	BA	3079	1/1	0.98	0.15	54,54,54,54	0
56	MG	CA	1746	1/1	0.98	0.03	65,65,65,65	0
56	MG	BA	3080	1/1	0.98	0.14	44,44,44,44	0
56	MG	BB	216	1/1	0.98	0.10	38,38,38,38	0
56	MG	BA	3519	1/1	0.98	0.18	53,53,53,53	0
56	MG	DA	3394	1/1	0.98	0.05	36,36,36,36	0
56	MG	DA	3552	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3553	1/1	0.98	0.12	46,46,46,46	0
56	MG	BA	3320	1/1	0.98	0.17	58,58,58,58	0
56	MG	DA	3396	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3467	1/1	0.98	0.09	56,56,56,56	0
56	MG	BA	3180	1/1	0.98	0.16	41,41,41,41	0
56	MG	BA	3241	1/1	0.98	0.15	38,38,38,38	0
56	MG	BA	3809	1/1	0.98	0.09	40,40,40,40	0
56	MG	BA	3368	1/1	0.98	0.12	63,63,63,63	0
56	MG	BA	3525	1/1	0.98	0.05	40,40,40,40	0
56	MG	DA	3406	1/1	0.98	0.05	48,48,48,48	0
56	MG	DA	3408	1/1	0.98	0.09	71,71,71,71	0
56	MG	DA	3409	1/1	0.98	0.07	64,64,64,64	0
56	MG	BA	3813	1/1	0.98	0.04	66,66,66,66	0
56	MG	DA	3411	1/1	0.98	0.12	55,55,55,55	0
56	MG	BA	3007	1/1	0.98	0.11	91,91,91,91	0
56	MG	AA	1924	1/1	0.98	0.05	80,80,80,80	0
56	MG	BB	229	1/1	0.98	0.03	67,67,67,67	0
56	MG	BA	3816	1/1	0.98	0.05	85,85,85,85	0
56	MG	BA	3528	1/1	0.98	0.06	71,71,71,71	0
56	MG	BA	3606	1/1	0.98	0.07	63,63,63,63	0
56	MG	BD	303	1/1	0.98	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3720	1/1	0.98	0.08	22,22,22,22	0
56	MG	D0	103	1/1	0.98	0.10	55,55,55,55	0
56	MG	BD	305	1/1	0.98	0.08	54,54,54,54	0
56	MG	DA	3422	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3822	1/1	0.98	0.12	66,66,66,66	0
56	MG	BA	3721	1/1	0.98	0.09	23,23,23,23	0
56	MG	BA	3722	1/1	0.98	0.08	61,61,61,61	0
56	MG	DA	3581	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3059	1/1	0.98	0.13	25,25,25,25	0
56	MG	BE	305	1/1	0.98	0.05	22,22,22,22	0
56	MG	DA	3584	1/1	0.98	0.06	76,76,76,76	0
56	MG	DA	3428	1/1	0.98	0.06	53,53,53,53	0
56	MG	DA	3054	1/1	0.98	0.14	78,78,78,78	0
56	MG	AA	1878	1/1	0.98	0.07	46,46,46,46	0
57	ZN	DY	201	1/1	0.98	0.04	123,123,123,123	0
56	MG	BA	3609	1/1	0.98	0.06	53,53,53,53	0
57	ZN	D5	102	1/1	0.98	0.04	88,88,88,88	0
56	MG	DA	3589	1/1	0.98	0.06	81,81,81,81	0
56	MG	BF	303	1/1	0.98	0.05	41,41,41,41	0
56	MG	DA	3387	1/1	0.99	0.04	40,40,40,40	0
56	MG	BA	3666	1/1	0.99	0.03	28,28,28,28	0
56	MG	DA	3389	1/1	0.99	0.04	66,66,66,66	0
56	MG	BA	3667	1/1	0.99	0.03	27,27,27,27	0
56	MG	DA	3477	1/1	0.99	0.03	78,78,78,78	0
56	MG	BA	3168	1/1	0.99	0.14	27,27,27,27	0
56	MG	BA	3669	1/1	0.99	0.04	34,34,34,34	0
56	MG	DA	3571	1/1	0.99	0.03	57,57,57,57	0
56	MG	BA	3670	1/1	0.99	0.05	57,57,57,57	0
56	MG	BA	3671	1/1	0.99	0.03	41,41,41,41	0
56	MG	BA	3798	1/1	0.99	0.12	45,45,45,45	0
56	MG	BA	3574	1/1	0.99	0.07	36,36,36,36	0
56	MG	DA	3397	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3872	1/1	0.99	0.04	24,24,24,24	0
56	MG	DA	3486	1/1	0.99	0.09	42,42,42,42	0
56	MG	BA	3601	1/1	0.99	0.04	24,24,24,24	0
56	MG	BA	3674	1/1	0.99	0.04	27,27,27,27	0
56	MG	DA	3677	1/1	0.99	0.13	51,51,51,51	0
56	MG	BA	3676	1/1	0.99	0.04	20,20,20,20	0
56	MG	DA	3402	1/1	0.99	0.07	38,38,38,38	0
56	MG	BA	3876	1/1	0.99	0.05	54,54,54,54	0
56	MG	DA	3404	1/1	0.99	0.08	56,56,56,56	0
56	MG	BA	3677	1/1	0.99	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3679	1/1	0.99	0.03	34,34,34,34	0
56	MG	BA	3064	1/1	0.99	0.14	41,41,41,41	0
56	MG	DA	3496	1/1	0.99	0.07	47,47,47,47	0
56	MG	BA	3681	1/1	0.99	0.07	52,52,52,52	0
56	MG	DA	3498	1/1	0.99	0.03	51,51,51,51	0
56	MG	BA	3682	1/1	0.99	0.07	28,28,28,28	0
56	MG	AA	1861	1/1	0.99	0.06	71,71,71,71	0
56	MG	DA	3501	1/1	0.99	0.07	81,81,81,81	0
56	MG	BA	3451	1/1	0.99	0.12	47,47,47,47	0
56	MG	BA	3810	1/1	0.99	0.03	27,27,27,27	0
56	MG	BA	3164	1/1	0.99	0.14	26,26,26,26	0
56	MG	BA	3686	1/1	0.99	0.04	26,26,26,26	0
56	MG	BA	3541	1/1	0.99	0.03	35,35,35,35	0
56	MG	DA	3599	1/1	0.99	0.13	50,50,50,50	0
56	MG	BA	3559	1/1	0.99	0.06	53,53,53,53	0
56	MG	BA	3690	1/1	0.99	0.05	27,27,27,27	0
56	MG	BA	3751	1/1	0.99	0.07	56,56,56,56	0
56	MG	BA	3817	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3134	1/1	0.99	0.07	35,35,35,35	0
56	MG	BA	3694	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3513	1/1	0.99	0.07	59,59,59,59	0
56	MG	BA	3695	1/1	0.99	0.02	29,29,29,29	0
56	MG	BA	3821	1/1	0.99	0.04	76,76,76,76	0
56	MG	BA	3640	1/1	0.99	0.03	33,33,33,33	0
56	MG	BA	3243	1/1	0.99	0.19	35,35,35,35	0
56	MG	BA	3758	1/1	0.99	0.07	60,60,60,60	0
56	MG	BA	3698	1/1	0.99	0.04	44,44,44,44	0
56	MG	BA	3699	1/1	0.99	0.04	38,38,38,38	0
56	MG	BA	3610	1/1	0.99	0.06	41,41,41,41	0
56	MG	BA	3762	1/1	0.99	0.04	48,48,48,48	0
56	MG	DA	3433	1/1	0.99	0.10	46,46,46,46	0
56	MG	BA	3701	1/1	0.99	0.07	26,26,26,26	0
56	MG	BA	3643	1/1	0.99	0.02	54,54,54,54	0
56	MG	DA	3526	1/1	0.99	0.03	64,64,64,64	0
56	MG	BA	3443	1/1	0.99	0.06	41,41,41,41	0
56	MG	BA	3645	1/1	0.99	0.05	46,46,46,46	0
56	MG	AA	1935	1/1	0.99	0.09	56,56,56,56	0
56	MG	BA	3586	1/1	0.99	0.04	52,52,52,52	0
56	MG	BA	3707	1/1	0.99	0.03	25,25,25,25	0
56	MG	BA	3587	1/1	0.99	0.08	48,48,48,48	0
56	MG	BA	3838	1/1	0.99	0.05	28,28,28,28	0
56	MG	BA	3530	1/1	0.99	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3650	1/1	0.99	0.04	46,46,46,46	0
56	MG	BA	3773	1/1	0.99	0.03	44,44,44,44	0
56	MG	DA	3446	1/1	0.99	0.10	40,40,40,40	0
56	MG	DA	3447	1/1	0.99	0.06	62,62,62,62	0
56	MG	BA	3566	1/1	0.99	0.06	54,54,54,54	0
56	MG	BA	3590	1/1	0.99	0.06	56,56,56,56	0
56	MG	BA	3618	1/1	0.99	0.04	46,46,46,46	0
56	MG	BA	3715	1/1	0.99	0.09	21,21,21,21	0
56	MG	BA	3846	1/1	0.99	0.06	27,27,27,27	0
56	MG	BA	3434	1/1	0.99	0.19	22,22,22,22	0
56	MG	DA	3638	1/1	0.99	0.08	48,48,48,48	0
56	MG	BA	3518	1/1	0.99	0.12	33,33,33,33	0
56	MG	AA	1929	1/1	0.99	0.10	48,48,48,48	0
56	MG	DA	3642	1/1	0.99	0.04	71,71,71,71	0
56	MG	BA	3534	1/1	0.99	0.08	44,44,44,44	0
56	MG	BA	3595	1/1	0.99	0.03	45,45,45,45	0
56	MG	DA	3458	1/1	0.99	0.05	49,49,49,49	0
56	MG	BA	3551	1/1	0.99	0.03	68,68,68,68	0
56	MG	BA	3660	1/1	0.99	0.02	28,28,28,28	0
56	MG	BA	3854	1/1	0.99	0.05	25,25,25,25	0
56	MG	DA	3080	1/1	0.99	0.26	36,36,36,36	0
56	MG	BA	3723	1/1	0.99	0.04	51,51,51,51	0
56	MG	BA	3390	1/1	0.99	0.08	28,28,28,28	0
57	ZN	BY	201	1/1	0.99	0.04	70,70,70,70	0
56	MG	BA	3787	1/1	0.99	0.04	35,35,35,35	0
57	ZN	B6	101	1/1	0.99	0.03	48,48,48,48	0
57	ZN	B9	101	1/1	0.99	0.02	51,51,51,51	0
56	MG	BA	3598	1/1	0.99	0.04	54,54,54,54	0
56	MG	BA	3789	1/1	0.99	0.04	41,41,41,41	0
56	MG	BA	3860	1/1	0.99	0.02	57,57,57,57	0
56	MG	BA	3664	1/1	0.99	0.06	31,31,31,31	0
56	MG	BA	3862	1/1	0.99	0.09	59,59,59,59	0
56	MG	DA	3385	1/1	0.99	0.05	48,48,48,48	0
56	MG	BA	3627	1/1	0.99	0.07	56,56,56,56	0
56	MG	B6	102	1/1	1.00	0.07	73,73,73,73	0
56	MG	BA	3675	1/1	1.00	0.03	33,33,33,33	0
56	MG	DA	3641	1/1	1.00	0.04	50,50,50,50	0
56	MG	BA	3711	1/1	1.00	0.05	24,24,24,24	0
56	MG	B8	102	1/1	1.00	0.03	49,49,49,49	0
56	MG	BA	3691	1/1	1.00	0.03	31,31,31,31	0
56	MG	BA	3692	1/1	1.00	0.03	30,30,30,30	0
56	MG	BA	3825	1/1	1.00	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3747	1/1	1.00	0.04	20,20,20,20	0
56	MG	BA	3565	1/1	1.00	0.03	34,34,34,34	0
56	MG	DA	3420	1/1	1.00	0.03	38,38,38,38	0
57	ZN	B5	104	1/1	1.00	0.04	75,75,75,75	0
56	MG	BA	3583	1/1	1.00	0.04	22,22,22,22	0
56	MG	BA	3678	1/1	1.00	0.03	22,22,22,22	0
56	MG	BA	3662	1/1	1.00	0.02	30,30,30,30	0
56	MG	BA	3630	1/1	1.00	0.05	23,23,23,23	0
56	MG	BA	3631	1/1	1.00	0.01	25,25,25,25	0
56	MG	DA	3407	1/1	1.00	0.03	44,44,44,44	0
56	MG	BB	221	1/1	1.00	0.03	44,44,44,44	0
56	MG	BA	3689	1/1	1.00	0.02	25,25,25,25	0
56	MG	BA	3755	1/1	1.00	0.04	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.