



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2024 – 12:48 PM EDT

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

This is a wwPDB 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

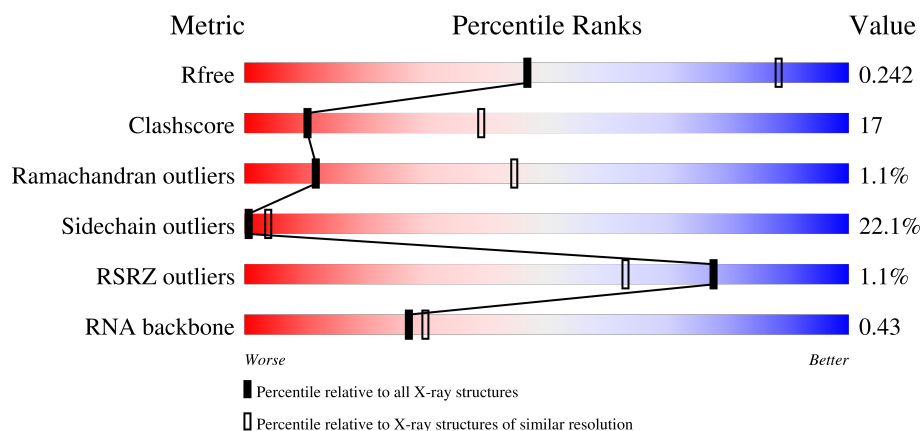
1 Overall quality at a glance

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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (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	<div> <div>25%</div> <div>43%</div> <div>23%</div> <div>6%</div> <div>•</div> </div>
1	CA	1522	<div> <div>29%</div> <div>43%</div> <div>20%</div> <div>•</div> <div>•</div> </div>
2	AB	256	<div> <div>36%</div> <div>42%</div> <div>12%</div> <div>9%</div> <div>•</div> </div>
2	CB	256	<div> <div>31%</div> <div>49%</div> <div>11%</div> <div>8%</div> <div>•</div> </div>


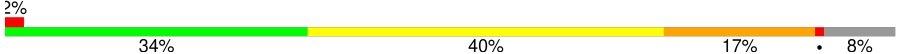
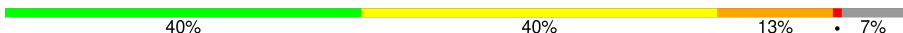


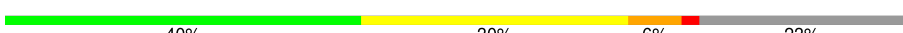
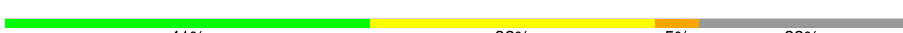









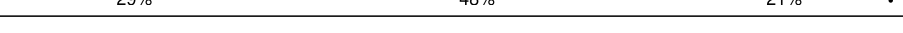



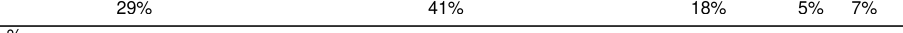
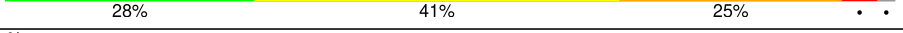
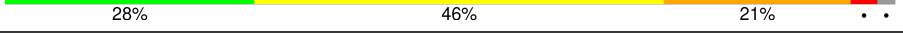


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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


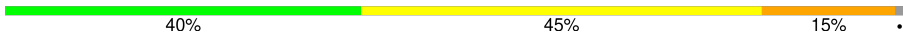









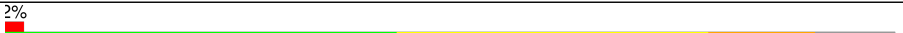













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Mol	Chain	Length	Quality of chain
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	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	1658	-	-	-	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
56	MG	DA	3258	-	-	-	X

2 Entry composition [i](#)

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			
			657	407	129	121	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called YAEJ.

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

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

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

- Molecule 24 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
30	DG	180	Total	C	N	O	S	0	0	0
			1361	874	241	243	3			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
50	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
51	D5	59	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

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

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

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

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

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

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

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

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

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

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

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

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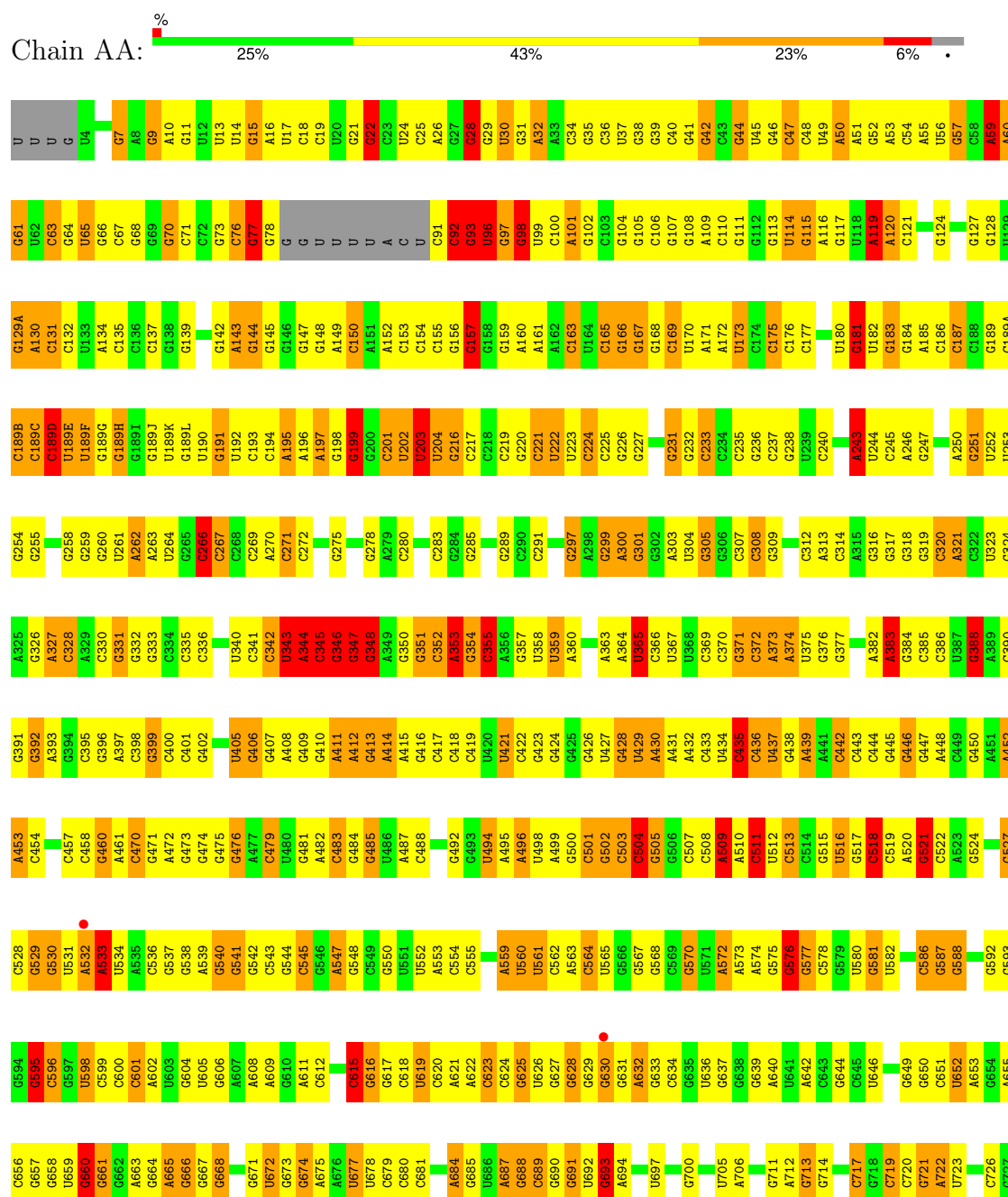
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	D1	3	Total 3	O 3	0	0
58	D3	1	Total 1	O 1	0	0
58	D6	2	Total 2	O 2	0	0
58	D7	2	Total 2	O 2	0	0
58	D8	4	Total 4	O 4	0	0

3 Residue-property plots

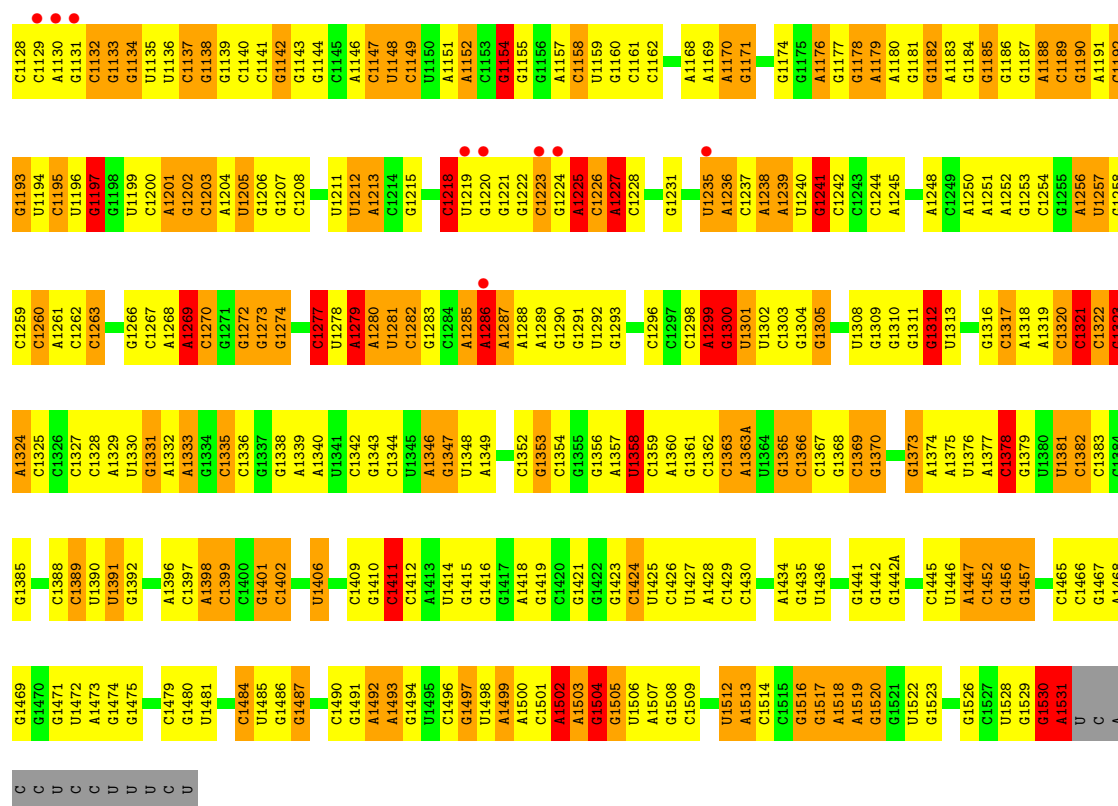
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

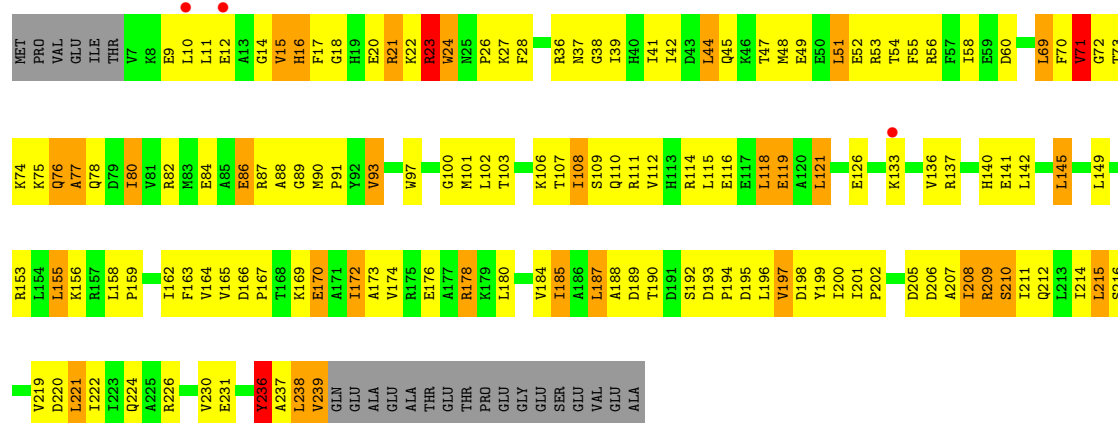




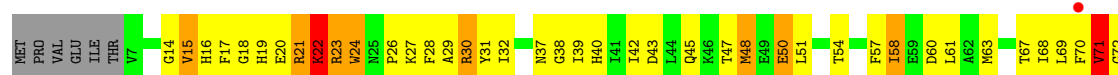


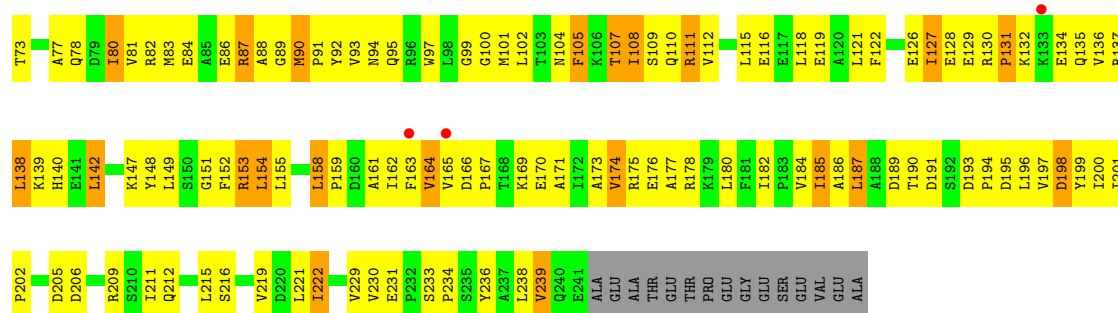


• Molecule 2: 30S Ribosomal Protein S2

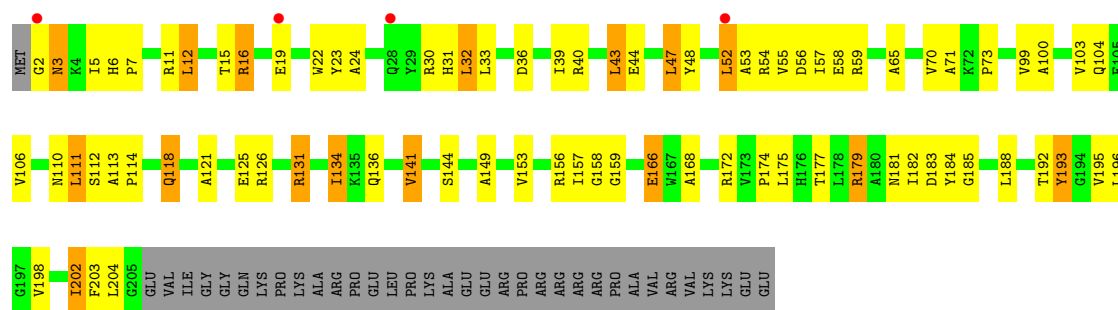


• Molecule 2: 30S Ribosomal Protein S2

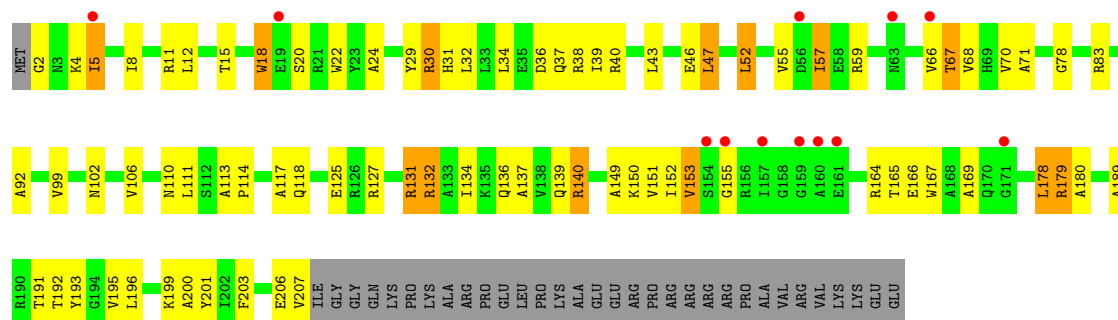




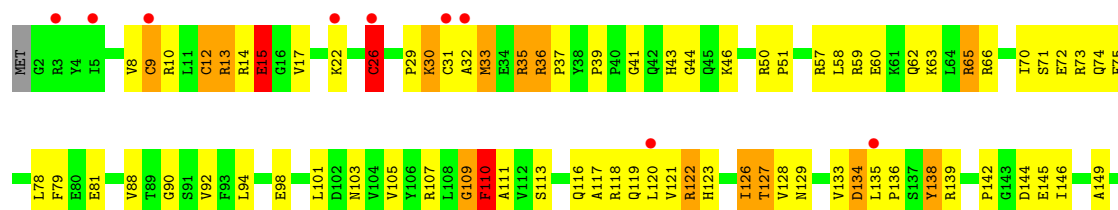
• Molecule 3: 30S Ribosomal Protein S3

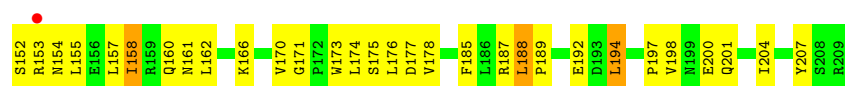


• Molecule 3: 30S Ribosomal Protein S3

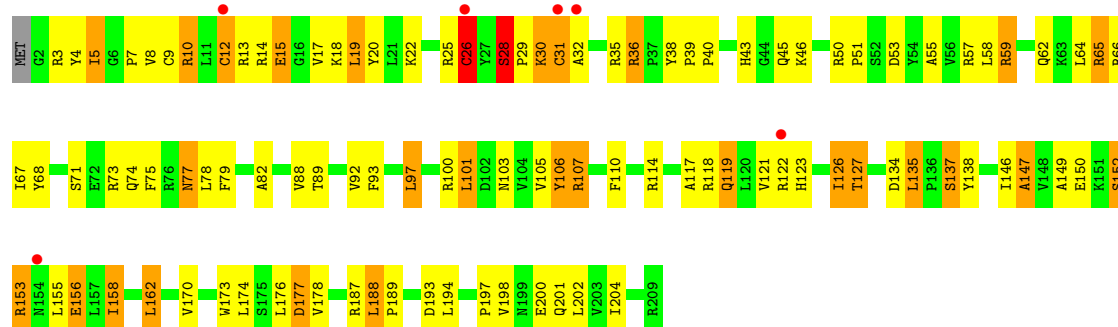


• Molecule 4: 30S Ribosomal Protein S4

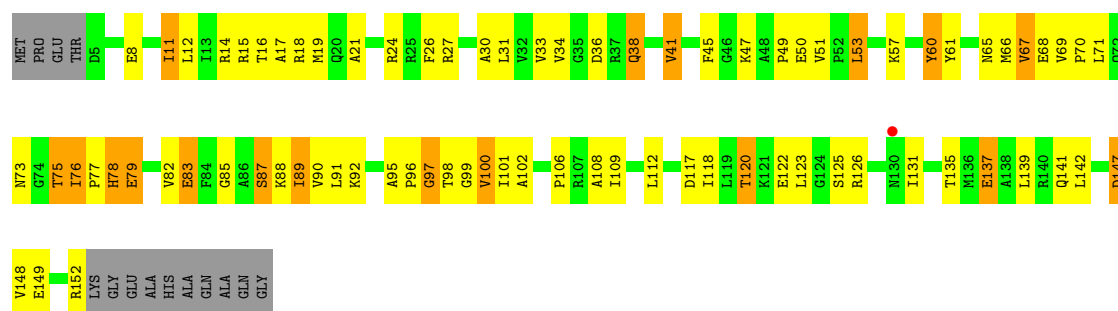
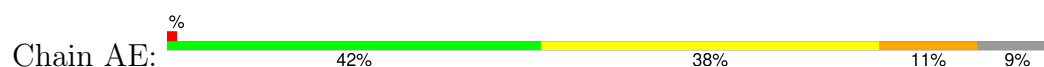




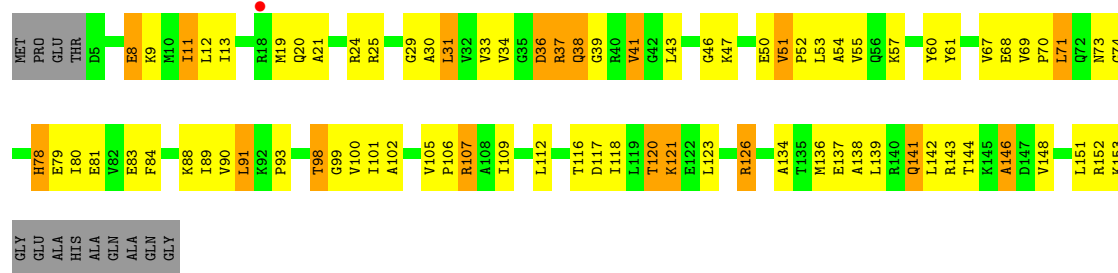
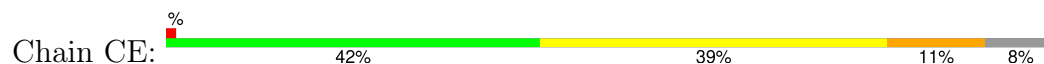
• Molecule 4: 30S Ribosomal Protein S4



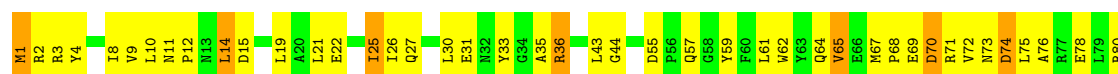
• Molecule 5: 30S Ribosomal Protein S5

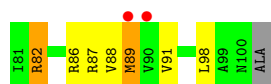


• Molecule 5: 30S Ribosomal Protein S5



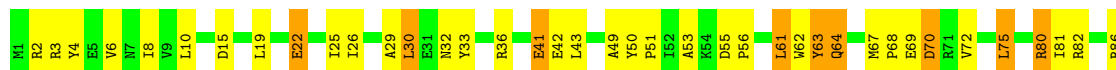
• Molecule 6: 30S Ribosomal Protein S6





• Molecule 6: 30S Ribosomal Protein S6

Chain CF: 57% 33% 9% .



• Molecule 7: 30S Ribosomal Protein S7

Chain AG: 56% 33% 10% .



• Molecule 7: 30S Ribosomal Protein S7

Chain CG: 56% 33% 9% ..



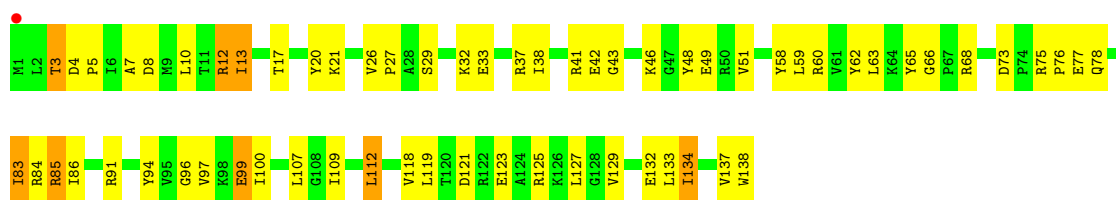
• Molecule 8: 30S Ribosomal Protein S8

Chain AH: 52% 41% 7%

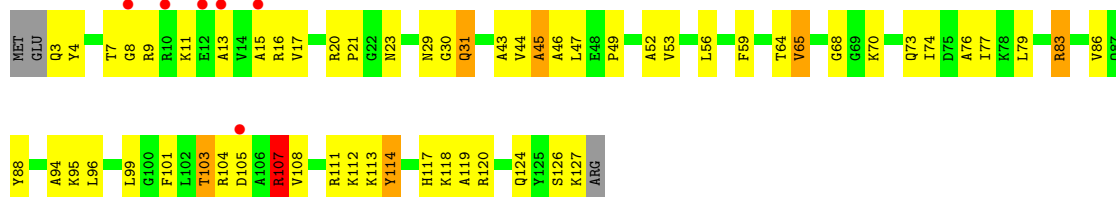


• Molecule 8: 30S Ribosomal Protein S8

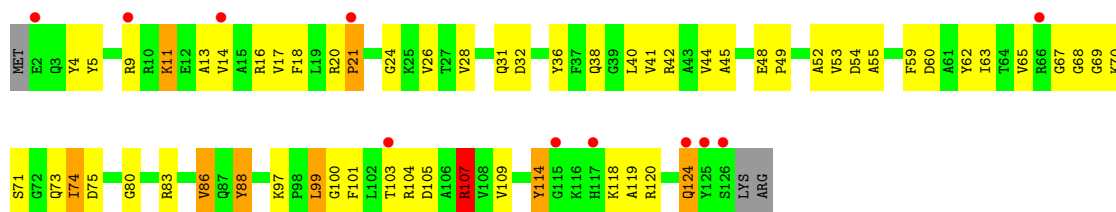
Chain CH: 54% 40% 6%



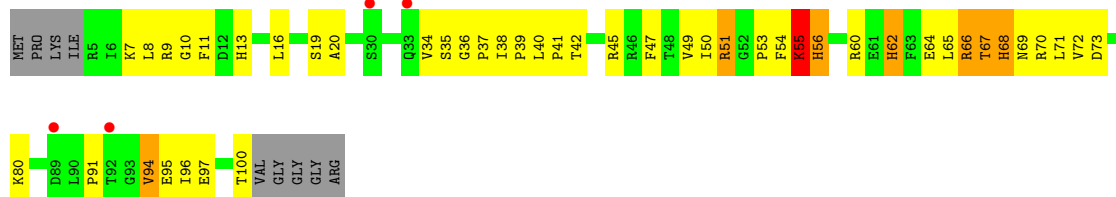
• Molecule 9: 30S Ribosomal Protein S9



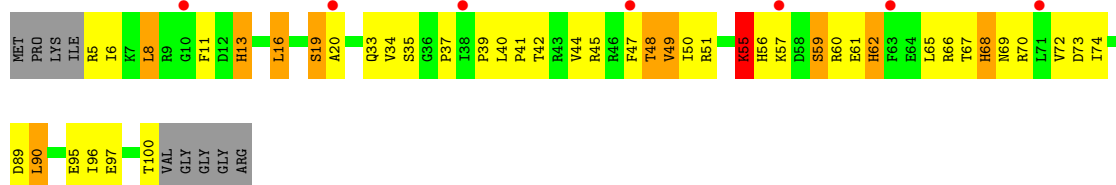
• Molecule 9: 30S Ribosomal Protein S9



• Molecule 10: 30S Ribosomal Protein S10

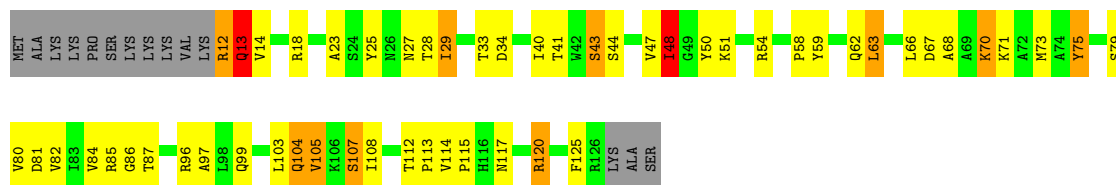


• Molecule 10: 30S Ribosomal Protein S10



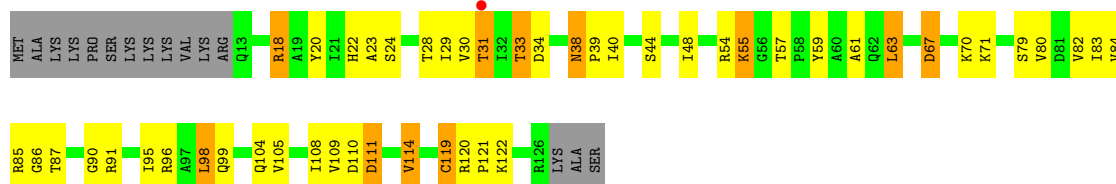
• Molecule 11: 30S Ribosomal Protein S11

Chain AK: 



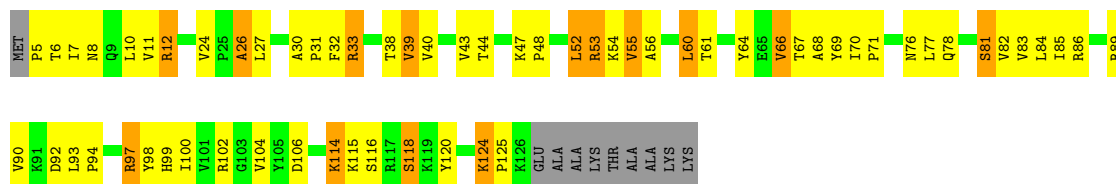
• Molecule 11: 30S Ribosomal Protein S11

Chain CK: 



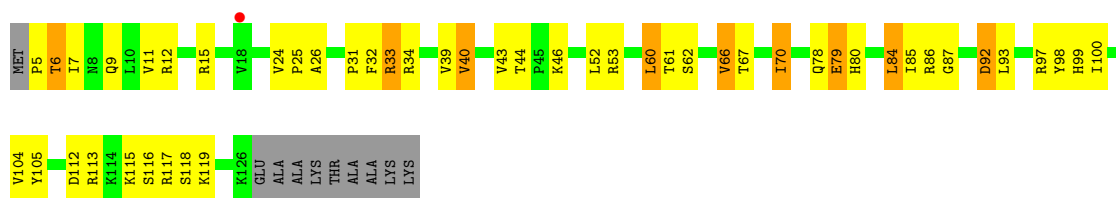
• Molecule 12: 30S Ribosomal Protein S12

Chain AL: 



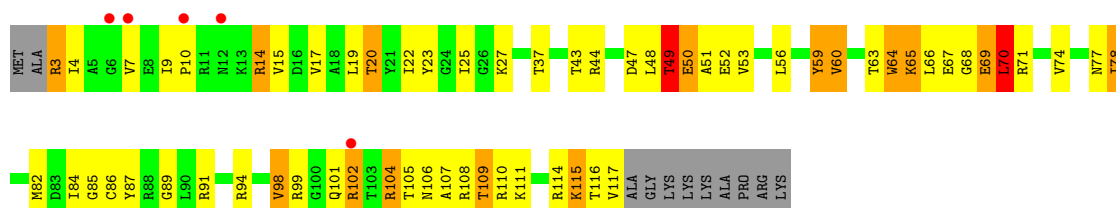
• Molecule 12: 30S Ribosomal Protein S12

Chain CL: 

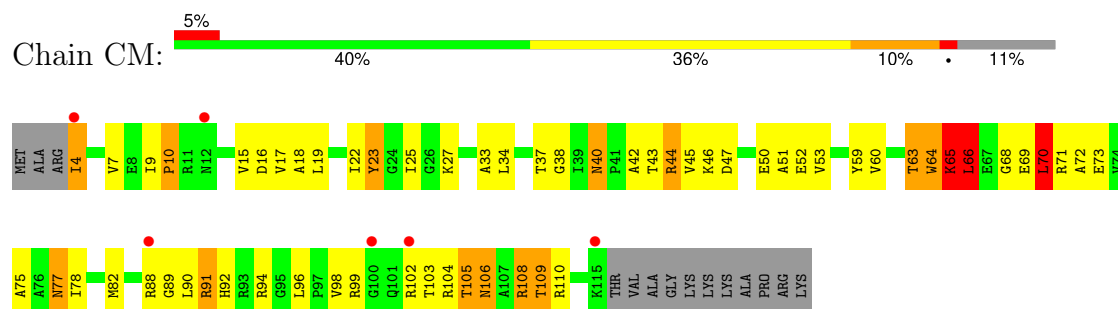


• Molecule 13: 30S Ribosomal Protein S13

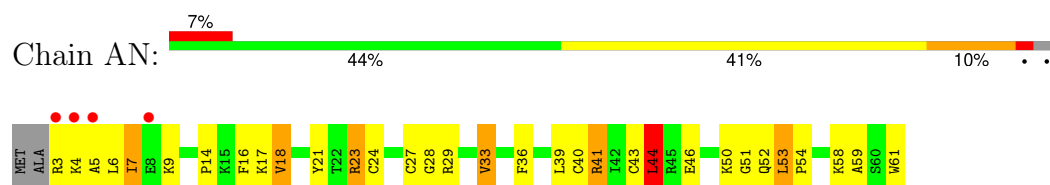
Chain AM: 



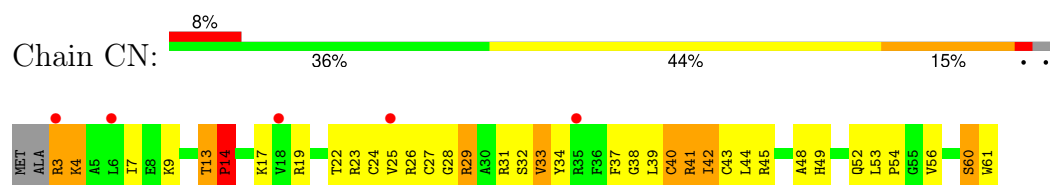
- Molecule 13: 30S Ribosomal Protein S13



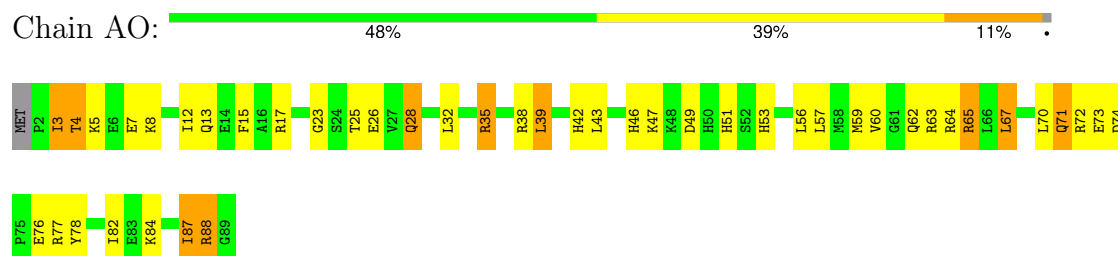
- Molecule 14: 30S Ribosomal Protein S14



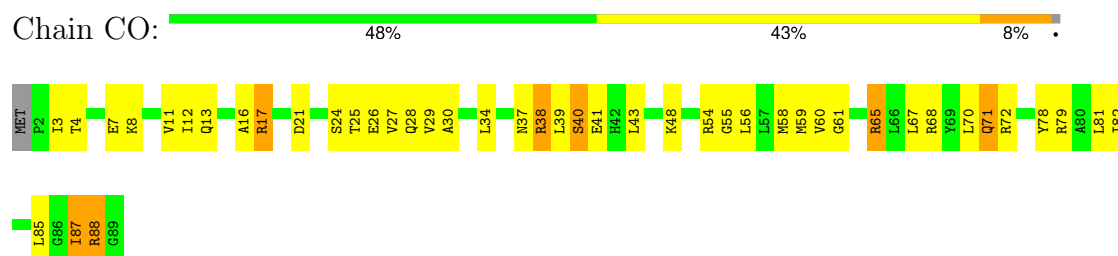
- Molecule 14: 30S Ribosomal Protein S14



- Molecule 15: 30S Ribosomal Protein S15

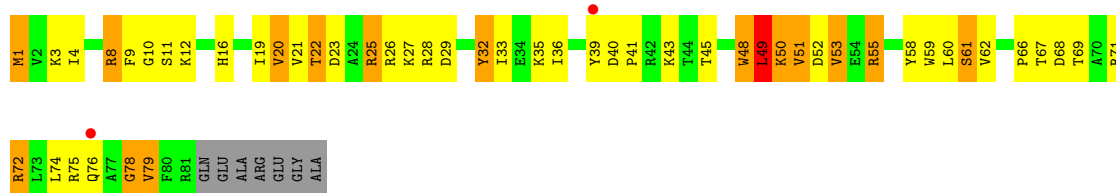


- Molecule 15: 30S Ribosomal Protein S15



- Molecule 16: 30S Ribosomal Protein S16





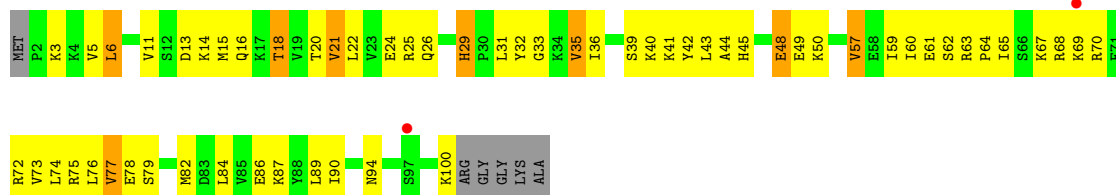
• Molecule 16: 30S Ribosomal Protein S16

Chain CP: 40% 40% 13% 7%



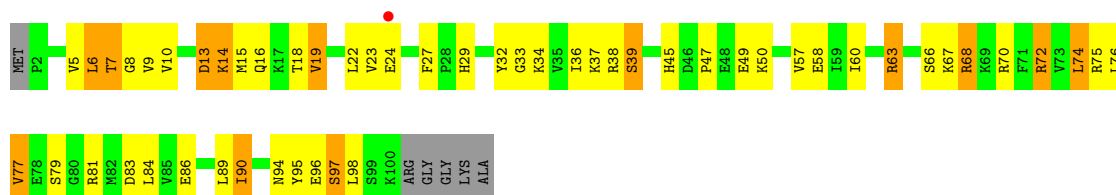
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ: 2% 38% 49% 8% 6%



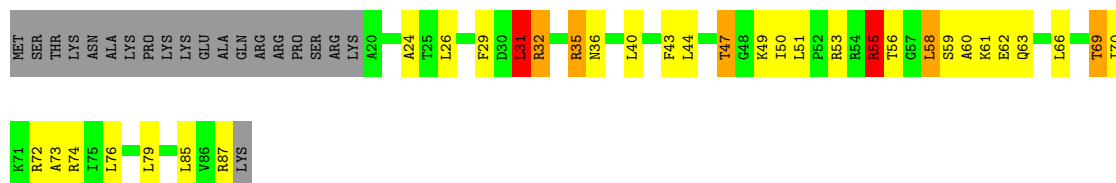
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ: 44% 38% 12% 6%



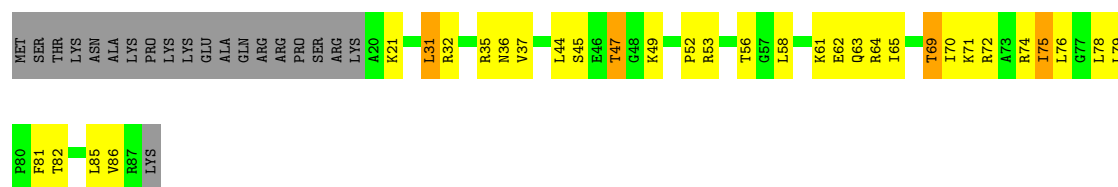
• Molecule 18: 30S Ribosomal Protein S18

Chain AR: 40% 30% 6% 23%



• Molecule 18: 30S Ribosomal Protein S18

Chain CR: 




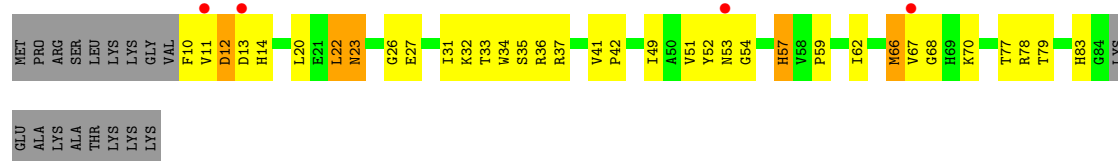
• Molecule 19: 30S Ribosomal Protein S19

Chain AS: 



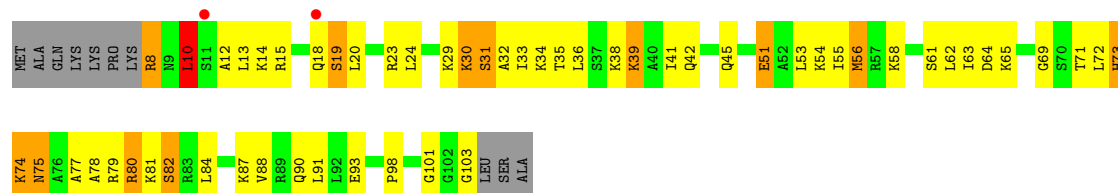
• Molecule 19: 30S Ribosomal Protein S19

Chain CS: 



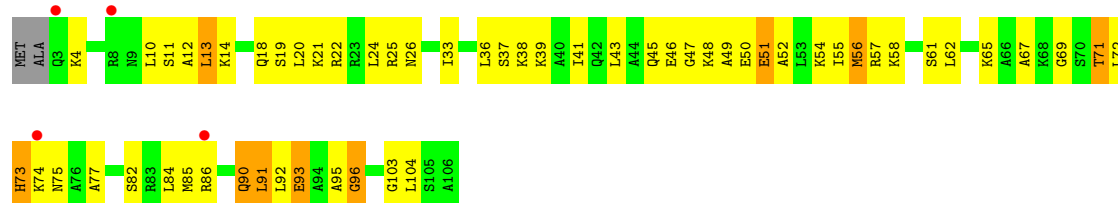
• Molecule 20: 30S Ribosomal Protein S20

Chain AT: 



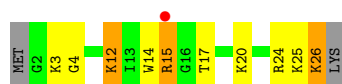
• Molecule 20: 30S Ribosomal Protein S20

Chain CT: 



• Molecule 21: 30S Ribosomal Protein THX

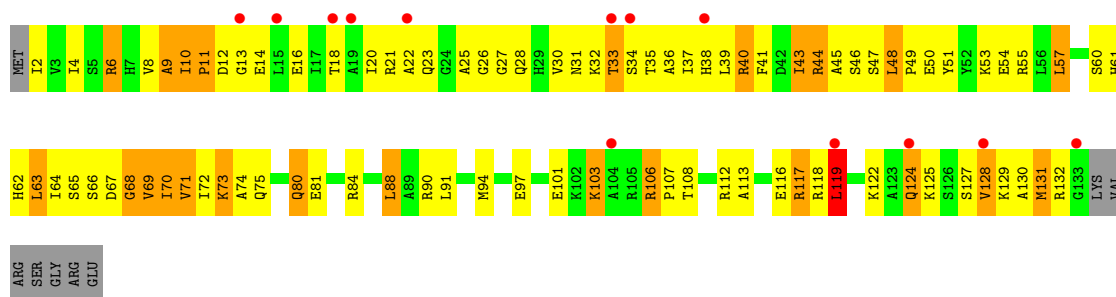
Chain AU: 



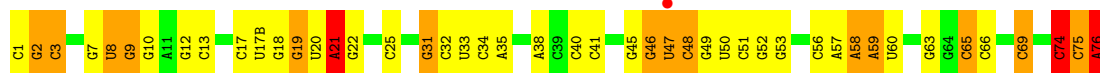
• Molecule 21: 30S Ribosomal Protein THX



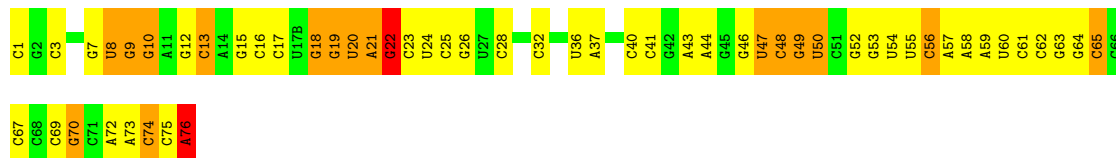
• Molecule 22: YAEJ



• Molecule 23: P-site fMet-tRNA



• Molecule 23: P-site fMet-tRNA

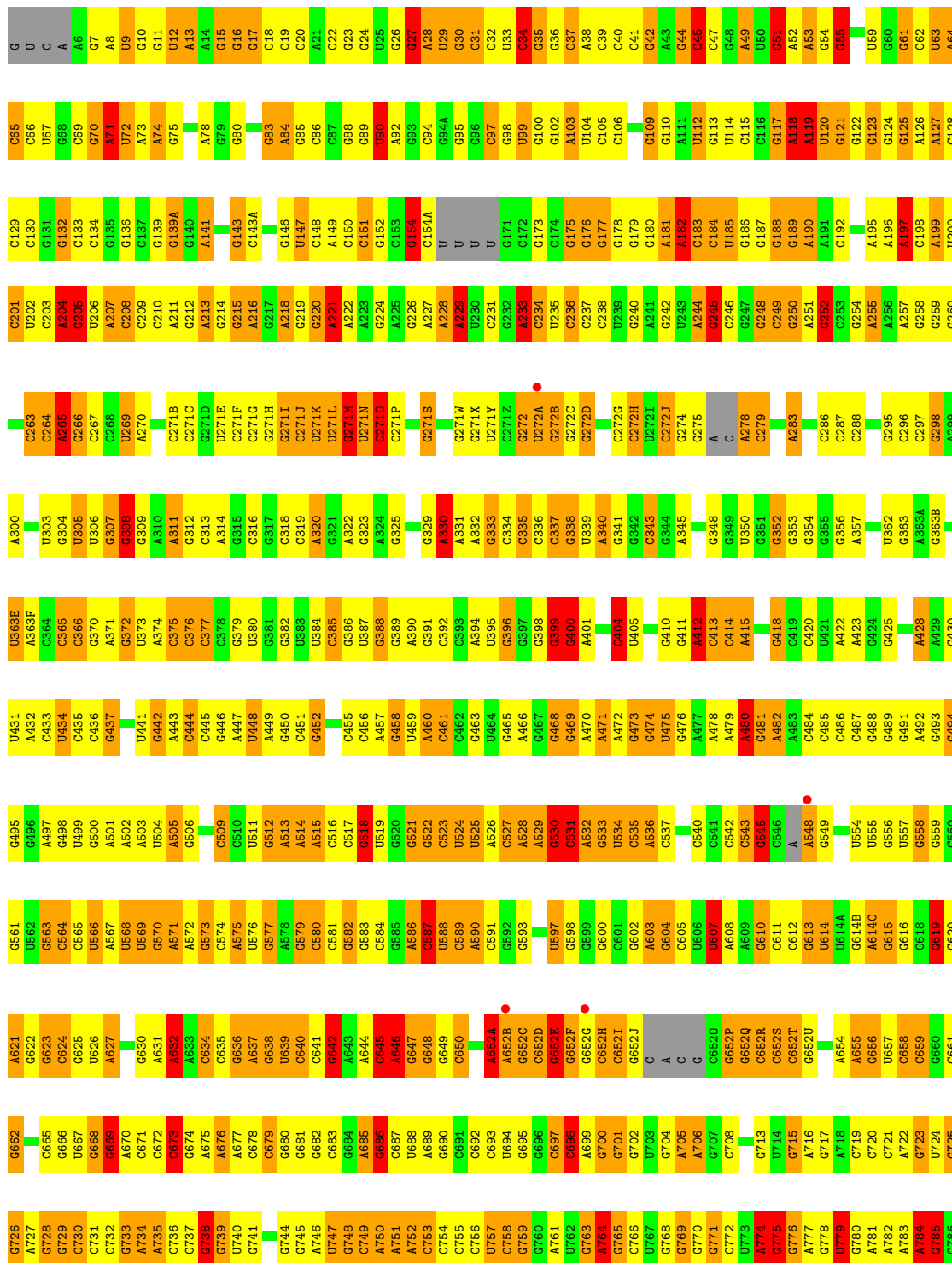


• Molecule 24: mRNA



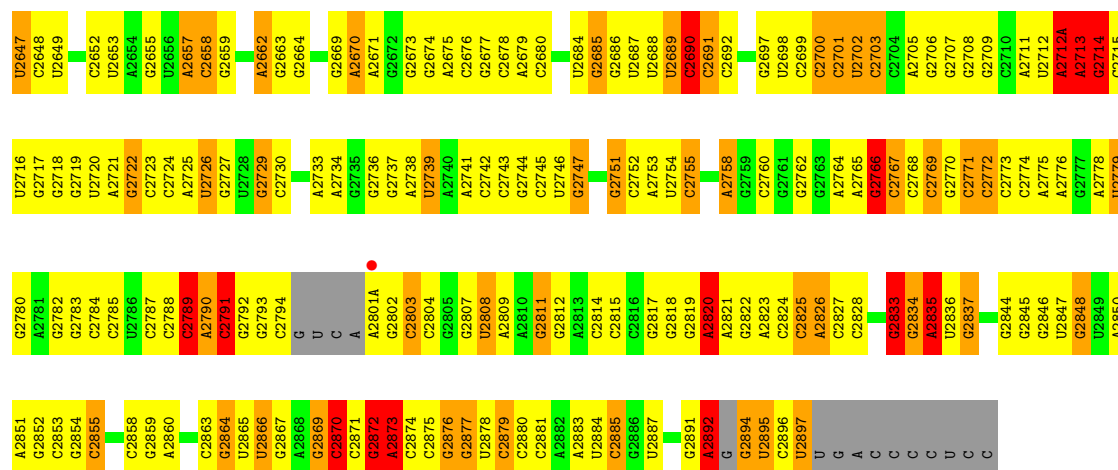
• Molecule 24: mRNA





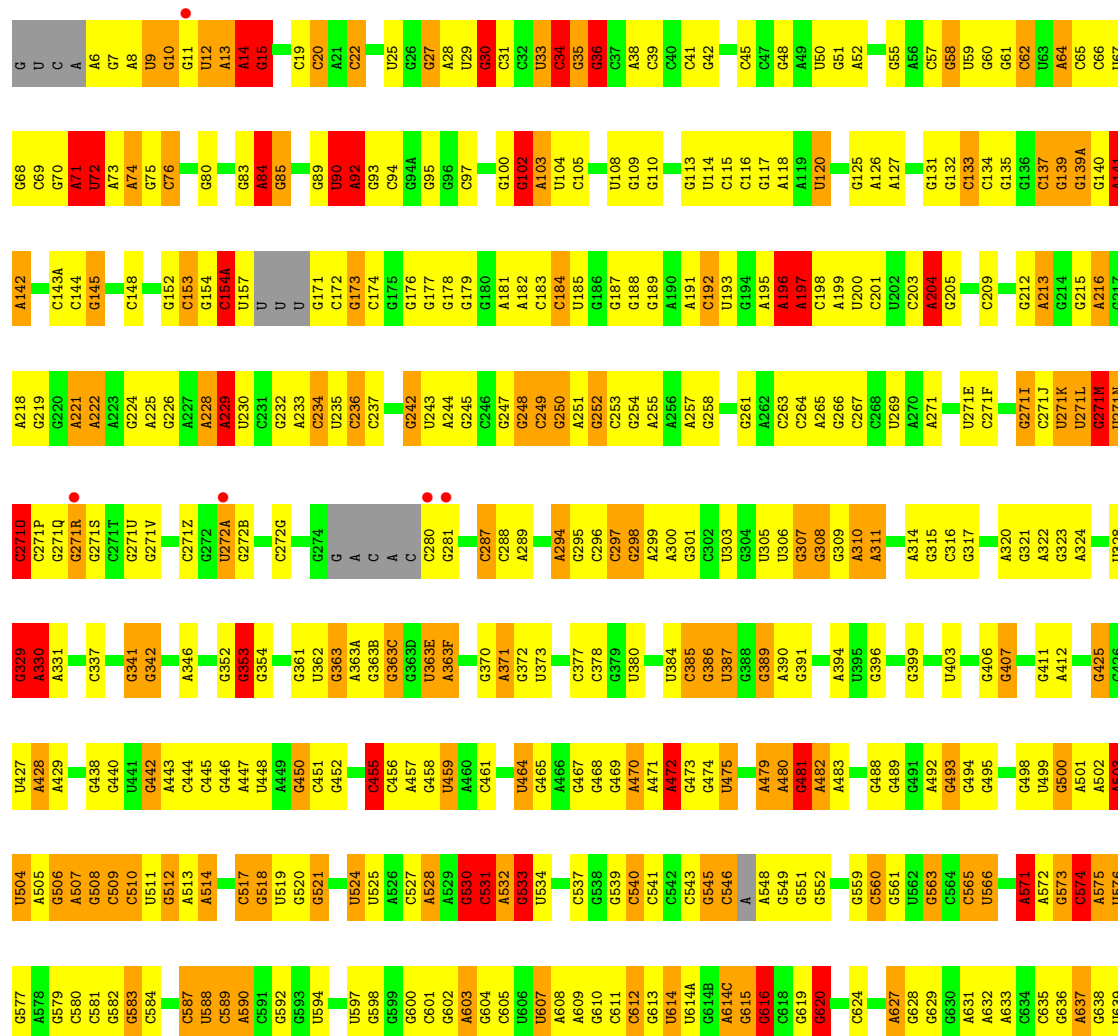






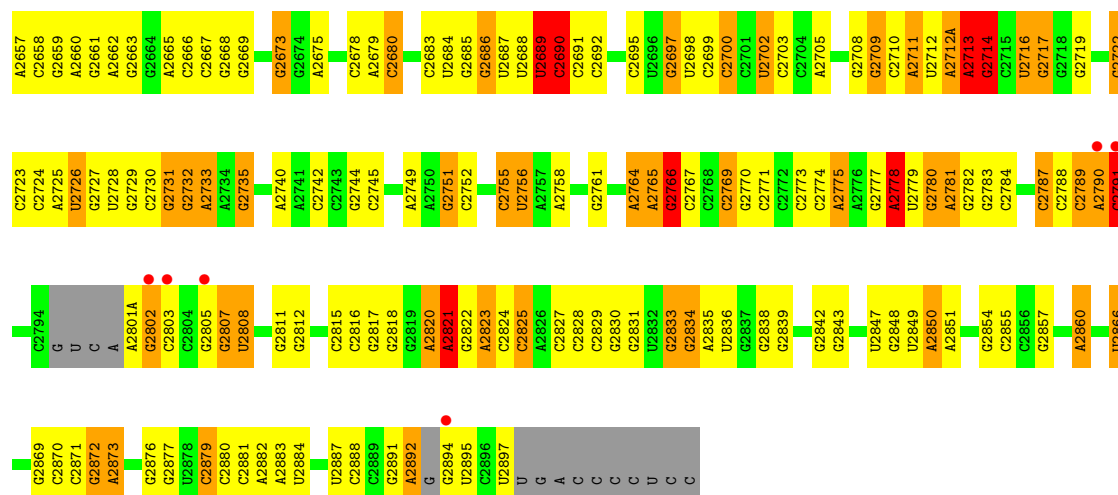
Molecule 25: 23S Ribosomal RNA

Chain DA: 29% 41% 18% 5% 7%





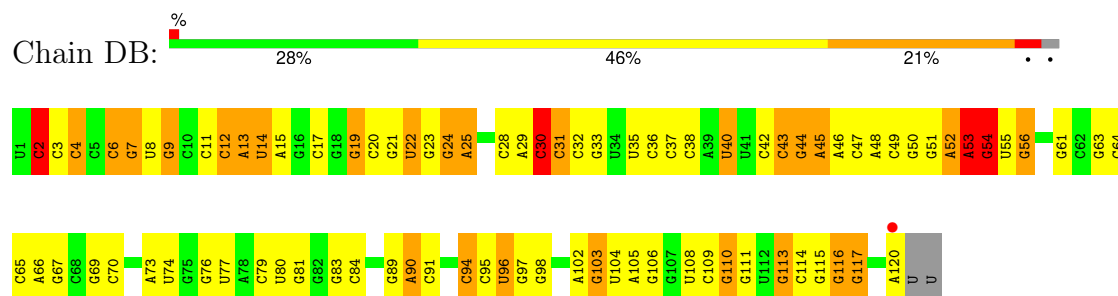
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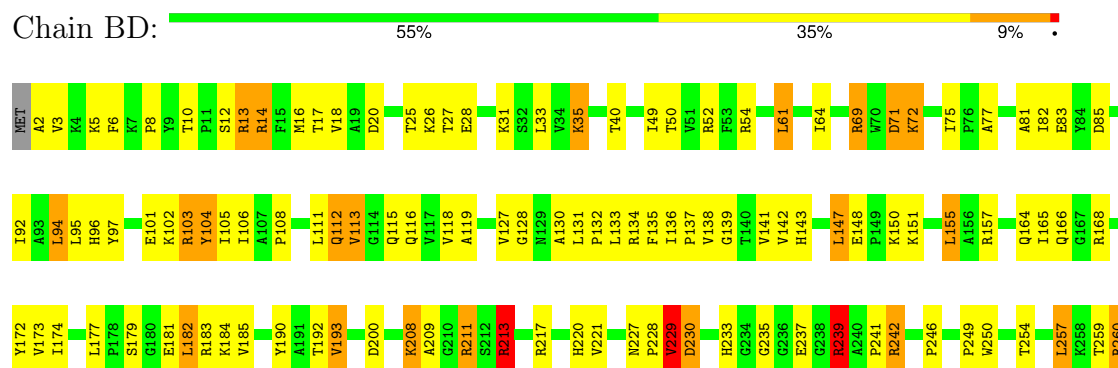
• Molecule 26: 5S Ribosomal RNA



• Molecule 26: 5S Ribosomal RNA



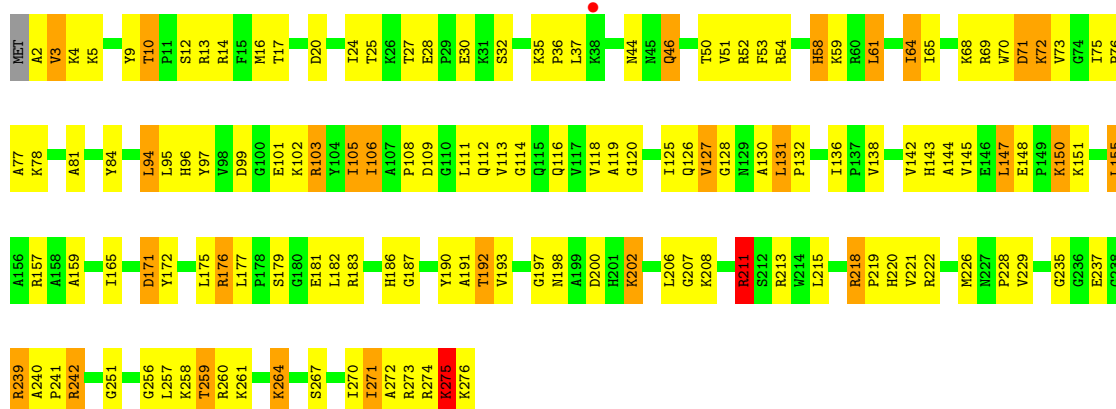
• Molecule 27: 50S Ribosomal Protein L2





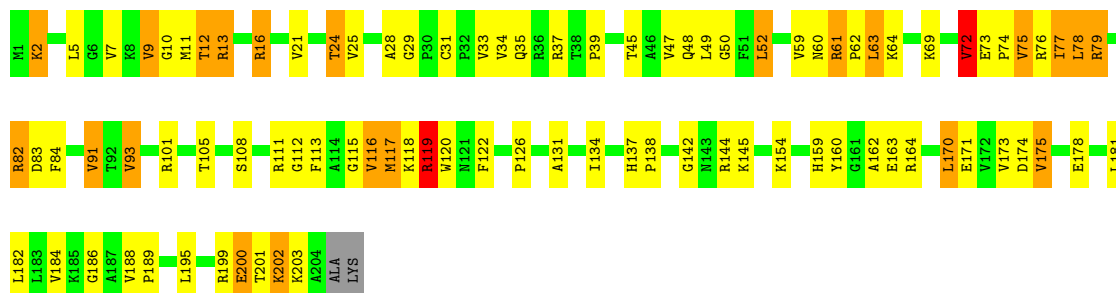
• Molecule 27: 50S Ribosomal Protein L2

Chain DD: 49% 41% 10% .



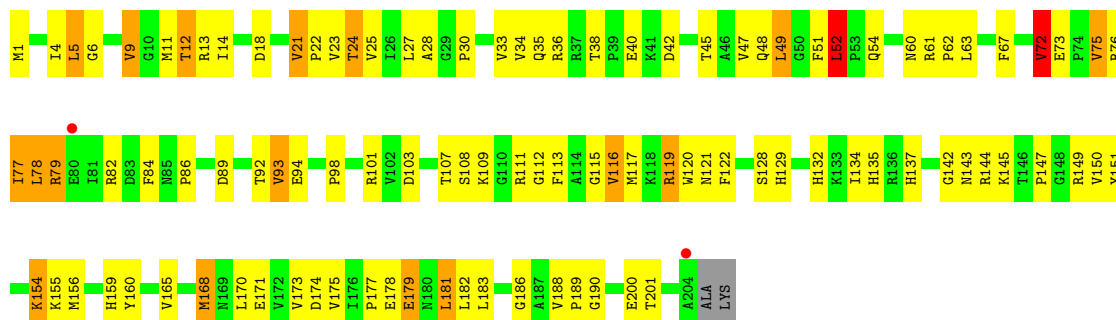
• Molecule 28: 50S Ribosomal Protein L3

Chain BE: 55% 33% 11% ..



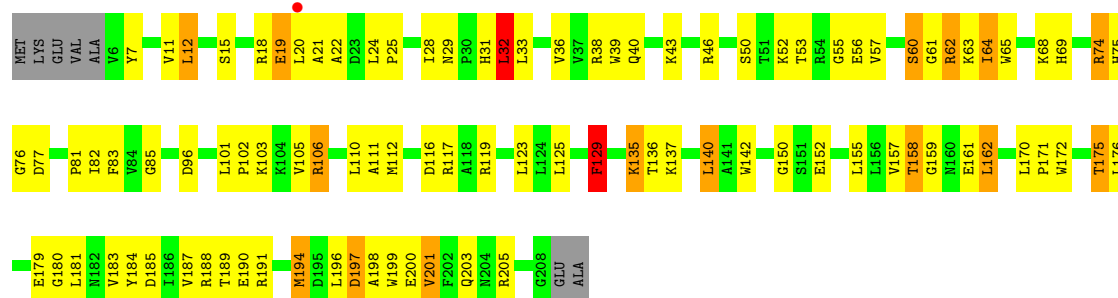
• Molecule 28: 50S Ribosomal Protein L3

Chain DE: 48% 42% 8% ..

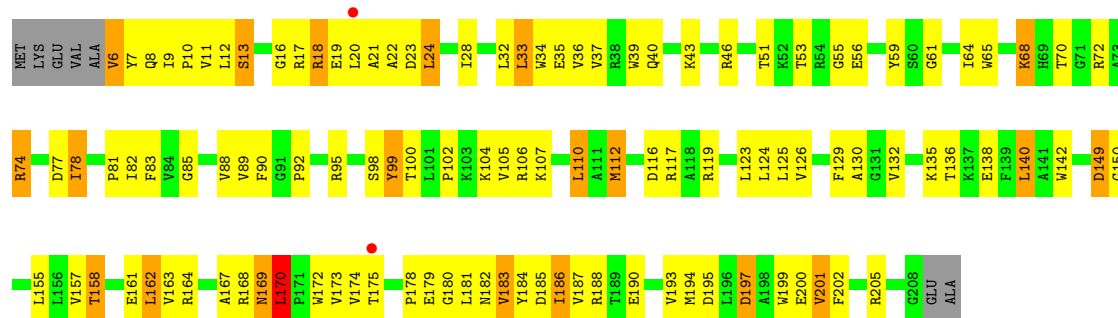


• Molecule 29: 50S Ribosomal Protein L4

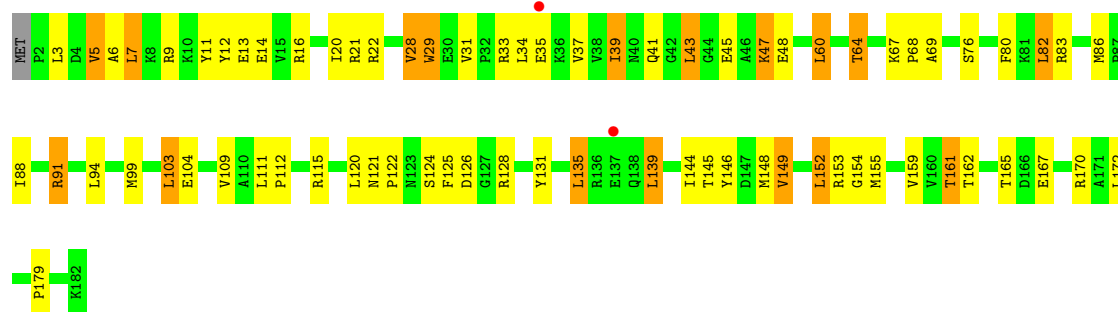
Chain BF: 50% 38% 7% ..



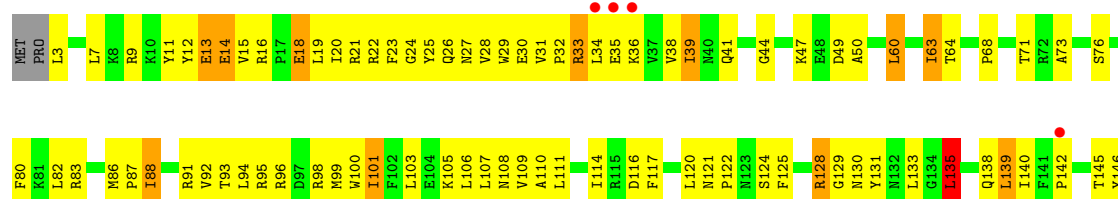
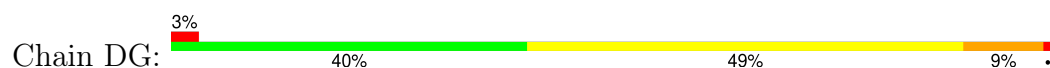
• Molecule 29: 50S Ribosomal Protein L4



• Molecule 30: 50S Ribosomal Protein L5

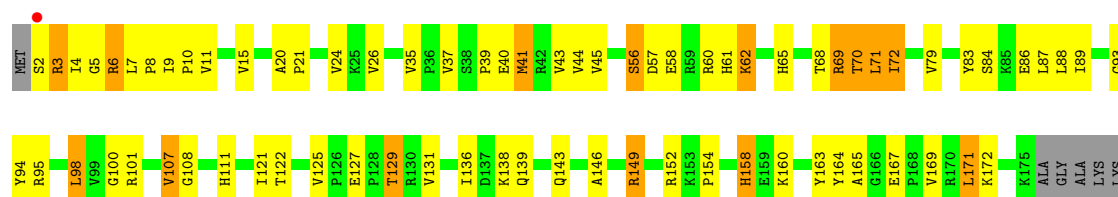


• Molecule 30: 50S Ribosomal Protein L5





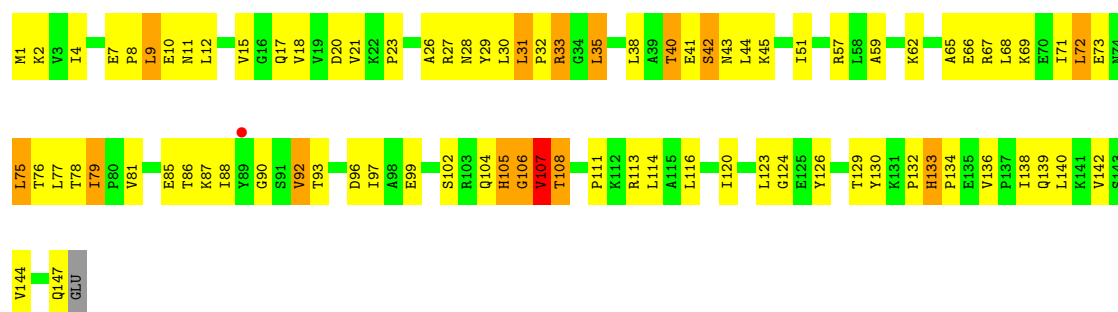
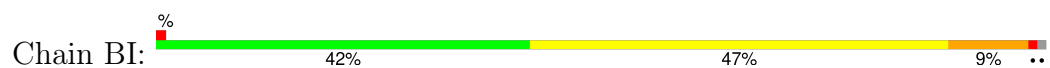
• Molecule 31: 50S Ribosomal Protein L6



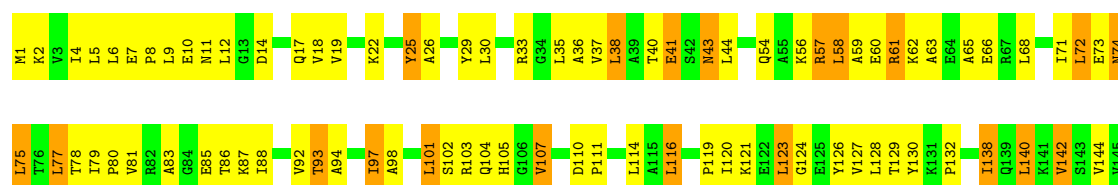
• Molecule 31: 50S Ribosomal Protein L6



• Molecule 32: 50S Ribosomal Protein L9



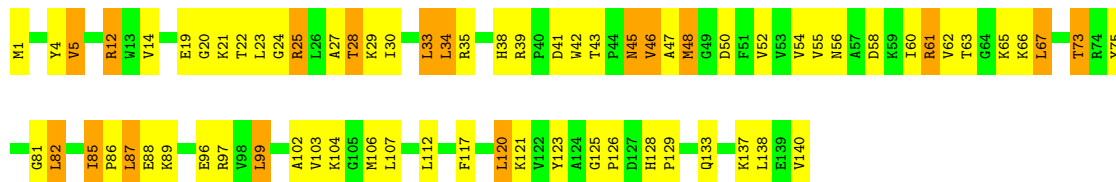
• Molecule 32: 50S Ribosomal Protein L9





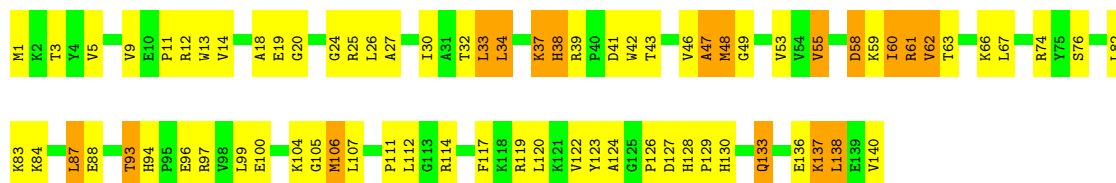
• Molecule 33: 50S Ribosomal Protein L13

Chain BN: 49% 39% 12%



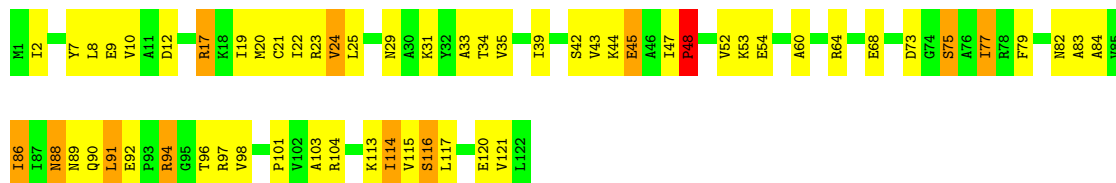
• Molecule 33: 50S Ribosomal Protein L13

Chain DN: 46% 41% 12%



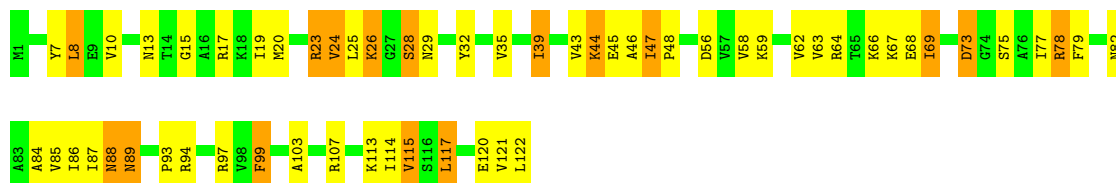
• Molecule 34: 50S Ribosomal Protein L14

Chain BO: 52% 39% 9%



• Molecule 34: 50S Ribosomal Protein L14

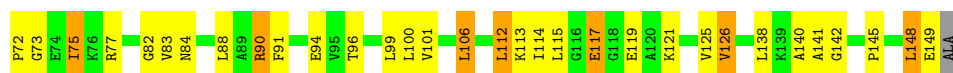
Chain DO: 52% 34% 13%



• Molecule 35: 50S Ribosomal Protein L15

Chain BP: 50% 36% 13%

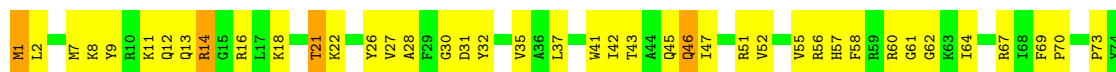




• Molecule 35: 50S Ribosomal Protein L15



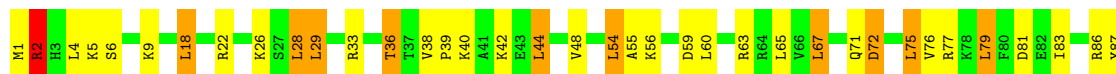
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 36: 50S Ribosomal Protein L16

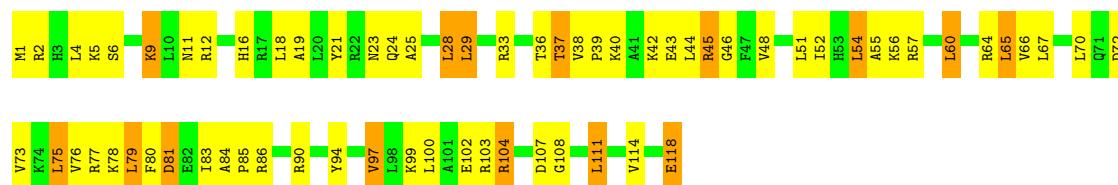


• Molecule 37: 50S Ribosomal Protein L17

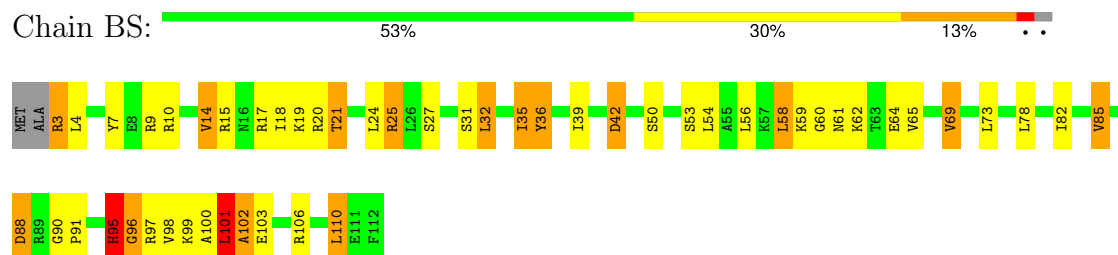


• Molecule 37: 50S Ribosomal Protein L17

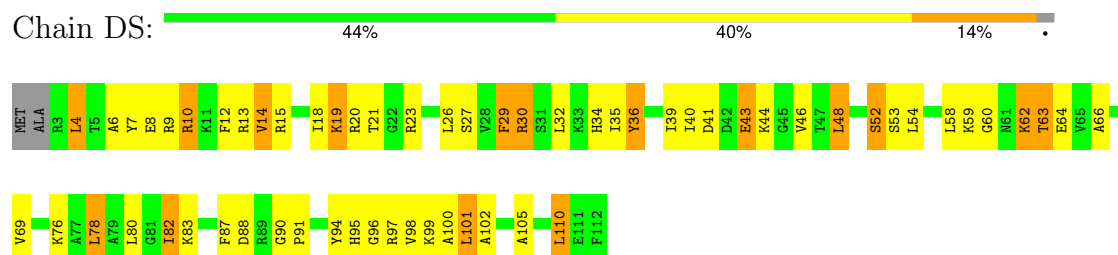




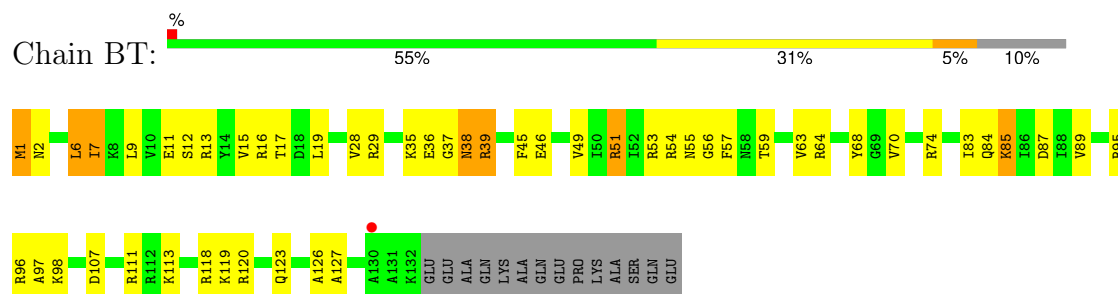
• Molecule 38: 50S Ribosomal Protein L18



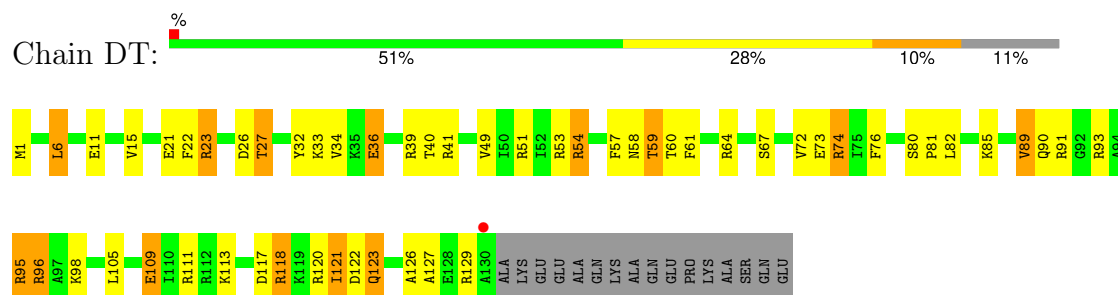
• Molecule 38: 50S Ribosomal Protein L18



• Molecule 39: 50S Ribosomal Protein L19

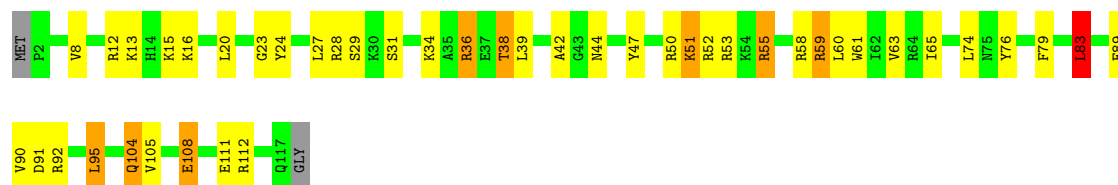


• Molecule 39: 50S Ribosomal Protein L19

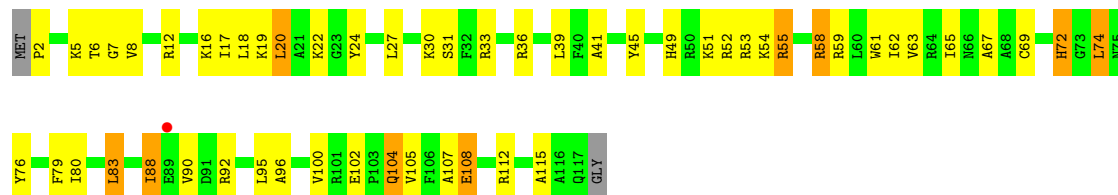


• Molecule 40: 50S Ribosomal Protein L20

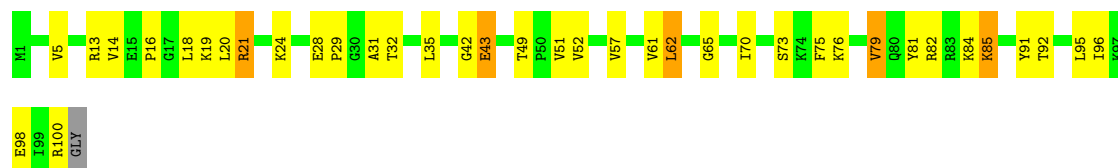




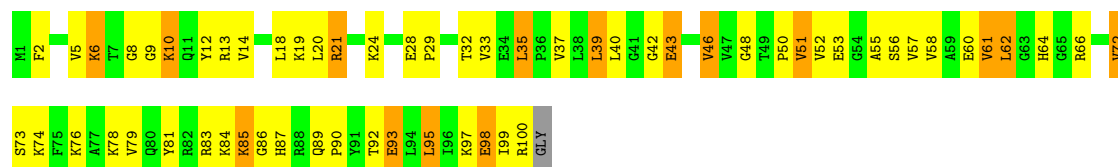
• Molecule 40: 50S Ribosomal Protein L20



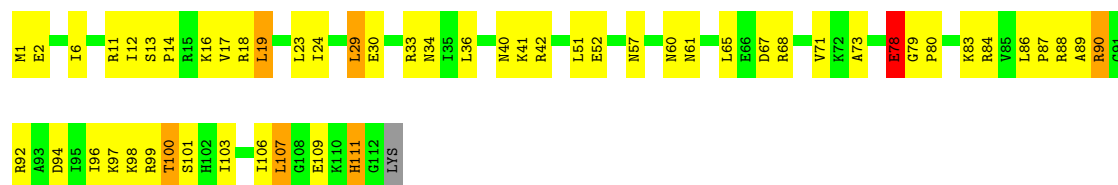
• Molecule 41: 50S Ribosomal Protein L21



• Molecule 41: 50S Ribosomal Protein L21

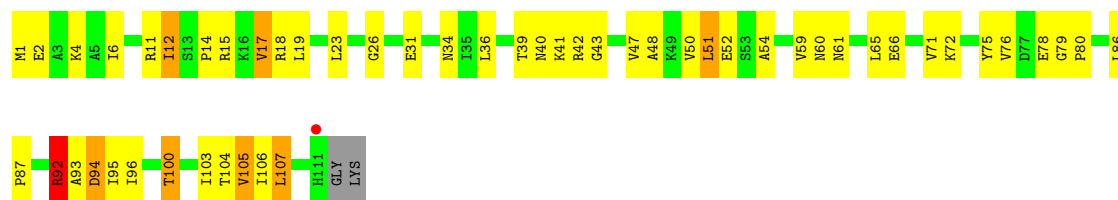


• Molecule 42: 50S Ribosomal Protein L22



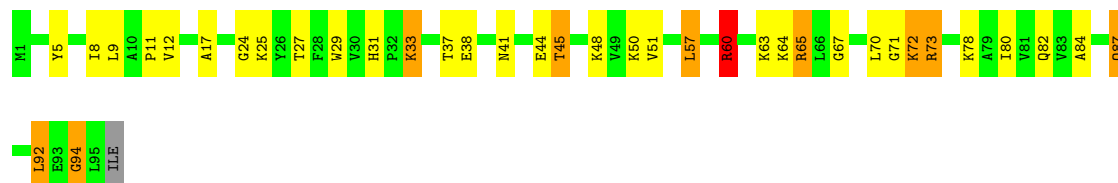
• Molecule 42: 50S Ribosomal Protein L22





• Molecule 43: 50S Ribosomal Protein L23

Chain BX: 60% 28% 9% ..



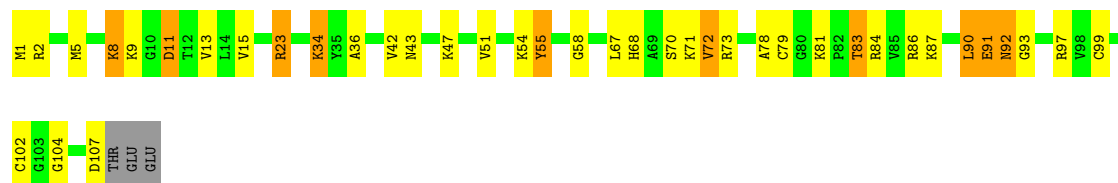
• Molecule 43: 50S Ribosomal Protein L23

Chain DX: 69% 26% ...



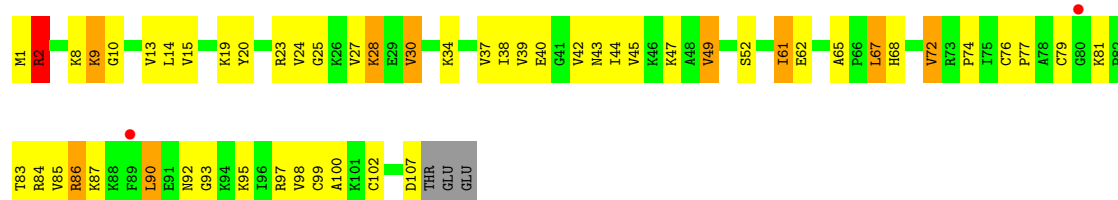
• Molecule 44: 50S Ribosomal Protein L24

Chain BY: 61% 27% 9% .



• Molecule 44: 50S Ribosomal Protein L24

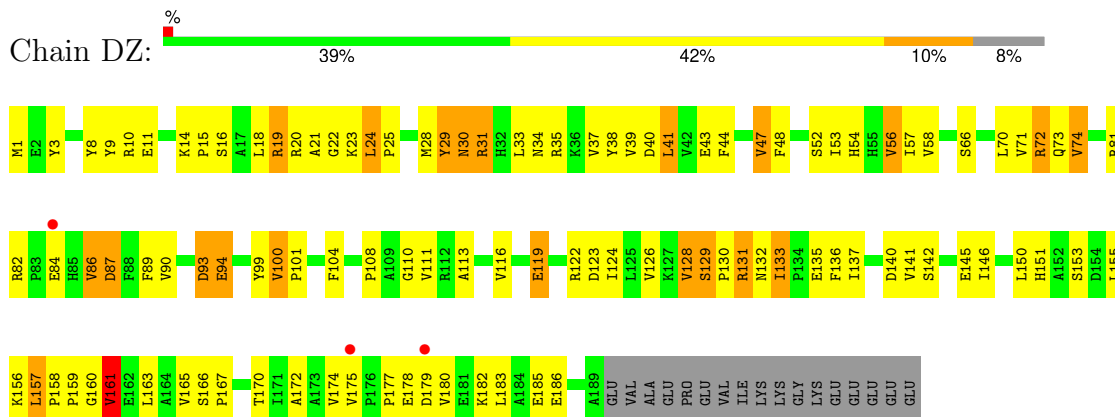
Chain DY: 48% 40% 8% ..



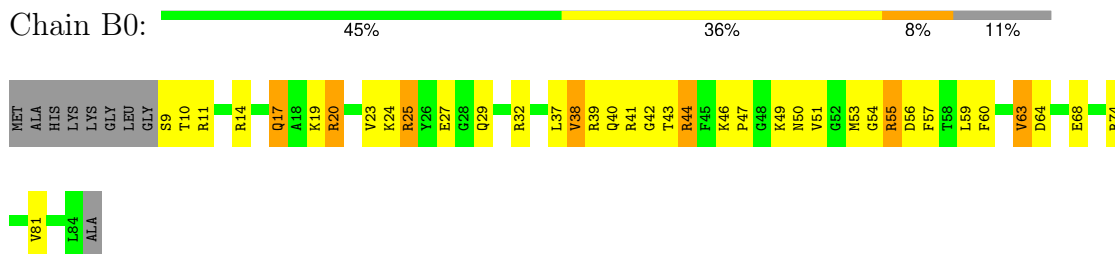
• Molecule 45: 50S Ribosomal Protein L25

Chain BZ: 44% 40% 6% 10%

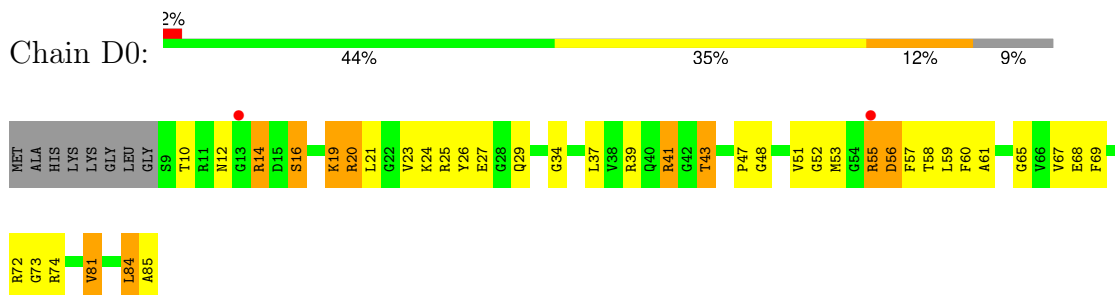
- Molecule 45: 50S Ribosomal Protein L25



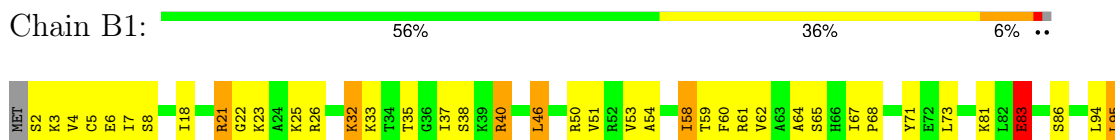
- Molecule 46: 50S Ribosomal Protein L27



- Molecule 46: 50S Ribosomal Protein L27

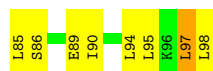
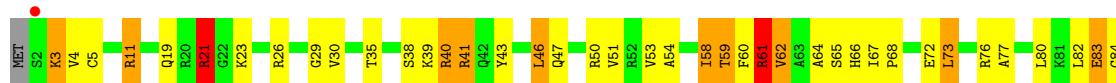


- Molecule 47: 50S Ribosomal Protein L28

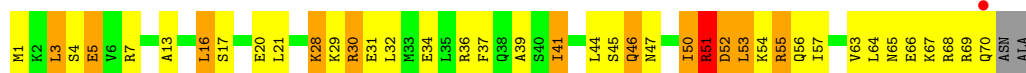
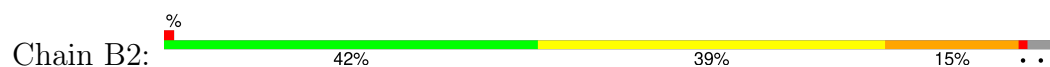




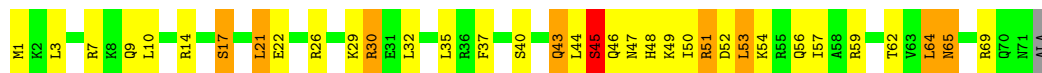
• Molecule 47: 50S Ribosomal Protein L28



• Molecule 48: 50S Ribosomal Protein L29



• Molecule 48: 50S Ribosomal Protein L29



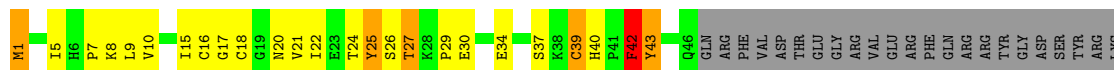
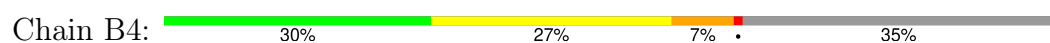
• Molecule 49: 50S Ribosomal Protein L30



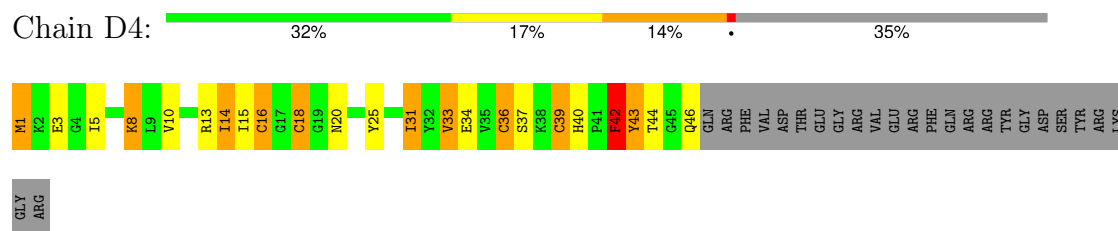
• Molecule 49: 50S Ribosomal Protein L30



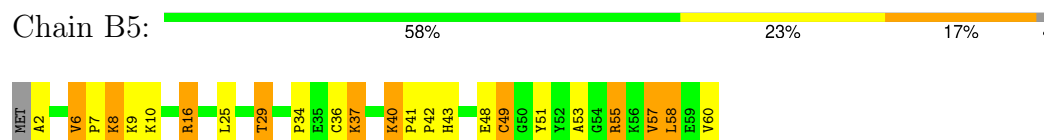
• Molecule 50: 50S Ribosomal Protein L31



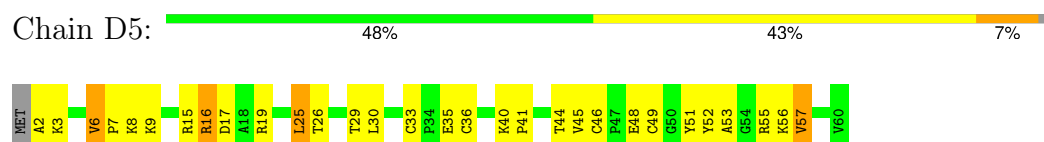
- Molecule 50: 50S Ribosomal Protein L31



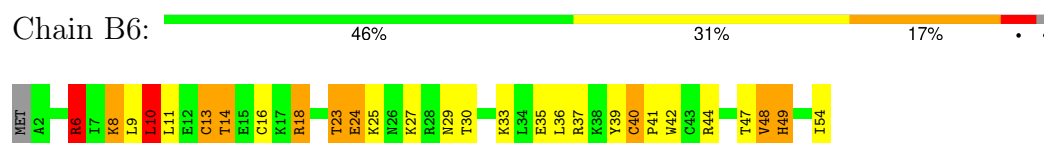
- Molecule 51: 50S Ribosomal Protein L32



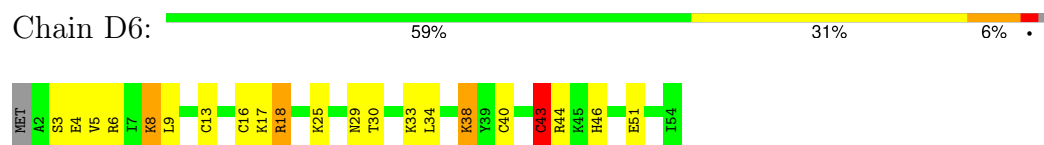
- Molecule 51: 50S Ribosomal Protein L32



- Molecule 52: 50S Ribosomal Protein L33



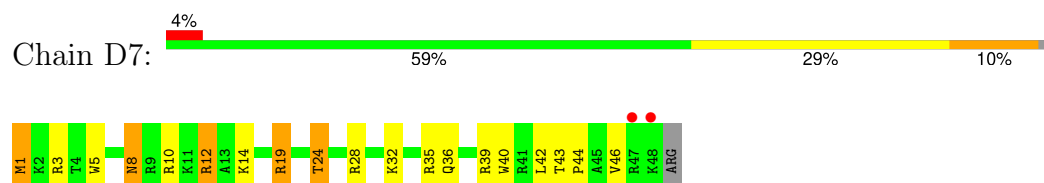
- Molecule 52: 50S Ribosomal Protein L33



- Molecule 53: 50S Ribosomal Protein L34

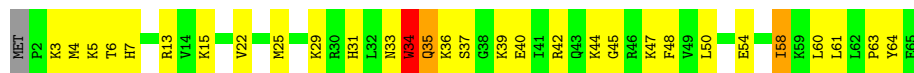


- Molecule 53: 50S Ribosomal Protein L34



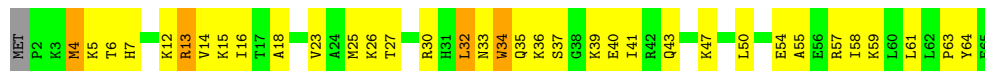
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:  52% 42%



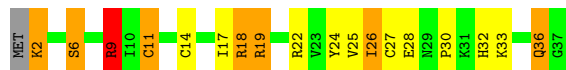
- Molecule 54: 50S Ribosomal Protein L35

Chain D8:  45% 48% 6%




- Molecule 55: 50S Ribosomal Protein L36

Chain B9:  49% 27% 19%



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:  8% 41% 49% 5% 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	0.97	30/35273 (0.1%)	1.68	779/55046 (1.4%)
1	CA	0.89	15/35152 (0.0%)	1.51	525/54858 (1.0%)
2	AB	0.67	3/1844 (0.2%)	0.87	1/2498 (0.0%)
2	CB	0.55	0/1852	0.79	1/2510 (0.0%)
3	AC	0.56	0/1458	0.84	0/1981
3	CC	0.53	0/1477	0.75	0/2006
4	AD	0.66	2/1550 (0.1%)	0.93	4/2106 (0.2%)
4	CD	0.70	3/1567 (0.2%)	0.95	4/2125 (0.2%)
5	AE	0.64	0/1121	0.90	0/1517
5	CE	0.68	0/1131	0.92	0/1529
6	AF	0.62	0/794	0.86	1/1082 (0.1%)
6	CF	0.60	0/797	0.81	0/1085
7	AG	0.53	0/1169	0.73	0/1580
7	CG	0.53	0/1166	0.77	0/1576
8	AH	0.63	0/1065	0.83	0/1445
8	CH	0.57	0/1069	0.80	0/1450
9	AI	0.60	0/879	0.96	1/1195 (0.1%)
9	CI	0.53	0/864	0.80	1/1177 (0.1%)
10	AJ	0.57	0/672	0.81	0/919
10	CJ	0.55	0/670	0.84	0/917
11	AK	0.70	0/858	0.91	1/1163 (0.1%)
11	CK	0.58	0/843	0.77	0/1144
12	AL	0.70	0/925	0.87	0/1251
12	CL	0.64	0/921	0.88	0/1247
13	AM	0.66	1/824 (0.1%)	0.92	1/1120 (0.1%)
13	CM	0.55	0/794	0.81	1/1081 (0.1%)
14	AN	0.59	0/482	0.86	2/642 (0.3%)
14	CN	0.60	0/478	0.86	0/638
15	AO	0.62	0/735	0.87	1/981 (0.1%)
15	CO	0.59	0/735	0.84	0/981
16	AP	0.60	0/662	0.99	3/898 (0.3%)
16	CP	0.60	0/677	0.91	0/917

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1

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

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

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

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

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

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

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(D)	C	Sidechain
2	AB	14	GLY	Peptide
2	AB	23	ARG	Peptide
2	AB	71	VAL	Peptide
2	AB	76	GLN	Peptide

5.2 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	882	0
1	CA	31406	0	15852	823	0
2	AB	1809	0	1781	104	0
2	CB	1817	0	1785	126	0
3	AC	1434	0	1299	59	0
3	CC	1453	0	1320	64	0
4	AD	1520	0	1407	80	0
4	CD	1537	0	1430	81	1
5	AE	1105	0	1130	50	0
5	CE	1115	0	1145	55	0
6	AF	781	0	741	36	1
6	CF	784	0	739	30	0
7	AG	1152	0	1098	58	0
7	CG	1149	0	1096	52	0
8	AH	1045	0	1033	52	0
8	CH	1049	0	1037	52	0
9	AI	863	0	760	54	0
9	CI	849	0	735	54	0
10	AJ	659	0	552	38	0
10	CJ	657	0	547	40	0
11	AK	843	0	841	34	0
11	CK	828	0	822	31	0
12	AL	909	0	927	50	0
12	CL	905	0	916	30	0
13	AM	814	0	765	47	0
13	CM	784	0	730	51	0
14	AN	473	0	491	39	0
14	CN	469	0	482	37	0
15	AO	724	0	749	34	0
15	CO	724	0	749	30	0
16	AP	646	0	636	42	0
16	CP	661	0	653	45	0
17	AQ	823	0	891	52	0
17	CQ	819	0	880	38	0
18	AR	514	0	530	27	0
18	CR	514	0	530	21	0
19	AS	560	0	466	24	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	41	0
20	CT	773	0	836	32	0
21	AU	217	0	234	7	0
21	CU	180	0	173	4	0
22	AY	1031	0	1087	85	0
23	AV	1644	0	836	23	0
23	CV	1644	0	836	38	0
24	AX	131	0	66	4	0
24	CX	131	0	66	2	0
25	BA	59281	0	29884	1053	0
25	DA	58627	0	29570	1197	0
26	BB	2573	0	1306	47	0
26	DB	2573	0	1306	83	0
27	BD	2131	0	2207	97	0
27	DD	2136	0	2218	104	0
28	BE	1555	0	1607	65	0
28	DE	1555	0	1607	72	0
29	BF	1576	0	1616	71	0
29	DF	1578	0	1623	96	0
30	BG	1368	0	1324	52	0
30	DG	1361	0	1316	76	0
31	BH	1317	0	1376	52	0
31	DH	1317	0	1376	59	0
32	BI	1066	0	1095	47	0
32	DI	1057	0	1087	56	0
33	BN	1112	0	1180	49	0
33	DN	1112	0	1180	64	0
34	BO	923	0	981	37	0
34	DO	923	0	981	38	0
35	BP	1131	0	1201	61	0
35	DP	1131	0	1201	66	0
36	BQ	1122	0	1179	46	0
36	DQ	1122	0	1179	66	0
37	BR	968	0	1033	42	0
37	DR	968	0	1033	56	0
38	BS	865	0	905	53	0
38	DS	873	0	927	64	0
39	BT	1072	0	1116	31	0
39	DT	1058	0	1098	35	0
40	BU	959	0	1019	35	0
40	DU	959	0	1019	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	BV	766	0	827	24	0
41	DV	770	0	838	40	0
42	BW	890	0	951	33	0
42	DW	877	0	932	32	0
43	BX	742	0	799	36	0
43	DX	732	0	777	17	0
44	BY	785	0	828	25	0
44	DY	781	0	829	42	0
45	BZ	1454	0	1452	66	0
45	DZ	1451	0	1421	72	0
46	B0	594	0	604	30	0
46	D0	607	0	622	39	0
47	B1	745	0	804	33	0
47	D1	745	0	804	37	0
48	B2	588	0	643	28	0
48	D2	584	0	623	26	0
49	B3	458	0	503	16	0
49	D3	453	0	501	28	0
50	B4	349	0	336	22	0
50	D4	349	0	336	19	0
51	B5	455	0	472	20	0
51	D5	451	0	461	25	0
52	B6	449	0	462	25	0
52	D6	437	0	440	16	0
53	B7	418	0	467	22	0
53	D7	402	0	434	11	0
54	B8	509	0	565	24	0
54	D8	509	0	565	26	0
55	B9	297	0	316	16	0
55	D9	292	0	313	14	0
56	AA	348	0	0	0	0
56	AD	2	0	0	0	0
56	AE	1	0	0	0	0
56	AF	1	0	0	0	0
56	AI	2	0	0	0	0
56	AK	1	0	0	0	0
56	AT	1	0	0	0	0
56	AV	18	0	0	0	0
56	AY	1	0	0	0	0
56	B0	5	0	0	0	0
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	1	0
58	CQ	2	0	0	1	0
58	CT	2	0	0	0	0
58	CV	13	0	0	0	0
58	CX	1	0	0	0	0
58	D1	3	0	0	1	0
58	D3	1	0	0	0	0
58	D6	2	0	0	0	0
58	D7	2	0	0	0	0
58	D8	4	0	0	1	0
58	DA	1028	0	0	63	0
58	DB	40	0	0	2	0
58	DD	8	0	0	0	0
58	DE	11	0	0	1	0
58	DF	4	0	0	0	0
58	DG	1	0	0	0	0
58	DN	3	0	0	0	0
58	DO	5	0	0	1	0
58	DP	4	0	0	0	0
58	DR	5	0	0	1	0
58	DT	3	0	0	0	0
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	7600	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 7600 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	49
2	CB	233/256 (91%)	182 (78%)	45 (19%)	6 (3%)	4	27
3	AC	202/239 (84%)	165 (82%)	33 (16%)	4 (2%)	6	32
3	CC	204/239 (85%)	168 (82%)	36 (18%)	0	100	100
4	AD	206/209 (99%)	166 (81%)	35 (17%)	5 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	5	29
5	AE	146/162 (90%)	120 (82%)	26 (18%)	0	100	100
5	CE	147/162 (91%)	129 (88%)	13 (9%)	5 (3%)	3	21
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%)	19	54
7	CG	152/156 (97%)	131 (86%)	20 (13%)	1 (1%)	19	54
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	19	54
8	CH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	AI	123/128 (96%)	105 (85%)	15 (12%)	3 (2%)	5	29
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	22
11	AK	113/129 (88%)	101 (89%)	11 (10%)	1 (1%)	14	49
11	CK	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
12	AL	120/132 (91%)	108 (90%)	10 (8%)	2 (2%)	7	36
12	CL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	7	36
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%)	7	35
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%)	13	47
17	CQ	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	13	47
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%)	10	41
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	38
27	BD	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	19	54
28	BE	202/206 (98%)	189 (94%)	9 (4%)	4 (2%)	6	32
28	DE	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	8	38
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	30
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%)	11	43
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	40
33	BN	138/140 (99%)	124 (90%)	11 (8%)	3 (2%)	5	30
33	DN	138/140 (99%)	117 (85%)	19 (14%)	2 (1%)	9	40
34	BO	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	51
34	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	BP	147/150 (98%)	128 (87%)	17 (12%)	2 (1%)	9	40
35	DP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	40
36	BQ	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	9	40
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	34
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%)	13	47
44	DY	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	13	47
45	BZ	184/206 (89%)	161 (88%)	21 (11%)	2 (1%)	12	44
45	DZ	187/206 (91%)	163 (87%)	21 (11%)	3 (2%)	8	37
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%)	12	44
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	B2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	8	38
48	D2	69/72 (96%)	60 (87%)	9 (13%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	7	35
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	30
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%)	12	44

5 of 130 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CI	62/99 (63%)	52 (84%)	10 (16%)	2	9
10	AJ	52/92 (56%)	38 (73%)	14 (27%)	0	1
10	CJ	52/92 (56%)	36 (69%)	16 (31%)	0	1
11	AK	83/99 (84%)	60 (72%)	23 (28%)	0	1
11	CK	81/99 (82%)	61 (75%)	20 (25%)	0	2
12	AL	92/109 (84%)	73 (79%)	19 (21%)	1	5
12	CL	91/109 (84%)	71 (78%)	20 (22%)	1	4
13	AM	66/101 (65%)	44 (67%)	22 (33%)	0	0
13	CM	62/101 (61%)	39 (63%)	23 (37%)	0	0
14	AN	46/50 (92%)	40 (87%)	6 (13%)	3	16
14	CN	45/50 (90%)	30 (67%)	15 (33%)	0	0
15	AO	77/80 (96%)	61 (79%)	16 (21%)	1	5
15	CO	77/80 (96%)	64 (83%)	13 (17%)	1	8
16	AP	63/74 (85%)	44 (70%)	19 (30%)	0	1
16	CP	65/74 (88%)	49 (75%)	16 (25%)	0	2
17	AQ	94/97 (97%)	79 (84%)	15 (16%)	2	10
17	CQ	93/97 (96%)	77 (83%)	16 (17%)	1	8
18	AR	49/77 (64%)	41 (84%)	8 (16%)	2	9
18	CR	49/77 (64%)	36 (74%)	13 (26%)	0	1
19	AS	43/80 (54%)	34 (79%)	9 (21%)	1	5
19	CS	42/80 (52%)	28 (67%)	14 (33%)	0	0
20	AT	66/82 (80%)	47 (71%)	19 (29%)	0	1
20	CT	72/82 (88%)	56 (78%)	16 (22%)	1	4
21	AU	20/22 (91%)	14 (70%)	6 (30%)	0	1
21	CU	14/22 (64%)	13 (93%)	1 (7%)	12	42
22	AY	108/115 (94%)	74 (68%)	34 (32%)	0	0
27	BD	214/218 (98%)	169 (79%)	45 (21%)	1	5
27	DD	215/218 (99%)	167 (78%)	48 (22%)	1	4
28	BE	163/166 (98%)	126 (77%)	37 (23%)	0	3
28	DE	163/166 (98%)	128 (78%)	35 (22%)	1	4
29	BF	158/166 (95%)	123 (78%)	35 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DF	159/166 (96%)	128 (80%)	31 (20%)	1	6
30	BG	128/156 (82%)	103 (80%)	25 (20%)	1	6
30	DG	127/156 (81%)	95 (75%)	32 (25%)	0	2
31	BH	141/148 (95%)	113 (80%)	28 (20%)	1	5
31	DH	141/148 (95%)	111 (79%)	30 (21%)	1	5
32	BI	105/124 (85%)	75 (71%)	30 (29%)	0	1
32	DI	104/124 (84%)	76 (73%)	28 (27%)	0	1
33	BN	117/119 (98%)	93 (80%)	24 (20%)	1	5
33	DN	117/119 (98%)	90 (77%)	27 (23%)	0	3
34	BO	98/100 (98%)	73 (74%)	25 (26%)	0	2
34	DO	98/100 (98%)	70 (71%)	28 (29%)	0	1
35	BP	114/116 (98%)	87 (76%)	27 (24%)	0	3
35	DP	114/116 (98%)	90 (79%)	24 (21%)	1	5
36	BQ	111/111 (100%)	91 (82%)	20 (18%)	1	7
36	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	9
37	BR	101/101 (100%)	79 (78%)	22 (22%)	1	4
37	DR	101/101 (100%)	79 (78%)	22 (22%)	1	4
38	BS	84/88 (96%)	66 (79%)	18 (21%)	1	5
38	DS	86/88 (98%)	68 (79%)	18 (21%)	1	5
39	BT	111/127 (87%)	90 (81%)	21 (19%)	1	6
39	DT	110/127 (87%)	82 (74%)	28 (26%)	0	2
40	BU	93/94 (99%)	77 (83%)	16 (17%)	1	8
40	DU	93/94 (99%)	77 (83%)	16 (17%)	1	8
41	BV	80/82 (98%)	66 (82%)	14 (18%)	1	8
41	DV	81/82 (99%)	56 (69%)	25 (31%)	0	1
42	BW	91/92 (99%)	71 (78%)	20 (22%)	1	4
42	DW	89/92 (97%)	74 (83%)	15 (17%)	1	8
43	BX	75/78 (96%)	63 (84%)	12 (16%)	2	10
43	DX	73/78 (94%)	61 (84%)	12 (16%)	2	9
44	BY	80/91 (88%)	63 (79%)	17 (21%)	1	5
44	DY	79/91 (87%)	59 (75%)	20 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BZ	156/179 (87%)	128 (82%)	28 (18%)	1	7
45	DZ	152/179 (85%)	119 (78%)	33 (22%)	1	4
46	B0	59/67 (88%)	47 (80%)	12 (20%)	1	5
46	D0	61/67 (91%)	47 (77%)	14 (23%)	0	3
47	B1	78/83 (94%)	61 (78%)	17 (22%)	1	4
47	D1	78/83 (94%)	58 (74%)	20 (26%)	0	2
48	B2	65/67 (97%)	49 (75%)	16 (25%)	0	2
48	D2	63/67 (94%)	50 (79%)	13 (21%)	1	5
49	B3	49/52 (94%)	44 (90%)	5 (10%)	6	26
49	D3	49/52 (94%)	40 (82%)	9 (18%)	1	7
50	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
50	D4	39/63 (62%)	25 (64%)	14 (36%)	0	0
51	B5	50/52 (96%)	41 (82%)	9 (18%)	1	7
51	D5	49/52 (94%)	39 (80%)	10 (20%)	1	5
52	B6	50/52 (96%)	34 (68%)	16 (32%)	0	0
52	D6	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	B7	41/42 (98%)	32 (78%)	9 (22%)	1	4
53	D7	38/42 (90%)	30 (79%)	8 (21%)	1	5
54	B8	52/55 (94%)	45 (86%)	7 (14%)	3	15
54	D8	52/55 (94%)	43 (83%)	9 (17%)	1	8
55	B9	32/34 (94%)	26 (81%)	6 (19%)	1	6
55	D9	32/34 (94%)	25 (78%)	7 (22%)	1	4
All	All	8835/10181 (87%)	6886 (78%)	1949 (22%)	1	4

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

Mol	Chain	Res	Type
50	B4	37	SER
43	DX	38	GLU
8	CH	119	LEU
41	DV	98	GLU
50	D4	5	ILE

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

Mol	Chain	Res	Type
11	CK	99	GLN
28	DE	135	HIS
13	CM	40	ASN
18	CR	63	GLN
33	DN	133	GLN

5.3.3 RNA ⓘ

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

5 of 2119 RNA backbone outliers are listed below:

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

5 of 188 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
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%)	-0.27	8 (0%) 87 78	43, 93, 137, 172	0
1	CA	1461/1522 (95%)	-0.14	12 (0%) 82 70	55, 104, 145, 167	0
2	AB	233/256 (91%)	0.22	3 (1%) 74 60	72, 113, 134, 153	0
2	CB	235/256 (91%)	0.26	4 (1%) 69 53	100, 125, 139, 147	0
3	AC	204/239 (85%)	0.22	4 (1%) 64 49	97, 112, 125, 133	0
3	CC	206/239 (86%)	0.43	12 (5%) 30 20	110, 125, 136, 142	0
4	AD	208/209 (99%)	0.39	10 (4%) 36 25	76, 103, 118, 125	0
4	CD	208/209 (99%)	0.28	6 (2%) 54 38	85, 98, 114, 120	0
5	AE	148/162 (91%)	-0.16	1 (0%) 84 73	67, 89, 108, 134	0
5	CE	149/162 (91%)	0.01	1 (0%) 84 73	83, 99, 110, 131	0
6	AF	100/101 (99%)	-0.17	2 (2%) 64 49	68, 88, 104, 110	0
6	CF	100/101 (99%)	-0.11	0 100 100	78, 96, 110, 117	0
7	AG	154/156 (98%)	0.01	0 100 100	87, 102, 120, 133	0
7	CG	154/156 (98%)	0.19	8 (5%) 34 23	107, 119, 133, 144	0
8	AH	138/138 (100%)	-0.24	1 (0%) 84 73	73, 91, 100, 111	0
8	CH	138/138 (100%)	-0.06	1 (0%) 84 73	82, 100, 111, 116	0
9	AI	125/128 (97%)	0.46	6 (4%) 36 25	71, 114, 126, 137	0
9	CI	125/128 (97%)	0.66	11 (8%) 17 12	101, 130, 138, 142	0
10	AJ	96/105 (91%)	0.63	4 (4%) 41 28	88, 119, 136, 140	0
10	CJ	96/105 (91%)	1.02	7 (7%) 22 16	111, 133, 141, 143	0
11	AK	115/129 (89%)	-0.16	0 100 100	53, 87, 104, 113	0
11	CK	114/129 (88%)	0.15	1 (0%) 81 68	78, 103, 118, 127	0
12	AL	122/132 (92%)	-0.19	0 100 100	61, 84, 100, 111	0
12	CL	122/132 (92%)	-0.05	1 (0%) 82 70	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%)	0.18	5 (4%)	40	27	66, 100, 113, 118	0
13	CM	112/126 (88%)	0.43	6 (5%)	32	22	102, 127, 135, 139	0
14	AN	59/61 (96%)	0.39	4 (6%)	25	17	94, 106, 114, 121	0
14	CN	59/61 (96%)	0.93	5 (8%)	18	12	116, 125, 133, 135	0
15	AO	88/89 (98%)	-0.17	0	100	100	65, 86, 106, 117	0
15	CO	88/89 (98%)	-0.07	0	100	100	74, 96, 114, 118	0
16	AP	81/88 (92%)	0.21	2 (2%)	58	42	83, 100, 122, 127	0
16	CP	82/88 (93%)	0.15	0	100	100	84, 94, 112, 122	0
17	AQ	99/105 (94%)	-0.12	2 (2%)	64	49	68, 89, 104, 113	0
17	CQ	99/105 (94%)	-0.11	1 (1%)	79	66	77, 95, 110, 113	0
18	AR	68/88 (77%)	-0.30	0	100	100	69, 84, 102, 106	0
18	CR	68/88 (77%)	-0.22	0	100	100	82, 92, 111, 115	0
19	AS	81/93 (87%)	0.22	4 (4%)	36	25	96, 110, 130, 141	0
19	CS	75/93 (80%)	0.48	4 (5%)	33	22	107, 131, 142, 146	0
20	AT	96/106 (90%)	0.14	2 (2%)	63	47	77, 97, 113, 118	0
20	CT	104/106 (98%)	0.07	4 (3%)	44	30	81, 101, 123, 139	0
21	AU	25/27 (92%)	0.90	1 (4%)	43	29	80, 98, 105, 107	0
21	CU	23/27 (85%)	1.54	6 (26%)	2	2	115, 126, 132, 134	0
22	AY	132/140 (94%)	0.69	13 (9%)	14	10	69, 110, 138, 152	0
23	AV	77/77 (100%)	-0.43	1 (1%)	74	60	55, 82, 112, 132	0
23	CV	77/77 (100%)	-0.26	0	100	100	73, 109, 133, 150	0
24	AX	6/16 (37%)	0.09	0	100	100	67, 73, 127, 128	0
24	CX	6/16 (37%)	0.51	0	100	100	89, 96, 142, 147	0
25	BA	2752/2915 (94%)	-0.99	9 (0%)	90	84	23, 43, 115, 170	0
25	DA	2722/2915 (93%)	-0.61	13 (0%)	87	78	44, 74, 127, 170	0
26	BB	120/122 (98%)	-0.75	1 (0%)	82	70	36, 64, 90, 125	0
26	DB	120/122 (98%)	0.06	1 (0%)	82	70	73, 114, 129, 146	0
27	BD	275/276 (99%)	-0.80	1 (0%)	89	81	27, 43, 62, 110	0
27	DD	275/276 (99%)	-0.48	1 (0%)	89	81	41, 62, 82, 100	0
28	BE	204/206 (99%)	-0.83	0	100	100	22, 45, 71, 94	0
28	DE	204/206 (99%)	-0.41	2 (0%)	79	66	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%)	-0.72	1 (0%) 87 78	26, 49, 87, 115	0
29	DF	203/210 (96%)	-0.24	2 (0%) 79 66	47, 88, 114, 127	0
30	BG	181/182 (99%)	-0.28	2 (1%) 77 63	58, 77, 105, 116	0
30	DG	180/182 (98%)	0.27	5 (2%) 55 39	101, 117, 127, 136	0
31	BH	174/180 (96%)	-0.59	1 (0%) 85 76	38, 65, 84, 98	0
31	DH	174/180 (96%)	0.09	1 (0%) 85 76	96, 116, 130, 140	0
32	BI	147/148 (99%)	-0.31	1 (0%) 84 73	50, 95, 112, 128	0
32	DI	146/148 (98%)	0.01	0 100 100	68, 108, 126, 131	0
33	BN	140/140 (100%)	-0.84	0 100 100	30, 42, 69, 83	0
33	DN	140/140 (100%)	-0.24	0 100 100	64, 86, 107, 117	0
34	BO	122/122 (100%)	-0.86	0 100 100	33, 52, 71, 82	0
34	DO	122/122 (100%)	-0.50	0 100 100	57, 73, 88, 96	0
35	BP	149/150 (99%)	-0.51	0 100 100	25, 55, 86, 108	0
35	DP	149/150 (99%)	-0.13	1 (0%) 84 73	52, 91, 116, 127	0
36	BQ	141/141 (100%)	-0.69	0 100 100	33, 50, 70, 90	0
36	DQ	141/141 (100%)	-0.03	2 (1%) 73 58	67, 90, 106, 114	0
37	BR	118/118 (100%)	-0.90	0 100 100	27, 41, 59, 67	0
37	DR	118/118 (100%)	-0.51	0 100 100	49, 65, 86, 95	0
38	BS	110/112 (98%)	-0.55	0 100 100	44, 62, 86, 97	0
38	DS	110/112 (98%)	0.04	0 100 100	90, 109, 119, 127	0
39	BT	132/146 (90%)	-0.61	1 (0%) 82 70	41, 55, 94, 127	0
39	DT	130/146 (89%)	-0.37	1 (0%) 82 70	62, 77, 108, 123	0
40	BU	116/118 (98%)	-0.90	0 100 100	25, 36, 55, 71	0
40	DU	116/118 (98%)	-0.26	1 (0%) 81 68	54, 82, 103, 108	0
41	BV	100/101 (99%)	-0.94	0 100 100	28, 46, 73, 90	0
41	DV	100/101 (99%)	-0.20	0 100 100	56, 98, 119, 123	0
42	BW	112/113 (99%)	-0.94	0 100 100	28, 37, 63, 89	0
42	DW	111/113 (98%)	-0.54	1 (0%) 81 68	49, 63, 89, 114	0
43	BX	95/96 (98%)	-0.69	0 100 100	34, 46, 77, 92	0
43	DX	95/96 (98%)	-0.29	1 (1%) 77 63	61, 77, 100, 107	0
44	BY	107/110 (97%)	-0.65	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%)	0.05	2 (1%) 66 50	77, 96, 112, 124	0
45	BZ	186/206 (90%)	-0.32	0 100 100	49, 76, 104, 126	0
45	DZ	189/206 (91%)	0.14	3 (1%) 70 55	98, 114, 131, 139	0
46	B0	76/85 (89%)	-0.74	0 100 100	32, 42, 59, 83	0
46	D0	77/85 (90%)	0.03	2 (2%) 57 41	73, 85, 101, 124	0
47	B1	97/98 (98%)	-0.57	0 100 100	32, 51, 90, 104	0
47	D1	97/98 (98%)	-0.30	1 (1%) 79 66	50, 72, 105, 115	0
48	B2	70/72 (97%)	-0.53	1 (1%) 73 58	41, 60, 78, 103	0
48	D2	71/72 (98%)	-0.17	0 100 100	78, 94, 106, 110	0
49	B3	59/60 (98%)	-0.92	0 100 100	33, 41, 76, 93	0
49	D3	58/60 (96%)	-0.14	1 (1%) 69 53	71, 84, 114, 128	0
50	B4	46/71 (64%)	-0.46	0 100 100	78, 96, 112, 114	0
50	D4	46/71 (64%)	0.03	0 100 100	118, 126, 136, 138	0
51	B5	59/60 (98%)	-0.93	0 100 100	25, 41, 62, 74	0
51	D5	59/60 (98%)	-0.36	0 100 100	47, 66, 85, 106	0
52	B6	53/54 (98%)	-0.84	0 100 100	42, 49, 66, 76	0
52	D6	53/54 (98%)	-0.27	0 100 100	67, 81, 93, 101	0
53	B7	48/49 (97%)	-0.55	2 (4%) 41 28	25, 33, 68, 88	0
53	D7	48/49 (97%)	-0.35	2 (4%) 41 28	41, 53, 82, 105	0
54	B8	64/65 (98%)	-0.82	0 100 100	35, 41, 49, 72	0
54	D8	64/65 (98%)	-0.17	0 100 100	60, 71, 83, 94	0
55	B9	36/37 (97%)	-0.66	0 100 100	33, 46, 58, 72	0
55	D9	35/37 (94%)	0.49	3 (8%) 18 12	73, 88, 103, 115	0
All	All	20489/21572 (94%)	-0.35	229 (1%) 77 63	22, 83, 131, 172	0

The worst 5 of 229 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DG	35	GLU	6.6
8	CH	1	MET	6.4
9	CI	126	SER	5.0
53	D7	48	LYS	4.8
13	AM	6	GLY	4.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
56	MG	AA	1686	1/1	0.28	0.33	112,112,112,112	0
56	MG	CA	1796	1/1	0.37	0.22	102,102,102,102	0
56	MG	CA	1708	1/1	0.52	0.47	91,91,91,91	0
56	MG	CA	1701	1/1	0.52	0.24	109,109,109,109	0
56	MG	AA	1811	1/1	0.54	0.23	120,120,120,120	0
56	MG	CA	1604	1/1	0.55	0.34	114,114,114,114	0
56	MG	AA	1695	1/1	0.56	0.32	102,102,102,102	0
56	MG	BA	3742	1/1	0.57	0.23	72,72,72,72	0
56	MG	CA	1671	1/1	0.58	0.14	82,82,82,82	0
56	MG	DA	3432	1/1	0.58	0.14	85,85,85,85	0
56	MG	AA	1699	1/1	0.60	0.17	109,109,109,109	0
56	MG	CA	1747	1/1	0.60	0.21	96,96,96,96	0
56	MG	DA	3616	1/1	0.60	0.16	115,115,115,115	0
56	MG	AA	1816	1/1	0.61	0.18	107,107,107,107	0
56	MG	AA	1932	1/1	0.61	0.12	116,116,116,116	0
56	MG	AD	303	1/1	0.61	0.26	93,93,93,93	0
56	MG	AA	1742	1/1	0.61	0.23	93,93,93,93	0
56	MG	AA	1689	1/1	0.62	0.20	77,77,77,77	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	CA	1797	1/1	0.63	0.17	121,121,121,121	0
56	MG	CV	105	1/1	0.63	0.27	106,106,106,106	0
56	MG	CA	1782	1/1	0.64	0.16	96,96,96,96	0
56	MG	DA	3570	1/1	0.64	0.23	79,79,79,79	0
56	MG	CA	1723	1/1	0.64	0.20	96,96,96,96	0
56	MG	DA	3335	1/1	0.65	0.17	74,74,74,74	0
56	MG	DA	3369	1/1	0.65	0.29	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3102	1/1	0.65	0.19	51,51,51,51	0
56	MG	CA	1780	1/1	0.65	0.15	90,90,90,90	0
56	MG	BA	3736	1/1	0.65	0.18	59,59,59,59	0
56	MG	DA	3258	1/1	0.66	0.44	91,91,91,91	0
56	MG	AA	1711	1/1	0.66	0.20	76,76,76,76	0
56	MG	DA	3232	1/1	0.66	0.28	91,91,91,91	0
56	MG	DA	3309	1/1	0.67	0.20	88,88,88,88	0
56	MG	AA	1915	1/1	0.67	0.13	121,121,121,121	0
56	MG	DA	3025	1/1	0.67	0.20	76,76,76,76	0
56	MG	DA	3158	1/1	0.67	0.22	82,82,82,82	0
56	MG	AA	1813	1/1	0.67	0.16	121,121,121,121	0
56	MG	BA	3853	1/1	0.67	0.14	76,76,76,76	0
56	MG	AA	1683	1/1	0.68	0.30	106,106,106,106	0
56	MG	DA	3017	1/1	0.68	0.33	69,69,69,69	0
56	MG	AA	1685	1/1	0.68	0.26	91,91,91,91	0
56	MG	AA	1844	1/1	0.69	0.20	86,86,86,86	0
56	MG	CA	1659	1/1	0.69	0.18	85,85,85,85	0
56	MG	CA	1703	1/1	0.69	0.25	100,100,100,100	0
56	MG	DB	208	1/1	0.69	0.26	98,98,98,98	0
56	MG	AA	1709	1/1	0.70	0.22	86,86,86,86	0
56	MG	CA	1702	1/1	0.70	0.20	114,114,114,114	0
56	MG	DA	3472	1/1	0.70	0.21	78,78,78,78	0
56	MG	DA	3259	1/1	0.70	0.30	78,78,78,78	0
56	MG	AV	108	1/1	0.70	0.12	98,98,98,98	0
56	MG	AA	1743	1/1	0.70	0.20	80,80,80,80	0
56	MG	CA	1815	1/1	0.71	0.23	119,119,119,119	0
56	MG	DA	3284	1/1	0.71	0.32	75,75,75,75	0
56	MG	AA	1718	1/1	0.71	0.10	70,70,70,70	0
56	MG	CX	101	1/1	0.71	0.19	99,99,99,99	0
56	MG	CA	1614	1/1	0.71	0.20	81,81,81,81	0
56	MG	CA	1722	1/1	0.72	0.24	76,76,76,76	0
56	MG	BA	3430	1/1	0.72	0.17	69,69,69,69	0
56	MG	AA	1657	1/1	0.72	0.36	67,67,67,67	0
56	MG	AA	1620	1/1	0.72	0.22	74,74,74,74	0
56	MG	BA	3799	1/1	0.72	0.12	72,72,72,72	0
56	MG	AA	1653	1/1	0.72	0.39	82,82,82,82	0
56	MG	CA	1788	1/1	0.72	0.11	118,118,118,118	0
56	MG	AA	1803	1/1	0.72	0.55	92,92,92,92	0
56	MG	DA	3654	1/1	0.72	0.12	118,118,118,118	0
56	MG	AA	1884	1/1	0.72	0.12	82,82,82,82	0
56	MG	D0	102	1/1	0.72	0.13	99,99,99,99	0
56	MG	DA	3013	1/1	0.73	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1675	1/1	0.73	0.35	78,78,78,78	0
56	MG	CA	1793	1/1	0.73	0.17	73,73,73,73	0
56	MG	DA	3065	1/1	0.73	0.49	59,59,59,59	0
56	MG	DA	3152	1/1	0.73	0.26	69,69,69,69	0
56	MG	DA	3519	1/1	0.73	0.15	93,93,93,93	0
56	MG	BA	3826	1/1	0.73	0.19	92,92,92,92	0
56	MG	AA	1723	1/1	0.73	0.26	102,102,102,102	0
56	MG	AA	1741	1/1	0.73	0.32	85,85,85,85	0
56	MG	DA	3666	1/1	0.73	0.17	100,100,100,100	0
56	MG	AA	1823	1/1	0.73	0.34	77,77,77,77	0
56	MG	DB	212	1/1	0.73	0.10	111,111,111,111	0
56	MG	AA	1838	1/1	0.73	0.15	72,72,72,72	0
56	MG	AA	1812	1/1	0.74	0.14	122,122,122,122	0
56	MG	DA	3541	1/1	0.74	0.24	106,106,106,106	0
56	MG	AA	1659	1/1	0.74	0.28	97,97,97,97	0
56	MG	DA	3590	1/1	0.74	0.19	89,89,89,89	0
56	MG	BA	3395	1/1	0.74	0.25	100,100,100,100	0
56	MG	DA	3620	1/1	0.74	0.14	95,95,95,95	0
56	MG	AA	1796	1/1	0.74	0.33	77,77,77,77	0
56	MG	AA	1698	1/1	0.74	0.29	97,97,97,97	0
56	MG	DB	203	1/1	0.74	0.22	105,105,105,105	0
56	MG	DB	204	1/1	0.74	0.20	107,107,107,107	0
56	MG	CA	1705	1/1	0.74	0.23	112,112,112,112	0
56	MG	AA	1612	1/1	0.74	0.25	60,60,60,60	0
56	MG	DA	3509	1/1	0.74	0.10	122,122,122,122	0
56	MG	DA	3294	1/1	0.75	0.21	82,82,82,82	0
56	MG	DA	3296	1/1	0.75	0.25	80,80,80,80	0
56	MG	CA	1813	1/1	0.75	0.19	113,113,113,113	0
56	MG	AA	1819	1/1	0.75	0.45	91,91,91,91	0
56	MG	AA	1901	1/1	0.75	0.09	119,119,119,119	0
56	MG	BA	3237	1/1	0.75	0.16	59,59,59,59	0
56	MG	DA	3009	1/1	0.75	0.20	90,90,90,90	0
56	MG	AA	1737	1/1	0.75	0.29	88,88,88,88	0
56	MG	AA	1923	1/1	0.75	0.13	115,115,115,115	0
56	MG	CA	1639	1/1	0.75	0.35	96,96,96,96	0
56	MG	BA	3500	1/1	0.75	0.25	93,93,93,93	0
56	MG	DA	3148	1/1	0.75	0.28	80,80,80,80	0
56	MG	CA	1664	1/1	0.75	0.35	76,76,76,76	0
56	MG	DA	3157	1/1	0.75	0.29	82,82,82,82	0
56	MG	BA	3542	1/1	0.75	0.12	79,79,79,79	0
56	MG	DA	3657	1/1	0.75	0.14	89,89,89,89	0
56	MG	DA	3199	1/1	0.75	0.57	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1697	1/1	0.75	0.28	117,117,117,117	0
56	MG	AA	1756	1/1	0.75	0.21	90,90,90,90	0
56	MG	AA	1795	1/1	0.75	0.40	70,70,70,70	0
56	MG	DA	3265	1/1	0.75	0.19	68,68,68,68	0
56	MG	BA	3778	1/1	0.75	0.12	92,92,92,92	0
56	MG	DA	3052	1/1	0.76	0.41	79,79,79,79	0
56	MG	DA	3532	1/1	0.76	0.18	90,90,90,90	0
56	MG	CA	1770	1/1	0.76	0.17	93,93,93,93	0
56	MG	DA	3557	1/1	0.76	0.27	93,93,93,93	0
56	MG	DA	3564	1/1	0.76	0.19	88,88,88,88	0
56	MG	BA	3396	1/1	0.76	0.28	95,95,95,95	0
56	MG	AI	202	1/1	0.76	0.17	90,90,90,90	0
56	MG	AA	1611	1/1	0.76	0.20	97,97,97,97	0
56	MG	DA	3306	1/1	0.76	0.13	106,106,106,106	0
56	MG	DA	3634	1/1	0.76	0.13	70,70,70,70	0
56	MG	BA	3035	1/1	0.76	0.15	82,82,82,82	0
56	MG	DA	3318	1/1	0.76	0.17	83,83,83,83	0
56	MG	CA	1649	1/1	0.76	0.13	78,78,78,78	0
56	MG	DA	3678	1/1	0.76	0.12	89,89,89,89	0
56	MG	DA	3343	1/1	0.76	0.34	70,70,70,70	0
56	MG	DA	3213	1/1	0.76	0.17	89,89,89,89	0
56	MG	DB	207	1/1	0.76	0.23	79,79,79,79	0
56	MG	CA	1745	1/1	0.76	0.13	99,99,99,99	0
56	MG	DA	3255	1/1	0.76	0.15	72,72,72,72	0
56	MG	BA	3588	1/1	0.76	0.23	78,78,78,78	0
56	MG	CA	1795	1/1	0.77	0.16	100,100,100,100	0
56	MG	DA	3348	1/1	0.77	0.24	77,77,77,77	0
56	MG	BA	3397	1/1	0.77	0.14	66,66,66,66	0
56	MG	DA	3040	1/1	0.77	0.17	78,78,78,78	0
56	MG	BA	3885	1/1	0.77	0.13	91,91,91,91	0
56	MG	CA	1799	1/1	0.77	0.11	94,94,94,94	0
56	MG	CA	1662	1/1	0.77	0.22	92,92,92,92	0
56	MG	BA	3012	1/1	0.77	0.35	69,69,69,69	0
56	MG	CA	1669	1/1	0.77	0.45	78,78,78,78	0
56	MG	BA	3591	1/1	0.77	0.19	64,64,64,64	0
56	MG	AE	201	1/1	0.77	0.38	83,83,83,83	0
56	MG	DA	3206	1/1	0.77	0.22	92,92,92,92	0
56	MG	CA	1700	1/1	0.77	0.36	90,90,90,90	0
56	MG	AA	1880	1/1	0.78	0.29	79,79,79,79	0
56	MG	CA	1748	1/1	0.78	0.20	75,75,75,75	0
56	MG	DA	3177	1/1	0.78	0.29	75,75,75,75	0
56	MG	AA	1903	1/1	0.78	0.14	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3855	1/1	0.78	0.24	103,103,103,103	0
56	MG	BA	3399	1/1	0.78	0.20	95,95,95,95	0
56	MG	AA	1687	1/1	0.78	0.34	105,105,105,105	0
56	MG	DA	3372	1/1	0.78	0.19	78,78,78,78	0
56	MG	DA	3664	1/1	0.78	0.11	97,97,97,97	0
56	MG	AV	112	1/1	0.78	0.20	79,79,79,79	0
56	MG	CA	1717	1/1	0.78	0.25	77,77,77,77	0
56	MG	CA	1684	1/1	0.78	0.19	70,70,70,70	0
56	MG	DA	3510	1/1	0.78	0.26	77,77,77,77	0
56	MG	CA	1621	1/1	0.78	0.22	100,100,100,100	0
56	MG	CA	1736	1/1	0.78	0.18	97,97,97,97	0
56	MG	AV	113	1/1	0.78	0.20	84,84,84,84	0
56	MG	CA	1812	1/1	0.78	0.11	114,114,114,114	0
56	MG	CA	1658	1/1	0.79	0.41	91,91,91,91	0
56	MG	AA	1720	1/1	0.79	0.30	92,92,92,92	0
56	MG	AK	201	1/1	0.79	0.19	107,107,107,107	0
56	MG	AA	1937	1/1	0.79	0.14	79,79,79,79	0
56	MG	AA	1733	1/1	0.79	0.13	94,94,94,94	0
56	MG	BA	3446	1/1	0.79	0.21	87,87,87,87	0
56	MG	CA	1718	1/1	0.79	0.28	88,88,88,88	0
56	MG	DA	3228	1/1	0.79	0.35	90,90,90,90	0
56	MG	BA	3294	1/1	0.79	0.21	67,67,67,67	0
56	MG	CA	1695	1/1	0.79	0.14	94,94,94,94	0
56	MG	CA	1638	1/1	0.79	0.30	99,99,99,99	0
56	MG	BA	3820	1/1	0.79	0.17	93,93,93,93	0
56	MG	DA	3497	1/1	0.79	0.11	70,70,70,70	0
56	MG	DA	3081	1/1	0.79	0.24	65,65,65,65	0
56	MG	DA	3282	1/1	0.79	0.40	75,75,75,75	0
56	MG	AA	1747	1/1	0.79	0.10	93,93,93,93	0
56	MG	DA	3289	1/1	0.79	0.18	86,86,86,86	0
56	MG	DA	3533	1/1	0.79	0.13	95,95,95,95	0
56	MG	DA	3539	1/1	0.79	0.12	102,102,102,102	0
56	MG	AA	1688	1/1	0.80	0.17	96,96,96,96	0
56	MG	AA	1805	1/1	0.80	0.41	89,89,89,89	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	DA	3082	1/1	0.80	0.30	89,89,89,89	0
56	MG	AV	111	1/1	0.80	0.31	85,85,85,85	0
56	MG	CA	1675	1/1	0.80	0.17	77,77,77,77	0
56	MG	BA	3743	1/1	0.80	0.21	71,71,71,71	0
56	MG	DA	3614	1/1	0.80	0.14	98,98,98,98	0
56	MG	CA	1692	1/1	0.80	0.39	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1737	1/1	0.80	0.30	90,90,90,90	0
56	MG	DA	3182	1/1	0.80	0.13	68,68,68,68	0
56	MG	DA	3186	1/1	0.80	0.36	76,76,76,76	0
56	MG	BA	3760	1/1	0.80	0.13	68,68,68,68	0
56	MG	DA	3364	1/1	0.80	0.18	94,94,94,94	0
56	MG	DA	3201	1/1	0.80	0.13	80,80,80,80	0
56	MG	DA	3674	1/1	0.80	0.10	105,105,105,105	0
56	MG	CA	1635	1/1	0.80	0.55	72,72,72,72	0
56	MG	DA	3696	1/1	0.80	0.18	96,96,96,96	0
56	MG	BA	3439	1/1	0.80	0.28	82,82,82,82	0
56	MG	BA	3790	1/1	0.80	0.09	75,75,75,75	0
56	MG	CA	1771	1/1	0.80	0.26	78,78,78,78	0
56	MG	AA	1724	1/1	0.80	0.21	92,92,92,92	0
56	MG	DB	209	1/1	0.80	0.27	86,86,86,86	0
56	MG	BA	3388	1/1	0.80	0.14	77,77,77,77	0
56	MG	DU	201	1/1	0.80	0.20	72,72,72,72	0
56	MG	AA	1602	1/1	0.80	0.16	104,104,104,104	0
56	MG	DA	3430	1/1	0.81	0.22	83,83,83,83	0
56	MG	AY	201	1/1	0.81	0.12	111,111,111,111	0
56	MG	CA	1742	1/1	0.81	0.19	89,89,89,89	0
56	MG	DA	3224	1/1	0.81	0.22	75,75,75,75	0
56	MG	CA	1687	1/1	0.81	0.20	81,81,81,81	0
56	MG	AA	1736	1/1	0.81	0.17	82,82,82,82	0
56	MG	DA	3241	1/1	0.81	0.27	76,76,76,76	0
56	MG	DA	3254	1/1	0.81	0.12	71,71,71,71	0
56	MG	CA	1618	1/1	0.81	0.27	78,78,78,78	0
56	MG	CA	1752	1/1	0.81	0.19	58,58,58,58	0
56	MG	AA	1678	1/1	0.81	0.24	90,90,90,90	0
56	MG	DA	3049	1/1	0.81	0.23	76,76,76,76	0
56	MG	DA	3279	1/1	0.81	0.19	74,74,74,74	0
56	MG	CA	1699	1/1	0.81	0.16	97,97,97,97	0
56	MG	AA	1851	1/1	0.81	0.09	80,80,80,80	0
56	MG	DA	3607	1/1	0.81	0.11	90,90,90,90	0
56	MG	AA	1859	1/1	0.81	0.13	91,91,91,91	0
56	MG	AA	1704	1/1	0.81	0.23	79,79,79,79	0
56	MG	DA	3092	1/1	0.81	0.27	92,92,92,92	0
56	MG	AA	1820	1/1	0.81	0.22	86,86,86,86	0
56	MG	AA	1821	1/1	0.81	0.24	78,78,78,78	0
56	MG	BA	3111	1/1	0.81	0.34	66,66,66,66	0
56	MG	AA	1800	1/1	0.81	0.25	76,76,76,76	0
56	MG	BA	3256	1/1	0.81	0.25	77,77,77,77	0
56	MG	BA	3558	1/1	0.81	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3287	1/1	0.81	0.26	82,82,82,82	0
56	MG	DA	3356	1/1	0.81	0.28	85,85,85,85	0
56	MG	DA	3197	1/1	0.81	0.34	82,82,82,82	0
56	MG	DA	3366	1/1	0.81	0.09	81,81,81,81	0
56	MG	BB	203	1/1	0.81	0.17	63,63,63,63	0
56	MG	CA	1683	1/1	0.81	0.42	71,71,71,71	0
56	MG	DA	3373	1/1	0.81	0.40	75,75,75,75	0
56	MG	DA	3379	1/1	0.81	0.30	80,80,80,80	0
56	MG	DA	3380	1/1	0.81	0.23	84,84,84,84	0
56	MG	DA	3381	1/1	0.81	0.22	88,88,88,88	0
56	MG	DA	3347	1/1	0.82	0.35	77,77,77,77	0
56	MG	CA	1733	1/1	0.82	0.17	90,90,90,90	0
56	MG	DA	3084	1/1	0.82	0.14	76,76,76,76	0
56	MG	DA	3360	1/1	0.82	0.22	61,61,61,61	0
56	MG	DA	3362	1/1	0.82	0.21	75,75,75,75	0
56	MG	DA	3363	1/1	0.82	0.22	64,64,64,64	0
56	MG	BA	3481	1/1	0.82	0.10	87,87,87,87	0
56	MG	DA	3114	1/1	0.82	0.28	70,70,70,70	0
56	MG	DA	3116	1/1	0.82	0.25	79,79,79,79	0
56	MG	AA	1647	1/1	0.82	0.27	77,77,77,77	0
56	MG	BA	3501	1/1	0.82	0.11	80,80,80,80	0
56	MG	CA	1645	1/1	0.82	0.33	74,74,74,74	0
56	MG	AA	1727	1/1	0.82	0.31	73,73,73,73	0
56	MG	AA	1746	1/1	0.82	0.28	81,81,81,81	0
56	MG	DA	3400	1/1	0.82	0.23	53,53,53,53	0
56	MG	DA	3180	1/1	0.82	0.20	75,75,75,75	0
56	MG	BA	3236	1/1	0.82	0.09	50,50,50,50	0
56	MG	DA	3465	1/1	0.82	0.12	104,104,104,104	0
56	MG	DA	3185	1/1	0.82	0.14	58,58,58,58	0
56	MG	DA	3478	1/1	0.82	0.16	90,90,90,90	0
56	MG	AA	1808	1/1	0.82	0.24	75,75,75,75	0
56	MG	BA	3605	1/1	0.82	0.10	75,75,75,75	0
56	MG	AA	1669	1/1	0.82	0.28	84,84,84,84	0
56	MG	AA	1618	1/1	0.82	0.27	61,61,61,61	0
56	MG	AA	1759	1/1	0.82	0.17	60,60,60,60	0
56	MG	DA	3207	1/1	0.82	0.22	74,74,74,74	0
56	MG	DA	3208	1/1	0.82	0.34	91,91,91,91	0
56	MG	CA	1784	1/1	0.82	0.15	96,96,96,96	0
56	MG	BA	3300	1/1	0.82	0.27	70,70,70,70	0
56	MG	DA	3227	1/1	0.82	0.27	79,79,79,79	0
56	MG	BA	3331	1/1	0.82	0.21	66,66,66,66	0
56	MG	BA	3339	1/1	0.82	0.22	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1688	1/1	0.82	0.24	68,68,68,68	0
56	MG	BA	3353	1/1	0.82	0.19	57,57,57,57	0
56	MG	BA	3808	1/1	0.82	0.11	70,70,70,70	0
56	MG	AA	1655	1/1	0.82	0.24	77,77,77,77	0
56	MG	DA	3629	1/1	0.82	0.23	104,104,104,104	0
56	MG	DA	3631	1/1	0.82	0.19	94,94,94,94	0
56	MG	AV	107	1/1	0.82	0.28	87,87,87,87	0
56	MG	AA	1817	1/1	0.82	0.30	93,93,93,93	0
56	MG	DA	3268	1/1	0.82	0.18	64,64,64,64	0
56	MG	DA	3272	1/1	0.82	0.21	68,68,68,68	0
56	MG	AA	1622	1/1	0.82	0.33	56,56,56,56	0
56	MG	AA	1913	1/1	0.82	0.08	109,109,109,109	0
56	MG	AA	1799	1/1	0.82	0.19	95,95,95,95	0
56	MG	BB	208	1/1	0.82	0.14	54,54,54,54	0
56	MG	BB	228	1/1	0.82	0.10	69,69,69,69	0
56	MG	CA	1706	1/1	0.82	0.46	75,75,75,75	0
56	MG	DB	206	1/1	0.82	0.22	77,77,77,77	0
56	MG	BA	3435	1/1	0.82	0.14	84,84,84,84	0
56	MG	CA	1612	1/1	0.82	0.27	84,84,84,84	0
56	MG	AA	1922	1/1	0.82	0.11	106,106,106,106	0
56	MG	BA	3026	1/1	0.82	0.20	92,92,92,92	0
56	MG	DA	3072	1/1	0.82	0.18	65,65,65,65	0
56	MG	BA	3476	1/1	0.82	0.13	50,50,50,50	0
56	MG	DA	3119	1/1	0.83	0.21	39,39,39,39	0
56	MG	AA	1670	1/1	0.83	0.25	88,88,88,88	0
56	MG	BA	3844	1/1	0.83	0.08	99,99,99,99	0
56	MG	CA	1707	1/1	0.83	0.24	72,72,72,72	0
56	MG	CA	1661	1/1	0.83	0.24	101,101,101,101	0
56	MG	DA	3165	1/1	0.83	0.32	65,65,65,65	0
56	MG	CA	1803	1/1	0.83	0.08	102,102,102,102	0
56	MG	DA	3178	1/1	0.83	0.23	77,77,77,77	0
56	MG	BA	3523	1/1	0.83	0.17	76,76,76,76	0
56	MG	AA	1729	1/1	0.83	0.24	79,79,79,79	0
56	MG	CA	1666	1/1	0.83	0.26	73,73,73,73	0
56	MG	CV	104	1/1	0.83	0.24	92,92,92,92	0
56	MG	AA	1601	1/1	0.83	0.20	65,65,65,65	0
56	MG	BA	3892	1/1	0.83	0.20	94,94,94,94	0
56	MG	AA	1629	1/1	0.83	0.28	68,68,68,68	0
56	MG	DA	3203	1/1	0.83	0.30	91,91,91,91	0
56	MG	DA	3625	1/1	0.83	0.12	80,80,80,80	0
56	MG	BA	3414	1/1	0.83	0.16	72,72,72,72	0
56	MG	BB	209	1/1	0.83	0.24	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3420	1/1	0.83	0.16	65,65,65,65	0
56	MG	AA	1703	1/1	0.83	0.12	74,74,74,74	0
56	MG	DA	3367	1/1	0.83	0.15	75,75,75,75	0
56	MG	AA	1810	1/1	0.83	0.23	84,84,84,84	0
56	MG	CA	1694	1/1	0.83	0.31	80,80,80,80	0
56	MG	AA	1794	1/1	0.83	0.36	68,68,68,68	0
56	MG	DA	3374	1/1	0.83	0.21	75,75,75,75	0
56	MG	BA	3444	1/1	0.83	0.28	74,74,74,74	0
56	MG	AA	1690	1/1	0.83	0.10	65,65,65,65	0
56	MG	BA	3372	1/1	0.83	0.16	77,77,77,77	0
56	MG	DA	3398	1/1	0.83	0.09	58,58,58,58	0
56	MG	BA	3792	1/1	0.83	0.15	48,48,48,48	0
56	MG	BA	3384	1/1	0.83	0.13	72,72,72,72	0
56	MG	DA	3109	1/1	0.83	0.28	74,74,74,74	0
56	MG	BA	3499	1/1	0.83	0.28	73,73,73,73	0
56	MG	DB	213	1/1	0.83	0.15	115,115,115,115	0
56	MG	DE	304	1/1	0.83	0.20	70,70,70,70	0
56	MG	AA	1693	1/1	0.83	0.18	103,103,103,103	0
56	MG	DA	3117	1/1	0.83	0.27	70,70,70,70	0
56	MG	DA	3588	1/1	0.84	0.11	109,109,109,109	0
56	MG	AA	1893	1/1	0.84	0.10	95,95,95,95	0
56	MG	AA	1898	1/1	0.84	0.07	98,98,98,98	0
56	MG	DA	3171	1/1	0.84	0.12	66,66,66,66	0
56	MG	AA	1900	1/1	0.84	0.12	110,110,110,110	0
56	MG	DA	3618	1/1	0.84	0.16	80,80,80,80	0
56	MG	DA	3269	1/1	0.84	0.29	85,85,85,85	0
56	MG	CA	1689	1/1	0.84	0.36	84,84,84,84	0
56	MG	CA	1785	1/1	0.84	0.15	87,87,87,87	0
56	MG	DA	3280	1/1	0.84	0.14	80,80,80,80	0
56	MG	AA	1856	1/1	0.84	0.17	66,66,66,66	0
56	MG	BA	3342	1/1	0.84	0.32	66,66,66,66	0
56	MG	BA	3188	1/1	0.84	0.27	74,74,74,74	0
56	MG	AD	302	1/1	0.84	0.31	79,79,79,79	0
56	MG	AA	1726	1/1	0.84	0.22	55,55,55,55	0
56	MG	CA	1798	1/1	0.84	0.13	94,94,94,94	0
56	MG	AA	1666	1/1	0.84	0.22	70,70,70,70	0
56	MG	AA	1853	1/1	0.84	0.20	93,93,93,93	0
56	MG	DB	202	1/1	0.84	0.43	73,73,73,73	0
56	MG	CA	1808	1/1	0.84	0.10	102,102,102,102	0
56	MG	BA	3448	1/1	0.84	0.10	60,60,60,60	0
56	MG	BA	3628	1/1	0.84	0.14	66,66,66,66	0
56	MG	CA	1814	1/1	0.84	0.10	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1633	1/1	0.84	0.28	81,81,81,81	0
56	MG	DA	3126	1/1	0.84	0.12	69,69,69,69	0
56	MG	DA	3146	1/1	0.84	0.16	66,66,66,66	0
56	MG	CA	1762	1/1	0.84	0.16	76,76,76,76	0
56	MG	CA	1676	1/1	0.84	0.23	83,83,83,83	0
56	MG	BA	3708	1/1	0.84	0.11	85,85,85,85	0
56	MG	DA	3365	1/1	0.84	0.11	71,71,71,71	0
57	ZN	AN	101	1/1	0.84	0.14	164,164,164,164	0
56	MG	CA	1716	1/1	0.85	0.10	66,66,66,66	0
56	MG	BA	3364	1/1	0.85	0.08	69,69,69,69	0
56	MG	BB	204	1/1	0.85	0.18	57,57,57,57	0
56	MG	AA	1863	1/1	0.85	0.18	54,54,54,54	0
56	MG	DA	3293	1/1	0.85	0.29	94,94,94,94	0
56	MG	AA	1694	1/1	0.85	0.23	74,74,74,74	0
56	MG	AA	1942	1/1	0.85	0.17	93,93,93,93	0
56	MG	DA	3297	1/1	0.85	0.24	81,81,81,81	0
56	MG	DA	3304	1/1	0.85	0.09	67,67,67,67	0
56	MG	BA	3054	1/1	0.85	0.21	58,58,58,58	0
56	MG	DA	3191	1/1	0.85	0.21	77,77,77,77	0
56	MG	DA	3585	1/1	0.85	0.18	104,104,104,104	0
56	MG	DA	3056	1/1	0.85	0.17	59,59,59,59	0
56	MG	DA	3331	1/1	0.85	0.32	77,77,77,77	0
56	MG	AA	1697	1/1	0.85	0.10	75,75,75,75	0
56	MG	AA	1731	1/1	0.85	0.25	70,70,70,70	0
56	MG	DA	3202	1/1	0.85	0.19	73,73,73,73	0
56	MG	AA	1755	1/1	0.85	0.12	70,70,70,70	0
56	MG	BA	3491	1/1	0.85	0.13	41,41,41,41	0
56	MG	DA	3083	1/1	0.85	0.22	82,82,82,82	0
56	MG	CA	1622	1/1	0.85	0.43	80,80,80,80	0
56	MG	DA	3210	1/1	0.85	0.25	74,74,74,74	0
56	MG	CA	1806	1/1	0.85	0.09	102,102,102,102	0
56	MG	DA	3098	1/1	0.85	0.17	39,39,39,39	0
56	MG	BA	3235	1/1	0.85	0.10	55,55,55,55	0
56	MG	CA	1757	1/1	0.85	0.14	94,94,94,94	0
56	MG	CA	1760	1/1	0.85	0.27	103,103,103,103	0
56	MG	DA	3371	1/1	0.85	0.11	65,65,65,65	0
56	MG	DA	3233	1/1	0.85	0.20	80,80,80,80	0
56	MG	DA	3682	1/1	0.85	0.09	90,90,90,90	0
56	MG	DA	3685	1/1	0.85	0.10	96,96,96,96	0
56	MG	DA	3690	1/1	0.85	0.09	107,107,107,107	0
56	MG	DA	3240	1/1	0.85	0.21	74,74,74,74	0
56	MG	CA	1678	1/1	0.85	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1714	1/1	0.85	0.20	74,74,74,74	0
56	MG	DA	3122	1/1	0.85	0.29	65,65,65,65	0
56	MG	DB	205	1/1	0.85	0.09	79,79,79,79	0
56	MG	BA	3886	1/1	0.85	0.12	94,94,94,94	0
56	MG	BA	3423	1/1	0.85	0.14	85,85,85,85	0
56	MG	CV	108	1/1	0.85	0.18	79,79,79,79	0
56	MG	CA	1776	1/1	0.85	0.27	90,90,90,90	0
56	MG	DA	3004	1/1	0.85	0.44	75,75,75,75	0
56	MG	DA	3448	1/1	0.85	0.10	73,73,73,73	0
56	MG	DA	3005	1/1	0.85	0.10	73,73,73,73	0
56	MG	DA	3008	1/1	0.85	0.09	108,108,108,108	0
56	MG	DA	3473	1/1	0.85	0.23	81,81,81,81	0
56	MG	DA	3170	1/1	0.85	0.09	96,96,96,96	0
56	MG	BA	3652	1/1	0.86	0.07	53,53,53,53	0
56	MG	DA	3016	1/1	0.86	0.14	42,42,42,42	0
56	MG	AA	1902	1/1	0.86	0.06	121,121,121,121	0
56	MG	AA	1831	1/1	0.86	0.15	63,63,63,63	0
56	MG	BA	3741	1/1	0.86	0.08	63,63,63,63	0
56	MG	AA	1834	1/1	0.86	0.14	76,76,76,76	0
56	MG	AA	1651	1/1	0.86	0.18	80,80,80,80	0
56	MG	AA	1809	1/1	0.86	0.19	83,83,83,83	0
56	MG	BA	3764	1/1	0.86	0.09	85,85,85,85	0
56	MG	DA	3069	1/1	0.86	0.31	83,83,83,83	0
56	MG	DA	3488	1/1	0.86	0.24	73,73,73,73	0
56	MG	CA	1660	1/1	0.86	0.15	92,92,92,92	0
56	MG	BA	3777	1/1	0.86	0.19	65,65,65,65	0
56	MG	AA	1846	1/1	0.86	0.16	90,90,90,90	0
56	MG	DA	3511	1/1	0.86	0.11	77,77,77,77	0
56	MG	AA	1930	1/1	0.86	0.12	58,58,58,58	0
56	MG	DA	3522	1/1	0.86	0.17	76,76,76,76	0
56	MG	DA	3529	1/1	0.86	0.23	82,82,82,82	0
56	MG	AA	1764	1/1	0.86	0.10	72,72,72,72	0
56	MG	BA	3193	1/1	0.86	0.22	45,45,45,45	0
56	MG	BA	3229	1/1	0.86	0.09	41,41,41,41	0
56	MG	BA	3230	1/1	0.86	0.16	57,57,57,57	0
56	MG	DA	3544	1/1	0.86	0.10	79,79,79,79	0
56	MG	DA	3549	1/1	0.86	0.13	87,87,87,87	0
56	MG	AA	1775	1/1	0.86	0.08	77,77,77,77	0
56	MG	CA	1677	1/1	0.86	0.10	88,88,88,88	0
56	MG	AA	1784	1/1	0.86	0.29	69,69,69,69	0
56	MG	CA	1682	1/1	0.86	0.31	73,73,73,73	0
56	MG	AA	1716	1/1	0.86	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3244	1/1	0.86	0.14	60,60,60,60	0
56	MG	DA	3295	1/1	0.86	0.22	75,75,75,75	0
56	MG	CA	1790	1/1	0.86	0.17	64,64,64,64	0
56	MG	BA	3866	1/1	0.86	0.09	82,82,82,82	0
56	MG	DA	3299	1/1	0.86	0.27	57,57,57,57	0
56	MG	BA	3463	1/1	0.86	0.09	57,57,57,57	0
56	MG	AA	1732	1/1	0.86	0.18	65,65,65,65	0
56	MG	DA	3628	1/1	0.86	0.20	80,80,80,80	0
56	MG	BA	3258	1/1	0.86	0.12	71,71,71,71	0
56	MG	DA	3311	1/1	0.86	0.26	68,68,68,68	0
56	MG	DA	3317	1/1	0.86	0.10	84,84,84,84	0
56	MG	BA	3896	1/1	0.86	0.11	72,72,72,72	0
56	MG	BA	3281	1/1	0.86	0.18	72,72,72,72	0
56	MG	DA	3659	1/1	0.86	0.19	77,77,77,77	0
56	MG	AA	1865	1/1	0.86	0.28	81,81,81,81	0
56	MG	DA	3175	1/1	0.86	0.26	75,75,75,75	0
56	MG	DA	3673	1/1	0.86	0.13	111,111,111,111	0
56	MG	AA	1874	1/1	0.86	0.20	95,95,95,95	0
56	MG	AA	1725	1/1	0.86	0.28	65,65,65,65	0
56	MG	DA	3349	1/1	0.86	0.18	72,72,72,72	0
56	MG	CA	1811	1/1	0.86	0.07	102,102,102,102	0
56	MG	BA	3312	1/1	0.86	0.19	54,54,54,54	0
56	MG	B2	101	1/1	0.86	0.29	63,63,63,63	0
56	MG	AA	1603	1/1	0.86	0.11	78,78,78,78	0
56	MG	CA	1605	1/1	0.86	0.21	59,59,59,59	0
56	MG	CA	1816	1/1	0.86	0.09	110,110,110,110	0
56	MG	AA	1752	1/1	0.86	0.13	88,88,88,88	0
56	MG	AA	1680	1/1	0.86	0.13	65,65,65,65	0
56	MG	DA	3368	1/1	0.86	0.22	80,80,80,80	0
56	MG	AV	109	1/1	0.86	0.18	81,81,81,81	0
56	MG	CA	1619	1/1	0.86	0.19	71,71,71,71	0
56	MG	DA	3204	1/1	0.86	0.08	76,76,76,76	0
56	MG	CA	1710	1/1	0.86	0.15	95,95,95,95	0
56	MG	DB	214	1/1	0.86	0.14	83,83,83,83	0
56	MG	AA	1739	1/1	0.86	0.21	99,99,99,99	0
56	MG	DA	3375	1/1	0.86	0.14	84,84,84,84	0
56	MG	D0	101	1/1	0.86	0.39	79,79,79,79	0
56	MG	AA	1827	1/1	0.86	0.13	69,69,69,69	0
56	MG	CA	1629	1/1	0.86	0.44	74,74,74,74	0
56	MG	B2	102	1/1	0.87	0.13	66,66,66,66	0
56	MG	DA	3070	1/1	0.87	0.18	74,74,74,74	0
56	MG	DA	3236	1/1	0.87	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3467	1/1	0.87	0.12	91,91,91,91	0
56	MG	AA	1858	1/1	0.87	0.10	90,90,90,90	0
56	MG	DA	3073	1/1	0.87	0.18	63,63,63,63	0
56	MG	DA	3242	1/1	0.87	0.18	77,77,77,77	0
56	MG	DA	3253	1/1	0.87	0.28	67,67,67,67	0
56	MG	DA	3491	1/1	0.87	0.11	101,101,101,101	0
56	MG	AA	1807	1/1	0.87	0.16	84,84,84,84	0
56	MG	BA	3355	1/1	0.87	0.16	62,62,62,62	0
56	MG	DA	3256	1/1	0.87	0.18	73,73,73,73	0
56	MG	CA	1693	1/1	0.87	0.17	83,83,83,83	0
56	MG	AA	1833	1/1	0.87	0.15	70,70,70,70	0
56	MG	DA	3086	1/1	0.87	0.22	32,32,32,32	0
56	MG	DA	3525	1/1	0.87	0.21	77,77,77,77	0
56	MG	CA	1617	1/1	0.87	0.35	61,61,61,61	0
56	MG	DA	3093	1/1	0.87	0.31	77,77,77,77	0
56	MG	BA	3483	1/1	0.87	0.18	70,70,70,70	0
56	MG	DA	3278	1/1	0.87	0.10	66,66,66,66	0
56	MG	BA	3486	1/1	0.87	0.08	60,60,60,60	0
56	MG	BA	3796	1/1	0.87	0.23	83,83,83,83	0
56	MG	AA	1905	1/1	0.87	0.06	130,130,130,130	0
56	MG	DA	3550	1/1	0.87	0.26	42,42,42,42	0
56	MG	BA	3806	1/1	0.87	0.18	57,57,57,57	0
56	MG	BA	3807	1/1	0.87	0.16	64,64,64,64	0
56	MG	CA	1634	1/1	0.87	0.29	63,63,63,63	0
56	MG	DA	3579	1/1	0.87	0.15	104,104,104,104	0
56	MG	DA	3125	1/1	0.87	0.16	65,65,65,65	0
56	MG	BA	3248	1/1	0.87	0.25	24,24,24,24	0
56	MG	DA	3139	1/1	0.87	0.41	64,64,64,64	0
56	MG	DA	3598	1/1	0.87	0.22	69,69,69,69	0
56	MG	CA	1804	1/1	0.87	0.12	103,103,103,103	0
56	MG	AA	1674	1/1	0.87	0.29	74,74,74,74	0
56	MG	AA	1684	1/1	0.87	0.20	102,102,102,102	0
56	MG	BA	3099	1/1	0.87	0.17	32,32,32,32	0
56	MG	BA	3283	1/1	0.87	0.09	47,47,47,47	0
56	MG	DA	3163	1/1	0.87	0.40	68,68,68,68	0
56	MG	DA	3626	1/1	0.87	0.13	103,103,103,103	0
56	MG	CA	1711	1/1	0.87	0.32	70,70,70,70	0
56	MG	DA	3167	1/1	0.87	0.18	67,67,67,67	0
56	MG	CA	1651	1/1	0.87	0.15	54,54,54,54	0
56	MG	DA	3320	1/1	0.87	0.17	56,56,56,56	0
56	MG	BA	3286	1/1	0.87	0.20	61,61,61,61	0
56	MG	DA	3656	1/1	0.87	0.09	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3863	1/1	0.87	0.08	72,72,72,72	0
56	MG	BA	3400	1/1	0.87	0.19	122,122,122,122	0
56	MG	AT	201	1/1	0.87	0.06	111,111,111,111	0
56	MG	DA	3179	1/1	0.87	0.12	67,67,67,67	0
56	MG	AA	1679	1/1	0.87	0.22	84,84,84,84	0
56	MG	DA	3354	1/1	0.87	0.18	43,43,43,43	0
56	MG	BA	3888	1/1	0.87	0.07	99,99,99,99	0
56	MG	AA	1788	1/1	0.87	0.26	62,62,62,62	0
56	MG	CA	1740	1/1	0.87	0.13	73,73,73,73	0
56	MG	BA	3648	1/1	0.87	0.11	49,49,49,49	0
56	MG	DA	3693	1/1	0.87	0.14	103,103,103,103	0
56	MG	AA	1789	1/1	0.87	0.12	77,77,77,77	0
56	MG	DB	201	1/1	0.87	0.25	61,61,61,61	0
56	MG	DA	3010	1/1	0.87	0.16	78,78,78,78	0
56	MG	CA	1672	1/1	0.87	0.23	76,76,76,76	0
56	MG	BA	3326	1/1	0.87	0.16	100,100,100,100	0
56	MG	BA	3329	1/1	0.87	0.24	85,85,85,85	0
56	MG	DA	3023	1/1	0.87	0.19	56,56,56,56	0
56	MG	AA	1825	1/1	0.87	0.27	64,64,64,64	0
56	MG	DA	3035	1/1	0.87	0.18	76,76,76,76	0
56	MG	BA	3445	1/1	0.87	0.20	68,68,68,68	0
56	MG	BF	305	1/1	0.87	0.21	52,52,52,52	0
56	MG	BO	201	1/1	0.87	0.19	62,62,62,62	0
56	MG	DA	3216	1/1	0.87	0.10	46,46,46,46	0
56	MG	DA	3219	1/1	0.87	0.17	67,67,67,67	0
56	MG	DO	201	1/1	0.87	0.15	80,80,80,80	0
56	MG	DA	3220	1/1	0.87	0.11	83,83,83,83	0
56	MG	DV	201	1/1	0.87	0.12	62,62,62,62	0
56	MG	DX	101	1/1	0.87	0.11	55,55,55,55	0
56	MG	AA	1615	1/1	0.87	0.16	75,75,75,75	0
56	MG	DA	3060	1/1	0.87	0.21	90,90,90,90	0
56	MG	CA	1773	1/1	0.87	0.12	124,124,124,124	0
57	ZN	D9	101	1/1	0.87	0.13	117,117,117,117	0
56	MG	DA	3471	1/1	0.88	0.13	87,87,87,87	0
56	MG	BA	3319	1/1	0.88	0.10	59,59,59,59	0
56	MG	BA	3322	1/1	0.88	0.29	54,54,54,54	0
56	MG	DA	3475	1/1	0.88	0.18	78,78,78,78	0
56	MG	CA	1654	1/1	0.88	0.19	74,74,74,74	0
56	MG	AA	1617	1/1	0.88	0.12	58,58,58,58	0
56	MG	BA	3327	1/1	0.88	0.21	80,80,80,80	0
56	MG	DA	3494	1/1	0.88	0.19	70,70,70,70	0
56	MG	DA	3074	1/1	0.88	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3507	1/1	0.88	0.12	109,109,109,109	0
56	MG	AA	1728	1/1	0.88	0.28	81,81,81,81	0
56	MG	CA	1765	1/1	0.88	0.21	61,61,61,61	0
56	MG	BA	3848	1/1	0.88	0.14	43,43,43,43	0
56	MG	AA	1719	1/1	0.88	0.11	70,70,70,70	0
56	MG	DA	3521	1/1	0.88	0.22	60,60,60,60	0
56	MG	DA	3264	1/1	0.88	0.17	74,74,74,74	0
56	MG	BA	3488	1/1	0.88	0.18	35,35,35,35	0
56	MG	BA	3857	1/1	0.88	0.10	78,78,78,78	0
56	MG	AA	1879	1/1	0.88	0.28	71,71,71,71	0
56	MG	BA	3182	1/1	0.88	0.25	25,25,25,25	0
56	MG	DA	3274	1/1	0.88	0.30	70,70,70,70	0
56	MG	AA	1744	1/1	0.88	0.17	68,68,68,68	0
56	MG	AA	1668	1/1	0.88	0.18	65,65,65,65	0
56	MG	BA	3356	1/1	0.88	0.20	66,66,66,66	0
56	MG	CA	1786	1/1	0.88	0.15	80,80,80,80	0
56	MG	CA	1787	1/1	0.88	0.12	98,98,98,98	0
56	MG	DA	3287	1/1	0.88	0.23	62,62,62,62	0
56	MG	BA	3533	1/1	0.88	0.12	61,61,61,61	0
56	MG	BA	3357	1/1	0.88	0.16	82,82,82,82	0
56	MG	DA	3583	1/1	0.88	0.08	96,96,96,96	0
56	MG	BA	3363	1/1	0.88	0.31	63,63,63,63	0
56	MG	DA	3129	1/1	0.88	0.17	53,53,53,53	0
56	MG	BA	3571	1/1	0.88	0.09	31,31,31,31	0
56	MG	DA	3142	1/1	0.88	0.21	50,50,50,50	0
56	MG	AA	1835	1/1	0.88	0.14	88,88,88,88	0
56	MG	DA	3611	1/1	0.88	0.11	80,80,80,80	0
56	MG	AF	201	1/1	0.88	0.24	79,79,79,79	0
56	MG	DA	3303	1/1	0.88	0.24	54,54,54,54	0
56	MG	DA	3617	1/1	0.88	0.09	86,86,86,86	0
56	MG	BB	219	1/1	0.88	0.28	85,85,85,85	0
56	MG	BB	222	1/1	0.88	0.16	70,70,70,70	0
56	MG	CA	1802	1/1	0.88	0.08	115,115,115,115	0
56	MG	DA	3310	1/1	0.88	0.29	72,72,72,72	0
56	MG	DA	3162	1/1	0.88	0.26	54,54,54,54	0
56	MG	AA	1722	1/1	0.88	0.17	68,68,68,68	0
56	MG	BA	3387	1/1	0.88	0.20	48,48,48,48	0
56	MG	DA	3319	1/1	0.88	0.35	69,69,69,69	0
56	MG	AA	1751	1/1	0.88	0.14	74,74,74,74	0
56	MG	DA	3325	1/1	0.88	0.29	62,62,62,62	0
56	MG	BP	202	1/1	0.88	0.08	62,62,62,62	0
56	MG	BA	3392	1/1	0.88	0.26	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1637	1/1	0.88	0.18	73,73,73,73	0
56	MG	CA	1601	1/1	0.88	0.37	79,79,79,79	0
56	MG	CA	1603	1/1	0.88	0.31	72,72,72,72	0
56	MG	BA	3714	1/1	0.88	0.10	62,62,62,62	0
56	MG	AA	1848	1/1	0.88	0.21	71,71,71,71	0
56	MG	DA	3355	1/1	0.88	0.24	55,55,55,55	0
56	MG	CA	1606	1/1	0.88	0.28	77,77,77,77	0
56	MG	DA	3689	1/1	0.88	0.11	104,104,104,104	0
56	MG	CA	1610	1/1	0.88	0.22	63,63,63,63	0
56	MG	BA	3737	1/1	0.88	0.10	60,60,60,60	0
56	MG	DA	3187	1/1	0.88	0.26	109,109,109,109	0
56	MG	AA	1850	1/1	0.88	0.17	85,85,85,85	0
56	MG	AA	1798	1/1	0.88	0.21	54,54,54,54	0
56	MG	DA	3198	1/1	0.88	0.32	80,80,80,80	0
56	MG	AA	1908	1/1	0.88	0.14	97,97,97,97	0
56	MG	DA	3007	1/1	0.88	0.09	82,82,82,82	0
56	MG	BA	3271	1/1	0.88	0.06	44,44,44,44	0
56	MG	CA	1714	1/1	0.88	0.12	74,74,74,74	0
56	MG	BA	3280	1/1	0.88	0.10	58,58,58,58	0
56	MG	AA	1911	1/1	0.88	0.07	106,106,106,106	0
56	MG	AA	1658	1/1	0.88	0.34	73,73,73,73	0
56	MG	AA	1642	1/1	0.88	0.30	73,73,73,73	0
56	MG	AA	1921	1/1	0.88	0.09	97,97,97,97	0
56	MG	AA	1758	1/1	0.88	0.14	72,72,72,72	0
56	MG	BA	3797	1/1	0.88	0.11	91,91,91,91	0
56	MG	DO	202	1/1	0.88	0.06	95,95,95,95	0
56	MG	AA	1717	1/1	0.88	0.11	76,76,76,76	0
56	MG	CA	1738	1/1	0.88	0.10	98,98,98,98	0
56	MG	DA	3051	1/1	0.88	0.10	60,60,60,60	0
56	MG	CA	1641	1/1	0.88	0.21	80,80,80,80	0
56	MG	CA	1642	1/1	0.88	0.29	84,84,84,84	0
56	MG	D6	102	1/1	0.88	0.17	82,82,82,82	0
56	MG	BA	3048	1/1	0.88	0.14	54,54,54,54	0
56	MG	DA	3062	1/1	0.88	0.15	65,65,65,65	0
56	MG	AA	1696	1/1	0.89	0.26	95,95,95,95	0
56	MG	CA	1630	1/1	0.89	0.36	70,70,70,70	0
56	MG	BA	3120	1/1	0.89	0.18	51,51,51,51	0
56	MG	DA	3499	1/1	0.89	0.12	68,68,68,68	0
56	MG	BA	3149	1/1	0.89	0.09	35,35,35,35	0
56	MG	BA	3158	1/1	0.89	0.14	48,48,48,48	0
56	MG	BA	3406	1/1	0.89	0.12	64,64,64,64	0
56	MG	BA	3589	1/1	0.89	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3134	1/1	0.89	0.21	61,61,61,61	0
56	MG	DA	3136	1/1	0.89	0.42	67,67,67,67	0
56	MG	CA	1713	1/1	0.89	0.22	71,71,71,71	0
56	MG	DA	3524	1/1	0.89	0.09	99,99,99,99	0
56	MG	BA	3408	1/1	0.89	0.19	44,44,44,44	0
56	MG	DA	3283	1/1	0.89	0.32	76,76,76,76	0
56	MG	BA	3593	1/1	0.89	0.10	54,54,54,54	0
56	MG	CA	1644	1/1	0.89	0.23	69,69,69,69	0
56	MG	DA	3535	1/1	0.89	0.14	96,96,96,96	0
56	MG	DA	3149	1/1	0.89	0.16	51,51,51,51	0
56	MG	DA	3150	1/1	0.89	0.10	65,65,65,65	0
56	MG	BA	3600	1/1	0.89	0.15	36,36,36,36	0
56	MG	CA	1818	1/1	0.89	0.11	87,87,87,87	0
56	MG	CA	1719	1/1	0.89	0.15	85,85,85,85	0
56	MG	DA	3555	1/1	0.89	0.15	94,94,94,94	0
56	MG	BA	3314	1/1	0.89	0.23	65,65,65,65	0
56	MG	BA	3608	1/1	0.89	0.12	81,81,81,81	0
56	MG	DA	3164	1/1	0.89	0.17	87,87,87,87	0
56	MG	CA	1731	1/1	0.89	0.20	84,84,84,84	0
56	MG	DA	3002	1/1	0.89	0.25	69,69,69,69	0
56	MG	AA	1706	1/1	0.89	0.20	62,62,62,62	0
56	MG	CA	1655	1/1	0.89	0.19	66,66,66,66	0
56	MG	DA	3174	1/1	0.89	0.27	68,68,68,68	0
56	MG	AA	1745	1/1	0.89	0.23	64,64,64,64	0
56	MG	DA	3176	1/1	0.89	0.22	67,67,67,67	0
56	MG	AA	1894	1/1	0.89	0.19	83,83,83,83	0
56	MG	BA	3194	1/1	0.89	0.32	70,70,70,70	0
56	MG	BB	207	1/1	0.89	0.24	44,44,44,44	0
56	MG	BA	3713	1/1	0.89	0.17	85,85,85,85	0
56	MG	BA	3228	1/1	0.89	0.30	59,59,59,59	0
56	MG	DA	3183	1/1	0.89	0.08	106,106,106,106	0
56	MG	DA	3338	1/1	0.89	0.27	69,69,69,69	0
56	MG	DA	3339	1/1	0.89	0.18	74,74,74,74	0
56	MG	BB	217	1/1	0.89	0.17	80,80,80,80	0
56	MG	DA	3345	1/1	0.89	0.09	67,67,67,67	0
56	MG	DA	3346	1/1	0.89	0.21	70,70,70,70	0
56	MG	BA	3716	1/1	0.89	0.15	40,40,40,40	0
56	MG	DA	3647	1/1	0.89	0.21	70,70,70,70	0
56	MG	CA	1756	1/1	0.89	0.26	84,84,84,84	0
56	MG	DA	3655	1/1	0.89	0.10	75,75,75,75	0
56	MG	DA	3029	1/1	0.89	0.25	68,68,68,68	0
56	MG	DA	3033	1/1	0.89	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3728	1/1	0.89	0.15	68,68,68,68	0
56	MG	BA	3441	1/1	0.89	0.13	47,47,47,47	0
56	MG	AA	1762	1/1	0.89	0.10	74,74,74,74	0
56	MG	DA	3671	1/1	0.89	0.08	92,92,92,92	0
56	MG	AA	1899	1/1	0.89	0.08	115,115,115,115	0
56	MG	AA	1643	1/1	0.89	0.28	59,59,59,59	0
56	MG	BX	101	1/1	0.89	0.65	78,78,78,78	0
56	MG	DA	3205	1/1	0.89	0.13	68,68,68,68	0
56	MG	DA	3058	1/1	0.89	0.20	83,83,83,83	0
56	MG	AA	1767	1/1	0.89	0.14	59,59,59,59	0
56	MG	BA	3010	1/1	0.89	0.23	56,56,56,56	0
56	MG	BA	3474	1/1	0.89	0.13	56,56,56,56	0
56	MG	DA	3066	1/1	0.89	0.36	68,68,68,68	0
56	MG	CA	1777	1/1	0.89	0.12	82,82,82,82	0
56	MG	CA	1778	1/1	0.89	0.27	81,81,81,81	0
56	MG	BA	3776	1/1	0.89	0.30	68,68,68,68	0
56	MG	AA	1948	1/1	0.89	0.08	88,88,88,88	0
56	MG	BA	3477	1/1	0.89	0.24	45,45,45,45	0
56	MG	DA	3078	1/1	0.89	0.40	75,75,75,75	0
56	MG	AA	1710	1/1	0.89	0.25	76,76,76,76	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	CA	1608	1/1	0.89	0.35	80,80,80,80	0
56	MG	DA	3234	1/1	0.89	0.18	62,62,62,62	0
56	MG	AA	1627	1/1	0.89	0.44	83,83,83,83	0
56	MG	DE	301	1/1	0.89	0.11	64,64,64,64	0
56	MG	AA	1842	1/1	0.89	0.18	89,89,89,89	0
56	MG	BA	3264	1/1	0.89	0.13	59,59,59,59	0
56	MG	AA	1866	1/1	0.89	0.22	86,86,86,86	0
56	MG	DA	3245	1/1	0.89	0.20	39,39,39,39	0
56	MG	DA	3249	1/1	0.89	0.21	55,55,55,55	0
56	MG	BA	3081	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3098	1/1	0.89	0.11	51,51,51,51	0
56	MG	DA	3101	1/1	0.89	0.23	53,53,53,53	0
56	MG	D5	101	1/1	0.89	0.26	62,62,62,62	0
56	MG	AA	1638	1/1	0.89	0.14	78,78,78,78	0
56	MG	DA	3481	1/1	0.89	0.37	85,85,85,85	0
57	ZN	CN	101	1/1	0.89	0.09	165,165,165,165	0
56	MG	AA	1626	1/1	0.89	0.27	62,62,62,62	0
56	MG	DA	3099	1/1	0.90	0.19	42,42,42,42	0
56	MG	BB	206	1/1	0.90	0.26	61,61,61,61	0
56	MG	AA	1608	1/1	0.90	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3112	1/1	0.90	0.21	61,61,61,61	0
56	MG	DA	3113	1/1	0.90	0.17	59,59,59,59	0
56	MG	AA	1826	1/1	0.90	0.20	63,63,63,63	0
56	MG	DA	3266	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3078	1/1	0.90	0.20	49,49,49,49	0
56	MG	BA	3262	1/1	0.90	0.19	57,57,57,57	0
56	MG	AA	1692	1/1	0.90	0.20	67,67,67,67	0
56	MG	DA	3514	1/1	0.90	0.16	76,76,76,76	0
56	MG	CA	1686	1/1	0.90	0.09	72,72,72,72	0
56	MG	DA	3276	1/1	0.90	0.17	63,63,63,63	0
56	MG	DA	3277	1/1	0.90	0.13	67,67,67,67	0
56	MG	DA	3123	1/1	0.90	0.22	61,61,61,61	0
56	MG	DA	3124	1/1	0.90	0.29	50,50,50,50	0
56	MG	DA	3527	1/1	0.90	0.15	81,81,81,81	0
56	MG	BA	3614	1/1	0.90	0.21	58,58,58,58	0
56	MG	DA	3530	1/1	0.90	0.09	72,72,72,72	0
56	MG	BA	3095	1/1	0.90	0.18	48,48,48,48	0
56	MG	BA	3274	1/1	0.90	0.08	35,35,35,35	0
56	MG	DA	3132	1/1	0.90	0.20	66,66,66,66	0
56	MG	BG	201	1/1	0.90	0.18	54,54,54,54	0
56	MG	AA	1785	1/1	0.90	0.18	68,68,68,68	0
56	MG	BA	3656	1/1	0.90	0.08	63,63,63,63	0
56	MG	DA	3290	1/1	0.90	0.18	79,79,79,79	0
56	MG	BA	3411	1/1	0.90	0.17	55,55,55,55	0
56	MG	DA	3554	1/1	0.90	0.20	49,49,49,49	0
56	MG	DA	3144	1/1	0.90	0.24	71,71,71,71	0
56	MG	AA	1630	1/1	0.90	0.28	98,98,98,98	0
56	MG	DA	3560	1/1	0.90	0.14	64,64,64,64	0
56	MG	BA	3419	1/1	0.90	0.26	62,62,62,62	0
56	MG	B5	102	1/1	0.90	0.11	58,58,58,58	0
56	MG	BA	3100	1/1	0.90	0.17	48,48,48,48	0
56	MG	DA	3302	1/1	0.90	0.17	76,76,76,76	0
56	MG	CA	1602	1/1	0.90	0.24	72,72,72,72	0
56	MG	DA	3587	1/1	0.90	0.09	86,86,86,86	0
56	MG	DA	3153	1/1	0.90	0.46	66,66,66,66	0
56	MG	AA	1712	1/1	0.90	0.15	72,72,72,72	0
56	MG	BA	3427	1/1	0.90	0.19	48,48,48,48	0
56	MG	DA	3603	1/1	0.90	0.14	100,100,100,100	0
56	MG	CA	1817	1/1	0.90	0.11	111,111,111,111	0
56	MG	BA	3428	1/1	0.90	0.13	63,63,63,63	0
56	MG	BA	3107	1/1	0.90	0.11	44,44,44,44	0
56	MG	DA	3615	1/1	0.90	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1702	1/1	0.90	0.23	71,71,71,71	0
56	MG	BA	3436	1/1	0.90	0.19	70,70,70,70	0
56	MG	BA	3746	1/1	0.90	0.17	77,77,77,77	0
56	MG	DA	3001	1/1	0.90	0.15	58,58,58,58	0
56	MG	DA	3326	1/1	0.90	0.18	62,62,62,62	0
56	MG	BA	3118	1/1	0.90	0.36	44,44,44,44	0
56	MG	DA	3334	1/1	0.90	0.20	83,83,83,83	0
56	MG	BA	3440	1/1	0.90	0.24	56,56,56,56	0
56	MG	AA	1914	1/1	0.90	0.06	104,104,104,104	0
56	MG	DA	3633	1/1	0.90	0.18	62,62,62,62	0
56	MG	BA	3121	1/1	0.90	0.13	40,40,40,40	0
56	MG	DA	3341	1/1	0.90	0.15	60,60,60,60	0
56	MG	BA	3135	1/1	0.90	0.26	58,58,58,58	0
56	MG	AV	105	1/1	0.90	0.24	64,64,64,64	0
56	MG	BA	3153	1/1	0.90	0.14	56,56,56,56	0
56	MG	AV	106	1/1	0.90	0.26	68,68,68,68	0
56	MG	CA	1631	1/1	0.90	0.35	66,66,66,66	0
56	MG	CA	1728	1/1	0.90	0.20	83,83,83,83	0
56	MG	DA	3352	1/1	0.90	0.22	68,68,68,68	0
56	MG	DA	3018	1/1	0.90	0.23	51,51,51,51	0
56	MG	DA	3020	1/1	0.90	0.28	75,75,75,75	0
56	MG	CA	1632	1/1	0.90	0.21	77,77,77,77	0
56	MG	DA	3357	1/1	0.90	0.13	51,51,51,51	0
56	MG	BA	3328	1/1	0.90	0.14	68,68,68,68	0
56	MG	BA	3475	1/1	0.90	0.07	42,42,42,42	0
56	MG	DA	3032	1/1	0.90	0.14	51,51,51,51	0
56	MG	BA	3801	1/1	0.90	0.21	93,93,93,93	0
56	MG	DA	3691	1/1	0.90	0.09	91,91,91,91	0
56	MG	CA	1637	1/1	0.90	0.22	80,80,80,80	0
56	MG	DA	3694	1/1	0.90	0.06	95,95,95,95	0
56	MG	AA	1661	1/1	0.90	0.26	56,56,56,56	0
56	MG	DA	3044	1/1	0.90	0.25	62,62,62,62	0
56	MG	CA	1741	1/1	0.90	0.12	92,92,92,92	0
56	MG	BA	3187	1/1	0.90	0.10	47,47,47,47	0
56	MG	AA	1663	1/1	0.90	0.14	76,76,76,76	0
56	MG	BA	3812	1/1	0.90	0.08	87,87,87,87	0
56	MG	AA	1636	1/1	0.90	0.37	65,65,65,65	0
56	MG	AA	1887	1/1	0.90	0.07	90,90,90,90	0
56	MG	BA	3211	1/1	0.90	0.17	46,46,46,46	0
56	MG	BA	3217	1/1	0.90	0.15	38,38,38,38	0
56	MG	CA	1652	1/1	0.90	0.23	75,75,75,75	0
56	MG	AA	1749	1/1	0.90	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1931	1/1	0.90	0.07	103,103,103,103	0
56	MG	DA	3383	1/1	0.90	0.21	76,76,76,76	0
56	MG	DE	303	1/1	0.90	0.23	63,63,63,63	0
56	MG	AA	1768	1/1	0.90	0.12	88,88,88,88	0
56	MG	BA	3511	1/1	0.90	0.22	48,48,48,48	0
56	MG	BA	3365	1/1	0.90	0.15	69,69,69,69	0
56	MG	DT	203	1/1	0.90	0.31	73,73,73,73	0
56	MG	BA	3874	1/1	0.90	0.08	90,90,90,90	0
56	MG	AA	1769	1/1	0.90	0.15	84,84,84,84	0
56	MG	BA	3373	1/1	0.90	0.23	69,69,69,69	0
56	MG	BA	3017	1/1	0.90	0.12	64,64,64,64	0
56	MG	CA	1779	1/1	0.90	0.22	95,95,95,95	0
56	MG	BA	3568	1/1	0.90	0.12	70,70,70,70	0
56	MG	DA	3247	1/1	0.90	0.09	58,58,58,58	0
56	MG	AA	1822	1/1	0.90	0.20	77,77,77,77	0
56	MG	AA	1772	1/1	0.90	0.12	77,77,77,77	0
56	MG	BA	3389	1/1	0.90	0.33	38,38,38,38	0
56	MG	DA	3159	1/1	0.91	0.13	66,66,66,66	0
56	MG	DA	3370	1/1	0.91	0.28	67,67,67,67	0
56	MG	BA	3775	1/1	0.91	0.11	74,74,74,74	0
56	MG	BA	3433	1/1	0.91	0.15	30,30,30,30	0
56	MG	CA	1791	1/1	0.91	0.17	85,85,85,85	0
56	MG	CA	1643	1/1	0.91	0.20	53,53,53,53	0
56	MG	AA	1936	1/1	0.91	0.09	84,84,84,84	0
56	MG	BA	3087	1/1	0.91	0.12	77,77,77,77	0
56	MG	CA	1646	1/1	0.91	0.13	73,73,73,73	0
56	MG	BA	3779	1/1	0.91	0.14	80,80,80,80	0
56	MG	BA	3780	1/1	0.91	0.12	86,86,86,86	0
56	MG	BA	3089	1/1	0.91	0.30	54,54,54,54	0
56	MG	CA	1653	1/1	0.91	0.15	78,78,78,78	0
56	MG	BA	3284	1/1	0.91	0.10	41,41,41,41	0
56	MG	BA	3793	1/1	0.91	0.16	69,69,69,69	0
56	MG	AA	1625	1/1	0.91	0.18	69,69,69,69	0
56	MG	DA	3181	1/1	0.91	0.24	59,59,59,59	0
56	MG	AA	1939	1/1	0.91	0.14	105,105,105,105	0
56	MG	DA	3454	1/1	0.91	0.16	91,91,91,91	0
56	MG	DA	3460	1/1	0.91	0.15	67,67,67,67	0
56	MG	AA	1875	1/1	0.91	0.18	59,59,59,59	0
56	MG	AA	1943	1/1	0.91	0.14	92,92,92,92	0
56	MG	BA	3301	1/1	0.91	0.21	70,70,70,70	0
56	MG	BA	3457	1/1	0.91	0.08	59,59,59,59	0
56	MG	DA	3189	1/1	0.91	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3474	1/1	0.91	0.11	76,76,76,76	0
56	MG	CA	1665	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3194	1/1	0.91	0.34	65,65,65,65	0
56	MG	DA	3196	1/1	0.91	0.16	77,77,77,77	0
56	MG	AA	1635	1/1	0.91	0.16	65,65,65,65	0
56	MG	BA	3470	1/1	0.91	0.16	52,52,52,52	0
56	MG	CT	201	1/1	0.91	0.14	67,67,67,67	0
56	MG	CV	101	1/1	0.91	0.23	59,59,59,59	0
56	MG	CV	102	1/1	0.91	0.21	85,85,85,85	0
56	MG	AA	1797	1/1	0.91	0.22	65,65,65,65	0
56	MG	AA	1676	1/1	0.91	0.45	72,72,72,72	0
56	MG	CV	107	1/1	0.91	0.18	70,70,70,70	0
56	MG	CA	1674	1/1	0.91	0.23	79,79,79,79	0
56	MG	CV	110	1/1	0.91	0.06	100,100,100,100	0
56	MG	BA	3828	1/1	0.91	0.05	99,99,99,99	0
56	MG	AA	1828	1/1	0.91	0.09	70,70,70,70	0
56	MG	DA	3211	1/1	0.91	0.23	83,83,83,83	0
56	MG	BA	3323	1/1	0.91	0.09	45,45,45,45	0
56	MG	AA	1892	1/1	0.91	0.08	84,84,84,84	0
56	MG	CA	1679	1/1	0.91	0.16	65,65,65,65	0
56	MG	BA	3482	1/1	0.91	0.08	73,73,73,73	0
56	MG	AA	1708	1/1	0.91	0.21	79,79,79,79	0
56	MG	BA	3484	1/1	0.91	0.23	49,49,49,49	0
56	MG	AA	1619	1/1	0.91	0.33	68,68,68,68	0
56	MG	DA	3230	1/1	0.91	0.11	68,68,68,68	0
56	MG	BA	3144	1/1	0.91	0.12	34,34,34,34	0
56	MG	BA	3875	1/1	0.91	0.17	74,74,74,74	0
56	MG	BA	3148	1/1	0.91	0.16	50,50,50,50	0
56	MG	DA	3547	1/1	0.91	0.10	83,83,83,83	0
56	MG	BA	3492	1/1	0.91	0.24	61,61,61,61	0
56	MG	DA	3019	1/1	0.91	0.20	65,65,65,65	0
56	MG	AA	1802	1/1	0.91	0.17	67,67,67,67	0
56	MG	BA	3889	1/1	0.91	0.08	80,80,80,80	0
56	MG	DA	3243	1/1	0.91	0.26	78,78,78,78	0
56	MG	DA	3559	1/1	0.91	0.18	76,76,76,76	0
56	MG	DA	3024	1/1	0.91	0.19	60,60,60,60	0
56	MG	DA	3563	1/1	0.91	0.08	73,73,73,73	0
56	MG	AA	1613	1/1	0.91	0.39	68,68,68,68	0
56	MG	DA	3566	1/1	0.91	0.11	84,84,84,84	0
56	MG	BA	3895	1/1	0.91	0.08	78,78,78,78	0
56	MG	DA	3574	1/1	0.91	0.14	53,53,53,53	0
56	MG	DA	3576	1/1	0.91	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3578	1/1	0.91	0.14	50,50,50,50	0
56	MG	BA	3345	1/1	0.91	0.20	74,74,74,74	0
56	MG	DA	3582	1/1	0.91	0.11	85,85,85,85	0
56	MG	BA	3352	1/1	0.91	0.28	68,68,68,68	0
56	MG	DA	3034	1/1	0.91	0.19	77,77,77,77	0
56	MG	BA	3515	1/1	0.91	0.25	49,49,49,49	0
56	MG	DA	3036	1/1	0.91	0.20	57,57,57,57	0
56	MG	BA	3521	1/1	0.91	0.10	68,68,68,68	0
56	MG	BA	3522	1/1	0.91	0.10	62,62,62,62	0
56	MG	BA	3154	1/1	0.91	0.14	53,53,53,53	0
56	MG	DA	3606	1/1	0.91	0.06	76,76,76,76	0
56	MG	BA	3524	1/1	0.91	0.08	81,81,81,81	0
56	MG	DA	3609	1/1	0.91	0.08	75,75,75,75	0
56	MG	BA	3529	1/1	0.91	0.12	49,49,49,49	0
56	MG	DA	3053	1/1	0.91	0.18	55,55,55,55	0
56	MG	DA	3270	1/1	0.91	0.14	70,70,70,70	0
56	MG	DA	3055	1/1	0.91	0.16	57,57,57,57	0
56	MG	BA	3155	1/1	0.91	0.25	58,58,58,58	0
56	MG	AV	104	1/1	0.91	0.31	81,81,81,81	0
56	MG	DA	3059	1/1	0.91	0.13	67,67,67,67	0
56	MG	DA	3622	1/1	0.91	0.13	74,74,74,74	0
56	MG	AA	1665	1/1	0.91	0.32	73,73,73,73	0
56	MG	BF	304	1/1	0.91	0.13	44,44,44,44	0
56	MG	CA	1712	1/1	0.91	0.20	83,83,83,83	0
56	MG	AA	1681	1/1	0.91	0.12	91,91,91,91	0
56	MG	AA	1616	1/1	0.91	0.18	65,65,65,65	0
56	MG	BA	3578	1/1	0.91	0.16	68,68,68,68	0
56	MG	BP	201	1/1	0.91	0.20	33,33,33,33	0
56	MG	DA	3639	1/1	0.91	0.14	82,82,82,82	0
56	MG	AA	1654	1/1	0.91	0.19	80,80,80,80	0
56	MG	BQ	203	1/1	0.91	0.09	62,62,62,62	0
56	MG	DA	3077	1/1	0.91	0.26	74,74,74,74	0
56	MG	BU	201	1/1	0.91	0.14	38,38,38,38	0
56	MG	AA	1776	1/1	0.91	0.16	89,89,89,89	0
56	MG	CA	1727	1/1	0.91	0.12	74,74,74,74	0
56	MG	BZ	301	1/1	0.91	0.11	54,54,54,54	0
56	MG	AA	1778	1/1	0.91	0.27	83,83,83,83	0
56	MG	DA	3085	1/1	0.91	0.18	64,64,64,64	0
56	MG	AA	1782	1/1	0.91	0.15	51,51,51,51	0
56	MG	DA	3088	1/1	0.91	0.07	73,73,73,73	0
56	MG	DA	3676	1/1	0.91	0.15	94,94,94,94	0
56	MG	CA	1734	1/1	0.91	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3225	1/1	0.91	0.14	46,46,46,46	0
56	MG	AA	1639	1/1	0.91	0.27	74,74,74,74	0
56	MG	AV	114	1/1	0.91	0.11	67,67,67,67	0
56	MG	DA	3100	1/1	0.91	0.21	45,45,45,45	0
56	MG	DA	3312	1/1	0.91	0.10	52,52,52,52	0
56	MG	BA	3001	1/1	0.91	0.08	35,35,35,35	0
56	MG	DA	3102	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3234	1/1	0.91	0.21	43,43,43,43	0
56	MG	BA	3629	1/1	0.91	0.12	64,64,64,64	0
56	MG	BA	3002	1/1	0.91	0.14	65,65,65,65	0
56	MG	BA	3651	1/1	0.91	0.09	49,49,49,49	0
56	MG	AA	1855	1/1	0.91	0.17	80,80,80,80	0
56	MG	AA	1640	1/1	0.91	0.20	43,43,43,43	0
56	MG	BA	3658	1/1	0.91	0.16	44,44,44,44	0
56	MG	CA	1615	1/1	0.91	0.19	74,74,74,74	0
56	MG	BA	3693	1/1	0.91	0.07	38,38,38,38	0
56	MG	AA	1786	1/1	0.91	0.28	69,69,69,69	0
56	MG	AA	1672	1/1	0.91	0.12	78,78,78,78	0
56	MG	CA	1766	1/1	0.91	0.08	106,106,106,106	0
56	MG	CA	1768	1/1	0.91	0.12	94,94,94,94	0
56	MG	DD	304	1/1	0.91	0.21	65,65,65,65	0
56	MG	BA	3407	1/1	0.91	0.10	44,44,44,44	0
56	MG	BA	3255	1/1	0.91	0.19	16,16,16,16	0
56	MG	DA	3135	1/1	0.91	0.20	66,66,66,66	0
56	MG	DF	301	1/1	0.91	0.14	71,71,71,71	0
56	MG	DF	303	1/1	0.91	0.11	77,77,77,77	0
56	MG	CA	1624	1/1	0.91	0.26	64,64,64,64	0
56	MG	BA	3719	1/1	0.91	0.12	71,71,71,71	0
56	MG	BA	3032	1/1	0.91	0.10	45,45,45,45	0
56	MG	AA	1754	1/1	0.91	0.22	59,59,59,59	0
56	MG	BA	3260	1/1	0.91	0.25	60,60,60,60	0
56	MG	AA	1791	1/1	0.91	0.17	99,99,99,99	0
56	MG	BA	3422	1/1	0.91	0.18	82,82,82,82	0
56	MG	AA	1734	1/1	0.91	0.08	80,80,80,80	0
56	MG	CA	1636	1/1	0.91	0.35	50,50,50,50	0
56	MG	BA	3076	1/1	0.91	0.36	39,39,39,39	0
56	MG	DA	3154	1/1	0.91	0.16	65,65,65,65	0
56	MG	BA	3272	1/1	0.91	0.05	72,72,72,72	0
56	MG	AA	1873	1/1	0.91	0.16	60,60,60,60	0
56	MG	AA	1682	1/1	0.92	0.11	118,118,118,118	0
56	MG	AA	1852	1/1	0.92	0.10	93,93,93,93	0
56	MG	AA	1646	1/1	0.92	0.29	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1657	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3150	1/1	0.92	0.24	54,54,54,54	0
56	MG	DA	3489	1/1	0.92	0.08	68,68,68,68	0
56	MG	AA	1607	1/1	0.92	0.18	44,44,44,44	0
56	MG	BA	3607	1/1	0.92	0.25	59,59,59,59	0
56	MG	DA	3244	1/1	0.92	0.14	64,64,64,64	0
56	MG	BA	3020	1/1	0.92	0.08	44,44,44,44	0
56	MG	DA	3504	1/1	0.92	0.08	94,94,94,94	0
56	MG	BA	3613	1/1	0.92	0.11	40,40,40,40	0
56	MG	DA	3090	1/1	0.92	0.33	76,76,76,76	0
56	MG	DA	3252	1/1	0.92	0.14	58,58,58,58	0
56	MG	CA	1663	1/1	0.92	0.30	63,63,63,63	0
56	MG	BA	3431	1/1	0.92	0.24	75,75,75,75	0
56	MG	AA	1748	1/1	0.92	0.12	90,90,90,90	0
56	MG	AA	1664	1/1	0.92	0.12	51,51,51,51	0
56	MG	BA	3162	1/1	0.92	0.17	36,36,36,36	0
56	MG	BA	3171	1/1	0.92	0.22	38,38,38,38	0
56	MG	DA	3260	1/1	0.92	0.15	71,71,71,71	0
56	MG	DA	3261	1/1	0.92	0.18	69,69,69,69	0
56	MG	BB	210	1/1	0.92	0.11	53,53,53,53	0
56	MG	DA	3107	1/1	0.92	0.13	58,58,58,58	0
56	MG	CA	1792	1/1	0.92	0.08	82,82,82,82	0
56	MG	DA	3267	1/1	0.92	0.18	66,66,66,66	0
56	MG	BB	214	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3325	1/1	0.92	0.22	83,83,83,83	0
56	MG	AA	1815	1/1	0.92	0.11	69,69,69,69	0
56	MG	DA	3271	1/1	0.92	0.16	68,68,68,68	0
56	MG	DA	3545	1/1	0.92	0.08	83,83,83,83	0
56	MG	BA	3044	1/1	0.92	0.09	46,46,46,46	0
56	MG	BA	3680	1/1	0.92	0.07	46,46,46,46	0
56	MG	DA	3118	1/1	0.92	0.21	50,50,50,50	0
56	MG	BB	230	1/1	0.92	0.14	56,56,56,56	0
56	MG	CA	1681	1/1	0.92	0.23	70,70,70,70	0
56	MG	BD	302	1/1	0.92	0.16	51,51,51,51	0
56	MG	AA	1801	1/1	0.92	0.24	65,65,65,65	0
56	MG	BA	3050	1/1	0.92	0.14	60,60,60,60	0
56	MG	AA	1904	1/1	0.92	0.05	118,118,118,118	0
56	MG	BA	3453	1/1	0.92	0.31	63,63,63,63	0
56	MG	DA	3285	1/1	0.92	0.22	62,62,62,62	0
56	MG	DA	3567	1/1	0.92	0.20	77,77,77,77	0
56	MG	BA	3455	1/1	0.92	0.21	22,22,22,22	0
56	MG	DA	3133	1/1	0.92	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3575	1/1	0.92	0.13	65,65,65,65	0
56	MG	BA	3199	1/1	0.92	0.20	29,29,29,29	0
56	MG	DA	3577	1/1	0.92	0.08	95,95,95,95	0
56	MG	CA	1690	1/1	0.92	0.27	74,74,74,74	0
56	MG	DA	3291	1/1	0.92	0.16	50,50,50,50	0
56	MG	DA	3580	1/1	0.92	0.09	76,76,76,76	0
56	MG	BA	3209	1/1	0.92	0.17	25,25,25,25	0
56	MG	DA	3138	1/1	0.92	0.27	58,58,58,58	0
56	MG	BA	3469	1/1	0.92	0.23	77,77,77,77	0
56	MG	DA	3140	1/1	0.92	0.31	44,44,44,44	0
56	MG	BA	3058	1/1	0.92	0.09	46,46,46,46	0
56	MG	BA	3472	1/1	0.92	0.22	58,58,58,58	0
56	MG	BA	3072	1/1	0.92	0.32	48,48,48,48	0
56	MG	DA	3601	1/1	0.92	0.10	53,53,53,53	0
56	MG	CA	1698	1/1	0.92	0.41	114,114,114,114	0
56	MG	AA	1691	1/1	0.92	0.29	121,121,121,121	0
56	MG	CV	103	1/1	0.92	0.17	88,88,88,88	0
56	MG	B3	101	1/1	0.92	0.17	57,57,57,57	0
56	MG	AA	1818	1/1	0.92	0.17	73,73,73,73	0
56	MG	AA	1790	1/1	0.92	0.13	70,70,70,70	0
56	MG	BA	3479	1/1	0.92	0.20	63,63,63,63	0
56	MG	BA	3083	1/1	0.92	0.10	48,48,48,48	0
56	MG	AA	1912	1/1	0.92	0.06	106,106,106,106	0
56	MG	DA	3160	1/1	0.92	0.22	69,69,69,69	0
56	MG	AV	103	1/1	0.92	0.21	53,53,53,53	0
56	MG	DA	3321	1/1	0.92	0.20	50,50,50,50	0
56	MG	BA	3090	1/1	0.92	0.19	46,46,46,46	0
56	MG	BA	3369	1/1	0.92	0.13	65,65,65,65	0
56	MG	DA	3330	1/1	0.92	0.20	78,78,78,78	0
56	MG	CA	1709	1/1	0.92	0.32	82,82,82,82	0
56	MG	DA	3166	1/1	0.92	0.29	66,66,66,66	0
56	MG	AA	1843	1/1	0.92	0.10	73,73,73,73	0
56	MG	DA	3336	1/1	0.92	0.36	71,71,71,71	0
56	MG	CA	1611	1/1	0.92	0.14	74,74,74,74	0
56	MG	DA	3645	1/1	0.92	0.13	93,93,93,93	0
56	MG	BA	3784	1/1	0.92	0.13	88,88,88,88	0
56	MG	DA	3648	1/1	0.92	0.20	53,53,53,53	0
56	MG	CA	1613	1/1	0.92	0.20	75,75,75,75	0
56	MG	DA	3342	1/1	0.92	0.19	70,70,70,70	0
56	MG	AA	1804	1/1	0.92	0.12	115,115,115,115	0
56	MG	AA	1845	1/1	0.92	0.21	59,59,59,59	0
56	MG	BA	3497	1/1	0.92	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3498	1/1	0.92	0.09	54,54,54,54	0
56	MG	BA	3249	1/1	0.92	0.21	24,24,24,24	0
56	MG	AA	1919	1/1	0.92	0.15	63,63,63,63	0
56	MG	AA	1777	1/1	0.92	0.18	61,61,61,61	0
56	MG	BA	3505	1/1	0.92	0.08	64,64,64,64	0
56	MG	CA	1625	1/1	0.92	0.24	71,71,71,71	0
56	MG	DA	3028	1/1	0.92	0.29	56,56,56,56	0
56	MG	DA	3681	1/1	0.92	0.08	71,71,71,71	0
56	MG	CA	1628	1/1	0.92	0.27	51,51,51,51	0
56	MG	DA	3358	1/1	0.92	0.08	60,60,60,60	0
56	MG	CA	1732	1/1	0.92	0.12	81,81,81,81	0
56	MG	DA	3361	1/1	0.92	0.14	60,60,60,60	0
56	MG	BA	3104	1/1	0.92	0.15	50,50,50,50	0
56	MG	DA	3190	1/1	0.92	0.16	70,70,70,70	0
56	MG	BA	3259	1/1	0.92	0.20	66,66,66,66	0
56	MG	DA	3193	1/1	0.92	0.20	67,67,67,67	0
56	MG	AA	1881	1/1	0.92	0.19	50,50,50,50	0
56	MG	BA	3819	1/1	0.92	0.08	71,71,71,71	0
56	MG	AA	1882	1/1	0.92	0.06	55,55,55,55	0
56	MG	BA	3115	1/1	0.92	0.24	52,52,52,52	0
56	MG	BA	3827	1/1	0.92	0.06	77,77,77,77	0
56	MG	AA	1641	1/1	0.92	0.19	44,44,44,44	0
56	MG	CA	1743	1/1	0.92	0.30	86,86,86,86	0
56	MG	AA	1849	1/1	0.92	0.13	59,59,59,59	0
56	MG	AA	1888	1/1	0.92	0.08	97,97,97,97	0
56	MG	BA	3849	1/1	0.92	0.07	83,83,83,83	0
56	MG	BA	3122	1/1	0.92	0.24	56,56,56,56	0
56	MG	CA	1754	1/1	0.92	0.19	70,70,70,70	0
56	MG	CA	1755	1/1	0.92	0.08	93,93,93,93	0
56	MG	DA	3061	1/1	0.92	0.35	78,78,78,78	0
56	MG	BA	3125	1/1	0.92	0.19	48,48,48,48	0
56	MG	DA	3386	1/1	0.92	0.14	47,47,47,47	0
56	MG	DA	3064	1/1	0.92	0.09	66,66,66,66	0
56	MG	BA	3413	1/1	0.92	0.19	58,58,58,58	0
56	MG	DA	3218	1/1	0.92	0.13	71,71,71,71	0
56	MG	AA	1779	1/1	0.92	0.16	60,60,60,60	0
56	MG	DA	3067	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3441	1/1	0.92	0.10	72,72,72,72	0
56	MG	DA	3221	1/1	0.92	0.10	82,82,82,82	0
56	MG	DA	3222	1/1	0.92	0.24	73,73,73,73	0
56	MG	BA	3576	1/1	0.92	0.13	66,66,66,66	0
56	MG	BA	3870	1/1	0.92	0.08	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3871	1/1	0.92	0.10	46,46,46,46	0
56	MG	DA	3469	1/1	0.92	0.12	84,84,84,84	0
56	MG	D7	101	1/1	0.92	0.23	63,63,63,63	0
56	MG	BA	3417	1/1	0.92	0.32	44,44,44,44	0
56	MG	DA	3231	1/1	0.92	0.13	74,74,74,74	0
56	MG	BA	3140	1/1	0.92	0.32	53,53,53,53	0
56	MG	BA	3867	1/1	0.93	0.10	60,60,60,60	0
56	MG	AA	1707	1/1	0.93	0.28	64,64,64,64	0
56	MG	DA	3392	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3393	1/1	0.93	0.16	63,63,63,63	0
56	MG	BA	3509	1/1	0.93	0.21	54,54,54,54	0
56	MG	AA	1926	1/1	0.93	0.07	90,90,90,90	0
56	MG	DA	3410	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3414	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3423	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3424	1/1	0.93	0.12	72,72,72,72	0
56	MG	BA	3513	1/1	0.93	0.12	60,60,60,60	0
56	MG	BA	3514	1/1	0.93	0.17	58,58,58,58	0
56	MG	DA	3200	1/1	0.93	0.14	53,53,53,53	0
56	MG	DA	3443	1/1	0.93	0.11	70,70,70,70	0
56	MG	AA	1780	1/1	0.93	0.19	55,55,55,55	0
56	MG	DA	3453	1/1	0.93	0.08	77,77,77,77	0
56	MG	BA	3516	1/1	0.93	0.20	56,56,56,56	0
56	MG	DA	3456	1/1	0.93	0.11	56,56,56,56	0
56	MG	BA	3517	1/1	0.93	0.16	58,58,58,58	0
56	MG	DA	3461	1/1	0.93	0.18	50,50,50,50	0
56	MG	AA	1757	1/1	0.93	0.13	58,58,58,58	0
56	MG	AA	1606	1/1	0.93	0.16	35,35,35,35	0
56	MG	BA	3381	1/1	0.93	0.26	19,19,19,19	0
56	MG	DA	3470	1/1	0.93	0.11	73,73,73,73	0
56	MG	AV	118	1/1	0.93	0.06	83,83,83,83	0
56	MG	BA	3109	1/1	0.93	0.13	58,58,58,58	0
56	MG	DA	3209	1/1	0.93	0.20	89,89,89,89	0
56	MG	BA	3240	1/1	0.93	0.14	57,57,57,57	0
56	MG	AA	1673	1/1	0.93	0.20	74,74,74,74	0
56	MG	AA	1761	1/1	0.93	0.15	58,58,58,58	0
56	MG	DA	3215	1/1	0.93	0.23	46,46,46,46	0
56	MG	DA	3482	1/1	0.93	0.12	63,63,63,63	0
56	MG	BA	3003	1/1	0.93	0.13	59,59,59,59	0
56	MG	BA	3251	1/1	0.93	0.16	51,51,51,51	0
56	MG	BB	211	1/1	0.93	0.23	66,66,66,66	0
56	MG	BA	3572	1/1	0.93	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3004	1/1	0.93	0.10	57,57,57,57	0
56	MG	DA	3037	1/1	0.93	0.24	83,83,83,83	0
56	MG	AA	1667	1/1	0.93	0.09	71,71,71,71	0
56	MG	DA	3041	1/1	0.93	0.33	54,54,54,54	0
56	MG	AA	1941	1/1	0.93	0.07	94,94,94,94	0
56	MG	DA	3047	1/1	0.93	0.14	65,65,65,65	0
56	MG	BA	3401	1/1	0.93	0.08	57,57,57,57	0
56	MG	BA	3402	1/1	0.93	0.11	55,55,55,55	0
56	MG	BA	3592	1/1	0.93	0.08	52,52,52,52	0
56	MG	BF	301	1/1	0.93	0.09	40,40,40,40	0
56	MG	BA	3403	1/1	0.93	0.08	51,51,51,51	0
56	MG	DA	3237	1/1	0.93	0.16	61,61,61,61	0
56	MG	BA	3405	1/1	0.93	0.17	62,62,62,62	0
56	MG	DA	3057	1/1	0.93	0.26	66,66,66,66	0
56	MG	AA	1650	1/1	0.93	0.28	65,65,65,65	0
56	MG	BA	3129	1/1	0.93	0.06	49,49,49,49	0
56	MG	BA	3132	1/1	0.93	0.16	44,44,44,44	0
56	MG	AA	1832	1/1	0.93	0.21	75,75,75,75	0
56	MG	BA	3265	1/1	0.93	0.08	67,67,67,67	0
56	MG	AA	1944	1/1	0.93	0.11	97,97,97,97	0
56	MG	DA	3251	1/1	0.93	0.16	62,62,62,62	0
56	MG	CA	1720	1/1	0.93	0.10	84,84,84,84	0
56	MG	BA	3416	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3642	1/1	0.93	0.13	78,78,78,78	0
56	MG	CA	1724	1/1	0.93	0.08	88,88,88,88	0
56	MG	CA	1725	1/1	0.93	0.15	79,79,79,79	0
56	MG	B0	102	1/1	0.93	0.06	50,50,50,50	0
56	MG	BA	3141	1/1	0.93	0.12	38,38,38,38	0
56	MG	BA	3418	1/1	0.93	0.24	59,59,59,59	0
56	MG	BA	3142	1/1	0.93	0.24	44,44,44,44	0
56	MG	DA	3262	1/1	0.93	0.25	67,67,67,67	0
56	MG	DA	3263	1/1	0.93	0.33	67,67,67,67	0
56	MG	B5	101	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3079	1/1	0.93	0.12	57,57,57,57	0
56	MG	AA	1945	1/1	0.93	0.09	107,107,107,107	0
56	MG	DA	3568	1/1	0.93	0.11	82,82,82,82	0
56	MG	BA	3421	1/1	0.93	0.31	75,75,75,75	0
56	MG	AA	1860	1/1	0.93	0.10	85,85,85,85	0
56	MG	AA	1614	1/1	0.93	0.21	72,72,72,72	0
56	MG	CA	1739	1/1	0.93	0.13	79,79,79,79	0
56	MG	BA	3426	1/1	0.93	0.07	46,46,46,46	0
56	MG	AA	1735	1/1	0.93	0.41	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3273	1/1	0.93	0.26	62,62,62,62	0
56	MG	DA	3089	1/1	0.93	0.11	82,82,82,82	0
56	MG	AA	1793	1/1	0.93	0.17	72,72,72,72	0
56	MG	CA	1607	1/1	0.93	0.11	73,73,73,73	0
56	MG	BA	3051	1/1	0.93	0.21	41,41,41,41	0
56	MG	CA	1609	1/1	0.93	0.15	70,70,70,70	0
56	MG	BA	3053	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3281	1/1	0.93	0.15	70,70,70,70	0
56	MG	DA	3592	1/1	0.93	0.07	69,69,69,69	0
56	MG	DA	3596	1/1	0.93	0.12	67,67,67,67	0
56	MG	BA	3726	1/1	0.93	0.20	48,48,48,48	0
56	MG	BA	3296	1/1	0.93	0.06	43,43,43,43	0
56	MG	BA	3733	1/1	0.93	0.10	49,49,49,49	0
56	MG	DA	3103	1/1	0.93	0.19	45,45,45,45	0
56	MG	DA	3104	1/1	0.93	0.27	60,60,60,60	0
56	MG	DA	3106	1/1	0.93	0.25	48,48,48,48	0
56	MG	BA	3297	1/1	0.93	0.13	53,53,53,53	0
56	MG	BA	3157	1/1	0.93	0.21	42,42,42,42	0
56	MG	DA	3110	1/1	0.93	0.26	60,60,60,60	0
56	MG	DA	3292	1/1	0.93	0.17	69,69,69,69	0
56	MG	DA	3111	1/1	0.93	0.18	51,51,51,51	0
56	MG	BA	3738	1/1	0.93	0.26	42,42,42,42	0
56	MG	AA	1868	1/1	0.93	0.21	62,62,62,62	0
56	MG	BA	3302	1/1	0.93	0.07	53,53,53,53	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	BA	3303	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3161	1/1	0.93	0.15	49,49,49,49	0
56	MG	DA	3627	1/1	0.93	0.06	81,81,81,81	0
56	MG	DA	3301	1/1	0.93	0.25	62,62,62,62	0
56	MG	CA	1623	1/1	0.93	0.20	68,68,68,68	0
56	MG	BA	3753	1/1	0.93	0.18	31,31,31,31	0
56	MG	BA	3313	1/1	0.93	0.17	66,66,66,66	0
56	MG	AA	1910	1/1	0.93	0.08	87,87,87,87	0
56	MG	DA	3308	1/1	0.93	0.12	60,60,60,60	0
56	MG	DA	3640	1/1	0.93	0.10	63,63,63,63	0
56	MG	BA	3770	1/1	0.93	0.11	49,49,49,49	0
56	MG	BA	3772	1/1	0.93	0.07	26,26,26,26	0
56	MG	BA	3169	1/1	0.93	0.27	14,14,14,14	0
56	MG	DA	3649	1/1	0.93	0.08	73,73,73,73	0
56	MG	DA	3652	1/1	0.93	0.10	85,85,85,85	0
56	MG	BA	3063	1/1	0.93	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3454	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3174	1/1	0.93	0.25	62,62,62,62	0
56	MG	CA	1783	1/1	0.93	0.07	78,78,78,78	0
56	MG	BA	3456	1/1	0.93	0.13	73,73,73,73	0
56	MG	AA	1837	1/1	0.93	0.09	66,66,66,66	0
56	MG	DA	3137	1/1	0.93	0.15	39,39,39,39	0
56	MG	DA	3669	1/1	0.93	0.06	93,93,93,93	0
56	MG	BA	3781	1/1	0.93	0.07	84,84,84,84	0
56	MG	DA	3329	1/1	0.93	0.24	63,63,63,63	0
56	MG	BA	3782	1/1	0.93	0.15	75,75,75,75	0
56	MG	AA	1713	1/1	0.93	0.07	60,60,60,60	0
56	MG	CA	1640	1/1	0.93	0.16	72,72,72,72	0
56	MG	BA	3788	1/1	0.93	0.08	48,48,48,48	0
56	MG	AA	1770	1/1	0.93	0.10	76,76,76,76	0
56	MG	DA	3337	1/1	0.93	0.09	65,65,65,65	0
56	MG	DA	3688	1/1	0.93	0.07	80,80,80,80	0
56	MG	BA	3192	1/1	0.93	0.14	53,53,53,53	0
56	MG	AA	1677	1/1	0.93	0.18	84,84,84,84	0
56	MG	BA	3082	1/1	0.93	0.10	45,45,45,45	0
56	MG	DA	3692	1/1	0.93	0.12	46,46,46,46	0
56	MG	BA	3333	1/1	0.93	0.24	58,58,58,58	0
56	MG	CA	1648	1/1	0.93	0.31	73,73,73,73	0
56	MG	BA	3337	1/1	0.93	0.10	51,51,51,51	0
56	MG	BA	3195	1/1	0.93	0.17	19,19,19,19	0
56	MG	BA	3196	1/1	0.93	0.25	66,66,66,66	0
56	MG	BA	3344	1/1	0.93	0.17	62,62,62,62	0
56	MG	AA	1660	1/1	0.93	0.20	59,59,59,59	0
56	MG	DA	3161	1/1	0.93	0.15	45,45,45,45	0
56	MG	DA	3353	1/1	0.93	0.12	80,80,80,80	0
56	MG	CA	1807	1/1	0.93	0.05	100,100,100,100	0
56	MG	BA	3347	1/1	0.93	0.23	20,20,20,20	0
56	MG	CA	1656	1/1	0.93	0.48	77,77,77,77	0
56	MG	BA	3350	1/1	0.93	0.08	69,69,69,69	0
56	MG	AA	1918	1/1	0.93	0.08	68,68,68,68	0
56	MG	BA	3823	1/1	0.93	0.09	78,78,78,78	0
56	MG	DD	303	1/1	0.93	0.09	59,59,59,59	0
56	MG	AA	1753	1/1	0.93	0.27	86,86,86,86	0
56	MG	AA	1740	1/1	0.93	0.28	72,72,72,72	0
56	MG	BA	3222	1/1	0.93	0.21	28,28,28,28	0
56	MG	BA	3833	1/1	0.93	0.08	41,41,41,41	0
56	MG	CD	302	1/1	0.93	0.15	53,53,53,53	0
56	MG	BA	3835	1/1	0.93	0.17	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3837	1/1	0.93	0.09	33,33,33,33	0
56	MG	BA	3841	1/1	0.93	0.15	91,91,91,91	0
56	MG	BA	3494	1/1	0.93	0.10	62,62,62,62	0
56	MG	CA	1670	1/1	0.93	0.14	69,69,69,69	0
56	MG	BA	3495	1/1	0.93	0.13	56,56,56,56	0
56	MG	CV	106	1/1	0.93	0.21	78,78,78,78	0
56	MG	BA	3496	1/1	0.93	0.18	61,61,61,61	0
56	MG	BA	3223	1/1	0.93	0.10	59,59,59,59	0
56	MG	D1	101	1/1	0.93	0.25	61,61,61,61	0
56	MG	BA	3359	1/1	0.93	0.17	72,72,72,72	0
56	MG	DA	3188	1/1	0.93	0.17	77,77,77,77	0
56	MG	BA	3361	1/1	0.93	0.26	60,60,60,60	0
56	MG	BA	3362	1/1	0.93	0.19	51,51,51,51	0
56	MG	AA	1671	1/1	0.93	0.09	94,94,94,94	0
56	MG	DA	3192	1/1	0.93	0.29	71,71,71,71	0
56	MG	BA	3724	1/1	0.94	0.09	88,88,88,88	0
56	MG	DA	3459	1/1	0.94	0.24	46,46,46,46	0
56	MG	DA	3226	1/1	0.94	0.28	62,62,62,62	0
56	MG	CA	1715	1/1	0.94	0.08	66,66,66,66	0
56	MG	DA	3462	1/1	0.94	0.08	50,50,50,50	0
56	MG	DA	3464	1/1	0.94	0.10	82,82,82,82	0
56	MG	BA	3045	1/1	0.94	0.08	35,35,35,35	0
56	MG	DA	3229	1/1	0.94	0.20	52,52,52,52	0
56	MG	B0	103	1/1	0.94	0.11	68,68,68,68	0
56	MG	B1	101	1/1	0.94	0.07	60,60,60,60	0
56	MG	B1	103	1/1	0.94	0.14	36,36,36,36	0
56	MG	AA	1609	1/1	0.94	0.28	61,61,61,61	0
56	MG	CA	1721	1/1	0.94	0.11	75,75,75,75	0
56	MG	BA	3340	1/1	0.94	0.21	55,55,55,55	0
56	MG	BA	3734	1/1	0.94	0.14	40,40,40,40	0
56	MG	DA	3476	1/1	0.94	0.11	71,71,71,71	0
56	MG	DA	3239	1/1	0.94	0.24	62,62,62,62	0
56	MG	BA	3049	1/1	0.94	0.31	49,49,49,49	0
56	MG	BA	3458	1/1	0.94	0.24	44,44,44,44	0
56	MG	DA	3483	1/1	0.94	0.09	84,84,84,84	0
56	MG	B5	103	1/1	0.94	0.10	61,61,61,61	0
56	MG	B8	101	1/1	0.94	0.15	49,49,49,49	0
56	MG	DA	3490	1/1	0.94	0.19	45,45,45,45	0
56	MG	DA	3068	1/1	0.94	0.34	44,44,44,44	0
56	MG	CA	1729	1/1	0.94	0.12	80,80,80,80	0
56	MG	BA	3461	1/1	0.94	0.15	58,58,58,58	0
56	MG	BA	3123	1/1	0.94	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3502	1/1	0.94	0.07	68,68,68,68	0
56	MG	AA	1773	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3128	1/1	0.94	0.25	60,60,60,60	0
56	MG	AA	1847	1/1	0.94	0.14	98,98,98,98	0
56	MG	BA	3130	1/1	0.94	0.10	30,30,30,30	0
56	MG	AA	1774	1/1	0.94	0.29	69,69,69,69	0
56	MG	AA	1700	1/1	0.94	0.10	116,116,116,116	0
56	MG	BA	3768	1/1	0.94	0.08	90,90,90,90	0
56	MG	BA	3137	1/1	0.94	0.28	55,55,55,55	0
56	MG	BA	3478	1/1	0.94	0.28	67,67,67,67	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	DA	3087	1/1	0.94	0.13	40,40,40,40	0
56	MG	AA	1644	1/1	0.94	0.17	48,48,48,48	0
56	MG	AA	1631	1/1	0.94	0.20	59,59,59,59	0
56	MG	CA	1751	1/1	0.94	0.08	86,86,86,86	0
56	MG	CA	1616	1/1	0.94	0.30	54,54,54,54	0
56	MG	BA	3250	1/1	0.94	0.20	27,27,27,27	0
56	MG	DA	3536	1/1	0.94	0.20	54,54,54,54	0
56	MG	DA	3095	1/1	0.94	0.23	41,41,41,41	0
56	MG	BA	3068	1/1	0.94	0.09	56,56,56,56	0
56	MG	BA	3071	1/1	0.94	0.12	41,41,41,41	0
56	MG	BA	3145	1/1	0.94	0.17	26,26,26,26	0
56	MG	BA	3370	1/1	0.94	0.11	64,64,64,64	0
56	MG	DA	3548	1/1	0.94	0.09	72,72,72,72	0
56	MG	CA	1761	1/1	0.94	0.18	68,68,68,68	0
56	MG	DA	3275	1/1	0.94	0.23	42,42,42,42	0
56	MG	BA	3371	1/1	0.94	0.17	66,66,66,66	0
56	MG	CA	1764	1/1	0.94	0.07	75,75,75,75	0
56	MG	DA	3105	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3558	1/1	0.94	0.23	59,59,59,59	0
56	MG	BA	3147	1/1	0.94	0.23	54,54,54,54	0
56	MG	AA	1621	1/1	0.94	0.07	54,54,54,54	0
56	MG	CA	1627	1/1	0.94	0.22	50,50,50,50	0
56	MG	BA	3376	1/1	0.94	0.12	43,43,43,43	0
56	MG	BA	3379	1/1	0.94	0.14	39,39,39,39	0
56	MG	AA	1738	1/1	0.94	0.07	84,84,84,84	0
56	MG	CA	1774	1/1	0.94	0.12	111,111,111,111	0
56	MG	BA	3077	1/1	0.94	0.11	45,45,45,45	0
56	MG	BA	3800	1/1	0.94	0.05	111,111,111,111	0
56	MG	AA	1814	1/1	0.94	0.18	81,81,81,81	0
56	MG	BA	3805	1/1	0.94	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1763	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3266	1/1	0.94	0.16	59,59,59,59	0
56	MG	BA	3391	1/1	0.94	0.14	27,27,27,27	0
56	MG	BA	3811	1/1	0.94	0.08	85,85,85,85	0
56	MG	BA	3512	1/1	0.94	0.19	56,56,56,56	0
56	MG	BA	3814	1/1	0.94	0.13	86,86,86,86	0
56	MG	AA	1648	1/1	0.94	0.17	65,65,65,65	0
56	MG	DA	3298	1/1	0.94	0.22	55,55,55,55	0
56	MG	AA	1920	1/1	0.94	0.10	86,86,86,86	0
56	MG	DA	3300	1/1	0.94	0.26	55,55,55,55	0
56	MG	DA	3591	1/1	0.94	0.11	86,86,86,86	0
56	MG	BA	3273	1/1	0.94	0.10	63,63,63,63	0
56	MG	BA	3084	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3398	1/1	0.94	0.23	62,62,62,62	0
56	MG	DA	3600	1/1	0.94	0.15	57,57,57,57	0
56	MG	BA	3275	1/1	0.94	0.09	55,55,55,55	0
56	MG	DA	3305	1/1	0.94	0.24	76,76,76,76	0
56	MG	DA	3604	1/1	0.94	0.06	97,97,97,97	0
56	MG	DA	3605	1/1	0.94	0.07	101,101,101,101	0
56	MG	BA	3277	1/1	0.94	0.15	65,65,65,65	0
56	MG	DA	3307	1/1	0.94	0.10	65,65,65,65	0
56	MG	AA	1836	1/1	0.94	0.14	59,59,59,59	0
56	MG	DA	3610	1/1	0.94	0.16	97,97,97,97	0
56	MG	CA	1650	1/1	0.94	0.25	61,61,61,61	0
56	MG	BA	3088	1/1	0.94	0.27	45,45,45,45	0
56	MG	BA	3165	1/1	0.94	0.29	17,17,17,17	0
56	MG	BA	3842	1/1	0.94	0.08	85,85,85,85	0
56	MG	DA	3316	1/1	0.94	0.15	80,80,80,80	0
56	MG	CA	1801	1/1	0.94	0.09	83,83,83,83	0
56	MG	BA	3166	1/1	0.94	0.19	30,30,30,30	0
56	MG	AI	201	1/1	0.94	0.34	66,66,66,66	0
56	MG	BA	3544	1/1	0.94	0.10	45,45,45,45	0
56	MG	BA	3850	1/1	0.94	0.11	82,82,82,82	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	AA	1783	1/1	0.94	0.22	61,61,61,61	0
56	MG	BA	3288	1/1	0.94	0.10	77,77,77,77	0
56	MG	BA	3290	1/1	0.94	0.13	63,63,63,63	0
56	MG	BA	3859	1/1	0.94	0.10	31,31,31,31	0
56	MG	BA	3172	1/1	0.94	0.22	44,44,44,44	0
56	MG	DA	3333	1/1	0.94	0.23	50,50,50,50	0
56	MG	DA	3636	1/1	0.94	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1605	1/1	0.94	0.21	81,81,81,81	0
56	MG	BA	3179	1/1	0.94	0.28	45,45,45,45	0
56	MG	BA	3579	1/1	0.94	0.17	64,64,64,64	0
56	MG	BA	3181	1/1	0.94	0.28	69,69,69,69	0
56	MG	CA	1668	1/1	0.94	0.13	59,59,59,59	0
56	MG	CA	1819	1/1	0.94	0.08	96,96,96,96	0
56	MG	AA	1925	1/1	0.94	0.05	86,86,86,86	0
56	MG	BA	3185	1/1	0.94	0.18	57,57,57,57	0
56	MG	DA	3168	1/1	0.94	0.30	53,53,53,53	0
56	MG	DA	3169	1/1	0.94	0.15	51,51,51,51	0
56	MG	BA	3879	1/1	0.94	0.12	53,53,53,53	0
56	MG	BA	3023	1/1	0.94	0.08	46,46,46,46	0
56	MG	CA	1673	1/1	0.94	0.15	54,54,54,54	0
56	MG	BA	3304	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3351	1/1	0.94	0.12	57,57,57,57	0
56	MG	BA	3025	1/1	0.94	0.07	68,68,68,68	0
56	MG	AA	1623	1/1	0.94	0.12	59,59,59,59	0
56	MG	BA	3029	1/1	0.94	0.23	33,33,33,33	0
56	MG	BA	3893	1/1	0.94	0.09	30,30,30,30	0
56	MG	CV	109	1/1	0.94	0.06	102,102,102,102	0
56	MG	BA	3316	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3317	1/1	0.94	0.13	61,61,61,61	0
56	MG	AV	101	1/1	0.94	0.23	48,48,48,48	0
56	MG	DA	3184	1/1	0.94	0.21	57,57,57,57	0
56	MG	BA	3616	1/1	0.94	0.18	40,40,40,40	0
56	MG	BA	3033	1/1	0.94	0.12	55,55,55,55	0
56	MG	CA	1685	1/1	0.94	0.21	64,64,64,64	0
56	MG	AA	1652	1/1	0.94	0.28	69,69,69,69	0
56	MG	BA	3633	1/1	0.94	0.06	52,52,52,52	0
56	MG	BA	3635	1/1	0.94	0.15	75,75,75,75	0
56	MG	BA	3041	1/1	0.94	0.07	43,43,43,43	0
56	MG	BA	3203	1/1	0.94	0.22	44,44,44,44	0
56	MG	BA	3204	1/1	0.94	0.27	52,52,52,52	0
56	MG	BA	3205	1/1	0.94	0.23	43,43,43,43	0
56	MG	BA	3206	1/1	0.94	0.18	31,31,31,31	0
56	MG	BA	3657	1/1	0.94	0.17	51,51,51,51	0
56	MG	CA	1696	1/1	0.94	0.12	99,99,99,99	0
56	MG	BA	3117	1/1	0.94	0.28	46,46,46,46	0
56	MG	DA	3378	1/1	0.94	0.07	64,64,64,64	0
56	MG	BA	3659	1/1	0.94	0.09	60,60,60,60	0
56	MG	BD	301	1/1	0.94	0.07	65,65,65,65	0
56	MG	DA	3026	1/1	0.94	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3027	1/1	0.94	0.28	72,72,72,72	0
56	MG	DD	301	1/1	0.94	0.10	84,84,84,84	0
56	MG	BA	3661	1/1	0.94	0.17	53,53,53,53	0
56	MG	BE	303	1/1	0.94	0.08	32,32,32,32	0
56	MG	BA	3332	1/1	0.94	0.20	74,74,74,74	0
56	MG	DA	3390	1/1	0.94	0.09	55,55,55,55	0
56	MG	BF	302	1/1	0.94	0.15	41,41,41,41	0
56	MG	BA	3683	1/1	0.94	0.06	31,31,31,31	0
56	MG	DF	302	1/1	0.94	0.16	75,75,75,75	0
56	MG	AA	1662	1/1	0.94	0.22	71,71,71,71	0
56	MG	BA	3704	1/1	0.94	0.06	44,44,44,44	0
56	MG	BA	3706	1/1	0.94	0.17	29,29,29,29	0
56	MG	DR	201	1/1	0.94	0.12	44,44,44,44	0
56	MG	DT	202	1/1	0.94	0.06	38,38,38,38	0
56	MG	DA	3413	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3334	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3417	1/1	0.94	0.14	46,46,46,46	0
56	MG	BA	3449	1/1	0.94	0.22	34,34,34,34	0
56	MG	DA	3042	1/1	0.94	0.10	47,47,47,47	0
56	MG	DA	3425	1/1	0.94	0.14	50,50,50,50	0
56	MG	DA	3217	1/1	0.94	0.22	68,68,68,68	0
56	MG	BQ	202	1/1	0.94	0.12	46,46,46,46	0
56	MG	DA	3046	1/1	0.94	0.18	79,79,79,79	0
56	MG	BA	3450	1/1	0.94	0.11	42,42,42,42	0
56	MG	D8	201	1/1	0.94	0.13	67,67,67,67	0
56	MG	BA	3452	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3335	1/1	0.94	0.25	47,47,47,47	0
57	ZN	D6	101	1/1	0.94	0.08	106,106,106,106	0
56	MG	DA	3223	1/1	0.94	0.25	70,70,70,70	0
56	MG	DA	3442	1/1	0.95	0.10	56,56,56,56	0
56	MG	BA	3013	1/1	0.95	0.14	57,57,57,57	0
56	MG	BA	3015	1/1	0.95	0.26	59,59,59,59	0
56	MG	DA	3449	1/1	0.95	0.10	45,45,45,45	0
56	MG	BA	3877	1/1	0.95	0.16	21,21,21,21	0
56	MG	BA	3246	1/1	0.95	0.21	53,53,53,53	0
56	MG	BA	3881	1/1	0.95	0.05	75,75,75,75	0
56	MG	DA	3031	1/1	0.95	0.15	49,49,49,49	0
56	MG	AA	1906	1/1	0.95	0.10	89,89,89,89	0
56	MG	BA	3611	1/1	0.95	0.14	43,43,43,43	0
56	MG	DA	3225	1/1	0.95	0.20	43,43,43,43	0
56	MG	BA	3612	1/1	0.95	0.06	61,61,61,61	0
56	MG	BA	3437	1/1	0.95	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3466	1/1	0.95	0.09	75,75,75,75	0
56	MG	BA	3018	1/1	0.95	0.27	53,53,53,53	0
56	MG	BA	3615	1/1	0.95	0.11	68,68,68,68	0
56	MG	BA	3341	1/1	0.95	0.07	53,53,53,53	0
56	MG	BA	3619	1/1	0.95	0.07	86,86,86,86	0
56	MG	BA	3622	1/1	0.95	0.08	65,65,65,65	0
56	MG	DA	3043	1/1	0.95	0.12	61,61,61,61	0
56	MG	AA	1907	1/1	0.95	0.10	78,78,78,78	0
56	MG	BA	3343	1/1	0.95	0.24	37,37,37,37	0
56	MG	BA	3022	1/1	0.95	0.07	85,85,85,85	0
56	MG	BA	3254	1/1	0.95	0.22	21,21,21,21	0
56	MG	DA	3050	1/1	0.95	0.24	67,67,67,67	0
56	MG	BA	3638	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3447	1/1	0.95	0.13	45,45,45,45	0
56	MG	DA	3485	1/1	0.95	0.08	42,42,42,42	0
56	MG	BA	3644	1/1	0.95	0.06	72,72,72,72	0
56	MG	BB	213	1/1	0.95	0.09	58,58,58,58	0
56	MG	BA	3646	1/1	0.95	0.11	44,44,44,44	0
56	MG	BB	215	1/1	0.95	0.17	62,62,62,62	0
56	MG	DA	3493	1/1	0.95	0.08	80,80,80,80	0
56	MG	BA	3647	1/1	0.95	0.10	61,61,61,61	0
56	MG	BB	218	1/1	0.95	0.14	57,57,57,57	0
56	MG	BA	3346	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3649	1/1	0.95	0.12	60,60,60,60	0
56	MG	BB	224	1/1	0.95	0.12	57,57,57,57	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
56	MG	BB	226	1/1	0.95	0.07	61,61,61,61	0
56	MG	DA	3508	1/1	0.95	0.08	87,87,87,87	0
56	MG	BA	3086	1/1	0.95	0.14	51,51,51,51	0
56	MG	DA	3257	1/1	0.95	0.21	51,51,51,51	0
56	MG	BA	3348	1/1	0.95	0.08	62,62,62,62	0
56	MG	DA	3512	1/1	0.95	0.15	49,49,49,49	0
56	MG	AV	102	1/1	0.95	0.23	66,66,66,66	0
56	MG	AA	1885	1/1	0.95	0.10	90,90,90,90	0
56	MG	BA	3159	1/1	0.95	0.15	43,43,43,43	0
56	MG	AA	1886	1/1	0.95	0.05	79,79,79,79	0
56	MG	BA	3027	1/1	0.95	0.11	44,44,44,44	0
56	MG	BA	3672	1/1	0.95	0.07	41,41,41,41	0
56	MG	BA	3094	1/1	0.95	0.12	45,45,45,45	0
56	MG	BF	306	1/1	0.95	0.15	48,48,48,48	0
56	MG	BA	3358	1/1	0.95	0.27	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3460	1/1	0.95	0.15	52,52,52,52	0
56	MG	BO	202	1/1	0.95	0.12	42,42,42,42	0
56	MG	BA	3697	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3702	1/1	0.95	0.18	49,49,49,49	0
56	MG	DA	3537	1/1	0.95	0.19	68,68,68,68	0
56	MG	BA	3703	1/1	0.95	0.05	65,65,65,65	0
56	MG	AA	1938	1/1	0.95	0.08	84,84,84,84	0
56	MG	BT	201	1/1	0.95	0.09	53,53,53,53	0
56	MG	BA	3096	1/1	0.95	0.15	37,37,37,37	0
56	MG	BA	3468	1/1	0.95	0.11	54,54,54,54	0
56	MG	BA	3269	1/1	0.95	0.09	55,55,55,55	0
56	MG	BA	3270	1/1	0.95	0.29	53,53,53,53	0
56	MG	BA	3471	1/1	0.95	0.12	49,49,49,49	0
56	MG	B0	105	1/1	0.95	0.18	76,76,76,76	0
56	MG	BA	3718	1/1	0.95	0.06	87,87,87,87	0
56	MG	DA	3556	1/1	0.95	0.06	58,58,58,58	0
56	MG	DA	3096	1/1	0.95	0.16	41,41,41,41	0
56	MG	B1	102	1/1	0.95	0.07	45,45,45,45	0
56	MG	BA	3030	1/1	0.95	0.12	36,36,36,36	0
56	MG	BA	3031	1/1	0.95	0.15	29,29,29,29	0
56	MG	DA	3561	1/1	0.95	0.17	70,70,70,70	0
56	MG	DA	3562	1/1	0.95	0.18	69,69,69,69	0
56	MG	DA	3286	1/1	0.95	0.32	69,69,69,69	0
56	MG	BA	3366	1/1	0.95	0.14	52,52,52,52	0
56	MG	AA	1624	1/1	0.95	0.25	57,57,57,57	0
56	MG	CA	1750	1/1	0.95	0.10	56,56,56,56	0
56	MG	BA	3731	1/1	0.95	0.10	53,53,53,53	0
56	MG	DA	3569	1/1	0.95	0.07	76,76,76,76	0
56	MG	BA	3101	1/1	0.95	0.13	26,26,26,26	0
56	MG	AA	1867	1/1	0.95	0.39	80,80,80,80	0
56	MG	B7	101	1/1	0.95	0.09	51,51,51,51	0
56	MG	BA	3735	1/1	0.95	0.07	58,58,58,58	0
56	MG	AA	1890	1/1	0.95	0.10	89,89,89,89	0
56	MG	BA	3480	1/1	0.95	0.26	59,59,59,59	0
56	MG	BA	3037	1/1	0.95	0.07	37,37,37,37	0
56	MG	BA	3740	1/1	0.95	0.10	48,48,48,48	0
56	MG	BA	3186	1/1	0.95	0.20	27,27,27,27	0
56	MG	DA	3115	1/1	0.95	0.30	75,75,75,75	0
56	MG	BA	3039	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3586	1/1	0.95	0.17	50,50,50,50	0
56	MG	BA	3380	1/1	0.95	0.11	44,44,44,44	0
56	MG	CA	1767	1/1	0.95	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3744	1/1	0.95	0.23	44,44,44,44	0
56	MG	DA	3121	1/1	0.95	0.20	37,37,37,37	0
56	MG	CA	1769	1/1	0.95	0.09	93,93,93,93	0
56	MG	DA	3593	1/1	0.95	0.07	75,75,75,75	0
56	MG	BA	3485	1/1	0.95	0.19	52,52,52,52	0
56	MG	BA	3750	1/1	0.95	0.08	65,65,65,65	0
56	MG	CA	1772	1/1	0.95	0.08	77,77,77,77	0
56	MG	BA	3752	1/1	0.95	0.10	28,28,28,28	0
56	MG	AA	1829	1/1	0.95	0.09	63,63,63,63	0
56	MG	BA	3754	1/1	0.95	0.12	68,68,68,68	0
56	MG	DA	3313	1/1	0.95	0.10	74,74,74,74	0
56	MG	BA	3757	1/1	0.95	0.08	28,28,28,28	0
56	MG	BA	3383	1/1	0.95	0.19	45,45,45,45	0
56	MG	BA	3761	1/1	0.95	0.07	77,77,77,77	0
56	MG	BA	3112	1/1	0.95	0.13	56,56,56,56	0
56	MG	BA	3765	1/1	0.95	0.08	59,59,59,59	0
56	MG	DA	3613	1/1	0.95	0.17	60,60,60,60	0
56	MG	CA	1781	1/1	0.95	0.11	103,103,103,103	0
56	MG	BA	3385	1/1	0.95	0.11	58,58,58,58	0
56	MG	BA	3493	1/1	0.95	0.08	62,62,62,62	0
56	MG	BA	3386	1/1	0.95	0.17	54,54,54,54	0
56	MG	DA	3143	1/1	0.95	0.19	50,50,50,50	0
56	MG	DA	3327	1/1	0.95	0.14	64,64,64,64	0
56	MG	DA	3328	1/1	0.95	0.10	59,59,59,59	0
56	MG	BA	3043	1/1	0.95	0.32	42,42,42,42	0
56	MG	AV	110	1/1	0.95	0.26	80,80,80,80	0
56	MG	BA	3289	1/1	0.95	0.14	61,61,61,61	0
56	MG	DA	3332	1/1	0.95	0.38	63,63,63,63	0
56	MG	CA	1626	1/1	0.95	0.21	50,50,50,50	0
56	MG	CA	1789	1/1	0.95	0.07	66,66,66,66	0
56	MG	AA	1871	1/1	0.95	0.10	71,71,71,71	0
56	MG	BA	3291	1/1	0.95	0.12	61,61,61,61	0
56	MG	BA	3393	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3394	1/1	0.95	0.16	58,58,58,58	0
56	MG	AA	1830	1/1	0.95	0.20	57,57,57,57	0
56	MG	BA	3197	1/1	0.95	0.15	41,41,41,41	0
56	MG	BA	3786	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3510	1/1	0.95	0.08	60,60,60,60	0
56	MG	DA	3344	1/1	0.95	0.22	88,88,88,88	0
56	MG	AA	1645	1/1	0.95	0.21	54,54,54,54	0
56	MG	BA	3791	1/1	0.95	0.15	29,29,29,29	0
56	MG	DA	3651	1/1	0.95	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3299	1/1	0.95	0.05	58,58,58,58	0
56	MG	DA	3653	1/1	0.95	0.13	59,59,59,59	0
56	MG	BA	3200	1/1	0.95	0.16	35,35,35,35	0
56	MG	AA	1750	1/1	0.95	0.07	79,79,79,79	0
56	MG	DA	3350	1/1	0.95	0.12	72,72,72,72	0
56	MG	AV	117	1/1	0.95	0.06	69,69,69,69	0
56	MG	AA	1806	1/1	0.95	0.20	59,59,59,59	0
56	MG	AA	1792	1/1	0.95	0.19	44,44,44,44	0
56	MG	CA	1810	1/1	0.95	0.07	92,92,92,92	0
56	MG	BA	3311	1/1	0.95	0.09	59,59,59,59	0
56	MG	BA	3802	1/1	0.95	0.10	71,71,71,71	0
56	MG	BA	3056	1/1	0.95	0.06	50,50,50,50	0
56	MG	BA	3057	1/1	0.95	0.07	30,30,30,30	0
56	MG	AA	1730	1/1	0.95	0.17	61,61,61,61	0
56	MG	BA	3410	1/1	0.95	0.30	54,54,54,54	0
56	MG	DA	3679	1/1	0.95	0.07	76,76,76,76	0
56	MG	BA	3531	1/1	0.95	0.07	59,59,59,59	0
56	MG	BA	3221	1/1	0.95	0.20	17,17,17,17	0
56	MG	DA	3683	1/1	0.95	0.12	94,94,94,94	0
56	MG	DA	3684	1/1	0.95	0.09	98,98,98,98	0
56	MG	BA	3535	1/1	0.95	0.14	68,68,68,68	0
56	MG	BA	3818	1/1	0.95	0.15	86,86,86,86	0
56	MG	BA	3536	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3133	1/1	0.95	0.14	27,27,27,27	0
56	MG	BA	3318	1/1	0.95	0.14	63,63,63,63	0
56	MG	BA	3824	1/1	0.95	0.08	90,90,90,90	0
56	MG	BA	3548	1/1	0.95	0.14	39,39,39,39	0
56	MG	AA	1787	1/1	0.95	0.15	66,66,66,66	0
56	MG	BA	3562	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3567	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3321	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3569	1/1	0.95	0.21	49,49,49,49	0
56	MG	DA	3376	1/1	0.95	0.22	69,69,69,69	0
56	MG	DA	3377	1/1	0.95	0.18	89,89,89,89	0
56	MG	BA	3570	1/1	0.95	0.10	60,60,60,60	0
56	MG	BA	3065	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3843	1/1	0.95	0.09	78,78,78,78	0
56	MG	CA	1667	1/1	0.95	0.22	66,66,66,66	0
56	MG	DA	3003	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3067	1/1	0.95	0.11	40,40,40,40	0
56	MG	AA	1883	1/1	0.95	0.06	86,86,86,86	0
56	MG	DB	216	1/1	0.95	0.05	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3577	1/1	0.95	0.09	78,78,78,78	0
56	MG	BA	3008	1/1	0.95	0.11	84,84,84,84	0
56	MG	DA	3391	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3851	1/1	0.95	0.06	35,35,35,35	0
56	MG	DE	302	1/1	0.95	0.15	55,55,55,55	0
56	MG	AA	1928	1/1	0.95	0.06	71,71,71,71	0
56	MG	DA	3011	1/1	0.95	0.06	66,66,66,66	0
56	MG	BA	3584	1/1	0.95	0.10	54,54,54,54	0
56	MG	DA	3401	1/1	0.95	0.22	36,36,36,36	0
56	MG	DA	3403	1/1	0.95	0.29	60,60,60,60	0
56	MG	BA	3585	1/1	0.95	0.06	35,35,35,35	0
56	MG	BA	3073	1/1	0.95	0.23	39,39,39,39	0
56	MG	DQ	202	1/1	0.95	0.22	77,77,77,77	0
56	MG	BA	3075	1/1	0.95	0.14	47,47,47,47	0
56	MG	DA	3415	1/1	0.95	0.28	33,33,33,33	0
56	MG	AA	1705	1/1	0.95	0.05	55,55,55,55	0
56	MG	DA	3418	1/1	0.95	0.11	52,52,52,52	0
56	MG	DA	3421	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3238	1/1	0.95	0.20	55,55,55,55	0
56	MG	DA	3212	1/1	0.95	0.28	66,66,66,66	0
56	MG	DA	3021	1/1	0.95	0.17	58,58,58,58	0
56	MG	D0	104	1/1	0.95	0.18	86,86,86,86	0
56	MG	DA	3427	1/1	0.95	0.12	45,45,45,45	0
56	MG	DA	3429	1/1	0.95	0.05	73,73,73,73	0
56	MG	DA	3214	1/1	0.95	0.13	64,64,64,64	0
56	MG	BA	3239	1/1	0.95	0.15	49,49,49,49	0
56	MG	DA	3434	1/1	0.95	0.08	48,48,48,48	0
56	MG	DA	3435	1/1	0.95	0.09	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	BA	3596	1/1	0.95	0.05	39,39,39,39	0
56	MG	BA	3506	1/1	0.96	0.12	61,61,61,61	0
56	MG	DA	3128	1/1	0.96	0.30	59,59,59,59	0
56	MG	BA	3507	1/1	0.96	0.14	53,53,53,53	0
56	MG	DA	3130	1/1	0.96	0.07	52,52,52,52	0
56	MG	DA	3131	1/1	0.96	0.18	46,46,46,46	0
56	MG	DA	3515	1/1	0.96	0.23	51,51,51,51	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	BA	3878	1/1	0.96	0.11	81,81,81,81	0
56	MG	DA	3520	1/1	0.96	0.06	67,67,67,67	0
56	MG	BA	3183	1/1	0.96	0.28	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3880	1/1	0.96	0.09	84,84,84,84	0
56	MG	BA	3126	1/1	0.96	0.24	40,40,40,40	0
56	MG	BA	3882	1/1	0.96	0.05	73,73,73,73	0
56	MG	BA	3883	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3528	1/1	0.96	0.05	88,88,88,88	0
56	MG	BA	3014	1/1	0.96	0.17	49,49,49,49	0
56	MG	BA	3085	1/1	0.96	0.12	35,35,35,35	0
56	MG	DA	3531	1/1	0.96	0.20	66,66,66,66	0
56	MG	BA	3046	1/1	0.96	0.10	49,49,49,49	0
56	MG	DA	3141	1/1	0.96	0.22	60,60,60,60	0
56	MG	DA	3534	1/1	0.96	0.11	73,73,73,73	0
56	MG	AA	1869	1/1	0.96	0.18	81,81,81,81	0
56	MG	CA	1809	1/1	0.96	0.05	101,101,101,101	0
56	MG	AA	1610	1/1	0.96	0.14	48,48,48,48	0
56	MG	DA	3538	1/1	0.96	0.08	96,96,96,96	0
56	MG	DA	3145	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3717	1/1	0.96	0.08	21,21,21,21	0
56	MG	BA	3894	1/1	0.96	0.11	52,52,52,52	0
56	MG	AA	1946	1/1	0.96	0.11	81,81,81,81	0
56	MG	DA	3546	1/1	0.96	0.08	73,73,73,73	0
56	MG	BA	3424	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3314	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3151	1/1	0.96	0.12	45,45,45,45	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	BA	3425	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3155	1/1	0.96	0.17	56,56,56,56	0
56	MG	DA	3156	1/1	0.96	0.15	57,57,57,57	0
56	MG	AA	1947	1/1	0.96	0.06	63,63,63,63	0
56	MG	DA	3323	1/1	0.96	0.08	57,57,57,57	0
56	MG	BB	205	1/1	0.96	0.22	29,29,29,29	0
56	MG	BA	3093	1/1	0.96	0.13	42,42,42,42	0
56	MG	AA	1760	1/1	0.96	0.18	64,64,64,64	0
56	MG	BA	3526	1/1	0.96	0.09	40,40,40,40	0
56	MG	AA	1857	1/1	0.96	0.12	62,62,62,62	0
56	MG	BA	3351	1/1	0.96	0.16	51,51,51,51	0
56	MG	BA	3532	1/1	0.96	0.11	34,34,34,34	0
56	MG	AA	1632	1/1	0.96	0.33	51,51,51,51	0
56	MG	CA	1680	1/1	0.96	0.26	70,70,70,70	0
56	MG	BA	3278	1/1	0.96	0.21	59,59,59,59	0
56	MG	BA	3739	1/1	0.96	0.09	42,42,42,42	0
56	MG	BA	3097	1/1	0.96	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1927	1/1	0.96	0.06	85,85,85,85	0
56	MG	BA	3543	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3172	1/1	0.96	0.18	51,51,51,51	0
56	MG	DA	3173	1/1	0.96	0.20	62,62,62,62	0
56	MG	DA	3340	1/1	0.96	0.29	55,55,55,55	0
56	MG	BA	3282	1/1	0.96	0.09	59,59,59,59	0
56	MG	BB	223	1/1	0.96	0.09	38,38,38,38	0
56	MG	AA	1909	1/1	0.96	0.07	91,91,91,91	0
56	MG	BA	3745	1/1	0.96	0.08	75,75,75,75	0
56	MG	BA	3554	1/1	0.96	0.07	55,55,55,55	0
56	MG	CA	1691	1/1	0.96	0.37	53,53,53,53	0
56	MG	BA	3555	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3556	1/1	0.96	0.11	52,52,52,52	0
56	MG	BA	3146	1/1	0.96	0.16	49,49,49,49	0
56	MG	BD	304	1/1	0.96	0.23	20,20,20,20	0
56	MG	DA	3012	1/1	0.96	0.06	76,76,76,76	0
56	MG	BE	301	1/1	0.96	0.17	36,36,36,36	0
56	MG	BE	302	1/1	0.96	0.21	51,51,51,51	0
56	MG	BA	3560	1/1	0.96	0.20	39,39,39,39	0
56	MG	BE	304	1/1	0.96	0.26	14,14,14,14	0
56	MG	BA	3285	1/1	0.96	0.09	55,55,55,55	0
56	MG	BA	3564	1/1	0.96	0.07	63,63,63,63	0
56	MG	BA	3061	1/1	0.96	0.14	45,45,45,45	0
56	MG	DA	3359	1/1	0.96	0.09	59,59,59,59	0
56	MG	BA	3763	1/1	0.96	0.05	84,84,84,84	0
56	MG	BA	3210	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3028	1/1	0.96	0.07	33,33,33,33	0
56	MG	DA	3612	1/1	0.96	0.10	87,87,87,87	0
56	MG	BG	202	1/1	0.96	0.05	82,82,82,82	0
56	MG	BA	3767	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3213	1/1	0.96	0.12	37,37,37,37	0
56	MG	BA	3769	1/1	0.96	0.07	55,55,55,55	0
56	MG	DA	3030	1/1	0.96	0.08	66,66,66,66	0
56	MG	BA	3214	1/1	0.96	0.06	49,49,49,49	0
56	MG	BA	3771	1/1	0.96	0.08	79,79,79,79	0
56	MG	DA	3621	1/1	0.96	0.09	73,73,73,73	0
56	MG	BA	3367	1/1	0.96	0.24	50,50,50,50	0
56	MG	BA	3774	1/1	0.96	0.18	72,72,72,72	0
56	MG	AA	1876	1/1	0.96	0.06	89,89,89,89	0
56	MG	BA	3292	1/1	0.96	0.13	47,47,47,47	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3293	1/1	0.96	0.07	45,45,45,45	0
56	MG	BZ	302	1/1	0.96	0.09	62,62,62,62	0
56	MG	BA	3103	1/1	0.96	0.38	54,54,54,54	0
56	MG	DA	3632	1/1	0.96	0.27	69,69,69,69	0
56	MG	BA	3295	1/1	0.96	0.16	45,45,45,45	0
56	MG	DA	3045	1/1	0.96	0.14	62,62,62,62	0
56	MG	BA	3375	1/1	0.96	0.11	47,47,47,47	0
56	MG	DA	3637	1/1	0.96	0.05	57,57,57,57	0
56	MG	BA	3151	1/1	0.96	0.10	38,38,38,38	0
56	MG	DA	3048	1/1	0.96	0.14	74,74,74,74	0
56	MG	DA	3643	1/1	0.96	0.08	89,89,89,89	0
56	MG	DA	3384	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3152	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3298	1/1	0.96	0.23	50,50,50,50	0
56	MG	CA	1726	1/1	0.96	0.18	70,70,70,70	0
56	MG	BA	3785	1/1	0.96	0.09	69,69,69,69	0
56	MG	BA	3224	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3464	1/1	0.96	0.08	53,53,53,53	0
56	MG	DA	3395	1/1	0.96	0.07	58,58,58,58	0
56	MG	CA	1730	1/1	0.96	0.24	69,69,69,69	0
56	MG	BA	3594	1/1	0.96	0.09	44,44,44,44	0
56	MG	BA	3466	1/1	0.96	0.15	50,50,50,50	0
56	MG	DA	3658	1/1	0.96	0.15	79,79,79,79	0
56	MG	BA	3597	1/1	0.96	0.06	66,66,66,66	0
56	MG	DA	3662	1/1	0.96	0.07	53,53,53,53	0
56	MG	DA	3405	1/1	0.96	0.14	43,43,43,43	0
56	MG	BA	3382	1/1	0.96	0.10	68,68,68,68	0
56	MG	DA	3412	1/1	0.96	0.07	52,52,52,52	0
56	MG	DA	3670	1/1	0.96	0.05	83,83,83,83	0
56	MG	BA	3603	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3672	1/1	0.96	0.11	87,87,87,87	0
56	MG	B9	102	1/1	0.96	0.15	43,43,43,43	0
56	MG	DA	3063	1/1	0.96	0.19	50,50,50,50	0
56	MG	AA	1649	1/1	0.96	0.09	60,60,60,60	0
56	MG	BA	3227	1/1	0.96	0.26	41,41,41,41	0
56	MG	BA	3105	1/1	0.96	0.12	45,45,45,45	0
56	MG	DA	3680	1/1	0.96	0.08	79,79,79,79	0
56	MG	AA	1896	1/1	0.96	0.06	88,88,88,88	0
56	MG	BA	3069	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3803	1/1	0.96	0.16	71,71,71,71	0
56	MG	DA	3238	1/1	0.96	0.13	65,65,65,65	0
56	MG	CA	1744	1/1	0.96	0.13	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3686	1/1	0.96	0.08	74,74,74,74	0
56	MG	BA	3804	1/1	0.96	0.07	59,59,59,59	0
56	MG	BA	3305	1/1	0.96	0.06	35,35,35,35	0
56	MG	BA	3308	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	3075	1/1	0.96	0.07	84,84,84,84	0
56	MG	CA	1749	1/1	0.96	0.16	92,92,92,92	0
56	MG	BA	3231	1/1	0.96	0.21	31,31,31,31	0
56	MG	DA	3246	1/1	0.96	0.20	48,48,48,48	0
56	MG	DA	3695	1/1	0.96	0.07	107,107,107,107	0
56	MG	BA	3233	1/1	0.96	0.11	22,22,22,22	0
56	MG	BA	3617	1/1	0.96	0.07	58,58,58,58	0
56	MG	CA	1753	1/1	0.96	0.22	61,61,61,61	0
56	MG	AA	1781	1/1	0.96	0.36	68,68,68,68	0
56	MG	DA	3450	1/1	0.96	0.11	59,59,59,59	0
56	MG	AA	1656	1/1	0.96	0.11	72,72,72,72	0
56	MG	BA	3815	1/1	0.96	0.04	51,51,51,51	0
56	MG	BA	3626	1/1	0.96	0.05	70,70,70,70	0
56	MG	BA	3160	1/1	0.96	0.11	41,41,41,41	0
56	MG	BA	3114	1/1	0.96	0.22	37,37,37,37	0
56	MG	DB	211	1/1	0.96	0.09	83,83,83,83	0
56	MG	AA	1721	1/1	0.96	0.21	84,84,84,84	0
56	MG	CA	1763	1/1	0.96	0.11	62,62,62,62	0
56	MG	BA	3116	1/1	0.96	0.17	37,37,37,37	0
56	MG	DB	215	1/1	0.96	0.06	94,94,94,94	0
56	MG	BA	3636	1/1	0.96	0.08	63,63,63,63	0
56	MG	BA	3006	1/1	0.96	0.13	55,55,55,55	0
56	MG	BA	3639	1/1	0.96	0.06	63,63,63,63	0
56	MG	BA	3832	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3641	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3167	1/1	0.96	0.09	31,31,31,31	0
56	MG	BA	3836	1/1	0.96	0.09	23,23,23,23	0
56	MG	BA	3038	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3489	1/1	0.96	0.10	55,55,55,55	0
56	MG	BA	3119	1/1	0.96	0.09	50,50,50,50	0
56	MG	AA	1917	1/1	0.96	0.07	71,71,71,71	0
56	MG	BA	3404	1/1	0.96	0.09	52,52,52,52	0
56	MG	DA	3480	1/1	0.96	0.13	70,70,70,70	0
56	MG	DO	203	1/1	0.96	0.15	79,79,79,79	0
56	MG	DQ	201	1/1	0.96	0.08	43,43,43,43	0
56	MG	BA	3040	1/1	0.96	0.09	46,46,46,46	0
56	MG	DA	3108	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3176	1/1	0.96	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3653	1/1	0.96	0.20	38,38,38,38	0
56	MG	DA	3487	1/1	0.96	0.06	70,70,70,70	0
56	MG	BA	3654	1/1	0.96	0.08	59,59,59,59	0
56	MG	BA	3852	1/1	0.96	0.19	59,59,59,59	0
56	MG	BA	3177	1/1	0.96	0.18	46,46,46,46	0
56	MG	BA	3178	1/1	0.96	0.16	43,43,43,43	0
56	MG	AA	1841	1/1	0.96	0.15	75,75,75,75	0
56	MG	BA	3257	1/1	0.96	0.19	48,48,48,48	0
56	MG	BA	3412	1/1	0.96	0.07	56,56,56,56	0
56	MG	BA	3668	1/1	0.96	0.07	29,29,29,29	0
56	MG	D6	103	1/1	0.96	0.06	93,93,93,93	0
56	MG	AA	1765	1/1	0.96	0.14	48,48,48,48	0
56	MG	BA	3869	1/1	0.96	0.06	64,64,64,64	0
56	MG	CA	1647	1/1	0.96	0.19	71,71,71,71	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	3503	1/1	0.96	0.09	51,51,51,51	0
57	ZN	D4	101	1/1	0.96	0.11	178,178,178,178	0
56	MG	BA	3504	1/1	0.96	0.14	57,57,57,57	0
56	MG	AA	1701	1/1	0.96	0.11	57,57,57,57	0
56	MG	DA	3551	1/1	0.97	0.14	42,42,42,42	0
56	MG	BA	3124	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3055	1/1	0.97	0.07	37,37,37,37	0
56	MG	BA	3091	1/1	0.97	0.13	60,60,60,60	0
56	MG	BA	3354	1/1	0.97	0.15	34,34,34,34	0
56	MG	BA	3127	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3655	1/1	0.97	0.08	46,46,46,46	0
56	MG	BA	3226	1/1	0.97	0.23	36,36,36,36	0
56	MG	BA	3839	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3840	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3092	1/1	0.97	0.21	34,34,34,34	0
56	MG	BA	3432	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3565	1/1	0.97	0.08	50,50,50,50	0
56	MG	AA	1771	1/1	0.97	0.10	68,68,68,68	0
56	MG	BA	3520	1/1	0.97	0.18	38,38,38,38	0
56	MG	BA	3847	1/1	0.97	0.19	82,82,82,82	0
56	MG	CA	1620	1/1	0.97	0.12	70,70,70,70	0
56	MG	BA	3173	1/1	0.97	0.13	31,31,31,31	0
56	MG	DA	3572	1/1	0.97	0.20	45,45,45,45	0
56	MG	DA	3573	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3360	1/1	0.97	0.07	51,51,51,51	0
56	MG	AA	1916	1/1	0.97	0.05	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3071	1/1	0.97	0.25	44,44,44,44	0
56	MG	CA	1758	1/1	0.97	0.18	56,56,56,56	0
56	MG	CA	1759	1/1	0.97	0.09	76,76,76,76	0
56	MG	BA	3438	1/1	0.97	0.11	62,62,62,62	0
56	MG	BA	3685	1/1	0.97	0.08	40,40,40,40	0
56	MG	DA	3076	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3687	1/1	0.97	0.11	23,23,23,23	0
56	MG	DA	3584	1/1	0.97	0.07	76,76,76,76	0
56	MG	BA	3131	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3856	1/1	0.97	0.10	68,68,68,68	0
56	MG	BA	3527	1/1	0.97	0.09	90,90,90,90	0
56	MG	BA	3858	1/1	0.97	0.13	70,70,70,70	0
56	MG	BA	3009	1/1	0.97	0.08	83,83,83,83	0
56	MG	AA	1839	1/1	0.97	0.06	69,69,69,69	0
56	MG	BA	3865	1/1	0.97	0.05	97,97,97,97	0
56	MG	BA	3034	1/1	0.97	0.08	23,23,23,23	0
56	MG	DA	3595	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3705	1/1	0.97	0.17	79,79,79,79	0
56	MG	DA	3235	1/1	0.97	0.14	53,53,53,53	0
56	MG	BA	3136	1/1	0.97	0.18	32,32,32,32	0
56	MG	AA	1840	1/1	0.97	0.10	83,83,83,83	0
56	MG	DA	3602	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3709	1/1	0.97	0.09	49,49,49,49	0
56	MG	DA	3091	1/1	0.97	0.06	47,47,47,47	0
56	MG	BA	3873	1/1	0.97	0.05	74,74,74,74	0
56	MG	BA	3710	1/1	0.97	0.08	58,58,58,58	0
56	MG	BA	3712	1/1	0.97	0.08	48,48,48,48	0
56	MG	BA	3066	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3097	1/1	0.97	0.28	31,31,31,31	0
56	MG	DA	3399	1/1	0.97	0.24	47,47,47,47	0
56	MG	BA	3537	1/1	0.97	0.15	47,47,47,47	0
56	MG	BA	3184	1/1	0.97	0.19	31,31,31,31	0
56	MG	BA	3036	1/1	0.97	0.08	54,54,54,54	0
56	MG	DA	3248	1/1	0.97	0.15	53,53,53,53	0
56	MG	BA	3242	1/1	0.97	0.20	47,47,47,47	0
56	MG	DA	3411	1/1	0.97	0.13	55,55,55,55	0
56	MG	DA	3250	1/1	0.97	0.36	62,62,62,62	0
56	MG	DA	3619	1/1	0.97	0.06	39,39,39,39	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
56	MG	BA	3725	1/1	0.97	0.09	69,69,69,69	0
56	MG	DA	3416	1/1	0.97	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3547	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3887	1/1	0.97	0.14	17,17,17,17	0
56	MG	DA	3419	1/1	0.97	0.10	35,35,35,35	0
56	MG	AA	1870	1/1	0.97	0.09	85,85,85,85	0
56	MG	BA	3729	1/1	0.97	0.06	59,59,59,59	0
56	MG	BA	3891	1/1	0.97	0.08	74,74,74,74	0
56	MG	DA	3630	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3549	1/1	0.97	0.10	19,19,19,19	0
56	MG	DA	3426	1/1	0.97	0.05	42,42,42,42	0
56	MG	BA	3732	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3552	1/1	0.97	0.10	39,39,39,39	0
56	MG	DA	3635	1/1	0.97	0.04	88,88,88,88	0
56	MG	CA	1794	1/1	0.97	0.09	59,59,59,59	0
56	MG	DA	3431	1/1	0.97	0.08	33,33,33,33	0
56	MG	AA	1895	1/1	0.97	0.06	87,87,87,87	0
56	MG	BA	3306	1/1	0.97	0.07	45,45,45,45	0
56	MG	BA	3378	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3437	1/1	0.97	0.12	70,70,70,70	0
56	MG	DA	3646	1/1	0.97	0.13	62,62,62,62	0
56	MG	BA	3557	1/1	0.97	0.05	62,62,62,62	0
56	MG	BA	3307	1/1	0.97	0.06	48,48,48,48	0
56	MG	BA	3070	1/1	0.97	0.14	51,51,51,51	0
56	MG	BA	3561	1/1	0.97	0.10	64,64,64,64	0
56	MG	BA	3309	1/1	0.97	0.14	56,56,56,56	0
56	MG	BA	3459	1/1	0.97	0.10	49,49,49,49	0
56	MG	BA	3310	1/1	0.97	0.10	54,54,54,54	0
56	MG	BA	3190	1/1	0.97	0.22	42,42,42,42	0
56	MG	DA	3451	1/1	0.97	0.12	39,39,39,39	0
56	MG	DA	3452	1/1	0.97	0.14	60,60,60,60	0
56	MG	BA	3462	1/1	0.97	0.15	47,47,47,47	0
56	MG	DA	3127	1/1	0.97	0.21	37,37,37,37	0
56	MG	DA	3660	1/1	0.97	0.07	78,78,78,78	0
56	MG	BA	3191	1/1	0.97	0.15	78,78,78,78	0
56	MG	DA	3663	1/1	0.97	0.05	81,81,81,81	0
56	MG	DA	3457	1/1	0.97	0.10	102,102,102,102	0
56	MG	DA	3665	1/1	0.97	0.04	87,87,87,87	0
56	MG	BB	212	1/1	0.97	0.07	62,62,62,62	0
56	MG	DA	3667	1/1	0.97	0.06	74,74,74,74	0
56	MG	DA	3668	1/1	0.97	0.09	100,100,100,100	0
56	MG	BA	3749	1/1	0.97	0.11	76,76,76,76	0
56	MG	AA	1634	1/1	0.97	0.27	47,47,47,47	0
56	MG	BA	3465	1/1	0.97	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3463	1/1	0.97	0.08	68,68,68,68	0
56	MG	BA	3575	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3252	1/1	0.97	0.24	20,20,20,20	0
56	MG	BA	3756	1/1	0.97	0.08	56,56,56,56	0
56	MG	BA	3467	1/1	0.97	0.09	56,56,56,56	0
56	MG	DA	3468	1/1	0.97	0.04	80,80,80,80	0
56	MG	BA	3315	1/1	0.97	0.20	54,54,54,54	0
56	MG	AA	1940	1/1	0.97	0.06	92,92,92,92	0
56	MG	BB	225	1/1	0.97	0.15	56,56,56,56	0
56	MG	BA	3580	1/1	0.97	0.05	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	3582	1/1	0.97	0.08	30,30,30,30	0
56	MG	BA	3106	1/1	0.97	0.07	28,28,28,28	0
56	MG	AA	1897	1/1	0.97	0.11	74,74,74,74	0
56	MG	BA	3042	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3147	1/1	0.97	0.06	70,70,70,70	0
56	MG	BA	3473	1/1	0.97	0.20	22,22,22,22	0
56	MG	BA	3320	1/1	0.97	0.18	58,58,58,58	0
56	MG	BA	3019	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3198	1/1	0.97	0.12	17,17,17,17	0
56	MG	AV	115	1/1	0.97	0.08	65,65,65,65	0
56	MG	BA	3324	1/1	0.97	0.22	62,62,62,62	0
56	MG	BA	3113	1/1	0.97	0.07	46,46,46,46	0
56	MG	BA	3599	1/1	0.97	0.05	52,52,52,52	0
56	MG	BA	3202	1/1	0.97	0.13	42,42,42,42	0
56	MG	BF	307	1/1	0.97	0.05	42,42,42,42	0
56	MG	DA	3495	1/1	0.97	0.04	62,62,62,62	0
56	MG	AA	1872	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3604	1/1	0.97	0.08	80,80,80,80	0
56	MG	DA	3500	1/1	0.97	0.09	68,68,68,68	0
56	MG	DB	210	1/1	0.97	0.16	91,91,91,91	0
56	MG	AA	1854	1/1	0.97	0.08	73,73,73,73	0
56	MG	DA	3503	1/1	0.97	0.15	80,80,80,80	0
56	MG	BA	3267	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3330	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	3268	1/1	0.97	0.10	52,52,52,52	0
56	MG	BA	3047	1/1	0.97	0.14	32,32,32,32	0
56	MG	DA	3015	1/1	0.97	0.15	66,66,66,66	0
56	MG	BA	3487	1/1	0.97	0.14	53,53,53,53	0
56	MG	DA	3315	1/1	0.97	0.24	47,47,47,47	0
56	MG	BQ	204	1/1	0.97	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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	BA	3024	1/1	0.97	0.14	36,36,36,36	0
56	MG	BA	3207	1/1	0.97	0.17	41,41,41,41	0
56	MG	BV	201	1/1	0.97	0.30	39,39,39,39	0
56	MG	BA	3208	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3795	1/1	0.97	0.19	84,84,84,84	0
56	MG	BA	3409	1/1	0.97	0.06	45,45,45,45	0
56	MG	BA	3336	1/1	0.97	0.08	46,46,46,46	0
56	MG	DA	3523	1/1	0.97	0.06	86,86,86,86	0
56	MG	BA	3620	1/1	0.97	0.05	49,49,49,49	0
56	MG	BA	3156	1/1	0.97	0.28	54,54,54,54	0
56	MG	DT	201	1/1	0.97	0.11	73,73,73,73	0
56	MG	BA	3624	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3625	1/1	0.97	0.05	41,41,41,41	0
56	MG	AA	1864	1/1	0.97	0.09	67,67,67,67	0
56	MG	AA	1824	1/1	0.97	0.23	33,33,33,33	0
56	MG	BA	3276	1/1	0.97	0.13	57,57,57,57	0
56	MG	BA	3415	1/1	0.97	0.07	50,50,50,50	0
56	MG	BA	3634	1/1	0.97	0.06	46,46,46,46	0
56	MG	D0	103	1/1	0.97	0.11	55,55,55,55	0
56	MG	AA	1766	1/1	0.97	0.15	53,53,53,53	0
56	MG	DA	3038	1/1	0.97	0.07	50,50,50,50	0
56	MG	BA	3052	1/1	0.97	0.11	35,35,35,35	0
56	MG	BA	3637	1/1	0.97	0.05	62,62,62,62	0
56	MG	BA	3279	1/1	0.97	0.08	50,50,50,50	0
56	MG	BA	3502	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3816	1/1	0.97	0.05	85,85,85,85	0
57	ZN	AD	301	1/1	0.97	0.17	93,93,93,93	0
56	MG	BA	3215	1/1	0.97	0.21	16,16,16,16	0
56	MG	AA	1929	1/1	0.97	0.11	48,48,48,48	0
56	MG	BA	3219	1/1	0.97	0.24	43,43,43,43	0
56	MG	CA	1735	1/1	0.97	0.08	78,78,78,78	0
56	MG	BA	3220	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3005	1/1	0.97	0.06	59,59,59,59	0
56	MG	BA	3508	1/1	0.97	0.20	41,41,41,41	0
56	MG	AA	1604	1/1	0.98	0.06	42,42,42,42	0
56	MG	DA	3589	1/1	0.98	0.06	81,81,81,81	0
56	MG	DA	3428	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	BA	3574	1/1	0.98	0.07	36,36,36,36	0
56	MG	BA	3232	1/1	0.98	0.21	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3594	1/1	0.98	0.15	44,44,44,44	0
56	MG	CA	1746	1/1	0.98	0.04	65,65,65,65	0
56	MG	AA	1889	1/1	0.98	0.04	71,71,71,71	0
56	MG	DA	3597	1/1	0.98	0.05	57,57,57,57	0
56	MG	BA	3663	1/1	0.98	0.05	21,21,21,21	0
56	MG	DA	3599	1/1	0.98	0.14	50,50,50,50	0
56	MG	DA	3436	1/1	0.98	0.14	50,50,50,50	0
56	MG	DA	3039	1/1	0.98	0.06	50,50,50,50	0
56	MG	BA	3665	1/1	0.98	0.05	44,44,44,44	0
56	MG	BA	3783	1/1	0.98	0.08	74,74,74,74	0
56	MG	DA	3440	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3016	1/1	0.98	0.30	52,52,52,52	0
56	MG	AA	1877	1/1	0.98	0.05	70,70,70,70	0
56	MG	BA	3673	1/1	0.98	0.11	43,43,43,43	0
56	MG	DA	3608	1/1	0.98	0.05	82,82,82,82	0
56	MG	DA	3444	1/1	0.98	0.04	54,54,54,54	0
56	MG	DA	3445	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3787	1/1	0.98	0.04	35,35,35,35	0
56	MG	BA	3201	1/1	0.98	0.23	54,54,54,54	0
56	MG	BA	3170	1/1	0.98	0.24	43,43,43,43	0
56	MG	BA	3684	1/1	0.98	0.10	42,42,42,42	0
56	MG	AA	1891	1/1	0.98	0.04	75,75,75,75	0
56	MG	AA	1933	1/1	0.98	0.06	54,54,54,54	0
56	MG	BA	3794	1/1	0.98	0.10	80,80,80,80	0
56	MG	DA	3455	1/1	0.98	0.05	61,61,61,61	0
56	MG	BA	3688	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3143	1/1	0.98	0.21	20,20,20,20	0
56	MG	DA	3054	1/1	0.98	0.14	78,78,78,78	0
56	MG	BA	3241	1/1	0.98	0.16	38,38,38,38	0
56	MG	BB	216	1/1	0.98	0.10	38,38,38,38	0
56	MG	BA	3700	1/1	0.98	0.10	26,26,26,26	0
56	MG	BA	3701	1/1	0.98	0.07	26,26,26,26	0
56	MG	BA	3368	1/1	0.98	0.12	63,63,63,63	0
56	MG	BB	220	1/1	0.98	0.09	44,44,44,44	0
56	MG	AA	1934	1/1	0.98	0.04	48,48,48,48	0
56	MG	BA	3519	1/1	0.98	0.18	53,53,53,53	0
56	MG	BA	3021	1/1	0.98	0.04	35,35,35,35	0
56	MG	BA	3245	1/1	0.98	0.17	42,42,42,42	0
56	MG	BA	3074	1/1	0.98	0.09	52,52,52,52	0
56	MG	BA	3247	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3374	1/1	0.98	0.22	24,24,24,24	0
56	MG	DA	3195	1/1	0.98	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BB	229	1/1	0.98	0.03	67,67,67,67	0
56	MG	BA	3809	1/1	0.98	0.09	40,40,40,40	0
56	MG	BA	3525	1/1	0.98	0.06	40,40,40,40	0
56	MG	AA	1924	1/1	0.98	0.05	80,80,80,80	0
56	MG	DA	3479	1/1	0.98	0.04	68,68,68,68	0
56	MG	DA	3644	1/1	0.98	0.05	80,80,80,80	0
56	MG	BD	303	1/1	0.98	0.15	29,29,29,29	0
56	MG	BA	3813	1/1	0.98	0.04	66,66,66,66	0
56	MG	BD	305	1/1	0.98	0.08	54,54,54,54	0
56	MG	BA	3602	1/1	0.98	0.07	22,22,22,22	0
56	MG	DA	3484	1/1	0.98	0.05	45,45,45,45	0
56	MG	DA	3650	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3007	1/1	0.98	0.11	91,91,91,91	0
56	MG	BA	3528	1/1	0.98	0.06	71,71,71,71	0
56	MG	BA	3377	1/1	0.98	0.11	50,50,50,50	0
56	MG	BE	305	1/1	0.98	0.05	22,22,22,22	0
56	MG	BA	3606	1/1	0.98	0.07	63,63,63,63	0
56	MG	BA	3720	1/1	0.98	0.09	22,22,22,22	0
56	MG	DA	3492	1/1	0.98	0.08	63,63,63,63	0
56	MG	BF	303	1/1	0.98	0.05	41,41,41,41	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	DA	3661	1/1	0.98	0.10	61,61,61,61	0
56	MG	BA	3722	1/1	0.98	0.08	61,61,61,61	0
56	MG	BA	3530	1/1	0.98	0.13	49,49,49,49	0
56	MG	BA	3180	1/1	0.98	0.16	41,41,41,41	0
56	MG	DA	3501	1/1	0.98	0.07	81,81,81,81	0
56	MG	BA	3609	1/1	0.98	0.06	53,53,53,53	0
56	MG	BA	3829	1/1	0.98	0.19	82,82,82,82	0
56	MG	BA	3830	1/1	0.98	0.06	31,31,31,31	0
56	MG	BA	3831	1/1	0.98	0.10	22,22,22,22	0
56	MG	CA	1800	1/1	0.98	0.04	105,105,105,105	0
56	MG	DA	3094	1/1	0.98	0.11	34,34,34,34	0
56	MG	BA	3727	1/1	0.98	0.05	66,66,66,66	0
56	MG	BQ	201	1/1	0.98	0.03	18,18,18,18	0
56	MG	BA	3212	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3675	1/1	0.98	0.09	75,75,75,75	0
56	MG	BA	3834	1/1	0.98	0.10	27,27,27,27	0
56	MG	CA	1805	1/1	0.98	0.04	88,88,88,88	0
56	MG	DA	3513	1/1	0.98	0.08	59,59,59,59	0
56	MG	AA	1878	1/1	0.98	0.07	46,46,46,46	0
56	MG	BA	3730	1/1	0.98	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3253	1/1	0.98	0.12	20,20,20,20	0
56	MG	DA	3517	1/1	0.98	0.10	64,64,64,64	0
56	MG	BA	3429	1/1	0.98	0.18	54,54,54,54	0
56	MG	AA	1628	1/1	0.98	0.20	22,22,22,22	0
56	MG	BA	3538	1/1	0.98	0.06	33,33,33,33	0
56	MG	DA	3687	1/1	0.98	0.03	64,64,64,64	0
56	MG	BV	202	1/1	0.98	0.20	67,67,67,67	0
56	MG	BA	3539	1/1	0.98	0.07	22,22,22,22	0
56	MG	BA	3540	1/1	0.98	0.05	19,19,19,19	0
56	MG	BA	3079	1/1	0.98	0.16	54,54,54,54	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	B0	101	1/1	0.98	0.05	43,43,43,43	0
56	MG	BA	3338	1/1	0.98	0.25	63,63,63,63	0
56	MG	BA	3623	1/1	0.98	0.07	75,75,75,75	0
56	MG	B0	104	1/1	0.98	0.07	58,58,58,58	0
56	MG	BA	3216	1/1	0.98	0.12	28,28,28,28	0
56	MG	BA	3080	1/1	0.98	0.14	44,44,44,44	0
56	MG	BA	3218	1/1	0.98	0.12	20,20,20,20	0
56	MG	AA	1862	1/1	0.98	0.04	45,45,45,45	0
56	MG	DA	3120	1/1	0.98	0.08	42,42,42,42	0
56	MG	BA	3059	1/1	0.98	0.16	25,25,25,25	0
56	MG	BA	3632	1/1	0.98	0.07	59,59,59,59	0
56	MG	BA	3748	1/1	0.98	0.05	28,28,28,28	0
56	MG	DA	3540	1/1	0.98	0.18	57,57,57,57	0
56	MG	B3	102	1/1	0.98	0.18	56,56,56,56	0
56	MG	DA	3542	1/1	0.98	0.07	84,84,84,84	0
56	MG	DA	3543	1/1	0.98	0.04	74,74,74,74	0
56	MG	BA	3261	1/1	0.98	0.09	69,69,69,69	0
56	MG	BA	3550	1/1	0.98	0.14	27,27,27,27	0
56	MG	BA	3861	1/1	0.98	0.04	66,66,66,66	0
56	MG	BA	3862	1/1	0.98	0.09	59,59,59,59	0
56	MG	DD	302	1/1	0.98	0.27	48,48,48,48	0
56	MG	BA	3490	1/1	0.98	0.16	49,49,49,49	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	BA	3060	1/1	0.98	0.06	52,52,52,52	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	DA	3006	1/1	0.98	0.07	56,56,56,56	0
56	MG	BA	3263	1/1	0.98	0.07	41,41,41,41	0
56	MG	BA	3868	1/1	0.98	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3442	1/1	0.98	0.16	45,45,45,45	0
56	MG	DA	3394	1/1	0.98	0.05	36,36,36,36	0
56	MG	BA	3758	1/1	0.98	0.07	60,60,60,60	0
56	MG	DA	3396	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3759	1/1	0.98	0.15	40,40,40,40	0
56	MG	BA	3872	1/1	0.98	0.05	24,24,24,24	0
56	MG	BA	3011	1/1	0.98	0.15	54,54,54,54	0
56	MG	DA	3014	1/1	0.98	0.15	38,38,38,38	0
56	MG	BA	3189	1/1	0.98	0.22	49,49,49,49	0
56	MG	BA	3762	1/1	0.98	0.05	48,48,48,48	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	3349	1/1	0.98	0.08	52,52,52,52	0
56	MG	BA	3645	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3062	1/1	0.98	0.15	34,34,34,34	0
56	MG	BA	3766	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3108	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3022	1/1	0.98	0.15	46,46,46,46	0
56	MG	BA	3563	1/1	0.98	0.12	45,45,45,45	0
56	MG	AV	116	1/1	0.98	0.05	84,84,84,84	0
56	MG	BA	3884	1/1	0.98	0.05	66,66,66,66	0
56	MG	BA	3134	1/1	0.98	0.07	35,35,35,35	0
56	MG	DA	3581	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3451	1/1	0.98	0.12	47,47,47,47	0
56	MG	DA	3422	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3110	1/1	0.98	0.22	51,51,51,51	0
57	ZN	DY	201	1/1	0.98	0.04	123,123,123,123	0
56	MG	AA	1633	1/1	0.98	0.24	32,32,32,32	0
57	ZN	D5	102	1/1	0.98	0.04	88,88,88,88	0
56	MG	BA	3163	1/1	0.98	0.20	40,40,40,40	0
56	MG	BA	3890	1/1	0.98	0.05	70,70,70,70	0
56	MG	BA	3650	1/1	0.99	0.04	46,46,46,46	0
56	MG	DA	3433	1/1	0.99	0.10	46,46,46,46	0
56	MG	BA	3876	1/1	0.99	0.06	54,54,54,54	0
56	MG	BA	3559	1/1	0.99	0.07	53,53,53,53	0
56	MG	DA	3677	1/1	0.99	0.13	51,51,51,51	0
56	MG	BA	3598	1/1	0.99	0.04	54,54,54,54	0
56	MG	BA	3707	1/1	0.99	0.03	25,25,25,25	0
56	MG	BA	3817	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3243	1/1	0.99	0.19	35,35,35,35	0
56	MG	AA	1861	1/1	0.99	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3601	1/1	0.99	0.04	24,24,24,24	0
56	MG	BA	3821	1/1	0.99	0.04	76,76,76,76	0
56	MG	BA	3534	1/1	0.99	0.08	44,44,44,44	0
56	MG	BA	3627	1/1	0.99	0.07	56,56,56,56	0
56	MG	BA	3064	1/1	0.99	0.14	41,41,41,41	0
56	MG	DA	3446	1/1	0.99	0.10	40,40,40,40	0
56	MG	DA	3447	1/1	0.99	0.05	62,62,62,62	0
56	MG	DA	3526	1/1	0.99	0.03	64,64,64,64	0
56	MG	BA	3825	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3715	1/1	0.99	0.09	21,21,21,21	0
56	MG	BA	3443	1/1	0.99	0.06	41,41,41,41	0
56	MG	BA	3660	1/1	0.99	0.02	28,28,28,28	0
56	MG	BA	3566	1/1	0.99	0.06	54,54,54,54	0
56	MG	BA	3434	1/1	0.99	0.20	22,22,22,22	0
56	MG	BA	3773	1/1	0.99	0.04	44,44,44,44	0
56	MG	BA	3664	1/1	0.99	0.06	31,31,31,31	0
56	MG	BA	3551	1/1	0.99	0.03	68,68,68,68	0
56	MG	BA	3666	1/1	0.99	0.03	28,28,28,28	0
56	MG	DA	3458	1/1	0.99	0.05	49,49,49,49	0
56	MG	BA	3723	1/1	0.99	0.05	51,51,51,51	0
56	MG	BA	3667	1/1	0.99	0.03	27,27,27,27	0
56	MG	DA	3385	1/1	0.99	0.05	48,48,48,48	0
56	MG	BA	3586	1/1	0.99	0.04	52,52,52,52	0
56	MG	DA	3387	1/1	0.99	0.05	40,40,40,40	0
56	MG	BA	3838	1/1	0.99	0.05	28,28,28,28	0
56	MG	DA	3389	1/1	0.99	0.05	66,66,66,66	0
56	MG	BA	3669	1/1	0.99	0.04	34,34,34,34	0
56	MG	BA	3670	1/1	0.99	0.05	57,57,57,57	0
56	MG	BA	3671	1/1	0.99	0.04	41,41,41,41	0
56	MG	BA	3587	1/1	0.99	0.08	48,48,48,48	0
56	MG	BA	3610	1/1	0.99	0.06	41,41,41,41	0
56	MG	BA	3674	1/1	0.99	0.04	27,27,27,27	0
56	MG	BA	3676	1/1	0.99	0.04	20,20,20,20	0
56	MG	DA	3397	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3846	1/1	0.99	0.06	27,27,27,27	0
56	MG	BA	3677	1/1	0.99	0.07	29,29,29,29	0
56	MG	BA	3679	1/1	0.99	0.03	34,34,34,34	0
56	MG	DA	3477	1/1	0.99	0.03	78,78,78,78	0
56	MG	BA	3789	1/1	0.99	0.04	41,41,41,41	0
56	MG	DA	3638	1/1	0.99	0.08	48,48,48,48	0
56	MG	DA	3402	1/1	0.99	0.07	38,38,38,38	0
56	MG	BA	3168	1/1	0.99	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3642	1/1	0.99	0.04	71,71,71,71	0
56	MG	DA	3404	1/1	0.99	0.09	56,56,56,56	0
56	MG	BA	3681	1/1	0.99	0.07	52,52,52,52	0
56	MG	DA	3080	1/1	0.99	0.26	36,36,36,36	0
56	MG	BA	3682	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3164	1/1	0.99	0.14	26,26,26,26	0
56	MG	DA	3486	1/1	0.99	0.09	42,42,42,42	0
56	MG	BA	3854	1/1	0.99	0.05	25,25,25,25	0
56	MG	BA	3640	1/1	0.99	0.03	33,33,33,33	0
56	MG	BA	3590	1/1	0.99	0.05	56,56,56,56	0
56	MG	BA	3686	1/1	0.99	0.04	26,26,26,26	0
56	MG	BA	3175	1/1	0.99	0.21	34,34,34,34	0
56	MG	DA	3571	1/1	0.99	0.04	57,57,57,57	0
56	MG	BA	3798	1/1	0.99	0.12	45,45,45,45	0
56	MG	BA	3860	1/1	0.99	0.02	57,57,57,57	0
56	MG	BA	3643	1/1	0.99	0.02	54,54,54,54	0
56	MG	BA	3690	1/1	0.99	0.05	27,27,27,27	0
56	MG	DA	3496	1/1	0.99	0.07	47,47,47,47	0
56	MG	BA	3541	1/1	0.99	0.03	35,35,35,35	0
56	MG	DA	3498	1/1	0.99	0.04	51,51,51,51	0
56	MG	BA	3694	1/1	0.99	0.04	29,29,29,29	0
56	MG	BA	3696	1/1	0.99	0.06	30,30,30,30	0
56	MG	BA	3518	1/1	0.99	0.13	33,33,33,33	0
57	ZN	BY	201	1/1	0.99	0.04	70,70,70,70	0
56	MG	BA	3698	1/1	0.99	0.04	44,44,44,44	0
57	ZN	B6	101	1/1	0.99	0.03	48,48,48,48	0
56	MG	BA	3751	1/1	0.99	0.07	56,56,56,56	0
56	MG	BA	3699	1/1	0.99	0.04	38,38,38,38	0
56	MG	AA	1935	1/1	0.99	0.09	56,56,56,56	0
56	MG	BA	3618	1/1	0.99	0.04	46,46,46,46	0
56	MG	BA	3810	1/1	0.99	0.04	27,27,27,27	0
56	MG	BA	3595	1/1	0.99	0.03	45,45,45,45	0
56	MG	BA	3390	1/1	0.99	0.08	28,28,28,28	0
56	MG	BA	3675	1/1	1.00	0.04	33,33,33,33	0
56	MG	B6	102	1/1	1.00	0.07	73,73,73,73	0
56	MG	BA	3691	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3641	1/1	1.00	0.04	50,50,50,50	0
56	MG	BA	3692	1/1	1.00	0.03	30,30,30,30	0
56	MG	B8	102	1/1	1.00	0.04	49,49,49,49	0
56	MG	BA	3565	1/1	1.00	0.03	34,34,34,34	0
56	MG	BA	3583	1/1	1.00	0.04	22,22,22,22	0
56	MG	BA	3755	1/1	1.00	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3695	1/1	1.00	0.02	29,29,29,29	0
56	MG	BA	3678	1/1	1.00	0.03	22,22,22,22	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	3662	1/1	1.00	0.02	30,30,30,30	0
57	ZN	B9	101	1/1	1.00	0.02	51,51,51,51	0
56	MG	BA	3630	1/1	1.00	0.05	23,23,23,23	0
56	MG	BA	3631	1/1	1.00	0.02	25,25,25,25	0
56	MG	BA	3747	1/1	1.00	0.04	20,20,20,20	0
56	MG	BA	3711	1/1	1.00	0.05	24,24,24,24	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

6.5 Other polymers ⓘ

There are no such residues in this entry.