



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 18, 2024 – 12:29 AM EST

PDB ID : 4V8C
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex with paromomycin).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.30 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
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

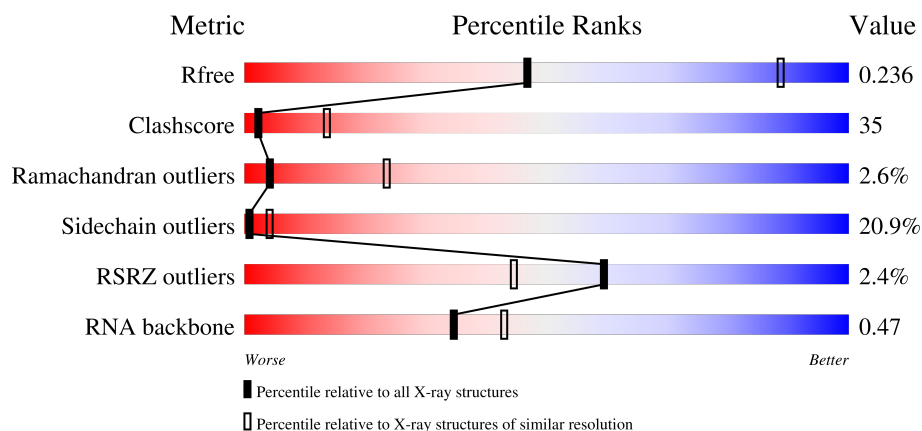
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.






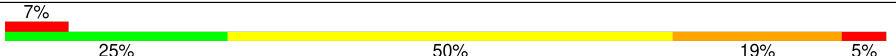
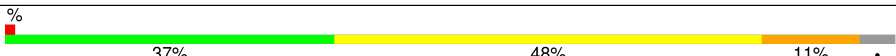
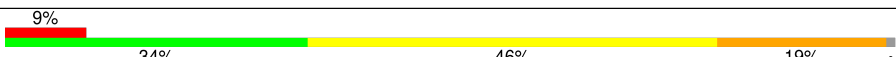
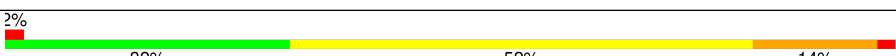
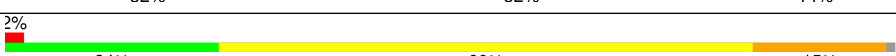
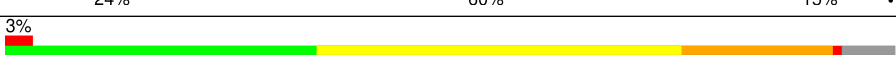
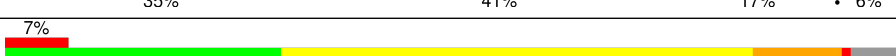
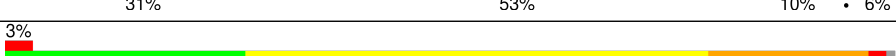
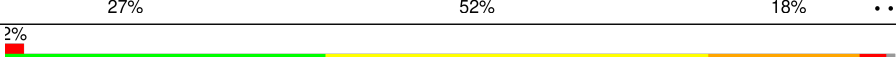

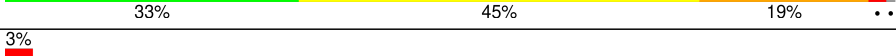


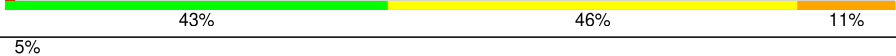
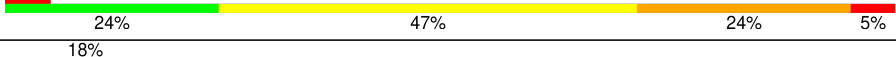
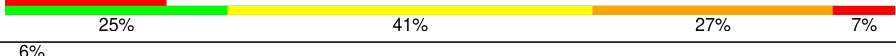
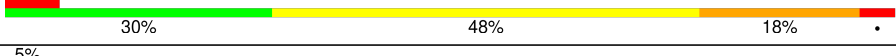
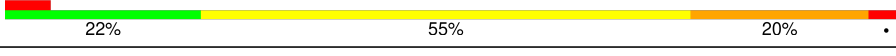
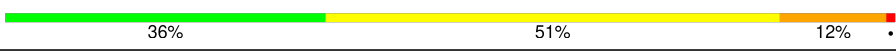



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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	2912	<div> <div>28%</div> <div>50%</div> <div>20%</div> <div>•</div> </div>
1	BA	2912	<div> <div>27%</div> <div>51%</div> <div>20%</div> <div>•</div> </div>
2	AB	122	<div> <div>%</div> <div>32%</div> <div>48%</div> <div>18%</div> <div>•</div> </div>
2	BB	122	<div> <div>%</div> <div>25%</div> <div>56%</div> <div>19%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	210	
5	BF	210	
6	AG	182	
6	BG	182	
7	AH	180	
7	BH	180	
8	AK	148	
8	BK	148	
9	AM	140	
9	BM	140	
10	AN	122	
10	BN	122	
11	AO	150	
11	BO	150	
12	AP	141	
12	BP	141	
13	A0	118	
13	B0	118	
14	AQ	112	
14	BQ	112	
15	AR	146	

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Mol	Chain	Length	Quality of chain
15	BR	146	
16	A1	118	
16	B1	118	
17	A2	101	
17	B2	101	
18	AS	113	
18	BS	113	
19	AT	96	
19	BT	96	
20	AU	110	
20	BU	110	
21	AV	206	
21	BV	206	
22	A3	85	
22	B3	85	
23	AZ	98	
23	BZ	98	
24	AW	72	
24	BW	72	
25	AX	60	
25	BX	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1506	
31	DA	1506	
32	CE	256	
32	DE	256	
33	CF	239	
33	DF	239	
34	CG	208	
34	DG	208	
35	CH	162	
35	DH	162	
36	CI	101	
36	DI	101	
37	CJ	156	
37	DJ	156	
38	CK	138	
38	DK	138	
39	CL	128	
39	DL	128	
40	CM	105	




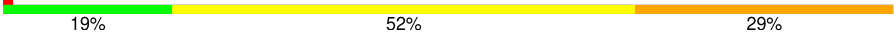
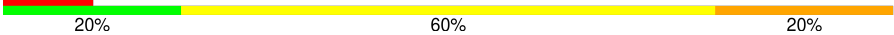
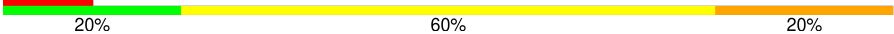
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Mol	Chain	Length	Quality of chain
40	DM	105	
41	CN	129	
41	DN	129	
42	CO	132	
42	DO	132	
43	CP	126	
43	DP	126	
44	CQ	61	
44	DQ	61	
45	CR	89	
45	DR	89	
46	CS	88	
46	DS	88	
47	CT	105	
47	DT	105	
48	CU	88	
48	DU	88	
49	CV	93	
49	DV	93	
50	CW	106	
50	DW	106	
51	CX	27	
51	DX	27	
52	CB	87	
52	DB	87	

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Mol	Chain	Length	Quality of chain
53	CC	77	
53	CD	77	
53	DC	77	
53	DD	77	
54	C1	10	
54	D1	10	

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
55	MG	AA	3309	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299682 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 RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	BA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	expression tag	GB AP008226.1
AA	654A	A	G	conflict	GB AP008226.1
AA	654E	C	G	conflict	GB AP008226.1
AA	654P	G	C	conflict	GB AP008226.1
AA	654T	A	C	conflict	GB AP008226.1
AA	1058	U	G	conflict	GB AP008226.1
AA	1080	A	C	conflict	GB AP008226.1
BA	158	U	-	expression tag	GB AP008226.1
BA	654A	A	G	conflict	GB AP008226.1
BA	654E	C	G	conflict	GB AP008226.1
BA	654P	G	C	conflict	GB AP008226.1
BA	654T	A	C	conflict	GB AP008226.1
BA	1058	U	G	conflict	GB AP008226.1
BA	1080	A	C	conflict	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	B0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	B3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	B4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

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

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CB	87	Total	C	N	O	P	9	0	0
			1861	829	333	612	87			
52	DB	87	Total	C	N	O	P	8	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	18	C	U	conflict	GB AP012306.1
CD	18	C	U	conflict	GB AP012306.1
DC	18	C	U	conflict	GB AP012306.1
DD	18	C	U	conflict	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
54	D1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

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

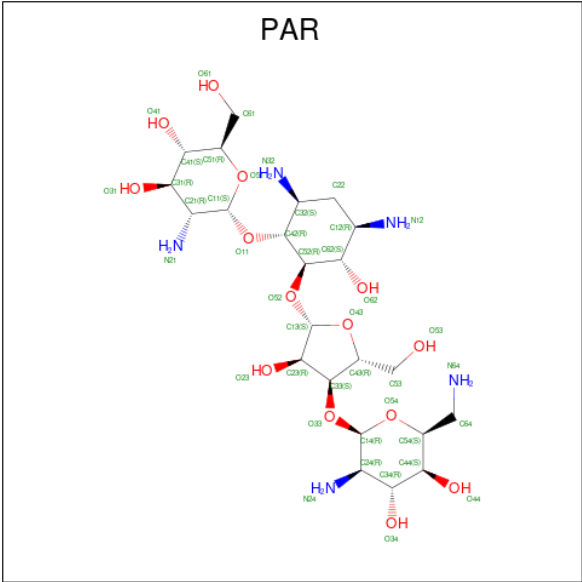
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	626	Total Mg 626 626	0	0
55	AB	17	Total Mg 17 17	0	0
55	AD	1	Total Mg 1 1	0	0
55	AE	4	Total Mg 4 4	0	0
55	AF	3	Total Mg 3 3	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A2	1	Total Mg 1 1	0	0
55	AU	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	AZ	1	Total Mg 1 1	0	0
55	A5	2	Total Mg 2 2	0	0
55	A6	1	Total Mg 1 1	0	0
55	A7	2	Total Mg 2 2	0	0
55	BA	528	Total Mg 528 528	0	0
55	BB	15	Total Mg 15 15	0	0
55	BD	1	Total Mg 1 1	0	0
55	BE	3	Total Mg 3 3	0	0
55	BP	1	Total Mg 1 1	0	0
55	BR	2	Total Mg 2 2	0	0
55	B1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B3	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	CA	240	Total 240	Mg 240	0	0
55	CG	2	Total 2	Mg 2	0	0
55	CN	2	Total 2	Mg 2	0	0
55	CQ	2	Total 2	Mg 2	0	0
55	CT	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	CC	7	Total 7	Mg 7	0	0
55	CD	1	Total 1	Mg 1	0	0
55	C1	1	Total 1	Mg 1	0	0
55	DA	204	Total 204	Mg 204	0	0
55	DG	2	Total 2	Mg 2	0	0
55	DH	1	Total 1	Mg 1	0	0
55	DS	1	Total 1	Mg 1	0	0
55	DB	2	Total 2	Mg 2	0	0
55	DC	8	Total 8	Mg 8	0	0

- Molecule 56 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	CA	1	Total	C	N	O	0	0
			42	23	5	14		
56	DA	1	Total	C	N	O	0	0
			42	23	5	14		

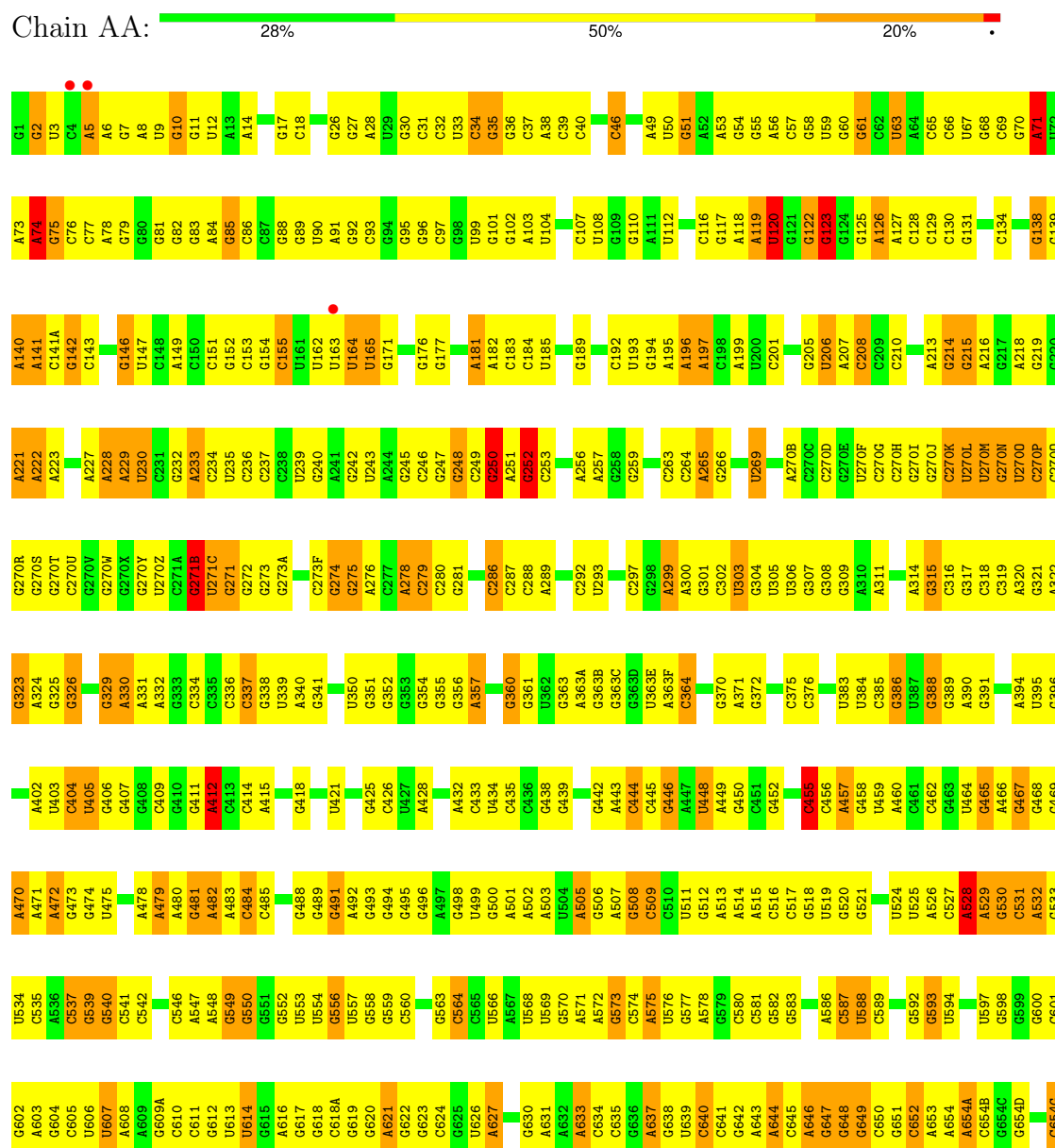
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CG	1	Total	Zn	0	0
			1	1		
57	CQ	1	Total	Zn	0	0
			1	1		
57	DG	1	Total	Zn	0	0
			1	1		
57	DQ	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

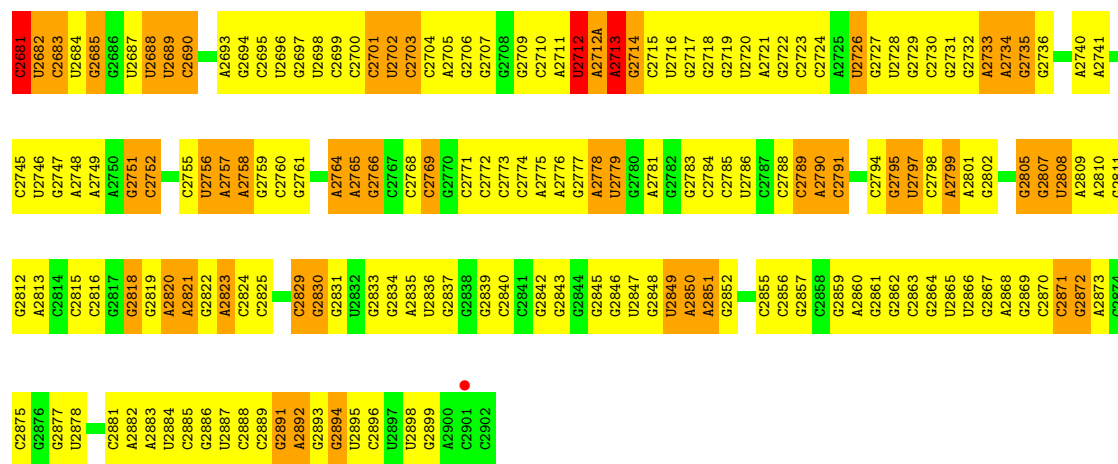
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA (2912-MER)

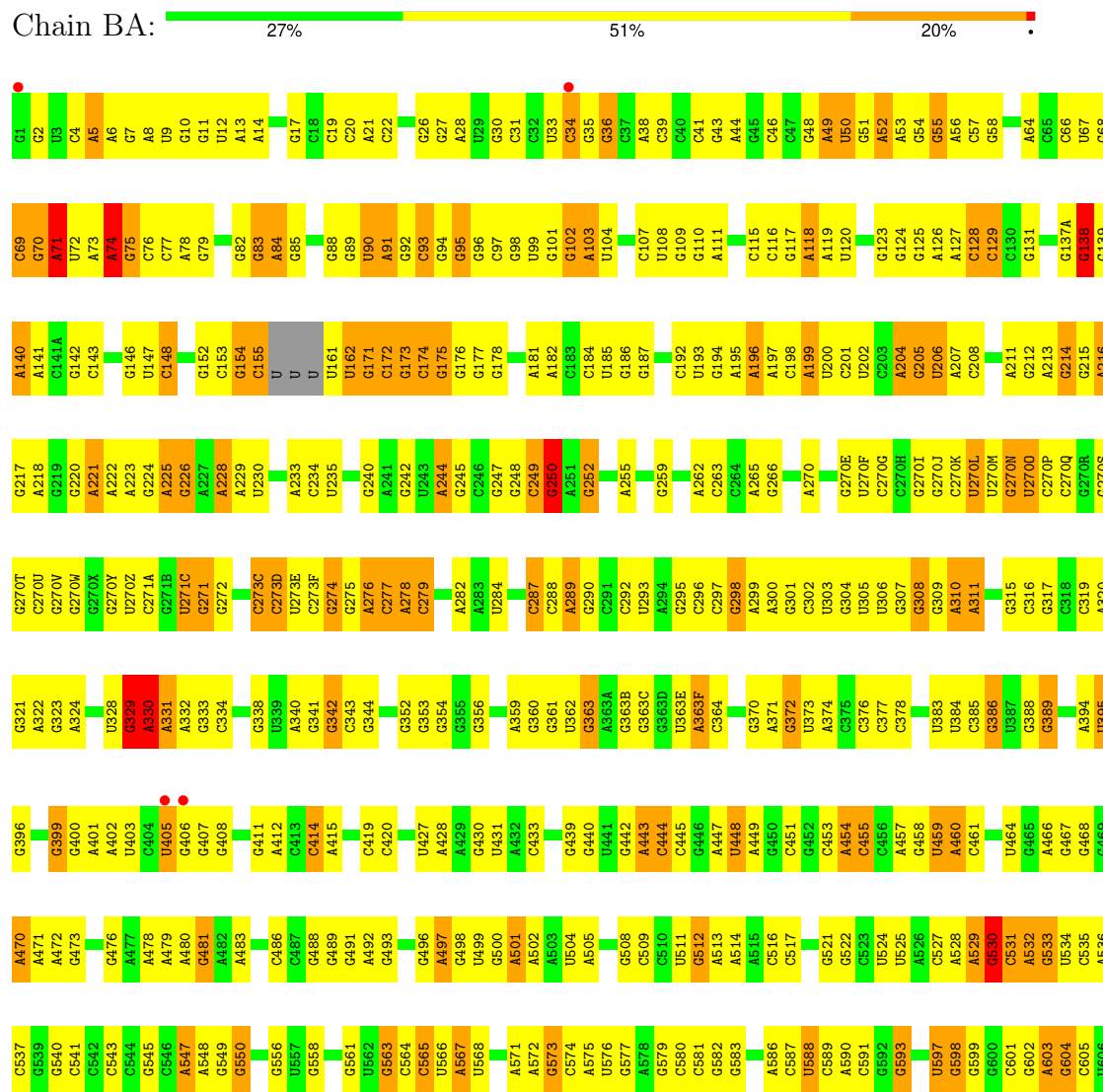


C1588	C1589	G1526	G1527	C1462	C1463	U1397	C1327	A1253	A1182	C1118	G1056	A988	G919	G853	G789	A789	U709	G654H
C1590	C1591	A1528	A1529	C1464	C1465	C1399	C1328	G1256	G1183	C1119	A1057	G889	U922	G854	C790	C790	G710	C654I
C1592	C1593	G1530	G1466	C1401	C1467	C1400	C1330	C1257	G1185	G1122	U1058	A990	C923	C855	C792	C792	G715	C654J
C1594	C1595	C1532	C1468	C1402	C1467	C1403	C1332	G1258	G1187	G1125	U1060	C992	C924	C857	C793	C793	G717	C654L
C1596	C1597	C1533	A1469	C1404	A1470	C1405	A1336	G1261	A1189	A1126	G1062	C994	A926	C859	C796	C796	A718	C654M
A1598	C1598	A1471	A1477	C1406	A1478	U1406	C1338	A1262	G1190	A1128	C1064	A996	G928	U860	C797	C797	C720	G654N
C1600	A1608	C1474	C1475	C1407	G1476	C1408	G1339	A1263	G1191	A1129	U1065	C998	G929	U861	C798	C798	G728	G654P
C1612	A1609	C1544	C1476	C1408	C1477	C1409	G1340	A1264	G1192	U1130	U1066	C999	G930	C862	C730	C730	G729	G654R
C1614	A1610	C1545	C1478	C1409	C1478	C1410	U1341	A1265	G1193	A1132	G1067	A1000	G931	C864	C731	C731	G730	G654S
C1615	C1611	C1546	C1479	C1411	C1479	C1412	U1342	A1266	G1194	U1133	A1069	A1001	G932	C865	C732	C732	G731	A655
C1616	C1617	C1547	C1480	C1412	C1480	C1413	U1343	A1267	G1195	U1134	A1070	A1002	G933	C866	C733	C733	G732	A655T
C1617	C1549	C1550	U1489	C1413	C1481	C1414	U1344	A1268	G1197	U1135	A1071	G1003	G934	C867	C734	C734	A734	G656
C1618	C1550	C1551	U1490	C1414	C1482	C1415	U1345	A1269	G1198	U1136	A1072	C1006	G935	C868	C735	C735	A735	U657
C1627	A1553	C1552	G1491	C1415	C1483	C1416	U1346	A1270	G1199	U1137	A1073	C1007	G936	C869	C736	C736	A736	U658
A1632	A1554	C1553	G1492	C1416	C1484	C1417	U1347	A1271	G1200	U1138	A1074	A1010	G937	C870	C737	C737	U740	G660
C1633	C1554	C1554	C1493	C1417	C1485	C1418	U1348	A1272	G1201	U1139	A1075	A1011	G938	C871	C738	C738	G738	C661
A1634	C1555	C1555	C1494	C1418	C1486	C1419	U1349	A1273	G1202	U1140	C1076	A1012	G939	C872	C739	C739	G739	C662
C1635	C1556	C1556	C1495	C1419	C1487	C1420	U1350	A1274	G1203	U1141	C1077	G1013	G940	C873	C740	C740	A740	C663
C1636	C1557	C1557	C1496	C1420	A1353	C1421	U1351	A1275	G1204	U1142	A1078	G1014	G941	C874	C741	C741	A741	C664
C1637	C1558	C1558	C1497	C1421	A1354	C1422	U1352	A1276	G1205	U1143	A1079	G1015	G942	C875	C742	C742	A742	C665
C1638	C1559	C1559	C1498	C1422	A1355	C1423	U1353	A1277	G1206	U1144	A1080	G1016	G943	C876	C743	C743	U747	C666
C1639	C1560	C1560	C1499	C1423	A1356	C1424	U1354	A1278	G1207	U1145	A1081	G1017	G944	C877	C744	C744	G748	C667
C1640	C1561	C1561	C1500	C1424	C1357	C1425	U1355	A1279	G1208	U1146	U1082	G1018	G945	C878	C745	C745	G748	C668
C1641	C1562	C1562	C1501	C1425	C1358	C1426	U1356	A1280	G1209	U1147	U1083	A1019	G946	C879	C746	C746	A751	C669
C1642	C1563	C1563	C1502	C1426	C1359	C1427	U1357	A1281	G1210	U1148	U1084	G1020	G947	C880	C747	C747	A752	C670
C1643	C1564	C1564	C1503	C1427	C1360	C1428	U1358	A1282	G1211	U1149	U1085	A1021	G948	C881	C748	C748	A753	C671
C1647	C1565	C1565	C1504	C1428	C1361	C1429	U1359	A1283	G1212	U1150	A1086	A1022	G949	C882	C749	C749	A754	C672
C1648	C1566	C1566	C1505	C1429	C1362	C1430	U1360	A1284	G1213	U1151	A1087	G1023	G950	C883	C750	C750	C755	C673
C1649	C1567	C1567	C1506	C1430	C1363	C1431	U1361	A1285	G1214	U1152	A1088	A1024	G951	C884	C751	C751	C755	C674
C1650	C1568	C1568	C1507	C1431	C1364	C1432	U1362	A1286	G1215	U1153	A1089	G1025	G952	C885	C752	C752	C755	C675
C1651	C1569	C1569	C1508	C1432	C1365	C1433	U1363	A1287	G1216	U1154	U1090	G1026	G953	C886	C753	C753	C755	C676
C1652	C1570	C1570	C1509	C1433	C1366	C1434	U1364	A1288	G1217	U1155	U1091	G1027	G954	C887	C754	C754	C755	C677
C1653	C1571	C1571	C1510	C1434	C1367	C1435	U1365	A1289	G1218	U1156	U1092	A1028	G955	C888	C755	C755	C755	C678
C1654	C1572	C1572	C1511	C1435	C1368	C1436	U1366	A1290	G1219	U1157	U1093	A1029	G956	C889	C756	C756	C755	C679
C1655	C1573	C1573	C1512	C1436	C1369	C1437	U1367	A1291	G1220	U1158	U1094	U1033	G957	C890	C757	C757	C755	C680
C1656	C1574	C1574	C1513	C1437	C1370	C1438	U1368	A1292	G1221	U1159	U1095	U1034	G958	C891	C758	C758	C755	C681
C1657	C1575	C1575	C1514	C1438	C1371	C1439	U1369	A1293	G1222	U1160	U1096	U1035	G959	C892	C759	C759	C755	C682
C1658	C1576	C1576	C1515	C1439	C1372	C1440	U1370	A1294	G1223	U1161	U1097	U1036	G960	C893	C760	C760	C755	C683
C1659	C1577	C1577	C1516	C1440	C1373	C1441	U1371	A1295	G1224	U1162	U1098	U1037	G961	C894	C761	C761	C755	C684
C1660	C1578	C1578	C1517	C1441	C1374	C1442	U1372	A1296	G1225	U1163	U1099	U1038	G962	C895	C762	C762	C755	C685
C1661	C1579	C1579	C1518	C1442	C1375	C1443	U1373	A1297	G1226	U1164	U1100	U1039	G963	C896	C763	C763	C755	C686
C1662	C1580	C1580	C1519	C1443	C1376	C1444	U1374	A1298	G1227	U1165	U1101	U1040	G964	C897	C764	C764	C755	C687
C1663	C1581	C1581	C1520	C1444	C1377	C1445	U1375	A1299	G1228	U1166	U1102	U1041	G965	C898	C765	C765	C755	C688
C1664	C1582	C1582	C1521	C1445	C1378	C1446	U1376	A1300	G1229	U1167	U1103	U1042	G966	C899	C766	C766	C755	C689
C1665	C1583	C1583	C1522	C1446	C1379	C1447	U1377	A1301	G1230	U1168	U1104	U1043	G967	C900	C767	C767	C755	C690
C1666	C1584	C1584	C1523	C1447	C1380	C1448	U1378	A1302	G1231	U1169	U1105	U1044	G968	C901	C768	C768	C755	C691
C1667	C1585	C1585	C1524	C1448	C1381	C1449	U1379	A1303	G1232	U1170	U1106	U1045	G969	C902	C769	C769	C755	C692
C1668	C1586	C1586	C1525	C1449	C1382	C1450	U1380	A1304	G1233	U1171	U1107	U1046	G970	C903	C770	C770	C755	C693
C1669	C1587	C1587	C1526	C1450	C1383	C1451	U1381	A1305	G1234	U1172	U1108	U1047	G971	C904	C771	C771	C755	C694
C1670	C1588	C1588	C1527	C1451	C1384	C1452	U1382	A1306	G1235	U1173	U1109	U1048	G972	C905	C772	C772	C755	C695
C1671	C1589	C1589	C1528	C1452	C1385	C1453	U1383	A1307	G1236	U1174	U1110	U1049	G973	C906	C773	C773	C755	C696
C1672	C1590	C1590	C1529	C1453	C1386	C1454	U1384	A1308	G1237	U1175	U1111	U1050	G974	C907	C774	C774	C755	C697
C1673	C1591	C1591	C1530	C1454	C1387	C1455	U1385	A1309	G1238	U1176	U1112	U1051	G975	C908	C775	C775	C755	C698
C1674	C1592	C1592	C1531	C1455	C1388	C1456	U1386	A1310	G1239	U1177	U1113	U1052	G976	C909	C776	C776	C755	C699
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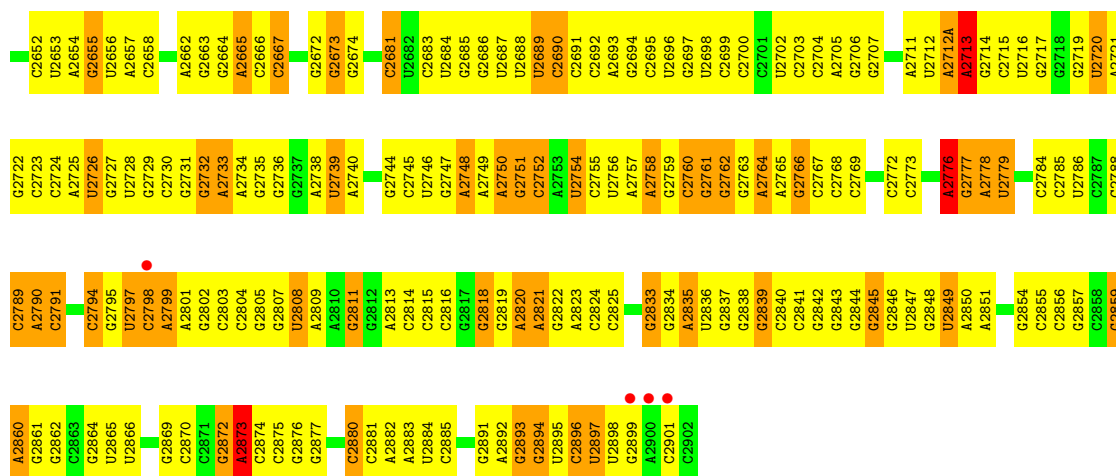


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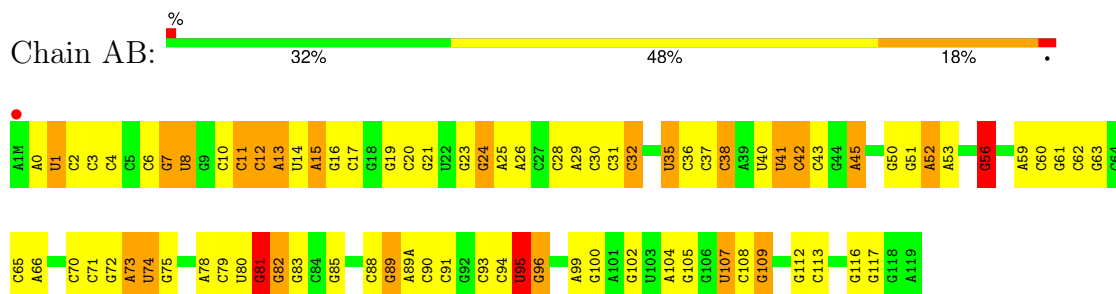


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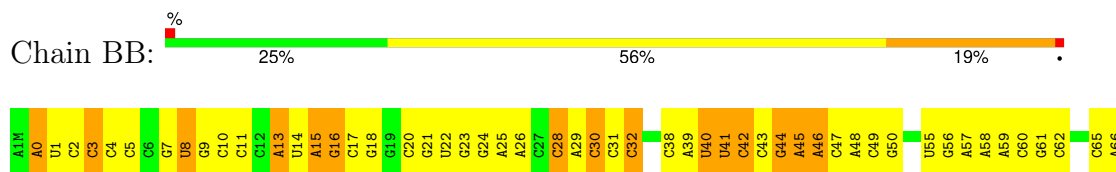
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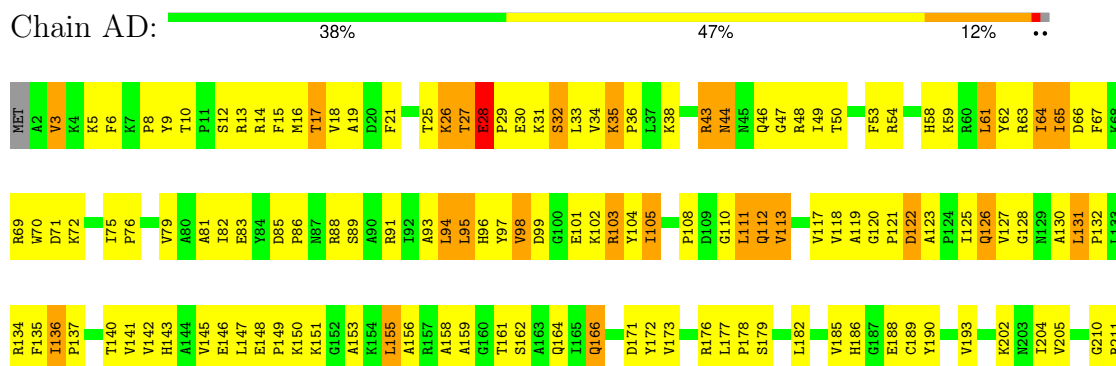
• Molecule 2: 5S RIBOSOMAL RNA



• Molecule 2: 5S RIBOSOMAL RNA

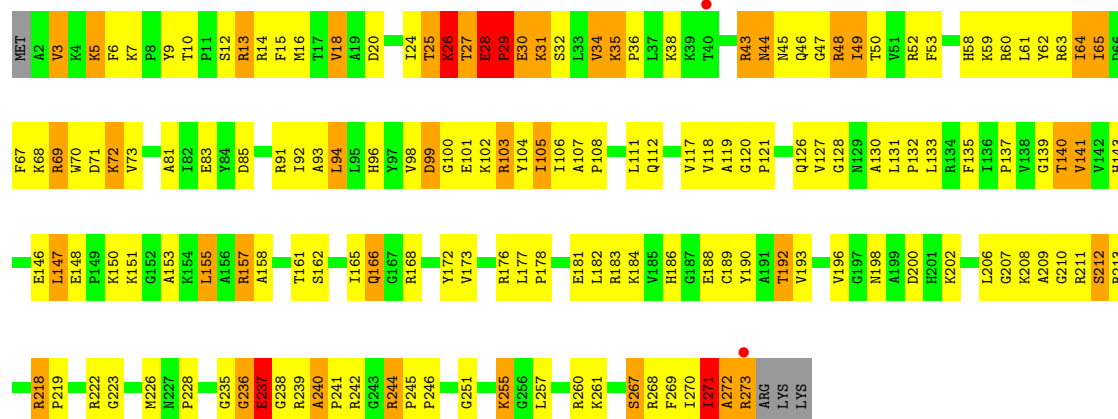
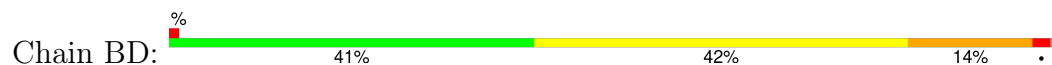


• Molecule 3: 50S ribosomal protein L2

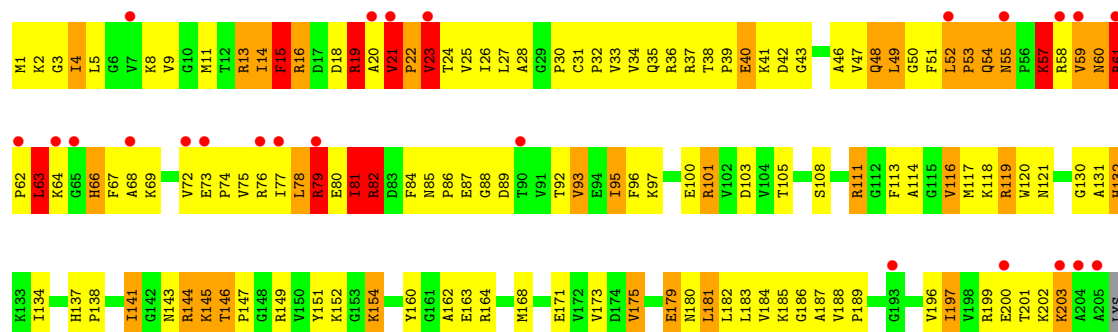




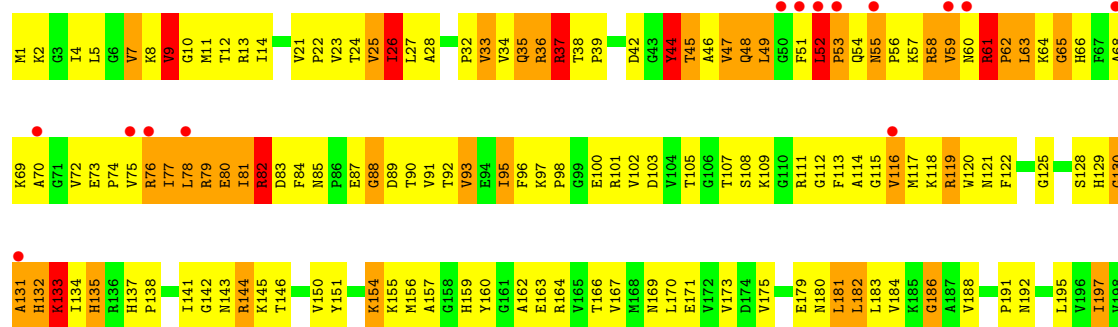
• Molecule 3: 50S ribosomal protein L2

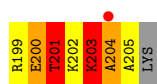


• Molecule 4: 50S ribosomal protein L3

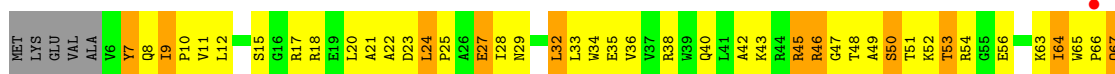


• Molecule 4: 50S ribosomal protein L3

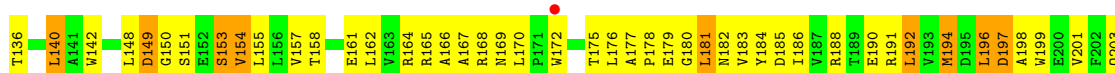




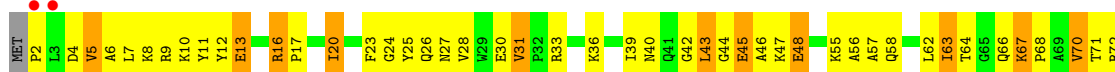
• Molecule 5: 50S ribosomal protein L4



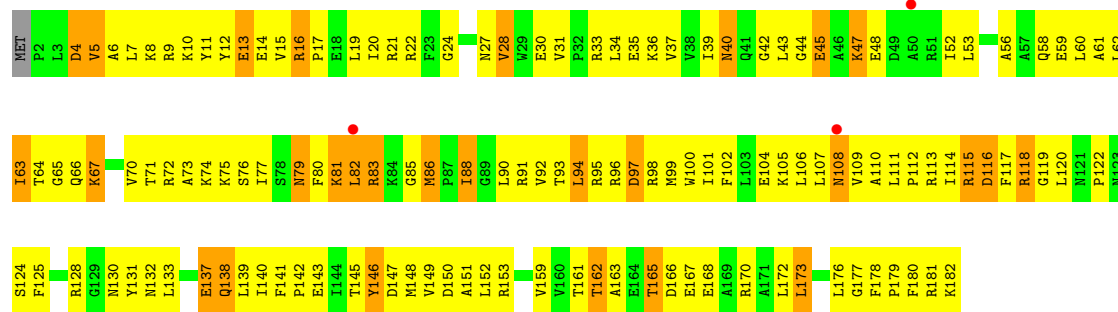
• Molecule 5: 50S ribosomal protein L4



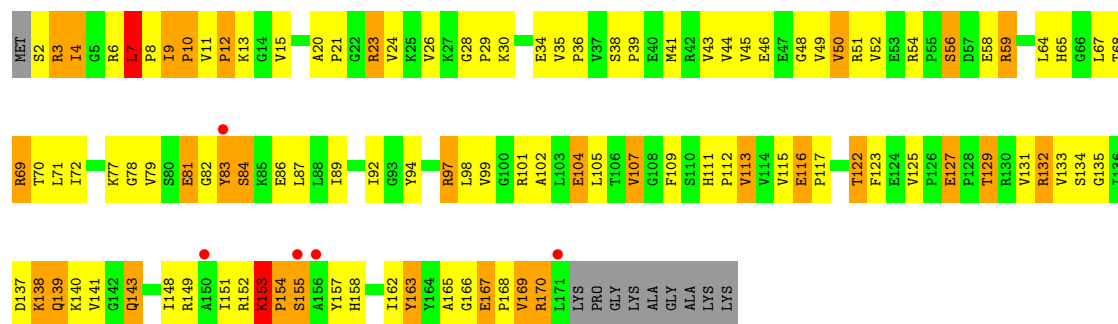
• Molecule 6: 50S ribosomal protein L5



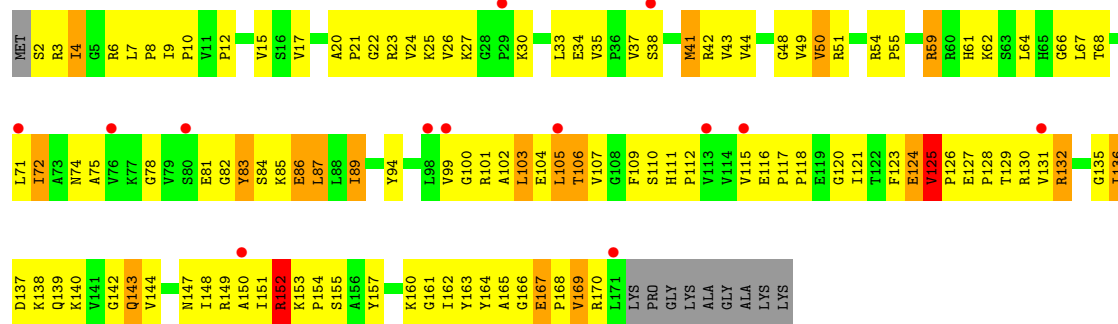
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

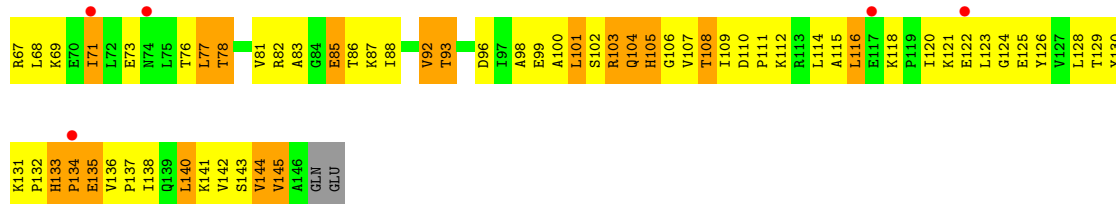


• Molecule 7: 50S ribosomal protein L6

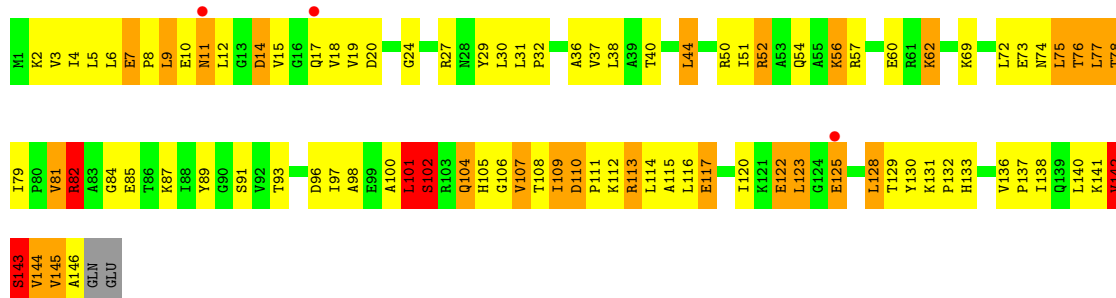


• Molecule 8: 50S ribosomal protein L9

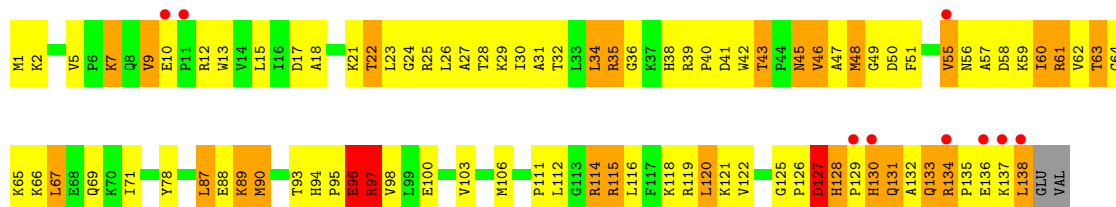




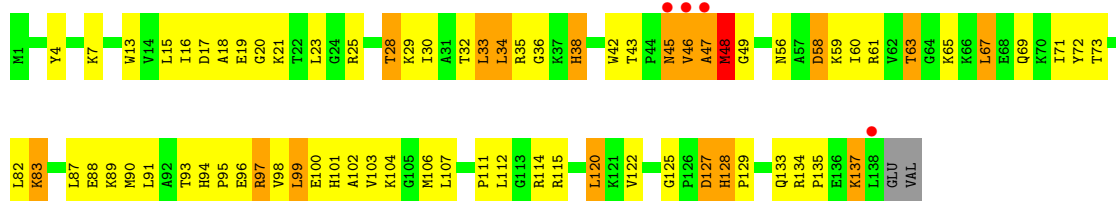
• Molecule 8: 50S ribosomal protein L9



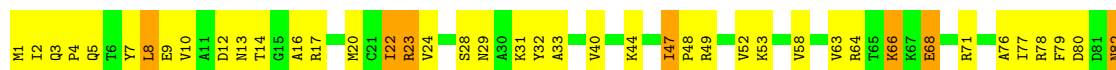
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

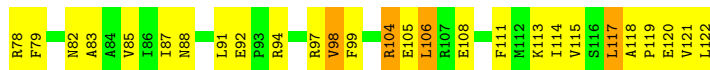
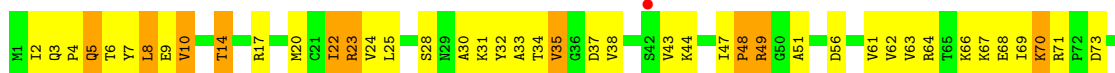
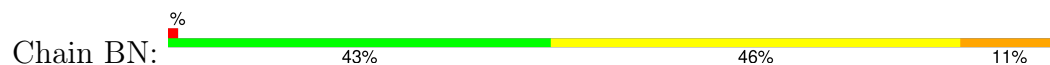


• Molecule 10: 50S ribosomal protein L14

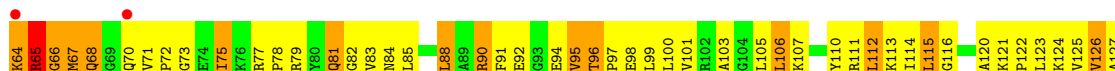
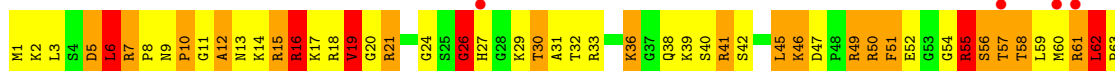




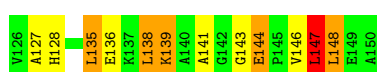
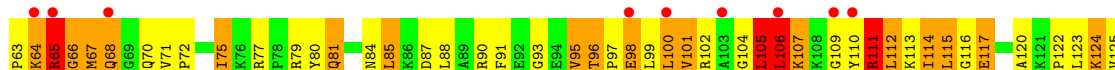
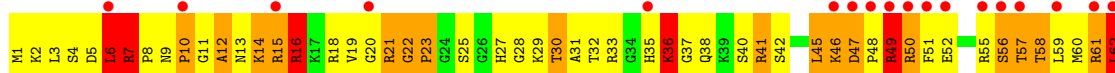
- Molecule 10: 50S ribosomal protein L14



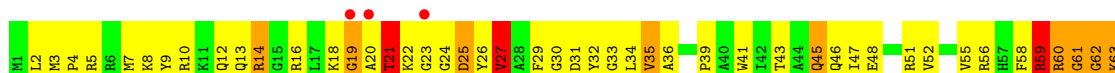
- Molecule 11: 50S ribosomal protein L15

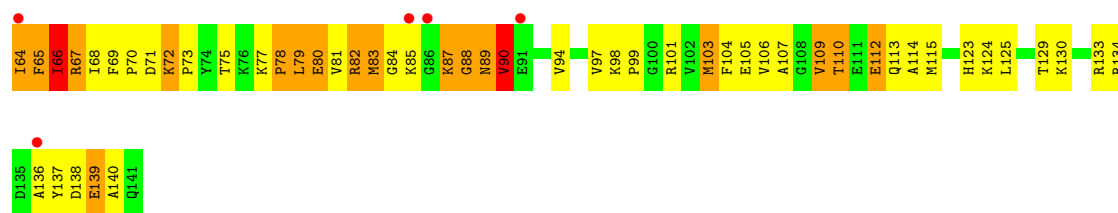


- Molecule 11: 50S ribosomal protein L15

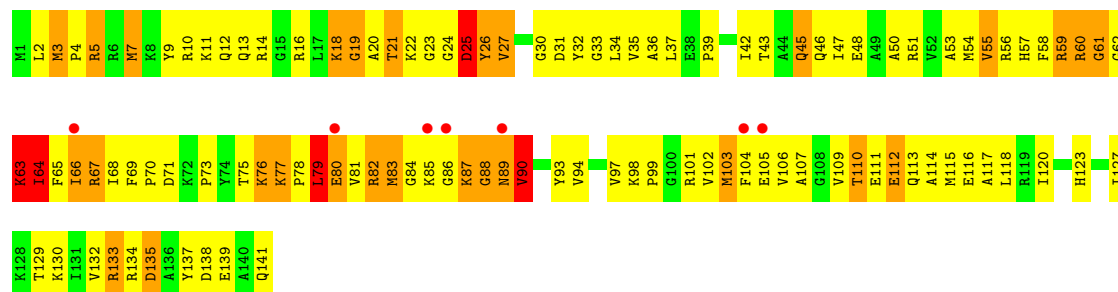


- Molecule 12: 50S ribosomal protein L16



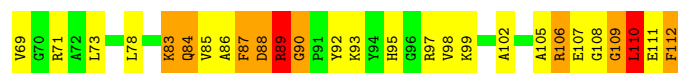
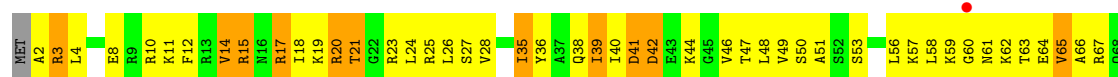


• Molecule 12: 50S ribosomal protein L16

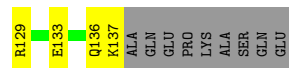
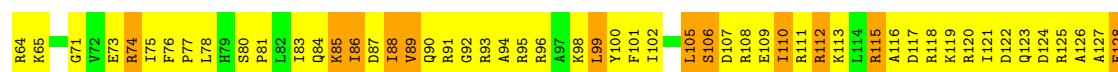
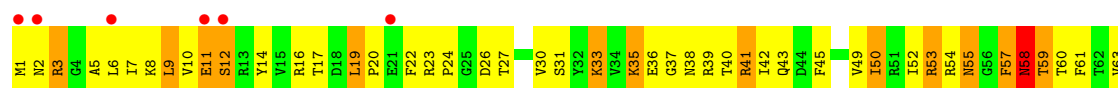




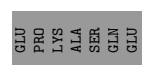
- Molecule 14: 50S ribosomal protein L18



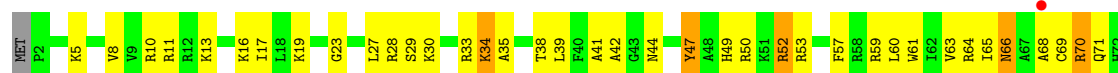
- Molecule 15: 50S ribosomal protein L19

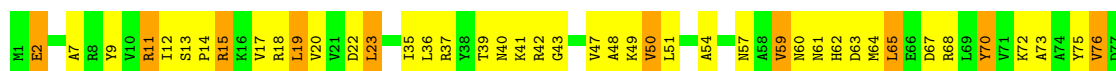


- Molecule 15: 50S ribosomal protein L19

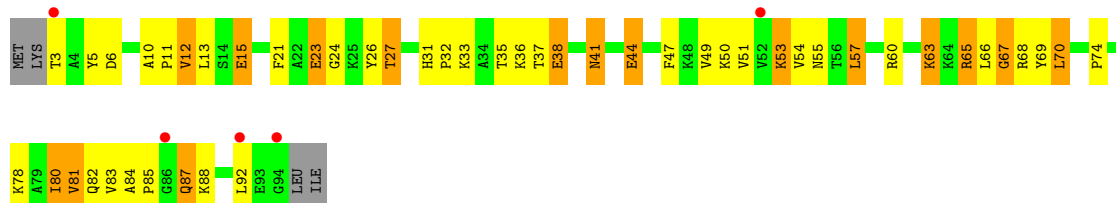


- Molecule 16: 50S ribosomal protein L20

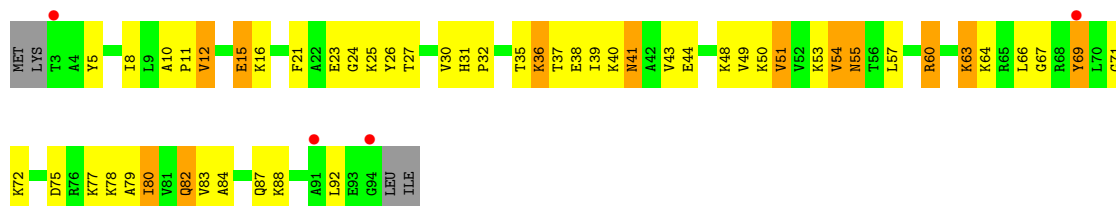
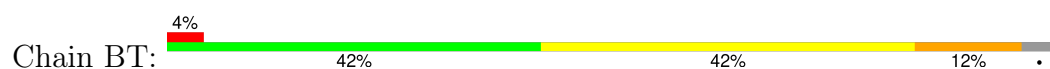




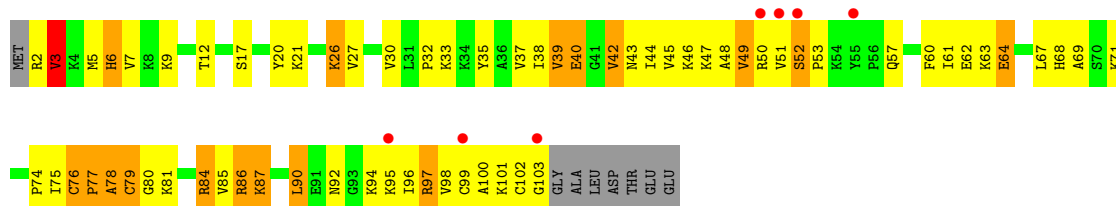
• Molecule 19: 50S ribosomal protein L23



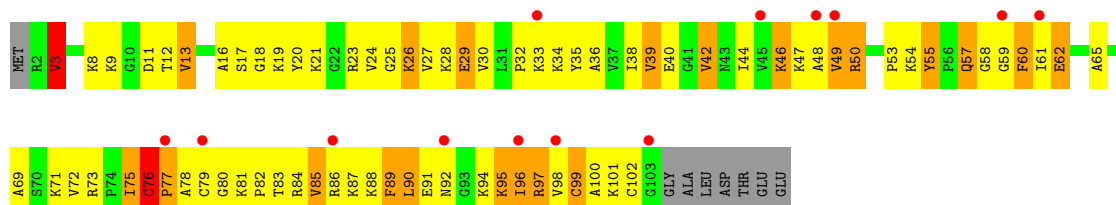
• Molecule 19: 50S ribosomal protein L23



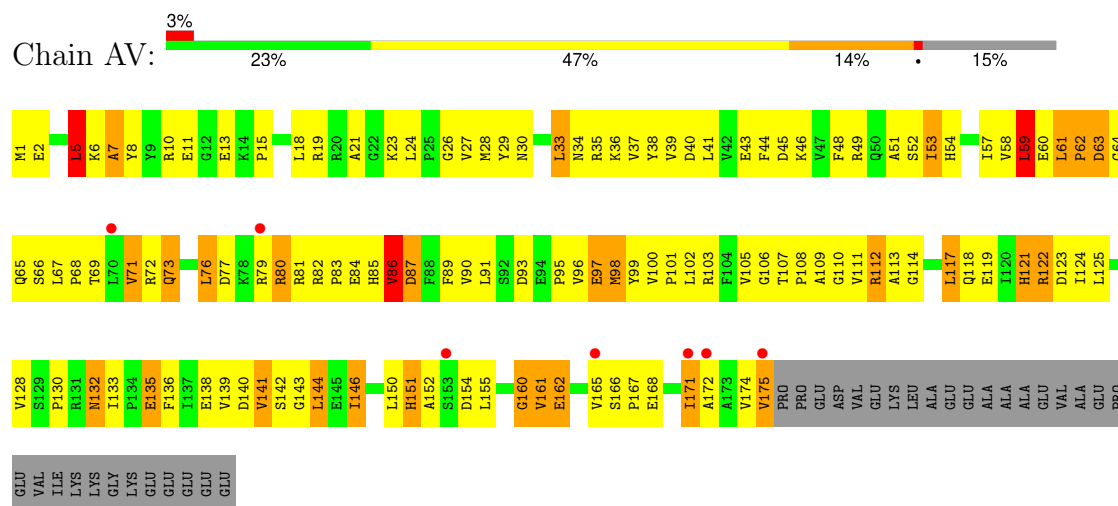
• Molecule 20: 50S ribosomal protein L24



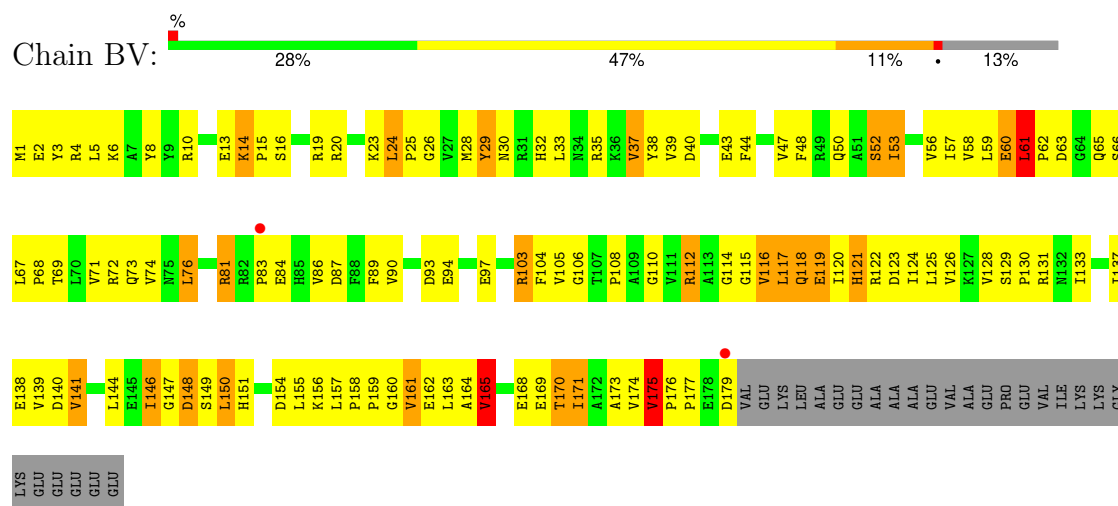
• Molecule 20: 50S ribosomal protein L24



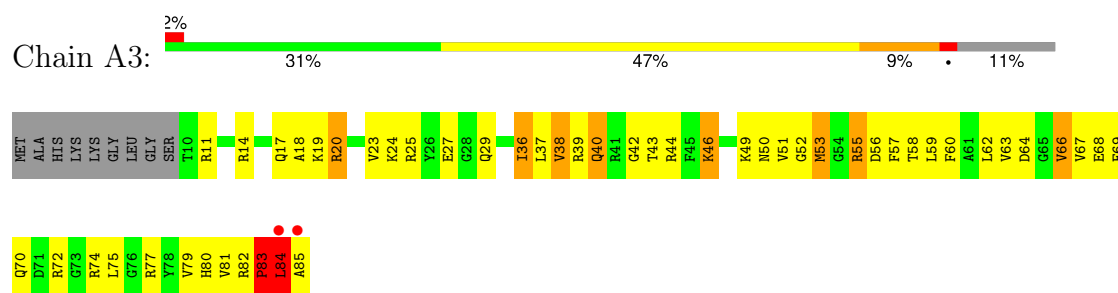
• Molecule 21: 50S ribosomal protein L25



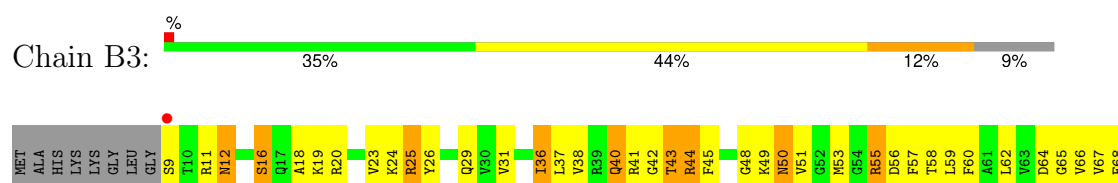
• Molecule 21: 50S ribosomal protein L25

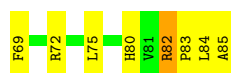


• Molecule 22: 50S ribosomal protein L27

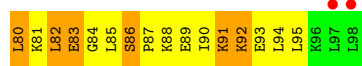
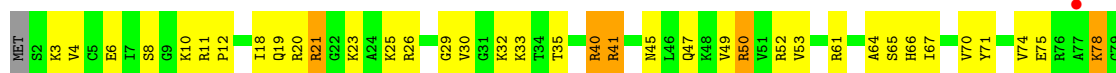


• Molecule 22: 50S ribosomal protein L27

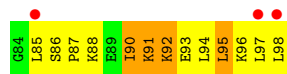
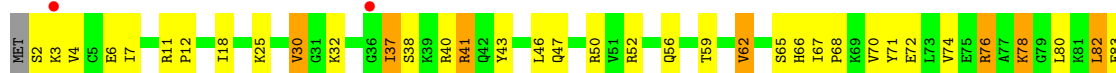




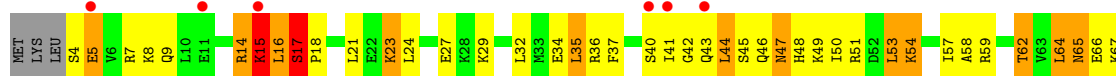
- Molecule 23: 50S ribosomal protein L28



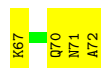
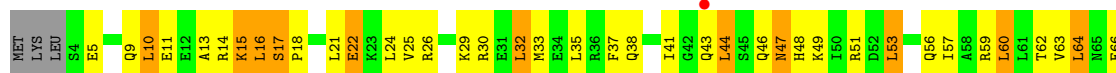
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

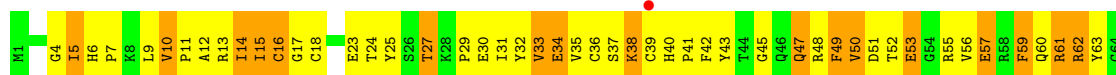
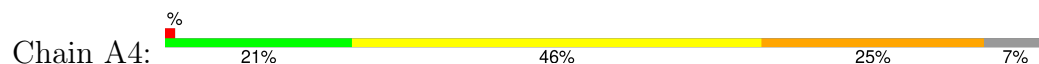




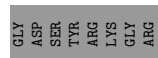
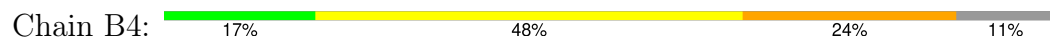
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



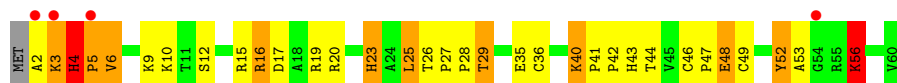
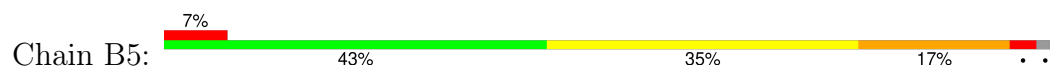
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

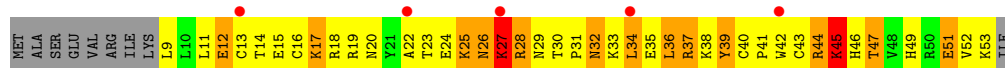


- Molecule 27: 50S ribosomal protein L32

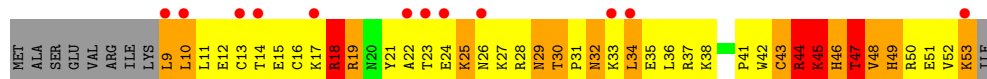


- Molecule 28: 50S ribosomal protein L33





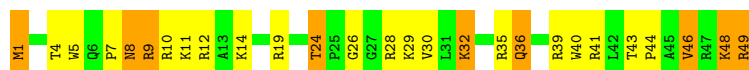
• Molecule 28: 50S ribosomal protein L33



• Molecule 29: 50S ribosomal protein L34



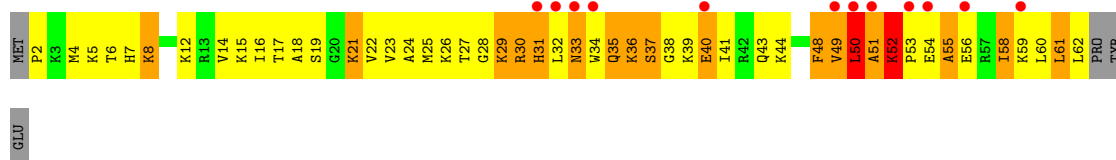
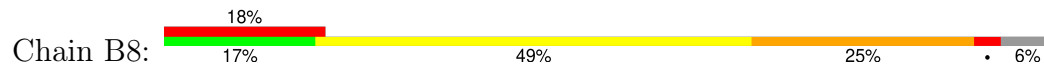
• Molecule 29: 50S ribosomal protein L34



• Molecule 30: 50S ribosomal protein L35



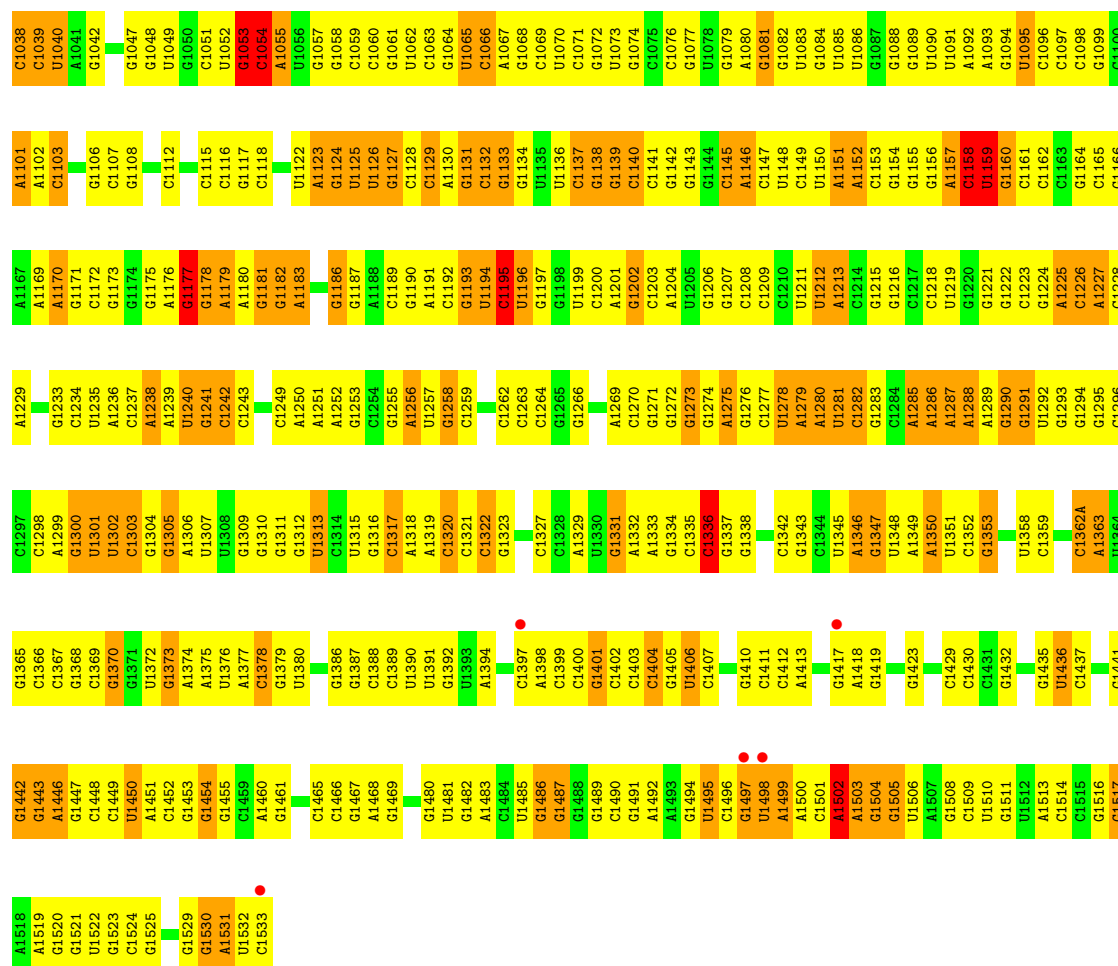
• Molecule 30: 50S ribosomal protein L35



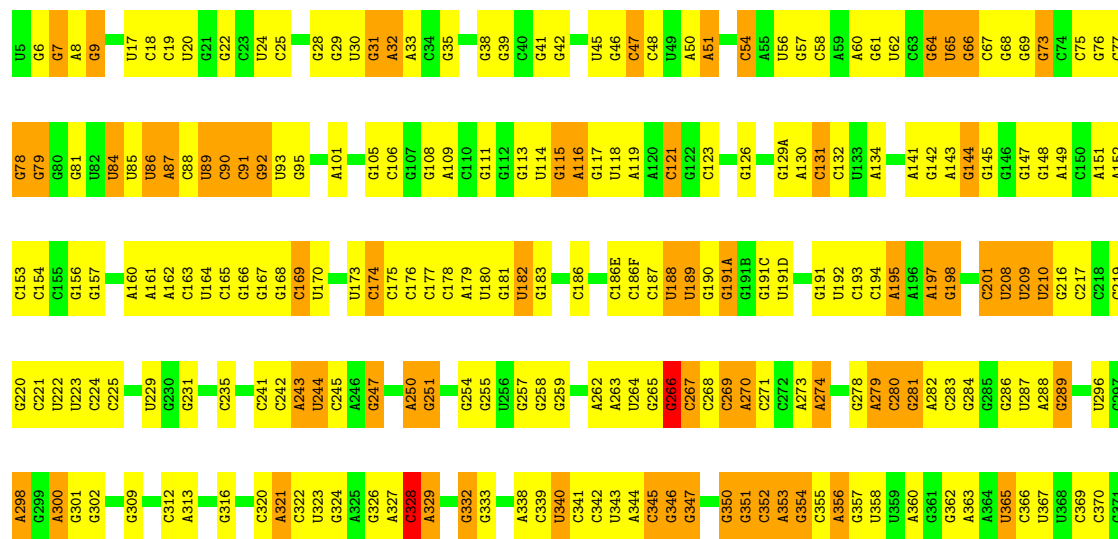
• Molecule 31: 16S ribosomal RNA



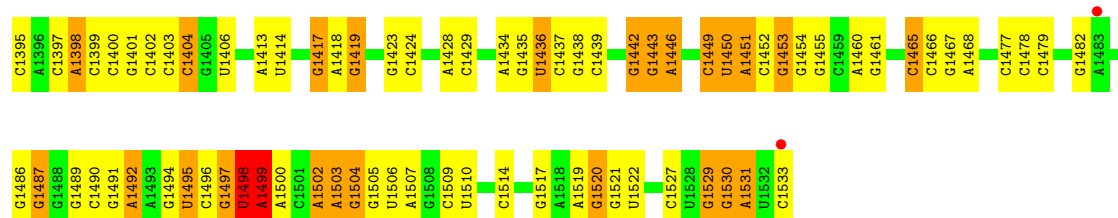
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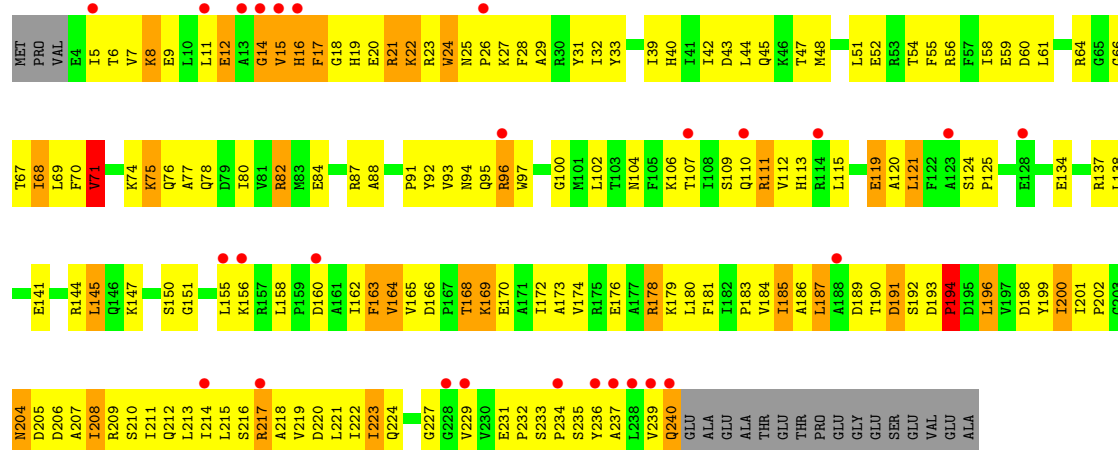


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G1334	G1207	G1142	G1082	G1021	C962	G895	A816	C745	U669		C529	U375	G376
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U1381	G1255	C1192	G1127	C1063	A1005	A946	C879	A802	G735	A583	C436		
C1320	G1256	G1193	C1128	G1064	C1006	G947	C883	G803	C736	G661	U437		
C1321	A1256	U1194	C1129	U1065	C1007	G948	U884	U804	G737	G662	G438		
G1322	C1257	C1195	A1130	U1066	G1008	A949	C885		G738	A663	A439		
C1323	U1257	U1196	G1131	A1067	G1009	U950	U886	C811	C739	C519	A440		
A1324	G1258	G1197	C1132	G1068	G1010	G951	C887		U740	A665	C442		
C1325	C1259	G1198	G1133	C1069	G1011	U952	U888						
G1326	C1260	U1199	G1134	U1070	U1012	G953	C879						
C1327	A1261	C1200	G1135	C1071	G1013	G954							
G1328	C1262	A1201	U1136	G1072	A1014	U955	C883						
U1333	C1263	G1202	U1137	U1073	A1015	U956	U885						
A1394			G1138		A1016	U957							
					G1017	A958							



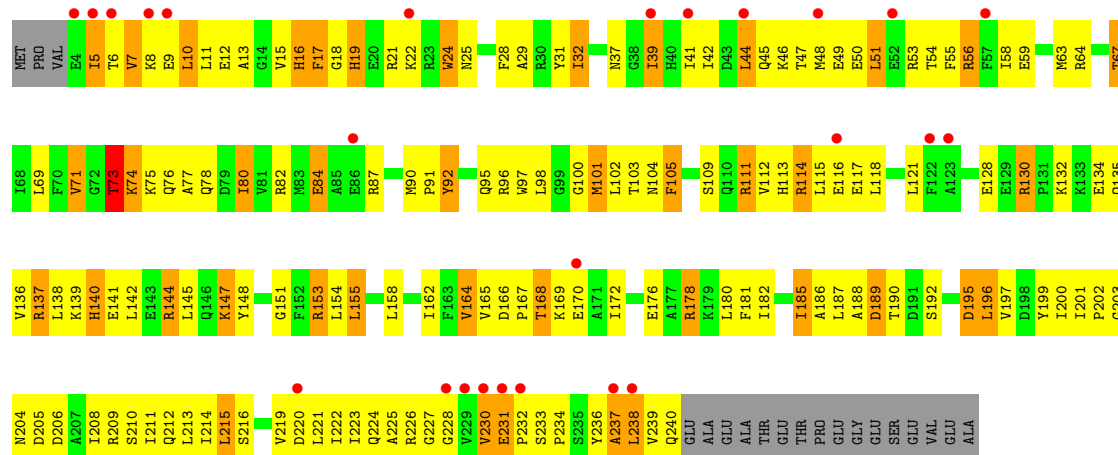
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain CE: 11% 30% 50% 12% 7%



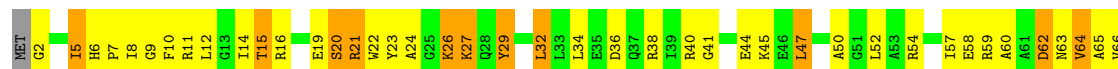
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

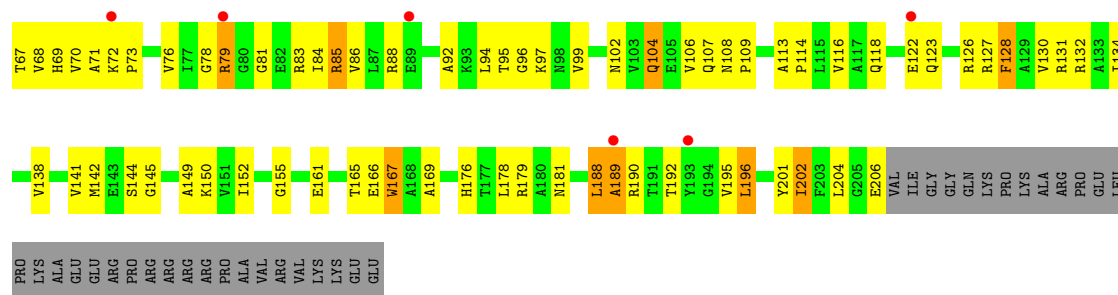
Chain DE: 10% 30% 46% 16% 7%



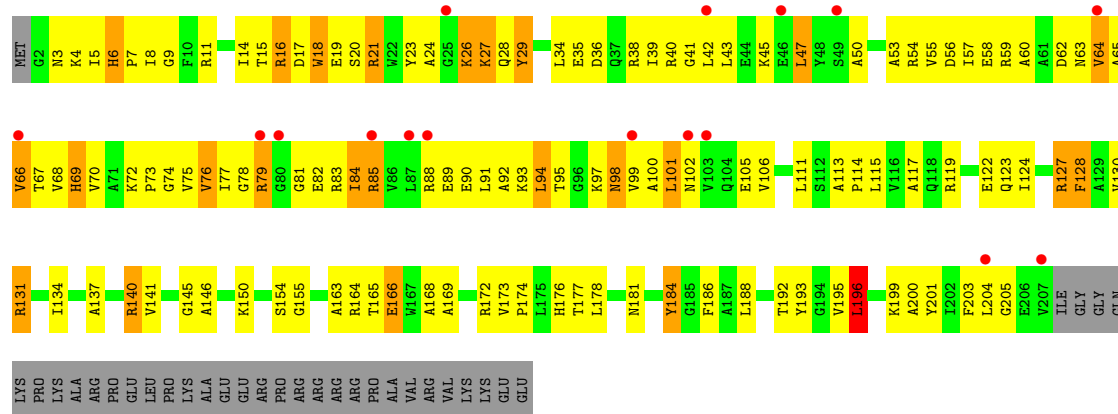
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain CF: 3% 39% 38% 8% 14%

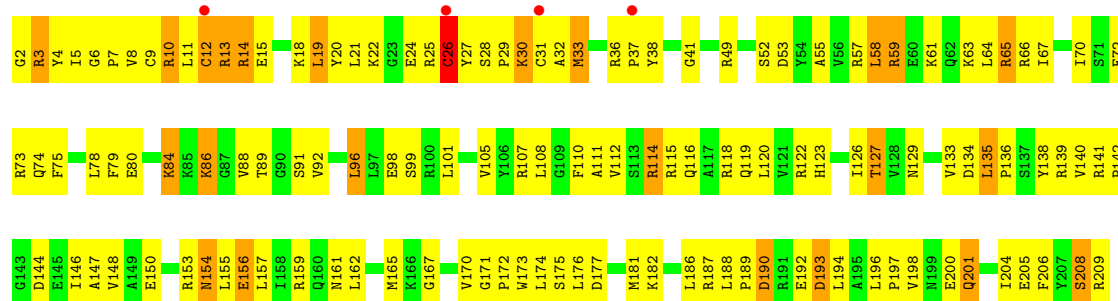




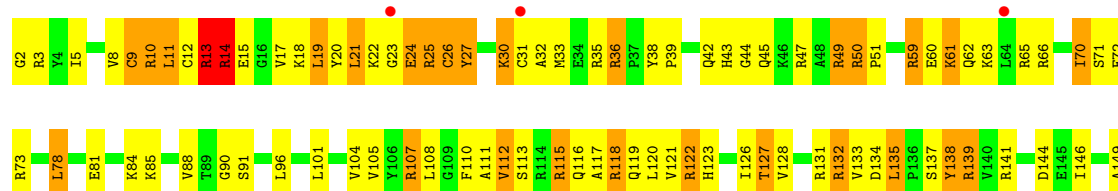
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



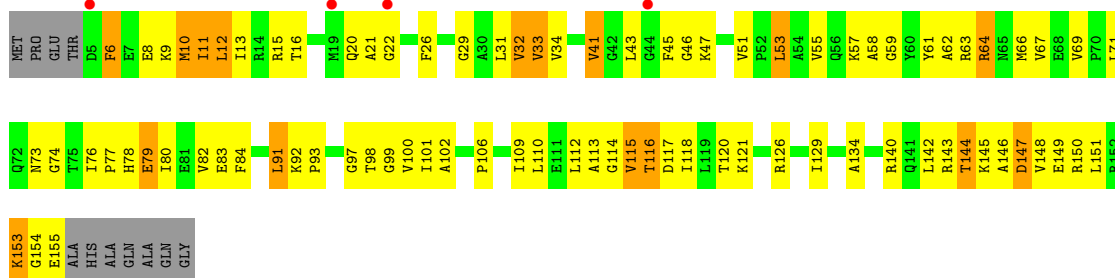
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



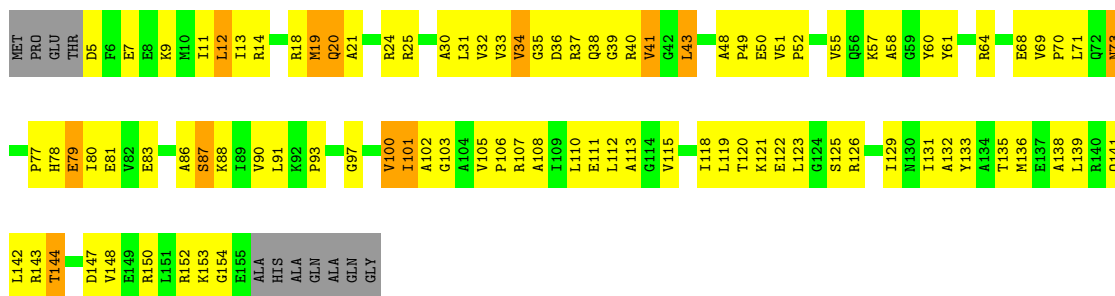
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



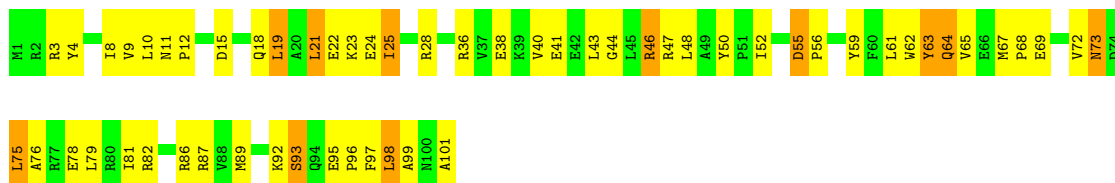
- Molecule 35: 30S RIBOSOMAL PROTEIN S5



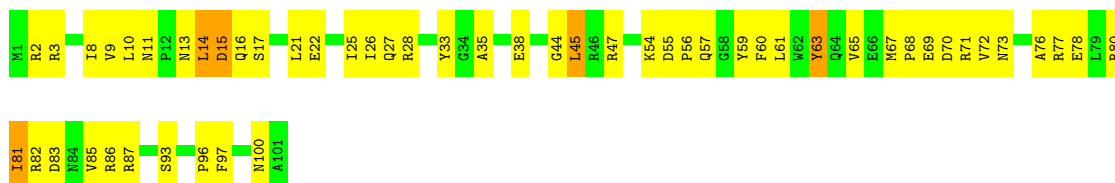
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



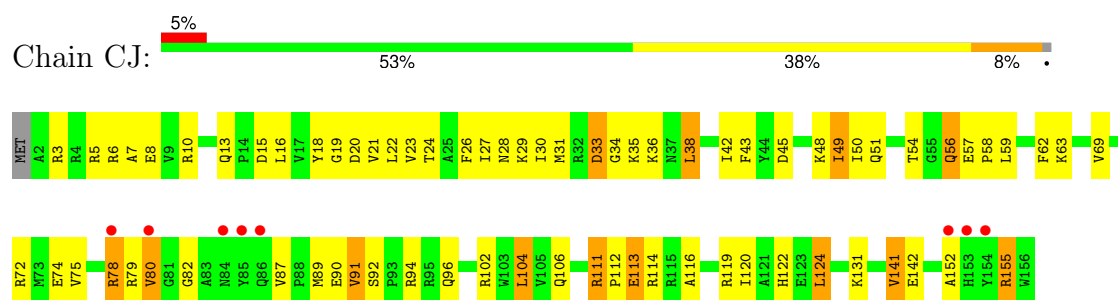
- Molecule 36: 30S RIBOSOMAL PROTEIN S6



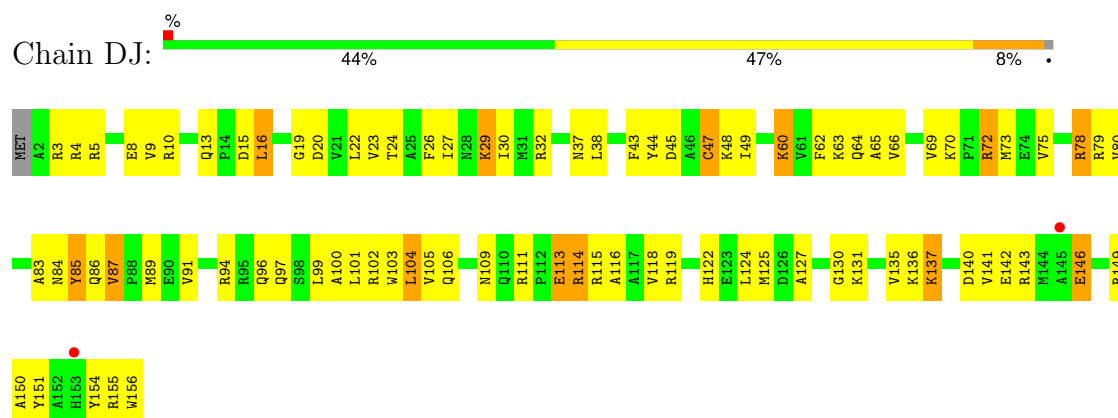
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



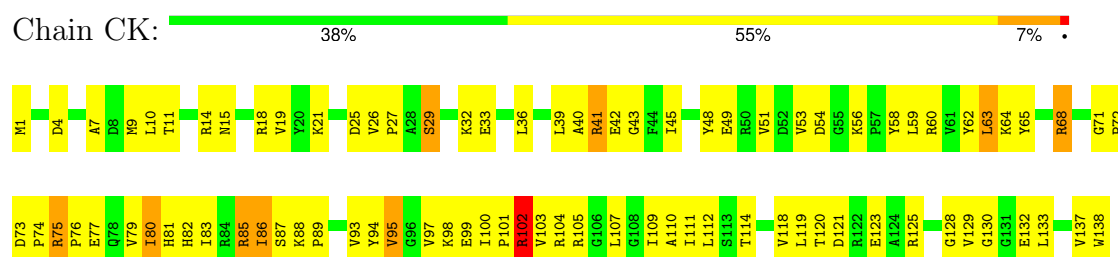
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



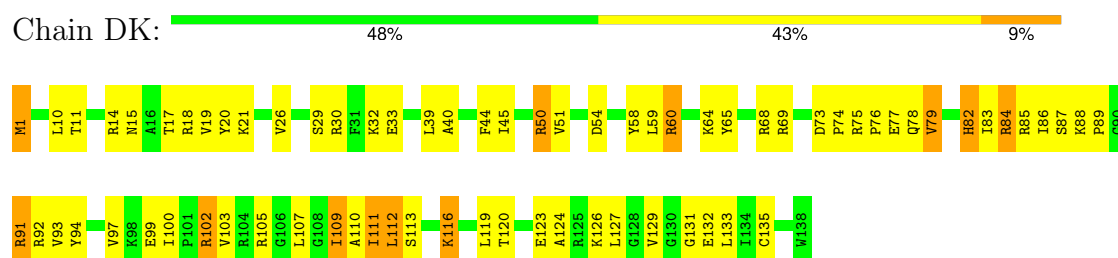
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



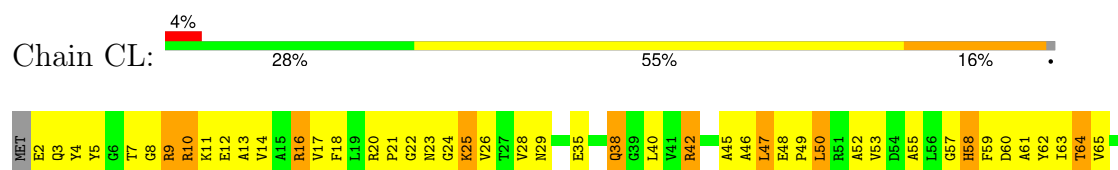
• Molecule 38: 30S RIBOSOMAL PROTEIN S8



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

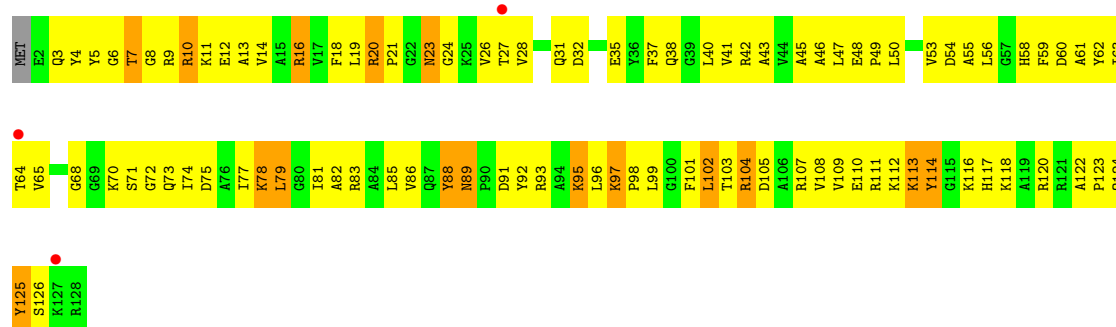


• Molecule 39: 30S RIBOSOMAL PROTEIN S9

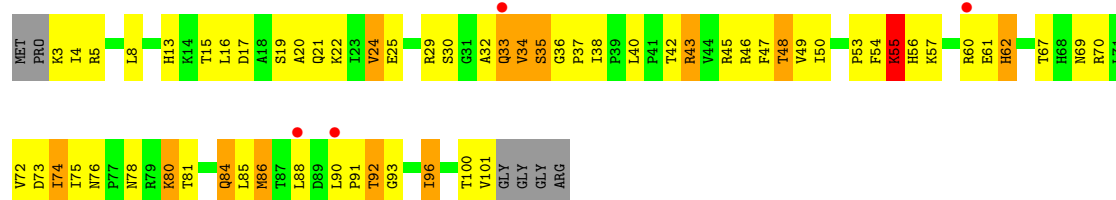




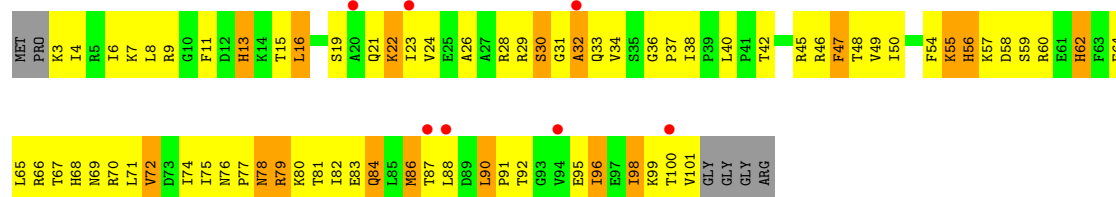
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



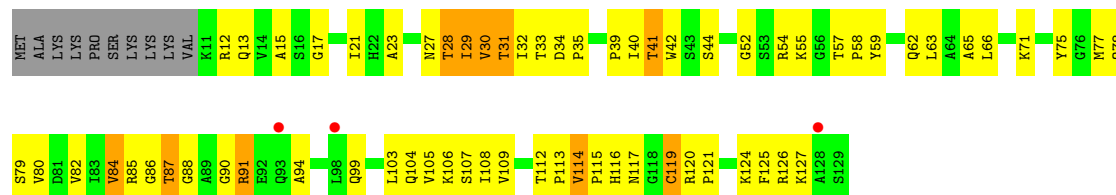
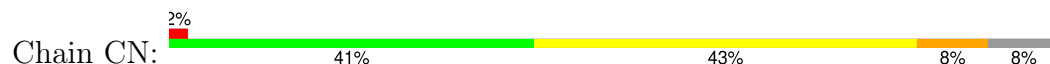
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



• Molecule 40: 30S RIBOSOMAL PROTEIN S10

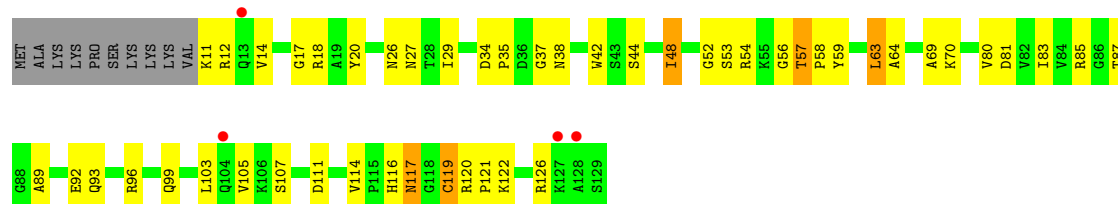


• Molecule 41: 30S RIBOSOMAL PROTEIN S11



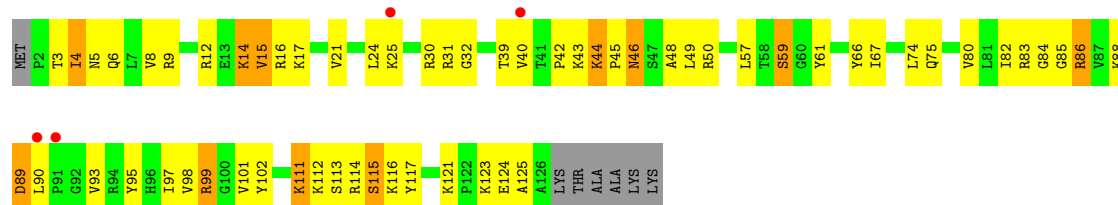
- Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain DN: 



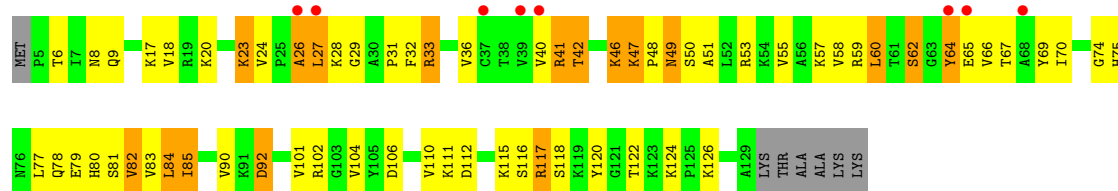
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain CO: 



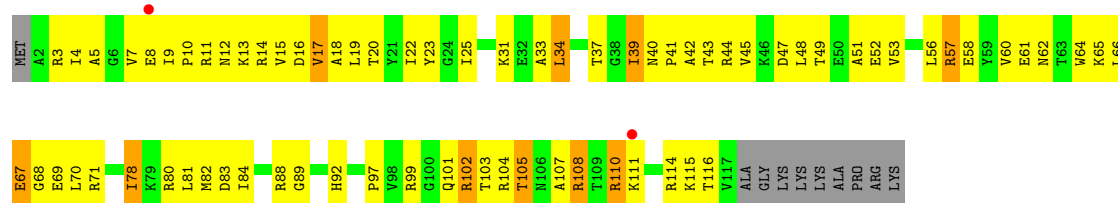
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain DO: 



- Molecule 43: 30S RIBOSOMAL PROTEIN S13

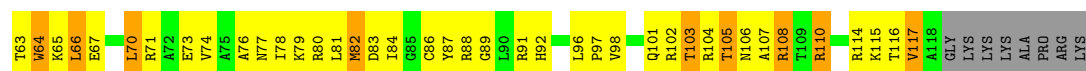
Chain CP: 



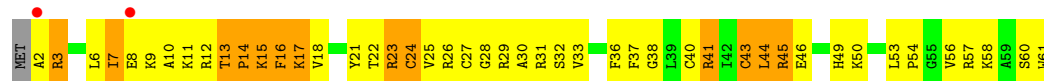
- Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain DP: 

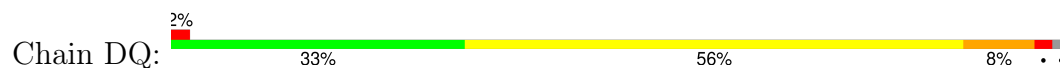




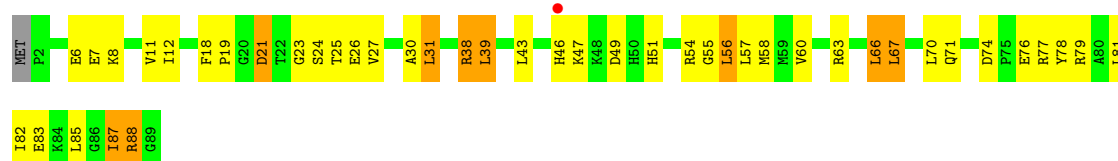
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



• Molecule 44: 30S RIBOSOMAL PROTEIN S14



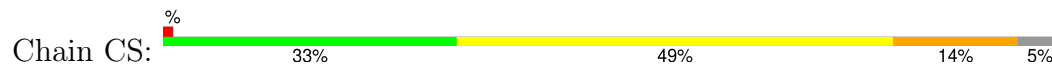
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



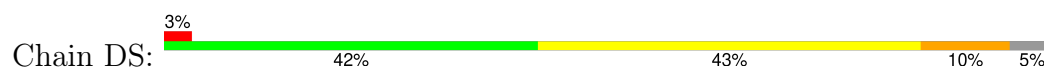
• Molecule 45: 30S RIBOSOMAL PROTEIN S15

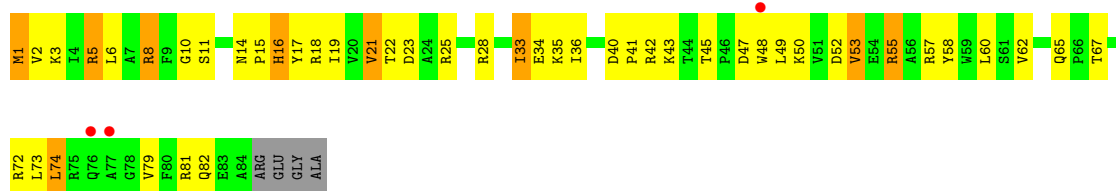


• Molecule 46: 30S RIBOSOMAL PROTEIN S16



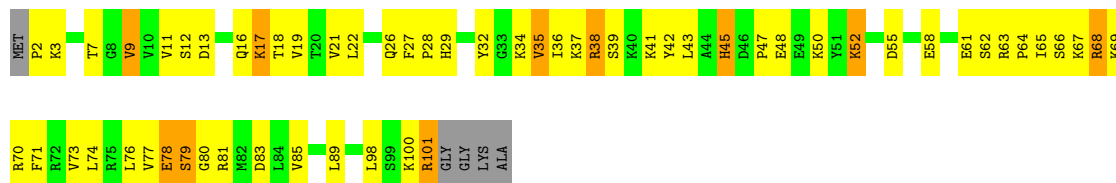
• Molecule 46: 30S RIBOSOMAL PROTEIN S16





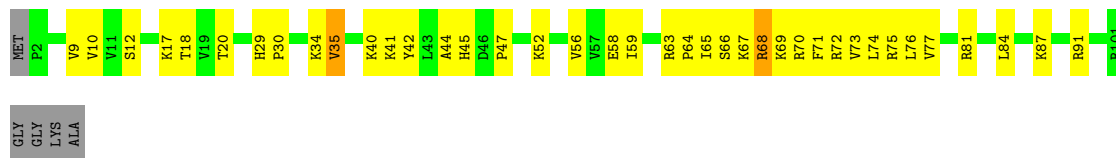
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain CT: 39% 47% 10% 5%



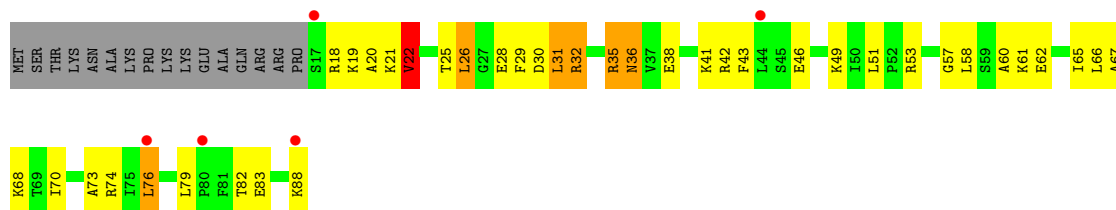
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain DT: 58% 35% 5%



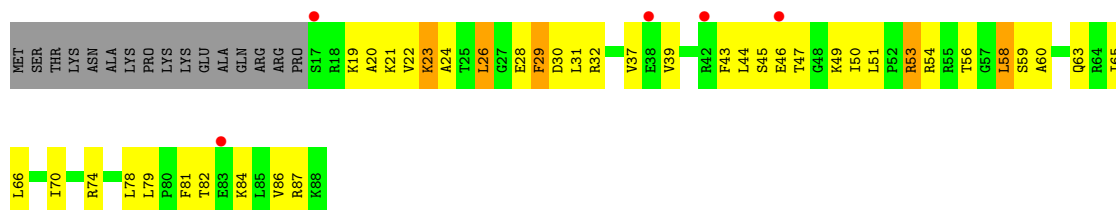
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain CU: 6% 38% 36% 7% 18%

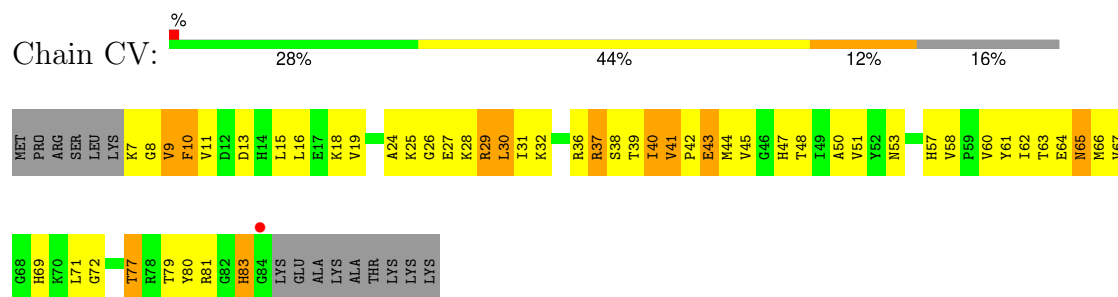


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

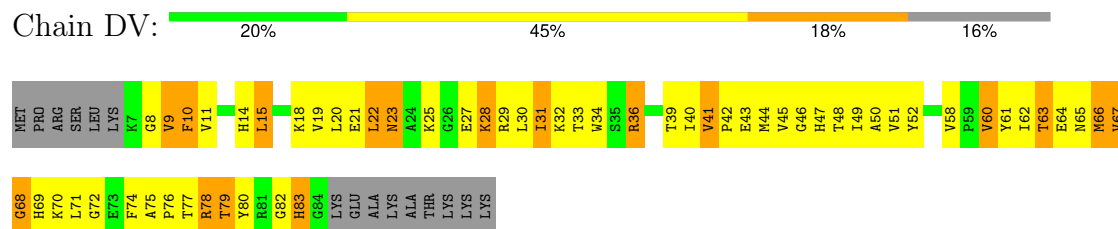
Chain DU: 6% 36% 40% 6% 18%



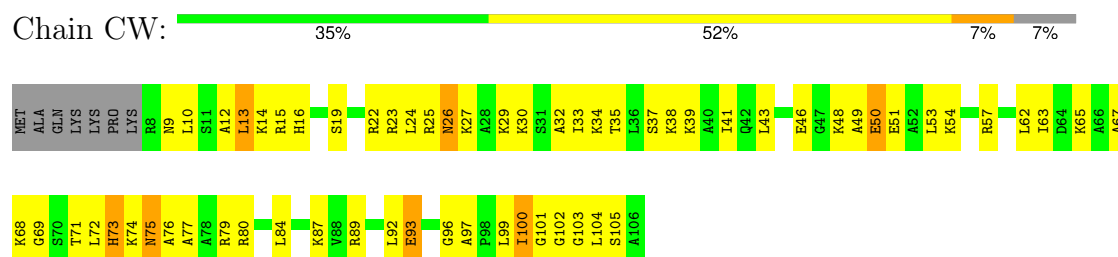
• Molecule 49: 30S RIBOSOMAL PROTEIN S19



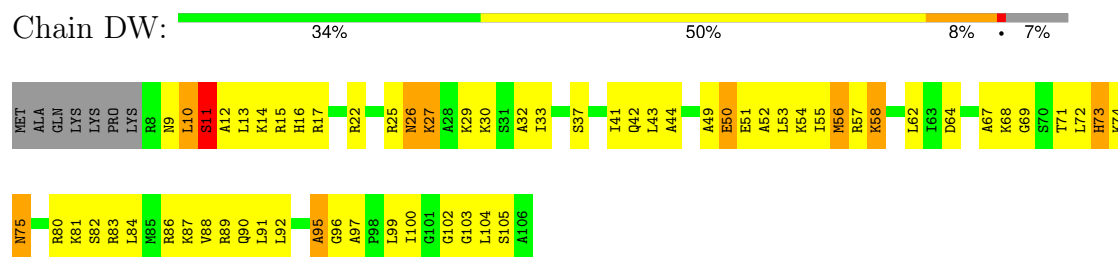
● Molecule 49: 30S RIBOSOMAL PROTEIN S19



● Molecule 50: 30S RIBOSOMAL PROTEIN S20



● Molecule 50: 30S RIBOSOMAL PROTEIN S20



● Molecule 51: 30S RIBOSOMAL PROTEIN THX

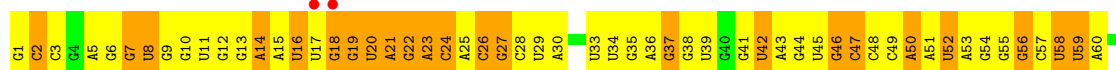
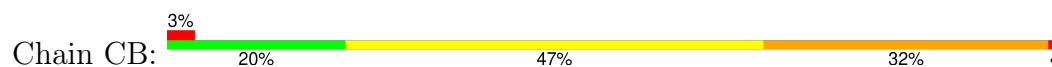


● Molecule 51: 30S RIBOSOMAL PROTEIN THX

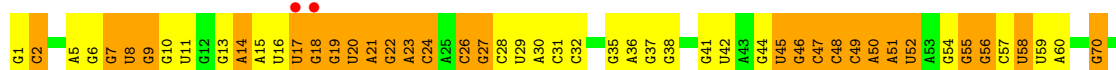




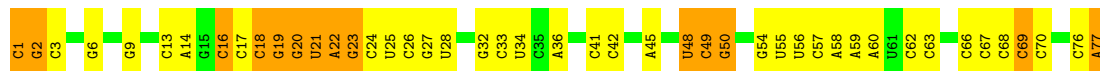
- Molecule 52: TRNA-LEU



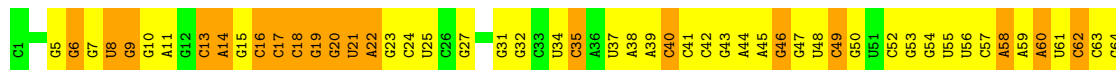
- Molecule 52: TRNA-LEU



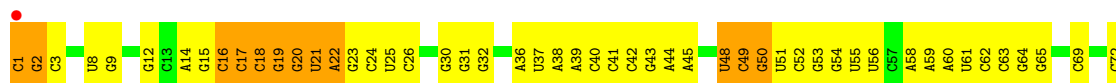
- Molecule 53: TRNA-FMET



- Molecule 53: TRNA-FMET

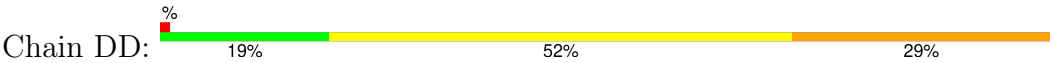


- Molecule 53: TRNA-FMET





● Molecule 53: TRNA-FMET



● Molecule 54: MRNA



● Molecule 54: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 448.15Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.73 – 3.30 189.73 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (189.73-3.30) 95.4 (189.73-3.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.199 , 0.237 0.197 , 0.236	Depositor DCC
R_{free} test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å ²)	102.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.6	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	0.95	EDS
Total number of atoms	299682	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: PAR, MG, ZN

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	0.62	12/70233 (0.0%)	1.11	353/109643 (0.3%)
1	BA	0.56	6/70167 (0.0%)	1.03	240/109541 (0.2%)
2	AB	0.53	0/2928	1.07	13/4568 (0.3%)
2	BB	0.45	0/2928	0.93	6/4568 (0.1%)
3	AD	0.55	0/2165	0.81	3/2919 (0.1%)
3	BD	0.47	0/2165	0.73	1/2919 (0.0%)
4	AE	0.44	0/1601	0.73	1/2160 (0.0%)
4	BE	0.41	0/1601	0.72	1/2160 (0.0%)
5	AF	0.45	0/1620	0.72	0/2194
5	BF	0.38	0/1662	0.67	0/2249
6	AG	0.36	0/1499	0.60	0/2016
6	BG	0.30	0/1499	0.55	0/2016
7	AH	0.41	0/1332	0.71	0/1802
7	BH	0.29	0/1332	0.58	0/1802
8	AK	0.38	0/1151	0.72	1/1558 (0.1%)
8	BK	0.36	0/1151	0.66	1/1558 (0.1%)
9	AM	0.45	0/1131	0.71	0/1525
9	BM	0.32	0/1131	0.58	0/1525
10	AN	0.41	0/943	0.66	0/1269
10	BN	0.40	0/943	0.61	0/1269
11	AO	0.39	0/1162	0.71	1/1544 (0.1%)
11	BO	0.33	0/1162	0.64	1/1544 (0.1%)
12	AP	0.41	0/1143	0.59	0/1527
12	BP	0.33	0/1143	0.52	0/1527
13	A0	0.41	0/982	0.71	1/1312 (0.1%)
13	B0	0.40	0/974	0.67	0/1302
14	AQ	0.40	0/892	0.69	1/1187 (0.1%)
14	BQ	0.34	0/892	0.62	1/1187 (0.1%)
15	AR	0.45	0/1155	0.70	0/1542
15	BR	0.41	0/1155	0.63	0/1542
16	A1	0.46	0/982	0.67	0/1306
16	B1	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.44	0/790	0.71	0/1057
17	B2	0.33	0/790	0.59	0/1057
18	AS	0.43	0/911	0.69	0/1220
18	BS	0.42	0/911	0.65	0/1220
19	AT	0.52	0/739	0.69	0/993
19	BT	0.48	0/739	0.66	0/993
20	AU	0.48	0/798	0.72	0/1064
20	BU	0.43	0/798	0.72	0/1064
21	AV	0.35	0/1427	0.67	2/1935 (0.1%)
21	BV	0.28	0/1460	0.56	0/1982
22	A3	0.46	0/615	0.69	0/819
22	B3	0.40	0/621	0.64	0/827
23	AZ	0.46	0/770	0.78	0/1022
23	BZ	0.43	0/770	0.75	0/1022
24	AW	0.51	0/560	0.75	0/741
24	BW	0.40	0/583	0.62	0/771
25	AX	0.35	0/474	0.61	0/635
25	BX	0.33	0/474	0.54	0/635
26	A4	0.39	0/545	0.73	1/733 (0.1%)
26	B4	0.34	0/527	0.65	0/709
27	A5	0.45	0/473	0.67	0/639
27	B5	0.40	0/473	0.73	0/639
28	A6	0.47	0/396	0.68	0/529
28	B6	0.36	0/396	0.60	0/529
29	A7	0.50	0/438	0.71	0/575
29	B7	0.40	0/438	0.62	0/575
30	A8	0.56	0/494	0.87	0/649
30	B8	0.40	0/494	0.58	0/649
31	CA	0.49	1/36234 (0.0%)	0.94	68/56554 (0.1%)
31	DA	0.46	0/36237	0.90	64/56558 (0.1%)
32	CE	0.31	0/1959	0.55	0/2642
32	DE	0.30	0/1959	0.54	0/2642
33	CF	0.34	0/1629	0.54	0/2195
33	DF	0.32	0/1636	0.57	1/2205 (0.0%)
34	CG	0.42	1/1733 (0.1%)	0.62	0/2318
34	DG	0.38	0/1733	0.63	0/2318
35	CH	0.38	0/1171	0.58	0/1576
35	DH	0.34	0/1171	0.58	0/1576
36	CI	0.38	0/856	0.58	0/1154
36	DI	0.36	0/856	0.55	0/1154
37	CJ	0.31	0/1276	0.48	0/1709
37	DJ	0.32	0/1276	0.48	0/1709
38	CK	0.36	0/1136	0.64	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.31	0/1136	0.54	0/1527
39	CL	0.30	0/1029	0.52	0/1379
39	DL	0.29	0/1029	0.53	0/1379
40	CM	0.32	0/814	0.61	1/1095 (0.1%)
40	DM	0.31	0/814	0.59	0/1095
41	CN	0.37	0/900	0.61	0/1213
41	DN	0.36	0/900	0.59	0/1213
42	CO	0.45	0/991	0.75	1/1327 (0.1%)
42	DO	0.41	0/991	0.65	0/1327
43	CP	0.33	0/938	0.59	0/1258
43	DP	0.29	0/943	0.53	0/1265
44	CQ	0.42	1/501 (0.2%)	0.68	1/664 (0.2%)
44	DQ	0.32	0/501	0.57	0/664
45	CR	0.38	0/745	0.64	0/992
45	DR	0.35	0/745	0.53	0/992
46	CS	0.31	0/721	0.55	0/970
46	DS	0.38	0/721	0.60	0/970
47	CT	0.36	0/847	0.56	0/1131
47	DT	0.34	0/847	0.55	0/1131
48	CU	0.35	0/596	0.62	0/790
48	DU	0.36	0/596	0.57	0/790
49	CV	0.34	0/638	0.57	0/860
49	DV	0.29	0/638	0.63	0/860
50	CW	0.32	0/765	0.55	0/1007
50	DW	0.35	0/765	0.63	0/1007
51	CX	0.29	0/221	0.49	0/288
51	DX	0.27	0/221	0.48	0/288
52	CB	0.44	0/2080	0.80	1/3242 (0.0%)
52	DB	0.46	0/2080	0.80	3/3242 (0.1%)
53	CC	0.46	0/1835	0.85	0/2859
53	CD	0.28	0/1835	0.66	2/2859 (0.1%)
53	DC	0.44	0/1835	0.83	0/2859
53	DD	0.27	0/1835	0.63	1/2859 (0.0%)
54	C1	0.69	0/226	0.84	0/348
54	D1	0.58	0/226	0.81	0/348
All	All	0.51	21/324077 (0.0%)	0.93	771/485305 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	6
3	BD	0	3
4	AE	0	1
4	BE	0	6
5	BF	0	2
6	AG	0	1
6	BG	0	1
7	AH	0	2
7	BH	0	4
8	AK	0	5
8	BK	0	5
9	AM	0	1
11	AO	0	3
11	BO	0	3
13	B0	0	1
14	AQ	0	2
14	BQ	0	3
15	AR	0	2
16	A1	0	2
17	A2	0	1
20	BU	0	2
21	AV	0	3
21	BV	0	3
22	A3	0	2
24	AW	0	2
24	BW	0	1
26	A4	0	3
26	B4	0	1
27	A5	0	3
27	B5	0	1
28	A6	0	1
28	B6	0	1
30	A8	0	2
32	CE	0	3
32	DE	0	4
33	CF	0	1
33	DF	0	1
34	DG	0	1
38	CK	0	1
40	CM	0	1
40	DM	0	1
42	CO	0	2
44	CQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	DQ	0	1
45	CR	0	1
50	DW	0	1
All	All	0	98

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1143	A	N7-C5	-9.76	1.33	1.39
1	BA	1342	A	N7-C5	-8.93	1.33	1.39
1	BA	2873	A	N7-C5	-8.51	1.34	1.39
1	BA	2287	A	N9-C4	-8.15	1.32	1.37
1	AA	1021	A	N9-C4	-8.08	1.32	1.37

The worst 5 of 771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	1025	U	C5-C4-O4	-13.19	117.99	125.90
1	BA	933	A	C6-C5-N7	-12.57	123.50	132.30
1	AA	1899	G	N3-C4-N9	-12.39	118.57	126.00
1	BA	1899	G	N3-C4-N9	-12.35	118.59	126.00
1	BA	2720	U	C2-N3-C4	-11.91	119.85	127.00

There are no chirality outliers.

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	122	ASP	Peptide
3	AD	236	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	28	GLU	Peptide
3	AD	47	GLY	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	62707	0	31613	2746	0
1	BA	62647	0	31583	2774	1
2	AB	2617	0	1328	105	0
2	BB	2617	0	1328	133	0
3	AD	2115	0	2195	263	0
3	BD	2115	0	2195	244	0
4	AE	1568	0	1634	288	0
4	BE	1568	0	1634	286	0
5	AF	1585	0	1632	143	0
5	BF	1627	0	1680	208	0
6	AG	1474	0	1535	200	0
6	BG	1474	0	1535	164	0
7	AH	1307	0	1382	158	0
7	BH	1307	0	1382	148	2
8	AK	1136	0	1223	128	0
8	BK	1136	0	1223	102	0
9	AM	1104	0	1180	139	0
9	BM	1104	0	1180	102	0
10	AN	933	0	996	53	0
10	BN	933	0	996	68	0
11	AO	1145	0	1228	245	0
11	BO	1145	0	1228	306	0
12	AP	1122	0	1179	208	0
12	BP	1122	0	1179	250	0
13	A0	968	0	1033	81	0
13	B0	960	0	1021	82	0
14	AQ	882	0	943	101	0
14	BQ	882	0	943	104	0
15	AR	1141	0	1202	128	0
15	BR	1141	0	1202	132	0
16	A1	964	0	1022	109	0
16	B1	964	0	1022	108	0
17	A2	779	0	852	98	1
17	B2	779	0	852	182	0
18	AS	900	0	964	86	0
18	BS	900	0	964	56	0
19	AT	725	0	778	60	0
19	BT	725	0	778	60	0
20	AU	785	0	878	95	0
20	BU	785	0	878	113	0
21	AV	1397	0	1430	140	0
21	BV	1428	0	1454	142	0
22	A3	607	0	628	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B3	613	0	633	59	0
23	AZ	763	0	848	61	0
23	BZ	763	0	848	59	0
24	AW	558	0	610	47	0
24	BW	581	0	629	63	0
25	AX	469	0	518	36	0
25	BX	469	0	518	33	0
26	A4	533	0	522	78	0
26	B4	515	0	510	109	0
27	A5	459	0	480	78	1
27	B5	459	0	480	72	0
28	A6	389	0	404	90	0
28	B6	389	0	404	110	0
29	A7	430	0	480	28	0
29	B7	430	0	480	32	0
30	A8	488	0	560	105	0
30	B8	488	0	560	153	0
31	CA	32369	0	16339	1550	2
31	DA	32372	0	16338	1515	1
32	CE	1924	0	1975	186	0
32	DE	1924	0	1975	206	0
33	CF	1605	0	1668	123	0
33	DF	1612	0	1677	160	0
34	CG	1703	0	1764	180	0
34	DG	1703	0	1763	158	1
35	CH	1155	0	1213	81	0
35	DH	1155	0	1213	91	0
36	CI	843	0	857	59	1
36	DI	843	0	857	48	0
37	CJ	1257	0	1296	72	0
37	DJ	1257	0	1296	90	0
38	CK	1116	0	1177	100	0
38	DK	1116	0	1177	62	0
39	CL	1010	0	1037	111	0
39	DL	1010	0	1037	130	0
40	CM	801	0	849	86	0
40	DM	801	0	849	95	0
41	CN	885	0	904	76	0
41	DN	885	0	904	45	0
42	CO	975	0	1062	63	0
42	DO	975	0	1062	89	0
43	CP	928	0	987	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DP	933	0	992	108	0
44	CQ	492	0	529	55	0
44	DQ	492	0	529	56	0
45	CR	734	0	771	55	0
45	DR	734	0	771	44	0
46	CS	705	0	725	63	0
46	DS	705	0	725	45	0
47	CT	834	0	904	79	0
47	DT	834	0	904	44	0
48	CU	591	0	662	31	0
48	DU	591	0	662	43	0
49	CV	624	0	636	74	0
49	DV	624	0	636	100	0
50	CW	763	0	861	76	0
50	DW	763	0	861	71	0
51	CX	217	0	234	20	0
51	DX	217	0	234	28	0
52	CB	1861	0	938	84	0
52	DB	1861	0	938	82	0
53	CC	1643	0	837	69	0
53	CD	1643	0	837	98	0
53	DC	1643	0	837	78	0
53	DD	1643	0	837	111	0
54	C1	205	0	103	9	0
54	D1	205	0	103	9	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	2	0	0	0	0
55	AA	626	0	0	0	0
55	AB	17	0	0	0	0
55	AD	1	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	AZ	1	0	0	0	0
55	B1	1	0	0	0	0
55	B3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B5	1	0	0	0	0
55	BA	528	0	0	0	0
55	BB	15	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BP	1	0	0	0	0
55	BR	2	0	0	0	0
55	C1	1	0	0	0	0
55	CA	240	0	0	0	0
55	CB	5	0	0	0	0
55	CC	7	0	0	0	0
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CN	2	0	0	0	0
55	CQ	2	0	0	0	0
55	CT	1	0	0	0	0
55	DA	204	0	0	0	0
55	DB	2	0	0	0	0
55	DC	8	0	0	0	0
55	DG	2	0	0	0	0
55	DH	1	0	0	0	0
55	DS	1	0	0	0	0
56	CA	42	0	45	4	0
56	DA	42	0	45	5	0
57	CG	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	299682	0	201028	17558	5

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 35.

The worst 5 of 17558 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)
11:BO:62:LEU:CD1	30:B8:30:ARG:HH11	1.03	1.63
11:BO:71:VAL:CG1	11:BO:72:PRO:HD3	1.32	1.59
4:AE:23:VAL:HG12	4:AE:185:LYS:CA	1.33	1.59
1:BA:2015:A:C1'	27:B5:2:ALA:HA	1.42	1.48
4:BE:51:PHE:CG	4:BE:52:LEU:HB3	1.45	1.47

All (5) 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)
1:BA:276:A:OP2	31:DA:86:U:O2'[3_555]	1.96	0.24
7:BH:100:GLY:O	31:CA:85:U:O2'[3_545]	2.02	0.18
36:CI:15:ASP:OD2	34:DG:27:TYR:OH[4_555]	2.06	0.14
7:BH:132:ARG:O	31:CA:84:U:N3[3_545]	2.18	0.02
17:A2:51:VAL:N	27:A5:60:VAL:O[4_465]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/276 (98%)	244 (90%)	20 (7%)	6 (2%)	5	26
3	BD	270/276 (98%)	246 (91%)	15 (6%)	9 (3%)	3	19
4	AE	203/206 (98%)	149 (73%)	37 (18%)	17 (8%)	0	4
4	BE	203/206 (98%)	149 (73%)	34 (17%)	20 (10%)	0	3
5	AF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
5	BF	206/210 (98%)	172 (84%)	29 (14%)	5 (2%)	5	25
6	AG	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	2	16
6	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	22	53
7	AH	168/180 (93%)	135 (80%)	25 (15%)	8 (5%)	2	12
7	BH	168/180 (93%)	129 (77%)	37 (22%)	2 (1%)	11	38
8	AK	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	1	10
8	BK	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	5	27
9	AM	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	2	14
9	BM	136/140 (97%)	120 (88%)	12 (9%)	4 (3%)	3	22
10	AN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	BN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AO	148/150 (99%)	101 (68%)	31 (21%)	16 (11%)	0	2
11	BO	148/150 (99%)	95 (64%)	32 (22%)	21 (14%)	0	1
12	AP	139/141 (99%)	101 (73%)	19 (14%)	19 (14%)	0	1
12	BP	139/141 (99%)	88 (63%)	34 (24%)	17 (12%)	0	1
13	A0	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	14	44
13	B0	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	AQ	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	7	30
14	BQ	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	2	17
15	AR	135/146 (92%)	111 (82%)	22 (16%)	2 (2%)	8	33
15	BR	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
16	A1	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	14	44
16	B1	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	14	44
17	A2	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	3	21
17	B2	99/101 (98%)	73 (74%)	13 (13%)	13 (13%)	0	1
18	AS	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	14	44
18	BS	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
19	AT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	5	26
19	BT	90/96 (94%)	81 (90%)	8 (9%)	1 (1%)	12	40
20	AU	100/110 (91%)	84 (84%)	10 (10%)	6 (6%)	1	9
20	BU	100/110 (91%)	67 (67%)	27 (27%)	6 (6%)	1	9
21	AV	173/206 (84%)	131 (76%)	35 (20%)	7 (4%)	2	16
21	BV	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	2	13
22	A3	74/85 (87%)	68 (92%)	4 (5%)	2 (3%)	4	22
22	B3	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	AZ	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	3	20
23	BZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	12	40
24	AW	64/72 (89%)	60 (94%)	1 (2%)	3 (5%)	2	13
24	BW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8	33
25	AX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	BX	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	A4	64/71 (90%)	42 (66%)	20 (31%)	2 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B4	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	3	19
27	A5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	7	30
27	B5	57/60 (95%)	48 (84%)	6 (10%)	3 (5%)	1	10
28	A6	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	13
28	B6	43/54 (80%)	26 (60%)	11 (26%)	6 (14%)	0	1
29	A7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	B7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	A8	59/65 (91%)	54 (92%)	4 (7%)	1 (2%)	7	31
30	B8	59/65 (91%)	42 (71%)	10 (17%)	7 (12%)	0	1
32	CE	235/256 (92%)	190 (81%)	44 (19%)	1 (0%)	30	61
32	DE	235/256 (92%)	186 (79%)	45 (19%)	4 (2%)	7	31
33	CF	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
33	DF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	13	42
34	CG	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	25	56
34	DG	206/208 (99%)	177 (86%)	28 (14%)	1 (0%)	25	56
35	CH	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	19	50
35	DH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
36	DI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
37	CJ	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
37	DJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
38	CK	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	19	50
38	DK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	CL	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
39	DL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	CM	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
40	DM	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	5	27
41	CN	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
41	DN	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
42	CO	123/132 (93%)	108 (88%)	13 (11%)	2 (2%)	8	32
42	DO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	CP	114/126 (90%)	90 (79%)	24 (21%)	0	100	100
43	DP	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	14	44
44	CQ	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	19
44	DQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	31
45	CR	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
45	DR	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
46	CS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
46	DS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	CT	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	6	28
47	DT	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
48	CU	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	9	34
48	DU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	CV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	4	23
49	DV	76/93 (82%)	58 (76%)	13 (17%)	5 (7%)	1	7
50	CW	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	13	42
50	DW	97/106 (92%)	81 (84%)	15 (16%)	1 (1%)	13	42
51	CX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
51	DX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
All	All	11336/12052 (94%)	9645 (85%)	1396 (12%)	295 (3%)	4	23

5 of 295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	237	GLU
3	AD	271	ILE
4	AE	15	PHE
4	AE	19	ARG
4	AE	23	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/218 (98%)	176 (82%)	38 (18%)	1	7
3	BD	214/218 (98%)	163 (76%)	51 (24%)	0	3
4	AE	165/166 (99%)	119 (72%)	46 (28%)	0	1
4	BE	165/166 (99%)	127 (77%)	38 (23%)	0	3
5	AF	161/166 (97%)	125 (78%)	36 (22%)	1	3
5	BF	165/166 (99%)	124 (75%)	41 (25%)	0	2
6	AG	155/156 (99%)	121 (78%)	34 (22%)	1	3
6	BG	155/156 (99%)	116 (75%)	39 (25%)	0	2
7	AH	142/148 (96%)	110 (78%)	32 (22%)	1	3
7	BH	142/148 (96%)	118 (83%)	24 (17%)	1	8
8	AK	122/124 (98%)	99 (81%)	23 (19%)	1	6
8	BK	122/124 (98%)	89 (73%)	33 (27%)	0	1
9	AM	117/119 (98%)	88 (75%)	29 (25%)	0	2
9	BM	117/119 (98%)	95 (81%)	22 (19%)	1	6
10	AN	100/100 (100%)	86 (86%)	14 (14%)	3	13
10	BN	100/100 (100%)	80 (80%)	20 (20%)	1	5
11	AO	116/116 (100%)	81 (70%)	35 (30%)	0	1
11	BO	116/116 (100%)	76 (66%)	40 (34%)	0	1
12	AP	111/111 (100%)	86 (78%)	25 (22%)	1	3
12	BP	111/111 (100%)	86 (78%)	25 (22%)	1	3
13	A0	101/101 (100%)	80 (79%)	21 (21%)	1	4
13	B0	100/101 (99%)	81 (81%)	19 (19%)	1	5
14	AQ	87/88 (99%)	69 (79%)	18 (21%)	1	4
14	BQ	87/88 (99%)	66 (76%)	21 (24%)	0	3
15	AR	120/127 (94%)	91 (76%)	29 (24%)	0	2
15	BR	120/127 (94%)	84 (70%)	36 (30%)	0	1
16	A1	93/94 (99%)	77 (83%)	16 (17%)	1	8
16	B1	93/94 (99%)	80 (86%)	13 (14%)	3	13
17	A2	82/82 (100%)	59 (72%)	23 (28%)	0	1
17	B2	82/82 (100%)	54 (66%)	28 (34%)	0	1
18	AS	92/92 (100%)	72 (78%)	20 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
18	BS	92/92 (100%)	66 (72%)	26 (28%)	0	1	
19	AT	74/78 (95%)	58 (78%)	16 (22%)	1	3	
19	BT	74/78 (95%)	60 (81%)	14 (19%)	1	6	
20	AU	85/91 (93%)	68 (80%)	17 (20%)	1	5	
20	BU	85/91 (93%)	61 (72%)	24 (28%)	0	1	
21	AV	154/179 (86%)	123 (80%)	31 (20%)	1	4	
21	BV	158/179 (88%)	130 (82%)	28 (18%)	1	7	
22	A3	61/67 (91%)	52 (85%)	9 (15%)	2	11	
22	B3	62/67 (92%)	50 (81%)	12 (19%)	1	5	
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	2	12	
23	BZ	82/83 (99%)	66 (80%)	16 (20%)	1	5	
24	AW	62/67 (92%)	46 (74%)	16 (26%)	0	2	
24	BW	64/67 (96%)	51 (80%)	13 (20%)	1	4	
25	AX	51/52 (98%)	47 (92%)	4 (8%)	10	33	
25	BX	51/52 (98%)	38 (74%)	13 (26%)	0	2	
26	A4	59/63 (94%)	42 (71%)	17 (29%)	0	1	
26	B4	57/63 (90%)	41 (72%)	16 (28%)	0	1	
27	A5	51/52 (98%)	37 (72%)	14 (28%)	0	1	
27	B5	51/52 (98%)	38 (74%)	13 (26%)	0	2	
28	A6	44/52 (85%)	28 (64%)	16 (36%)	0	0	
28	B6	44/52 (85%)	29 (66%)	15 (34%)	0	1	
29	A7	42/42 (100%)	35 (83%)	7 (17%)	2	8	
29	B7	42/42 (100%)	30 (71%)	12 (29%)	0	1	
30	A8	51/55 (93%)	41 (80%)	10 (20%)	1	5	
30	B8	51/55 (93%)	37 (72%)	14 (28%)	0	1	
32	CE	205/220 (93%)	164 (80%)	41 (20%)	1	5	
32	DE	205/220 (93%)	168 (82%)	37 (18%)	1	7	
33	CF	159/188 (85%)	132 (83%)	27 (17%)	1	8	
33	DF	160/188 (85%)	129 (81%)	31 (19%)	1	5	
34	CG	180/180 (100%)	150 (83%)	30 (17%)	2	8	
34	DG	180/180 (100%)	141 (78%)	39 (22%)	1	3	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	CH	116/123 (94%)	94 (81%)	22 (19%)	1	5
35	DH	116/123 (94%)	97 (84%)	19 (16%)	2	9
36	CI	90/90 (100%)	78 (87%)	12 (13%)	3	14
36	DI	90/90 (100%)	78 (87%)	12 (13%)	3	14
37	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	8
37	DJ	126/127 (99%)	100 (79%)	26 (21%)	1	4
38	CK	119/119 (100%)	106 (89%)	13 (11%)	5	20
38	DK	119/119 (100%)	102 (86%)	17 (14%)	2	12
39	CL	98/99 (99%)	69 (70%)	29 (30%)	0	1
39	DL	98/99 (99%)	72 (74%)	26 (26%)	0	2
40	CM	89/92 (97%)	69 (78%)	20 (22%)	1	3
40	DM	89/92 (97%)	65 (73%)	24 (27%)	0	1
41	CN	90/99 (91%)	77 (86%)	13 (14%)	2	12
41	DN	90/99 (91%)	79 (88%)	11 (12%)	4	16
42	CO	104/109 (95%)	88 (85%)	16 (15%)	2	10
42	DO	104/109 (95%)	85 (82%)	19 (18%)	1	6
43	CP	94/101 (93%)	76 (81%)	18 (19%)	1	5
43	DP	94/101 (93%)	77 (82%)	17 (18%)	1	6
44	CQ	49/50 (98%)	34 (69%)	15 (31%)	0	1
44	DQ	49/50 (98%)	37 (76%)	12 (24%)	0	2
45	CR	79/80 (99%)	69 (87%)	10 (13%)	3	15
45	DR	79/80 (99%)	68 (86%)	11 (14%)	3	13
46	CS	72/74 (97%)	58 (81%)	14 (19%)	1	5
46	DS	72/74 (97%)	58 (81%)	14 (19%)	1	5
47	CT	95/97 (98%)	83 (87%)	12 (13%)	3	16
47	DT	95/97 (98%)	88 (93%)	7 (7%)	11	34
48	CU	63/77 (82%)	51 (81%)	12 (19%)	1	5
48	DU	63/77 (82%)	50 (79%)	13 (21%)	1	4
49	CV	67/80 (84%)	50 (75%)	17 (25%)	0	2
49	DV	67/80 (84%)	53 (79%)	14 (21%)	1	4
50	CW	76/82 (93%)	64 (84%)	12 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	DW	76/82 (93%)	62 (82%)	14 (18%)	1	6
51	CX	20/22 (91%)	15 (75%)	5 (25%)	0	2
51	DX	20/22 (91%)	18 (90%)	2 (10%)	6	23
All	All	9579/9996 (96%)	7581 (79%)	1998 (21%)	1	4

5 of 1998 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	BP	76	LYS
37	DJ	8	GLU
21	BV	165	VAL
35	DH	101	ILE
42	DO	102	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such sidechains are listed below:

Mol	Chain	Res	Type
35	DH	141	GLN
37	DJ	97	GLN
49	DV	83	HIS
7	BH	74	ASN
6	BG	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	700 (24%)	52 (1%)
1	BA	2908/2912 (99%)	711 (24%)	53 (1%)
2	AB	121/122 (99%)	29 (23%)	0
2	BB	121/122 (99%)	29 (23%)	0
31	CA	1506/1506 (100%)	346 (22%)	35 (2%)
31	DA	1505/1506 (99%)	353 (23%)	49 (3%)
52	CB	86/87 (98%)	37 (43%)	4 (4%)
52	DB	86/87 (98%)	33 (38%)	3 (3%)
53	CC	77/77 (100%)	17 (22%)	4 (5%)
53	CD	76/77 (98%)	27 (35%)	1 (1%)
53	DC	77/77 (100%)	17 (22%)	4 (5%)
53	DD	76/77 (98%)	26 (34%)	1 (1%)
54	C1	9/10 (90%)	2 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	D1	9/10 (90%)	2 (22%)	0
All	All	9568/9582 (99%)	2329 (24%)	206 (2%)

5 of 2329 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	G
1	AA	5	A
1	AA	10	G
1	AA	34	C
1	AA	35	G

5 of 206 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	428	G
52	CB	23	A
52	DB	23	A
31	CA	530	G
31	CA	992	U

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 1703 ligands modelled in this entry, 1701 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PAR	CA	1841	-	44,45,45	0.53	0	63,67,67	1.41	9 (14%)
56	PAR	DA	1805	-	44,45,45	0.55	0	63,67,67	1.70	16 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PAR	CA	1841	-	-	8/18/94/94	0/4/4/4
56	PAR	DA	1805	-	-	6/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	1805	PAR	C13-O52-C52	-4.51	107.28	117.98
56	DA	1805	PAR	C11-O51-C51	3.99	121.51	113.72
56	DA	1805	PAR	O54-C54-C64	3.94	113.64	106.07
56	CA	1841	PAR	C41-C31-C21	-3.78	104.72	110.99
56	CA	1841	PAR	O54-C54-C64	3.75	113.28	106.07

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	CA	1841	PAR	C23-C13-O52-C52
56	CA	1841	PAR	C44-C54-C64-N64
56	CA	1841	PAR	O54-C54-C64-N64
56	DA	1805	PAR	C23-C13-O52-C52
56	CA	1841	PAR	O43-C43-C53-O53

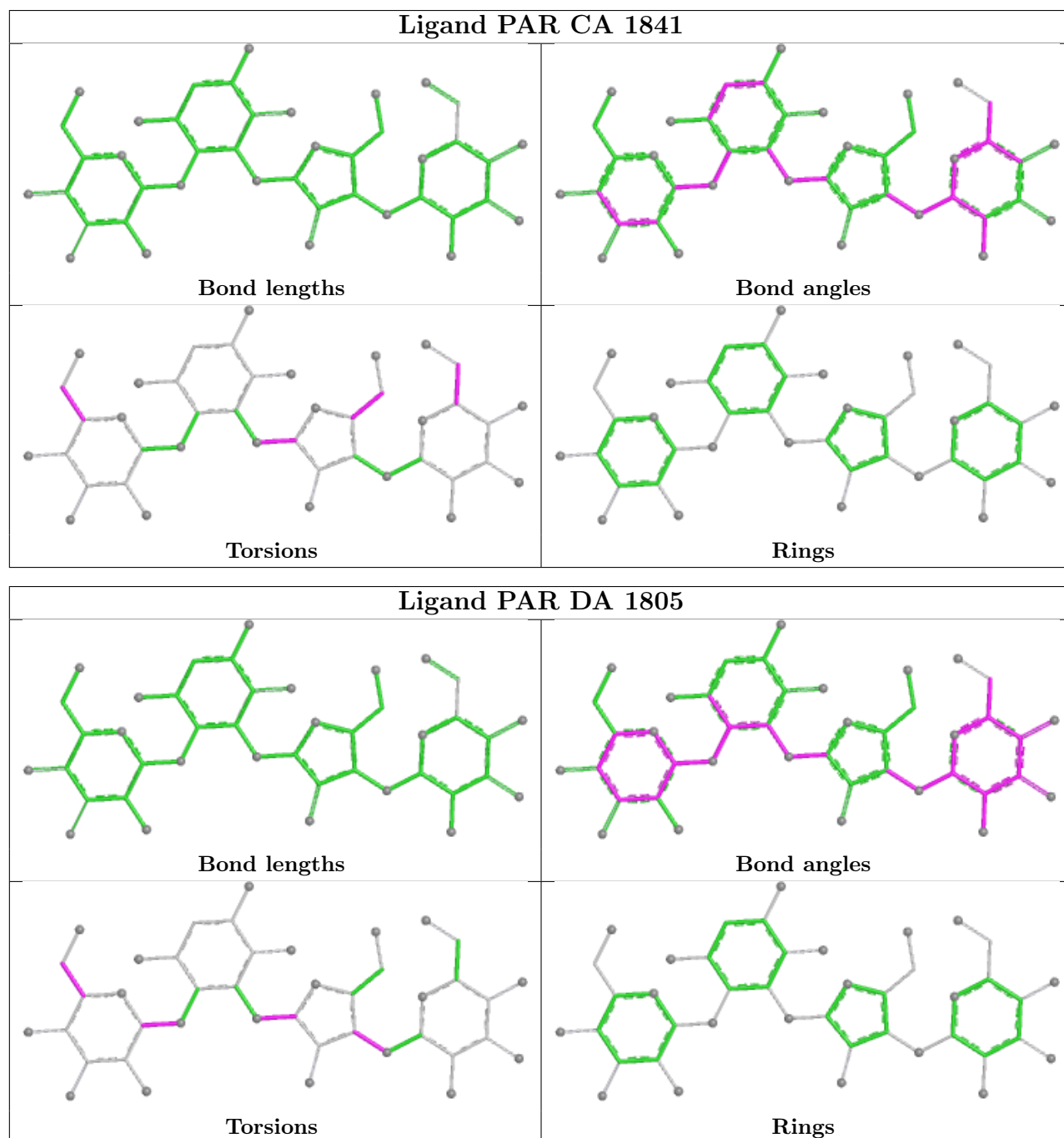
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1841	PAR	4	0
56	DA	1805	PAR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	2912/2912 (100%)	-0.72	13 (0%) 89 83	50, 80, 215, 247	0
1	BA	2909/2912 (99%)	-0.60	10 (0%) 90 85	60, 95, 235, 249	0
2	AB	122/122 (100%)	-0.68	1 (0%) 82 72	81, 105, 124, 182	0
2	BB	122/122 (100%)	-0.62	1 (0%) 82 72	98, 133, 156, 203	0
3	AD	272/276 (98%)	-0.45	0 100 100	47, 72, 94, 112	0
3	BD	272/276 (98%)	-0.20	2 (0%) 84 75	56, 82, 103, 138	0
4	AE	205/206 (99%)	0.41	24 (11%) 10 11	55, 91, 137, 149	0
4	BE	205/206 (99%)	0.16	15 (7%) 22 19	66, 104, 153, 172	0
5	AF	202/210 (96%)	-0.49	2 (0%) 79 68	52, 84, 123, 137	0
5	BF	208/210 (99%)	0.46	18 (8%) 17 16	64, 108, 166, 191	0
6	AG	181/182 (99%)	-0.22	4 (2%) 62 47	95, 115, 143, 157	0
6	BG	181/182 (99%)	0.00	3 (1%) 69 55	125, 148, 169, 176	0
7	AH	170/180 (94%)	0.26	5 (2%) 54 40	89, 119, 138, 160	0
7	BH	170/180 (94%)	0.35	13 (7%) 21 19	161, 203, 224, 232	0
8	AK	146/148 (98%)	0.33	5 (3%) 48 35	85, 134, 151, 157	0
8	BK	146/148 (98%)	0.17	3 (2%) 63 48	91, 134, 158, 167	0
9	AM	138/140 (98%)	0.41	9 (6%) 26 21	70, 95, 131, 144	0
9	BM	138/140 (98%)	0.19	4 (2%) 54 40	86, 118, 148, 158	0
10	AN	122/122 (100%)	-0.49	0 100 100	63, 82, 98, 111	0
10	BN	122/122 (100%)	-0.08	1 (0%) 82 72	76, 98, 116, 133	0
11	AO	150/150 (100%)	0.12	7 (4%) 37 28	45, 90, 122, 167	0
11	BO	150/150 (100%)	1.03	27 (18%) 4 4	44, 101, 149, 186	0
12	AP	141/141 (100%)	0.40	8 (5%) 30 25	58, 91, 116, 142	0
12	BP	141/141 (100%)	0.50	7 (4%) 35 28	58, 107, 142, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.45	0 100 100	64, 90, 109, 123	0
13	B0	117/118 (99%)	-0.60	0 100 100	68, 90, 113, 128	0
14	AQ	111/112 (99%)	0.07	2 (1%) 67 53	83, 103, 126, 142	0
14	BQ	111/112 (99%)	0.01	1 (0%) 81 70	95, 132, 156, 175	0
15	AR	137/146 (93%)	-0.21	6 (4%) 39 30	75, 97, 147, 178	0
15	BR	137/146 (93%)	0.02	5 (3%) 46 34	86, 107, 167, 187	0
16	A1	117/118 (99%)	-0.19	2 (1%) 69 55	61, 84, 116, 145	0
16	B1	117/118 (99%)	0.16	2 (1%) 69 55	71, 106, 146, 165	0
17	A2	101/101 (100%)	0.06	2 (1%) 64 50	61, 105, 126, 145	0
17	B2	101/101 (100%)	1.11	15 (14%) 7 6	73, 131, 148, 158	0
18	AS	113/113 (100%)	-0.27	3 (2%) 56 41	55, 80, 111, 163	0
18	BS	113/113 (100%)	-0.14	2 (1%) 67 53	69, 84, 121, 162	0
19	AT	92/96 (95%)	-0.02	5 (5%) 32 26	63, 78, 102, 118	0
19	BT	92/96 (95%)	-0.12	4 (4%) 40 30	78, 96, 119, 134	0
20	AU	102/110 (92%)	0.34	7 (6%) 24 20	82, 107, 157, 172	0
20	BU	102/110 (92%)	0.93	13 (12%) 9 9	97, 123, 176, 191	0
21	AV	175/206 (84%)	0.48	7 (4%) 43 32	93, 133, 193, 198	0
21	BV	179/206 (86%)	-0.04	2 (1%) 77 66	128, 166, 212, 218	0
22	A3	76/85 (89%)	-0.20	2 (2%) 57 42	65, 84, 98, 136	0
22	B3	77/85 (90%)	-0.17	1 (1%) 74 61	79, 101, 122, 155	0
23	AZ	97/98 (98%)	-0.25	3 (3%) 51 38	61, 81, 137, 165	0
23	BZ	97/98 (98%)	0.26	5 (5%) 34 27	69, 91, 141, 162	0
24	AW	66/72 (91%)	0.11	6 (9%) 16 15	69, 87, 106, 136	0
24	BW	69/72 (95%)	0.13	1 (1%) 73 60	90, 114, 148, 183	0
25	AX	59/60 (98%)	-0.08	2 (3%) 48 35	73, 90, 120, 135	0
25	BX	59/60 (98%)	0.15	1 (1%) 69 55	86, 114, 146, 166	0
26	A4	66/71 (92%)	0.10	1 (1%) 71 58	127, 161, 179, 187	0
26	B4	63/71 (88%)	0.13	0 100 100	154, 190, 200, 207	0
27	A5	59/60 (98%)	0.24	3 (5%) 34 27	55, 95, 180, 185	0
27	B5	59/60 (98%)	0.28	4 (6%) 25 20	65, 94, 181, 192	0
28	A6	45/54 (83%)	0.95	5 (11%) 12 11	122, 152, 173, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	45/54 (83%)	1.30	12 (26%) 2 1	141, 173, 188, 192	0
29	A7	49/49 (100%)	-0.67	0 100 100	50, 60, 106, 137	0
29	B7	49/49 (100%)	-0.37	0 100 100	60, 69, 129, 148	0
30	A8	61/65 (93%)	-0.09	3 (4%) 36 28	64, 78, 95, 120	0
30	B8	61/65 (93%)	0.92	12 (19%) 3 3	78, 95, 110, 142	0
31	CA	1506/1506 (100%)	-0.62	11 (0%) 84 75	64, 112, 193, 248	0
31	DA	1506/1506 (100%)	-0.62	6 (0%) 89 83	76, 122, 195, 248	0
32	CE	237/256 (92%)	0.78	27 (11%) 11 11	115, 149, 188, 198	0
32	DE	237/256 (92%)	0.84	25 (10%) 13 13	127, 165, 200, 215	0
33	CF	205/239 (85%)	0.26	6 (2%) 54 40	98, 124, 158, 166	0
33	DF	206/239 (86%)	0.47	16 (7%) 20 18	128, 151, 180, 188	0
34	CG	208/208 (100%)	0.08	4 (1%) 66 51	95, 119, 143, 154	0
34	DG	208/208 (100%)	-0.06	3 (1%) 73 60	91, 116, 137, 151	0
35	CH	151/162 (93%)	-0.01	4 (2%) 57 42	87, 109, 132, 166	0
35	DH	151/162 (93%)	-0.15	0 100 100	104, 125, 148, 169	0
36	CI	101/101 (100%)	-0.01	0 100 100	89, 112, 130, 153	0
36	DI	101/101 (100%)	-0.11	0 100 100	87, 109, 130, 156	0
37	CJ	155/156 (99%)	0.21	8 (5%) 34 27	111, 128, 158, 167	0
37	DJ	155/156 (99%)	-0.00	2 (1%) 74 61	116, 136, 164, 170	0
38	CK	138/138 (100%)	-0.23	0 100 100	95, 116, 130, 137	0
38	DK	138/138 (100%)	-0.31	0 100 100	109, 129, 143, 151	0
39	CL	127/128 (99%)	0.15	5 (3%) 44 33	99, 147, 167, 173	0
39	DL	127/128 (99%)	-0.16	3 (2%) 59 44	120, 158, 174, 178	0
40	CM	99/105 (94%)	0.50	4 (4%) 43 32	93, 146, 176, 179	0
40	DM	99/105 (94%)	0.51	7 (7%) 23 20	127, 164, 180, 185	0
41	CN	119/129 (92%)	-0.04	3 (2%) 58 43	79, 110, 142, 169	0
41	DN	119/129 (92%)	0.05	4 (3%) 48 35	90, 116, 148, 172	0
42	CO	125/132 (94%)	-0.08	4 (3%) 50 37	76, 87, 119, 164	0
42	DO	125/132 (94%)	0.23	8 (6%) 27 22	88, 112, 137, 175	0
43	CP	116/126 (92%)	-0.04	2 (1%) 69 55	98, 132, 151, 160	0
43	DP	117/126 (92%)	-0.27	2 (1%) 69 55	117, 160, 174, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	CQ	60/61 (98%)	-0.02	2 (3%)	49	36	95, 115, 129, 139	0
44	DQ	60/61 (98%)	-0.23	1 (1%)	69	55	129, 146, 159, 166	0
45	CR	88/89 (98%)	-0.48	1 (1%)	77	66	86, 108, 129, 133	0
45	DR	88/89 (98%)	-0.36	0	100	100	85, 118, 142, 148	0
46	CS	84/88 (95%)	-0.52	1 (1%)	76	64	104, 121, 148, 179	0
46	DS	84/88 (95%)	-0.08	3 (3%)	46	34	94, 111, 134, 166	0
47	CT	100/105 (95%)	-0.54	0	100	100	94, 115, 132, 146	0
47	DT	100/105 (95%)	-0.36	0	100	100	95, 117, 141, 155	0
48	CU	72/88 (81%)	0.37	5 (6%)	24	20	91, 112, 146, 173	0
48	DU	72/88 (81%)	0.24	5 (6%)	24	20	97, 120, 156, 173	0
49	CV	78/93 (83%)	-0.23	1 (1%)	74	61	112, 136, 151, 158	0
49	DV	78/93 (83%)	-0.30	0	100	100	150, 167, 187, 191	0
50	CW	99/106 (93%)	-0.57	0	100	100	106, 130, 158, 169	0
50	DW	99/106 (93%)	-0.30	0	100	100	97, 124, 158, 172	0
51	CX	25/27 (92%)	-0.60	0	100	100	101, 124, 142, 160	0
51	DX	25/27 (92%)	-0.55	0	100	100	126, 149, 163, 175	0
52	CB	87/87 (100%)	0.22	3 (3%)	48	35	91, 155, 201, 213	2 (2%)
52	DB	87/87 (100%)	-0.08	3 (3%)	48	35	97, 156, 203, 216	2 (2%)
53	CC	77/77 (100%)	-0.32	0	100	100	82, 118, 149, 164	0
53	CD	77/77 (100%)	0.09	0	100	100	86, 232, 246, 248	0
53	DC	77/77 (100%)	-0.50	1 (1%)	74	61	87, 120, 153, 167	0
53	DD	77/77 (100%)	0.21	1 (1%)	74	61	91, 234, 245, 249	0
54	C1	10/10 (100%)	0.07	1 (10%)	14	13	85, 102, 117, 131	0
54	D1	10/10 (100%)	-0.32	1 (10%)	14	13	88, 109, 119, 137	0
All	All	21107/21634 (97%)	-0.24	504 (2%)	59	44	44, 110, 191, 249	4 (0%)

The worst 5 of 504 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	B5	2	ALA	7.7
32	DE	4	GLU	7.6
9	AM	134	ARG	7.5
7	AH	155	SER	7.4
9	AM	138	LEU	7.3

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1779	1/1	0.28	0.12	113,113,113,113	0
55	MG	BA	3420	1/1	0.37	0.15	136,136,136,136	0
55	MG	DA	1740	1/1	0.43	0.18	113,113,113,113	0
55	MG	CA	1704	1/1	0.44	0.23	113,113,113,113	0
55	MG	BA	3277	1/1	0.45	0.26	109,109,109,109	0
55	MG	AA	3437	1/1	0.47	0.24	122,122,122,122	0
55	MG	AA	3433	1/1	0.48	0.14	152,152,152,152	0
55	MG	DA	1703	1/1	0.48	0.19	115,115,115,115	0
55	MG	BA	3407	1/1	0.48	0.26	96,96,96,96	0
55	MG	CB	101	1/1	0.49	0.14	108,108,108,108	0
55	MG	CG	302	1/1	0.50	0.26	122,122,122,122	0
55	MG	CA	1728	1/1	0.50	0.17	117,117,117,117	0
55	MG	DA	1804	1/1	0.50	0.24	123,123,123,123	0
55	MG	CB	104	1/1	0.52	0.22	101,101,101,101	0
55	MG	AA	3422	1/1	0.53	0.31	106,106,106,106	0
55	MG	BA	3095	1/1	0.53	0.30	112,112,112,112	0
55	MG	AA	3224	1/1	0.53	0.34	93,93,93,93	0
55	MG	CA	1720	1/1	0.53	0.18	102,102,102,102	0
55	MG	BA	3337	1/1	0.54	0.31	100,100,100,100	0
55	MG	BA	3507	1/1	0.54	0.34	102,102,102,102	0
55	MG	AA	3620	1/1	0.54	0.19	115,115,115,115	0
55	MG	BA	3459	1/1	0.55	0.12	115,115,115,115	0
55	MG	AA	3407	1/1	0.55	0.23	110,110,110,110	0
55	MG	AA	3373	1/1	0.55	0.27	106,106,106,106	0
55	MG	AA	3393	1/1	0.56	0.17	98,98,98,98	0
55	MG	CA	1828	1/1	0.56	0.28	98,98,98,98	0
55	MG	BA	3384	1/1	0.56	0.30	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1614	1/1	0.56	0.21	101,101,101,101	0
55	MG	CC	101	1/1	0.57	0.18	108,108,108,108	0
55	MG	BA	3301	1/1	0.57	0.35	106,106,106,106	0
55	MG	AA	3362	1/1	0.58	0.17	89,89,89,89	0
55	MG	CA	1701	1/1	0.58	0.15	105,105,105,105	0
55	MG	BA	3402	1/1	0.58	0.12	95,95,95,95	0
55	MG	CA	1714	1/1	0.58	0.25	118,118,118,118	0
55	MG	AB	214	1/1	0.58	0.19	102,102,102,102	0
55	MG	CA	1767	1/1	0.59	0.16	120,120,120,120	0
55	MG	AA	3594	1/1	0.59	0.24	105,105,105,105	0
55	MG	AA	3325	1/1	0.59	0.28	100,100,100,100	0
55	MG	CA	1672	1/1	0.59	0.18	106,106,106,106	0
55	MG	DA	1784	1/1	0.59	0.17	103,103,103,103	0
55	MG	BA	3472	1/1	0.59	0.37	83,83,83,83	0
55	MG	CA	1823	1/1	0.60	0.15	110,110,110,110	0
55	MG	BA	3463	1/1	0.60	0.30	114,114,114,114	0
55	MG	DC	107	1/1	0.60	0.12	105,105,105,105	0
55	MG	BA	3446	1/1	0.61	0.21	98,98,98,98	0
55	MG	BA	3401	1/1	0.61	0.13	100,100,100,100	0
55	MG	BA	3151	1/1	0.61	0.33	96,96,96,96	0
55	MG	BA	3371	1/1	0.61	0.20	129,129,129,129	0
55	MG	BA	3313	1/1	0.61	0.13	106,106,106,106	0
55	MG	BA	3050	1/1	0.62	0.12	103,103,103,103	0
55	MG	DA	1793	1/1	0.62	0.33	108,108,108,108	0
55	MG	CA	1615	1/1	0.62	0.30	104,104,104,104	0
55	MG	AA	3385	1/1	0.62	0.25	88,88,88,88	0
55	MG	CA	1783	1/1	0.63	0.14	106,106,106,106	0
55	MG	DA	1751	1/1	0.63	0.22	124,124,124,124	0
55	MG	DA	1630	1/1	0.63	0.28	102,102,102,102	0
55	MG	BA	3525	1/1	0.63	0.34	98,98,98,98	0
55	MG	DA	1794	1/1	0.63	0.16	91,91,91,91	0
55	MG	DA	1713	1/1	0.63	0.24	111,111,111,111	0
55	MG	DA	1719	1/1	0.63	0.23	112,112,112,112	0
55	MG	CA	1694	1/1	0.64	0.11	104,104,104,104	0
55	MG	DA	1666	1/1	0.64	0.12	115,115,115,115	0
55	MG	BB	212	1/1	0.64	0.17	104,104,104,104	0
55	MG	AA	3391	1/1	0.64	0.07	106,106,106,106	0
55	MG	AA	3497	1/1	0.64	0.29	95,95,95,95	0
55	MG	BA	3349	1/1	0.64	0.23	93,93,93,93	0
55	MG	BA	3464	1/1	0.65	0.18	104,104,104,104	0
55	MG	BA	3332	1/1	0.65	0.23	100,100,100,100	0
55	MG	BA	3075	1/1	0.65	0.19	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1825	1/1	0.65	0.19	114,114,114,114	0
55	MG	AA	3097	1/1	0.65	0.20	106,106,106,106	0
55	MG	CA	1753	1/1	0.65	0.11	107,107,107,107	0
55	MG	AA	3221	1/1	0.65	0.26	47,47,47,47	0
55	MG	AA	3587	1/1	0.66	0.33	77,77,77,77	0
55	MG	DA	1766	1/1	0.66	0.27	116,116,116,116	0
55	MG	CA	1765	1/1	0.66	0.21	109,109,109,109	0
55	MG	BA	3519	1/1	0.66	0.23	107,107,107,107	0
55	MG	AA	3509	1/1	0.66	0.27	95,95,95,95	0
55	MG	DA	1802	1/1	0.66	0.20	102,102,102,102	0
55	MG	CA	1692	1/1	0.66	0.12	127,127,127,127	0
55	MG	BA	3021	1/1	0.66	0.17	105,105,105,105	0
55	MG	BA	3094	1/1	0.67	0.33	79,79,79,79	0
55	MG	BA	3036	1/1	0.67	0.27	85,85,85,85	0
55	MG	CA	1832	1/1	0.67	0.28	106,106,106,106	0
55	MG	CA	1621	1/1	0.67	0.33	107,107,107,107	0
55	MG	CA	1630	1/1	0.67	0.18	112,112,112,112	0
55	MG	AA	3439	1/1	0.67	0.17	97,97,97,97	0
55	MG	AA	3193	1/1	0.67	0.22	96,96,96,96	0
55	MG	BA	3118	1/1	0.68	0.25	110,110,110,110	0
55	MG	CA	1736	1/1	0.68	0.26	88,88,88,88	0
55	MG	AE	304	1/1	0.68	0.27	87,87,87,87	0
55	MG	CA	1759	1/1	0.68	0.26	117,117,117,117	0
55	MG	BA	3164	1/1	0.68	0.11	99,99,99,99	0
55	MG	AA	3231	1/1	0.68	0.20	106,106,106,106	0
55	MG	AA	3260	1/1	0.68	0.25	91,91,91,91	0
55	MG	DA	1746	1/1	0.68	0.18	104,104,104,104	0
55	MG	DA	1747	1/1	0.68	0.21	105,105,105,105	0
55	MG	AA	3370	1/1	0.68	0.10	106,106,106,106	0
55	MG	AA	3295	1/1	0.68	0.31	102,102,102,102	0
55	MG	DA	1771	1/1	0.68	0.16	114,114,114,114	0
55	MG	BA	3081	1/1	0.68	0.15	91,91,91,91	0
55	MG	AA	3441	1/1	0.68	0.10	101,101,101,101	0
55	MG	AA	3446	1/1	0.68	0.17	93,93,93,93	0
55	MG	BA	3104	1/1	0.68	0.24	115,115,115,115	0
55	MG	CA	1715	1/1	0.68	0.19	115,115,115,115	0
55	MG	BA	3398	1/1	0.68	0.16	96,96,96,96	0
55	MG	CA	1735	1/1	0.69	0.20	101,101,101,101	0
55	MG	BB	213	1/1	0.69	0.10	97,97,97,97	0
55	MG	DA	1702	1/1	0.69	0.17	99,99,99,99	0
55	MG	AA	3075	1/1	0.69	0.33	85,85,85,85	0
55	MG	AA	3454	1/1	0.69	0.27	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1718	1/1	0.69	0.21	132,132,132,132	0
55	MG	AA	3461	1/1	0.69	0.22	105,105,105,105	0
55	MG	AA	3469	1/1	0.69	0.35	103,103,103,103	0
55	MG	BA	3317	1/1	0.69	0.30	91,91,91,91	0
55	MG	CA	1684	1/1	0.69	0.16	101,101,101,101	0
55	MG	AA	3253	1/1	0.69	0.26	81,81,81,81	0
55	MG	AA	3432	1/1	0.69	0.15	87,87,87,87	0
55	MG	AA	3354	1/1	0.69	0.21	84,84,84,84	0
55	MG	AA	3361	1/1	0.69	0.18	93,93,93,93	0
55	MG	AA	3604	1/1	0.69	0.25	93,93,93,93	0
55	MG	BA	3520	1/1	0.69	0.26	101,101,101,101	0
55	MG	AA	3209	1/1	0.69	0.22	81,81,81,81	0
55	MG	AA	3396	1/1	0.69	0.30	104,104,104,104	0
55	MG	CD	101	1/1	0.69	0.09	105,105,105,105	0
55	MG	BA	3435	1/1	0.70	0.22	108,108,108,108	0
55	MG	BB	206	1/1	0.70	0.10	102,102,102,102	0
55	MG	CA	1647	1/1	0.70	0.20	92,92,92,92	0
55	MG	BA	3445	1/1	0.70	0.09	95,95,95,95	0
55	MG	CA	1810	1/1	0.70	0.24	108,108,108,108	0
55	MG	CA	1683	1/1	0.70	0.18	104,104,104,104	0
55	MG	CA	1731	1/1	0.70	0.24	98,98,98,98	0
55	MG	BA	3107	1/1	0.70	0.25	89,89,89,89	0
55	MG	BB	214	1/1	0.70	0.14	99,99,99,99	0
55	MG	AA	3381	1/1	0.70	0.26	90,90,90,90	0
55	MG	AA	3599	1/1	0.70	0.34	87,87,87,87	0
55	MG	BB	210	1/1	0.71	0.17	96,96,96,96	0
55	MG	BA	3334	1/1	0.71	0.10	103,103,103,103	0
55	MG	AA	3307	1/1	0.71	0.34	76,76,76,76	0
55	MG	AA	3481	1/1	0.71	0.21	112,112,112,112	0
55	MG	AA	3402	1/1	0.71	0.16	92,92,92,92	0
55	MG	CA	1716	1/1	0.71	0.24	117,117,117,117	0
55	MG	AA	3273	1/1	0.71	0.20	101,101,101,101	0
55	MG	BA	3470	1/1	0.71	0.17	81,81,81,81	0
55	MG	AA	3409	1/1	0.71	0.19	104,104,104,104	0
55	MG	DA	1762	1/1	0.71	0.17	109,109,109,109	0
55	MG	AA	3067	1/1	0.71	0.28	108,108,108,108	0
55	MG	AA	3425	1/1	0.71	0.31	94,94,94,94	0
55	MG	BA	3090	1/1	0.71	0.20	109,109,109,109	0
55	MG	CA	1754	1/1	0.71	0.23	114,114,114,114	0
55	MG	DA	1605	1/1	0.71	0.33	82,82,82,82	0
55	MG	DA	1626	1/1	0.71	0.25	104,104,104,104	0
55	MG	AA	3456	1/1	0.71	0.32	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3357	1/1	0.71	0.18	99,99,99,99	0
55	MG	DA	1657	1/1	0.72	0.28	95,95,95,95	0
55	MG	DA	1756	1/1	0.72	0.33	106,106,106,106	0
55	MG	BA	3416	1/1	0.72	0.29	103,103,103,103	0
55	MG	CA	1679	1/1	0.72	0.24	101,101,101,101	0
55	MG	AB	216	1/1	0.72	0.22	106,106,106,106	0
55	MG	BA	3282	1/1	0.72	0.25	93,93,93,93	0
55	MG	BA	3121	1/1	0.72	0.35	99,99,99,99	0
55	MG	AA	3524	1/1	0.72	0.22	94,94,94,94	0
55	MG	BA	3116	1/1	0.72	0.23	107,107,107,107	0
55	MG	CA	1838	1/1	0.72	0.26	103,103,103,103	0
55	MG	DA	1631	1/1	0.72	0.28	102,102,102,102	0
55	MG	BA	3108	1/1	0.73	0.33	99,99,99,99	0
55	MG	BA	3389	1/1	0.73	0.11	96,96,96,96	0
55	MG	BA	3447	1/1	0.73	0.24	100,100,100,100	0
55	MG	BA	3454	1/1	0.73	0.27	105,105,105,105	0
55	MG	AA	3626	1/1	0.73	0.25	96,96,96,96	0
55	MG	DA	1728	1/1	0.73	0.20	112,112,112,112	0
55	MG	BB	215	1/1	0.73	0.10	101,101,101,101	0
55	MG	BA	3460	1/1	0.73	0.09	101,101,101,101	0
55	MG	AA	3556	1/1	0.73	0.33	96,96,96,96	0
55	MG	AA	3237	1/1	0.73	0.27	83,83,83,83	0
55	MG	CA	1628	1/1	0.73	0.31	85,85,85,85	0
55	MG	BA	3469	1/1	0.73	0.28	92,92,92,92	0
55	MG	CA	1750	1/1	0.73	0.27	104,104,104,104	0
55	MG	AA	3132	1/1	0.73	0.31	106,106,106,106	0
55	MG	AA	3498	1/1	0.73	0.28	95,95,95,95	0
55	MG	AA	3319	1/1	0.73	0.23	94,94,94,94	0
55	MG	BA	3423	1/1	0.73	0.20	91,91,91,91	0
55	MG	BA	3429	1/1	0.73	0.13	95,95,95,95	0
55	MG	AA	3421	1/1	0.73	0.17	94,94,94,94	0
55	MG	DA	1688	1/1	0.73	0.17	99,99,99,99	0
55	MG	AA	3242	1/1	0.74	0.10	93,93,93,93	0
55	MG	BA	3374	1/1	0.74	0.28	86,86,86,86	0
55	MG	BA	3281	1/1	0.74	0.22	92,92,92,92	0
55	MG	BA	3450	1/1	0.74	0.25	99,99,99,99	0
55	MG	BA	3078	1/1	0.74	0.14	95,95,95,95	0
55	MG	CA	1709	1/1	0.74	0.22	96,96,96,96	0
55	MG	BA	3114	1/1	0.74	0.15	103,103,103,103	0
55	MG	CA	1831	1/1	0.74	0.23	105,105,105,105	0
55	MG	AA	3235	1/1	0.74	0.18	84,84,84,84	0
55	MG	AA	3043	1/1	0.74	0.22	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3331	1/1	0.74	0.12	101,101,101,101	0
55	MG	CA	1724	1/1	0.74	0.24	97,97,97,97	0
55	MG	BA	3468	1/1	0.74	0.20	105,105,105,105	0
55	MG	AA	3356	1/1	0.74	0.21	86,86,86,86	0
55	MG	AA	3466	1/1	0.74	0.30	100,100,100,100	0
55	MG	DA	1774	1/1	0.74	0.24	103,103,103,103	0
55	MG	CA	1637	1/1	0.74	0.15	106,106,106,106	0
55	MG	AA	3309	1/1	0.74	0.46	90,90,90,90	0
55	MG	CA	1661	1/1	0.74	0.15	52,52,52,52	0
55	MG	BA	3174	1/1	0.74	0.29	82,82,82,82	0
55	MG	BA	3363	1/1	0.74	0.23	88,88,88,88	0
55	MG	BA	3438	1/1	0.74	0.09	88,88,88,88	0
55	MG	BA	3436	1/1	0.75	0.17	94,94,94,94	0
55	MG	DA	1698	1/1	0.75	0.16	103,103,103,103	0
55	MG	BA	3193	1/1	0.75	0.18	102,102,102,102	0
55	MG	BA	3273	1/1	0.75	0.28	102,102,102,102	0
55	MG	DA	1712	1/1	0.75	0.24	100,100,100,100	0
55	MG	CA	1834	1/1	0.75	0.19	90,90,90,90	0
55	MG	DA	1717	1/1	0.75	0.17	103,103,103,103	0
55	MG	CA	1607	1/1	0.75	0.21	93,93,93,93	0
55	MG	AA	3184	1/1	0.75	0.10	94,94,94,94	0
55	MG	BA	3502	1/1	0.75	0.10	91,91,91,91	0
55	MG	BA	3404	1/1	0.75	0.20	101,101,101,101	0
55	MG	DA	1741	1/1	0.75	0.27	93,93,93,93	0
55	MG	AA	3521	1/1	0.75	0.22	75,75,75,75	0
55	MG	CA	1766	1/1	0.75	0.31	108,108,108,108	0
55	MG	DA	1604	1/1	0.75	0.18	92,92,92,92	0
55	MG	BA	3027	1/1	0.75	0.17	107,107,107,107	0
55	MG	AA	3078	1/1	0.75	0.28	88,88,88,88	0
55	MG	AA	3490	1/1	0.75	0.28	97,97,97,97	0
55	MG	DA	1767	1/1	0.75	0.25	113,113,113,113	0
55	MG	AA	3197	1/1	0.75	0.28	74,74,74,74	0
55	MG	DA	1636	1/1	0.75	0.18	103,103,103,103	0
55	MG	DA	1642	1/1	0.75	0.22	110,110,110,110	0
55	MG	AA	3345	1/1	0.75	0.33	93,93,93,93	0
55	MG	DA	1661	1/1	0.75	0.20	98,98,98,98	0
55	MG	DA	1795	1/1	0.75	0.19	101,101,101,101	0
55	MG	DA	1663	1/1	0.75	0.18	103,103,103,103	0
55	MG	CA	1677	1/1	0.75	0.13	90,90,90,90	0
55	MG	DC	106	1/1	0.75	0.19	111,111,111,111	0
55	MG	DA	1684	1/1	0.75	0.21	92,92,92,92	0
55	MG	AA	3359	1/1	0.76	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3513	1/1	0.76	0.28	83,83,83,83	0
55	MG	BA	3148	1/1	0.76	0.26	91,91,91,91	0
55	MG	CA	1729	1/1	0.76	0.15	94,94,94,94	0
55	MG	CQ	101	1/1	0.76	0.22	102,102,102,102	0
55	MG	BA	3422	1/1	0.76	0.14	102,102,102,102	0
55	MG	AA	3191	1/1	0.76	0.19	95,95,95,95	0
55	MG	CA	1653	1/1	0.76	0.22	91,91,91,91	0
55	MG	CA	1748	1/1	0.76	0.21	87,87,87,87	0
55	MG	BA	3156	1/1	0.76	0.31	87,87,87,87	0
55	MG	AA	3413	1/1	0.76	0.18	109,109,109,109	0
55	MG	DA	1606	1/1	0.76	0.19	95,95,95,95	0
55	MG	BA	3172	1/1	0.76	0.20	85,85,85,85	0
55	MG	AA	3480	1/1	0.76	0.29	86,86,86,86	0
55	MG	BA	3019	1/1	0.76	0.12	100,100,100,100	0
55	MG	AA	3104	1/1	0.76	0.17	80,80,80,80	0
55	MG	AA	3369	1/1	0.76	0.33	93,93,93,93	0
55	MG	CA	1773	1/1	0.76	0.17	101,101,101,101	0
55	MG	BA	3387	1/1	0.76	0.28	107,107,107,107	0
55	MG	DA	1787	1/1	0.76	0.18	114,114,114,114	0
55	MG	AA	3120	1/1	0.76	0.16	86,86,86,86	0
55	MG	BA	3044	1/1	0.76	0.37	104,104,104,104	0
55	MG	DA	1681	1/1	0.76	0.18	106,106,106,106	0
55	MG	BR	202	1/1	0.76	0.14	105,105,105,105	0
55	MG	BA	3293	1/1	0.76	0.15	96,96,96,96	0
55	MG	AA	3328	1/1	0.76	0.28	82,82,82,82	0
55	MG	BA	3303	1/1	0.76	0.28	89,89,89,89	0
55	MG	DC	108	1/1	0.76	0.12	102,102,102,102	0
55	MG	AA	3390	1/1	0.77	0.13	109,109,109,109	0
55	MG	DA	1720	1/1	0.77	0.20	96,96,96,96	0
55	MG	CA	1649	1/1	0.77	0.23	86,86,86,86	0
55	MG	DA	1738	1/1	0.77	0.27	85,85,85,85	0
55	MG	AA	3414	1/1	0.77	0.22	94,94,94,94	0
55	MG	AA	3079	1/1	0.77	0.11	92,92,92,92	0
55	MG	DA	1745	1/1	0.77	0.23	106,106,106,106	0
55	MG	AA	3115	1/1	0.77	0.35	70,70,70,70	0
55	MG	BA	3462	1/1	0.77	0.14	123,123,123,123	0
55	MG	BA	3294	1/1	0.77	0.18	98,98,98,98	0
55	MG	BA	3372	1/1	0.77	0.30	105,105,105,105	0
55	MG	CA	1745	1/1	0.77	0.29	95,95,95,95	0
55	MG	DA	1763	1/1	0.77	0.32	89,89,89,89	0
55	MG	BA	3163	1/1	0.77	0.27	84,84,84,84	0
55	MG	DA	1683	1/1	0.77	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3434	1/1	0.77	0.31	90,90,90,90	0
55	MG	CA	1693	1/1	0.77	0.16	102,102,102,102	0
55	MG	AA	3102	1/1	0.77	0.18	90,90,90,90	0
55	MG	AA	3429	1/1	0.77	0.29	90,90,90,90	0
55	MG	AA	3103	1/1	0.77	0.28	97,97,97,97	0
55	MG	DA	1710	1/1	0.77	0.27	100,100,100,100	0
55	MG	BA	3329	1/1	0.77	0.16	66,66,66,66	0
55	MG	DA	1798	1/1	0.77	0.19	92,92,92,92	0
55	MG	AA	3327	1/1	0.77	0.27	84,84,84,84	0
55	MG	DA	1714	1/1	0.77	0.28	105,105,105,105	0
55	MG	DB	102	1/1	0.77	0.06	107,107,107,107	0
55	MG	DA	1716	1/1	0.77	0.23	105,105,105,105	0
55	MG	AA	3164	1/1	0.77	0.24	95,95,95,95	0
55	MG	CA	1778	1/1	0.77	0.33	95,95,95,95	0
55	MG	AA	3347	1/1	0.78	0.15	92,92,92,92	0
55	MG	BA	3299	1/1	0.78	0.13	82,82,82,82	0
55	MG	BA	3157	1/1	0.78	0.27	93,93,93,93	0
55	MG	DA	1613	1/1	0.78	0.26	88,88,88,88	0
55	MG	DA	1623	1/1	0.78	0.16	96,96,96,96	0
55	MG	CA	1711	1/1	0.78	0.18	98,98,98,98	0
55	MG	BA	3471	1/1	0.78	0.32	96,96,96,96	0
55	MG	BA	3032	1/1	0.78	0.26	110,110,110,110	0
55	MG	BA	3386	1/1	0.78	0.28	81,81,81,81	0
55	MG	DA	1637	1/1	0.78	0.23	97,97,97,97	0
55	MG	CA	1794	1/1	0.78	0.21	106,106,106,106	0
55	MG	DA	1754	1/1	0.78	0.15	98,98,98,98	0
55	MG	DA	1650	1/1	0.78	0.26	95,95,95,95	0
55	MG	DA	1757	1/1	0.78	0.19	104,104,104,104	0
55	MG	DA	1656	1/1	0.78	0.26	99,99,99,99	0
55	MG	AA	3348	1/1	0.78	0.12	94,94,94,94	0
55	MG	AA	3185	1/1	0.78	0.22	88,88,88,88	0
55	MG	CA	1727	1/1	0.78	0.24	103,103,103,103	0
55	MG	BA	3396	1/1	0.78	0.28	91,91,91,91	0
55	MG	CA	1829	1/1	0.78	0.15	102,102,102,102	0
55	MG	BA	3522	1/1	0.78	0.31	84,84,84,84	0
55	MG	AA	3087	1/1	0.78	0.34	76,76,76,76	0
55	MG	BA	3064	1/1	0.78	0.17	103,103,103,103	0
55	MG	BB	208	1/1	0.78	0.26	107,107,107,107	0
55	MG	BA	3068	1/1	0.78	0.22	93,93,93,93	0
55	MG	AA	3502	1/1	0.78	0.32	96,96,96,96	0
55	MG	AA	3506	1/1	0.78	0.10	80,80,80,80	0
55	MG	AA	3366	1/1	0.78	0.21	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CB	105	1/1	0.78	0.14	113,113,113,113	0
55	MG	BA	3352	1/1	0.78	0.25	102,102,102,102	0
55	MG	AA	3601	1/1	0.78	0.23	86,86,86,86	0
55	MG	DA	1601	1/1	0.78	0.22	107,107,107,107	0
55	MG	AA	3279	1/1	0.79	0.13	89,89,89,89	0
55	MG	BA	3494	1/1	0.79	0.31	88,88,88,88	0
55	MG	AA	3397	1/1	0.79	0.29	95,95,95,95	0
55	MG	AA	3289	1/1	0.79	0.30	84,84,84,84	0
55	MG	DA	1664	1/1	0.79	0.11	97,97,97,97	0
55	MG	BA	3357	1/1	0.79	0.22	71,71,71,71	0
55	MG	BA	3359	1/1	0.79	0.25	98,98,98,98	0
55	MG	AA	3264	1/1	0.79	0.24	80,80,80,80	0
55	MG	BA	3415	1/1	0.79	0.17	109,109,109,109	0
55	MG	CA	1768	1/1	0.79	0.18	105,105,105,105	0
55	MG	CA	1718	1/1	0.79	0.09	93,93,93,93	0
55	MG	BA	3368	1/1	0.79	0.21	106,106,106,106	0
55	MG	AA	3508	1/1	0.79	0.21	101,101,101,101	0
55	MG	BA	3175	1/1	0.79	0.12	100,100,100,100	0
55	MG	DA	1775	1/1	0.79	0.20	102,102,102,102	0
55	MG	DA	1783	1/1	0.79	0.21	86,86,86,86	0
55	MG	AB	204	1/1	0.79	0.26	96,96,96,96	0
55	MG	BA	3465	1/1	0.79	0.13	97,97,97,97	0
55	MG	CA	1815	1/1	0.79	0.23	91,91,91,91	0
55	MG	DA	1625	1/1	0.79	0.13	105,105,105,105	0
55	MG	CA	1816	1/1	0.79	0.11	95,95,95,95	0
55	MG	CA	1822	1/1	0.79	0.11	105,105,105,105	0
55	MG	AB	211	1/1	0.79	0.23	100,100,100,100	0
55	MG	BA	3043	1/1	0.79	0.40	108,108,108,108	0
55	MG	DA	1722	1/1	0.79	0.14	106,106,106,106	0
55	MG	AA	3463	1/1	0.79	0.21	90,90,90,90	0
55	MG	CA	1737	1/1	0.79	0.12	92,92,92,92	0
55	MG	BA	3098	1/1	0.79	0.08	106,106,106,106	0
55	MG	BA	3474	1/1	0.80	0.20	88,88,88,88	0
55	MG	AA	3251	1/1	0.80	0.11	68,68,68,68	0
55	MG	CA	1762	1/1	0.80	0.15	89,89,89,89	0
55	MG	AA	3468	1/1	0.80	0.11	95,95,95,95	0
55	MG	BA	3504	1/1	0.80	0.15	117,117,117,117	0
55	MG	BA	3072	1/1	0.80	0.20	104,104,104,104	0
55	MG	AA	3335	1/1	0.80	0.41	91,91,91,91	0
55	MG	DA	1769	1/1	0.80	0.20	79,79,79,79	0
55	MG	AA	3624	1/1	0.80	0.31	111,111,111,111	0
55	MG	CA	1730	1/1	0.80	0.21	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3383	1/1	0.80	0.39	95,95,95,95	0
55	MG	BA	3523	1/1	0.80	0.30	84,84,84,84	0
55	MG	CA	1787	1/1	0.80	0.15	100,100,100,100	0
55	MG	BA	3414	1/1	0.80	0.17	92,92,92,92	0
55	MG	DA	1725	1/1	0.80	0.29	96,96,96,96	0
55	MG	CC	107	1/1	0.80	0.12	93,93,93,93	0
55	MG	CA	1635	1/1	0.80	0.21	100,100,100,100	0
55	MG	DA	1739	1/1	0.80	0.11	113,113,113,113	0
55	MG	DA	1801	1/1	0.80	0.20	90,90,90,90	0
55	MG	AA	3479	1/1	0.80	0.14	94,94,94,94	0
55	MG	DA	1678	1/1	0.80	0.19	86,86,86,86	0
55	MG	DG	302	1/1	0.80	0.12	112,112,112,112	0
55	MG	DA	1603	1/1	0.80	0.27	89,89,89,89	0
55	MG	BA	3304	1/1	0.80	0.20	91,91,91,91	0
55	MG	AA	3358	1/1	0.80	0.40	89,89,89,89	0
55	MG	BA	3115	1/1	0.80	0.22	79,79,79,79	0
55	MG	AA	3126	1/1	0.81	0.20	83,83,83,83	0
55	MG	AA	3460	1/1	0.81	0.32	106,106,106,106	0
55	MG	BA	3410	1/1	0.81	0.31	94,94,94,94	0
55	MG	BA	3413	1/1	0.81	0.12	94,94,94,94	0
55	MG	AA	3108	1/1	0.81	0.32	66,66,66,66	0
55	MG	BA	3117	1/1	0.81	0.22	91,91,91,91	0
55	MG	AA	3526	1/1	0.81	0.32	90,90,90,90	0
55	MG	BA	3033	1/1	0.81	0.22	94,94,94,94	0
55	MG	BA	3124	1/1	0.81	0.11	102,102,102,102	0
55	MG	AA	3548	1/1	0.81	0.17	54,54,54,54	0
55	MG	BB	209	1/1	0.81	0.15	95,95,95,95	0
55	MG	AA	3416	1/1	0.81	0.18	95,95,95,95	0
55	MG	BA	3340	1/1	0.81	0.12	84,84,84,84	0
55	MG	AA	3194	1/1	0.81	0.20	102,102,102,102	0
55	MG	AA	3236	1/1	0.81	0.34	96,96,96,96	0
55	MG	BA	3058	1/1	0.81	0.33	89,89,89,89	0
55	MG	BA	3442	1/1	0.81	0.28	91,91,91,91	0
55	MG	AA	3275	1/1	0.81	0.22	87,87,87,87	0
55	MG	AA	3276	1/1	0.81	0.29	78,78,78,78	0
55	MG	AA	3050	1/1	0.81	0.41	108,108,108,108	0
55	MG	AA	3118	1/1	0.81	0.25	87,87,87,87	0
55	MG	BA	3453	1/1	0.81	0.17	93,93,93,93	0
55	MG	DA	1759	1/1	0.81	0.24	108,108,108,108	0
55	MG	DA	1760	1/1	0.81	0.21	100,100,100,100	0
55	MG	AA	3398	1/1	0.81	0.13	73,73,73,73	0
55	MG	BA	3373	1/1	0.81	0.24	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1760	1/1	0.81	0.18	91,91,91,91	0
55	MG	BA	3214	1/1	0.81	0.19	77,77,77,77	0
55	MG	AA	3367	1/1	0.81	0.32	87,87,87,87	0
55	MG	AA	3404	1/1	0.81	0.21	95,95,95,95	0
55	MG	BA	3385	1/1	0.81	0.20	97,97,97,97	0
55	MG	BA	3279	1/1	0.81	0.30	73,73,73,73	0
55	MG	DA	1778	1/1	0.81	0.19	118,118,118,118	0
55	MG	AB	207	1/1	0.81	0.08	103,103,103,103	0
55	MG	CA	1775	1/1	0.81	0.10	113,113,113,113	0
55	MG	AA	3096	1/1	0.81	0.16	89,89,89,89	0
55	MG	AB	212	1/1	0.81	0.31	94,94,94,94	0
55	MG	BA	3397	1/1	0.81	0.40	96,96,96,96	0
55	MG	AA	3448	1/1	0.81	0.24	106,106,106,106	0
55	MG	CA	1788	1/1	0.81	0.18	105,105,105,105	0
55	MG	CA	1687	1/1	0.81	0.20	78,78,78,78	0
55	MG	CA	1802	1/1	0.81	0.16	77,77,77,77	0
55	MG	CA	1689	1/1	0.81	0.14	115,115,115,115	0
55	MG	AA	3453	1/1	0.81	0.17	95,95,95,95	0
55	MG	AA	3298	1/1	0.81	0.17	73,73,73,73	0
55	MG	CA	1818	1/1	0.81	0.11	89,89,89,89	0
55	MG	BA	3500	1/1	0.81	0.16	104,104,104,104	0
55	MG	CA	1698	1/1	0.81	0.14	89,89,89,89	0
55	MG	BA	3003	1/1	0.82	0.28	99,99,99,99	0
55	MG	BA	3478	1/1	0.82	0.26	92,92,92,92	0
55	MG	CA	1793	1/1	0.82	0.12	96,96,96,96	0
55	MG	BA	3305	1/1	0.82	0.21	76,76,76,76	0
55	MG	BA	3308	1/1	0.82	0.17	108,108,108,108	0
55	MG	BA	3008	1/1	0.82	0.18	89,89,89,89	0
55	MG	BA	3503	1/1	0.82	0.14	69,69,69,69	0
55	MG	AA	3529	1/1	0.82	0.19	68,68,68,68	0
55	MG	BA	3020	1/1	0.82	0.23	76,76,76,76	0
55	MG	CA	1820	1/1	0.82	0.27	88,88,88,88	0
55	MG	AA	3401	1/1	0.82	0.22	93,93,93,93	0
55	MG	AA	3304	1/1	0.82	0.08	90,90,90,90	0
55	MG	BA	3521	1/1	0.82	0.31	79,79,79,79	0
55	MG	BA	3419	1/1	0.82	0.15	99,99,99,99	0
55	MG	AA	3558	1/1	0.82	0.23	89,89,89,89	0
55	MG	AA	3247	1/1	0.82	0.30	74,74,74,74	0
55	MG	AA	3148	1/1	0.82	0.26	83,83,83,83	0
55	MG	CA	1721	1/1	0.82	0.16	89,89,89,89	0
55	MG	BA	3342	1/1	0.82	0.13	80,80,80,80	0
55	MG	AA	3312	1/1	0.82	0.17	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3443	1/1	0.82	0.12	90,90,90,90	0
55	MG	CQ	102	1/1	0.82	0.12	97,97,97,97	0
55	MG	AA	3445	1/1	0.82	0.25	95,95,95,95	0
55	MG	DA	1743	1/1	0.82	0.21	94,94,94,94	0
55	MG	AA	3617	1/1	0.82	0.27	92,92,92,92	0
55	MG	BA	3063	1/1	0.82	0.20	89,89,89,89	0
55	MG	AA	3216	1/1	0.82	0.15	64,64,64,64	0
55	MG	BA	3370	1/1	0.82	0.21	98,98,98,98	0
55	MG	AA	3258	1/1	0.82	0.16	92,92,92,92	0
55	MG	CA	1740	1/1	0.82	0.18	72,72,72,72	0
55	MG	CA	1743	1/1	0.82	0.06	112,112,112,112	0
55	MG	CA	1609	1/1	0.82	0.30	78,78,78,78	0
55	MG	BA	3449	1/1	0.82	0.18	109,109,109,109	0
55	MG	AA	3451	1/1	0.82	0.12	76,76,76,76	0
55	MG	DA	1607	1/1	0.82	0.26	92,92,92,92	0
55	MG	BA	3451	1/1	0.82	0.15	89,89,89,89	0
55	MG	DA	1620	1/1	0.82	0.26	85,85,85,85	0
55	MG	DA	1768	1/1	0.82	0.15	82,82,82,82	0
55	MG	AB	203	1/1	0.82	0.33	69,69,69,69	0
55	MG	CA	1755	1/1	0.82	0.13	81,81,81,81	0
55	MG	CA	1758	1/1	0.82	0.14	97,97,97,97	0
55	MG	DA	1628	1/1	0.82	0.16	97,97,97,97	0
55	MG	AA	3080	1/1	0.82	0.29	104,104,104,104	0
55	MG	BA	3375	1/1	0.82	0.30	75,75,75,75	0
55	MG	AA	3420	1/1	0.82	0.26	88,88,88,88	0
55	MG	BA	3083	1/1	0.82	0.22	92,92,92,92	0
55	MG	DA	1641	1/1	0.82	0.26	95,95,95,95	0
55	MG	BA	3084	1/1	0.82	0.10	99,99,99,99	0
55	MG	DA	1643	1/1	0.82	0.25	81,81,81,81	0
55	MG	AA	3245	1/1	0.82	0.26	75,75,75,75	0
55	MG	DA	1655	1/1	0.82	0.21	96,96,96,96	0
55	MG	AA	3333	1/1	0.82	0.28	95,95,95,95	0
55	MG	CA	1770	1/1	0.82	0.26	90,90,90,90	0
55	MG	AA	3271	1/1	0.82	0.16	92,92,92,92	0
55	MG	AB	215	1/1	0.82	0.17	93,93,93,93	0
55	MG	BA	3101	1/1	0.82	0.13	94,94,94,94	0
55	MG	AA	3303	1/1	0.82	0.19	95,95,95,95	0
55	MG	AA	3465	1/1	0.82	0.12	71,71,71,71	0
55	MG	BA	3243	1/1	0.83	0.29	65,65,65,65	0
55	MG	CA	1685	1/1	0.83	0.15	103,103,103,103	0
55	MG	CA	1686	1/1	0.83	0.21	86,86,86,86	0
55	MG	BA	3256	1/1	0.83	0.13	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BB	204	1/1	0.83	0.21	90,90,90,90	0
55	MG	C1	101	1/1	0.83	0.10	98,98,98,98	0
55	MG	AA	3475	1/1	0.83	0.15	102,102,102,102	0
55	MG	BB	207	1/1	0.83	0.23	116,116,116,116	0
55	MG	BA	3399	1/1	0.83	0.12	104,104,104,104	0
55	MG	CA	1695	1/1	0.83	0.19	90,90,90,90	0
55	MG	AA	3114	1/1	0.83	0.34	56,56,56,56	0
55	MG	CA	1771	1/1	0.83	0.13	102,102,102,102	0
55	MG	DA	1609	1/1	0.83	0.18	116,116,116,116	0
55	MG	BA	3344	1/1	0.83	0.25	101,101,101,101	0
55	MG	DA	1619	1/1	0.83	0.24	77,77,77,77	0
55	MG	CA	1774	1/1	0.83	0.24	97,97,97,97	0
55	MG	BA	3348	1/1	0.83	0.21	98,98,98,98	0
55	MG	AA	3412	1/1	0.83	0.17	110,110,110,110	0
55	MG	BA	3037	1/1	0.83	0.11	75,75,75,75	0
55	MG	BA	3355	1/1	0.83	0.37	87,87,87,87	0
55	MG	CA	1785	1/1	0.83	0.32	89,89,89,89	0
55	MG	BA	3356	1/1	0.83	0.10	84,84,84,84	0
55	MG	AA	3426	1/1	0.83	0.14	80,80,80,80	0
55	MG	BA	3287	1/1	0.83	0.28	87,87,87,87	0
55	MG	BA	3092	1/1	0.83	0.28	95,95,95,95	0
55	MG	AA	3616	1/1	0.83	0.17	95,95,95,95	0
55	MG	CA	1616	1/1	0.83	0.17	103,103,103,103	0
55	MG	CA	1725	1/1	0.83	0.17	98,98,98,98	0
55	MG	AA	3094	1/1	0.83	0.21	62,62,62,62	0
55	MG	BA	3475	1/1	0.83	0.27	90,90,90,90	0
55	MG	AA	3123	1/1	0.83	0.26	52,52,52,52	0
55	MG	BA	3099	1/1	0.83	0.08	98,98,98,98	0
55	MG	AA	3300	1/1	0.83	0.09	81,81,81,81	0
55	MG	CA	1644	1/1	0.83	0.15	84,84,84,84	0
55	MG	AA	3554	1/1	0.83	0.18	74,74,74,74	0
55	MG	AA	3467	1/1	0.83	0.20	87,87,87,87	0
55	MG	CA	1830	1/1	0.83	0.25	94,94,94,94	0
55	MG	DA	1682	1/1	0.83	0.28	96,96,96,96	0
55	MG	CA	1738	1/1	0.83	0.12	103,103,103,103	0
55	MG	CA	1652	1/1	0.83	0.26	93,93,93,93	0
55	MG	AA	3149	1/1	0.83	0.22	57,57,57,57	0
55	MG	DA	1693	1/1	0.83	0.21	93,93,93,93	0
55	MG	BA	3189	1/1	0.83	0.19	61,61,61,61	0
55	MG	BA	3073	1/1	0.83	0.33	99,99,99,99	0
55	MG	DB	101	1/1	0.83	0.10	103,103,103,103	0
55	MG	CN	202	1/1	0.83	0.11	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3330	1/1	0.83	0.28	91,91,91,91	0
55	MG	BA	3201	1/1	0.83	0.20	94,94,94,94	0
55	MG	AA	3377	1/1	0.83	0.20	94,94,94,94	0
55	MG	BA	3312	1/1	0.84	0.19	98,98,98,98	0
55	MG	CA	1798	1/1	0.84	0.26	82,82,82,82	0
55	MG	BA	3040	1/1	0.84	0.16	94,94,94,94	0
55	MG	CA	1803	1/1	0.84	0.13	94,94,94,94	0
55	MG	CA	1804	1/1	0.84	0.10	107,107,107,107	0
55	MG	BA	3408	1/1	0.84	0.32	88,88,88,88	0
55	MG	BA	3512	1/1	0.84	0.29	75,75,75,75	0
55	MG	DA	1690	1/1	0.84	0.24	92,92,92,92	0
55	MG	BA	3513	1/1	0.84	0.18	104,104,104,104	0
55	MG	AA	3612	1/1	0.84	0.18	92,92,92,92	0
55	MG	CA	1819	1/1	0.84	0.12	109,109,109,109	0
55	MG	BA	3125	1/1	0.84	0.16	104,104,104,104	0
55	MG	DA	1708	1/1	0.84	0.34	102,102,102,102	0
55	MG	AA	3278	1/1	0.84	0.24	100,100,100,100	0
55	MG	AA	3499	1/1	0.84	0.38	93,93,93,93	0
55	MG	BA	3054	1/1	0.84	0.23	81,81,81,81	0
55	MG	AA	3351	1/1	0.84	0.20	82,82,82,82	0
55	MG	DA	1715	1/1	0.84	0.18	92,92,92,92	0
55	MG	BA	3159	1/1	0.84	0.25	83,83,83,83	0
55	MG	AA	3621	1/1	0.84	0.20	91,91,91,91	0
55	MG	AA	3423	1/1	0.84	0.14	74,74,74,74	0
55	MG	BA	3424	1/1	0.84	0.14	86,86,86,86	0
55	MG	AA	3625	1/1	0.84	0.17	89,89,89,89	0
55	MG	BA	3346	1/1	0.84	0.25	99,99,99,99	0
55	MG	BA	3347	1/1	0.84	0.12	85,85,85,85	0
55	MG	AA	3457	1/1	0.84	0.39	64,64,64,64	0
55	MG	DA	1729	1/1	0.84	0.29	84,84,84,84	0
55	MG	AA	3368	1/1	0.84	0.23	90,90,90,90	0
55	MG	AA	3059	1/1	0.84	0.27	80,80,80,80	0
55	MG	BA	3443	1/1	0.84	0.15	92,92,92,92	0
55	MG	CB	102	1/1	0.84	0.08	106,106,106,106	0
55	MG	AA	3514	1/1	0.84	0.21	67,67,67,67	0
55	MG	CA	1739	1/1	0.84	0.24	86,86,86,86	0
55	MG	AA	3355	1/1	0.84	0.24	94,94,94,94	0
55	MG	BA	3210	1/1	0.84	0.27	55,55,55,55	0
55	MG	AA	3371	1/1	0.84	0.25	89,89,89,89	0
55	MG	DA	1753	1/1	0.84	0.33	87,87,87,87	0
55	MG	BA	3233	1/1	0.84	0.28	74,74,74,74	0
55	MG	AA	3284	1/1	0.84	0.27	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3251	1/1	0.84	0.19	81,81,81,81	0
55	MG	AA	3286	1/1	0.84	0.22	86,86,86,86	0
55	MG	BA	3457	1/1	0.84	0.11	99,99,99,99	0
55	MG	CA	1756	1/1	0.84	0.05	113,113,113,113	0
55	MG	BA	3272	1/1	0.84	0.25	81,81,81,81	0
55	MG	CA	1640	1/1	0.84	0.18	85,85,85,85	0
55	MG	AA	3122	1/1	0.84	0.17	84,84,84,84	0
55	MG	AA	3553	1/1	0.84	0.25	87,87,87,87	0
55	MG	CA	1764	1/1	0.84	0.10	92,92,92,92	0
55	MG	AO	201	1/1	0.84	0.33	65,65,65,65	0
55	MG	DA	1624	1/1	0.84	0.20	95,95,95,95	0
55	MG	BA	3380	1/1	0.84	0.18	78,78,78,78	0
55	MG	AA	3384	1/1	0.84	0.33	87,87,87,87	0
55	MG	DA	1782	1/1	0.84	0.28	94,94,94,94	0
55	MG	AA	3341	1/1	0.84	0.15	95,95,95,95	0
55	MG	BA	3018	1/1	0.84	0.13	83,83,83,83	0
55	MG	AA	3557	1/1	0.84	0.29	100,100,100,100	0
55	MG	DA	1788	1/1	0.84	0.23	90,90,90,90	0
55	MG	AA	3444	1/1	0.84	0.22	58,58,58,58	0
55	MG	BA	3296	1/1	0.84	0.17	76,76,76,76	0
55	MG	DA	1640	1/1	0.84	0.11	101,101,101,101	0
55	MG	AA	3268	1/1	0.84	0.37	85,85,85,85	0
55	MG	AA	3270	1/1	0.84	0.23	69,69,69,69	0
55	MG	AA	3482	1/1	0.84	0.29	96,96,96,96	0
55	MG	CA	1782	1/1	0.84	0.29	94,94,94,94	0
55	MG	AA	3418	1/1	0.84	0.14	91,91,91,91	0
55	MG	CA	1784	1/1	0.84	0.28	101,101,101,101	0
55	MG	BA	3496	1/1	0.84	0.10	96,96,96,96	0
55	MG	BA	3498	1/1	0.84	0.13	99,99,99,99	0
55	MG	AA	3602	1/1	0.84	0.17	59,59,59,59	0
55	MG	AA	3392	1/1	0.84	0.09	93,93,93,93	0
55	MG	AA	3382	1/1	0.85	0.26	102,102,102,102	0
55	MG	AA	3098	1/1	0.85	0.25	81,81,81,81	0
55	MG	BA	3170	1/1	0.85	0.10	96,96,96,96	0
55	MG	BA	3062	1/1	0.85	0.25	110,110,110,110	0
55	MG	AA	3049	1/1	0.85	0.23	80,80,80,80	0
55	MG	AA	3459	1/1	0.85	0.23	81,81,81,81	0
55	MG	BA	3426	1/1	0.85	0.20	87,87,87,87	0
55	MG	DA	1618	1/1	0.85	0.18	104,104,104,104	0
55	MG	BA	3066	1/1	0.85	0.10	86,86,86,86	0
55	MG	AA	3386	1/1	0.85	0.16	74,74,74,74	0
55	MG	AA	3315	1/1	0.85	0.32	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AB	206	1/1	0.85	0.21	93,93,93,93	0
55	MG	AA	3316	1/1	0.85	0.17	83,83,83,83	0
55	MG	AB	209	1/1	0.85	0.18	108,108,108,108	0
55	MG	BA	3239	1/1	0.85	0.25	80,80,80,80	0
55	MG	BA	3444	1/1	0.85	0.25	96,96,96,96	0
55	MG	AA	3182	1/1	0.85	0.14	88,88,88,88	0
55	MG	BA	3367	1/1	0.85	0.36	91,91,91,91	0
55	MG	AA	3427	1/1	0.85	0.33	82,82,82,82	0
55	MG	AA	3535	1/1	0.85	0.07	103,103,103,103	0
55	MG	AA	3322	1/1	0.85	0.24	68,68,68,68	0
55	MG	AA	3288	1/1	0.85	0.23	90,90,90,90	0
55	MG	AA	3119	1/1	0.85	0.30	75,75,75,75	0
55	MG	AA	3474	1/1	0.85	0.17	65,65,65,65	0
55	MG	AA	3365	1/1	0.85	0.26	74,74,74,74	0
55	MG	AA	3068	1/1	0.85	0.40	72,72,72,72	0
55	MG	CA	1821	1/1	0.85	0.26	94,94,94,94	0
55	MG	AA	3583	1/1	0.85	0.24	103,103,103,103	0
55	MG	AA	3134	1/1	0.85	0.27	79,79,79,79	0
55	MG	CA	1625	1/1	0.85	0.13	71,71,71,71	0
55	MG	AA	3121	1/1	0.85	0.42	90,90,90,90	0
55	MG	AA	3336	1/1	0.85	0.12	82,82,82,82	0
55	MG	BA	3298	1/1	0.85	0.18	61,61,61,61	0
55	MG	BA	3025	1/1	0.85	0.11	80,80,80,80	0
55	MG	AA	3483	1/1	0.85	0.10	87,87,87,87	0
55	MG	BA	3028	1/1	0.85	0.25	85,85,85,85	0
55	MG	AA	3487	1/1	0.85	0.10	77,77,77,77	0
55	MG	AA	3252	1/1	0.85	0.25	94,94,94,94	0
55	MG	BA	3035	1/1	0.85	0.18	103,103,103,103	0
55	MG	AA	3611	1/1	0.85	0.14	100,100,100,100	0
55	MG	CA	1757	1/1	0.85	0.12	92,92,92,92	0
55	MG	CA	1655	1/1	0.85	0.30	95,95,95,95	0
55	MG	AA	3232	1/1	0.85	0.23	104,104,104,104	0
55	MG	DA	1803	1/1	0.85	0.21	100,100,100,100	0
55	MG	BA	3489	1/1	0.85	0.29	68,68,68,68	0
55	MG	AA	3614	1/1	0.85	0.24	78,78,78,78	0
55	MG	AA	3305	1/1	0.85	0.18	80,80,80,80	0
55	MG	AA	3255	1/1	0.85	0.14	88,88,88,88	0
55	MG	AA	3308	1/1	0.85	0.18	96,96,96,96	0
55	MG	BA	3051	1/1	0.85	0.09	90,90,90,90	0
55	MG	BA	3161	1/1	0.85	0.20	89,89,89,89	0
55	MG	DA	1674	1/1	0.86	0.18	76,76,76,76	0
55	MG	AA	3419	1/1	0.86	0.28	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1805	1/1	0.86	0.25	75,75,75,75	0
55	MG	CA	1809	1/1	0.86	0.19	79,79,79,79	0
55	MG	AA	3165	1/1	0.86	0.36	82,82,82,82	0
55	MG	BA	3074	1/1	0.86	0.10	83,83,83,83	0
55	MG	BA	3528	1/1	0.86	0.15	98,98,98,98	0
55	MG	BA	3427	1/1	0.86	0.19	100,100,100,100	0
55	MG	AA	3394	1/1	0.86	0.18	99,99,99,99	0
55	MG	AA	3452	1/1	0.86	0.26	76,76,76,76	0
55	MG	CA	1723	1/1	0.86	0.29	106,106,106,106	0
55	MG	BA	3200	1/1	0.86	0.20	65,65,65,65	0
55	MG	DA	1706	1/1	0.86	0.32	90,90,90,90	0
55	MG	AA	3017	1/1	0.86	0.18	64,64,64,64	0
55	MG	AA	3183	1/1	0.86	0.23	93,93,93,93	0
55	MG	A6	101	1/1	0.86	0.16	111,111,111,111	0
55	MG	AA	3564	1/1	0.86	0.18	76,76,76,76	0
55	MG	BA	3358	1/1	0.86	0.30	85,85,85,85	0
55	MG	BA	3091	1/1	0.86	0.25	86,86,86,86	0
55	MG	CA	1733	1/1	0.86	0.07	107,107,107,107	0
55	MG	CA	1734	1/1	0.86	0.18	86,86,86,86	0
55	MG	AA	3493	1/1	0.86	0.15	92,92,92,92	0
55	MG	BA	3093	1/1	0.86	0.10	78,78,78,78	0
55	MG	AA	3585	1/1	0.86	0.30	91,91,91,91	0
55	MG	AA	3249	1/1	0.86	0.32	76,76,76,76	0
55	MG	AA	3062	1/1	0.86	0.19	86,86,86,86	0
55	MG	AA	3598	1/1	0.86	0.15	87,87,87,87	0
55	MG	CA	1742	1/1	0.86	0.12	115,115,115,115	0
55	MG	DA	1730	1/1	0.86	0.18	102,102,102,102	0
55	MG	CA	1618	1/1	0.86	0.17	94,94,94,94	0
55	MG	AA	3228	1/1	0.86	0.23	79,79,79,79	0
55	MG	CA	1747	1/1	0.86	0.23	83,83,83,83	0
55	MG	CC	104	1/1	0.86	0.21	97,97,97,97	0
55	MG	CA	1624	1/1	0.86	0.09	97,97,97,97	0
55	MG	BA	3102	1/1	0.86	0.08	86,86,86,86	0
55	MG	AA	3500	1/1	0.86	0.17	103,103,103,103	0
55	MG	BA	3378	1/1	0.86	0.08	78,78,78,78	0
55	MG	AA	3501	1/1	0.86	0.11	99,99,99,99	0
55	MG	BA	3290	1/1	0.86	0.11	82,82,82,82	0
55	MG	AA	3081	1/1	0.86	0.35	51,51,51,51	0
55	MG	BA	3109	1/1	0.86	0.14	75,75,75,75	0
55	MG	AA	3063	1/1	0.86	0.27	85,85,85,85	0
55	MG	AA	3077	1/1	0.86	0.16	103,103,103,103	0
55	MG	CA	1651	1/1	0.86	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1614	1/1	0.86	0.22	93,93,93,93	0
55	MG	AA	3435	1/1	0.86	0.32	78,78,78,78	0
55	MG	AA	3510	1/1	0.86	0.42	84,84,84,84	0
55	MG	AA	3410	1/1	0.86	0.12	95,95,95,95	0
55	MG	DA	1621	1/1	0.86	0.31	99,99,99,99	0
55	MG	AA	3438	1/1	0.86	0.27	90,90,90,90	0
55	MG	DA	1770	1/1	0.86	0.29	95,95,95,95	0
55	MG	CA	1670	1/1	0.86	0.27	70,70,70,70	0
55	MG	BA	3122	1/1	0.86	0.24	95,95,95,95	0
55	MG	BA	3307	1/1	0.86	0.20	106,106,106,106	0
55	MG	DA	1627	1/1	0.86	0.14	105,105,105,105	0
55	MG	AA	3065	1/1	0.86	0.26	88,88,88,88	0
55	MG	BA	3045	1/1	0.86	0.26	88,88,88,88	0
55	MG	BA	3405	1/1	0.86	0.21	87,87,87,87	0
55	MG	DA	1635	1/1	0.86	0.19	79,79,79,79	0
55	MG	CA	1776	1/1	0.86	0.22	79,79,79,79	0
55	MG	AA	3339	1/1	0.86	0.18	85,85,85,85	0
55	MG	AA	3109	1/1	0.86	0.19	53,53,53,53	0
55	MG	AA	3342	1/1	0.86	0.27	70,70,70,70	0
55	MG	AA	3531	1/1	0.86	0.16	96,96,96,96	0
55	MG	AA	3532	1/1	0.86	0.29	88,88,88,88	0
55	MG	DA	1644	1/1	0.86	0.26	82,82,82,82	0
55	MG	AA	3313	1/1	0.86	0.22	70,70,70,70	0
55	MG	AA	3536	1/1	0.86	0.16	92,92,92,92	0
55	MG	AA	3540	1/1	0.86	0.47	63,63,63,63	0
55	MG	BA	3518	1/1	0.86	0.27	74,74,74,74	0
55	MG	BA	3338	1/1	0.86	0.22	71,71,71,71	0
55	MG	CA	1703	1/1	0.86	0.18	103,103,103,103	0
55	MG	BA	3421	1/1	0.86	0.08	102,102,102,102	0
55	MG	AA	3546	1/1	0.86	0.18	74,74,74,74	0
55	MG	DA	1695	1/1	0.87	0.25	88,88,88,88	0
55	MG	BA	3350	1/1	0.87	0.30	77,77,77,77	0
55	MG	CA	1681	1/1	0.87	0.17	80,80,80,80	0
55	MG	BA	3269	1/1	0.87	0.22	58,58,58,58	0
55	MG	DA	1705	1/1	0.87	0.21	97,97,97,97	0
55	MG	CA	1763	1/1	0.87	0.14	81,81,81,81	0
55	MG	BA	3270	1/1	0.87	0.26	81,81,81,81	0
55	MG	AB	208	1/1	0.87	0.22	92,92,92,92	0
55	MG	AA	3060	1/1	0.87	0.15	84,84,84,84	0
55	MG	AA	3383	1/1	0.87	0.18	85,85,85,85	0
55	MG	AA	3196	1/1	0.87	0.15	61,61,61,61	0
55	MG	BA	3431	1/1	0.87	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3280	1/1	0.87	0.36	74,74,74,74	0
55	MG	AA	3283	1/1	0.87	0.24	91,91,91,91	0
55	MG	AA	3512	1/1	0.87	0.12	97,97,97,97	0
55	MG	AA	3019	1/1	0.87	0.20	55,55,55,55	0
55	MG	BA	3441	1/1	0.87	0.18	93,93,93,93	0
55	MG	BB	205	1/1	0.87	0.23	86,86,86,86	0
55	MG	AA	3388	1/1	0.87	0.28	85,85,85,85	0
55	MG	DA	1615	1/1	0.87	0.17	96,96,96,96	0
55	MG	DA	1617	1/1	0.87	0.21	102,102,102,102	0
55	MG	BA	3144	1/1	0.87	0.15	95,95,95,95	0
55	MG	AA	3600	1/1	0.87	0.26	74,74,74,74	0
55	MG	AA	3389	1/1	0.87	0.20	72,72,72,72	0
55	MG	AA	3522	1/1	0.87	0.19	97,97,97,97	0
55	MG	BA	3377	1/1	0.87	0.28	81,81,81,81	0
55	MG	BA	3077	1/1	0.87	0.16	101,101,101,101	0
55	MG	AA	3478	1/1	0.87	0.19	75,75,75,75	0
55	MG	AA	3609	1/1	0.87	0.18	62,62,62,62	0
55	MG	AA	3032	1/1	0.87	0.18	65,65,65,65	0
55	MG	CA	1605	1/1	0.87	0.20	86,86,86,86	0
55	MG	DA	1629	1/1	0.87	0.07	92,92,92,92	0
55	MG	AA	3136	1/1	0.87	0.12	61,61,61,61	0
55	MG	AA	3449	1/1	0.87	0.11	63,63,63,63	0
55	MG	DA	1633	1/1	0.87	0.20	88,88,88,88	0
55	MG	AA	3137	1/1	0.87	0.10	51,51,51,51	0
55	MG	AA	3291	1/1	0.87	0.29	68,68,68,68	0
55	MG	DA	1761	1/1	0.87	0.29	84,84,84,84	0
55	MG	BA	3392	1/1	0.87	0.11	85,85,85,85	0
55	MG	BA	3393	1/1	0.87	0.16	84,84,84,84	0
55	MG	DA	1764	1/1	0.87	0.32	85,85,85,85	0
55	MG	AA	3619	1/1	0.87	0.22	87,87,87,87	0
55	MG	AA	3142	1/1	0.87	0.15	71,71,71,71	0
55	MG	AA	3321	1/1	0.87	0.19	65,65,65,65	0
55	MG	BA	3195	1/1	0.87	0.25	94,94,94,94	0
55	MG	AA	3248	1/1	0.87	0.30	74,74,74,74	0
55	MG	DA	1654	1/1	0.87	0.24	92,92,92,92	0
55	MG	AA	3227	1/1	0.87	0.38	90,90,90,90	0
55	MG	BA	3206	1/1	0.87	0.23	98,98,98,98	0
55	MG	CA	1639	1/1	0.87	0.24	86,86,86,86	0
55	MG	DA	1658	1/1	0.87	0.15	113,113,113,113	0
55	MG	DA	1660	1/1	0.87	0.16	102,102,102,102	0
55	MG	BA	3473	1/1	0.87	0.21	78,78,78,78	0
55	MG	BA	3335	1/1	0.87	0.15	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3375	1/1	0.87	0.15	88,88,88,88	0
55	MG	AB	202	1/1	0.87	0.15	92,92,92,92	0
55	MG	DA	1668	1/1	0.87	0.18	73,73,73,73	0
55	MG	DA	1669	1/1	0.87	0.29	68,68,68,68	0
55	MG	AA	3056	1/1	0.87	0.24	98,98,98,98	0
55	MG	AA	3380	1/1	0.87	0.08	96,96,96,96	0
55	MG	DA	1680	1/1	0.87	0.27	81,81,81,81	0
55	MG	BA	3495	1/1	0.87	0.23	81,81,81,81	0
55	MG	CG	301	1/1	0.87	0.25	94,94,94,94	0
55	MG	AB	205	1/1	0.87	0.18	83,83,83,83	0
55	MG	DH	201	1/1	0.87	0.19	105,105,105,105	0
55	MG	AA	3462	1/1	0.87	0.22	85,85,85,85	0
55	MG	AA	3003	1/1	0.87	0.27	64,64,64,64	0
55	MG	BA	3260	1/1	0.87	0.14	82,82,82,82	0
55	MG	DA	1692	1/1	0.87	0.24	81,81,81,81	0
55	MG	BA	3266	1/1	0.87	0.51	91,91,91,91	0
55	MG	AA	3329	1/1	0.88	0.14	94,94,94,94	0
55	MG	CC	103	1/1	0.88	0.20	104,104,104,104	0
55	MG	BA	3176	1/1	0.88	0.13	79,79,79,79	0
55	MG	BA	3177	1/1	0.88	0.24	75,75,75,75	0
55	MG	BA	3187	1/1	0.88	0.36	65,65,65,65	0
55	MG	BA	3320	1/1	0.88	0.27	77,77,77,77	0
55	MG	DA	1711	1/1	0.88	0.22	89,89,89,89	0
55	MG	BA	3324	1/1	0.88	0.28	75,75,75,75	0
55	MG	CA	1654	1/1	0.88	0.24	75,75,75,75	0
55	MG	BA	3326	1/1	0.88	0.16	84,84,84,84	0
55	MG	BA	3188	1/1	0.88	0.21	85,85,85,85	0
55	MG	AA	3330	1/1	0.88	0.14	60,60,60,60	0
55	MG	AA	3045	1/1	0.88	0.25	54,54,54,54	0
55	MG	BA	3194	1/1	0.88	0.18	70,70,70,70	0
55	MG	AA	3615	1/1	0.88	0.10	102,102,102,102	0
55	MG	BA	3196	1/1	0.88	0.18	84,84,84,84	0
55	MG	AA	3203	1/1	0.88	0.31	65,65,65,65	0
55	MG	AA	3173	1/1	0.88	0.12	67,67,67,67	0
55	MG	AA	3107	1/1	0.88	0.13	69,69,69,69	0
55	MG	AA	3489	1/1	0.88	0.41	86,86,86,86	0
55	MG	BA	3516	1/1	0.88	0.14	73,73,73,73	0
55	MG	DA	1734	1/1	0.88	0.21	88,88,88,88	0
55	MG	BA	3343	1/1	0.88	0.12	75,75,75,75	0
55	MG	AA	3542	1/1	0.88	0.16	93,93,93,93	0
55	MG	BA	3228	1/1	0.88	0.27	74,74,74,74	0
55	MG	BA	3034	1/1	0.88	0.21	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3218	1/1	0.88	0.24	73,73,73,73	0
55	MG	BA	3242	1/1	0.88	0.32	62,62,62,62	0
55	MG	AA	3492	1/1	0.88	0.10	94,94,94,94	0
55	MG	BA	3527	1/1	0.88	0.25	97,97,97,97	0
55	MG	DA	1748	1/1	0.88	0.32	91,91,91,91	0
55	MG	DA	1750	1/1	0.88	0.11	84,84,84,84	0
55	MG	AA	3274	1/1	0.88	0.15	72,72,72,72	0
55	MG	CA	1792	1/1	0.88	0.19	81,81,81,81	0
55	MG	AA	3424	1/1	0.88	0.22	54,54,54,54	0
55	MG	AA	3343	1/1	0.88	0.23	74,74,74,74	0
55	MG	AA	3317	1/1	0.88	0.25	85,85,85,85	0
55	MG	CA	1801	1/1	0.88	0.10	84,84,84,84	0
55	MG	AA	3155	1/1	0.88	0.32	71,71,71,71	0
55	MG	BA	3439	1/1	0.88	0.12	103,103,103,103	0
55	MG	BA	3048	1/1	0.88	0.12	74,74,74,74	0
55	MG	AA	3428	1/1	0.88	0.15	120,120,120,120	0
55	MG	BA	3365	1/1	0.88	0.19	90,90,90,90	0
55	MG	AA	3320	1/1	0.88	0.11	103,103,103,103	0
55	MG	BA	3119	1/1	0.88	0.12	79,79,79,79	0
55	MG	AA	3584	1/1	0.88	0.09	63,63,63,63	0
55	MG	AA	3376	1/1	0.88	0.19	85,85,85,85	0
55	MG	AA	3222	1/1	0.88	0.30	54,54,54,54	0
55	MG	AA	3590	1/1	0.88	0.26	81,81,81,81	0
55	MG	DA	1659	1/1	0.88	0.12	80,80,80,80	0
55	MG	AA	3378	1/1	0.88	0.28	84,84,84,84	0
55	MG	DA	1777	1/1	0.88	0.21	87,87,87,87	0
55	MG	CA	1613	1/1	0.88	0.05	94,94,94,94	0
55	MG	DA	1780	1/1	0.88	0.25	107,107,107,107	0
55	MG	AA	3117	1/1	0.88	0.22	54,54,54,54	0
55	MG	AA	3408	1/1	0.88	0.20	83,83,83,83	0
55	MG	BA	3070	1/1	0.88	0.19	81,81,81,81	0
55	MG	AA	3324	1/1	0.88	0.15	92,92,92,92	0
55	MG	AF	303	1/1	0.88	0.22	69,69,69,69	0
55	MG	DA	1790	1/1	0.88	0.27	100,100,100,100	0
55	MG	CA	1623	1/1	0.88	0.17	73,73,73,73	0
55	MG	DA	1677	1/1	0.88	0.14	82,82,82,82	0
55	MG	AA	3470	1/1	0.88	0.17	96,96,96,96	0
55	MG	DA	1796	1/1	0.88	0.15	97,97,97,97	0
55	MG	AO	203	1/1	0.88	0.17	43,43,43,43	0
55	MG	DA	1800	1/1	0.88	0.23	99,99,99,99	0
55	MG	CA	1741	1/1	0.88	0.17	80,80,80,80	0
55	MG	A2	201	1/1	0.88	0.32	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3225	1/1	0.88	0.20	95,95,95,95	0
55	MG	AA	3282	1/1	0.88	0.20	78,78,78,78	0
55	MG	DA	1686	1/1	0.88	0.23	97,97,97,97	0
55	MG	CA	1636	1/1	0.88	0.23	91,91,91,91	0
55	MG	BA	3390	1/1	0.88	0.27	77,77,77,77	0
55	MG	BA	3306	1/1	0.88	0.21	86,86,86,86	0
55	MG	DC	101	1/1	0.88	0.10	95,95,95,95	0
55	MG	CA	1751	1/1	0.88	0.17	78,78,78,78	0
55	MG	CA	1752	1/1	0.88	0.11	96,96,96,96	0
55	MG	AA	3261	1/1	0.88	0.26	85,85,85,85	0
55	MG	AA	3505	1/1	0.89	0.31	85,85,85,85	0
55	MG	AA	3262	1/1	0.89	0.21	33,33,33,33	0
55	MG	AA	3560	1/1	0.89	0.19	87,87,87,87	0
55	MG	BA	3333	1/1	0.89	0.20	73,73,73,73	0
55	MG	AA	3472	1/1	0.89	0.36	80,80,80,80	0
55	MG	BA	3418	1/1	0.89	0.14	73,73,73,73	0
55	MG	CA	1824	1/1	0.89	0.25	94,94,94,94	0
55	MG	AA	3576	1/1	0.89	0.26	46,46,46,46	0
55	MG	BA	3336	1/1	0.89	0.26	97,97,97,97	0
55	MG	CA	1719	1/1	0.89	0.09	85,85,85,85	0
55	MG	DA	1701	1/1	0.89	0.21	80,80,80,80	0
55	MG	BA	3526	1/1	0.89	0.21	92,92,92,92	0
55	MG	BA	3039	1/1	0.89	0.10	85,85,85,85	0
55	MG	BA	3212	1/1	0.89	0.26	70,70,70,70	0
55	MG	AA	3473	1/1	0.89	0.13	77,77,77,77	0
55	MG	BA	3341	1/1	0.89	0.24	82,82,82,82	0
55	MG	DA	1709	1/1	0.89	0.17	109,109,109,109	0
55	MG	CA	1726	1/1	0.89	0.16	103,103,103,103	0
55	MG	BA	3226	1/1	0.89	0.32	82,82,82,82	0
55	MG	BA	3106	1/1	0.89	0.16	85,85,85,85	0
55	MG	BA	3041	1/1	0.89	0.09	104,104,104,104	0
55	MG	AA	3072	1/1	0.89	0.05	101,101,101,101	0
55	MG	AA	3511	1/1	0.89	0.34	98,98,98,98	0
55	MG	BA	3111	1/1	0.89	0.14	82,82,82,82	0
55	MG	AA	3586	1/1	0.89	0.13	53,53,53,53	0
55	MG	AA	3285	1/1	0.89	0.23	80,80,80,80	0
55	MG	AA	3211	1/1	0.89	0.14	58,58,58,58	0
55	MG	BA	3263	1/1	0.89	0.18	84,84,84,84	0
55	MG	B1	201	1/1	0.89	0.38	82,82,82,82	0
55	MG	BA	3265	1/1	0.89	0.22	86,86,86,86	0
55	MG	DA	1726	1/1	0.89	0.32	79,79,79,79	0
55	MG	AA	3250	1/1	0.89	0.12	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3515	1/1	0.89	0.32	77,77,77,77	0
55	MG	BA	3056	1/1	0.89	0.20	96,96,96,96	0
55	MG	BA	3361	1/1	0.89	0.15	88,88,88,88	0
55	MG	AA	3187	1/1	0.89	0.24	87,87,87,87	0
55	MG	BA	3448	1/1	0.89	0.10	85,85,85,85	0
55	MG	BA	3060	1/1	0.89	0.09	51,51,51,51	0
55	MG	BA	3274	1/1	0.89	0.15	90,90,90,90	0
55	MG	BA	3275	1/1	0.89	0.26	52,52,52,52	0
55	MG	DA	1611	1/1	0.89	0.07	100,100,100,100	0
55	MG	DA	1612	1/1	0.89	0.08	73,73,73,73	0
55	MG	BA	3369	1/1	0.89	0.24	69,69,69,69	0
55	MG	AB	217	1/1	0.89	0.07	110,110,110,110	0
55	MG	BA	3456	1/1	0.89	0.20	88,88,88,88	0
55	MG	DA	1616	1/1	0.89	0.22	100,100,100,100	0
55	MG	AA	3405	1/1	0.89	0.36	90,90,90,90	0
55	MG	CA	1633	1/1	0.89	0.22	83,83,83,83	0
55	MG	BA	3127	1/1	0.89	0.33	55,55,55,55	0
55	MG	BA	3135	1/1	0.89	0.21	52,52,52,52	0
55	MG	AA	3099	1/1	0.89	0.22	64,64,64,64	0
55	MG	CA	1638	1/1	0.89	0.19	108,108,108,108	0
55	MG	AA	3092	1/1	0.89	0.19	71,71,71,71	0
55	MG	AA	3486	1/1	0.89	0.11	90,90,90,90	0
55	MG	AA	3431	1/1	0.89	0.18	89,89,89,89	0
55	MG	BA	3467	1/1	0.89	0.21	93,93,93,93	0
55	MG	DA	1765	1/1	0.89	0.11	93,93,93,93	0
55	MG	CA	1648	1/1	0.89	0.24	79,79,79,79	0
55	MG	AA	3340	1/1	0.89	0.18	83,83,83,83	0
55	MG	BA	3158	1/1	0.89	0.23	70,70,70,70	0
55	MG	BA	3297	1/1	0.89	0.13	63,63,63,63	0
55	MG	AA	3318	1/1	0.89	0.14	92,92,92,92	0
55	MG	DA	1634	1/1	0.89	0.16	77,77,77,77	0
55	MG	AA	3033	1/1	0.89	0.21	49,49,49,49	0
55	MG	BA	3010	1/1	0.89	0.22	68,68,68,68	0
55	MG	BA	3076	1/1	0.89	0.29	91,91,91,91	0
55	MG	AA	3537	1/1	0.89	0.09	105,105,105,105	0
55	MG	BA	3476	1/1	0.89	0.11	68,68,68,68	0
55	MG	CA	1675	1/1	0.89	0.13	97,97,97,97	0
55	MG	CA	1781	1/1	0.89	0.23	62,62,62,62	0
55	MG	AA	3076	1/1	0.89	0.18	82,82,82,82	0
55	MG	CA	1678	1/1	0.89	0.25	69,69,69,69	0
55	MG	DA	1652	1/1	0.89	0.17	85,85,85,85	0
55	MG	AA	3301	1/1	0.89	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1680	1/1	0.89	0.18	79,79,79,79	0
55	MG	BA	3490	1/1	0.89	0.13	52,52,52,52	0
55	MG	BA	3395	1/1	0.89	0.06	89,89,89,89	0
55	MG	AA	3259	1/1	0.89	0.17	81,81,81,81	0
55	MG	DA	1797	1/1	0.89	0.22	85,85,85,85	0
55	MG	AA	3048	1/1	0.89	0.14	86,86,86,86	0
55	MG	BA	3085	1/1	0.89	0.28	74,74,74,74	0
55	MG	BA	3179	1/1	0.89	0.30	61,61,61,61	0
55	MG	CA	1688	1/1	0.89	0.14	77,77,77,77	0
55	MG	BA	3088	1/1	0.89	0.16	94,94,94,94	0
55	MG	AA	3442	1/1	0.89	0.20	78,78,78,78	0
55	MG	DG	301	1/1	0.89	0.19	94,94,94,94	0
55	MG	AA	3349	1/1	0.89	0.13	84,84,84,84	0
55	MG	BA	3030	1/1	0.89	0.22	99,99,99,99	0
55	MG	BA	3509	1/1	0.89	0.34	73,73,73,73	0
55	MG	DA	1676	1/1	0.89	0.23	82,82,82,82	0
55	MG	BA	3328	1/1	0.89	0.09	61,61,61,61	0
55	MG	CA	1700	1/1	0.89	0.12	72,72,72,72	0
55	MG	AA	3129	1/1	0.89	0.29	73,73,73,73	0
55	MG	CA	1817	1/1	0.89	0.20	85,85,85,85	0
55	MG	AA	3280	1/1	0.90	0.14	94,94,94,94	0
55	MG	BA	3327	1/1	0.90	0.24	91,91,91,91	0
55	MG	BA	3221	1/1	0.90	0.15	37,37,37,37	0
55	MG	AA	3623	1/1	0.90	0.20	74,74,74,74	0
55	MG	CA	1712	1/1	0.90	0.14	92,92,92,92	0
55	MG	AA	3403	1/1	0.90	0.26	91,91,91,91	0
55	MG	DA	1723	1/1	0.90	0.17	83,83,83,83	0
55	MG	CA	1791	1/1	0.90	0.16	97,97,97,97	0
55	MG	AA	3052	1/1	0.90	0.22	73,73,73,73	0
55	MG	AA	3095	1/1	0.90	0.10	89,89,89,89	0
55	MG	BA	3024	1/1	0.90	0.14	110,110,110,110	0
55	MG	AB	201	1/1	0.90	0.25	96,96,96,96	0
55	MG	CA	1799	1/1	0.90	0.25	95,95,95,95	0
55	MG	AA	3455	1/1	0.90	0.26	49,49,49,49	0
55	MG	AA	3039	1/1	0.90	0.26	82,82,82,82	0
55	MG	AA	3363	1/1	0.90	0.26	95,95,95,95	0
55	MG	BA	3149	1/1	0.90	0.15	72,72,72,72	0
55	MG	BA	3150	1/1	0.90	0.24	96,96,96,96	0
55	MG	AA	3167	1/1	0.90	0.28	50,50,50,50	0
55	MG	BA	3152	1/1	0.90	0.21	73,73,73,73	0
55	MG	CA	1813	1/1	0.90	0.11	94,94,94,94	0
55	MG	BA	3155	1/1	0.90	0.30	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3485	1/1	0.90	0.21	46,46,46,46	0
55	MG	BA	3082	1/1	0.90	0.40	76,76,76,76	0
55	MG	BA	3345	1/1	0.90	0.13	87,87,87,87	0
55	MG	CA	1732	1/1	0.90	0.18	69,69,69,69	0
55	MG	AA	3169	1/1	0.90	0.18	89,89,89,89	0
55	MG	AA	3171	1/1	0.90	0.09	84,84,84,84	0
55	MG	AA	3326	1/1	0.90	0.12	64,64,64,64	0
55	MG	AA	3145	1/1	0.90	0.31	91,91,91,91	0
55	MG	BA	3278	1/1	0.90	0.29	92,92,92,92	0
55	MG	BA	3162	1/1	0.90	0.07	92,92,92,92	0
55	MG	AA	3415	1/1	0.90	0.28	87,87,87,87	0
55	MG	AA	3440	1/1	0.90	0.24	87,87,87,87	0
55	MG	BA	3505	1/1	0.90	0.13	94,94,94,94	0
55	MG	DA	1662	1/1	0.90	0.31	78,78,78,78	0
55	MG	BA	3506	1/1	0.90	0.16	74,74,74,74	0
55	MG	AA	3290	1/1	0.90	0.27	72,72,72,72	0
55	MG	AA	3091	1/1	0.90	0.23	78,78,78,78	0
55	MG	CA	1837	1/1	0.90	0.21	88,88,88,88	0
55	MG	BA	3288	1/1	0.90	0.15	98,98,98,98	0
55	MG	DA	1672	1/1	0.90	0.19	63,63,63,63	0
55	MG	CA	1839	1/1	0.90	0.19	68,68,68,68	0
55	MG	AA	3372	1/1	0.90	0.08	87,87,87,87	0
55	MG	CA	1665	1/1	0.90	0.35	74,74,74,74	0
55	MG	CA	1667	1/1	0.90	0.21	77,77,77,77	0
55	MG	AA	3353	1/1	0.90	0.27	86,86,86,86	0
55	MG	AA	3547	1/1	0.90	0.14	45,45,45,45	0
55	MG	BA	3047	1/1	0.90	0.14	80,80,80,80	0
55	MG	CA	1676	1/1	0.90	0.21	76,76,76,76	0
55	MG	AA	3503	1/1	0.90	0.23	81,81,81,81	0
55	MG	DA	1685	1/1	0.90	0.33	72,72,72,72	0
55	MG	BA	3180	1/1	0.90	0.23	57,57,57,57	0
55	MG	AA	3198	1/1	0.90	0.34	74,74,74,74	0
55	MG	AA	3332	1/1	0.90	0.11	62,62,62,62	0
55	MG	BA	3524	1/1	0.90	0.38	105,105,105,105	0
55	MG	BA	3052	1/1	0.90	0.15	58,58,58,58	0
55	MG	AA	3296	1/1	0.90	0.25	72,72,72,72	0
55	MG	BA	3055	1/1	0.90	0.22	99,99,99,99	0
55	MG	A3	101	1/1	0.90	0.34	74,74,74,74	0
55	MG	BA	3110	1/1	0.90	0.25	92,92,92,92	0
55	MG	AZ	101	1/1	0.90	0.10	77,77,77,77	0
55	MG	BA	3311	1/1	0.90	0.12	82,82,82,82	0
55	MG	CA	1690	1/1	0.90	0.17	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3381	1/1	0.90	0.24	80,80,80,80	0
55	MG	AA	3618	1/1	0.90	0.21	97,97,97,97	0
55	MG	AA	3074	1/1	0.90	0.30	68,68,68,68	0
55	MG	BA	3005	1/1	0.90	0.18	70,70,70,70	0
55	MG	CA	1696	1/1	0.90	0.17	90,90,90,90	0
55	MG	BA	3455	1/1	0.90	0.17	92,92,92,92	0
55	MG	AA	3477	1/1	0.90	0.25	86,86,86,86	0
55	MG	BA	3213	1/1	0.90	0.21	75,75,75,75	0
55	MG	DA	1665	1/1	0.91	0.26	82,82,82,82	0
55	MG	AA	3495	1/1	0.91	0.26	90,90,90,90	0
55	MG	AA	3559	1/1	0.91	0.16	83,83,83,83	0
55	MG	CA	1673	1/1	0.91	0.20	76,76,76,76	0
55	MG	CA	1674	1/1	0.91	0.19	102,102,102,102	0
55	MG	CA	1797	1/1	0.91	0.16	93,93,93,93	0
55	MG	BA	3133	1/1	0.91	0.16	50,50,50,50	0
55	MG	BA	3057	1/1	0.91	0.21	97,97,97,97	0
55	MG	AA	3337	1/1	0.91	0.23	99,99,99,99	0
55	MG	BA	3276	1/1	0.91	0.12	88,88,88,88	0
55	MG	BA	3477	1/1	0.91	0.14	94,94,94,94	0
55	MG	BA	3146	1/1	0.91	0.19	86,86,86,86	0
55	MG	BA	3479	1/1	0.91	0.39	95,95,95,95	0
55	MG	CA	1806	1/1	0.91	0.11	62,62,62,62	0
55	MG	BA	3484	1/1	0.91	0.24	65,65,65,65	0
55	MG	BA	3379	1/1	0.91	0.22	84,84,84,84	0
55	MG	AA	3023	1/1	0.91	0.33	56,56,56,56	0
55	MG	CA	1814	1/1	0.91	0.13	86,86,86,86	0
55	MG	AA	3575	1/1	0.91	0.21	42,42,42,42	0
55	MG	AE	303	1/1	0.91	0.12	91,91,91,91	0
55	MG	DA	1694	1/1	0.91	0.34	84,84,84,84	0
55	MG	AA	3266	1/1	0.91	0.30	49,49,49,49	0
55	MG	AF	301	1/1	0.91	0.13	80,80,80,80	0
55	MG	BA	3067	1/1	0.91	0.10	74,74,74,74	0
55	MG	AA	3058	1/1	0.91	0.20	64,64,64,64	0
55	MG	AA	3047	1/1	0.91	0.17	60,60,60,60	0
55	MG	BA	3291	1/1	0.91	0.34	67,67,67,67	0
55	MG	AA	3234	1/1	0.91	0.12	82,82,82,82	0
55	MG	AA	3344	1/1	0.91	0.20	68,68,68,68	0
55	MG	AU	201	1/1	0.91	0.14	85,85,85,85	0
55	MG	AA	3504	1/1	0.91	0.23	80,80,80,80	0
55	MG	AA	3272	1/1	0.91	0.27	65,65,65,65	0
55	MG	AA	3346	1/1	0.91	0.24	88,88,88,88	0
55	MG	AA	3507	1/1	0.91	0.26	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1705	1/1	0.91	0.08	95,95,95,95	0
55	MG	BA	3004	1/1	0.91	0.25	105,105,105,105	0
55	MG	CA	1835	1/1	0.91	0.15	87,87,87,87	0
55	MG	AA	3189	1/1	0.91	0.20	90,90,90,90	0
55	MG	AA	3037	1/1	0.91	0.25	69,69,69,69	0
55	MG	AA	3150	1/1	0.91	0.29	59,59,59,59	0
55	MG	BA	3406	1/1	0.91	0.12	97,97,97,97	0
55	MG	DA	1721	1/1	0.91	0.25	71,71,71,71	0
55	MG	AA	3241	1/1	0.91	0.31	80,80,80,80	0
55	MG	BA	3087	1/1	0.91	0.31	80,80,80,80	0
55	MG	AA	3277	1/1	0.91	0.12	82,82,82,82	0
55	MG	BA	3184	1/1	0.91	0.13	76,76,76,76	0
55	MG	DA	1727	1/1	0.91	0.24	86,86,86,86	0
55	MG	CT	201	1/1	0.91	0.16	102,102,102,102	0
55	MG	AA	3124	1/1	0.91	0.33	47,47,47,47	0
55	MG	BA	3314	1/1	0.91	0.16	71,71,71,71	0
55	MG	DA	1732	1/1	0.91	0.16	94,94,94,94	0
55	MG	BA	3316	1/1	0.91	0.13	67,67,67,67	0
55	MG	DA	1735	1/1	0.91	0.25	106,106,106,106	0
55	MG	DA	1736	1/1	0.91	0.22	65,65,65,65	0
55	MG	BA	3417	1/1	0.91	0.12	88,88,88,88	0
55	MG	AA	3163	1/1	0.91	0.12	55,55,55,55	0
55	MG	CC	102	1/1	0.91	0.19	69,69,69,69	0
55	MG	AA	3024	1/1	0.91	0.25	45,45,45,45	0
55	MG	BA	3192	1/1	0.91	0.27	72,72,72,72	0
55	MG	AA	3471	1/1	0.91	0.22	85,85,85,85	0
55	MG	AA	3040	1/1	0.91	0.23	68,68,68,68	0
55	MG	AA	3166	1/1	0.91	0.18	53,53,53,53	0
55	MG	AA	3130	1/1	0.91	0.14	67,67,67,67	0
55	MG	AA	3527	1/1	0.91	0.13	86,86,86,86	0
55	MG	AA	3131	1/1	0.91	0.18	90,90,90,90	0
55	MG	BA	3202	1/1	0.91	0.15	69,69,69,69	0
55	MG	BA	3205	1/1	0.91	0.21	70,70,70,70	0
55	MG	BA	3433	1/1	0.91	0.19	88,88,88,88	0
55	MG	CA	1604	1/1	0.91	0.20	77,77,77,77	0
55	MG	DA	1758	1/1	0.91	0.28	109,109,109,109	0
55	MG	DA	1610	1/1	0.91	0.12	97,97,97,97	0
55	MG	AA	3215	1/1	0.91	0.17	79,79,79,79	0
55	MG	AA	3051	1/1	0.91	0.26	71,71,71,71	0
55	MG	BA	3105	1/1	0.91	0.33	81,81,81,81	0
55	MG	CA	1612	1/1	0.91	0.09	102,102,102,102	0
55	MG	AA	3364	1/1	0.91	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3254	1/1	0.91	0.25	85,85,85,85	0
55	MG	CA	1746	1/1	0.91	0.16	98,98,98,98	0
55	MG	BA	3339	1/1	0.91	0.16	90,90,90,90	0
55	MG	BA	3215	1/1	0.91	0.20	66,66,66,66	0
55	MG	BA	3220	1/1	0.91	0.11	40,40,40,40	0
55	MG	AA	3172	1/1	0.91	0.13	94,94,94,94	0
55	MG	CA	1622	1/1	0.91	0.10	86,86,86,86	0
55	MG	BA	3222	1/1	0.91	0.11	54,54,54,54	0
55	MG	BA	3223	1/1	0.91	0.20	64,64,64,64	0
55	MG	BA	3225	1/1	0.91	0.15	78,78,78,78	0
55	MG	AA	3008	1/1	0.91	0.21	44,44,44,44	0
55	MG	CA	1629	1/1	0.91	0.11	95,95,95,95	0
55	MG	DA	1781	1/1	0.91	0.11	87,87,87,87	0
55	MG	AA	3292	1/1	0.91	0.22	76,76,76,76	0
55	MG	AA	3543	1/1	0.91	0.27	46,46,46,46	0
55	MG	BA	3235	1/1	0.91	0.19	74,74,74,74	0
55	MG	CA	1761	1/1	0.91	0.17	66,66,66,66	0
55	MG	AA	3177	1/1	0.91	0.27	46,46,46,46	0
55	MG	DA	1789	1/1	0.91	0.15	77,77,77,77	0
55	MG	BA	3241	1/1	0.91	0.24	52,52,52,52	0
55	MG	AA	3180	1/1	0.91	0.23	64,64,64,64	0
55	MG	AA	3447	1/1	0.91	0.26	75,75,75,75	0
55	MG	BA	3246	1/1	0.91	0.12	99,99,99,99	0
55	MG	CA	1643	1/1	0.91	0.20	91,91,91,91	0
55	MG	BA	3458	1/1	0.91	0.10	71,71,71,71	0
55	MG	CA	1645	1/1	0.91	0.25	60,60,60,60	0
55	MG	AA	3552	1/1	0.91	0.28	83,83,83,83	0
55	MG	AA	3055	1/1	0.91	0.26	67,67,67,67	0
55	MG	BA	3461	1/1	0.91	0.12	83,83,83,83	0
55	MG	BA	3258	1/1	0.91	0.18	64,64,64,64	0
55	MG	BA	3362	1/1	0.91	0.07	71,71,71,71	0
55	MG	AA	3411	1/1	0.91	0.23	85,85,85,85	0
55	MG	AA	3085	1/1	0.91	0.17	34,34,34,34	0
55	MG	BA	3053	1/1	0.91	0.20	65,65,65,65	0
55	MG	CA	1660	1/1	0.91	0.19	64,64,64,64	0
55	MG	BA	3123	1/1	0.91	0.07	77,77,77,77	0
55	MG	BA	3267	1/1	0.91	0.25	62,62,62,62	0
55	MG	DC	104	1/1	0.91	0.20	102,102,102,102	0
55	MG	CA	1666	1/1	0.91	0.20	70,70,70,70	0
55	MG	AA	3494	1/1	0.91	0.22	88,88,88,88	0
55	MG	CA	1668	1/1	0.91	0.37	79,79,79,79	0
55	MG	AB	213	1/1	0.92	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3066	1/1	0.92	0.25	48,48,48,48	0
55	MG	BA	3351	1/1	0.92	0.30	81,81,81,81	0
55	MG	BA	3440	1/1	0.92	0.08	80,80,80,80	0
55	MG	BA	3167	1/1	0.92	0.23	59,59,59,59	0
55	MG	BA	3097	1/1	0.92	0.12	60,60,60,60	0
55	MG	AA	3592	1/1	0.92	0.20	76,76,76,76	0
55	MG	AA	3528	1/1	0.92	0.25	76,76,76,76	0
55	MG	AA	3596	1/1	0.92	0.20	93,93,93,93	0
55	MG	CA	1722	1/1	0.92	0.21	74,74,74,74	0
55	MG	DA	1704	1/1	0.92	0.24	87,87,87,87	0
55	MG	B3	101	1/1	0.92	0.12	76,76,76,76	0
55	MG	B5	101	1/1	0.92	0.18	61,61,61,61	0
55	MG	CA	1601	1/1	0.92	0.16	56,56,56,56	0
55	MG	AA	3597	1/1	0.92	0.17	91,91,91,91	0
55	MG	BA	3360	1/1	0.92	0.21	83,83,83,83	0
55	MG	BA	3103	1/1	0.92	0.16	82,82,82,82	0
55	MG	AA	3311	1/1	0.92	0.20	68,68,68,68	0
55	MG	AA	3530	1/1	0.92	0.13	79,79,79,79	0
55	MG	BA	3182	1/1	0.92	0.15	47,47,47,47	0
55	MG	BA	3452	1/1	0.92	0.08	96,96,96,96	0
55	MG	CB	103	1/1	0.92	0.10	110,110,110,110	0
55	MG	BA	3183	1/1	0.92	0.13	80,80,80,80	0
55	MG	AA	3186	1/1	0.92	0.13	58,58,58,58	0
55	MG	CA	1617	1/1	0.92	0.20	72,72,72,72	0
55	MG	AA	3027	1/1	0.92	0.19	45,45,45,45	0
55	MG	CA	1620	1/1	0.92	0.12	74,74,74,74	0
55	MG	AA	3044	1/1	0.92	0.26	52,52,52,52	0
55	MG	CC	106	1/1	0.92	0.18	92,92,92,92	0
55	MG	AA	3256	1/1	0.92	0.13	66,66,66,66	0
55	MG	BA	3289	1/1	0.92	0.19	70,70,70,70	0
55	MG	BA	3191	1/1	0.92	0.28	77,77,77,77	0
55	MG	AA	3070	1/1	0.92	0.20	68,68,68,68	0
55	MG	AA	3430	1/1	0.92	0.07	105,105,105,105	0
55	MG	BA	3376	1/1	0.92	0.17	65,65,65,65	0
55	MG	DA	1731	1/1	0.92	0.27	70,70,70,70	0
55	MG	BA	3112	1/1	0.92	0.13	69,69,69,69	0
55	MG	DA	1733	1/1	0.92	0.20	98,98,98,98	0
55	MG	CA	1631	1/1	0.92	0.07	74,74,74,74	0
55	MG	AA	3013	1/1	0.92	0.12	44,44,44,44	0
55	MG	AA	3613	1/1	0.92	0.17	76,76,76,76	0
55	MG	BA	3197	1/1	0.92	0.08	76,76,76,76	0
55	MG	BA	3199	1/1	0.92	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3168	1/1	0.92	0.25	68,68,68,68	0
55	MG	BA	3302	1/1	0.92	0.21	75,75,75,75	0
55	MG	AA	3544	1/1	0.92	0.22	63,63,63,63	0
55	MG	BA	3065	1/1	0.92	0.25	101,101,101,101	0
55	MG	AA	3141	1/1	0.92	0.24	50,50,50,50	0
55	MG	AA	3406	1/1	0.92	0.13	83,83,83,83	0
55	MG	AA	3436	1/1	0.92	0.18	66,66,66,66	0
55	MG	AA	3113	1/1	0.92	0.28	49,49,49,49	0
55	MG	BA	3310	1/1	0.92	0.17	74,74,74,74	0
55	MG	BA	3394	1/1	0.92	0.27	88,88,88,88	0
55	MG	AA	3057	1/1	0.92	0.23	66,66,66,66	0
55	MG	BA	3481	1/1	0.92	0.18	49,49,49,49	0
55	MG	BA	3483	1/1	0.92	0.18	34,34,34,34	0
55	MG	AA	3201	1/1	0.92	0.17	85,85,85,85	0
55	MG	CA	1656	1/1	0.92	0.26	88,88,88,88	0
55	MG	CA	1658	1/1	0.92	0.18	50,50,50,50	0
55	MG	AA	3239	1/1	0.92	0.14	60,60,60,60	0
55	MG	AA	3125	1/1	0.92	0.25	55,55,55,55	0
55	MG	AA	3297	1/1	0.92	0.11	69,69,69,69	0
55	MG	BA	3139	1/1	0.92	0.14	58,58,58,58	0
55	MG	BA	3318	1/1	0.92	0.07	89,89,89,89	0
55	MG	BA	3141	1/1	0.92	0.17	72,72,72,72	0
55	MG	CA	1669	1/1	0.92	0.20	70,70,70,70	0
55	MG	BA	3142	1/1	0.92	0.22	70,70,70,70	0
55	MG	DA	1639	1/1	0.92	0.20	78,78,78,78	0
55	MG	BA	3499	1/1	0.92	0.13	78,78,78,78	0
55	MG	AA	3176	1/1	0.92	0.10	74,74,74,74	0
55	MG	DA	1772	1/1	0.92	0.18	68,68,68,68	0
55	MG	BA	3145	1/1	0.92	0.25	53,53,53,53	0
55	MG	BA	3231	1/1	0.92	0.29	47,47,47,47	0
55	MG	AA	3064	1/1	0.92	0.05	79,79,79,79	0
55	MG	BA	3411	1/1	0.92	0.29	83,83,83,83	0
55	MG	BA	3412	1/1	0.92	0.27	50,50,50,50	0
55	MG	CA	1790	1/1	0.92	0.07	89,89,89,89	0
55	MG	AA	3246	1/1	0.92	0.29	73,73,73,73	0
55	MG	AA	3570	1/1	0.92	0.22	41,41,41,41	0
55	MG	BA	3240	1/1	0.92	0.24	72,72,72,72	0
55	MG	DA	1785	1/1	0.92	0.17	93,93,93,93	0
55	MG	CA	1682	1/1	0.92	0.15	106,106,106,106	0
55	MG	AA	3387	1/1	0.92	0.34	80,80,80,80	0
55	MG	BA	3515	1/1	0.92	0.16	59,59,59,59	0
55	MG	AA	3417	1/1	0.92	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3517	1/1	0.92	0.16	61,61,61,61	0
55	MG	AA	3577	1/1	0.92	0.10	52,52,52,52	0
55	MG	BA	3245	1/1	0.92	0.21	72,72,72,72	0
55	MG	AA	3116	1/1	0.92	0.25	37,37,37,37	0
55	MG	BA	3247	1/1	0.92	0.26	74,74,74,74	0
55	MG	DA	1667	1/1	0.92	0.18	82,82,82,82	0
55	MG	BA	3248	1/1	0.92	0.18	54,54,54,54	0
55	MG	AA	3154	1/1	0.92	0.28	52,52,52,52	0
55	MG	BA	3255	1/1	0.92	0.22	52,52,52,52	0
55	MG	BA	3425	1/1	0.92	0.31	85,85,85,85	0
55	MG	BA	3089	1/1	0.92	0.15	83,83,83,83	0
55	MG	CA	1697	1/1	0.92	0.22	92,92,92,92	0
55	MG	BA	3257	1/1	0.92	0.35	86,86,86,86	0
55	MG	DA	1679	1/1	0.92	0.29	64,64,64,64	0
55	MG	DS	101	1/1	0.92	0.26	87,87,87,87	0
55	MG	AA	3016	1/1	0.92	0.16	48,48,48,48	0
55	MG	BB	201	1/1	0.92	0.09	90,90,90,90	0
55	MG	AA	3220	1/1	0.92	0.17	70,70,70,70	0
55	MG	BA	3261	1/1	0.92	0.19	65,65,65,65	0
55	MG	AA	3156	1/1	0.92	0.16	94,94,94,94	0
55	MG	BA	3042	1/1	0.92	0.10	86,86,86,86	0
55	MG	CA	1710	1/1	0.92	0.20	81,81,81,81	0
56	PAR	DA	1805	42/42	0.92	0.07	46,59,73,84	0
57	ZN	CG	303	1/1	0.92	0.24	95,95,95,95	0
55	MG	AA	3207	1/1	0.93	0.09	50,50,50,50	0
55	MG	AA	3595	1/1	0.93	0.30	79,79,79,79	0
55	MG	BA	3271	1/1	0.93	0.19	84,84,84,84	0
55	MG	AA	3101	1/1	0.93	0.13	79,79,79,79	0
55	MG	CA	1796	1/1	0.93	0.20	82,82,82,82	0
55	MG	BA	3147	1/1	0.93	0.23	63,63,63,63	0
55	MG	BA	3204	1/1	0.93	0.23	74,74,74,74	0
55	MG	AA	3147	1/1	0.93	0.29	89,89,89,89	0
55	MG	BA	3014	1/1	0.93	0.17	72,72,72,72	0
55	MG	BA	3207	1/1	0.93	0.15	46,46,46,46	0
55	MG	BA	3208	1/1	0.93	0.18	57,57,57,57	0
55	MG	BA	3015	1/1	0.93	0.15	71,71,71,71	0
55	MG	CA	1650	1/1	0.93	0.25	73,73,73,73	0
55	MG	AA	3214	1/1	0.93	0.31	47,47,47,47	0
55	MG	DA	1632	1/1	0.93	0.13	84,84,84,84	0
55	MG	AA	3090	1/1	0.93	0.18	45,45,45,45	0
55	MG	BA	3059	1/1	0.93	0.16	50,50,50,50	0
55	MG	CA	1811	1/1	0.93	0.18	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1812	1/1	0.93	0.27	84,84,84,84	0
55	MG	BA	3403	1/1	0.93	0.13	77,77,77,77	0
55	MG	DA	1638	1/1	0.93	0.15	74,74,74,74	0
55	MG	DA	1742	1/1	0.93	0.20	82,82,82,82	0
55	MG	BA	3286	1/1	0.93	0.12	85,85,85,85	0
55	MG	AA	3009	1/1	0.93	0.17	63,63,63,63	0
55	MG	BB	203	1/1	0.93	0.17	76,76,76,76	0
55	MG	AA	3026	1/1	0.93	0.08	40,40,40,40	0
55	MG	BA	3022	1/1	0.93	0.12	75,75,75,75	0
55	MG	DA	1749	1/1	0.93	0.21	101,101,101,101	0
55	MG	AA	3476	1/1	0.93	0.23	79,79,79,79	0
55	MG	AA	3240	1/1	0.93	0.14	80,80,80,80	0
55	MG	AA	3395	1/1	0.93	0.19	80,80,80,80	0
55	MG	AA	3561	1/1	0.93	0.12	82,82,82,82	0
55	MG	DA	1755	1/1	0.93	0.23	79,79,79,79	0
55	MG	BA	3353	1/1	0.93	0.22	84,84,84,84	0
55	MG	BB	211	1/1	0.93	0.30	71,71,71,71	0
55	MG	CA	1744	1/1	0.93	0.30	57,57,57,57	0
55	MG	CA	1827	1/1	0.93	0.11	89,89,89,89	0
55	MG	CA	1671	1/1	0.93	0.10	72,72,72,72	0
55	MG	AA	3563	1/1	0.93	0.19	52,52,52,52	0
55	MG	BA	3230	1/1	0.93	0.16	68,68,68,68	0
55	MG	AA	3004	1/1	0.93	0.19	40,40,40,40	0
55	MG	BA	3071	1/1	0.93	0.13	78,78,78,78	0
55	MG	CA	1833	1/1	0.93	0.11	95,95,95,95	0
55	MG	BE	302	1/1	0.93	0.14	76,76,76,76	0
55	MG	BA	3171	1/1	0.93	0.14	63,63,63,63	0
55	MG	BA	3113	1/1	0.93	0.17	84,84,84,84	0
55	MG	AA	3360	1/1	0.93	0.18	63,63,63,63	0
55	MG	AA	3533	1/1	0.93	0.13	67,67,67,67	0
55	MG	CA	1840	1/1	0.93	0.17	69,69,69,69	0
55	MG	AA	3534	1/1	0.93	0.17	49,49,49,49	0
55	MG	BA	3480	1/1	0.93	0.20	56,56,56,56	0
55	MG	CN	201	1/1	0.93	0.10	78,78,78,78	0
55	MG	AA	3379	1/1	0.93	0.24	66,66,66,66	0
55	MG	BA	3244	1/1	0.93	0.21	54,54,54,54	0
55	MG	CA	1608	1/1	0.93	0.15	68,68,68,68	0
55	MG	AA	3133	1/1	0.93	0.24	46,46,46,46	0
55	MG	CA	1611	1/1	0.93	0.15	97,97,97,97	0
55	MG	AA	3073	1/1	0.93	0.37	97,97,97,97	0
55	MG	AA	3223	1/1	0.93	0.27	71,71,71,71	0
55	MG	AA	3028	1/1	0.93	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1786	1/1	0.93	0.23	86,86,86,86	0
55	MG	CA	1691	1/1	0.93	0.16	56,56,56,56	0
55	MG	BA	3491	1/1	0.93	0.08	49,49,49,49	0
55	MG	AA	3022	1/1	0.93	0.12	49,49,49,49	0
55	MG	BA	3253	1/1	0.93	0.24	66,66,66,66	0
55	MG	AA	3588	1/1	0.93	0.18	68,68,68,68	0
55	MG	CC	105	1/1	0.93	0.10	105,105,105,105	0
55	MG	CA	1772	1/1	0.93	0.07	83,83,83,83	0
55	MG	DA	1697	1/1	0.93	0.06	111,111,111,111	0
55	MG	BA	3497	1/1	0.93	0.19	63,63,63,63	0
55	MG	DA	1700	1/1	0.93	0.23	94,94,94,94	0
55	MG	AA	3086	1/1	0.93	0.32	62,62,62,62	0
55	MG	AA	3591	1/1	0.93	0.13	74,74,74,74	0
55	MG	BA	3132	1/1	0.93	0.17	54,54,54,54	0
55	MG	CA	1777	1/1	0.93	0.16	92,92,92,92	0
55	MG	BA	3046	1/1	0.93	0.19	83,83,83,83	0
55	MG	BA	3325	1/1	0.93	0.30	50,50,50,50	0
55	MG	DA	1707	1/1	0.93	0.15	95,95,95,95	0
55	MG	CA	1626	1/1	0.93	0.12	88,88,88,88	0
55	MG	BA	3001	1/1	0.93	0.17	64,64,64,64	0
55	MG	DA	1608	1/1	0.93	0.15	92,92,92,92	0
55	MG	BA	3137	1/1	0.93	0.19	48,48,48,48	0
55	MG	BA	3002	1/1	0.93	0.17	66,66,66,66	0
55	MG	BA	3049	1/1	0.93	0.11	86,86,86,86	0
55	MG	CA	1786	1/1	0.93	0.10	74,74,74,74	0
55	MG	AA	3001	1/1	0.93	0.28	44,44,44,44	0
55	MG	CA	1634	1/1	0.93	0.21	60,60,60,60	0
55	MG	CA	1789	1/1	0.93	0.06	71,71,71,71	0
55	MG	BA	3511	1/1	0.93	0.25	68,68,68,68	0
55	MG	AA	3525	1/1	0.94	0.09	73,73,73,73	0
55	MG	AA	3195	1/1	0.94	0.16	62,62,62,62	0
55	MG	AA	3350	1/1	0.94	0.14	90,90,90,90	0
55	MG	A5	102	1/1	0.94	0.24	83,83,83,83	0
55	MG	AA	3310	1/1	0.94	0.12	65,65,65,65	0
55	MG	BA	3466	1/1	0.94	0.11	73,73,73,73	0
55	MG	BA	3218	1/1	0.94	0.24	51,51,51,51	0
55	MG	AA	3010	1/1	0.94	0.19	47,47,47,47	0
55	MG	CA	1702	1/1	0.94	0.09	71,71,71,71	0
55	MG	DA	1724	1/1	0.94	0.28	72,72,72,72	0
55	MG	BA	3069	1/1	0.94	0.11	70,70,70,70	0
55	MG	AA	3011	1/1	0.94	0.20	37,37,37,37	0
55	MG	AA	3054	1/1	0.94	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3224	1/1	0.94	0.16	51,51,51,51	0
55	MG	AA	3314	1/1	0.94	0.22	80,80,80,80	0
55	MG	AA	3238	1/1	0.94	0.24	82,82,82,82	0
55	MG	BA	3227	1/1	0.94	0.31	50,50,50,50	0
55	MG	CA	1800	1/1	0.94	0.10	104,104,104,104	0
55	MG	CA	1713	1/1	0.94	0.18	83,83,83,83	0
55	MG	BA	3315	1/1	0.94	0.13	91,91,91,91	0
55	MG	AA	3606	1/1	0.94	0.26	61,61,61,61	0
55	MG	AA	3105	1/1	0.94	0.19	61,61,61,61	0
55	MG	BA	3013	1/1	0.94	0.17	74,74,74,74	0
55	MG	AA	3093	1/1	0.94	0.27	65,65,65,65	0
55	MG	CA	1807	1/1	0.94	0.19	64,64,64,64	0
55	MG	BA	3323	1/1	0.94	0.27	74,74,74,74	0
55	MG	AA	3204	1/1	0.94	0.19	44,44,44,44	0
55	MG	BA	3237	1/1	0.94	0.17	47,47,47,47	0
55	MG	BA	3238	1/1	0.94	0.30	66,66,66,66	0
55	MG	AA	3484	1/1	0.94	0.10	44,44,44,44	0
55	MG	BA	3153	1/1	0.94	0.29	77,77,77,77	0
55	MG	AA	3205	1/1	0.94	0.23	55,55,55,55	0
55	MG	AA	3005	1/1	0.94	0.14	25,25,25,25	0
55	MG	AA	3281	1/1	0.94	0.21	74,74,74,74	0
55	MG	AA	3029	1/1	0.94	0.12	46,46,46,46	0
55	MG	DA	1752	1/1	0.94	0.21	89,89,89,89	0
55	MG	DA	1651	1/1	0.94	0.17	72,72,72,72	0
55	MG	AA	3210	1/1	0.94	0.19	72,72,72,72	0
55	MG	DA	1653	1/1	0.94	0.15	96,96,96,96	0
55	MG	AA	3111	1/1	0.94	0.26	36,36,36,36	0
55	MG	AA	3181	1/1	0.94	0.17	66,66,66,66	0
55	MG	AA	3112	1/1	0.94	0.34	45,45,45,45	0
55	MG	CA	1642	1/1	0.94	0.20	69,69,69,69	0
55	MG	BA	3029	1/1	0.94	0.23	75,75,75,75	0
55	MG	BA	3165	1/1	0.94	0.18	42,42,42,42	0
55	MG	CA	1826	1/1	0.94	0.19	81,81,81,81	0
55	MG	AA	3622	1/1	0.94	0.18	65,65,65,65	0
55	MG	AA	3014	1/1	0.94	0.20	38,38,38,38	0
55	MG	AA	3217	1/1	0.94	0.07	64,64,64,64	0
55	MG	AA	3555	1/1	0.94	0.19	67,67,67,67	0
55	MG	BA	3259	1/1	0.94	0.15	54,54,54,54	0
55	MG	BA	3510	1/1	0.94	0.24	67,67,67,67	0
55	MG	AA	3006	1/1	0.94	0.37	46,46,46,46	0
55	MG	AA	3157	1/1	0.94	0.19	39,39,39,39	0
55	MG	BA	3262	1/1	0.94	0.06	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1836	1/1	0.94	0.10	71,71,71,71	0
55	MG	AA	3162	1/1	0.94	0.19	45,45,45,45	0
55	MG	DA	1675	1/1	0.94	0.28	60,60,60,60	0
55	MG	BA	3428	1/1	0.94	0.07	89,89,89,89	0
55	MG	BA	3038	1/1	0.94	0.21	78,78,78,78	0
55	MG	BA	3178	1/1	0.94	0.20	62,62,62,62	0
55	MG	BA	3432	1/1	0.94	0.19	88,88,88,88	0
55	MG	CA	1662	1/1	0.94	0.28	81,81,81,81	0
55	MG	AA	3374	1/1	0.94	0.17	74,74,74,74	0
55	MG	AA	3334	1/1	0.94	0.36	76,76,76,76	0
55	MG	AA	3458	1/1	0.94	0.14	70,70,70,70	0
55	MG	AA	3293	1/1	0.94	0.08	77,77,77,77	0
55	MG	BA	3354	1/1	0.94	0.16	90,90,90,90	0
55	MG	AA	3034	1/1	0.94	0.25	52,52,52,52	0
55	MG	DA	1687	1/1	0.94	0.26	72,72,72,72	0
55	MG	BA	3185	1/1	0.94	0.25	68,68,68,68	0
55	MG	DA	1792	1/1	0.94	0.15	81,81,81,81	0
55	MG	DA	1689	1/1	0.94	0.20	72,72,72,72	0
55	MG	AA	3188	1/1	0.94	0.27	57,57,57,57	0
55	MG	DA	1691	1/1	0.94	0.25	82,82,82,82	0
55	MG	AA	3574	1/1	0.94	0.21	54,54,54,54	0
55	MG	AA	3025	1/1	0.94	0.18	40,40,40,40	0
55	MG	AA	3190	1/1	0.94	0.09	58,58,58,58	0
55	MG	AA	3464	1/1	0.94	0.22	83,83,83,83	0
55	MG	AA	3581	1/1	0.94	0.11	36,36,36,36	0
55	MG	AA	3226	1/1	0.94	0.13	77,77,77,77	0
55	MG	AA	3100	1/1	0.94	0.28	67,67,67,67	0
55	MG	AA	3192	1/1	0.94	0.18	63,63,63,63	0
55	MG	AE	301	1/1	0.94	0.14	65,65,65,65	0
55	MG	AA	3229	1/1	0.94	0.09	89,89,89,89	0
55	MG	AA	3267	1/1	0.94	0.17	62,62,62,62	0
55	MG	AA	3517	1/1	0.94	0.08	66,66,66,66	0
55	MG	DA	1602	1/1	0.94	0.23	85,85,85,85	0
55	MG	BA	3120	1/1	0.94	0.18	81,81,81,81	0
55	MG	BA	3203	1/1	0.94	0.25	53,53,53,53	0
55	MG	DC	102	1/1	0.94	0.18	74,74,74,74	0
55	MG	AA	3519	1/1	0.94	0.10	53,53,53,53	0
55	MG	DC	105	1/1	0.94	0.22	75,75,75,75	0
55	MG	AA	3306	1/1	0.94	0.22	65,65,65,65	0
55	MG	BP	201	1/1	0.94	0.09	65,65,65,65	0
55	MG	AO	202	1/1	0.94	0.34	80,80,80,80	0
55	MG	AA	3135	1/1	0.94	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3038	1/1	0.94	0.34	80,80,80,80	0
55	MG	BA	3134	1/1	0.95	0.16	63,63,63,63	0
55	MG	AA	3565	1/1	0.95	0.27	53,53,53,53	0
55	MG	DA	1645	1/1	0.95	0.19	51,51,51,51	0
55	MG	DA	1646	1/1	0.95	0.18	65,65,65,65	0
55	MG	AA	3569	1/1	0.95	0.19	60,60,60,60	0
55	MG	BA	3138	1/1	0.95	0.16	52,52,52,52	0
55	MG	DA	1737	1/1	0.95	0.26	74,74,74,74	0
55	MG	AA	3153	1/1	0.95	0.14	48,48,48,48	0
55	MG	AA	3572	1/1	0.95	0.27	54,54,54,54	0
55	MG	A1	201	1/1	0.95	0.29	64,64,64,64	0
55	MG	BA	3268	1/1	0.95	0.11	59,59,59,59	0
55	MG	BA	3400	1/1	0.95	0.19	74,74,74,74	0
55	MG	BA	3143	1/1	0.95	0.13	63,63,63,63	0
55	MG	AA	3012	1/1	0.95	0.18	40,40,40,40	0
55	MG	AA	3299	1/1	0.95	0.16	79,79,79,79	0
55	MG	AA	3139	1/1	0.95	0.15	54,54,54,54	0
55	MG	BR	201	1/1	0.95	0.06	77,77,77,77	0
55	MG	AA	3042	1/1	0.95	0.05	77,77,77,77	0
55	MG	AA	3002	1/1	0.95	0.19	41,41,41,41	0
55	MG	AA	3434	1/1	0.95	0.24	44,44,44,44	0
55	MG	AA	3243	1/1	0.95	0.18	51,51,51,51	0
55	MG	BA	3409	1/1	0.95	0.19	71,71,71,71	0
55	MG	CA	1603	1/1	0.95	0.15	73,73,73,73	0
55	MG	AA	3263	1/1	0.95	0.16	51,51,51,51	0
55	MG	AA	3174	1/1	0.95	0.25	40,40,40,40	0
55	MG	AA	3158	1/1	0.95	0.09	68,68,68,68	0
55	MG	DA	1673	1/1	0.95	0.13	88,88,88,88	0
55	MG	BA	3100	1/1	0.95	0.27	66,66,66,66	0
55	MG	CA	1769	1/1	0.95	0.04	79,79,79,79	0
55	MG	AA	3545	1/1	0.95	0.15	75,75,75,75	0
55	MG	BA	3219	1/1	0.95	0.13	48,48,48,48	0
55	MG	AA	3485	1/1	0.95	0.19	71,71,71,71	0
55	MG	BA	3009	1/1	0.95	0.17	48,48,48,48	0
55	MG	AA	3061	1/1	0.95	0.19	79,79,79,79	0
55	MG	BA	3488	1/1	0.95	0.09	59,59,59,59	0
55	MG	BA	3160	1/1	0.95	0.18	82,82,82,82	0
55	MG	BA	3012	1/1	0.95	0.28	63,63,63,63	0
55	MG	AA	3179	1/1	0.95	0.15	53,53,53,53	0
55	MG	AA	3593	1/1	0.95	0.33	95,95,95,95	0
55	MG	AA	3551	1/1	0.95	0.24	69,69,69,69	0
55	MG	BA	3061	1/1	0.95	0.05	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1773	1/1	0.95	0.29	69,69,69,69	0
55	MG	BA	3016	1/1	0.95	0.06	56,56,56,56	0
55	MG	BA	3168	1/1	0.95	0.15	60,60,60,60	0
55	MG	DA	1776	1/1	0.95	0.10	70,70,70,70	0
55	MG	BA	3232	1/1	0.95	0.18	55,55,55,55	0
55	MG	AA	3488	1/1	0.95	0.07	93,93,93,93	0
55	MG	CA	1706	1/1	0.95	0.14	91,91,91,91	0
55	MG	CA	1707	1/1	0.95	0.23	78,78,78,78	0
55	MG	AA	3331	1/1	0.95	0.21	76,76,76,76	0
55	MG	AA	3106	1/1	0.95	0.17	69,69,69,69	0
55	MG	DA	1696	1/1	0.95	0.19	66,66,66,66	0
55	MG	BA	3366	1/1	0.95	0.24	76,76,76,76	0
55	MG	BA	3173	1/1	0.95	0.23	50,50,50,50	0
55	MG	CA	1632	1/1	0.95	0.12	76,76,76,76	0
55	MG	AA	3071	1/1	0.95	0.23	56,56,56,56	0
55	MG	CA	1795	1/1	0.95	0.14	68,68,68,68	0
55	MG	AA	3233	1/1	0.95	0.12	55,55,55,55	0
55	MG	DA	1791	1/1	0.95	0.21	80,80,80,80	0
55	MG	AA	3127	1/1	0.95	0.22	53,53,53,53	0
55	MG	BA	3437	1/1	0.95	0.21	73,73,73,73	0
55	MG	AA	3128	1/1	0.95	0.17	56,56,56,56	0
55	MG	BA	3309	1/1	0.95	0.23	80,80,80,80	0
55	MG	BA	3026	1/1	0.95	0.22	72,72,72,72	0
55	MG	BA	3514	1/1	0.95	0.24	51,51,51,51	0
55	MG	AA	3496	1/1	0.95	0.18	87,87,87,87	0
55	MG	DA	1799	1/1	0.95	0.18	68,68,68,68	0
55	MG	AA	3294	1/1	0.95	0.39	93,93,93,93	0
55	MG	AA	3605	1/1	0.95	0.29	72,72,72,72	0
55	MG	AA	3219	1/1	0.95	0.23	81,81,81,81	0
55	MG	AD	301	1/1	0.95	0.07	99,99,99,99	0
55	MG	BA	3250	1/1	0.95	0.16	58,58,58,58	0
55	MG	AA	3608	1/1	0.95	0.12	41,41,41,41	0
55	MG	BA	3252	1/1	0.95	0.20	86,86,86,86	0
55	MG	BA	3382	1/1	0.95	0.18	89,89,89,89	0
55	MG	BA	3319	1/1	0.95	0.27	68,68,68,68	0
55	MG	AA	3151	1/1	0.95	0.26	58,58,58,58	0
55	MG	AA	3610	1/1	0.95	0.08	46,46,46,46	0
55	MG	BA	3128	1/1	0.95	0.11	56,56,56,56	0
55	MG	BA	3130	1/1	0.95	0.13	44,44,44,44	0
55	MG	CA	1657	1/1	0.95	0.19	63,63,63,63	0
55	MG	AA	3450	1/1	0.95	0.21	72,72,72,72	0
55	MG	CA	1659	1/1	0.95	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BB	202	1/1	0.95	0.06	103,103,103,103	0
55	MG	AF	302	1/1	0.95	0.14	93,93,93,93	0
56	PAR	CA	1841	42/42	0.95	0.07	40,56,74,83	0
55	MG	BA	3391	1/1	0.95	0.11	95,95,95,95	0
55	MG	CA	1663	1/1	0.95	0.10	52,52,52,52	0
55	MG	AA	3036	1/1	0.96	0.06	39,39,39,39	0
55	MG	BA	3284	1/1	0.96	0.08	61,61,61,61	0
55	MG	BA	3079	1/1	0.96	0.12	82,82,82,82	0
55	MG	AA	3015	1/1	0.96	0.20	44,44,44,44	0
55	MG	AA	3206	1/1	0.96	0.09	51,51,51,51	0
55	MG	DA	1622	1/1	0.96	0.10	98,98,98,98	0
55	MG	AA	3089	1/1	0.96	0.26	64,64,64,64	0
55	MG	AA	3208	1/1	0.96	0.12	44,44,44,44	0
55	MG	BA	3234	1/1	0.96	0.22	67,67,67,67	0
55	MG	AA	3030	1/1	0.96	0.13	45,45,45,45	0
55	MG	BA	3236	1/1	0.96	0.34	41,41,41,41	0
55	MG	BA	3086	1/1	0.96	0.52	82,82,82,82	0
55	MG	AA	3323	1/1	0.96	0.07	71,71,71,71	0
55	MG	AA	3170	1/1	0.96	0.15	41,41,41,41	0
55	MG	AA	3516	1/1	0.96	0.20	76,76,76,76	0
55	MG	BA	3136	1/1	0.96	0.10	43,43,43,43	0
55	MG	BA	3186	1/1	0.96	0.23	52,52,52,52	0
55	MG	CA	1641	1/1	0.96	0.10	65,65,65,65	0
55	MG	BA	3006	1/1	0.96	0.07	47,47,47,47	0
55	MG	BA	3007	1/1	0.96	0.06	83,83,83,83	0
55	MG	AA	3152	1/1	0.96	0.28	58,58,58,58	0
55	MG	BA	3190	1/1	0.96	0.11	73,73,73,73	0
55	MG	AA	3352	1/1	0.96	0.14	52,52,52,52	0
55	MG	AA	3212	1/1	0.96	0.15	52,52,52,52	0
55	MG	BA	3364	1/1	0.96	0.12	76,76,76,76	0
55	MG	DA	1779	1/1	0.96	0.20	91,91,91,91	0
55	MG	BA	3011	1/1	0.96	0.23	65,65,65,65	0
55	MG	BA	3096	1/1	0.96	0.20	89,89,89,89	0
55	MG	AA	3302	1/1	0.96	0.16	104,104,104,104	0
55	MG	AA	3523	1/1	0.96	0.12	91,91,91,91	0
55	MG	CA	1717	1/1	0.96	0.14	69,69,69,69	0
55	MG	DA	1647	1/1	0.96	0.10	71,71,71,71	0
55	MG	BA	3254	1/1	0.96	0.32	69,69,69,69	0
55	MG	AA	3031	1/1	0.96	0.20	52,52,52,52	0
55	MG	AA	3257	1/1	0.96	0.15	79,79,79,79	0
55	MG	BA	3482	1/1	0.96	0.14	65,65,65,65	0
55	MG	AA	3069	1/1	0.96	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BE	303	1/1	0.96	0.19	57,57,57,57	0
55	MG	BA	3017	1/1	0.96	0.19	50,50,50,50	0
55	MG	AA	3053	1/1	0.96	0.47	67,67,67,67	0
55	MG	AA	3562	1/1	0.96	0.12	82,82,82,82	0
55	MG	AA	3175	1/1	0.96	0.10	45,45,45,45	0
55	MG	BA	3154	1/1	0.96	0.09	46,46,46,46	0
55	MG	AA	3046	1/1	0.96	0.07	57,57,57,57	0
55	MG	BA	3492	1/1	0.96	0.18	47,47,47,47	0
55	MG	AA	3607	1/1	0.96	0.15	44,44,44,44	0
55	MG	BA	3023	1/1	0.96	0.26	70,70,70,70	0
55	MG	AA	3035	1/1	0.96	0.13	45,45,45,45	0
55	MG	AA	3143	1/1	0.96	0.17	35,35,35,35	0
55	MG	AA	3287	1/1	0.96	0.20	69,69,69,69	0
55	MG	AA	3144	1/1	0.96	0.27	45,45,45,45	0
55	MG	CA	1610	1/1	0.96	0.18	54,54,54,54	0
55	MG	DA	1671	1/1	0.96	0.25	77,77,77,77	0
55	MG	AA	3573	1/1	0.96	0.17	31,31,31,31	0
55	MG	BA	3501	1/1	0.96	0.07	88,88,88,88	0
55	MG	BA	3216	1/1	0.96	0.20	56,56,56,56	0
55	MG	AA	3338	1/1	0.96	0.18	51,51,51,51	0
55	MG	AA	3265	1/1	0.96	0.12	95,95,95,95	0
55	MG	AA	3082	1/1	0.96	0.21	50,50,50,50	0
55	MG	DC	103	1/1	0.96	0.23	78,78,78,78	0
55	MG	BA	3166	1/1	0.96	0.16	40,40,40,40	0
55	MG	CA	1808	1/1	0.96	0.17	67,67,67,67	0
55	MG	AA	3146	1/1	0.96	0.17	65,65,65,65	0
55	MG	AA	3578	1/1	0.96	0.20	50,50,50,50	0
55	MG	AA	3539	1/1	0.96	0.15	49,49,49,49	0
55	MG	AA	3582	1/1	0.96	0.14	44,44,44,44	0
55	MG	CA	1749	1/1	0.96	0.13	62,62,62,62	0
55	MG	AA	3041	1/1	0.96	0.17	66,66,66,66	0
57	ZN	CQ	103	1/1	0.96	0.08	144,144,144,144	0
57	ZN	DG	303	1/1	0.96	0.18	134,134,134,134	0
55	MG	AA	3549	1/1	0.97	0.35	50,50,50,50	0
55	MG	CA	1708	1/1	0.97	0.18	45,45,45,45	0
55	MG	AA	3571	1/1	0.97	0.10	52,52,52,52	0
55	MG	BA	3217	1/1	0.97	0.10	39,39,39,39	0
55	MG	BA	3295	1/1	0.97	0.09	58,58,58,58	0
55	MG	AA	3550	1/1	0.97	0.23	39,39,39,39	0
55	MG	AA	3020	1/1	0.97	0.15	39,39,39,39	0
55	MG	AA	3520	1/1	0.97	0.20	68,68,68,68	0
55	MG	AA	3018	1/1	0.97	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3300	1/1	0.97	0.16	56,56,56,56	0
55	MG	CA	1664	1/1	0.97	0.07	47,47,47,47	0
55	MG	AE	302	1/1	0.97	0.21	45,45,45,45	0
55	MG	AA	3244	1/1	0.97	0.23	45,45,45,45	0
55	MG	AA	3140	1/1	0.97	0.17	67,67,67,67	0
55	MG	BA	3126	1/1	0.97	0.12	51,51,51,51	0
55	MG	BA	3430	1/1	0.97	0.05	89,89,89,89	0
55	MG	BA	3388	1/1	0.97	0.23	87,87,87,87	0
55	MG	AA	3538	1/1	0.97	0.17	36,36,36,36	0
55	MG	BA	3264	1/1	0.97	0.14	59,59,59,59	0
55	MG	AA	3579	1/1	0.97	0.10	39,39,39,39	0
55	MG	AA	3603	1/1	0.97	0.24	41,41,41,41	0
55	MG	BA	3229	1/1	0.97	0.21	50,50,50,50	0
55	MG	AA	3161	1/1	0.97	0.15	42,42,42,42	0
55	MG	AA	3088	1/1	0.97	0.09	42,42,42,42	0
55	MG	CA	1627	1/1	0.97	0.14	65,65,65,65	0
55	MG	AA	3541	1/1	0.97	0.12	48,48,48,48	0
55	MG	AA	3399	1/1	0.97	0.14	60,60,60,60	0
55	MG	BA	3198	1/1	0.97	0.13	44,44,44,44	0
55	MG	AA	3199	1/1	0.97	0.27	46,46,46,46	0
55	MG	BA	3486	1/1	0.97	0.13	30,30,30,30	0
55	MG	BA	3487	1/1	0.97	0.11	66,66,66,66	0
55	MG	AA	3200	1/1	0.97	0.22	71,71,71,71	0
55	MG	AA	3491	1/1	0.97	0.16	85,85,85,85	0
55	MG	BA	3169	1/1	0.97	0.20	56,56,56,56	0
55	MG	AA	3083	1/1	0.97	0.17	34,34,34,34	0
55	MG	BA	3140	1/1	0.97	0.17	42,42,42,42	0
55	MG	BA	3493	1/1	0.97	0.13	39,39,39,39	0
55	MG	BA	3321	1/1	0.97	0.04	59,59,59,59	0
55	MG	A5	101	1/1	0.97	0.11	51,51,51,51	0
55	MG	AA	3589	1/1	0.97	0.13	60,60,60,60	0
55	MG	BD	301	1/1	0.97	0.16	39,39,39,39	0
55	MG	DA	1699	1/1	0.97	0.17	68,68,68,68	0
55	MG	AB	210	1/1	0.97	0.38	65,65,65,65	0
55	MG	A7	101	1/1	0.97	0.21	60,60,60,60	0
55	MG	CA	1646	1/1	0.97	0.18	75,75,75,75	0
55	MG	BA	3283	1/1	0.97	0.11	43,43,43,43	0
55	MG	DA	1648	1/1	0.97	0.11	69,69,69,69	0
55	MG	DA	1649	1/1	0.97	0.10	93,93,93,93	0
55	MG	BA	3209	1/1	0.97	0.16	46,46,46,46	0
55	MG	AA	3007	1/1	0.97	0.09	42,42,42,42	0
55	MG	BA	3211	1/1	0.97	0.14	57,57,57,57	0

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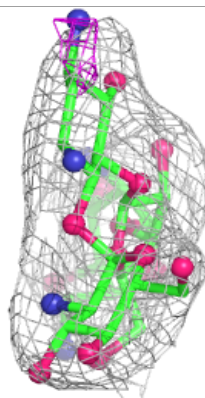
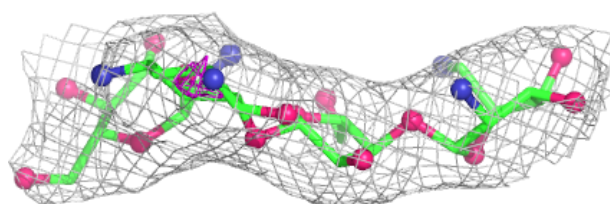
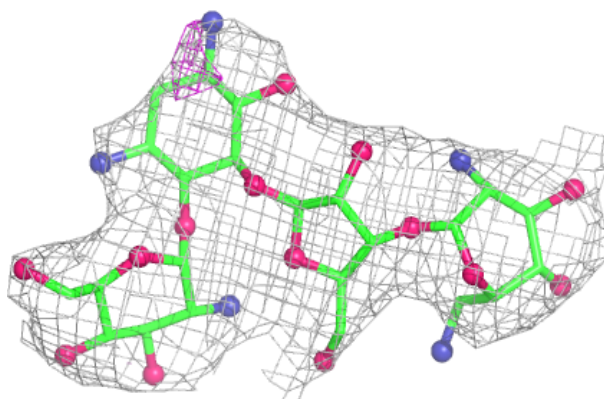
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3568	1/1	0.97	0.14	49,49,49,49	0
55	MG	AA	3518	1/1	0.97	0.26	90,90,90,90	0
55	MG	BA	3031	1/1	0.97	0.20	60,60,60,60	0
55	MG	CA	1602	1/1	0.97	0.09	74,74,74,74	0
55	MG	BA	3508	1/1	0.98	0.34	73,73,73,73	0
55	MG	CA	1780	1/1	0.98	0.22	55,55,55,55	0
55	MG	AA	3202	1/1	0.98	0.13	46,46,46,46	0
55	MG	AA	3566	1/1	0.98	0.13	27,27,27,27	0
55	MG	AA	3567	1/1	0.98	0.15	39,39,39,39	0
55	MG	BA	3322	1/1	0.98	0.16	79,79,79,79	0
55	MG	BA	3129	1/1	0.98	0.11	41,41,41,41	0
55	MG	DA	1744	1/1	0.98	0.27	57,57,57,57	0
55	MG	CA	1606	1/1	0.98	0.08	94,94,94,94	0
55	MG	AA	3213	1/1	0.98	0.27	59,59,59,59	0
55	MG	A7	102	1/1	0.98	0.23	68,68,68,68	0
55	MG	BA	3285	1/1	0.98	0.06	45,45,45,45	0
55	MG	BA	3249	1/1	0.98	0.12	40,40,40,40	0
55	MG	BA	3181	1/1	0.98	0.09	49,49,49,49	0
55	MG	AA	3580	1/1	0.98	0.07	78,78,78,78	0
55	MG	AA	3021	1/1	0.98	0.15	42,42,42,42	0
55	MG	AA	3269	1/1	0.98	0.26	55,55,55,55	0
55	MG	A0	201	1/1	0.98	0.11	62,62,62,62	0
55	MG	DA	1670	1/1	0.98	0.22	49,49,49,49	0
55	MG	BE	301	1/1	0.98	0.14	54,54,54,54	0
55	MG	BA	3292	1/1	0.98	0.27	51,51,51,51	0
55	MG	AA	3084	1/1	0.98	0.07	43,43,43,43	0
55	MG	CA	1619	1/1	0.98	0.14	59,59,59,59	0
55	MG	AA	3159	1/1	0.98	0.05	28,28,28,28	0
55	MG	AA	3400	1/1	0.98	0.21	39,39,39,39	0
55	MG	AA	3160	1/1	0.98	0.12	32,32,32,32	0
55	MG	AA	3230	1/1	0.98	0.07	34,34,34,34	0
55	MG	CA	1699	1/1	0.98	0.09	63,63,63,63	0
55	MG	BA	3080	1/1	0.98	0.11	72,72,72,72	0
55	MG	AA	3110	1/1	0.99	0.03	40,40,40,40	0
55	MG	BA	3131	1/1	0.99	0.10	49,49,49,49	0
55	MG	AA	3178	1/1	0.99	0.06	54,54,54,54	0
55	MG	AA	3138	1/1	0.99	0.25	45,45,45,45	0
57	ZN	DQ	101	1/1	0.99	0.05	118,118,118,118	0

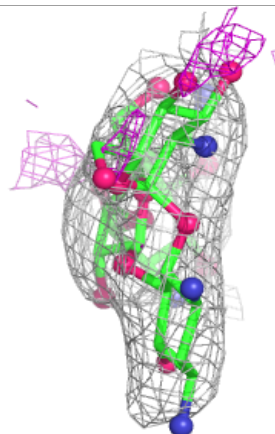
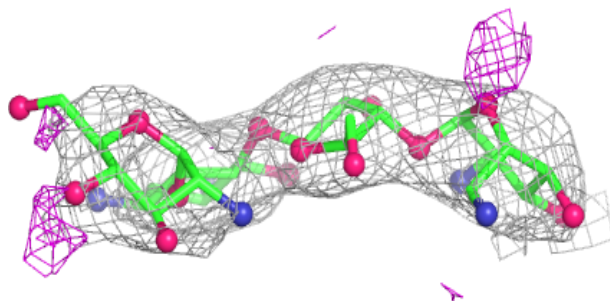
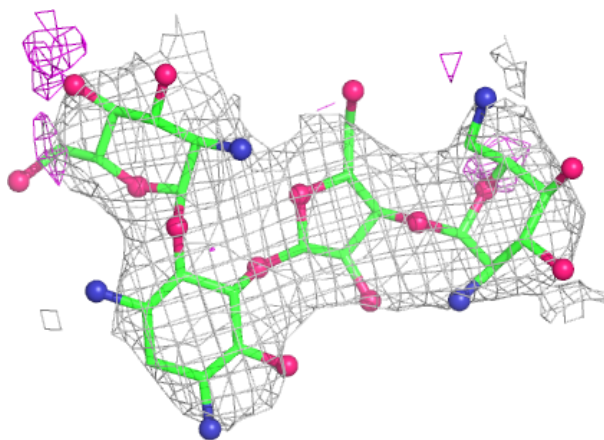
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR DA 1805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PAR CA 1841:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.