



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:18 PM UTC

PDB ID : 4V8C / pdb_00004v8c
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

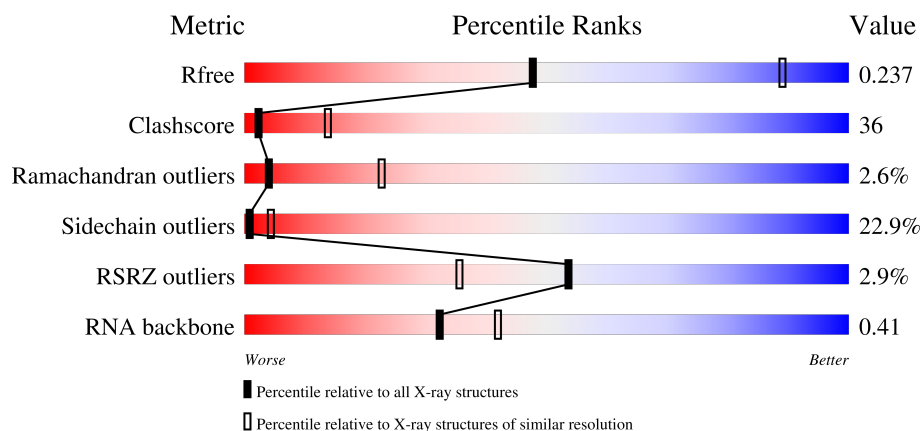
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



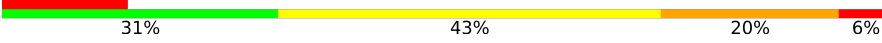
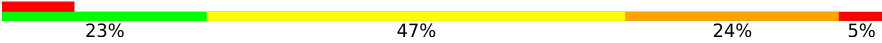
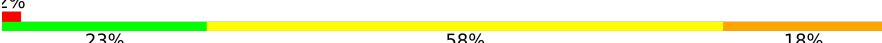
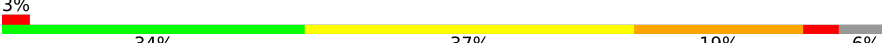
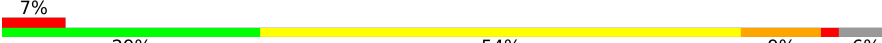
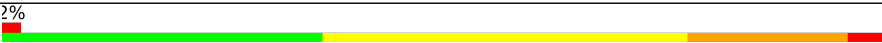
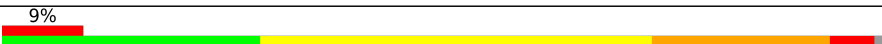
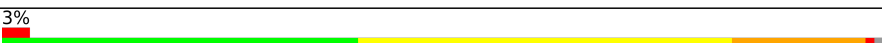
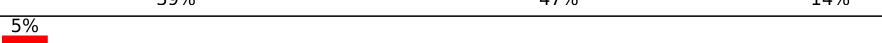
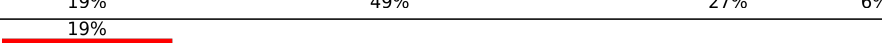
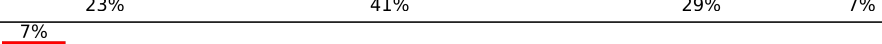
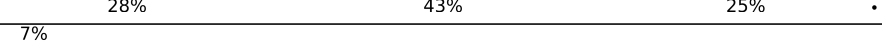
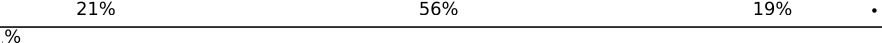
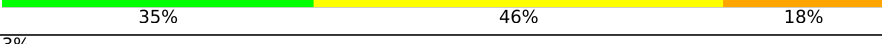
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	29% 52% 19%
1	BA	2912	28% 53% 19%
2	AB	122	% 31% 49% 20%
2	BB	122	% 25% 56% 20%

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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	 % 40% 42% 18%
53	CD	77	 19% 53% 27%
53	DC	77	 % 29% 55% 17%
53	DD	77	 % 19% 53% 27%
54	C1	10	 10% 20% 60% 20%
54	D1	10	 10% 20% 60% 20%

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

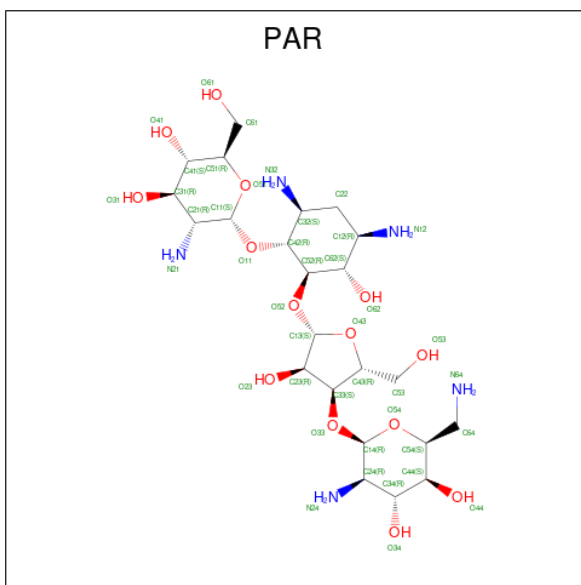
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	626	Total Mg 626 626	0	0
55	AB	17	Total Mg 17 17	0	0
55	AD	1	Total Mg 1 1	0	0
55	AE	4	Total Mg 4 4	0	0
55	AF	3	Total Mg 3 3	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A2	1	Total Mg 1 1	0	0
55	AU	1	Total Mg 1 1	0	0
55	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 (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

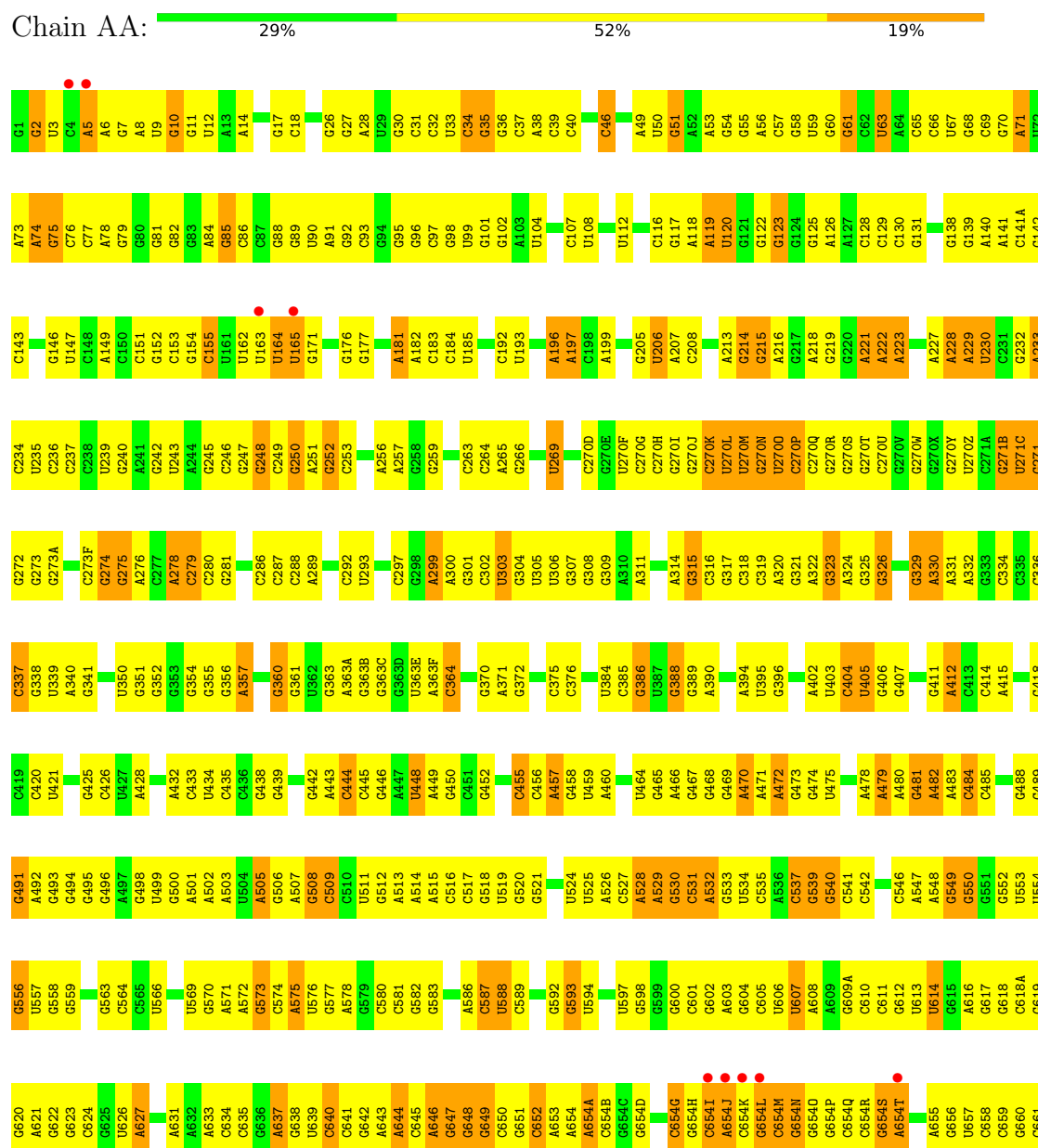
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

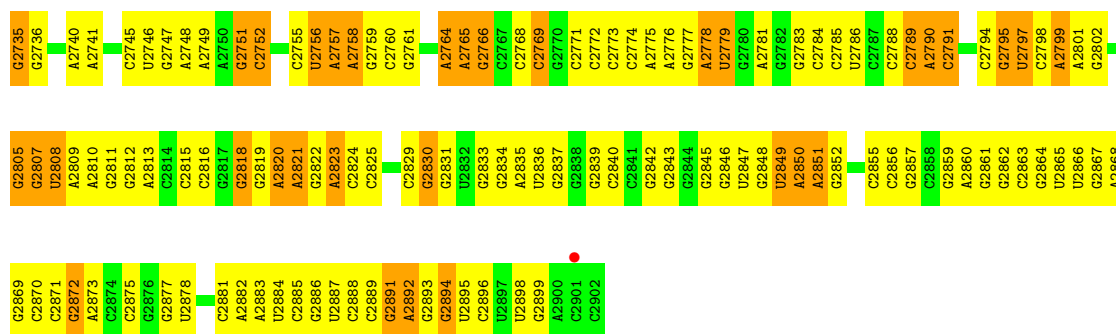
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (2912-MER)

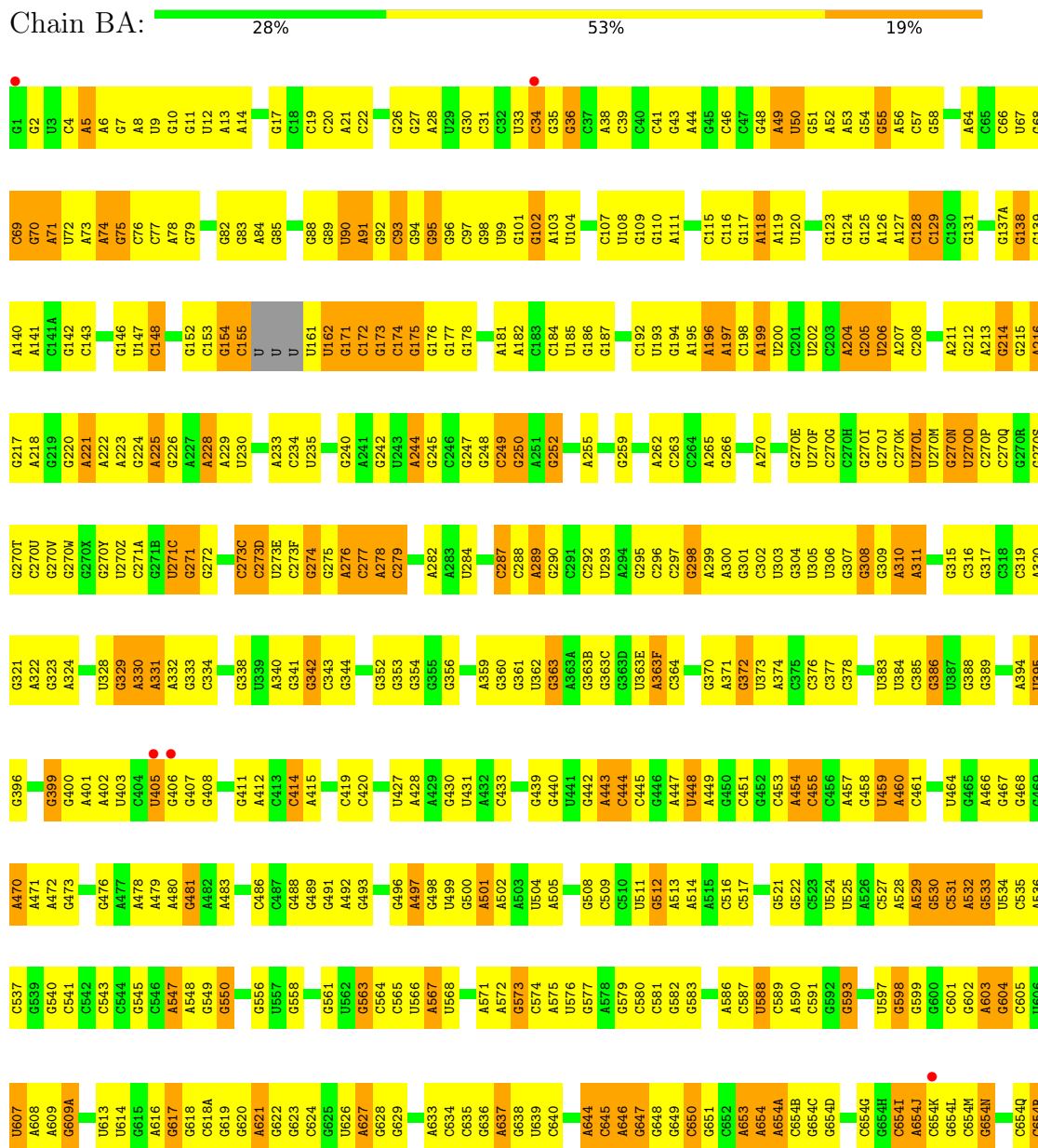


C1636	A1637	A1495	G1429	G1361	C1290	G1212	A1148	A1084	U1019	C955	C886	G818	A751	G662
A1638	A1496	C1430	C1430	G1365	C1291	G1215	G1149	A1085	A1020	G956	A887	A819	A752	G663
C1639	C1497	U1431	U1431	A1365	U1292	G1216	C1150	A1086	A1021	A957	C888	A820	C753	C664
C1640	C1498	C1432	C1432	G1368	C1293	C1217	G1151	A1087	G1022	U958	C889	A821	C754	C671
A1641	C1499	U1433	U1433	G1369	U1294	C1218	C1152	A1088	U1023	A959	A890	U822	C755	C672
G1642	G1501	G1435	G1435	G1372	G1295	G1219	C1153	A1089	G1024	A960	G892	G823	G760	C673
G1643	C1502	G1436	G1436	U1372	G1296	A1220	G1154	U1090	G1025	G961	C893	A824	A761	C674
G1647	U1503	C1437	C1437	A1373	C1297	A1227	A1156	G1092	U1026	G962	C894	G825	U762	A675
C1648	C1504	U1438	U1438	G1374	C1298	G1374	A1157	G1093	A1027	U963	A895	U826	G763	A676
G1649	C1505	A1439	A1439	C1375	U1300	G1228	G1158	U1094	A1028	C965	C897	U828	A764	C675
G1650	C1506	G1440	G1440	A1379	A1301	C1230	U1159	A1095	U1033	G966	C898	G831	G765	C683
G1651	A1507	G1441	G1441	G1380	A1302	G1231	G1160	A1096	G1036	C967	A899	G832	G766	G686
G1652	A1508	G1442	G1442	G1381	G1303	G1232	C1161	U1097	U1037	G968	A900	G833	G769	G690
G1653	C1509	G1443	G1443	G1382	G1310	C1233	G1162	A1098	G1038	C971	C902	U833	G770	C691
A1654	A1510	G1444	G1444	C1383	G1311	G1234	G1165	G1099	C1039	A972	G903	G834	G771	C692
A1655	G1511	A1444A	A1444A	C1384	U1312	U1234	U1166	C1100	G1042	A973	C904	C838	A774	C693
C1656	A1512	G1445	G1445	C1385	G1313	G1235	U1167	U1010	C1043	G974	U905	U839	G775	C694
C1657	C1513	G1446	G1446	C1386	U1314	G1236	G1168	C1102	G1044	G975	G906	C840	G776	C695
C1658	U1514	A1449	A1449	C1387	C1315	A1237	G1169	C1103	G1045	C976	U907	A841	G777	C696
U1659	C1515	G1449A	G1449A	C1388	U1316	G1238	G1170	A1045	G1046	G978	C908	G842	A778	C697
A1660	G1517	G1453	G1453	G1389	A1317	U1240	G1171	G1106	A1046	G979	A909	G843	G779	C698
G1661	C1518	U1454	U1454	G1390	C1318	A1241	G1172	G1107	G1047	A980	A910	C844	G780	C699
C1662	C1519	G1455	G1455	U1391	G1319	A1242	A1174	U108	A1048	A981	A911	C845	A781	C700
C1663	U1520	A1455	A1455	A1392	C1320	G1243	U1175	C1109	C1049	A982	C912	C846	G782	C701
A1664	G1521	C1458	C1458	A1393	A1321	G1244	G1176	G1110	A1050	C982	U913	U847	A783	G702
A1665	C1522	U1459	U1459	U1394	A1322	G1256	A1177	A1111	G1051	A983	C914	G848	G784	C703
C1666	G1525	A1460	A1460	A1395	U1323	G1257	C1178	G1112	C1052	A984	C915	A849	A785	A705
C1667	G1526	G1461	G1461	U1396	G1258	C1251	C1179	U1113	G1053	C985	G916	C850	G786	A706
A1668	G1527	C1462	C1462	C1397	U1326	G1252	C1180	G1117	A1054	C986	A917	U851	C787	C707
A1669	C1528	G1463	G1463	U1398	C1327	A1253	C1181	C1118	G1055	C987	A918	G852	A787	C708
C1670	A1529	C1464	C1464	C1399	U1328	G1256	U1182	C1119	G1056	A988	C919	G853	A789	C709
U1673	G1530	G1465	G1465	G1400	U1329	C1257	G1183	G1119	U1058	A990	U922	G854	G790	G710
G1674	C1531	C1467	C1467	A1402	A1331	G1258	C1185	G1122	G1059	C991	C923	C856	C791	G711
A1677	C1532	G1468	G1468	C1403	G1332	G1259	G1186	G1125	U1060	C992	G924	C857	G792	G715
G1678	C1533	A1469	A1469	C1404	A1336	G1260	G1187	A1126	U1061	C993	C925	U858	A793	A716
U1679	G1534	G1470	G1470	U1405	U1337	C1261	U1188	A1127	G1062	C994	A926	G859	G794	A717
C1680	A1536	A1471	A1471	U1406	G1337	A1262	A1189	G1128	G1063	C995	G928	U860	C795	A718
U1681	C1537	G1474	G1474	C1407	G1338	U1263	G1190	A1129	C1064	A996	G929	A861	C796	C719
C1684	G1538	C1475	C1475	C1408	G1339	G1264	G1191	U1129	U1065	C997	U930	G862	C797	C720
C1685	G1539	G1476	G1476	C1409	U1340	A1265	G1192	U1130	U1066	C998	G931	A863	G800	G728
C1686	C1540	A1477	A1477	G1410	U1341	G1266	G1193	G1131	A1067	U999	G932	G864	G801	G729
C1687	U1541	G1478	G1478	C1411	G1344	U1267	A1194	A1132	G1068	A1000	A933	C865	A802	C730
C1688	G1542	G1479	G1479	A1412	C1345	A1268	G1195	U1133	A1069	G1001	G938	A870	G805	C731
U1689	A1543	G1480	G1480	G1413	G1346	C1270	C1197	G1136	A1070	G1002	G941	U871	C806	C732
A1690	C1544	U1482	U1482	G1416	G1348	G1271	G1198	G1137	C1072	C1005	A941	A872	U807	A734
C1691	A1545	G1483	G1483	C1417	A1349	A1272	G1199	G1138	A1073	C1006	G942	G873	G808	G733
C1692	C1546	G1484	G1484	G1418	U1352	U1273	C1201	G1139	G1074	C1007	U943	G874	G809	A734
U1693	U1547	G1487	G1487	A1419	A1353	A1275	C1202	G1140	C1075	G944	G944	G875	G812	G738
C1694	C1548	G1488	G1488	U1420	U1354	U1276	G1203	U1141	C1076	A1010	A945	A879	U810	G739
A1695	G1549	U1489	U1489	G1421	G1355	A1277	A1204	U1142	A1077	G1011	G946	G880	U811	U740
G1695	C1550	G1490	G1490	G1424	G1356	G1278	G1206	A1142A	U1078	U1012	G946	G881	C812	C812
A1698	G1491	G1491	G1491	G1425	U1357	G1279	C1207	A1143	C1079	C1013	G950	G882	C814	G745
G1699	G1492	G1492	G1492	G1426	U1358	G1279	G1208	G1144	A1080	U1014	C951	G883	C815	A746
A1700	A1553	G1493	G1493	G1427	G1359	A1287	C1209	C1145	U1081	G1015	G952	G884	C816	G747
G1695	G1555	A1494	A1494	C1428	A1360	G1287	A1210	C1146	U1082	G1016	A953	C885	C817	G748



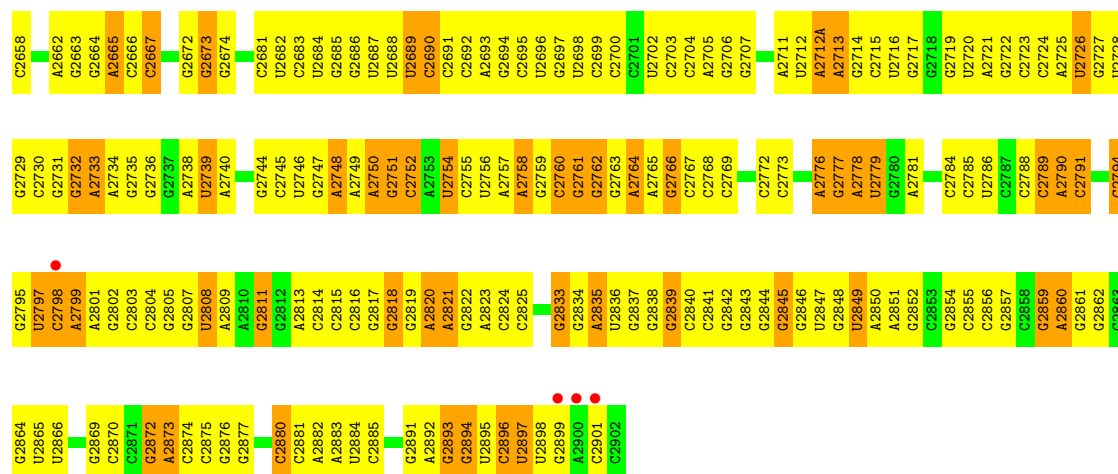


● Molecule 1: RNA (2912-MER)

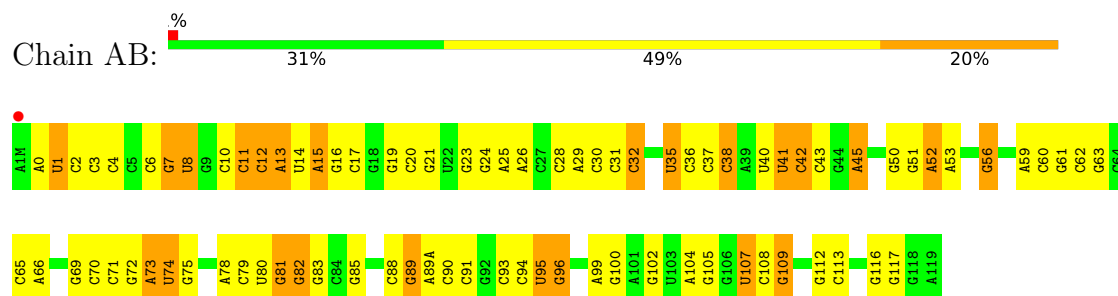


A1587	C1588	G1519	C1320	A1253	G1183	C1121	G1056	G993	G928	A866	A804	G723	G654S
C1589	C1590	U1390	A1321	A1254	G1184	G1122	A1057	C994	G929	C867	G805	G726	A654I
G1525	G1526	A1396	A1322	U1255	G1187	C1123	U1058	C995	U930	U868	C906	A727	A654V
G1527	G1528	U1397	U1323	G1256	G1188	C1124	G1059	A996	G931	G869	U807	G728	A655
A1596	A1597	G1401	G1324	C1257	A1189	G1125	U1060	G997	G932	U871	G808	G729	G656
C1598	C1599	G1402	U1325	G1258	A1190	A1126	U1061	C998	A933	A872	G809	C730	U657
G1600	G1601	C1403	U1326	G1259	G1191	A1127	G1062	U999	C934	G874	U810	C731	C658
C1602	C1603	G1404	C1327	G1260	G1192	A1128	G1063	A1000	C935	G875	U811	C732	C659
G1604	G1605	G1405	G1328	C1261	C1196	A1129	G1064	A1001	G936	G876	C812	A734	C661
U1609	U1610	C1406	C1329	U1262	G1197	U1130	U1065	G1002	U937	C877	U813		
G1606	G1607	C1407	U1330	G1263	U1198	U1131	U1066	G1003	G938	C878	C814		
A1614	A1615	U1331	A1332	G1264	U1199	A1132	A1067	C1004		U877	C815	U747	
C1616	C1617	G1333	A1336	G1266	C1200	C1135	A1068	C1006	A941	A878	C816	G748	
A1619	A1620	C1337	U1337	U1267	C1201	G1136	A1069	G942	G942	G879	C817		
G1625	G1626	G1338	U1338	U1268	C1202	G1137	A1070	C1007	U943	G880	G818		
C1627	C1628	C1339	G1339	A1269	G1203	A1071	G1071	U1008	G944	G881	A819	A751	
A1635	A1636	C1340	U1340	C1270	A1204	C1072	A1072	A1009	A945	G882	A820	A752	
G1635	G1636	U1341	U1341	G1271	U1205	A1073	G1073	A1010	G946	G883	A824	C753	
C1637	C1638	U1342	U1342	A1272	G1286	C1140	C1075	G1011	G947	C884	A824	C754	
A1639	A1640	G1343	G1343	U1273	C1207	U1141	C1076	U1012		C885	U826	C755	
G1640	G1641	U1344	U1344	A1274	C1208	A1142A	A1077	G1013	G952	C886	U827	C756	
A1642	A1643	C1345	C1345	U1275	C1209	A1143		G1014	A953	C887	U828	U757	
G1644	G1645	U1346	U1346	A1278	A1210	G1144	A1080	G1015	G954	C888	U829	G760	
C1646	C1647	G1347	G1347	G1279	U1211	G1147	U1081	G1016	C955	C889	G830	A761	
G1648	G1649	U1348	U1348	G1280	G1212	C1148	U1082	C1017	G956	C892	G831		
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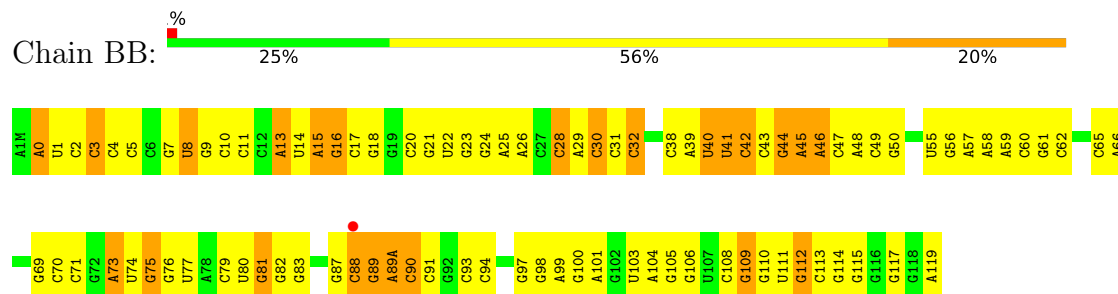
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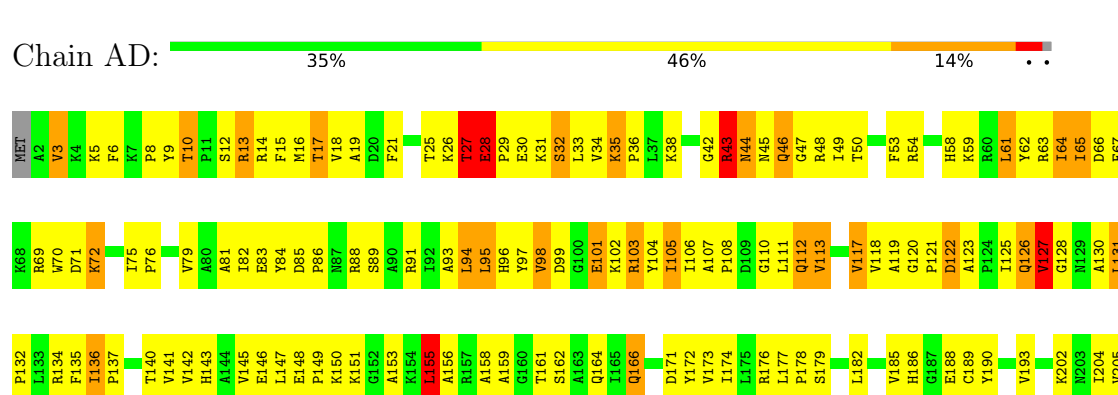
• Molecule 2: 5S RIBOSOMAL RNA



• Molecule 2: 5S RIBOSOMAL RNA

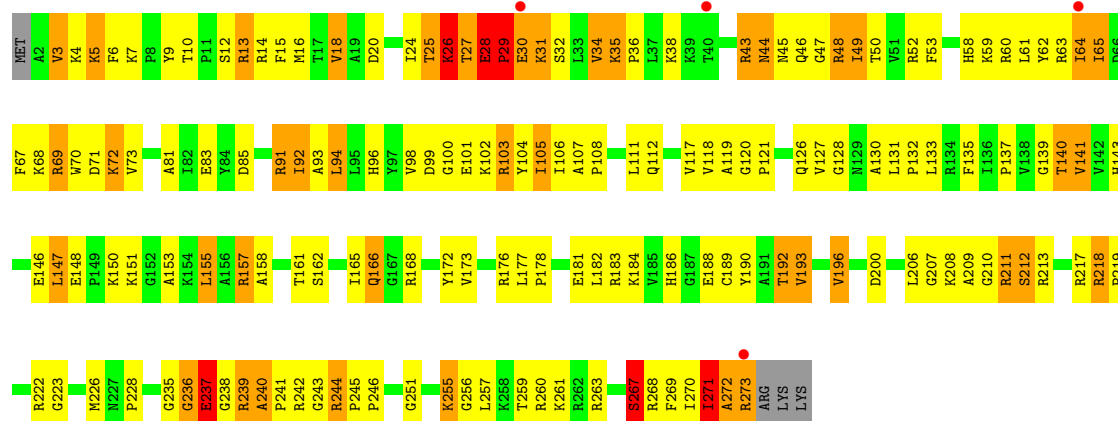


• Molecule 3: 50S ribosomal protein L2

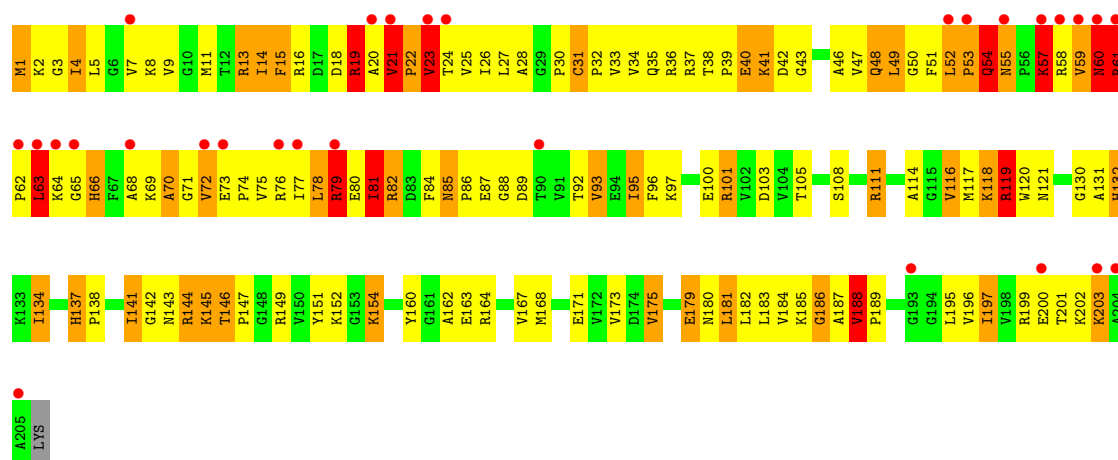




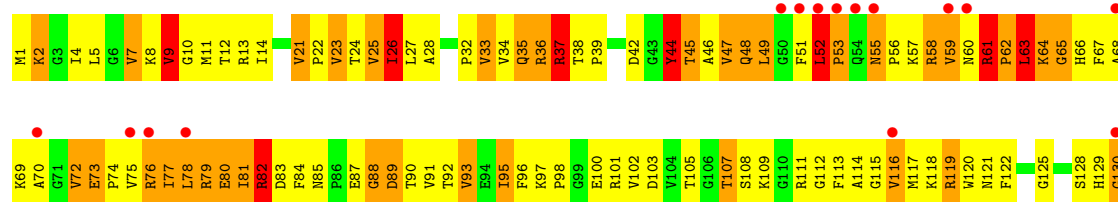
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

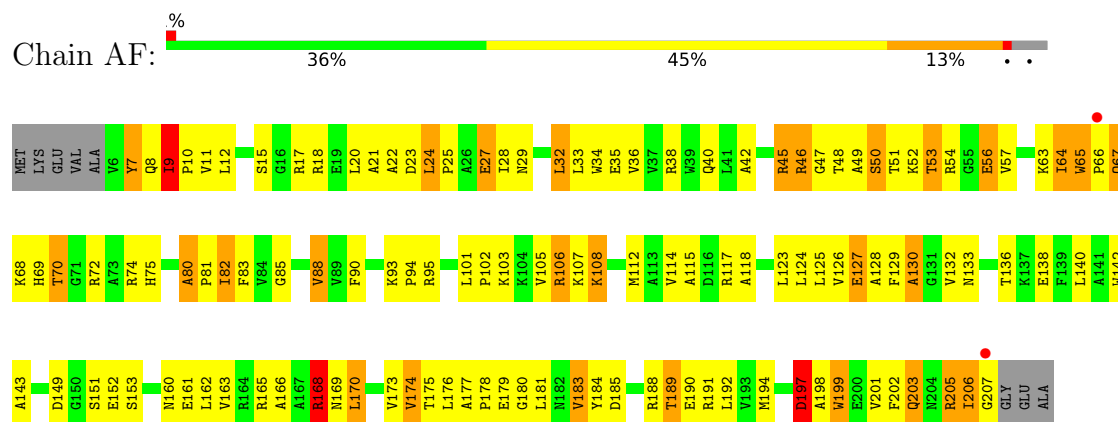


• Molecule 4: 50S ribosomal protein L3

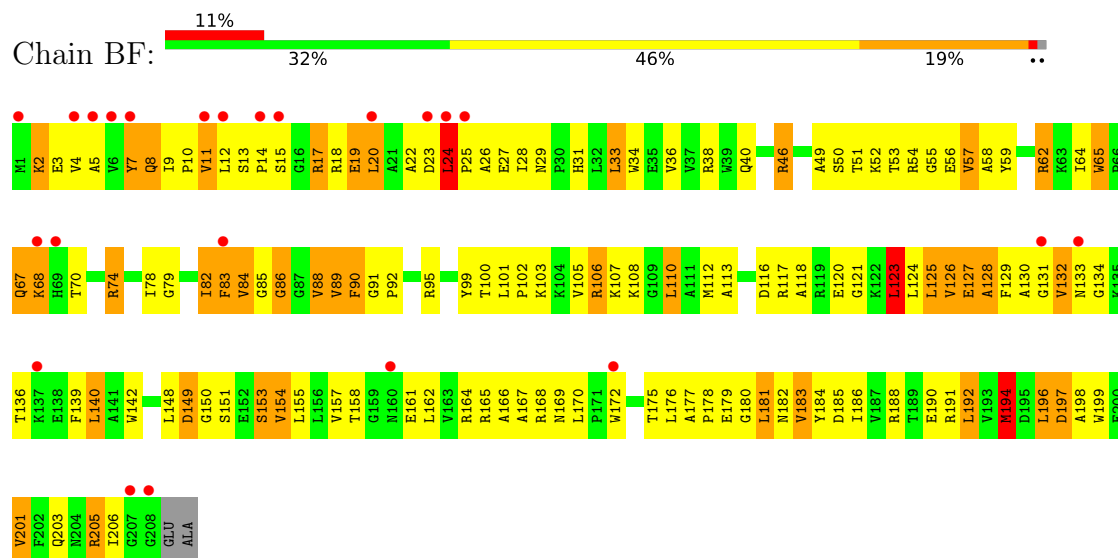




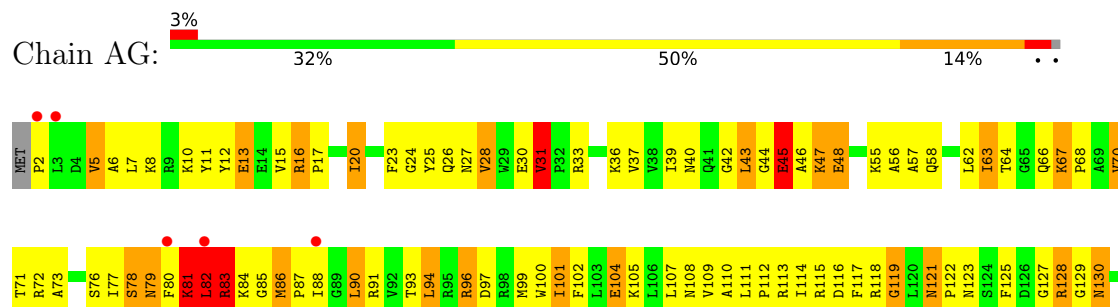
• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4

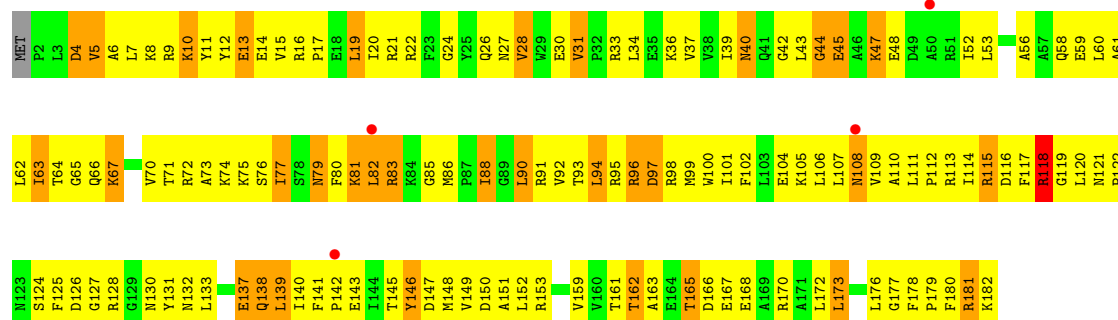


• Molecule 6: 50S ribosomal protein L5

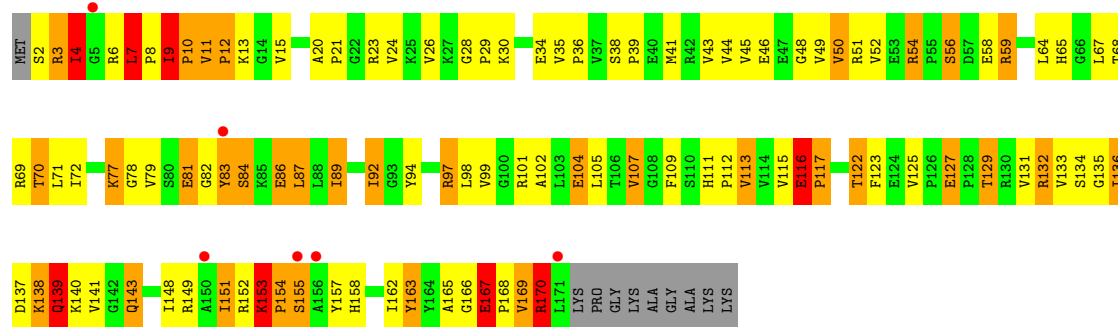




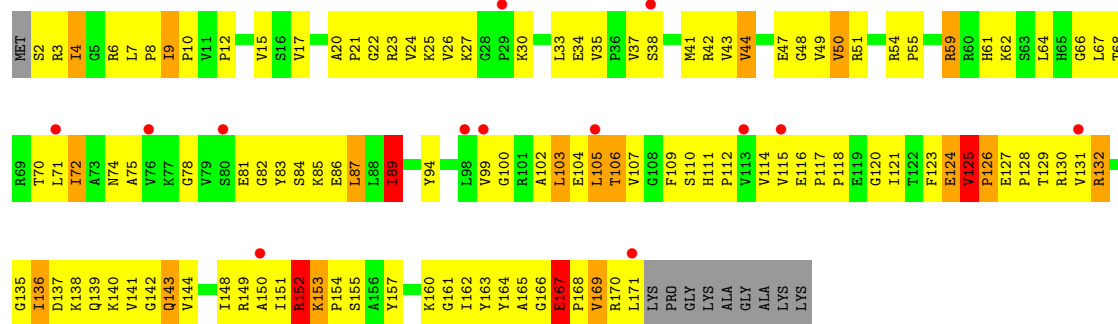
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

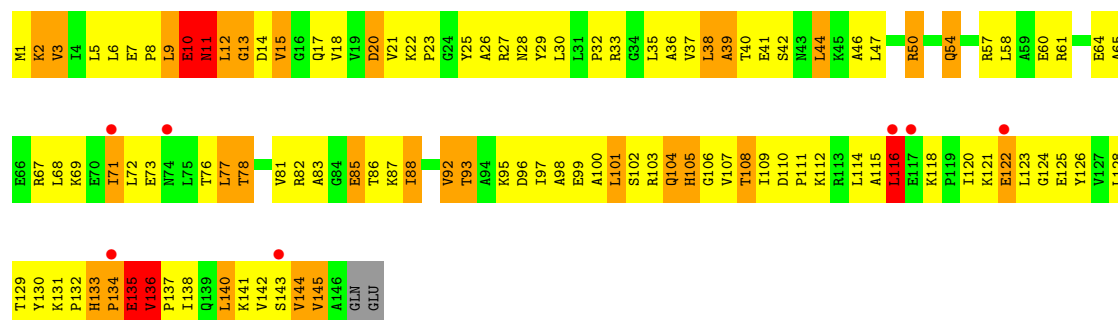


• Molecule 7: 50S ribosomal protein L6

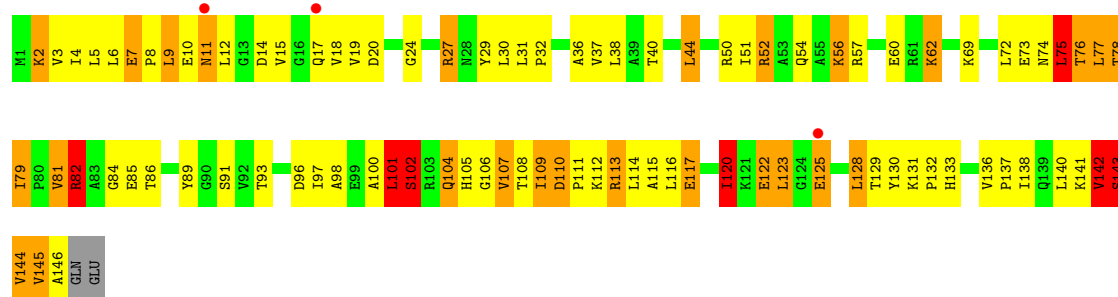


• Molecule 8: 50S ribosomal protein L9

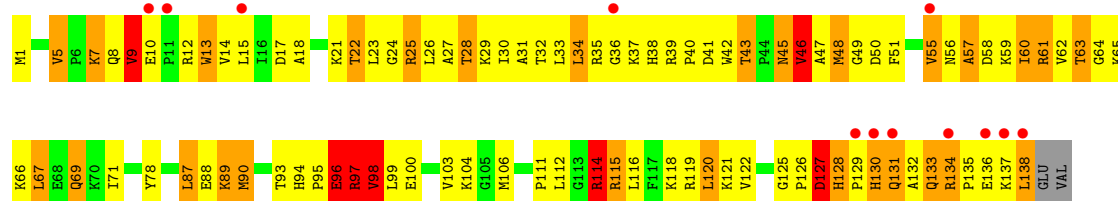




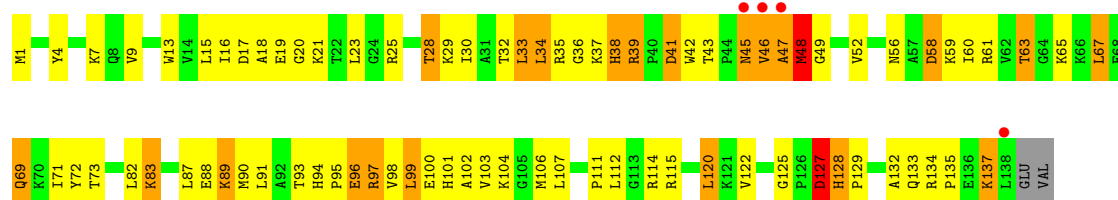
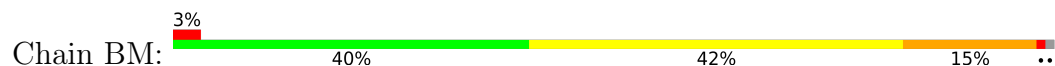
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13

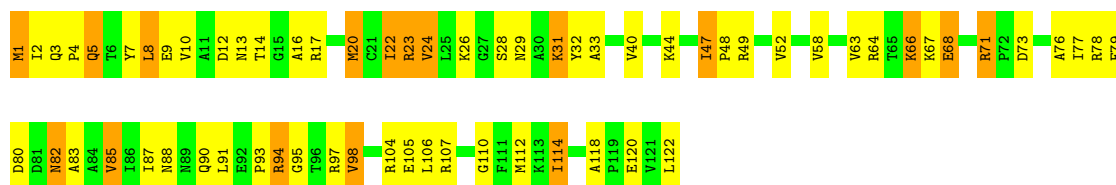


• Molecule 9: 50S ribosomal protein L13

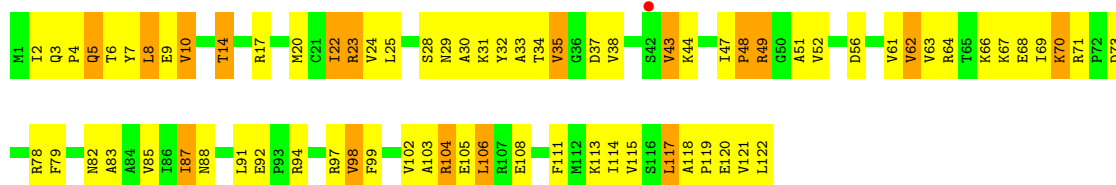
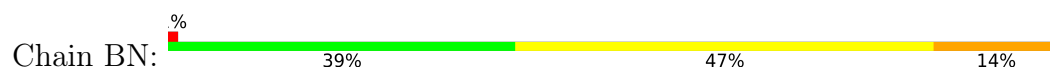


• Molecule 10: 50S ribosomal protein L14

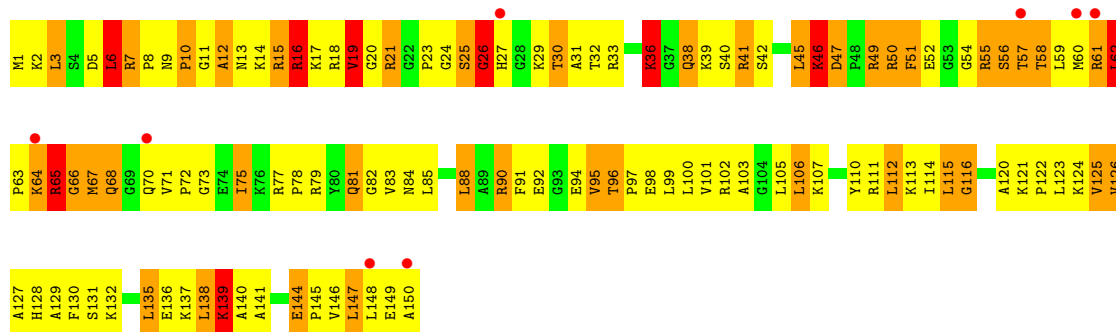
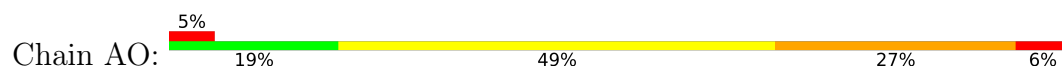




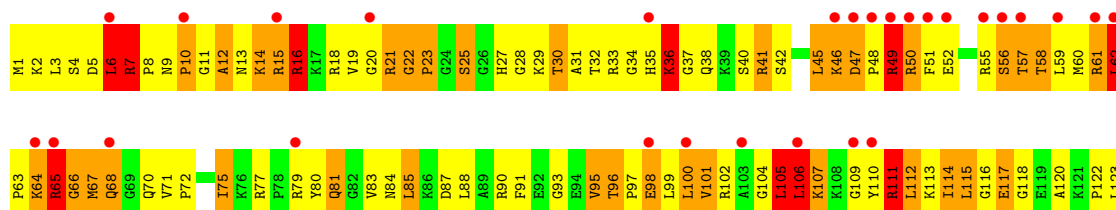
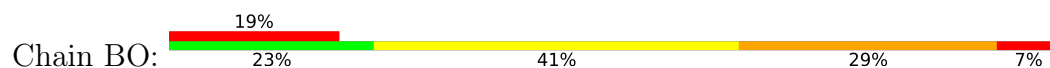
• Molecule 10: 50S ribosomal protein L14



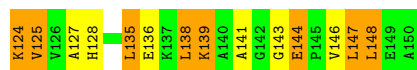
• Molecule 11: 50S ribosomal protein L15

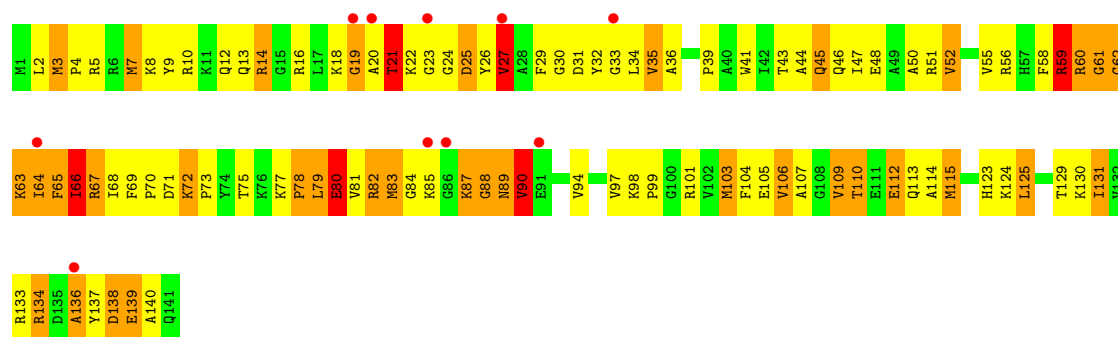


• Molecule 11: 50S ribosomal protein L15

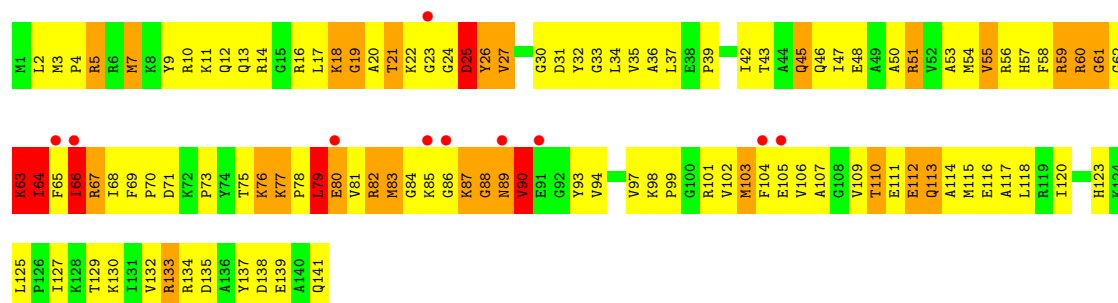


• Molecule 12: 50S ribosomal protein L16

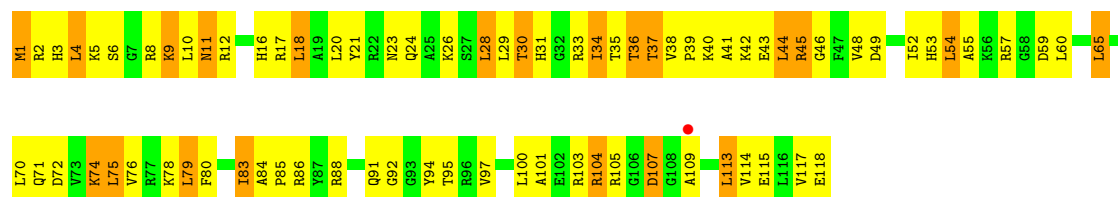




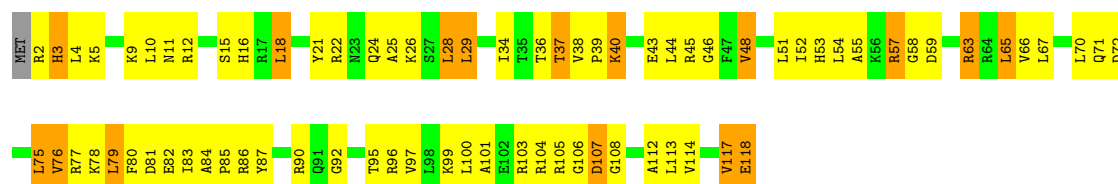
• Molecule 12: 50S ribosomal protein L16



• Molecule 13: 50S ribosomal protein L17

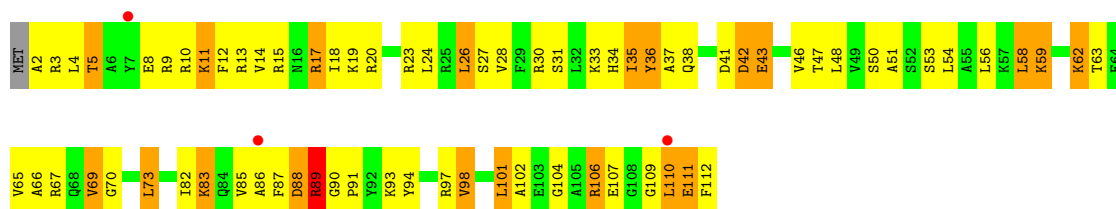


• Molecule 13: 50S ribosomal protein L17

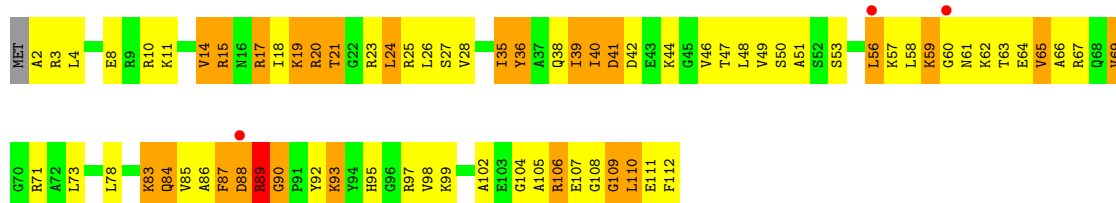


• Molecule 14: 50S ribosomal protein L18

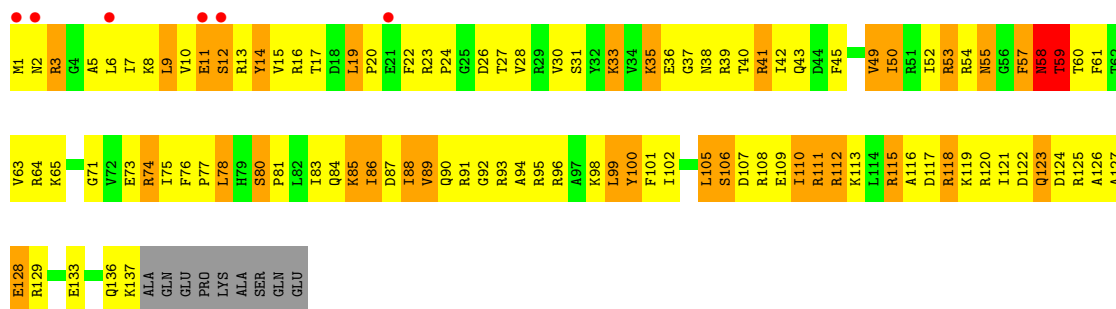
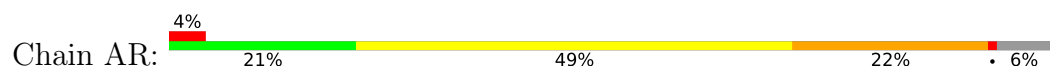




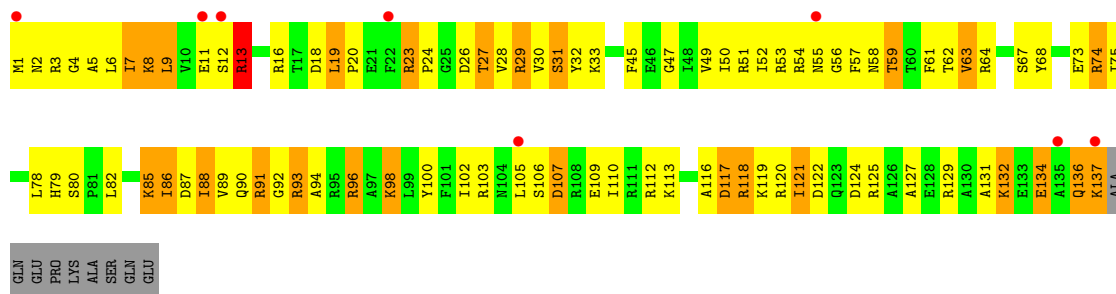
• Molecule 14: 50S ribosomal protein L18



• Molecule 15: 50S ribosomal protein L19

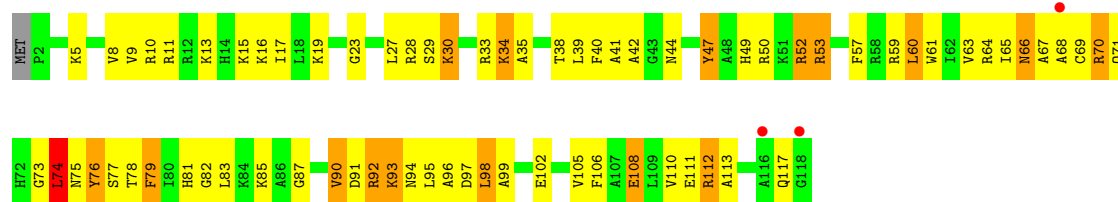


• Molecule 15: 50S ribosomal protein L19

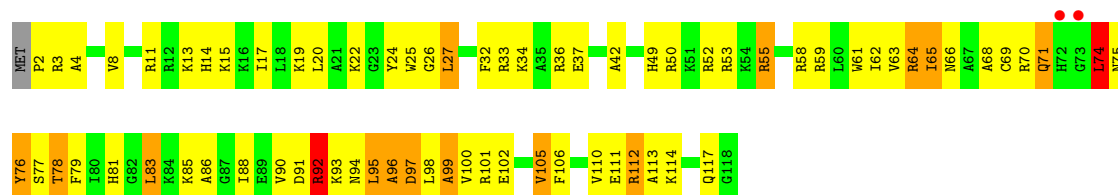


• Molecule 16: 50S ribosomal protein L20

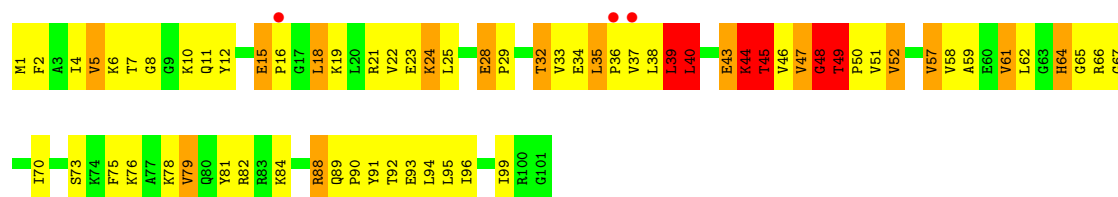




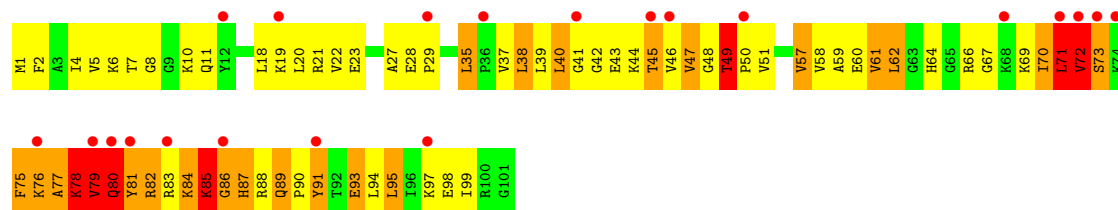
• Molecule 16: 50S ribosomal protein L20



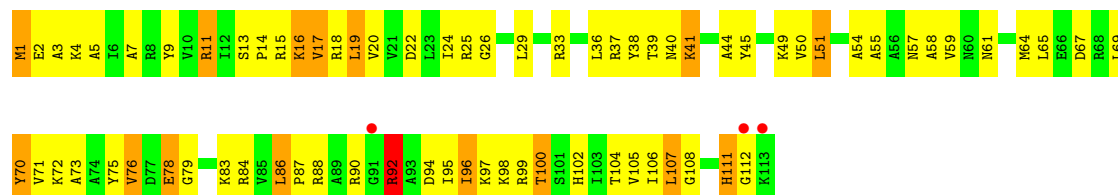
• Molecule 17: 50S ribosomal protein L21



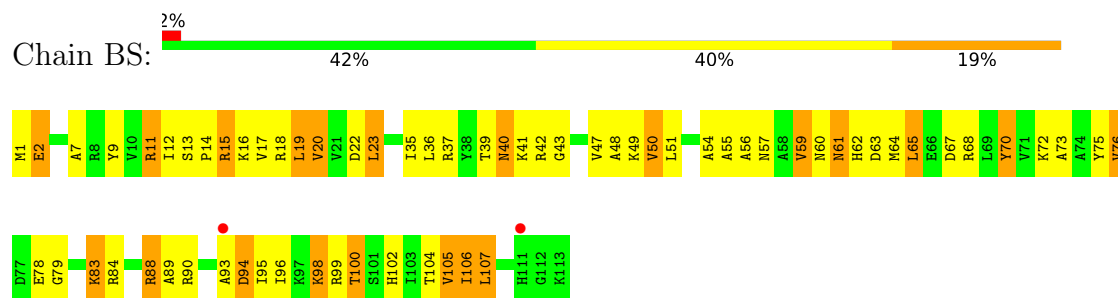
• Molecule 17: 50S ribosomal protein L21



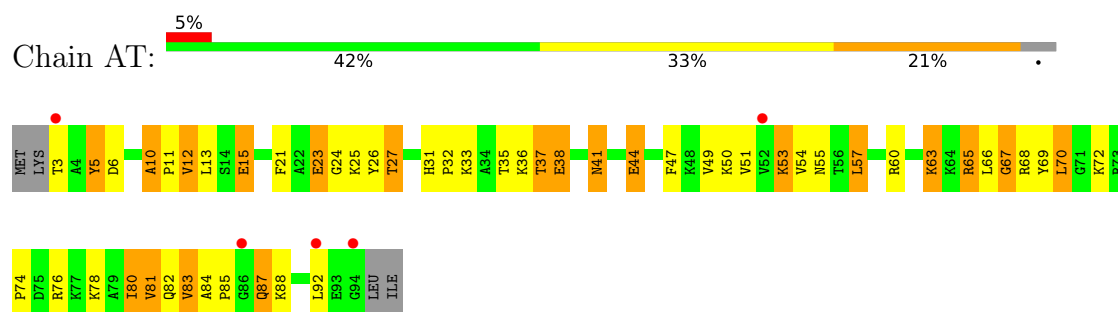
• Molecule 18: 50S ribosomal protein L22



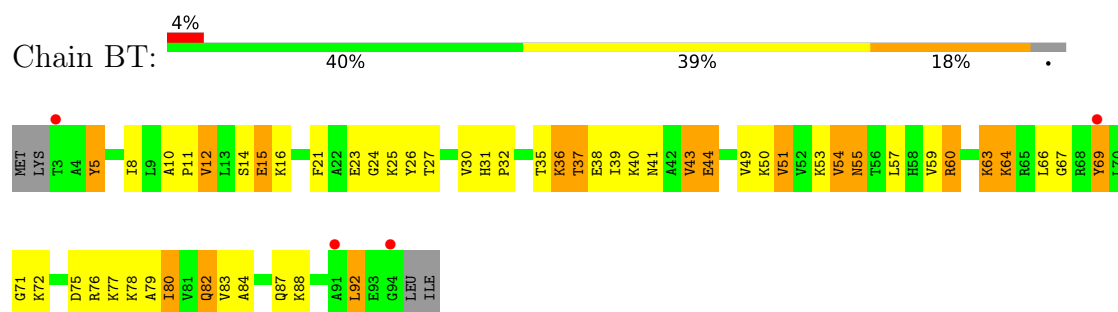
- Molecule 18: 50S ribosomal protein L22



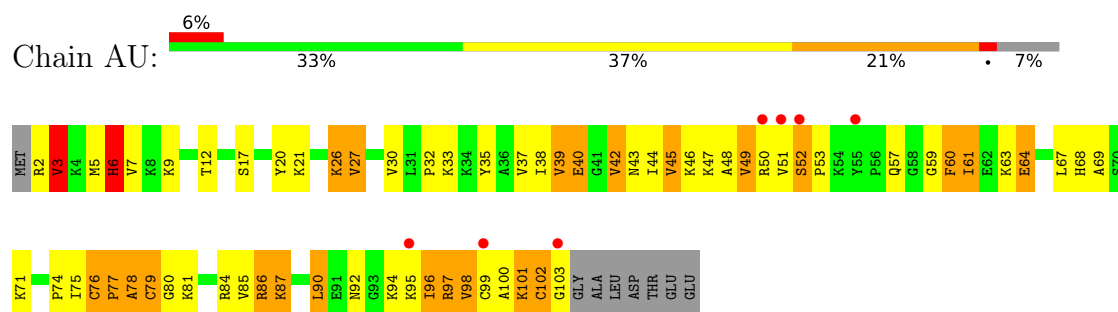
- Molecule 19: 50S ribosomal protein L23



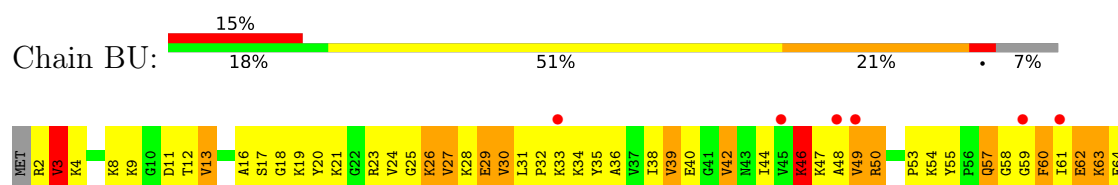
- Molecule 19: 50S ribosomal protein L23

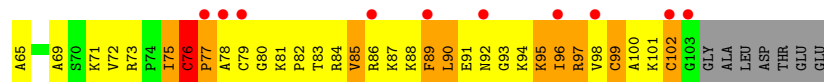


- Molecule 20: 50S ribosomal protein L24

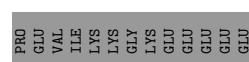
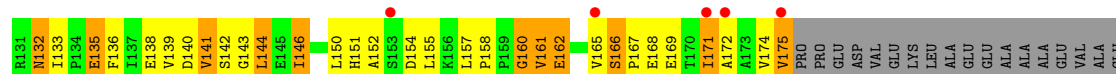
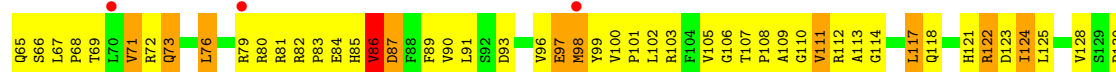
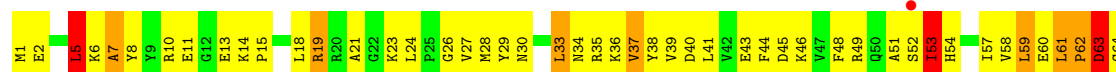


- Molecule 20: 50S ribosomal protein L24

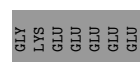
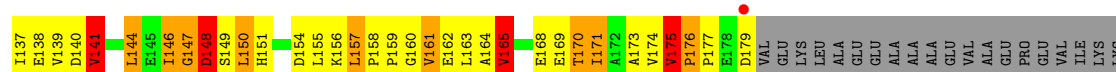




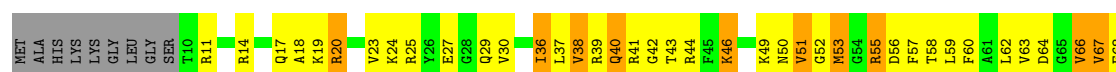
• Molecule 21: 50S ribosomal protein L25



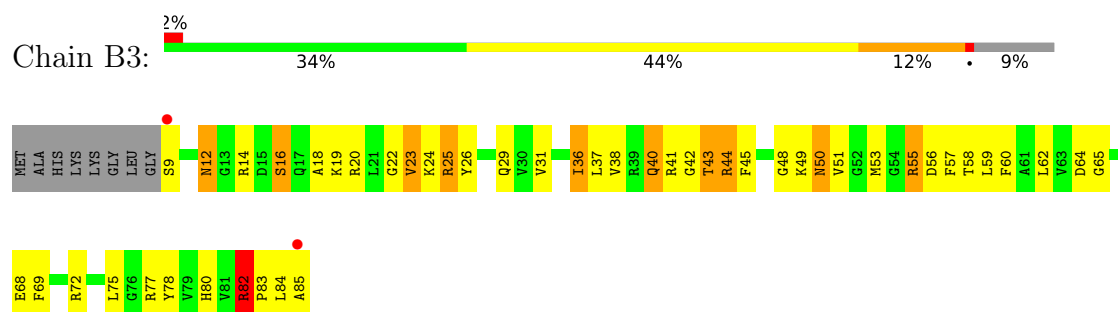
• Molecule 21: 50S ribosomal protein L25



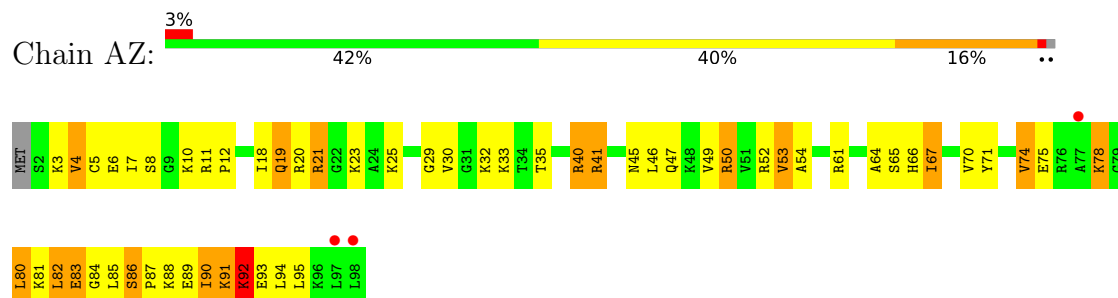
• Molecule 22: 50S ribosomal protein L27



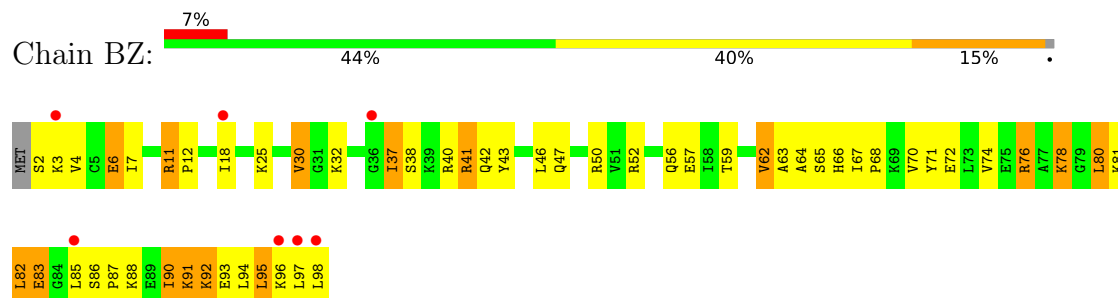
• Molecule 22: 50S ribosomal protein L27



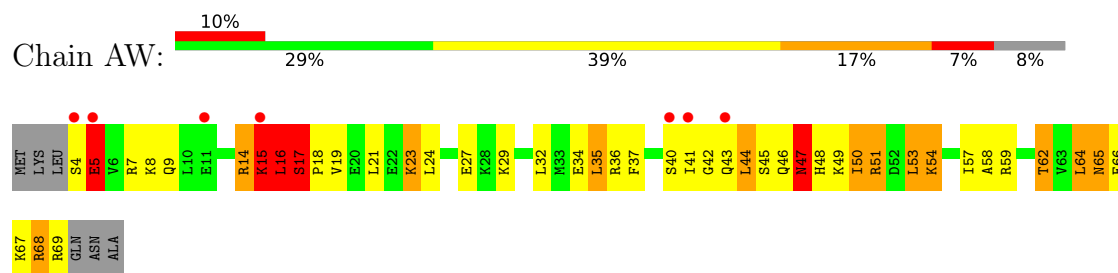
- Molecule 23: 50S ribosomal protein L28



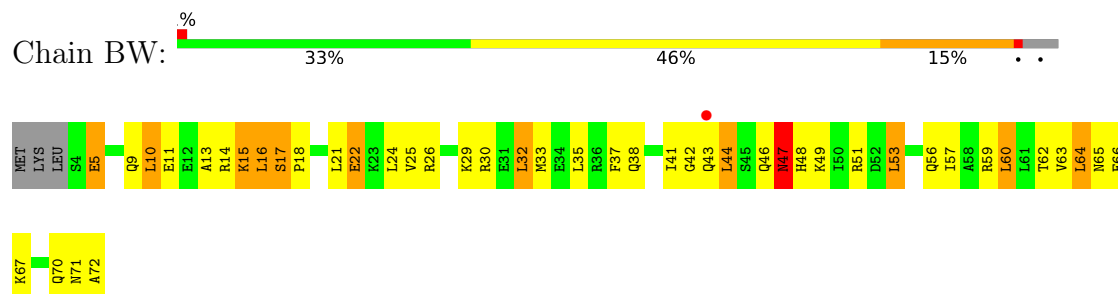
- Molecule 23: 50S ribosomal protein L28



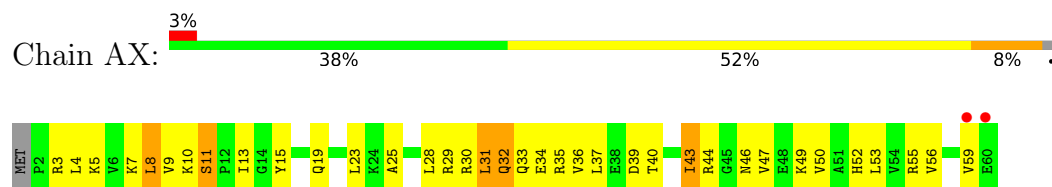
- Molecule 24: 50S ribosomal protein L29



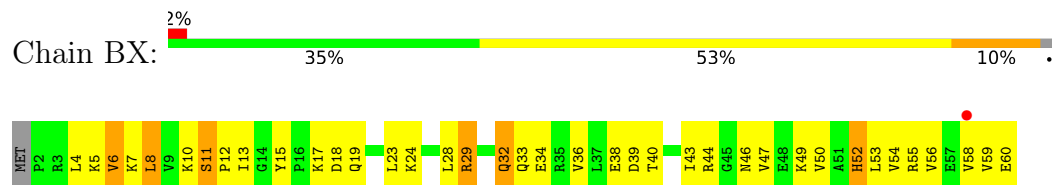
- Molecule 24: 50S ribosomal protein L29



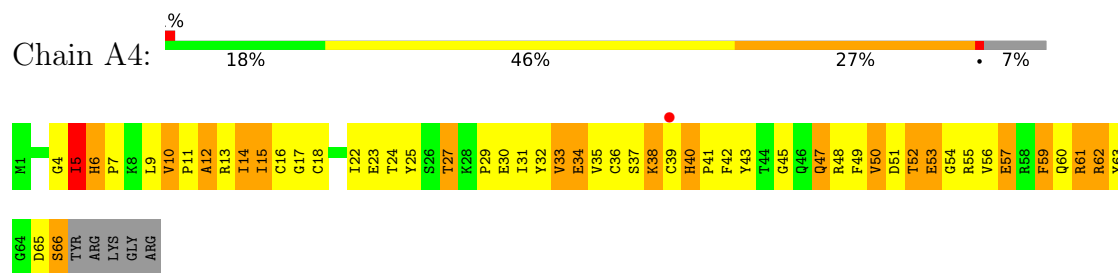
• Molecule 25: 50S ribosomal protein L30



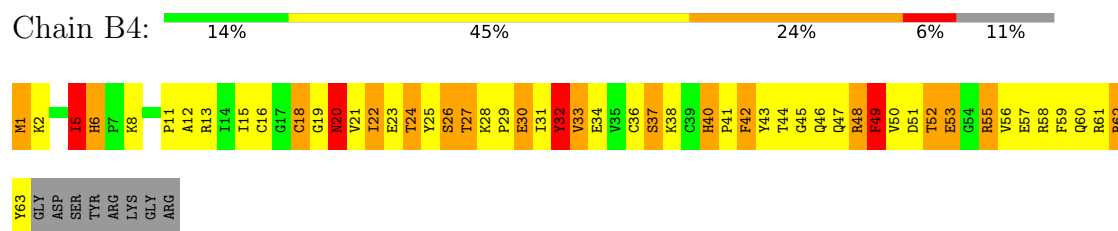
• Molecule 25: 50S ribosomal protein L30



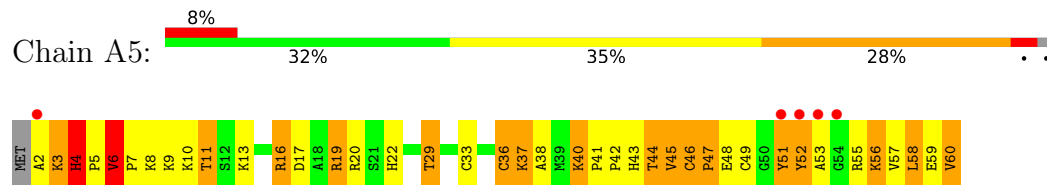
• Molecule 26: 50S ribosomal protein L31



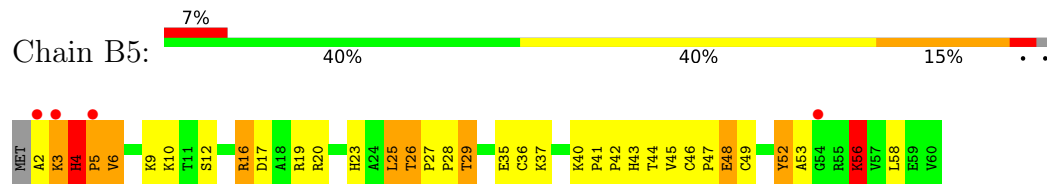
• Molecule 26: 50S ribosomal protein L31



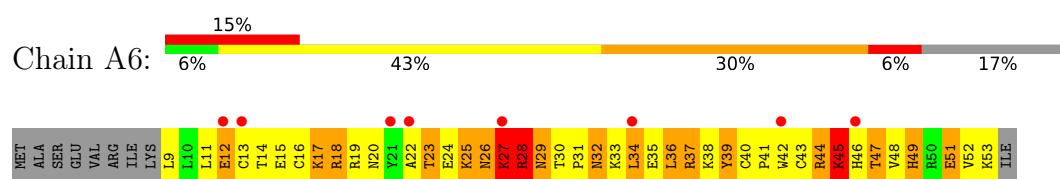
• Molecule 27: 50S ribosomal protein L32



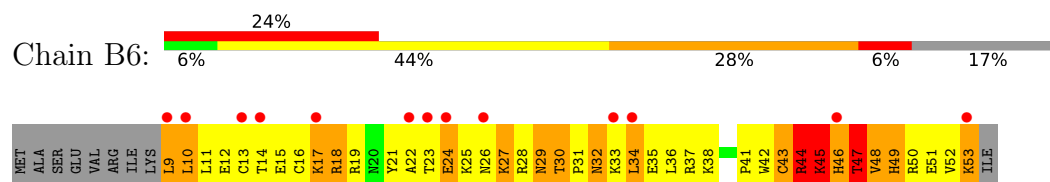
• Molecule 27: 50S ribosomal protein L32



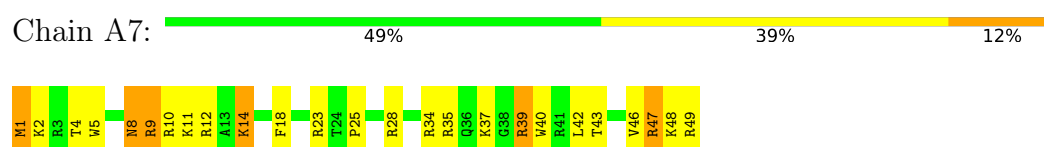
• Molecule 28: 50S ribosomal protein L33



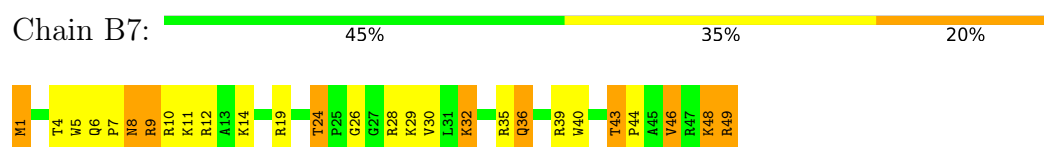
- Molecule 28: 50S ribosomal protein L33



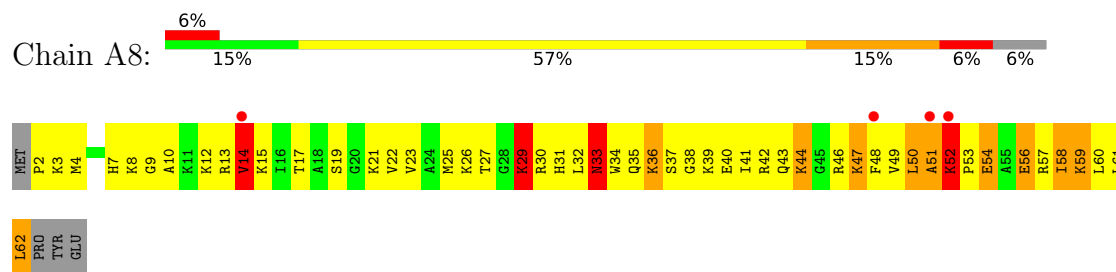
- Molecule 29: 50S ribosomal protein L34



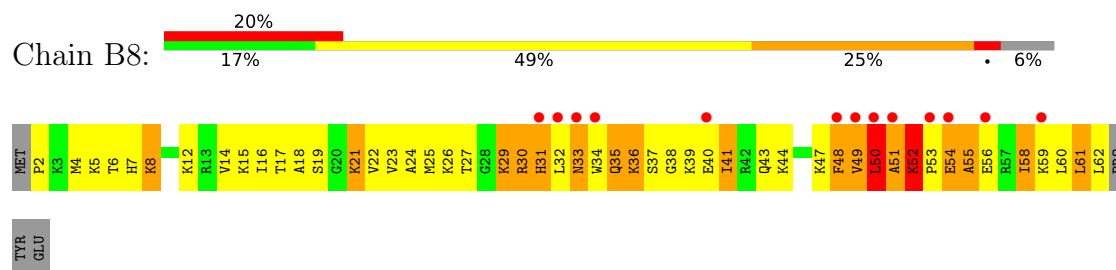
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



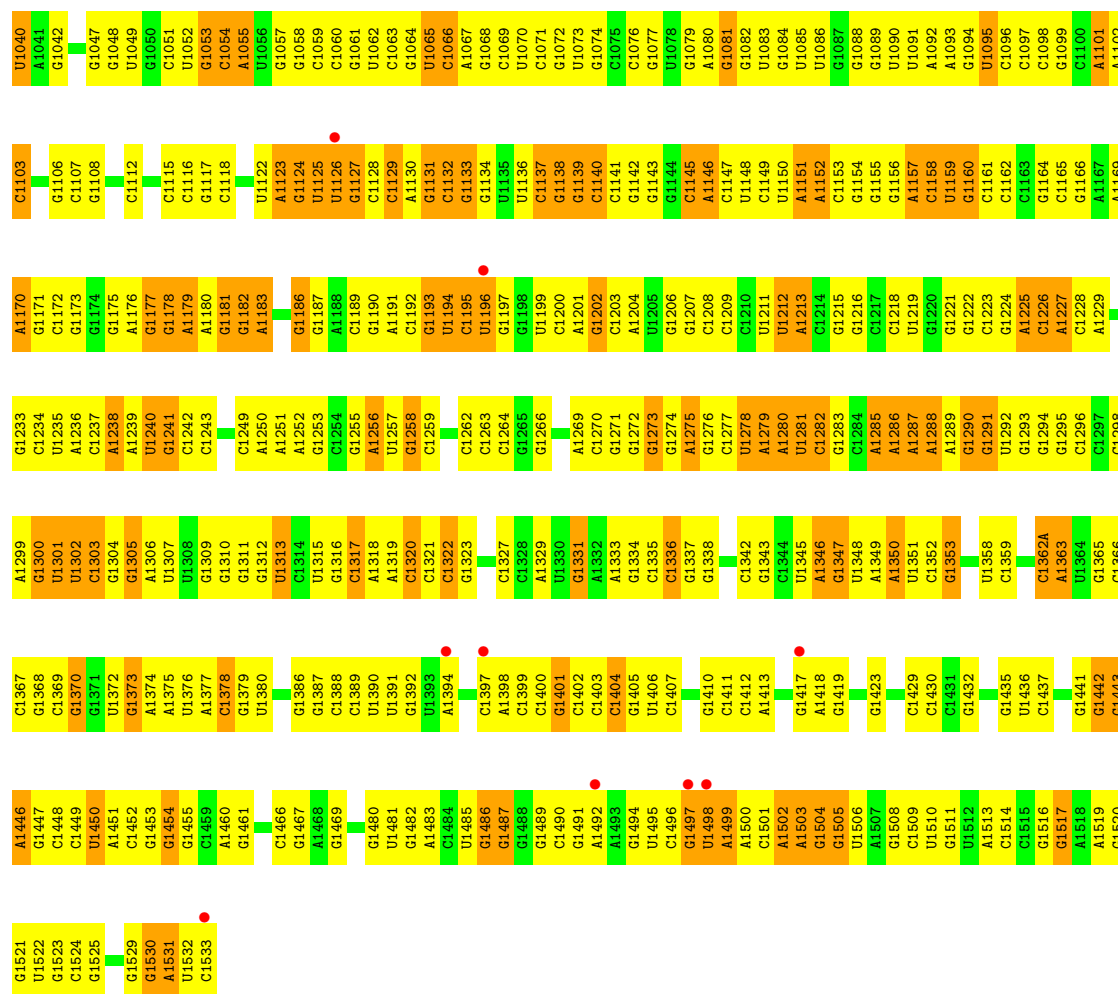
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 16S ribosomal RNA

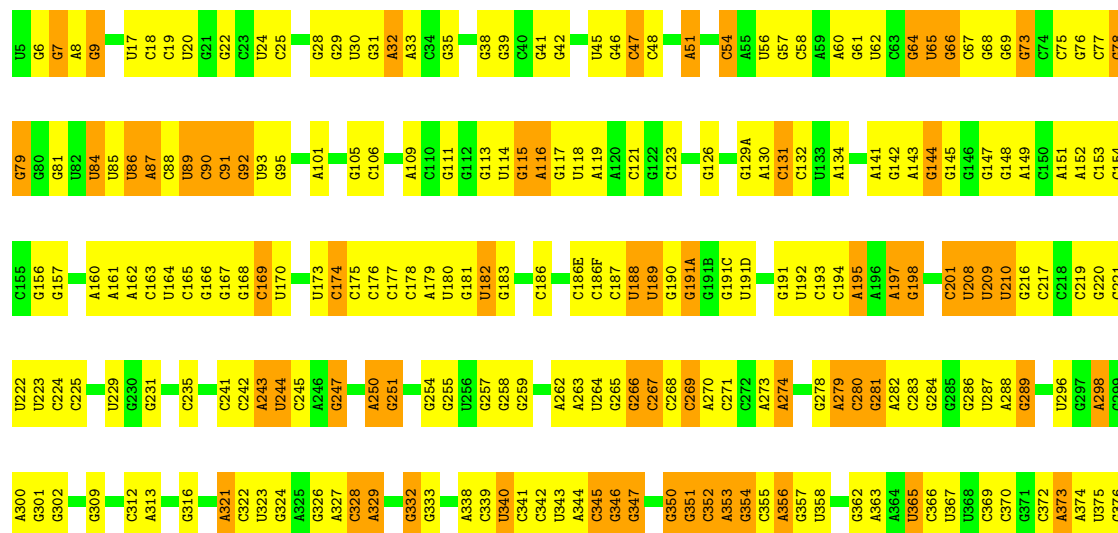


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G987	G988	U920	G837	A702	A702	C634	U565	G502	G424	A353	G281	G199	G148	G80	G7
G988	G989	U921	G838	G763	G703	G635	G566	C503		A354	A282	G200	G149	G81	A8
G989	G990	G922	U841	G765	A704	G636	G567	C504	U427	C355	C283	C201	C150	U82	G9
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A996			G853	G772	A711	G646	A575	A511		A433	G291	C219		U90	A17
U997			G854	G773	A712	U647	A576	C511	U437	U365	G292	C220	A150	C90	C18
G998			G855	G774	G713	A648	G576	C512	G438	C366	G293	C221	A161	C91	
C998A			G856		G714	U649	G577	C513	A439	U367	G297	U222	A162	C92	G22
U999			C857	A777	A715	G650	C578	C514	A440	U368	G298	U223	C163	U93	G23
A1000			G858	G778	A716	G651	C579	U516	C443	C369	G299	C224	U164	G95	G27
G1001			A859	G779	C717	U652	U580	G517	C444	C370	A300	C225	C165	G96	
G1002			A860	A780	G718	A853	G581	C518	G445	G371	G301	C226	G167	U97	G31
C1003				A781	C719	G654		C519		C372	G302	G227	G168	C99	A32
A1004			A864	A782	C720		G584	A520	A448	C373	A303		C169	A101	A33
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C1006					A722	U659	C586	C522	G450	G375		C233	A171	C103	G35
G1007			A767	G788	G723	G660	G587	A523	A451	G376	G309	C234	A172	G104	
C1008			U871	U789	G725	G661	G592	G524	A452	G377	G310	C235	U173	G105	G38
G1009			A872	A789	C726	G662		C525	A453		G311	G236	C174	C106	C39
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G1011			G874	A791	G728	G664	C596	C527	C455	U387	A313		C176	G41	G42
			C875	A792	A729	A665	C597	C528	C456	A382	C314	U244	C177	G11	
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G1021			C877	A794	G731	G668	C600	U531	C458	G384	G316	A246	A179	G13	U45
A1015			C878		C732		C601	U532	C464	C385	G317	G247	U180	U14	G46
U1016			C879	C797	A733	U672	A602	A532	A465	C386			G181	G47	C47
C1017			C880	G798	G734	G673	A603	A533	C466	U387	A321	G250	U182	C48	C48
G1019			C882	U804	C735	G674	U604	C536	A467	A389	G322	G251	G183	U49	U49
U1020			U884	C805	C736	A675	U605	C537	G474	C390	G324	G254	G184	U51	A50
G1022			G885		A737	A676	G606	G538	G475		A325	G255	A185	A51	A51
U1024			C811	C812	C738	U677	A607	A539	G476	A393	G326	U256	C186	G52	G52
G1025			A814	A814	U740	C679	A608	G540	G477	G394	G327	G257	C186A	A53	A53
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C1027			G894	A816	G742			G542	U480	G396	A329	G259	C186D	U56	U56
C1028			G895	C817				C543	G481	A397	C330	G260	C186E	G57	G57
C1028A			C896	G818	C745	A684	G615	C544	A482	C398	G331	U261	C186F	C58	C58
U1028B			A819	G818	A746	G685	G616	C545	C483		G332	A262	C187	A59	A59
G1029			U820	A819	C747	U686	G617	G546	G484	C401	G333	U263	U188	A60	A60
C1030			G821	G821	C748	A687	C618	A547	G485	G402	U343	U264	U189	G61	G61
G1031			A900	A820	C749	G688	U619	G548	U486	C403	C338	G265	G190	U62	U62
A1032			G902	G822	C750	C689	C620	C549	A487	U405	U340	G267	G191A	G63	G63
G1032A			G903	G823	U751	G690	A621	U552	C488	G406	C341	C268	G191B	G64	G64
G1032B			C904	C824	G752	G691	C622	A553	G490	G407	C342	C269	G191C	U65	U65
G1033			A908	G825	A753	U692	C624	C566	G491		U343	A270	G191D	G66	G66
U1034			U827	G826	C754	G693	G625	G557	G492	A411	A344	C271	G191E	C67	C67
A1035			A828	A828	G755	A694	U626	G558	G493	A412	C272	G272	U191F	G68	G68
G1036					C756	A695	G627	A559	U494	G413	G346	A273	G191	G69	G69
C1037			A913	C832	U757	A696	G628	U560	A495	C419	G348	G276	C193	C74	C74
U1038			A914	A832	G758	U697	G629	U561	A496	U420	A349	G277	C194	C75	C75
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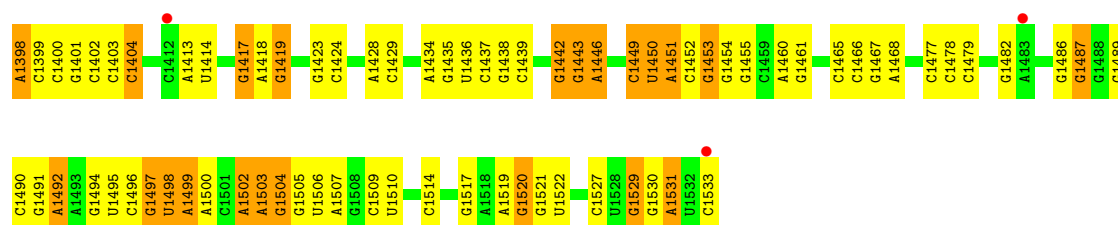


• Molecule 31: 16S ribosomal RNA

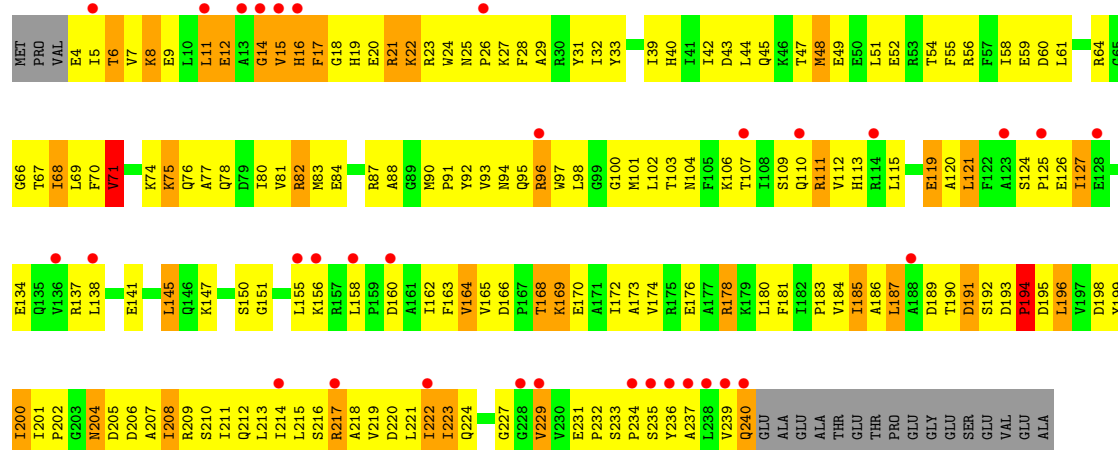
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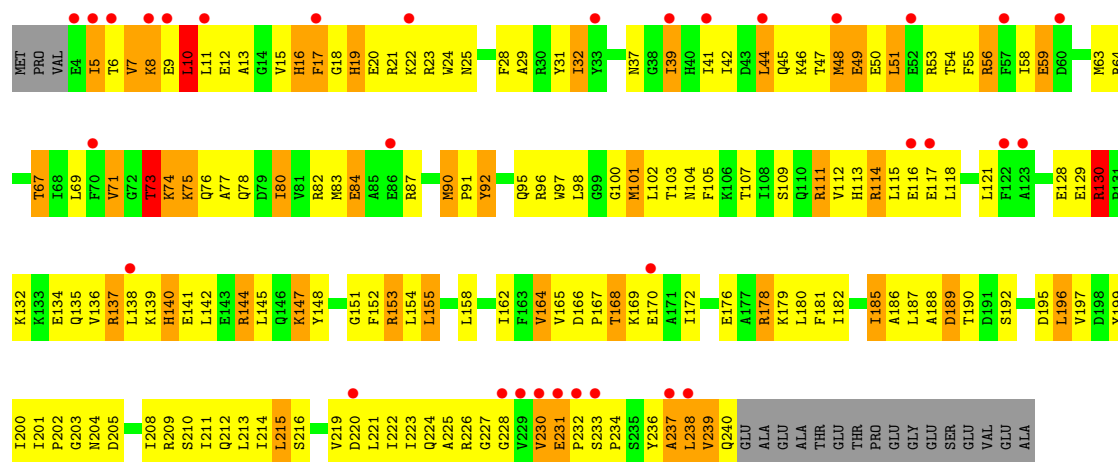
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G1338	C1210	G1145	G1084	G1024	A965	C899	C821	C750	U677		A533	A452	A383
A1339	U1211	A1146	U1085	U1025	G966	A900		U751	C680	G604	U534	A453	G384
	U1212	G1147	U1086	G1026	C967	A901	C824	G752		U605	A535	C385	
	A1213	U1148	G1087	C1027	A968	G902	C825	A753		G606	C536	C386	
	C1214	C1149	G1088	C1028	A969		C826	C754	U686	A607	C457	C387	
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C1344	C1217	A1152	U1091	G1029	C972	A908	C829	C757	C689		G540	A439	
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G1347	G1220	G1155	G1094	A1032	A975	C910	C832	A759	C692	C614	C543	C443	
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G1366	U1239	A1179	C1114		A994	C934	C858	C779		A632	A563	C417	
C1367	G1240	G1180	C1115	C1051	C995	A935	A859	A780	C719	G633	C564	C418	
G1368	G1241	G1181	C1116	U1052	A996	G936	C860	A781	C720	C634	A495	C419	
C1369	C1242	G1182	G1117	G1053	U997	A937	C861	A782	C721	U636	G567	U420	
G1370	C1243	A1183	G1118	C1054	G998	G938	C862		A722		C568	U421	
G1371	C1244	G1184	C1119	A1055	C999	G939	U863	A787	U723	C647	G570	C422	
U1372	A1245	G1185	G1120	U1056	U999	C940		U788	U724	A648	G571	G423	
A1374		G1186	U1121	G1057	A1000	G941	C869	U789	G725	G649	A572	G424	
		G1187	U1122	G1058	G1001	G942	U870	A790	G726	G650	C502	G425	
		A1188	A1123	C1059	G1002	U943	U871	G791	G727	C651	A573	G426	
		G1189	G1124	G1060	G1003	G944	A872	A792	G728	U652	C504	U427	
		G1190	U1125	G1061	A1004	G945	U873	A793	A729	A653	G575	G428	
		A1191	U1126	U1062	A1005	A946	C874	A794	G730	G654	G576	U429	
		C1192	G1127	C1063	C1006	G947			G731	A655	G577	A430	
		G1193	C1128	G1064	C1007	C948	C877	G799	C732	U655	U580	C433	
		A1194	U1129	U1065	C1008	A949	C878	G800	A733	G657	C581	U434	
		C1195	A1130	C1066	G1009	U950	C879	U801	G734	G660	U582	C435	
		U1196	G1131	A1067	G1010	G951		A802	C735	G661	A583	C436	
		G1197	C1132	C1068	G1011	U952	C883	G803	C736	G662	G584	U437	
		G1198	G1133	U1069	U1012	G953	U884	U804	A737	G663	C587	G438	
		U1199	G1134	G1070	G1013	G954	C885		C738	A663	G588	A439	
		C1200	U1135	C1071	A1014	U955		C811	G739	G664	C589	A440	
		G1201	U1136	G1072	A1015	U956	C890	C812	U740	A665	C590	G520	
		A1202	C1137	U1073	A1016	U957	U891	U813	G741	G666	U591	C443	
		C1203	G1138		G1017	A958	A892	A814	G742	G667	G592	C444	
		A1204	G1139		C1018	U959	C893	A815		G668	G593	G445	
		G1302	U1205	G1077	C1019	U960	A816	A816	C745	U669	C594	C446	
		A1303	C1140	A1080	U1020	U961	C895	C817	A746			A448	
		A1333	C1141										



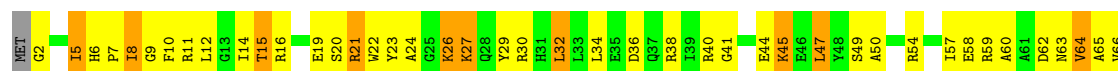
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

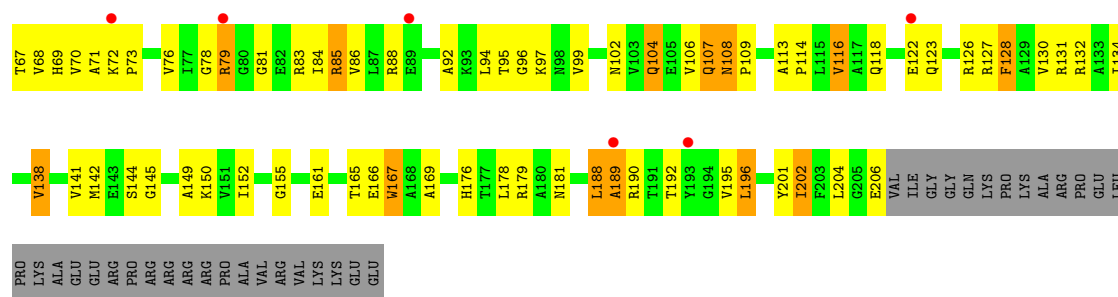


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

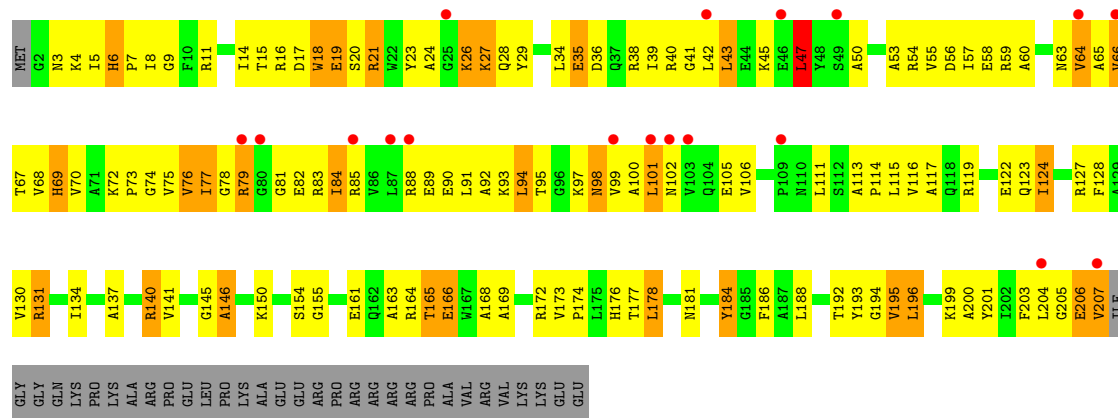


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

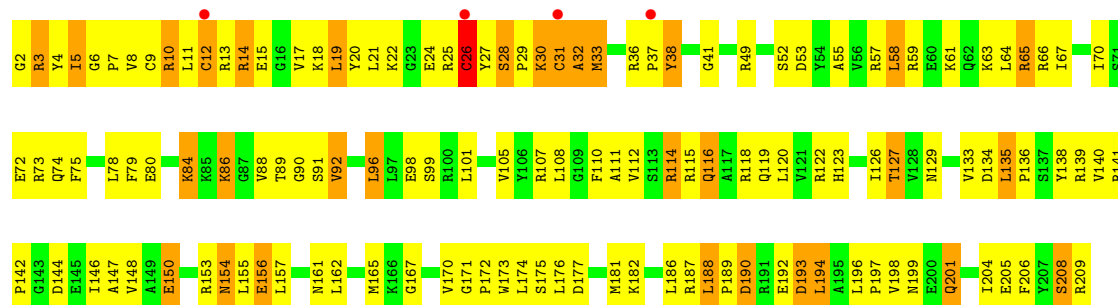




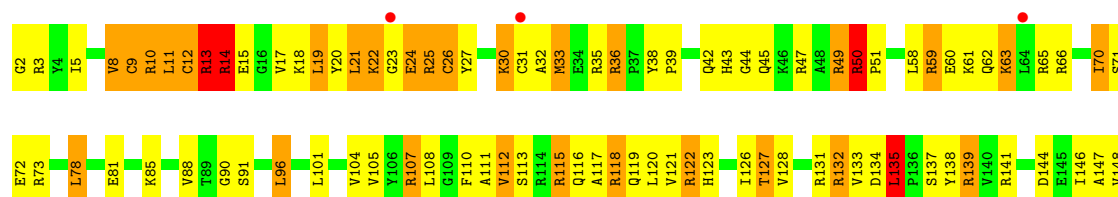
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



• Molecule 34: 30S RIBOSOMAL PROTEIN S4

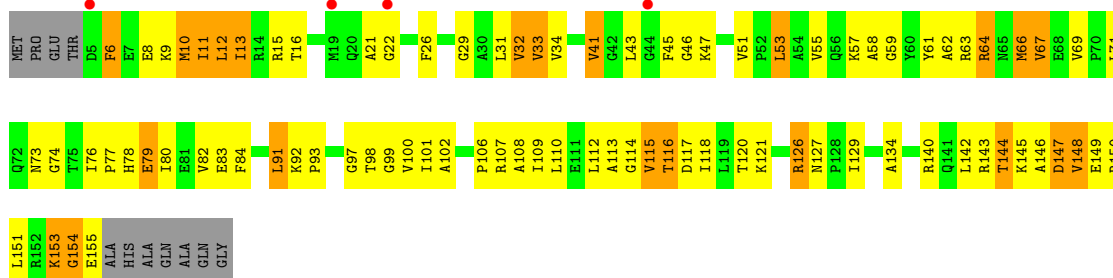


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

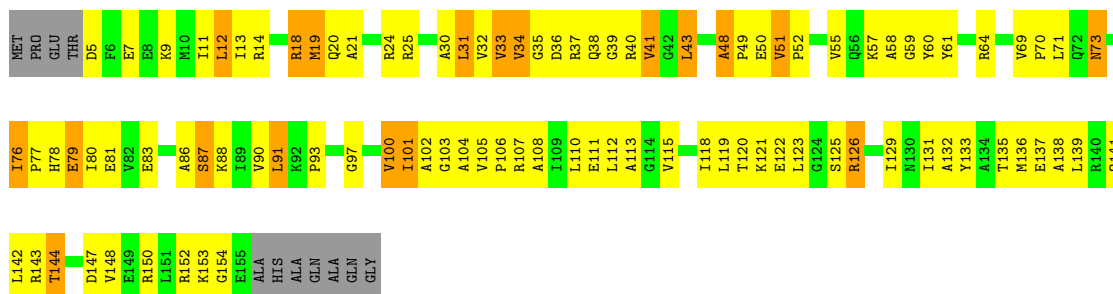




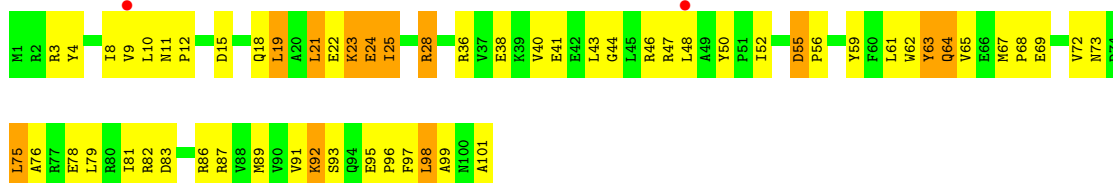
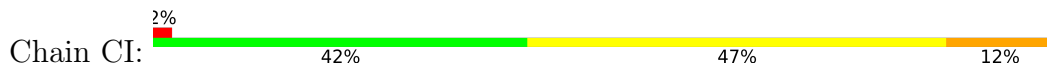
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



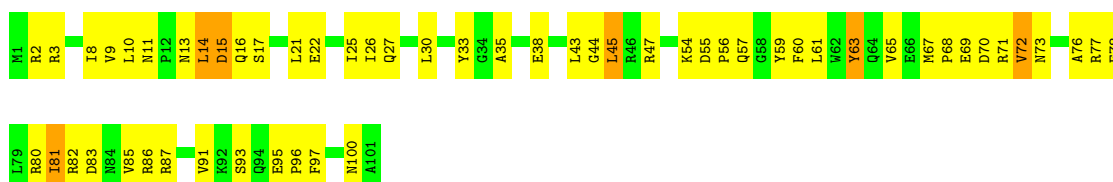
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



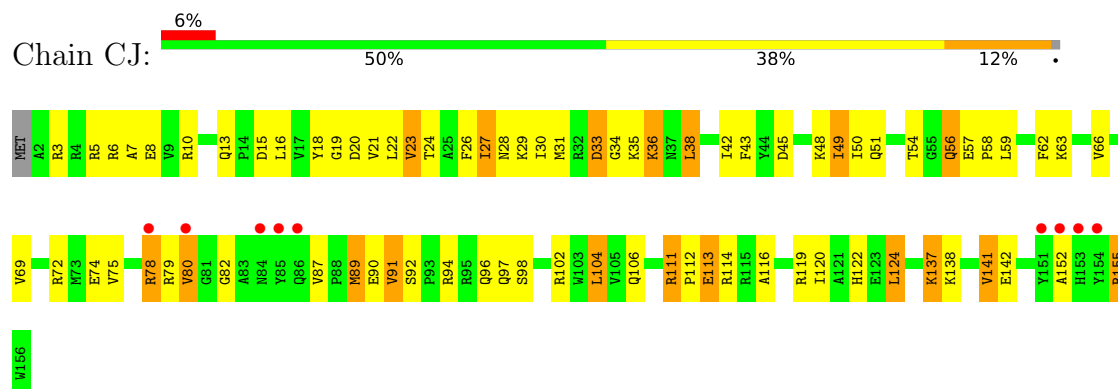
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



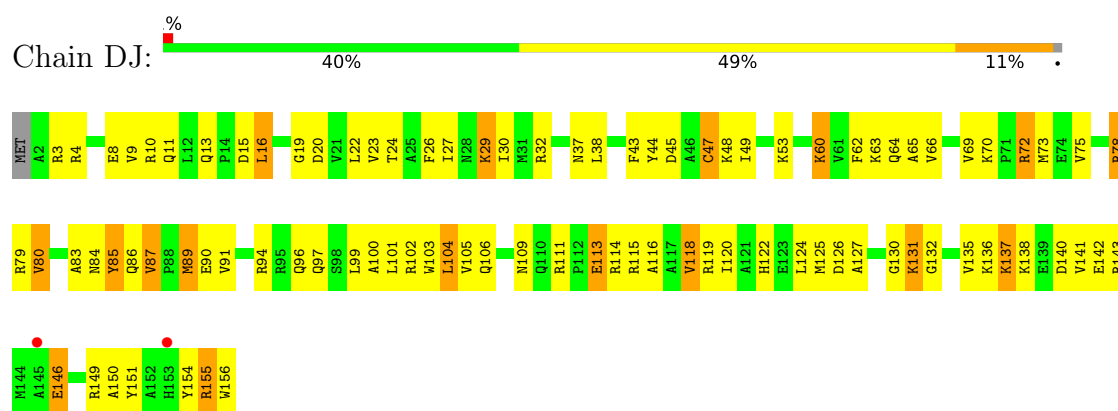
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



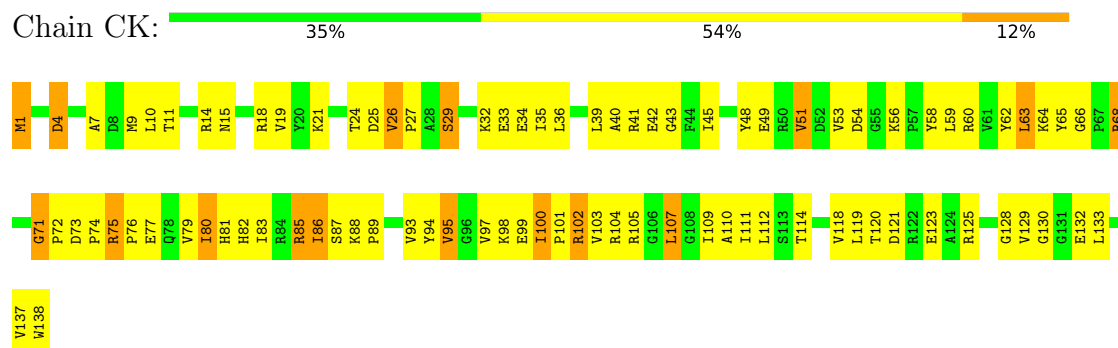
- Molecule 37: 30S RIBOSOMAL PROTEIN S7



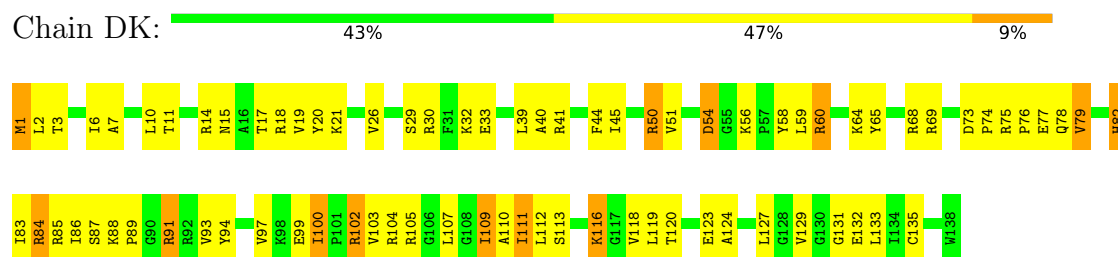
- Molecule 37: 30S RIBOSOMAL PROTEIN S7



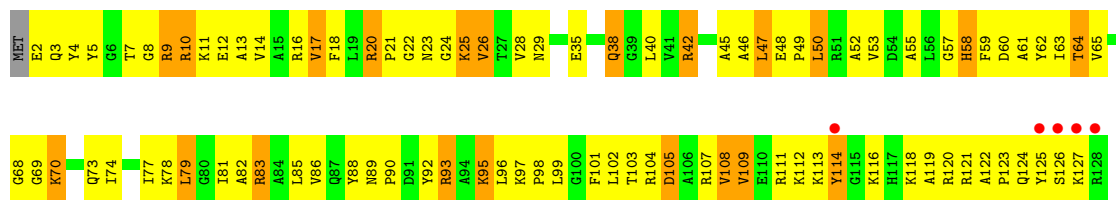
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



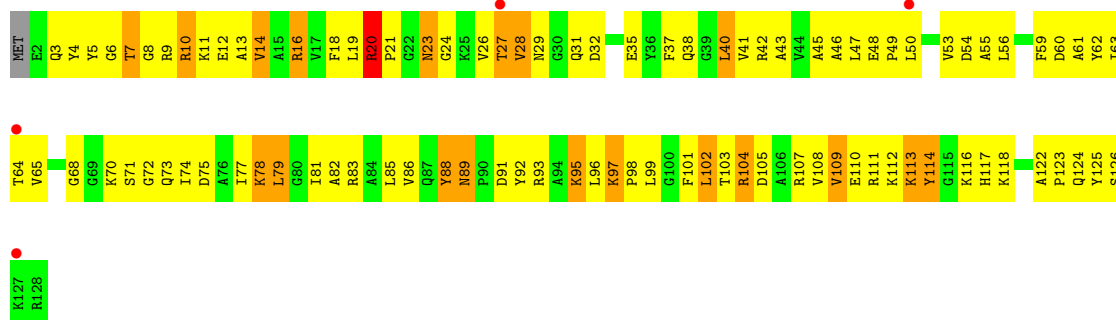
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



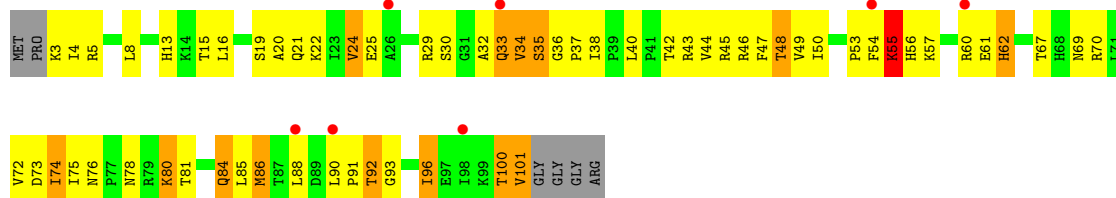
- Molecule 39: 30S RIBOSOMAL PROTEIN S9



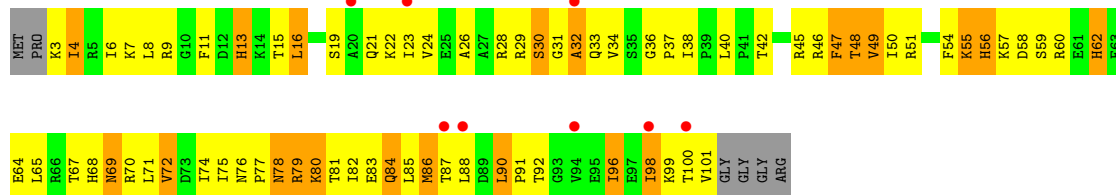
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



• Molecule 40: 30S RIBOSOMAL PROTEIN S10

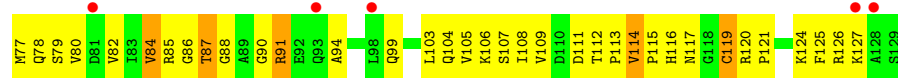
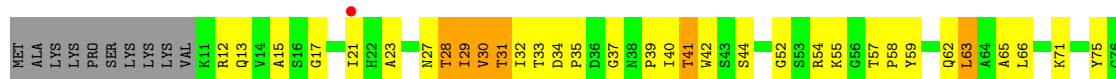


• Molecule 40: 30S RIBOSOMAL PROTEIN S10

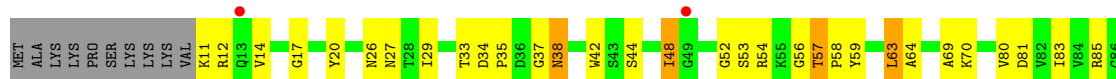


• Molecule 41: 30S RIBOSOMAL PROTEIN S11





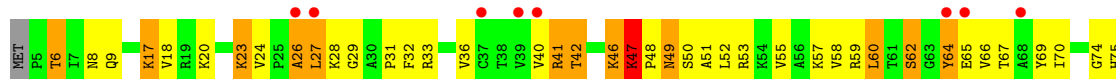
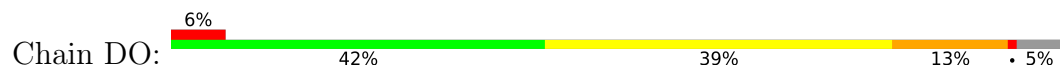
• Molecule 41: 30S RIBOSOMAL PROTEIN S11



• Molecule 42: 30S RIBOSOMAL PROTEIN S12



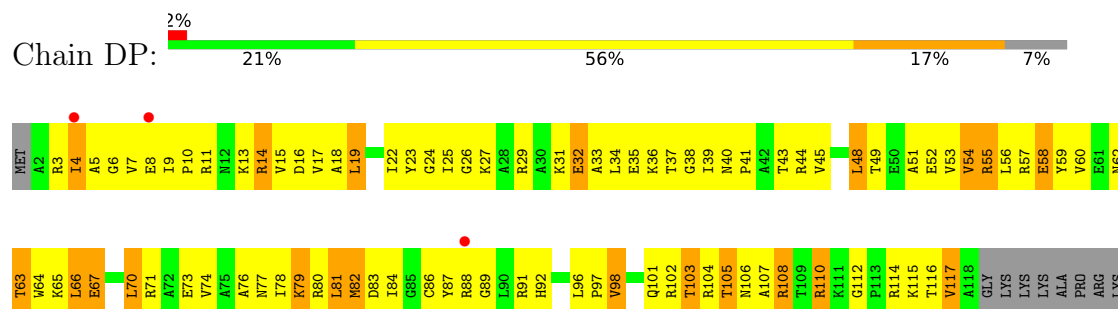
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



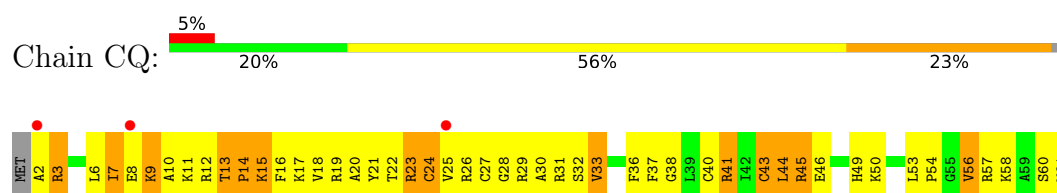
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



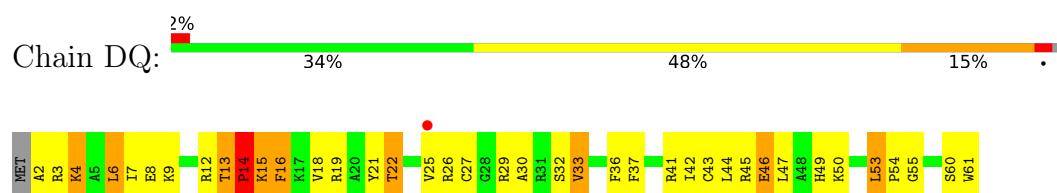
- Molecule 43: 30S RIBOSOMAL PROTEIN S13



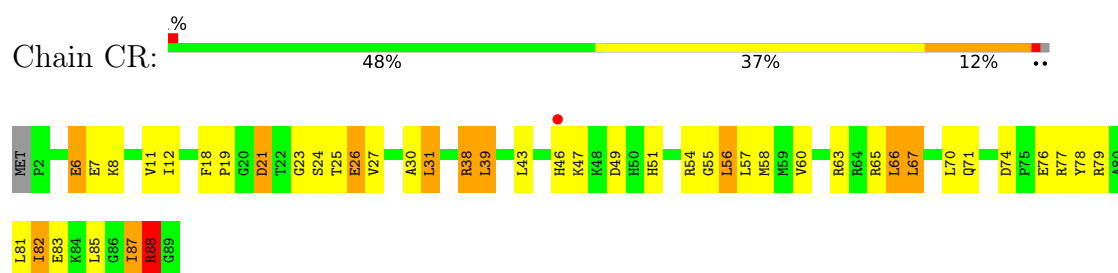
- Molecule 44: 30S RIBOSOMAL PROTEIN S14



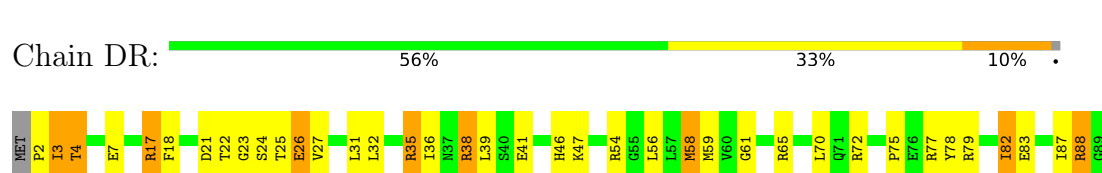
- Molecule 44: 30S RIBOSOMAL PROTEIN S14



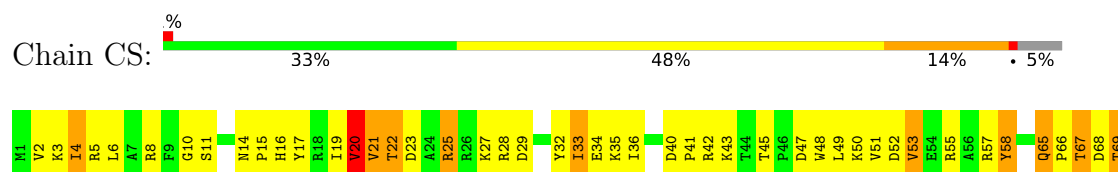
- Molecule 45: 30S RIBOSOMAL PROTEIN S15



- Molecule 45: 30S RIBOSOMAL PROTEIN S15

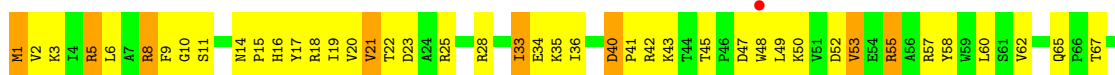


- Molecule 46: 30S RIBOSOMAL PROTEIN S16





• Molecule 46: 30S RIBOSOMAL PROTEIN S16



• Molecule 47: 30S RIBOSOMAL PROTEIN S17



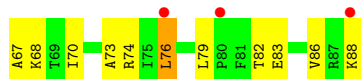
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

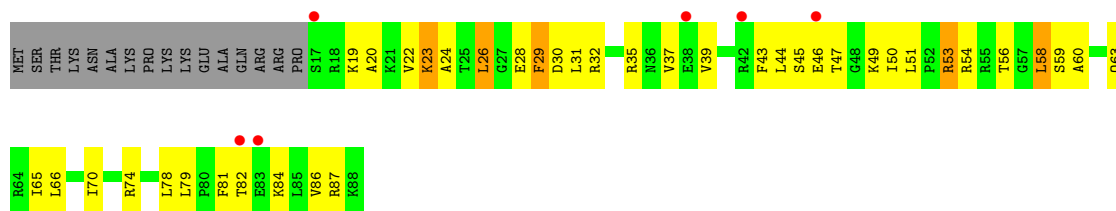


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

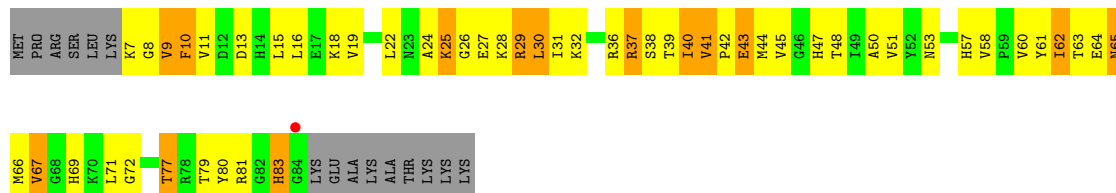


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

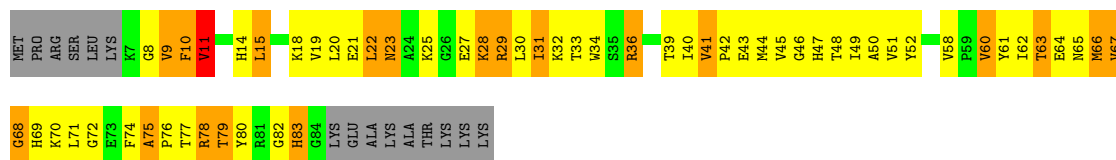
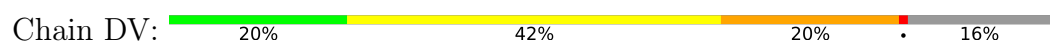




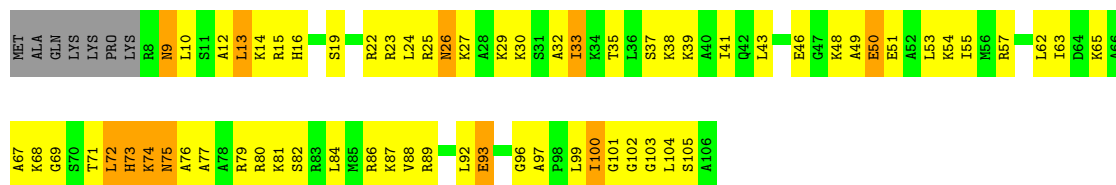
● Molecule 49: 30S RIBOSOMAL PROTEIN S19



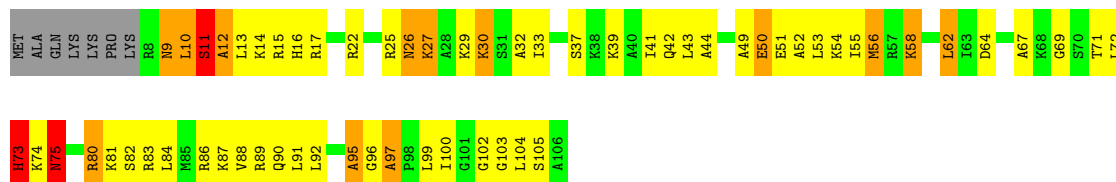
● Molecule 49: 30S RIBOSOMAL PROTEIN S19



● Molecule 50: 30S RIBOSOMAL PROTEIN S20



● Molecule 50: 30S RIBOSOMAL PROTEIN S20

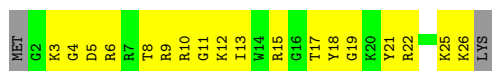


● Molecule 51: 30S RIBOSOMAL PROTEIN THX

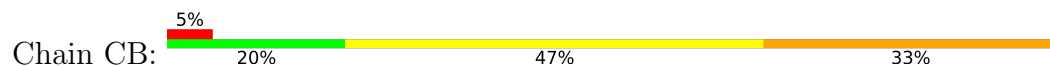




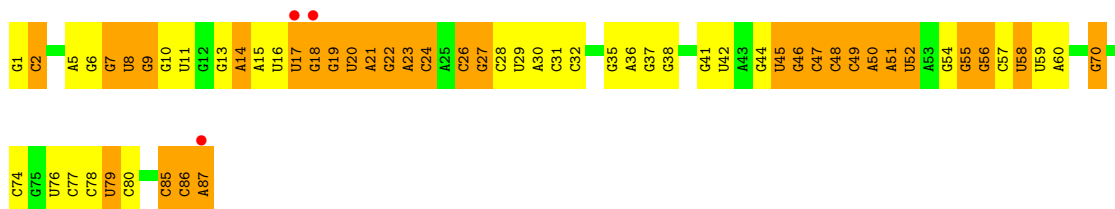
- Molecule 51: 30S RIBOSOMAL PROTEIN THX



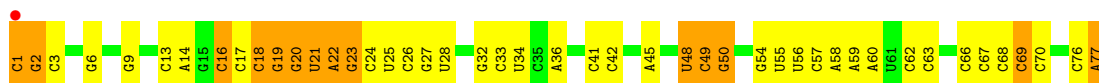
- Molecule 52: TRNA-LEU



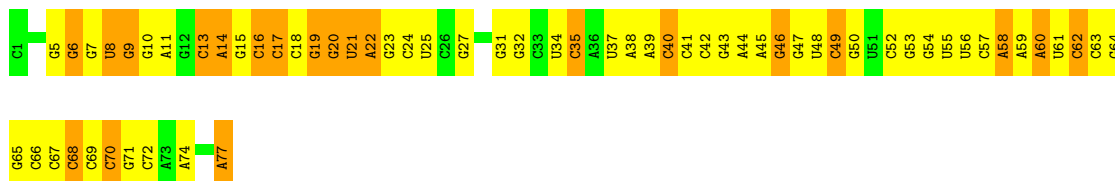
- Molecule 52: TRNA-LEU



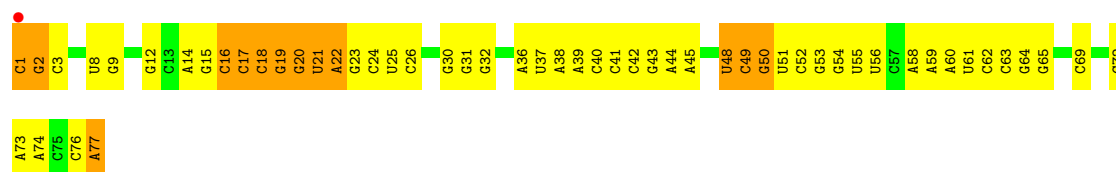
- Molecule 53: TRNA-FMET



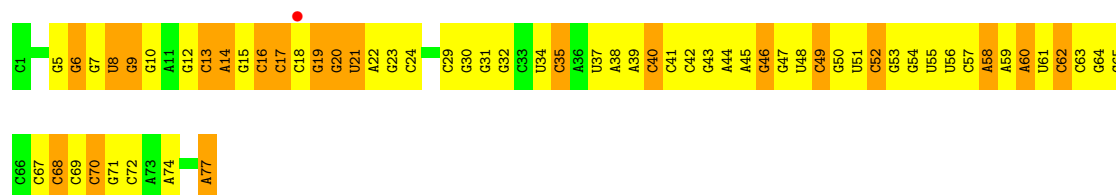
- Molecule 53: TRNA-FMET



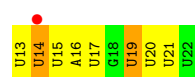
- Molecule 53: TRNA-FMET



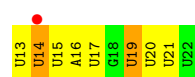
• Molecule 53: TRNA-FMET



• 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 , 0.237	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, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.35	0/70233	0.45	0/109643
1	BA	0.32	0/70167	0.43	2/109541 (0.0%)
2	AB	0.31	0/2928	0.43	0/4568
2	BB	0.27	0/2928	0.41	0/4568
3	AD	0.68	0/2165	1.21	17/2919 (0.6%)
3	BD	0.58	0/2165	1.10	6/2919 (0.2%)
4	AE	0.57	0/1601	1.19	15/2160 (0.7%)
4	BE	0.54	0/1601	1.20	14/2160 (0.6%)
5	AF	0.58	0/1620	1.13	13/2194 (0.6%)
5	BF	0.47	0/1662	1.07	10/2249 (0.4%)
6	AG	0.44	0/1499	1.00	8/2016 (0.4%)
6	BG	0.38	0/1499	0.92	7/2016 (0.3%)
7	AH	0.56	0/1332	1.26	22/1802 (1.2%)
7	BH	0.44	0/1332	1.14	10/1802 (0.6%)
8	AK	0.52	0/1151	1.10	6/1558 (0.4%)
8	BK	0.48	0/1151	1.00	5/1558 (0.3%)
9	AM	0.58	0/1131	1.13	12/1525 (0.8%)
9	BM	0.43	0/1131	0.96	6/1525 (0.4%)
10	AN	0.56	0/943	1.07	7/1269 (0.6%)
10	BN	0.51	0/943	0.93	1/1269 (0.1%)
11	AO	0.50	0/1162	1.14	10/1544 (0.6%)
11	BO	0.42	0/1162	0.94	2/1544 (0.1%)
12	AP	0.51	0/1143	1.00	9/1527 (0.6%)
12	BP	0.41	0/1143	0.88	2/1527 (0.1%)
13	A0	0.57	0/982	1.00	4/1312 (0.3%)
13	B0	0.55	0/974	1.03	1/1302 (0.1%)
14	AQ	0.47	0/892	0.95	1/1187 (0.1%)
14	BQ	0.45	0/892	0.91	2/1187 (0.2%)
15	AR	0.56	0/1155	1.09	8/1542 (0.5%)
15	BR	0.52	0/1155	1.01	5/1542 (0.3%)
16	A1	0.54	0/982	0.98	4/1306 (0.3%)
16	B1	0.50	0/982	0.96	4/1306 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.56	0/790	1.17	9/1057 (0.9%)
17	B2	0.43	0/790	0.96	2/1057 (0.2%)
18	AS	0.58	0/911	0.99	1/1220 (0.1%)
18	BS	0.58	0/911	0.97	1/1220 (0.1%)
19	AT	0.58	0/739	1.06	4/993 (0.4%)
19	BT	0.56	0/739	1.01	1/993 (0.1%)
20	AU	0.63	0/798	1.09	4/1064 (0.4%)
20	BU	0.60	0/798	1.07	3/1064 (0.3%)
21	AV	0.44	0/1427	1.06	6/1935 (0.3%)
21	BV	0.40	0/1460	1.01	11/1982 (0.6%)
22	A3	0.54	0/615	1.07	2/819 (0.2%)
22	B3	0.51	0/621	1.07	4/827 (0.5%)
23	AZ	0.58	0/770	1.10	1/1022 (0.1%)
23	BZ	0.56	0/770	1.07	2/1022 (0.2%)
24	AW	0.59	0/560	1.22	5/741 (0.7%)
24	BW	0.47	0/583	1.02	3/771 (0.4%)
25	AX	0.47	0/474	1.06	2/635 (0.3%)
25	BX	0.45	0/474	0.93	2/635 (0.3%)
26	A4	0.48	0/545	1.07	5/733 (0.7%)
26	B4	0.47	0/527	1.13	7/709 (1.0%)
27	A5	0.56	0/473	1.08	4/639 (0.6%)
27	B5	0.49	0/473	1.02	0/639
28	A6	0.55	0/396	1.16	6/529 (1.1%)
28	B6	0.51	0/396	0.92	0/529
29	A7	0.62	0/438	1.01	2/575 (0.3%)
29	B7	0.53	0/438	0.94	2/575 (0.3%)
30	A8	0.69	0/494	1.39	11/649 (1.7%)
30	B8	0.52	0/494	0.88	0/649
31	CA	0.28	0/36234	0.41	0/56554
31	DA	0.27	0/36237	0.40	0/56558
32	CE	0.41	0/1959	0.90	2/2642 (0.1%)
32	DE	0.38	0/1959	0.95	6/2642 (0.2%)
33	CF	0.43	0/1629	0.83	2/2195 (0.1%)
33	DF	0.43	0/1636	0.89	3/2205 (0.1%)
34	CG	0.49	0/1733	0.98	8/2318 (0.3%)
34	DG	0.45	0/1733	1.06	12/2318 (0.5%)
35	CH	0.50	0/1171	0.93	4/1576 (0.3%)
35	DH	0.44	0/1171	0.95	5/1576 (0.3%)
36	CI	0.50	0/856	0.90	0/1154
36	DI	0.46	0/856	0.83	0/1154
37	CJ	0.41	0/1276	0.85	2/1709 (0.1%)
37	DJ	0.40	0/1276	0.83	1/1709 (0.1%)
38	CK	0.45	0/1136	1.02	9/1527 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.41	0/1136	0.89	4/1527 (0.3%)
39	CL	0.40	0/1029	0.84	1/1379 (0.1%)
39	DL	0.37	0/1029	0.88	2/1379 (0.1%)
40	CM	0.43	0/814	0.93	1/1095 (0.1%)
40	DM	0.41	0/814	0.98	3/1095 (0.3%)
41	CN	0.50	0/900	0.94	0/1213
41	DN	0.48	0/900	0.98	4/1213 (0.3%)
42	CO	0.59	0/991	1.17	9/1327 (0.7%)
42	DO	0.53	0/991	1.00	2/1327 (0.2%)
43	CP	0.42	0/938	0.93	2/1258 (0.2%)
43	DP	0.40	0/943	0.85	4/1265 (0.3%)
44	CQ	0.51	0/501	0.98	1/664 (0.2%)
44	DQ	0.38	0/501	0.98	4/664 (0.6%)
45	CR	0.50	0/745	0.94	1/992 (0.1%)
45	DR	0.46	0/745	0.80	1/992 (0.1%)
46	CS	0.40	0/721	0.92	4/970 (0.4%)
46	DS	0.47	0/721	0.96	3/970 (0.3%)
47	CT	0.41	0/847	0.86	1/1131 (0.1%)
47	DT	0.41	0/847	0.87	0/1131
48	CU	0.47	0/596	0.92	1/790 (0.1%)
48	DU	0.45	0/596	0.89	1/790 (0.1%)
49	CV	0.45	0/638	0.92	2/860 (0.2%)
49	DV	0.39	0/638	1.09	4/860 (0.5%)
50	CW	0.40	0/765	0.90	2/1007 (0.2%)
50	DW	0.47	0/765	1.07	6/1007 (0.6%)
51	CX	0.37	0/221	0.83	0/288
51	DX	0.33	0/221	0.78	0/288
52	CB	0.25	0/2080	0.35	0/3242
52	DB	0.26	0/2080	0.35	0/3242
53	CC	0.27	0/1835	0.39	0/2859
53	CD	0.16	0/1835	0.30	0/2859
53	DC	0.26	0/1835	0.38	0/2859
53	DD	0.17	0/1835	0.30	0/2859
54	C1	0.40	0/226	0.35	0/348
54	D1	0.34	0/226	0.37	0/348
All	All	0.37	0/324077	0.63	430/485305 (0.1%)

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

There are no bond length outliers.

The worst 5 of 430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	DW	12	ALA	N-CA-C	-11.70	98.43	113.17
4	BE	67	PHE	N-CA-C	-11.36	99.07	113.16
25	AX	11	SER	CA-C-N	11.31	131.64	119.87
25	AX	11	SER	C-N-CA	11.31	131.64	119.87
34	CG	31	CYS	N-CA-C	-10.89	99.52	112.92

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	2747	0
1	BA	62647	0	31583	2777	1
2	AB	2617	0	1328	106	0
2	BB	2617	0	1328	134	0
3	AD	2115	0	2195	273	0
3	BD	2115	0	2195	246	0
4	AE	1568	0	1634	297	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BE	1568	0	1634	294	0
5	AF	1585	0	1632	150	0
5	BF	1627	0	1680	212	0
6	AG	1474	0	1535	205	0
6	BG	1474	0	1535	169	0
7	AH	1307	0	1382	160	0
7	BH	1307	0	1382	149	2
8	AK	1136	0	1223	130	0
8	BK	1136	0	1223	106	0
9	AM	1104	0	1180	140	0
9	BM	1104	0	1180	108	0
10	AN	933	0	996	60	0
10	BN	933	0	996	71	0
11	AO	1145	0	1228	253	0
11	BO	1145	0	1228	317	0
12	AP	1122	0	1179	215	0
12	BP	1122	0	1179	251	0
13	A0	968	0	1033	85	0
13	B0	960	0	1021	87	0
14	AQ	882	0	943	105	0
14	BQ	882	0	943	107	0
15	AR	1141	0	1202	134	0
15	BR	1141	0	1202	136	0
16	A1	964	0	1022	117	0
16	B1	964	0	1022	112	0
17	A2	779	0	852	100	1
17	B2	779	0	852	183	0
18	AS	900	0	964	86	0
18	BS	900	0	964	59	0
19	AT	725	0	778	62	0
19	BT	725	0	778	63	0
20	AU	785	0	878	96	0
20	BU	785	0	878	118	0
21	AV	1397	0	1430	148	0
21	BV	1428	0	1454	145	0
22	A3	607	0	628	66	0
22	B3	613	0	633	59	0
23	AZ	763	0	848	68	0
23	BZ	763	0	848	62	0
24	AW	558	0	610	48	0
24	BW	581	0	629	65	0
25	AX	469	0	518	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BX	469	0	518	34	0
26	A4	533	0	522	82	0
26	B4	515	0	510	111	0
27	A5	459	0	480	79	1
27	B5	459	0	480	72	0
28	A6	389	0	404	89	0
28	B6	389	0	404	110	0
29	A7	430	0	480	29	0
29	B7	430	0	480	32	0
30	A8	488	0	560	108	0
30	B8	488	0	560	156	0
31	CA	32369	0	16339	1553	2
31	DA	32372	0	16338	1514	1
32	CE	1924	0	1975	197	0
32	DE	1924	0	1975	215	0
33	CF	1605	0	1668	127	0
33	DF	1612	0	1677	168	0
34	CG	1703	0	1764	185	0
34	DG	1703	0	1763	162	1
35	CH	1155	0	1213	83	0
35	DH	1155	0	1213	95	0
36	CI	843	0	857	63	1
36	DI	843	0	857	48	0
37	CJ	1257	0	1296	76	0
37	DJ	1257	0	1296	94	0
38	CK	1116	0	1177	103	0
38	DK	1116	0	1177	66	0
39	CL	1010	0	1037	113	0
39	DL	1010	0	1037	131	0
40	CM	801	0	849	88	0
40	DM	801	0	849	97	0
41	CN	885	0	904	82	0
41	DN	885	0	904	45	0
42	CO	975	0	1062	65	0
42	DO	975	0	1062	90	0
43	CP	928	0	987	84	0
43	DP	933	0	992	110	0
44	CQ	492	0	529	60	0
44	DQ	492	0	529	60	0
45	CR	734	0	771	56	0
45	DR	734	0	771	46	0
46	CS	705	0	725	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DS	705	0	725	48	0
47	CT	834	0	904	82	0
47	DT	834	0	904	45	0
48	CU	591	0	662	33	0
48	DU	591	0	662	43	0
49	CV	624	0	636	77	0
49	DV	624	0	636	103	0
50	CW	763	0	861	78	0
50	DW	763	0	861	72	0
51	CX	217	0	234	20	0
51	DX	217	0	234	28	0
52	CB	1861	0	938	83	0
52	DB	1861	0	938	82	0
53	CC	1643	0	837	68	0
53	CD	1643	0	837	99	0
53	DC	1643	0	837	77	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17863	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 36.

The worst 5 of 17863 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4	24
6	AG	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	2	16
6	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	21	52
7	AH	168/180 (93%)	135 (80%)	25 (15%)	8 (5%)	2	12
7	BH	168/180 (93%)	129 (77%)	37 (22%)	2 (1%)	10	37
8	AK	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	1	9
8	BK	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	5	26
9	AM	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	2	13
9	BM	136/140 (97%)	120 (88%)	12 (9%)	4 (3%)	3	21
10	AN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	BN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	45
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	43
13	B0	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	AQ	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	6	29
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	32
15	BR	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
16	A1	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	14	43
16	B1	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	14	43
17	A2	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	3	20
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	43
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%)	11	39
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	15
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	19
23	BZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	11	39
24	AW	64/72 (89%)	60 (94%)	1 (2%)	3 (5%)	2	12
24	BW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8	32
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	20
26	B4	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	3	19
27	A5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	12
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	30
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	60
32	DE	235/256 (92%)	186 (79%)	45 (19%)	4 (2%)	7	30
33	CF	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
33	DF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	12	40
34	CG	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	24	55
34	DG	206/208 (99%)	177 (86%)	28 (14%)	1 (0%)	24	55
35	CH	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	18	49
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%)	18	49
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	26
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%)	7	31
42	DO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	7	31
43	CP	114/126 (90%)	90 (79%)	24 (21%)	0	100	100
43	DP	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	CQ	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
44	DQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
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	27
47	DT	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
48	CU	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	9	33
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%)	12	40
50	DW	97/106 (92%)	81 (84%)	15 (16%)	1 (1%)	12	40
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%)	170 (79%)	44 (21%)	1	6
3	BD	214/218 (98%)	158 (74%)	56 (26%)	0	2
4	AE	165/166 (99%)	118 (72%)	47 (28%)	0	2
4	BE	165/166 (99%)	122 (74%)	43 (26%)	0	2
5	AF	161/166 (97%)	123 (76%)	38 (24%)	1	4
5	BF	165/166 (99%)	126 (76%)	39 (24%)	1	4
6	AG	155/156 (99%)	122 (79%)	33 (21%)	1	5
6	BG	155/156 (99%)	115 (74%)	40 (26%)	0	2
7	AH	142/148 (96%)	106 (75%)	36 (25%)	0	3
7	BH	142/148 (96%)	116 (82%)	26 (18%)	2	7
8	AK	122/124 (98%)	92 (75%)	30 (25%)	1	3
8	BK	122/124 (98%)	88 (72%)	34 (28%)	0	2
9	AM	117/119 (98%)	85 (73%)	32 (27%)	0	2
9	BM	117/119 (98%)	91 (78%)	26 (22%)	1	5
10	AN	100/100 (100%)	84 (84%)	16 (16%)	2	11
10	BN	100/100 (100%)	75 (75%)	25 (25%)	0	3
11	AO	116/116 (100%)	78 (67%)	38 (33%)	0	1
11	BO	116/116 (100%)	74 (64%)	42 (36%)	0	1
12	AP	111/111 (100%)	83 (75%)	28 (25%)	0	3
12	BP	111/111 (100%)	86 (78%)	25 (22%)	1	5
13	A0	101/101 (100%)	73 (72%)	28 (28%)	0	2
13	B0	100/101 (99%)	79 (79%)	21 (21%)	1	5
14	AQ	87/88 (99%)	62 (71%)	25 (29%)	0	2
14	BQ	87/88 (99%)	64 (74%)	23 (26%)	0	2
15	AR	120/127 (94%)	86 (72%)	34 (28%)	0	2
15	BR	120/127 (94%)	84 (70%)	36 (30%)	0	1
16	A1	93/94 (99%)	74 (80%)	19 (20%)	1	6
16	B1	93/94 (99%)	78 (84%)	15 (16%)	2	12
17	A2	82/82 (100%)	55 (67%)	27 (33%)	0	1
17	B2	82/82 (100%)	56 (68%)	26 (32%)	0	1
18	AS	92/92 (100%)	73 (79%)	19 (21%)	1	6
18	BS	92/92 (100%)	64 (70%)	28 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AT	74/78 (95%)	54 (73%)	20 (27%)	0	2
19	BT	74/78 (95%)	56 (76%)	18 (24%)	1	3
20	AU	85/91 (93%)	65 (76%)	20 (24%)	1	4
20	BU	85/91 (93%)	57 (67%)	28 (33%)	0	1
21	AV	154/179 (86%)	124 (80%)	30 (20%)	1	6
21	BV	158/179 (88%)	127 (80%)	31 (20%)	1	6
22	A3	61/67 (91%)	48 (79%)	13 (21%)	1	5
22	B3	62/67 (92%)	50 (81%)	12 (19%)	1	6
23	AZ	82/83 (99%)	63 (77%)	19 (23%)	1	4
23	BZ	82/83 (99%)	61 (74%)	21 (26%)	0	2
24	AW	62/67 (92%)	43 (69%)	19 (31%)	0	1
24	BW	64/67 (96%)	50 (78%)	14 (22%)	1	5
25	AX	51/52 (98%)	45 (88%)	6 (12%)	5	20
25	BX	51/52 (98%)	40 (78%)	11 (22%)	1	5
26	A4	59/63 (94%)	42 (71%)	17 (29%)	0	2
26	B4	57/63 (90%)	39 (68%)	18 (32%)	0	1
27	A5	51/52 (98%)	36 (71%)	15 (29%)	0	2
27	B5	51/52 (98%)	37 (72%)	14 (28%)	0	2
28	A6	44/52 (85%)	28 (64%)	16 (36%)	0	1
28	B6	44/52 (85%)	29 (66%)	15 (34%)	0	1
29	A7	42/42 (100%)	34 (81%)	8 (19%)	1	7
29	B7	42/42 (100%)	30 (71%)	12 (29%)	0	2
30	A8	51/55 (93%)	41 (80%)	10 (20%)	1	6
30	B8	51/55 (93%)	36 (71%)	15 (29%)	0	2
32	CE	205/220 (93%)	162 (79%)	43 (21%)	1	5
32	DE	205/220 (93%)	163 (80%)	42 (20%)	1	6
33	CF	159/188 (85%)	129 (81%)	30 (19%)	1	7
33	DF	160/188 (85%)	124 (78%)	36 (22%)	1	5
34	CG	180/180 (100%)	149 (83%)	31 (17%)	2	10
34	DG	180/180 (100%)	141 (78%)	39 (22%)	1	5
35	CH	116/123 (94%)	91 (78%)	25 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DH	116/123 (94%)	92 (79%)	24 (21%)	1	6
36	CI	90/90 (100%)	75 (83%)	15 (17%)	2	11
36	DI	90/90 (100%)	74 (82%)	16 (18%)	2	8
37	CJ	126/127 (99%)	102 (81%)	24 (19%)	1	7
37	DJ	126/127 (99%)	96 (76%)	30 (24%)	1	4
38	CK	119/119 (100%)	102 (86%)	17 (14%)	3	14
38	DK	119/119 (100%)	103 (87%)	16 (13%)	4	16
39	CL	98/99 (99%)	70 (71%)	28 (29%)	0	2
39	DL	98/99 (99%)	69 (70%)	29 (30%)	0	1
40	CM	89/92 (97%)	68 (76%)	21 (24%)	1	4
40	DM	89/92 (97%)	64 (72%)	25 (28%)	0	2
41	CN	90/99 (91%)	76 (84%)	14 (16%)	2	12
41	DN	90/99 (91%)	78 (87%)	12 (13%)	4	17
42	CO	104/109 (95%)	89 (86%)	15 (14%)	3	14
42	DO	104/109 (95%)	82 (79%)	22 (21%)	1	5
43	CP	94/101 (93%)	72 (77%)	22 (23%)	1	4
43	DP	94/101 (93%)	74 (79%)	20 (21%)	1	5
44	CQ	49/50 (98%)	33 (67%)	16 (33%)	0	1
44	DQ	49/50 (98%)	37 (76%)	12 (24%)	1	3
45	CR	79/80 (99%)	65 (82%)	14 (18%)	2	8
45	DR	79/80 (99%)	67 (85%)	12 (15%)	3	13
46	CS	72/74 (97%)	59 (82%)	13 (18%)	2	8
46	DS	72/74 (97%)	58 (81%)	14 (19%)	1	6
47	CT	95/97 (98%)	82 (86%)	13 (14%)	3	16
47	DT	95/97 (98%)	84 (88%)	11 (12%)	5	21
48	CU	63/77 (82%)	50 (79%)	13 (21%)	1	6
48	DU	63/77 (82%)	51 (81%)	12 (19%)	1	7
49	CV	67/80 (84%)	48 (72%)	19 (28%)	0	2
49	DV	67/80 (84%)	52 (78%)	15 (22%)	1	5
50	CW	76/82 (93%)	61 (80%)	15 (20%)	1	6
50	DW	76/82 (93%)	59 (78%)	17 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	CX	20/22 (91%)	17 (85%)	3 (15%)	3	13
51	DX	20/22 (91%)	20 (100%)	0	100	100
All	All	9579/9996 (96%)	7383 (77%)	2196 (23%)	1	4

5 of 2196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	DF	94	LEU
34	DG	196	LEU
33	DF	84	ILE
42	DO	104	VAL
4	BE	175	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
49	CV	65	ASN
49	DV	56	GLN
32	DE	95	GLN
37	DJ	86	GLN
3	BD	166	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	701 (24%)	52 (1%)
1	BA	2908/2912 (99%)	714 (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%)	355 (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
54	D1	9/10 (90%)	2 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9568/9582 (99%)	2335 (24%)	206 (2%)

5 of 2335 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	DA	1805	-	44,45,45	0.55	0	63,67,67	1.70	16 (25%)
56	PAR	CA	1841	-	44,45,45	0.53	0	63,67,67	1.41	9 (14%)

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	DA	1805	-	-	6/18/94/94	0/4/4/4
56	PAR	CA	1841	-	-	8/18/94/94	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

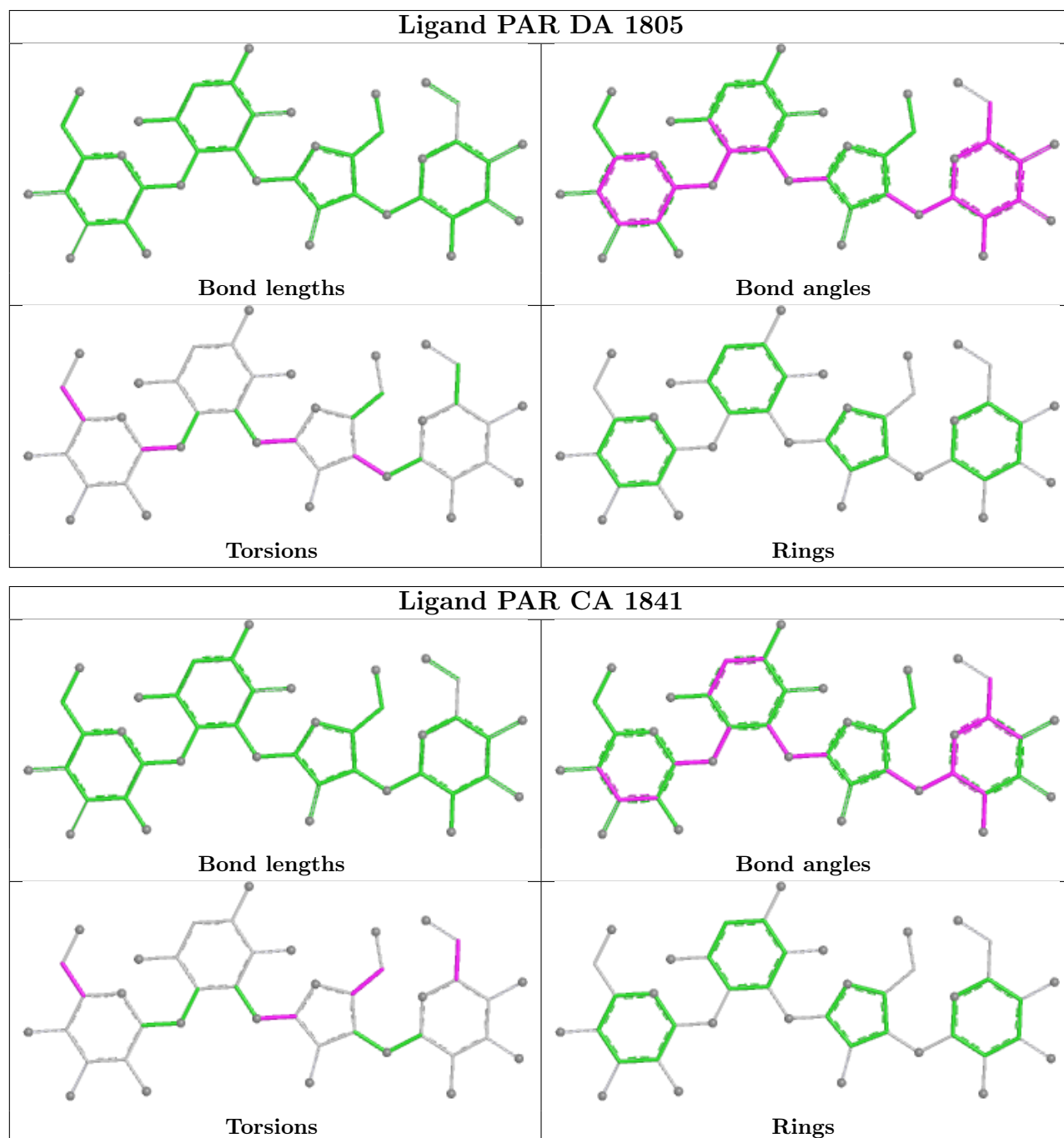
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1805	PAR	5	0
56	CA	1841	PAR	4	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%)	-0.68	14 (0%) 87 76	50, 80, 215, 247	0
1	BA	2909/2912 (99%)	-0.56	14 (0%) 87 76	60, 95, 235, 249	0
2	AB	122/122 (100%)	-0.64	1 (0%) 82 68	81, 105, 124, 182	0
2	BB	122/122 (100%)	-0.58	1 (0%) 82 68	98, 133, 156, 203	0
3	AD	272/276 (98%)	-0.30	0 100 100	47, 72, 94, 112	0
3	BD	272/276 (98%)	-0.06	4 (1%) 72 53	56, 82, 103, 138	0
4	AE	205/206 (99%)	0.55	29 (14%) 6 5	55, 91, 137, 149	0
4	BE	205/206 (99%)	0.30	17 (8%) 17 13	66, 104, 153, 172	0
5	AF	202/210 (96%)	-0.34	2 (0%) 79 63	52, 84, 123, 137	0
5	BF	208/210 (99%)	0.61	23 (11%) 10 9	64, 108, 166, 191	0
6	AG	181/182 (99%)	-0.08	5 (2%) 55 36	95, 115, 143, 157	0
6	BG	181/182 (99%)	0.15	4 (2%) 62 43	125, 148, 169, 176	0
7	AH	170/180 (94%)	0.40	6 (3%) 47 31	89, 119, 138, 160	0
7	BH	170/180 (94%)	0.50	13 (7%) 20 14	161, 203, 224, 232	0
8	AK	146/148 (98%)	0.47	7 (4%) 35 24	85, 134, 151, 157	0
8	BK	146/148 (98%)	0.31	3 (2%) 63 44	91, 134, 158, 167	0
9	AM	138/140 (98%)	0.55	12 (8%) 16 12	70, 95, 131, 144	0
9	BM	138/140 (98%)	0.34	4 (2%) 53 35	86, 118, 148, 158	0
10	AN	122/122 (100%)	-0.35	0 100 100	63, 82, 98, 111	0
10	BN	122/122 (100%)	0.06	1 (0%) 82 68	76, 98, 116, 133	0
11	AO	150/150 (100%)	0.27	8 (5%) 32 22	45, 90, 122, 167	0
11	BO	150/150 (100%)	1.17	28 (18%) 3 3	44, 101, 149, 186	0
12	AP	141/141 (100%)	0.55	10 (7%) 22 15	58, 91, 116, 142	0
12	BP	141/141 (100%)	0.65	10 (7%) 22 15	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%)	-0.31	1 (0%) 82 68	64, 90, 109, 123	0
13	B0	117/118 (99%)	-0.46	0 100 100	68, 90, 113, 128	0
14	AQ	111/112 (99%)	0.21	3 (2%) 56 37	83, 103, 126, 142	0
14	BQ	111/112 (99%)	0.15	3 (2%) 56 37	95, 132, 156, 175	0
15	AR	137/146 (93%)	-0.07	6 (4%) 39 25	75, 97, 147, 178	0
15	BR	137/146 (93%)	0.17	8 (5%) 29 19	86, 107, 167, 187	0
16	A1	117/118 (99%)	-0.05	3 (2%) 57 38	61, 84, 116, 145	0
16	B1	117/118 (99%)	0.30	2 (1%) 69 50	71, 106, 146, 165	0
17	A2	101/101 (100%)	0.20	3 (2%) 52 35	61, 105, 126, 145	0
17	B2	101/101 (100%)	1.26	21 (20%) 2 2	73, 131, 148, 158	0
18	AS	113/113 (100%)	-0.13	3 (2%) 56 37	55, 80, 111, 163	0
18	BS	113/113 (100%)	0.01	2 (1%) 67 49	69, 84, 121, 162	0
19	AT	92/96 (95%)	0.12	5 (5%) 31 21	63, 78, 102, 118	0
19	BT	92/96 (95%)	0.03	4 (4%) 40 25	78, 96, 119, 134	0
20	AU	102/110 (92%)	0.48	7 (6%) 23 16	82, 107, 157, 172	0
20	BU	102/110 (92%)	1.07	16 (15%) 5 4	97, 123, 176, 191	0
21	AV	175/206 (84%)	0.63	9 (5%) 33 22	93, 133, 193, 198	0
21	BV	179/206 (86%)	0.11	3 (1%) 69 50	128, 166, 212, 218	0
22	A3	76/85 (89%)	-0.06	2 (2%) 57 38	65, 84, 98, 136	0
22	B3	77/85 (90%)	-0.03	2 (2%) 57 38	79, 101, 122, 155	0
23	AZ	97/98 (98%)	-0.10	3 (3%) 51 35	61, 81, 137, 165	0
23	BZ	97/98 (98%)	0.41	7 (7%) 21 15	69, 91, 141, 162	0
24	AW	66/72 (91%)	0.25	7 (10%) 11 9	69, 87, 106, 136	0
24	BW	69/72 (95%)	0.28	1 (1%) 73 55	90, 114, 148, 183	0
25	AX	59/60 (98%)	0.06	2 (3%) 48 32	73, 90, 120, 135	0
25	BX	59/60 (98%)	0.29	1 (1%) 69 50	86, 114, 146, 166	0
26	A4	66/71 (92%)	0.25	1 (1%) 72 53	127, 161, 179, 187	0
26	B4	63/71 (88%)	0.28	0 100 100	154, 190, 200, 207	0
27	A5	59/60 (98%)	0.39	5 (8%) 16 13	55, 95, 180, 185	0
27	B5	59/60 (98%)	0.43	4 (6%) 23 16	65, 94, 181, 192	0
28	A6	45/54 (83%)	1.10	8 (17%) 4 3	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%)	1.45	13 (28%) 1 1	141, 173, 188, 192	0
29	A7	49/49 (100%)	-0.53	0 100 100	50, 60, 106, 137	0
29	B7	49/49 (100%)	-0.23	0 100 100	60, 69, 129, 148	0
30	A8	61/65 (93%)	0.05	4 (6%) 24 16	64, 78, 95, 120	0
30	B8	61/65 (93%)	1.06	13 (21%) 2 2	78, 95, 110, 142	0
31	CA	1506/1506 (100%)	-0.57	15 (0%) 79 63	64, 112, 193, 248	0
31	DA	1506/1506 (100%)	-0.57	7 (0%) 87 76	76, 122, 195, 248	0
32	CE	237/256 (92%)	0.93	33 (13%) 6 5	115, 149, 188, 198	0
32	DE	237/256 (92%)	0.99	33 (13%) 6 5	127, 165, 200, 215	0
33	CF	205/239 (85%)	0.40	6 (2%) 53 35	98, 124, 158, 166	0
33	DF	206/239 (86%)	0.62	18 (8%) 16 12	128, 151, 180, 188	0
34	CG	208/208 (100%)	0.23	4 (1%) 66 48	95, 119, 143, 154	0
34	DG	208/208 (100%)	0.09	3 (1%) 73 55	91, 116, 137, 151	0
35	CH	151/162 (93%)	0.13	4 (2%) 57 38	87, 109, 132, 166	0
35	DH	151/162 (93%)	-0.00	0 100 100	104, 125, 148, 169	0
36	CI	101/101 (100%)	0.14	2 (1%) 65 46	89, 112, 130, 153	0
36	DI	101/101 (100%)	0.04	0 100 100	87, 109, 130, 156	0
37	CJ	155/156 (99%)	0.35	9 (5%) 29 19	111, 128, 158, 167	0
37	DJ	155/156 (99%)	0.14	2 (1%) 75 56	116, 136, 164, 170	0
38	CK	138/138 (100%)	-0.09	0 100 100	95, 116, 130, 137	0
38	DK	138/138 (100%)	-0.16	0 100 100	109, 129, 143, 151	0
39	CL	127/128 (99%)	0.30	5 (3%) 43 29	99, 147, 167, 173	0
39	DL	127/128 (99%)	-0.01	4 (3%) 51 35	120, 158, 174, 178	0
40	CM	99/105 (94%)	0.65	7 (7%) 22 15	93, 146, 176, 179	0
40	DM	99/105 (94%)	0.66	8 (8%) 18 13	127, 164, 180, 185	0
41	CN	119/129 (92%)	0.11	6 (5%) 34 23	79, 110, 142, 169	0
41	DN	119/129 (92%)	0.20	6 (5%) 34 23	90, 116, 148, 172	0
42	CO	125/132 (94%)	0.06	4 (3%) 50 34	76, 87, 119, 164	0
42	DO	125/132 (94%)	0.38	8 (6%) 25 17	88, 112, 137, 175	0
43	CP	116/126 (92%)	0.10	2 (1%) 69 50	98, 132, 151, 160	0
43	DP	117/126 (92%)	-0.13	3 (2%) 57 38	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%)	0.12	3 (5%) 34 23	95, 115, 129, 139	0
44	DQ	60/61 (98%)	-0.09	1 (1%) 69 50	129, 146, 159, 166	0
45	CR	88/89 (98%)	-0.33	1 (1%) 78 60	86, 108, 129, 133	0
45	DR	88/89 (98%)	-0.21	0 100 100	85, 118, 142, 148	0
46	CS	84/88 (95%)	-0.37	1 (1%) 76 58	104, 121, 148, 179	0
46	DS	84/88 (95%)	0.07	3 (3%) 46 31	94, 111, 134, 166	0
47	CT	100/105 (95%)	-0.39	0 100 100	94, 115, 132, 146	0
47	DT	100/105 (95%)	-0.22	0 100 100	95, 117, 141, 155	0
48	CU	72/88 (81%)	0.51	5 (6%) 23 16	91, 112, 146, 173	0
48	DU	72/88 (81%)	0.38	6 (8%) 17 13	97, 120, 156, 173	0
49	CV	78/93 (83%)	-0.08	1 (1%) 75 56	112, 136, 151, 158	0
49	DV	78/93 (83%)	-0.16	0 100 100	150, 167, 187, 191	0
50	CW	99/106 (93%)	-0.42	0 100 100	106, 130, 158, 169	0
50	DW	99/106 (93%)	-0.15	0 100 100	97, 124, 158, 172	0
51	CX	25/27 (92%)	-0.46	0 100 100	101, 124, 142, 160	0
51	DX	25/27 (92%)	-0.40	0 100 100	126, 149, 163, 175	0
52	CB	87/87 (100%)	0.29	4 (4%) 37 25	91, 155, 201, 213	2 (2%)
52	DB	87/87 (100%)	-0.02	3 (3%) 48 32	97, 156, 203, 216	2 (2%)
53	CC	77/77 (100%)	-0.27	1 (1%) 75 56	82, 118, 149, 164	0
53	CD	77/77 (100%)	0.15	0 100 100	86, 232, 246, 248	0
53	DC	77/77 (100%)	-0.45	1 (1%) 75 56	87, 120, 153, 167	0
53	DD	77/77 (100%)	0.28	1 (1%) 75 56	91, 234, 245, 249	0
54	C1	10/10 (100%)	0.13	1 (10%) 12 10	85, 102, 117, 131	0
54	D1	10/10 (100%)	-0.28	1 (10%) 12 10	88, 109, 119, 137	0
All	All	21107/21634 (97%)	-0.14	610 (2%) 53 35	44, 110, 191, 249	4 (0%)

The worst 5 of 610 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	B5	2	ALA	7.9
7	AH	155	SER	7.7
32	DE	4	GLU	7.7
9	AM	134	ARG	7.5
9	AM	138	LEU	7.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1779	1/1	0.37	0.10	113,113,113,113	0
55	MG	BA	3407	1/1	0.41	0.26	96,96,96,96	0
55	MG	BA	3420	1/1	0.43	0.15	136,136,136,136	0
55	MG	BA	3277	1/1	0.44	0.26	109,109,109,109	0
55	MG	AA	3437	1/1	0.46	0.24	122,122,122,122	0
55	MG	AA	3224	1/1	0.47	0.35	93,93,93,93	0
55	MG	DA	1740	1/1	0.47	0.17	113,113,113,113	0
55	MG	DA	1703	1/1	0.48	0.19	115,115,115,115	0
55	MG	CA	1728	1/1	0.48	0.17	117,117,117,117	0
55	MG	CB	104	1/1	0.50	0.22	101,101,101,101	0
55	MG	AA	3422	1/1	0.50	0.31	106,106,106,106	0
55	MG	CG	302	1/1	0.50	0.26	122,122,122,122	0
55	MG	AA	3433	1/1	0.51	0.14	152,152,152,152	0
55	MG	BA	3337	1/1	0.51	0.31	100,100,100,100	0
55	MG	DA	1804	1/1	0.51	0.24	123,123,123,123	0
55	MG	CA	1823	1/1	0.53	0.15	110,110,110,110	0
55	MG	AA	3407	1/1	0.53	0.22	110,110,110,110	0
55	MG	AA	3393	1/1	0.53	0.16	98,98,98,98	0
55	MG	CC	101	1/1	0.55	0.18	108,108,108,108	0
55	MG	CA	1704	1/1	0.55	0.21	113,113,113,113	0
55	MG	CB	101	1/1	0.55	0.13	108,108,108,108	0
55	MG	AA	3620	1/1	0.55	0.19	115,115,115,115	0
55	MG	AB	214	1/1	0.56	0.18	102,102,102,102	0
55	MG	CA	1720	1/1	0.56	0.18	102,102,102,102	0
55	MG	CA	1714	1/1	0.57	0.24	118,118,118,118	0
55	MG	AA	3373	1/1	0.57	0.27	106,106,106,106	0
55	MG	BA	3402	1/1	0.58	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3472	1/1	0.58	0.36	83,83,83,83	0
55	MG	CA	1614	1/1	0.58	0.21	101,101,101,101	0
55	MG	DA	1794	1/1	0.58	0.16	91,91,91,91	0
55	MG	AA	3325	1/1	0.58	0.27	100,100,100,100	0
55	MG	BA	3095	1/1	0.59	0.29	112,112,112,112	0
55	MG	DA	1784	1/1	0.59	0.17	103,103,103,103	0
55	MG	BA	3401	1/1	0.59	0.13	100,100,100,100	0
55	MG	BA	3050	1/1	0.59	0.12	103,103,103,103	0
55	MG	BA	3459	1/1	0.60	0.12	115,115,115,115	0
55	MG	AA	3626	1/1	0.60	0.24	96,96,96,96	0
55	MG	DA	1630	1/1	0.60	0.28	102,102,102,102	0
55	MG	BA	3384	1/1	0.60	0.30	92,92,92,92	0
55	MG	CA	1672	1/1	0.60	0.18	106,106,106,106	0
55	MG	CA	1828	1/1	0.60	0.28	98,98,98,98	0
55	MG	DA	1793	1/1	0.60	0.33	108,108,108,108	0
55	MG	BA	3313	1/1	0.60	0.13	106,106,106,106	0
55	MG	BA	3446	1/1	0.60	0.20	98,98,98,98	0
55	MG	CA	1767	1/1	0.61	0.16	120,120,120,120	0
55	MG	BA	3507	1/1	0.61	0.34	102,102,102,102	0
55	MG	BA	3151	1/1	0.61	0.33	96,96,96,96	0
55	MG	BA	3301	1/1	0.61	0.34	106,106,106,106	0
55	MG	CA	1701	1/1	0.61	0.14	105,105,105,105	0
55	MG	AA	3601	1/1	0.62	0.21	86,86,86,86	0
55	MG	DA	1713	1/1	0.62	0.23	111,111,111,111	0
55	MG	DA	1718	1/1	0.62	0.21	132,132,132,132	0
55	MG	DA	1719	1/1	0.62	0.23	112,112,112,112	0
55	MG	AA	3391	1/1	0.62	0.07	106,106,106,106	0
55	MG	CA	1753	1/1	0.62	0.11	107,107,107,107	0
55	MG	BA	3371	1/1	0.62	0.19	129,129,129,129	0
55	MG	AA	3197	1/1	0.62	0.28	74,74,74,74	0
55	MG	BB	212	1/1	0.62	0.17	104,104,104,104	0
55	MG	DA	1666	1/1	0.63	0.12	115,115,115,115	0
55	MG	CA	1694	1/1	0.63	0.10	104,104,104,104	0
55	MG	AA	3097	1/1	0.63	0.20	106,106,106,106	0
55	MG	CA	1615	1/1	0.63	0.30	104,104,104,104	0
55	MG	AA	3594	1/1	0.63	0.24	105,105,105,105	0
55	MG	CA	1783	1/1	0.64	0.13	106,106,106,106	0
55	MG	AA	3370	1/1	0.64	0.10	106,106,106,106	0
55	MG	DA	1766	1/1	0.64	0.27	116,116,116,116	0
55	MG	BA	3525	1/1	0.64	0.34	98,98,98,98	0
55	MG	BA	3332	1/1	0.64	0.23	100,100,100,100	0
55	MG	BA	3463	1/1	0.64	0.31	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3509	1/1	0.64	0.25	95,95,95,95	0
55	MG	DC	107	1/1	0.64	0.12	105,105,105,105	0
55	MG	AA	3497	1/1	0.65	0.29	95,95,95,95	0
55	MG	CA	1684	1/1	0.65	0.16	101,101,101,101	0
55	MG	DA	1771	1/1	0.65	0.16	114,114,114,114	0
55	MG	BA	3519	1/1	0.65	0.23	107,107,107,107	0
55	MG	CA	1825	1/1	0.66	0.19	114,114,114,114	0
55	MG	BA	3435	1/1	0.66	0.21	108,108,108,108	0
55	MG	BA	3164	1/1	0.66	0.10	99,99,99,99	0
55	MG	AE	304	1/1	0.66	0.26	87,87,87,87	0
55	MG	BA	3036	1/1	0.66	0.28	85,85,85,85	0
55	MG	CA	1630	1/1	0.66	0.18	112,112,112,112	0
55	MG	BA	3464	1/1	0.66	0.17	104,104,104,104	0
55	MG	AA	3221	1/1	0.66	0.25	47,47,47,47	0
55	MG	AA	3441	1/1	0.66	0.09	101,101,101,101	0
55	MG	AA	3193	1/1	0.66	0.22	96,96,96,96	0
55	MG	AA	3273	1/1	0.67	0.20	101,101,101,101	0
55	MG	BA	3104	1/1	0.67	0.24	115,115,115,115	0
55	MG	AA	3075	1/1	0.67	0.32	85,85,85,85	0
55	MG	AA	3354	1/1	0.67	0.21	84,84,84,84	0
55	MG	AA	3191	1/1	0.67	0.19	95,95,95,95	0
55	MG	AA	3469	1/1	0.67	0.34	103,103,103,103	0
55	MG	CA	1692	1/1	0.67	0.12	127,127,127,127	0
55	MG	CA	1765	1/1	0.67	0.21	109,109,109,109	0
55	MG	BB	210	1/1	0.68	0.16	96,96,96,96	0
55	MG	AA	3209	1/1	0.68	0.22	81,81,81,81	0
55	MG	BB	214	1/1	0.68	0.15	99,99,99,99	0
55	MG	AA	3253	1/1	0.68	0.26	81,81,81,81	0
55	MG	CA	1715	1/1	0.68	0.19	115,115,115,115	0
55	MG	DA	1746	1/1	0.68	0.18	104,104,104,104	0
55	MG	DA	1751	1/1	0.68	0.21	124,124,124,124	0
55	MG	CA	1832	1/1	0.68	0.28	106,106,106,106	0
55	MG	BA	3494	1/1	0.68	0.30	88,88,88,88	0
55	MG	BA	3107	1/1	0.68	0.26	89,89,89,89	0
55	MG	CA	1735	1/1	0.68	0.20	101,101,101,101	0
55	MG	AA	3260	1/1	0.68	0.25	91,91,91,91	0
55	MG	BA	3520	1/1	0.68	0.25	101,101,101,101	0
55	MG	AA	3362	1/1	0.68	0.16	89,89,89,89	0
55	MG	BA	3470	1/1	0.69	0.17	81,81,81,81	0
55	MG	DA	1728	1/1	0.69	0.20	112,112,112,112	0
55	MG	BA	3349	1/1	0.69	0.23	93,93,93,93	0
55	MG	AA	3604	1/1	0.69	0.24	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3231	1/1	0.69	0.20	106,106,106,106	0
55	MG	DA	1626	1/1	0.69	0.25	104,104,104,104	0
55	MG	BA	3118	1/1	0.69	0.24	110,110,110,110	0
55	MG	BA	3460	1/1	0.69	0.09	101,101,101,101	0
55	MG	DA	1702	1/1	0.69	0.17	99,99,99,99	0
55	MG	AA	3295	1/1	0.69	0.30	102,102,102,102	0
55	MG	DA	1802	1/1	0.69	0.20	102,102,102,102	0
55	MG	AA	3409	1/1	0.69	0.18	104,104,104,104	0
55	MG	CA	1736	1/1	0.69	0.26	88,88,88,88	0
55	MG	BA	3317	1/1	0.70	0.30	91,91,91,91	0
55	MG	BA	3090	1/1	0.70	0.19	109,109,109,109	0
55	MG	CA	1621	1/1	0.70	0.33	107,107,107,107	0
55	MG	AA	3361	1/1	0.70	0.17	93,93,93,93	0
55	MG	AA	3498	1/1	0.70	0.28	95,95,95,95	0
55	MG	AA	3446	1/1	0.70	0.17	93,93,93,93	0
55	MG	CA	1810	1/1	0.70	0.24	108,108,108,108	0
55	MG	BA	3116	1/1	0.70	0.21	107,107,107,107	0
55	MG	AA	3524	1/1	0.70	0.21	94,94,94,94	0
55	MG	AA	3454	1/1	0.70	0.27	94,94,94,94	0
55	MG	BA	3156	1/1	0.70	0.31	87,87,87,87	0
55	MG	BA	3021	1/1	0.70	0.16	105,105,105,105	0
55	MG	BB	206	1/1	0.70	0.10	102,102,102,102	0
55	MG	CA	1716	1/1	0.70	0.24	117,117,117,117	0
55	MG	AA	3599	1/1	0.70	0.33	87,87,87,87	0
55	MG	DA	1605	1/1	0.70	0.32	82,82,82,82	0
55	MG	AA	3432	1/1	0.70	0.15	87,87,87,87	0
55	MG	BA	3081	1/1	0.70	0.14	91,91,91,91	0
55	MG	AA	3385	1/1	0.71	0.24	88,88,88,88	0
55	MG	DA	1657	1/1	0.71	0.28	95,95,95,95	0
55	MG	BA	3398	1/1	0.71	0.15	96,96,96,96	0
55	MG	CA	1759	1/1	0.71	0.26	117,117,117,117	0
55	MG	CA	1647	1/1	0.71	0.19	92,92,92,92	0
55	MG	AA	3414	1/1	0.71	0.22	94,94,94,94	0
55	MG	CA	1683	1/1	0.71	0.18	104,104,104,104	0
55	MG	AA	3235	1/1	0.71	0.18	84,84,84,84	0
55	MG	BA	3075	1/1	0.71	0.18	99,99,99,99	0
55	MG	AA	3466	1/1	0.71	0.28	100,100,100,100	0
55	MG	BA	3429	1/1	0.71	0.13	95,95,95,95	0
55	MG	AA	3425	1/1	0.71	0.31	94,94,94,94	0
55	MG	AA	3481	1/1	0.71	0.21	112,112,112,112	0
55	MG	AA	3237	1/1	0.71	0.27	83,83,83,83	0
55	MG	AA	3396	1/1	0.71	0.30	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BB	215	1/1	0.71	0.10	101,101,101,101	0
55	MG	AB	216	1/1	0.71	0.22	106,106,106,106	0
55	MG	CD	101	1/1	0.71	0.09	105,105,105,105	0
55	MG	CA	1731	1/1	0.71	0.24	98,98,98,98	0
55	MG	AA	3104	1/1	0.71	0.17	80,80,80,80	0
55	MG	AA	3421	1/1	0.72	0.17	94,94,94,94	0
55	MG	AA	3587	1/1	0.72	0.32	77,77,77,77	0
55	MG	DA	1604	1/1	0.72	0.18	92,92,92,92	0
55	MG	BA	3334	1/1	0.72	0.10	103,103,103,103	0
55	MG	AA	3357	1/1	0.72	0.17	99,99,99,99	0
55	MG	DA	1762	1/1	0.72	0.17	109,109,109,109	0
55	MG	AA	3439	1/1	0.72	0.16	97,97,97,97	0
55	MG	DA	1741	1/1	0.73	0.26	93,93,93,93	0
55	MG	CA	1628	1/1	0.73	0.31	85,85,85,85	0
55	MG	AA	3412	1/1	0.73	0.17	110,110,110,110	0
55	MG	DA	1795	1/1	0.73	0.19	101,101,101,101	0
55	MG	AA	3461	1/1	0.73	0.22	105,105,105,105	0
55	MG	CA	1766	1/1	0.73	0.30	108,108,108,108	0
55	MG	DC	106	1/1	0.73	0.20	111,111,111,111	0
55	MG	CA	1750	1/1	0.73	0.27	104,104,104,104	0
55	MG	AA	3369	1/1	0.74	0.33	93,93,93,93	0
55	MG	BA	3172	1/1	0.74	0.20	85,85,85,85	0
55	MG	BA	3174	1/1	0.74	0.29	82,82,82,82	0
55	MG	BA	3273	1/1	0.74	0.27	102,102,102,102	0
55	MG	CA	1745	1/1	0.74	0.29	95,95,95,95	0
55	MG	AA	3043	1/1	0.74	0.23	108,108,108,108	0
55	MG	BA	3281	1/1	0.74	0.22	92,92,92,92	0
55	MG	BA	3282	1/1	0.74	0.24	93,93,93,93	0
55	MG	AA	3115	1/1	0.74	0.34	70,70,70,70	0
55	MG	AA	3132	1/1	0.74	0.31	106,106,106,106	0
55	MG	AA	3307	1/1	0.74	0.34	76,76,76,76	0
55	MG	BA	3331	1/1	0.74	0.12	101,101,101,101	0
55	MG	CA	1679	1/1	0.74	0.24	101,101,101,101	0
55	MG	AA	3184	1/1	0.74	0.10	94,94,94,94	0
55	MG	BA	3469	1/1	0.74	0.27	92,92,92,92	0
55	MG	AA	3078	1/1	0.74	0.28	88,88,88,88	0
55	MG	AA	3067	1/1	0.74	0.28	108,108,108,108	0
55	MG	AA	3242	1/1	0.74	0.10	93,93,93,93	0
55	MG	CA	1838	1/1	0.74	0.25	103,103,103,103	0
55	MG	BA	3363	1/1	0.74	0.22	88,88,88,88	0
55	MG	CQ	101	1/1	0.74	0.22	102,102,102,102	0
55	MG	AA	3556	1/1	0.74	0.33	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3374	1/1	0.74	0.28	86,86,86,86	0
55	MG	AA	3103	1/1	0.74	0.28	97,97,97,97	0
55	MG	BA	3389	1/1	0.74	0.10	96,96,96,96	0
55	MG	CA	1724	1/1	0.74	0.24	97,97,97,97	0
55	MG	CA	1748	1/1	0.75	0.20	87,87,87,87	0
55	MG	AA	3521	1/1	0.75	0.22	75,75,75,75	0
55	MG	BA	3416	1/1	0.75	0.28	103,103,103,103	0
55	MG	CA	1754	1/1	0.75	0.23	114,114,114,114	0
55	MG	AA	3102	1/1	0.75	0.18	90,90,90,90	0
55	MG	BA	3502	1/1	0.75	0.10	91,91,91,91	0
55	MG	AA	3480	1/1	0.75	0.28	86,86,86,86	0
55	MG	BA	3078	1/1	0.75	0.14	95,95,95,95	0
55	MG	DA	1756	1/1	0.75	0.33	106,106,106,106	0
55	MG	AA	3413	1/1	0.75	0.18	109,109,109,109	0
55	MG	DA	1606	1/1	0.75	0.18	95,95,95,95	0
55	MG	DA	1767	1/1	0.75	0.25	113,113,113,113	0
55	MG	AA	3381	1/1	0.75	0.27	90,90,90,90	0
55	MG	DA	1774	1/1	0.75	0.23	103,103,103,103	0
55	MG	CA	1677	1/1	0.75	0.13	90,90,90,90	0
55	MG	DA	1637	1/1	0.75	0.23	97,97,97,97	0
55	MG	AA	3050	1/1	0.75	0.39	108,108,108,108	0
55	MG	AA	3120	1/1	0.75	0.17	86,86,86,86	0
55	MG	DA	1681	1/1	0.75	0.18	106,106,106,106	0
55	MG	DA	1698	1/1	0.75	0.16	103,103,103,103	0
55	MG	BA	3175	1/1	0.75	0.12	100,100,100,100	0
55	MG	BA	3193	1/1	0.75	0.18	102,102,102,102	0
55	MG	CA	1711	1/1	0.76	0.17	98,98,98,98	0
55	MG	BA	3019	1/1	0.76	0.12	100,100,100,100	0
55	MG	DA	1717	1/1	0.76	0.17	103,103,103,103	0
55	MG	BA	3352	1/1	0.76	0.26	102,102,102,102	0
55	MG	BA	3450	1/1	0.76	0.25	99,99,99,99	0
55	MG	DA	1720	1/1	0.76	0.20	96,96,96,96	0
55	MG	BA	3454	1/1	0.76	0.27	105,105,105,105	0
55	MG	DA	1738	1/1	0.76	0.26	85,85,85,85	0
55	MG	BR	202	1/1	0.76	0.14	105,105,105,105	0
55	MG	CA	1607	1/1	0.76	0.21	93,93,93,93	0
55	MG	AA	3348	1/1	0.76	0.12	94,94,94,94	0
55	MG	BA	3108	1/1	0.76	0.34	99,99,99,99	0
55	MG	AA	3319	1/1	0.76	0.23	94,94,94,94	0
55	MG	AA	3366	1/1	0.76	0.21	92,92,92,92	0
55	MG	BA	3387	1/1	0.76	0.27	107,107,107,107	0
55	MG	BA	3293	1/1	0.76	0.15	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3148	1/1	0.76	0.26	91,91,91,91	0
55	MG	AA	3490	1/1	0.76	0.28	97,97,97,97	0
55	MG	AA	3164	1/1	0.76	0.24	95,95,95,95	0
55	MG	DA	1636	1/1	0.76	0.17	103,103,103,103	0
55	MG	AA	3390	1/1	0.76	0.13	109,109,109,109	0
55	MG	AA	3506	1/1	0.76	0.10	80,80,80,80	0
55	MG	DA	1798	1/1	0.76	0.19	92,92,92,92	0
55	MG	BA	3094	1/1	0.76	0.33	79,79,79,79	0
55	MG	BA	3521	1/1	0.76	0.31	79,79,79,79	0
55	MG	BA	3422	1/1	0.76	0.13	102,102,102,102	0
55	MG	BA	3003	1/1	0.76	0.28	99,99,99,99	0
55	MG	BA	3471	1/1	0.77	0.32	96,96,96,96	0
55	MG	CA	1693	1/1	0.77	0.16	102,102,102,102	0
55	MG	BA	3163	1/1	0.77	0.27	84,84,84,84	0
55	MG	CB	105	1/1	0.77	0.14	113,113,113,113	0
55	MG	BA	3438	1/1	0.77	0.09	88,88,88,88	0
55	MG	CC	107	1/1	0.77	0.12	93,93,93,93	0
55	MG	BA	3445	1/1	0.77	0.09	95,95,95,95	0
55	MG	AA	3402	1/1	0.77	0.14	92,92,92,92	0
55	MG	DA	1745	1/1	0.77	0.23	106,106,106,106	0
55	MG	AA	3347	1/1	0.77	0.15	92,92,92,92	0
55	MG	DA	1747	1/1	0.77	0.20	105,105,105,105	0
55	MG	BA	3044	1/1	0.77	0.37	104,104,104,104	0
55	MG	DA	1754	1/1	0.77	0.16	98,98,98,98	0
55	MG	CA	1773	1/1	0.77	0.17	101,101,101,101	0
55	MG	AA	3328	1/1	0.77	0.27	82,82,82,82	0
55	MG	CA	1718	1/1	0.77	0.09	93,93,93,93	0
55	MG	BA	3523	1/1	0.77	0.30	84,84,84,84	0
55	MG	CA	1649	1/1	0.77	0.23	86,86,86,86	0
55	MG	DA	1664	1/1	0.77	0.11	97,97,97,97	0
55	MG	AA	3359	1/1	0.77	0.15	84,84,84,84	0
55	MG	DA	1787	1/1	0.77	0.18	114,114,114,114	0
55	MG	BA	3329	1/1	0.77	0.15	66,66,66,66	0
55	MG	DA	1688	1/1	0.77	0.16	99,99,99,99	0
55	MG	AA	3456	1/1	0.77	0.32	91,91,91,91	0
55	MG	CA	1834	1/1	0.77	0.19	90,90,90,90	0
55	MG	BA	3157	1/1	0.77	0.28	93,93,93,93	0
55	MG	DA	1712	1/1	0.77	0.23	100,100,100,100	0
55	MG	BA	3434	1/1	0.77	0.31	90,90,90,90	0
55	MG	DA	1716	1/1	0.77	0.23	105,105,105,105	0
55	MG	DC	108	1/1	0.77	0.12	102,102,102,102	0
55	MG	BA	3032	1/1	0.78	0.26	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3397	1/1	0.78	0.39	96,96,96,96	0
55	MG	AA	3502	1/1	0.78	0.31	96,96,96,96	0
55	MG	BA	3043	1/1	0.78	0.37	108,108,108,108	0
55	MG	BA	3462	1/1	0.78	0.15	123,123,123,123	0
55	MG	DA	1601	1/1	0.78	0.21	107,107,107,107	0
55	MG	BA	3279	1/1	0.78	0.30	73,73,73,73	0
55	MG	AA	3397	1/1	0.78	0.29	95,95,95,95	0
55	MG	BA	3465	1/1	0.78	0.14	97,97,97,97	0
55	MG	BA	3468	1/1	0.78	0.19	105,105,105,105	0
55	MG	CA	1709	1/1	0.78	0.22	96,96,96,96	0
55	MG	DA	1631	1/1	0.78	0.28	102,102,102,102	0
55	MG	BA	3098	1/1	0.78	0.08	106,106,106,106	0
55	MG	BA	3359	1/1	0.78	0.25	98,98,98,98	0
55	MG	DA	1656	1/1	0.78	0.26	99,99,99,99	0
55	MG	CA	1794	1/1	0.78	0.21	106,106,106,106	0
55	MG	DA	1663	1/1	0.78	0.18	103,103,103,103	0
55	MG	AA	3463	1/1	0.78	0.21	90,90,90,90	0
55	MG	BA	3064	1/1	0.78	0.16	103,103,103,103	0
55	MG	DA	1678	1/1	0.78	0.19	86,86,86,86	0
55	MG	BA	3372	1/1	0.78	0.30	105,105,105,105	0
55	MG	DA	1683	1/1	0.78	0.30	80,80,80,80	0
55	MG	DA	1684	1/1	0.78	0.21	92,92,92,92	0
55	MG	AA	3513	1/1	0.78	0.28	83,83,83,83	0
55	MG	CA	1637	1/1	0.78	0.15	106,106,106,106	0
55	MG	BA	3114	1/1	0.78	0.15	103,103,103,103	0
55	MG	CA	1729	1/1	0.78	0.14	94,94,94,94	0
55	MG	BA	3386	1/1	0.78	0.27	81,81,81,81	0
55	MG	CA	1661	1/1	0.78	0.14	52,52,52,52	0
55	MG	AA	3087	1/1	0.78	0.34	76,76,76,76	0
55	MG	DA	1714	1/1	0.79	0.29	105,105,105,105	0
55	MG	AA	3624	1/1	0.79	0.31	111,111,111,111	0
55	MG	BA	3357	1/1	0.79	0.22	71,71,71,71	0
55	MG	BA	3414	1/1	0.79	0.17	92,92,92,92	0
55	MG	CA	1698	1/1	0.79	0.14	89,89,89,89	0
55	MG	CA	1762	1/1	0.79	0.15	89,89,89,89	0
55	MG	BA	3294	1/1	0.79	0.19	98,98,98,98	0
55	MG	BA	3027	1/1	0.79	0.16	107,107,107,107	0
55	MG	BA	3368	1/1	0.79	0.21	106,106,106,106	0
55	MG	DA	1625	1/1	0.79	0.13	105,105,105,105	0
55	MG	CA	1768	1/1	0.79	0.19	105,105,105,105	0
55	MG	BA	3303	1/1	0.79	0.27	89,89,89,89	0
55	MG	CA	1778	1/1	0.79	0.33	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3448	1/1	0.79	0.24	106,106,106,106	0
55	MG	AA	3453	1/1	0.79	0.18	95,95,95,95	0
55	MG	DA	1642	1/1	0.79	0.22	110,110,110,110	0
55	MG	CA	1787	1/1	0.79	0.15	100,100,100,100	0
55	MG	BA	3121	1/1	0.79	0.34	99,99,99,99	0
55	MG	DA	1661	1/1	0.79	0.20	98,98,98,98	0
55	MG	AA	3356	1/1	0.79	0.20	86,86,86,86	0
55	MG	CA	1815	1/1	0.79	0.23	91,91,91,91	0
55	MG	DA	1783	1/1	0.79	0.21	86,86,86,86	0
55	MG	AA	3185	1/1	0.79	0.21	88,88,88,88	0
55	MG	BA	3447	1/1	0.79	0.24	100,100,100,100	0
55	MG	CA	1653	1/1	0.79	0.21	91,91,91,91	0
55	MG	CA	1829	1/1	0.79	0.15	102,102,102,102	0
55	MG	AA	3548	1/1	0.79	0.16	54,54,54,54	0
55	MG	BA	3396	1/1	0.79	0.28	91,91,91,91	0
55	MG	BA	3058	1/1	0.79	0.33	89,89,89,89	0
55	MG	BA	3340	1/1	0.79	0.12	84,84,84,84	0
55	MG	CA	1737	1/1	0.79	0.12	92,92,92,92	0
55	MG	BB	208	1/1	0.79	0.26	107,107,107,107	0
55	MG	AA	3416	1/1	0.79	0.18	95,95,95,95	0
55	MG	AA	3526	1/1	0.80	0.32	90,90,90,90	0
55	MG	BA	3355	1/1	0.80	0.36	87,87,87,87	0
55	MG	AB	211	1/1	0.80	0.22	100,100,100,100	0
55	MG	CA	1788	1/1	0.80	0.18	105,105,105,105	0
55	MG	CA	1793	1/1	0.80	0.12	96,96,96,96	0
55	MG	AA	3479	1/1	0.80	0.13	94,94,94,94	0
55	MG	DA	1757	1/1	0.80	0.20	104,104,104,104	0
55	MG	DA	1760	1/1	0.80	0.22	100,100,100,100	0
55	MG	DA	1603	1/1	0.80	0.27	89,89,89,89	0
55	MG	DA	1763	1/1	0.80	0.32	89,89,89,89	0
55	MG	CA	1804	1/1	0.80	0.10	107,107,107,107	0
55	MG	AA	3327	1/1	0.80	0.27	84,84,84,84	0
55	MG	DA	1769	1/1	0.80	0.20	79,79,79,79	0
55	MG	AA	3367	1/1	0.80	0.32	87,87,87,87	0
55	MG	AA	3289	1/1	0.80	0.31	84,84,84,84	0
55	MG	BA	3304	1/1	0.80	0.20	91,91,91,91	0
55	MG	BB	209	1/1	0.80	0.15	95,95,95,95	0
55	MG	BA	3373	1/1	0.80	0.24	88,88,88,88	0
55	MG	CA	1831	1/1	0.80	0.23	105,105,105,105	0
55	MG	BA	3408	1/1	0.80	0.31	88,88,88,88	0
55	MG	BB	213	1/1	0.80	0.09	97,97,97,97	0
55	MG	DA	1650	1/1	0.80	0.26	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3474	1/1	0.80	0.20	88,88,88,88	0
55	MG	BA	3346	1/1	0.80	0.24	99,99,99,99	0
55	MG	DB	102	1/1	0.80	0.06	107,107,107,107	0
55	MG	DA	1739	1/1	0.80	0.11	113,113,113,113	0
55	MG	BA	3170	1/1	0.80	0.10	96,96,96,96	0
55	MG	BA	3503	1/1	0.80	0.14	69,69,69,69	0
55	MG	AA	3468	1/1	0.81	0.10	95,95,95,95	0
55	MG	DA	1715	1/1	0.81	0.19	92,92,92,92	0
55	MG	AA	3236	1/1	0.81	0.33	96,96,96,96	0
55	MG	BA	3415	1/1	0.81	0.18	109,109,109,109	0
55	MG	AA	3118	1/1	0.81	0.25	87,87,87,87	0
55	MG	AA	3096	1/1	0.81	0.16	89,89,89,89	0
55	MG	CA	1755	1/1	0.81	0.13	81,81,81,81	0
55	MG	DA	1725	1/1	0.81	0.29	96,96,96,96	0
55	MG	AA	3309	1/1	0.81	0.47	90,90,90,90	0
55	MG	BA	3423	1/1	0.81	0.19	91,91,91,91	0
55	MG	AA	3398	1/1	0.81	0.13	73,73,73,73	0
55	MG	CA	1685	1/1	0.81	0.15	103,103,103,103	0
55	MG	CA	1687	1/1	0.81	0.20	78,78,78,78	0
55	MG	DA	1743	1/1	0.81	0.21	94,94,94,94	0
55	MG	DA	1613	1/1	0.81	0.25	88,88,88,88	0
55	MG	DA	1620	1/1	0.81	0.26	85,85,85,85	0
55	MG	DA	1623	1/1	0.81	0.16	96,96,96,96	0
55	MG	CA	1689	1/1	0.81	0.14	115,115,115,115	0
55	MG	AA	3126	1/1	0.81	0.19	83,83,83,83	0
55	MG	DA	1628	1/1	0.81	0.16	97,97,97,97	0
55	MG	CA	1775	1/1	0.81	0.10	113,113,113,113	0
55	MG	AA	3445	1/1	0.81	0.25	95,95,95,95	0
55	MG	AA	3079	1/1	0.81	0.10	92,92,92,92	0
55	MG	AA	3264	1/1	0.81	0.24	80,80,80,80	0
55	MG	AA	3508	1/1	0.81	0.21	101,101,101,101	0
55	MG	BA	3099	1/1	0.81	0.07	98,98,98,98	0
55	MG	BA	3101	1/1	0.81	0.12	94,94,94,94	0
55	MG	AA	3271	1/1	0.81	0.17	92,92,92,92	0
55	MG	AO	201	1/1	0.81	0.32	65,65,65,65	0
55	MG	DA	1775	1/1	0.81	0.21	102,102,102,102	0
55	MG	AA	3333	1/1	0.81	0.27	95,95,95,95	0
55	MG	AA	3345	1/1	0.81	0.33	93,93,93,93	0
55	MG	BA	3020	1/1	0.81	0.23	76,76,76,76	0
55	MG	AA	3460	1/1	0.81	0.32	106,106,106,106	0
55	MG	AA	3059	1/1	0.81	0.26	80,80,80,80	0
55	MG	CA	1727	1/1	0.81	0.23	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3124	1/1	0.81	0.11	102,102,102,102	0
55	MG	AA	3529	1/1	0.81	0.19	68,68,68,68	0
55	MG	AA	3276	1/1	0.81	0.28	78,78,78,78	0
55	MG	DG	302	1/1	0.81	0.12	112,112,112,112	0
55	MG	CA	1635	1/1	0.81	0.20	100,100,100,100	0
55	MG	BA	3404	1/1	0.81	0.18	101,101,101,101	0
55	MG	CN	202	1/1	0.81	0.09	99,99,99,99	0
55	MG	AA	3279	1/1	0.81	0.12	89,89,89,89	0
55	MG	DA	1710	1/1	0.82	0.26	100,100,100,100	0
55	MG	AA	3558	1/1	0.82	0.23	89,89,89,89	0
55	MG	AA	3404	1/1	0.82	0.21	95,95,95,95	0
55	MG	BA	3296	1/1	0.82	0.17	76,76,76,76	0
55	MG	CA	1739	1/1	0.82	0.24	86,86,86,86	0
55	MG	CQ	102	1/1	0.82	0.12	97,97,97,97	0
55	MG	CA	1740	1/1	0.82	0.18	72,72,72,72	0
55	MG	AA	3304	1/1	0.82	0.08	90,90,90,90	0
55	MG	BA	3115	1/1	0.82	0.22	79,79,79,79	0
55	MG	BA	3033	1/1	0.82	0.21	94,94,94,94	0
55	MG	DA	1722	1/1	0.82	0.13	106,106,106,106	0
55	MG	BA	3399	1/1	0.82	0.11	104,104,104,104	0
55	MG	BA	3308	1/1	0.82	0.17	108,108,108,108	0
55	MG	C1	101	1/1	0.82	0.10	98,98,98,98	0
55	MG	BA	3117	1/1	0.82	0.23	91,91,91,91	0
55	MG	CA	1756	1/1	0.82	0.05	113,113,113,113	0
55	MG	BA	3478	1/1	0.82	0.25	92,92,92,92	0
55	MG	BA	3035	1/1	0.82	0.19	103,103,103,103	0
55	MG	AA	3123	1/1	0.82	0.26	52,52,52,52	0
55	MG	AA	3183	1/1	0.82	0.22	93,93,93,93	0
55	MG	AA	3602	1/1	0.82	0.16	59,59,59,59	0
55	MG	AA	3384	1/1	0.82	0.33	87,87,87,87	0
55	MG	BA	3054	1/1	0.82	0.23	81,81,81,81	0
55	MG	AA	3275	1/1	0.82	0.22	87,87,87,87	0
55	MG	BA	3344	1/1	0.82	0.25	101,101,101,101	0
55	MG	AA	3358	1/1	0.82	0.40	89,89,89,89	0
55	MG	BA	3072	1/1	0.82	0.20	104,104,104,104	0
55	MG	AA	3080	1/1	0.82	0.28	104,104,104,104	0
55	MG	AA	3258	1/1	0.82	0.16	92,92,92,92	0
55	MG	DA	1640	1/1	0.82	0.11	101,101,101,101	0
55	MG	AA	3423	1/1	0.82	0.15	74,74,74,74	0
55	MG	DA	1643	1/1	0.82	0.24	81,81,81,81	0
55	MG	AB	215	1/1	0.82	0.16	93,93,93,93	0
55	MG	DA	1655	1/1	0.82	0.21	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1782	1/1	0.82	0.28	94,94,94,94	0
55	MG	CA	1802	1/1	0.82	0.15	77,77,77,77	0
55	MG	AA	3286	1/1	0.82	0.21	86,86,86,86	0
55	MG	BA	3210	1/1	0.82	0.26	55,55,55,55	0
55	MG	AA	3429	1/1	0.82	0.29	90,90,90,90	0
55	MG	CA	1818	1/1	0.82	0.10	89,89,89,89	0
55	MG	CA	1820	1/1	0.82	0.27	88,88,88,88	0
55	MG	CA	1822	1/1	0.82	0.09	105,105,105,105	0
55	MG	DA	1801	1/1	0.82	0.20	90,90,90,90	0
55	MG	BA	3451	1/1	0.82	0.14	89,89,89,89	0
55	MG	BA	3453	1/1	0.82	0.17	93,93,93,93	0
55	MG	AA	3094	1/1	0.82	0.20	62,62,62,62	0
55	MG	DB	101	1/1	0.82	0.10	103,103,103,103	0
55	MG	AA	3216	1/1	0.82	0.15	64,64,64,64	0
55	MG	AA	3475	1/1	0.82	0.15	102,102,102,102	0
55	MG	CA	1730	1/1	0.82	0.21	107,107,107,107	0
55	MG	AA	3298	1/1	0.82	0.16	73,73,73,73	0
55	MG	AA	3451	1/1	0.83	0.12	76,76,76,76	0
55	MG	BA	3442	1/1	0.83	0.27	91,91,91,91	0
55	MG	AA	3625	1/1	0.83	0.17	89,89,89,89	0
55	MG	BA	3062	1/1	0.83	0.25	110,110,110,110	0
55	MG	BA	3356	1/1	0.83	0.10	84,84,84,84	0
55	MG	CA	1770	1/1	0.83	0.26	90,90,90,90	0
55	MG	BA	3449	1/1	0.83	0.17	109,109,109,109	0
55	MG	CA	1774	1/1	0.83	0.23	97,97,97,97	0
55	MG	AA	3371	1/1	0.83	0.25	89,89,89,89	0
55	MG	BA	3066	1/1	0.83	0.10	86,86,86,86	0
55	MG	CA	1652	1/1	0.83	0.26	93,93,93,93	0
55	MG	BA	3068	1/1	0.83	0.20	93,93,93,93	0
55	MG	CA	1785	1/1	0.83	0.31	89,89,89,89	0
55	MG	CA	1655	1/1	0.83	0.30	95,95,95,95	0
55	MG	AB	206	1/1	0.83	0.20	93,93,93,93	0
55	MG	BA	3370	1/1	0.83	0.20	98,98,98,98	0
55	MG	AA	3341	1/1	0.83	0.15	95,95,95,95	0
55	MG	AB	212	1/1	0.83	0.31	94,94,94,94	0
55	MG	AA	3255	1/1	0.83	0.14	88,88,88,88	0
55	MG	BA	3083	1/1	0.83	0.21	92,92,92,92	0
55	MG	BA	3375	1/1	0.83	0.29	75,75,75,75	0
55	MG	CA	1816	1/1	0.83	0.11	95,95,95,95	0
55	MG	BA	3380	1/1	0.83	0.18	78,78,78,78	0
55	MG	AA	3418	1/1	0.83	0.14	91,91,91,91	0
55	MG	BA	3385	1/1	0.83	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3092	1/1	0.83	0.28	95,95,95,95	0
55	MG	AA	3194	1/1	0.83	0.19	102,102,102,102	0
55	MG	CA	1695	1/1	0.83	0.19	90,90,90,90	0
55	MG	BA	3287	1/1	0.83	0.28	87,87,87,87	0
55	MG	CA	1830	1/1	0.83	0.25	94,94,94,94	0
55	MG	AA	3134	1/1	0.83	0.27	79,79,79,79	0
55	MG	CA	1703	1/1	0.83	0.18	103,103,103,103	0
55	MG	AA	3142	1/1	0.83	0.15	71,71,71,71	0
55	MG	BA	3498	1/1	0.83	0.13	99,99,99,99	0
55	MG	BA	3500	1/1	0.83	0.16	104,104,104,104	0
55	MG	AA	3149	1/1	0.83	0.21	57,57,57,57	0
55	MG	BA	3299	1/1	0.83	0.12	82,82,82,82	0
55	MG	BA	3008	1/1	0.83	0.18	89,89,89,89	0
55	MG	BA	3512	1/1	0.83	0.29	75,75,75,75	0
55	MG	BA	3513	1/1	0.83	0.18	104,104,104,104	0
55	MG	DA	1759	1/1	0.83	0.25	108,108,108,108	0
55	MG	CA	1721	1/1	0.83	0.16	89,89,89,89	0
55	MG	AA	3553	1/1	0.83	0.25	87,87,87,87	0
55	MG	CA	1725	1/1	0.83	0.17	98,98,98,98	0
55	MG	AA	3122	1/1	0.83	0.17	84,84,84,84	0
55	MG	AA	3312	1/1	0.83	0.17	76,76,76,76	0
55	MG	BA	3522	1/1	0.83	0.30	84,84,84,84	0
55	MG	AA	3316	1/1	0.83	0.16	83,83,83,83	0
55	MG	BA	3410	1/1	0.83	0.31	94,94,94,94	0
55	MG	BB	204	1/1	0.83	0.20	90,90,90,90	0
55	MG	DA	1778	1/1	0.83	0.19	118,118,118,118	0
55	MG	BA	3413	1/1	0.83	0.12	94,94,94,94	0
55	MG	DA	1607	1/1	0.83	0.26	92,92,92,92	0
55	MG	AA	3245	1/1	0.83	0.25	75,75,75,75	0
55	MG	CA	1738	1/1	0.83	0.12	103,103,103,103	0
55	MG	DA	1788	1/1	0.83	0.23	90,90,90,90	0
55	MG	AA	3251	1/1	0.83	0.10	68,68,68,68	0
55	MG	AA	3278	1/1	0.83	0.24	100,100,100,100	0
55	MG	CA	1743	1/1	0.83	0.06	112,112,112,112	0
55	MG	BA	3419	1/1	0.83	0.14	99,99,99,99	0
55	MG	AA	3252	1/1	0.83	0.24	94,94,94,94	0
55	MG	BA	3037	1/1	0.83	0.11	75,75,75,75	0
55	MG	BA	3040	1/1	0.83	0.15	94,94,94,94	0
55	MG	AA	3182	1/1	0.83	0.14	88,88,88,88	0
55	MG	AA	3616	1/1	0.83	0.16	95,95,95,95	0
55	MG	CA	1609	1/1	0.83	0.30	78,78,78,78	0
55	MG	CA	1758	1/1	0.83	0.14	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1644	1/1	0.83	0.25	82,82,82,82	0
55	MG	AA	3335	1/1	0.83	0.39	91,91,91,91	0
55	MG	AA	3514	1/1	0.84	0.21	67,67,67,67	0
55	MG	AB	209	1/1	0.84	0.18	108,108,108,108	0
55	MG	AA	3355	1/1	0.84	0.24	94,94,94,94	0
55	MG	AA	3465	1/1	0.84	0.12	71,71,71,71	0
55	MG	CA	1670	1/1	0.84	0.25	70,70,70,70	0
55	MG	BA	3342	1/1	0.84	0.12	80,80,80,80	0
55	MG	AA	3121	1/1	0.84	0.41	90,90,90,90	0
55	MG	CB	102	1/1	0.84	0.08	106,106,106,106	0
55	MG	AA	3377	1/1	0.84	0.20	94,94,94,94	0
55	MG	BA	3348	1/1	0.84	0.21	98,98,98,98	0
55	MG	AA	3329	1/1	0.84	0.14	94,94,94,94	0
55	MG	BA	3504	1/1	0.84	0.15	117,117,117,117	0
55	MG	CA	1760	1/1	0.84	0.17	91,91,91,91	0
55	MG	CA	1686	1/1	0.84	0.20	86,86,86,86	0
55	MG	DA	1729	1/1	0.84	0.28	84,84,84,84	0
55	MG	AA	3474	1/1	0.84	0.17	65,65,65,65	0
55	MG	AA	3554	1/1	0.84	0.17	74,74,74,74	0
55	MG	BA	3084	1/1	0.84	0.10	99,99,99,99	0
55	MG	BA	3424	1/1	0.84	0.14	86,86,86,86	0
55	MG	AA	3382	1/1	0.84	0.25	102,102,102,102	0
55	MG	BA	3239	1/1	0.84	0.25	80,80,80,80	0
55	MG	DA	1609	1/1	0.84	0.18	116,116,116,116	0
55	MG	BA	3243	1/1	0.84	0.29	65,65,65,65	0
55	MG	DA	1619	1/1	0.84	0.24	77,77,77,77	0
55	MG	BA	3436	1/1	0.84	0.16	94,94,94,94	0
55	MG	DA	1621	1/1	0.84	0.31	99,99,99,99	0
55	MG	CA	1776	1/1	0.84	0.22	79,79,79,79	0
55	MG	DA	1624	1/1	0.84	0.20	95,95,95,95	0
55	MG	AA	3148	1/1	0.84	0.26	83,83,83,83	0
55	MG	BA	3018	1/1	0.84	0.13	83,83,83,83	0
55	MG	CA	1782	1/1	0.84	0.29	94,94,94,94	0
55	MG	BA	3444	1/1	0.84	0.25	96,96,96,96	0
55	MG	AA	3583	1/1	0.84	0.24	103,103,103,103	0
55	MG	AA	3443	1/1	0.84	0.11	90,90,90,90	0
55	MG	AA	3288	1/1	0.84	0.23	90,90,90,90	0
55	MG	AA	3336	1/1	0.84	0.12	82,82,82,82	0
55	MG	DA	1641	1/1	0.84	0.26	95,95,95,95	0
55	MG	BA	3290	1/1	0.84	0.11	82,82,82,82	0
55	MG	AA	3247	1/1	0.84	0.30	74,74,74,74	0
55	MG	CA	1803	1/1	0.84	0.13	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3420	1/1	0.84	0.25	88,88,88,88	0
55	MG	AA	3499	1/1	0.84	0.37	93,93,93,93	0
55	MG	BA	3455	1/1	0.84	0.17	92,92,92,92	0
55	MG	BA	3457	1/1	0.84	0.11	99,99,99,99	0
55	MG	AA	3062	1/1	0.84	0.19	86,86,86,86	0
55	MG	CA	1819	1/1	0.84	0.12	109,109,109,109	0
55	MG	AA	3617	1/1	0.84	0.27	92,92,92,92	0
55	MG	AA	3049	1/1	0.84	0.23	80,80,80,80	0
55	MG	AA	3621	1/1	0.84	0.20	91,91,91,91	0
55	MG	CA	1734	1/1	0.84	0.18	86,86,86,86	0
55	MG	AA	3300	1/1	0.84	0.08	81,81,81,81	0
55	MG	AA	3303	1/1	0.84	0.20	95,95,95,95	0
55	MG	AA	3426	1/1	0.84	0.14	80,80,80,80	0
55	MG	DA	1693	1/1	0.84	0.20	93,93,93,93	0
55	MG	BA	3125	1/1	0.84	0.17	104,104,104,104	0
55	MG	AB	204	1/1	0.84	0.25	96,96,96,96	0
55	MG	DA	1730	1/1	0.85	0.19	102,102,102,102	0
55	MG	AA	3487	1/1	0.85	0.11	77,77,77,77	0
55	MG	BA	3077	1/1	0.85	0.15	101,101,101,101	0
55	MG	BA	3256	1/1	0.85	0.13	102,102,102,102	0
55	MG	BA	3475	1/1	0.85	0.27	90,90,90,90	0
55	MG	BA	3269	1/1	0.85	0.21	58,58,58,58	0
55	MG	BA	3489	1/1	0.85	0.29	68,68,68,68	0
55	MG	CA	1757	1/1	0.85	0.12	92,92,92,92	0
55	MG	BA	3272	1/1	0.85	0.25	81,81,81,81	0
55	MG	AA	3401	1/1	0.85	0.22	93,93,93,93	0
55	MG	DA	1753	1/1	0.85	0.33	87,87,87,87	0
55	MG	CA	1618	1/1	0.85	0.17	94,94,94,94	0
55	MG	AA	3392	1/1	0.85	0.09	93,93,93,93	0
55	MG	CA	1764	1/1	0.85	0.09	92,92,92,92	0
55	MG	CA	1625	1/1	0.85	0.13	71,71,71,71	0
55	MG	BA	3122	1/1	0.85	0.24	95,95,95,95	0
55	MG	BA	3347	1/1	0.85	0.12	85,85,85,85	0
55	MG	AA	3339	1/1	0.85	0.18	85,85,85,85	0
55	MG	AA	3531	1/1	0.85	0.16	96,96,96,96	0
55	MG	CA	1771	1/1	0.85	0.14	102,102,102,102	0
55	MG	DA	1768	1/1	0.85	0.14	82,82,82,82	0
55	MG	CA	1640	1/1	0.85	0.17	85,85,85,85	0
55	MG	DA	1770	1/1	0.85	0.28	95,95,95,95	0
55	MG	CA	1644	1/1	0.85	0.14	84,84,84,84	0
55	MG	CA	1723	1/1	0.85	0.29	106,106,106,106	0
55	MG	CC	104	1/1	0.85	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3535	1/1	0.85	0.06	103,103,103,103	0
55	MG	AA	3137	1/1	0.85	0.10	51,51,51,51	0
55	MG	CA	1651	1/1	0.85	0.27	75,75,75,75	0
55	MG	AF	303	1/1	0.85	0.22	69,69,69,69	0
55	MG	AA	3427	1/1	0.85	0.33	82,82,82,82	0
55	MG	AA	3459	1/1	0.85	0.23	81,81,81,81	0
55	MG	AA	3444	1/1	0.85	0.22	58,58,58,58	0
55	MG	AA	3351	1/1	0.85	0.20	82,82,82,82	0
55	MG	AA	3283	1/1	0.85	0.23	91,91,91,91	0
55	MG	AB	203	1/1	0.85	0.34	69,69,69,69	0
55	MG	AA	3585	1/1	0.85	0.29	91,91,91,91	0
55	MG	DA	1618	1/1	0.85	0.18	104,104,104,104	0
55	MG	DA	1803	1/1	0.85	0.21	100,100,100,100	0
55	MG	BB	207	1/1	0.85	0.23	116,116,116,116	0
55	MG	BA	3312	1/1	0.85	0.18	98,98,98,98	0
55	MG	CA	1805	1/1	0.85	0.25	75,75,75,75	0
55	MG	AA	3482	1/1	0.85	0.29	96,96,96,96	0
55	MG	CA	1742	1/1	0.85	0.12	115,115,115,115	0
55	MG	BA	3201	1/1	0.85	0.20	94,94,94,94	0
55	MG	BA	3073	1/1	0.85	0.32	99,99,99,99	0
55	MG	DA	1686	1/1	0.86	0.23	97,97,97,97	0
55	MG	CA	1605	1/1	0.86	0.20	86,86,86,86	0
55	MG	DA	1690	1/1	0.86	0.23	92,92,92,92	0
55	MG	DA	1692	1/1	0.86	0.24	81,81,81,81	0
55	MG	BA	3214	1/1	0.86	0.18	77,77,77,77	0
55	MG	CA	1733	1/1	0.86	0.07	107,107,107,107	0
55	MG	BA	3358	1/1	0.86	0.30	85,85,85,85	0
55	MG	BA	3233	1/1	0.86	0.29	74,74,74,74	0
55	MG	DA	1705	1/1	0.86	0.21	97,97,97,97	0
55	MG	DA	1708	1/1	0.86	0.34	102,102,102,102	0
55	MG	AA	3383	1/1	0.86	0.19	85,85,85,85	0
55	MG	BA	3367	1/1	0.86	0.36	91,91,91,91	0
55	MG	AO	203	1/1	0.86	0.18	43,43,43,43	0
55	MG	CA	1624	1/1	0.86	0.09	97,97,97,97	0
55	MG	BA	3251	1/1	0.86	0.19	81,81,81,81	0
55	MG	CA	1741	1/1	0.86	0.17	80,80,80,80	0
55	MG	BA	3456	1/1	0.86	0.20	88,88,88,88	0
55	MG	AA	3165	1/1	0.86	0.36	82,82,82,82	0
55	MG	AA	3598	1/1	0.86	0.15	87,87,87,87	0
55	MG	AA	3173	1/1	0.86	0.12	67,67,67,67	0
55	MG	AA	3452	1/1	0.86	0.26	76,76,76,76	0
55	MG	AA	3114	1/1	0.86	0.35	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3228	1/1	0.86	0.23	79,79,79,79	0
55	MG	BA	3383	1/1	0.86	0.38	95,95,95,95	0
55	MG	AA	3609	1/1	0.86	0.18	62,62,62,62	0
55	MG	BA	3102	1/1	0.86	0.08	86,86,86,86	0
55	MG	AA	3611	1/1	0.86	0.14	100,100,100,100	0
55	MG	AA	3612	1/1	0.86	0.19	92,92,92,92	0
55	MG	AA	3019	1/1	0.86	0.18	55,55,55,55	0
55	MG	AA	3063	1/1	0.86	0.26	85,85,85,85	0
55	MG	AA	3619	1/1	0.86	0.23	87,87,87,87	0
55	MG	BA	3298	1/1	0.86	0.16	61,61,61,61	0
55	MG	AA	3394	1/1	0.86	0.18	99,99,99,99	0
55	MG	CA	1681	1/1	0.86	0.17	80,80,80,80	0
55	MG	DA	1614	1/1	0.86	0.21	93,93,93,93	0
55	MG	DA	1615	1/1	0.86	0.17	96,96,96,96	0
55	MG	AA	3270	1/1	0.86	0.23	69,69,69,69	0
55	MG	AA	3136	1/1	0.86	0.12	61,61,61,61	0
55	MG	BA	3045	1/1	0.86	0.25	88,88,88,88	0
55	MG	BA	3307	1/1	0.86	0.20	106,106,106,106	0
55	MG	DA	1761	1/1	0.86	0.29	84,84,84,84	0
55	MG	AA	3368	1/1	0.86	0.23	90,90,90,90	0
55	MG	AA	3119	1/1	0.86	0.29	75,75,75,75	0
55	MG	BA	3056	1/1	0.86	0.19	96,96,96,96	0
55	MG	BA	3144	1/1	0.86	0.14	95,95,95,95	0
55	MG	DA	1627	1/1	0.86	0.14	105,105,105,105	0
55	MG	AA	3305	1/1	0.86	0.19	80,80,80,80	0
55	MG	DA	1629	1/1	0.86	0.07	92,92,92,92	0
55	MG	BA	3518	1/1	0.86	0.27	74,74,74,74	0
55	MG	BA	3330	1/1	0.86	0.27	91,91,91,91	0
55	MG	CA	1784	1/1	0.86	0.28	101,101,101,101	0
55	MG	DA	1777	1/1	0.86	0.21	87,87,87,87	0
55	MG	AA	3274	1/1	0.86	0.14	72,72,72,72	0
55	MG	DA	1780	1/1	0.86	0.25	107,107,107,107	0
55	MG	BA	3063	1/1	0.86	0.20	89,89,89,89	0
55	MG	AA	3470	1/1	0.86	0.16	96,96,96,96	0
55	MG	BA	3159	1/1	0.86	0.24	83,83,83,83	0
55	MG	BA	3161	1/1	0.86	0.19	89,89,89,89	0
55	MG	CA	1798	1/1	0.86	0.26	82,82,82,82	0
55	MG	BA	3427	1/1	0.86	0.19	100,100,100,100	0
55	MG	DA	1654	1/1	0.86	0.24	92,92,92,92	0
55	MG	BB	205	1/1	0.86	0.21	86,86,86,86	0
55	MG	AA	3438	1/1	0.86	0.27	90,90,90,90	0
55	MG	AA	3405	1/1	0.86	0.36	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3070	1/1	0.86	0.17	81,81,81,81	0
55	MG	AA	3478	1/1	0.86	0.19	75,75,75,75	0
55	MG	AA	3098	1/1	0.86	0.26	81,81,81,81	0
55	MG	AA	3033	1/1	0.86	0.20	49,49,49,49	0
55	MG	BA	3443	1/1	0.86	0.15	92,92,92,92	0
55	MG	AA	3017	1/1	0.86	0.17	64,64,64,64	0
55	MG	DA	1682	1/1	0.86	0.28	96,96,96,96	0
55	MG	AA	3077	1/1	0.86	0.16	103,103,103,103	0
55	MG	AA	3483	1/1	0.86	0.09	87,87,87,87	0
55	MG	BA	3426	1/1	0.87	0.19	87,87,87,87	0
55	MG	AB	207	1/1	0.87	0.07	103,103,103,103	0
55	MG	AB	208	1/1	0.87	0.22	92,92,92,92	0
55	MG	AA	3489	1/1	0.87	0.41	86,86,86,86	0
55	MG	DA	1695	1/1	0.87	0.26	88,88,88,88	0
55	MG	AA	3108	1/1	0.87	0.30	66,66,66,66	0
55	MG	AA	3557	1/1	0.87	0.29	100,100,100,100	0
55	MG	BA	3179	1/1	0.87	0.28	61,61,61,61	0
55	MG	BA	3441	1/1	0.87	0.17	93,93,93,93	0
55	MG	DA	1706	1/1	0.87	0.32	90,90,90,90	0
55	MG	AA	3493	1/1	0.87	0.14	92,92,92,92	0
55	MG	BA	3194	1/1	0.87	0.19	70,70,70,70	0
55	MG	CG	301	1/1	0.87	0.25	94,94,94,94	0
55	MG	AA	3564	1/1	0.87	0.16	76,76,76,76	0
55	MG	AA	3435	1/1	0.87	0.32	78,78,78,78	0
55	MG	AA	3584	1/1	0.87	0.09	63,63,63,63	0
55	MG	AA	3462	1/1	0.87	0.22	85,85,85,85	0
55	MG	CA	1616	1/1	0.87	0.17	103,103,103,103	0
55	MG	AA	3386	1/1	0.87	0.15	74,74,74,74	0
55	MG	BA	3242	1/1	0.87	0.31	62,62,62,62	0
55	MG	CA	1623	1/1	0.87	0.17	73,73,73,73	0
55	MG	BA	3365	1/1	0.87	0.19	90,90,90,90	0
55	MG	AA	3500	1/1	0.87	0.17	103,103,103,103	0
55	MG	BA	3091	1/1	0.87	0.25	86,86,86,86	0
55	MG	AZ	101	1/1	0.87	0.10	77,77,77,77	0
55	MG	CA	1751	1/1	0.87	0.18	78,78,78,78	0
55	MG	CA	1752	1/1	0.87	0.11	96,96,96,96	0
55	MG	BA	3260	1/1	0.87	0.13	82,82,82,82	0
55	MG	A6	101	1/1	0.87	0.17	111,111,111,111	0
55	MG	CA	1639	1/1	0.87	0.24	86,86,86,86	0
55	MG	AA	3501	1/1	0.87	0.11	99,99,99,99	0
55	MG	AA	3342	1/1	0.87	0.27	70,70,70,70	0
55	MG	AA	3600	1/1	0.87	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1648	1/1	0.87	0.24	79,79,79,79	0
55	MG	DA	1750	1/1	0.87	0.11	84,84,84,84	0
55	MG	BA	3378	1/1	0.87	0.07	78,78,78,78	0
55	MG	AA	3320	1/1	0.87	0.11	103,103,103,103	0
55	MG	CA	1763	1/1	0.87	0.14	81,81,81,81	0
55	MG	AA	3321	1/1	0.87	0.19	65,65,65,65	0
55	MG	AA	3324	1/1	0.87	0.15	92,92,92,92	0
55	MG	CA	1654	1/1	0.87	0.24	75,75,75,75	0
55	MG	BA	3025	1/1	0.87	0.10	80,80,80,80	0
55	MG	AA	3510	1/1	0.87	0.42	84,84,84,84	0
55	MG	AA	3511	1/1	0.87	0.32	98,98,98,98	0
55	MG	AA	3248	1/1	0.87	0.29	74,74,74,74	0
55	MG	DA	1764	1/1	0.87	0.32	85,85,85,85	0
55	MG	DA	1765	1/1	0.87	0.11	93,93,93,93	0
55	MG	BA	3390	1/1	0.87	0.26	77,77,77,77	0
55	MG	AA	3614	1/1	0.87	0.24	78,78,78,78	0
55	MG	AA	3032	1/1	0.87	0.17	65,65,65,65	0
55	MG	AA	3291	1/1	0.87	0.29	68,68,68,68	0
55	MG	AA	3522	1/1	0.87	0.19	97,97,97,97	0
55	MG	DA	1635	1/1	0.87	0.18	79,79,79,79	0
55	MG	BA	3495	1/1	0.87	0.23	81,81,81,81	0
55	MG	AA	3060	1/1	0.87	0.15	84,84,84,84	0
55	MG	AA	3380	1/1	0.87	0.08	96,96,96,96	0
55	MG	AA	3117	1/1	0.87	0.21	54,54,54,54	0
55	MG	BA	3405	1/1	0.87	0.21	87,87,87,87	0
55	MG	BA	3127	1/1	0.87	0.33	55,55,55,55	0
55	MG	AA	3315	1/1	0.87	0.32	70,70,70,70	0
55	MG	AA	3428	1/1	0.87	0.15	120,120,120,120	0
55	MG	BA	3055	1/1	0.87	0.21	99,99,99,99	0
55	MG	BA	3516	1/1	0.87	0.14	73,73,73,73	0
55	MG	BA	3324	1/1	0.87	0.26	75,75,75,75	0
55	MG	BA	3326	1/1	0.87	0.16	84,84,84,84	0
55	MG	DA	1658	1/1	0.87	0.16	113,113,113,113	0
55	MG	AB	202	1/1	0.87	0.15	92,92,92,92	0
55	MG	BA	3418	1/1	0.87	0.14	73,73,73,73	0
55	MG	CA	1809	1/1	0.87	0.18	79,79,79,79	0
55	MG	AA	3537	1/1	0.87	0.09	105,105,105,105	0
55	MG	DA	1668	1/1	0.87	0.18	73,73,73,73	0
55	MG	BA	3158	1/1	0.87	0.22	70,70,70,70	0
55	MG	BA	3421	1/1	0.87	0.08	102,102,102,102	0
55	MG	AA	3056	1/1	0.87	0.24	98,98,98,98	0
55	MG	DC	101	1/1	0.87	0.10	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AB	205	1/1	0.87	0.18	83,83,83,83	0
55	MG	AA	3317	1/1	0.87	0.26	85,85,85,85	0
55	MG	CA	1821	1/1	0.87	0.26	94,94,94,94	0
55	MG	AA	3576	1/1	0.88	0.26	46,46,46,46	0
55	MG	BA	3195	1/1	0.88	0.25	94,94,94,94	0
55	MG	BA	3196	1/1	0.88	0.18	84,84,84,84	0
55	MG	BA	3200	1/1	0.88	0.19	65,65,65,65	0
55	MG	AA	3492	1/1	0.88	0.09	94,94,94,94	0
55	MG	AA	3415	1/1	0.88	0.27	87,87,87,87	0
55	MG	AA	3227	1/1	0.88	0.37	90,90,90,90	0
55	MG	BA	3228	1/1	0.88	0.27	74,74,74,74	0
55	MG	A2	201	1/1	0.88	0.33	101,101,101,101	0
55	MG	CC	103	1/1	0.88	0.19	104,104,104,104	0
55	MG	AA	3388	1/1	0.88	0.29	85,85,85,85	0
55	MG	AA	3419	1/1	0.88	0.28	89,89,89,89	0
55	MG	CA	1636	1/1	0.88	0.23	91,91,91,91	0
55	MG	AA	3389	1/1	0.88	0.19	72,72,72,72	0
55	MG	AA	3189	1/1	0.88	0.19	90,90,90,90	0
55	MG	AA	3313	1/1	0.88	0.23	70,70,70,70	0
55	MG	DA	1727	1/1	0.88	0.24	86,86,86,86	0
55	MG	AA	3505	1/1	0.88	0.30	85,85,85,85	0
55	MG	AA	3155	1/1	0.88	0.32	71,71,71,71	0
55	MG	BA	3377	1/1	0.88	0.28	81,81,81,81	0
55	MG	DA	1731	1/1	0.88	0.26	70,70,70,70	0
55	MG	BA	3270	1/1	0.88	0.25	81,81,81,81	0
55	MG	AA	3065	1/1	0.88	0.26	88,88,88,88	0
55	MG	DA	1612	1/1	0.88	0.08	73,73,73,73	0
55	MG	AA	3343	1/1	0.88	0.23	74,74,74,74	0
55	MG	AA	3107	1/1	0.88	0.13	69,69,69,69	0
55	MG	BA	3028	1/1	0.88	0.24	85,85,85,85	0
55	MG	DA	1617	1/1	0.88	0.22	102,102,102,102	0
55	MG	BA	3109	1/1	0.88	0.13	75,75,75,75	0
55	MG	DA	1748	1/1	0.88	0.32	91,91,91,91	0
55	MG	BA	3111	1/1	0.88	0.14	82,82,82,82	0
55	MG	AA	3268	1/1	0.88	0.37	85,85,85,85	0
55	MG	AA	3512	1/1	0.88	0.12	97,97,97,97	0
55	MG	AA	3467	1/1	0.88	0.19	87,87,87,87	0
55	MG	AA	3196	1/1	0.88	0.16	61,61,61,61	0
55	MG	CA	1680	1/1	0.88	0.18	79,79,79,79	0
55	MG	AA	3431	1/1	0.88	0.18	89,89,89,89	0
55	MG	BA	3496	1/1	0.88	0.09	96,96,96,96	0
55	MG	AA	3375	1/1	0.88	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3473	1/1	0.88	0.13	77,77,77,77	0
55	MG	AA	3376	1/1	0.88	0.19	85,85,85,85	0
55	MG	AA	3403	1/1	0.88	0.24	91,91,91,91	0
55	MG	AA	3092	1/1	0.88	0.18	71,71,71,71	0
55	MG	BA	3505	1/1	0.88	0.13	94,94,94,94	0
55	MG	BA	3506	1/1	0.88	0.16	74,74,74,74	0
55	MG	BA	3306	1/1	0.88	0.21	86,86,86,86	0
55	MG	BA	3051	1/1	0.88	0.09	90,90,90,90	0
55	MG	AA	3109	1/1	0.88	0.20	53,53,53,53	0
55	MG	AA	3536	1/1	0.88	0.16	92,92,92,92	0
55	MG	AA	3301	1/1	0.88	0.07	85,85,85,85	0
55	MG	AA	3542	1/1	0.88	0.15	93,93,93,93	0
55	MG	AA	3546	1/1	0.88	0.17	74,74,74,74	0
55	MG	AA	3408	1/1	0.88	0.20	83,83,83,83	0
55	MG	AA	3099	1/1	0.88	0.22	64,64,64,64	0
55	MG	AA	3410	1/1	0.88	0.11	95,95,95,95	0
55	MG	AA	3486	1/1	0.88	0.10	90,90,90,90	0
55	MG	BA	3528	1/1	0.88	0.14	98,98,98,98	0
55	MG	AA	3218	1/1	0.88	0.24	73,73,73,73	0
55	MG	AA	3076	1/1	0.88	0.17	82,82,82,82	0
55	MG	DA	1790	1/1	0.88	0.26	100,100,100,100	0
55	MG	BA	3335	1/1	0.88	0.16	100,100,100,100	0
55	MG	AA	3560	1/1	0.88	0.19	87,87,87,87	0
55	MG	BA	3338	1/1	0.88	0.21	71,71,71,71	0
55	MG	DA	1796	1/1	0.88	0.15	97,97,97,97	0
55	MG	BA	3074	1/1	0.88	0.09	83,83,83,83	0
55	MG	CA	1824	1/1	0.88	0.24	94,94,94,94	0
55	MG	BA	3431	1/1	0.88	0.16	84,84,84,84	0
55	MG	BA	3176	1/1	0.88	0.14	79,79,79,79	0
55	MG	BA	3343	1/1	0.88	0.12	75,75,75,75	0
55	MG	BA	3177	1/1	0.88	0.24	75,75,75,75	0
55	MG	AA	3045	1/1	0.88	0.24	54,54,54,54	0
55	MG	BA	3439	1/1	0.88	0.12	103,103,103,103	0
55	MG	CA	1833	1/1	0.88	0.10	95,95,95,95	0
55	MG	BA	3188	1/1	0.88	0.20	85,85,85,85	0
55	MG	BA	3189	1/1	0.88	0.17	61,61,61,61	0
55	MG	AB	217	1/1	0.88	0.07	110,110,110,110	0
55	MG	A3	101	1/1	0.89	0.32	74,74,74,74	0
55	MG	CA	1747	1/1	0.89	0.22	83,83,83,83	0
55	MG	AA	3048	1/1	0.89	0.14	86,86,86,86	0
55	MG	BA	3490	1/1	0.89	0.13	52,52,52,52	0
55	MG	BA	3225	1/1	0.89	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1709	1/1	0.89	0.17	109,109,109,109	0
55	MG	BA	3336	1/1	0.89	0.25	97,97,97,97	0
55	MG	AA	3091	1/1	0.89	0.22	78,78,78,78	0
55	MG	AA	3259	1/1	0.89	0.17	81,81,81,81	0
55	MG	BA	3004	1/1	0.89	0.23	105,105,105,105	0
55	MG	BA	3341	1/1	0.89	0.24	82,82,82,82	0
55	MG	BA	3241	1/1	0.89	0.24	52,52,52,52	0
55	MG	AA	3282	1/1	0.89	0.20	78,78,78,78	0
55	MG	BA	3010	1/1	0.89	0.22	68,68,68,68	0
55	MG	BA	3345	1/1	0.89	0.13	87,87,87,87	0
55	MG	CA	1676	1/1	0.89	0.20	76,76,76,76	0
55	MG	AA	3330	1/1	0.89	0.14	60,60,60,60	0
55	MG	CA	1678	1/1	0.89	0.25	69,69,69,69	0
55	MG	DA	1726	1/1	0.89	0.31	79,79,79,79	0
55	MG	BA	3509	1/1	0.89	0.34	73,73,73,73	0
55	MG	AA	3308	1/1	0.89	0.17	96,96,96,96	0
55	MG	AA	3365	1/1	0.89	0.24	74,74,74,74	0
55	MG	DA	1611	1/1	0.89	0.07	100,100,100,100	0
55	MG	BA	3263	1/1	0.89	0.18	84,84,84,84	0
55	MG	DA	1734	1/1	0.89	0.21	88,88,88,88	0
55	MG	BA	3265	1/1	0.89	0.21	86,86,86,86	0
55	MG	BA	3135	1/1	0.89	0.21	52,52,52,52	0
55	MG	AA	3003	1/1	0.89	0.26	64,64,64,64	0
55	MG	DA	1616	1/1	0.89	0.22	100,100,100,100	0
55	MG	AA	3284	1/1	0.89	0.26	81,81,81,81	0
55	MG	CA	1688	1/1	0.89	0.14	77,77,77,77	0
55	MG	BA	3150	1/1	0.89	0.24	96,96,96,96	0
55	MG	BA	3274	1/1	0.89	0.15	90,90,90,90	0
55	MG	BA	3076	1/1	0.89	0.29	91,91,91,91	0
55	MG	CA	1781	1/1	0.89	0.22	62,62,62,62	0
55	MG	AA	3262	1/1	0.89	0.21	33,33,33,33	0
55	MG	AA	3340	1/1	0.89	0.18	83,83,83,83	0
55	MG	AA	3023	1/1	0.89	0.32	56,56,56,56	0
55	MG	BA	3082	1/1	0.89	0.38	76,76,76,76	0
55	MG	AA	3457	1/1	0.89	0.38	64,64,64,64	0
55	MG	BA	3162	1/1	0.89	0.07	92,92,92,92	0
55	MG	CA	1791	1/1	0.89	0.16	97,97,97,97	0
55	MG	CA	1792	1/1	0.89	0.19	81,81,81,81	0
55	MG	BA	3034	1/1	0.89	0.22	81,81,81,81	0
55	MG	AA	3222	1/1	0.89	0.29	54,54,54,54	0
55	MG	AA	3047	1/1	0.89	0.16	60,60,60,60	0
55	MG	CA	1801	1/1	0.89	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3318	1/1	0.89	0.14	92,92,92,92	0
55	MG	BA	3093	1/1	0.89	0.10	78,78,78,78	0
55	MG	BA	3039	1/1	0.89	0.09	85,85,85,85	0
55	MG	CA	1719	1/1	0.89	0.09	85,85,85,85	0
55	MG	AA	3081	1/1	0.89	0.34	51,51,51,51	0
55	MG	B1	201	1/1	0.89	0.36	82,82,82,82	0
55	MG	BA	3041	1/1	0.89	0.08	104,104,104,104	0
55	MG	AA	3129	1/1	0.89	0.29	73,73,73,73	0
55	MG	CA	1817	1/1	0.89	0.19	85,85,85,85	0
55	MG	AA	3378	1/1	0.89	0.27	84,84,84,84	0
55	MG	DA	1659	1/1	0.89	0.12	80,80,80,80	0
55	MG	CA	1726	1/1	0.89	0.16	103,103,103,103	0
55	MG	CA	1613	1/1	0.89	0.05	94,94,94,94	0
55	MG	AA	3613	1/1	0.89	0.16	76,76,76,76	0
55	MG	BA	3048	1/1	0.89	0.11	74,74,74,74	0
55	MG	DA	1667	1/1	0.89	0.19	82,82,82,82	0
55	MG	BA	3106	1/1	0.89	0.16	85,85,85,85	0
55	MG	DA	1674	1/1	0.89	0.18	76,76,76,76	0
55	MG	DA	1676	1/1	0.89	0.23	82,82,82,82	0
55	MG	DA	1677	1/1	0.89	0.14	82,82,82,82	0
55	MG	BA	3392	1/1	0.89	0.09	85,85,85,85	0
55	MG	DA	1680	1/1	0.89	0.27	81,81,81,81	0
55	MG	BA	3393	1/1	0.89	0.16	84,84,84,84	0
55	MG	BA	3395	1/1	0.89	0.06	89,89,89,89	0
55	MG	BA	3320	1/1	0.89	0.27	77,77,77,77	0
55	MG	AA	3349	1/1	0.89	0.12	84,84,84,84	0
55	MG	AA	3198	1/1	0.89	0.34	74,74,74,74	0
55	MG	DH	201	1/1	0.89	0.19	105,105,105,105	0
55	MG	BA	3328	1/1	0.89	0.09	61,61,61,61	0
55	MG	AA	3322	1/1	0.89	0.23	68,68,68,68	0
55	MG	AA	3232	1/1	0.89	0.23	104,104,104,104	0
55	MG	BA	3206	1/1	0.89	0.23	98,98,98,98	0
55	MG	CA	1638	1/1	0.89	0.19	108,108,108,108	0
55	MG	BA	3476	1/1	0.89	0.11	68,68,68,68	0
55	MG	AA	3618	1/1	0.90	0.21	97,97,97,97	0
55	MG	CA	1840	1/1	0.90	0.16	69,69,69,69	0
55	MG	BA	3369	1/1	0.90	0.23	69,69,69,69	0
55	MG	AA	3547	1/1	0.90	0.14	45,45,45,45	0
55	MG	BA	3275	1/1	0.90	0.24	52,52,52,52	0
55	MG	BA	3152	1/1	0.90	0.21	73,73,73,73	0
55	MG	BA	3278	1/1	0.90	0.28	92,92,92,92	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($\text{\AA}^2$)	Q<0.9
55	MG	AA	3272	1/1	0.90	0.27	65,65,65,65	0
55	MG	AA	3250	1/1	0.90	0.12	99,99,99,99	0
55	MG	CA	1746	1/1	0.90	0.17	98,98,98,98	0
55	MG	DA	1711	1/1	0.90	0.22	89,89,89,89	0
55	MG	AA	3623	1/1	0.90	0.20	74,74,74,74	0
55	MG	CC	102	1/1	0.90	0.18	69,69,69,69	0
55	MG	CA	1633	1/1	0.90	0.22	83,83,83,83	0
55	MG	BA	3288	1/1	0.90	0.14	98,98,98,98	0
55	MG	AA	3095	1/1	0.90	0.10	89,89,89,89	0
55	MG	BA	3467	1/1	0.90	0.21	93,93,93,93	0
55	MG	AA	3055	1/1	0.90	0.25	67,67,67,67	0
55	MG	AA	3177	1/1	0.90	0.26	46,46,46,46	0
55	MG	AA	3254	1/1	0.90	0.25	85,85,85,85	0
55	MG	CA	1643	1/1	0.90	0.20	91,91,91,91	0
55	MG	BA	3030	1/1	0.90	0.22	99,99,99,99	0
55	MG	BA	3088	1/1	0.90	0.16	94,94,94,94	0
55	MG	BA	3473	1/1	0.90	0.21	78,78,78,78	0
55	MG	AA	3124	1/1	0.90	0.32	47,47,47,47	0
55	MG	AA	3363	1/1	0.90	0.26	95,95,95,95	0
55	MG	AA	3575	1/1	0.90	0.20	42,42,42,42	0
55	MG	BA	3305	1/1	0.90	0.19	76,76,76,76	0
55	MG	BA	3479	1/1	0.90	0.37	95,95,95,95	0
55	MG	BA	3485	1/1	0.90	0.21	46,46,46,46	0
55	MG	AA	3472	1/1	0.90	0.36	80,80,80,80	0
55	MG	CA	1667	1/1	0.90	0.20	77,77,77,77	0
55	MG	AA	3280	1/1	0.90	0.14	94,94,94,94	0
55	MG	AA	3145	1/1	0.90	0.32	91,91,91,91	0
55	MG	CA	1675	1/1	0.90	0.12	97,97,97,97	0
55	MG	BA	3311	1/1	0.90	0.12	82,82,82,82	0
55	MG	BA	3187	1/1	0.90	0.33	65,65,65,65	0
55	MG	AA	3203	1/1	0.90	0.32	65,65,65,65	0
55	MG	AA	3586	1/1	0.90	0.13	53,53,53,53	0
55	MG	AA	3039	1/1	0.90	0.26	82,82,82,82	0
55	MG	BA	3406	1/1	0.90	0.12	97,97,97,97	0
55	MG	AB	213	1/1	0.90	0.26	73,73,73,73	0
55	MG	AA	3447	1/1	0.90	0.25	75,75,75,75	0
55	MG	AA	3261	1/1	0.90	0.26	85,85,85,85	0
55	MG	BA	3047	1/1	0.90	0.14	80,80,80,80	0
55	MG	DA	1633	1/1	0.90	0.20	88,88,88,88	0
55	MG	DA	1634	1/1	0.90	0.16	77,77,77,77	0
55	MG	AA	3449	1/1	0.90	0.11	63,63,63,63	0
55	MG	AA	3211	1/1	0.90	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3068	1/1	0.90	0.39	72,72,72,72	0
55	MG	BA	3333	1/1	0.90	0.21	73,73,73,73	0
55	MG	BA	3212	1/1	0.90	0.25	70,70,70,70	0
55	MG	BA	3052	1/1	0.90	0.15	58,58,58,58	0
55	MG	BA	3220	1/1	0.90	0.12	40,40,40,40	0
55	MG	CA	1799	1/1	0.90	0.25	95,95,95,95	0
55	MG	BA	3221	1/1	0.90	0.16	37,37,37,37	0
55	MG	DA	1652	1/1	0.90	0.16	85,85,85,85	0
55	MG	BA	3222	1/1	0.90	0.11	54,54,54,54	0
55	MG	AA	3372	1/1	0.90	0.07	87,87,87,87	0
55	MG	BA	3524	1/1	0.90	0.37	105,105,105,105	0
55	MG	BA	3226	1/1	0.90	0.32	82,82,82,82	0
55	MG	BA	3526	1/1	0.90	0.21	92,92,92,92	0
55	MG	DA	1781	1/1	0.90	0.12	87,87,87,87	0
55	MG	AA	3424	1/1	0.90	0.22	54,54,54,54	0
55	MG	DA	1660	1/1	0.90	0.15	102,102,102,102	0
55	MG	AA	3532	1/1	0.90	0.28	88,88,88,88	0
55	MG	DA	1662	1/1	0.90	0.31	78,78,78,78	0
55	MG	AA	3290	1/1	0.90	0.26	72,72,72,72	0
55	MG	BA	3433	1/1	0.90	0.18	88,88,88,88	0
55	MG	BA	3060	1/1	0.90	0.07	51,51,51,51	0
55	MG	AU	201	1/1	0.90	0.14	85,85,85,85	0
55	MG	BA	3123	1/1	0.90	0.07	77,77,77,77	0
55	MG	DA	1669	1/1	0.90	0.29	68,68,68,68	0
55	MG	DA	1672	1/1	0.90	0.19	63,63,63,63	0
55	MG	DA	1800	1/1	0.90	0.24	99,99,99,99	0
55	MG	BA	3246	1/1	0.90	0.12	99,99,99,99	0
55	MG	AA	3187	1/1	0.90	0.23	87,87,87,87	0
55	MG	AA	3072	1/1	0.90	0.05	101,101,101,101	0
55	MG	AA	3540	1/1	0.90	0.47	63,63,63,63	0
55	MG	DG	301	1/1	0.90	0.19	94,94,94,94	0
55	MG	BA	3133	1/1	0.90	0.15	50,50,50,50	0
55	MG	AA	3296	1/1	0.90	0.25	72,72,72,72	0
55	MG	BA	3266	1/1	0.90	0.50	91,91,91,91	0
55	MG	CA	1604	1/1	0.90	0.19	77,77,77,77	0
55	MG	BA	3267	1/1	0.90	0.24	62,62,62,62	0
55	MG	BA	3142	1/1	0.90	0.21	70,70,70,70	0
55	MG	AA	3052	1/1	0.90	0.22	73,73,73,73	0
55	MG	BA	3005	1/1	0.90	0.18	70,70,70,70	0
55	MG	AA	3364	1/1	0.91	0.09	69,69,69,69	0
55	MG	AA	3024	1/1	0.91	0.25	45,45,45,45	0
55	MG	BA	3316	1/1	0.91	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1814	1/1	0.91	0.13	86,86,86,86	0
55	MG	BA	3199	1/1	0.91	0.24	76,76,76,76	0
55	MG	AA	3051	1/1	0.91	0.26	71,71,71,71	0
55	MG	CA	1690	1/1	0.91	0.16	102,102,102,102	0
55	MG	AA	3559	1/1	0.91	0.15	83,83,83,83	0
55	MG	BA	3202	1/1	0.91	0.15	69,69,69,69	0
55	MG	BA	3412	1/1	0.91	0.25	50,50,50,50	0
55	MG	BA	3327	1/1	0.91	0.24	91,91,91,91	0
55	MG	CA	1696	1/1	0.91	0.17	90,90,90,90	0
55	MG	AA	3277	1/1	0.91	0.11	82,82,82,82	0
55	MG	AA	3337	1/1	0.91	0.22	99,99,99,99	0
55	MG	AA	3574	1/1	0.91	0.21	54,54,54,54	0
55	MG	DA	1694	1/1	0.91	0.34	84,84,84,84	0
55	MG	BA	3417	1/1	0.91	0.12	88,88,88,88	0
55	MG	CA	1705	1/1	0.91	0.08	95,95,95,95	0
55	MG	DA	1701	1/1	0.91	0.20	80,80,80,80	0
55	MG	BA	3213	1/1	0.91	0.20	75,75,75,75	0
55	MG	BA	3110	1/1	0.91	0.25	92,92,92,92	0
55	MG	DA	1704	1/1	0.91	0.24	87,87,87,87	0
55	MG	BA	3215	1/1	0.91	0.20	66,66,66,66	0
55	MG	AA	3503	1/1	0.91	0.23	81,81,81,81	0
55	MG	AA	3504	1/1	0.91	0.23	80,80,80,80	0
55	MG	CA	1835	1/1	0.91	0.15	87,87,87,87	0
55	MG	BA	3527	1/1	0.91	0.25	97,97,97,97	0
55	MG	CA	1839	1/1	0.91	0.19	68,68,68,68	0
55	MG	AA	3028	1/1	0.91	0.23	54,54,54,54	0
55	MG	AA	3225	1/1	0.91	0.20	95,95,95,95	0
55	MG	BA	3425	1/1	0.91	0.30	85,85,85,85	0
55	MG	AA	3085	1/1	0.91	0.17	34,34,34,34	0
55	MG	BA	3339	1/1	0.91	0.16	90,90,90,90	0
55	MG	BA	3428	1/1	0.91	0.07	89,89,89,89	0
55	MG	CT	201	1/1	0.91	0.16	102,102,102,102	0
55	MG	BA	3053	1/1	0.91	0.20	65,65,65,65	0
55	MG	BA	3231	1/1	0.91	0.27	47,47,47,47	0
55	MG	DA	1721	1/1	0.91	0.24	71,71,71,71	0
55	MG	CB	103	1/1	0.91	0.09	110,110,110,110	0
55	MG	DA	1723	1/1	0.91	0.17	83,83,83,83	0
55	MG	BB	211	1/1	0.91	0.28	71,71,71,71	0
55	MG	BA	3119	1/1	0.91	0.10	79,79,79,79	0
55	MG	BA	3235	1/1	0.91	0.19	74,74,74,74	0
55	MG	AA	3130	1/1	0.91	0.14	67,67,67,67	0
55	MG	AA	3256	1/1	0.91	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3590	1/1	0.91	0.25	81,81,81,81	0
55	MG	CC	105	1/1	0.91	0.10	105,105,105,105	0
55	MG	DA	1732	1/1	0.91	0.16	94,94,94,94	0
55	MG	CC	106	1/1	0.91	0.17	92,92,92,92	0
55	MG	BA	3057	1/1	0.91	0.21	97,97,97,97	0
55	MG	BA	3440	1/1	0.91	0.08	80,80,80,80	0
55	MG	AA	3592	1/1	0.91	0.19	76,76,76,76	0
55	MG	AA	3074	1/1	0.91	0.30	68,68,68,68	0
55	MG	BA	3350	1/1	0.91	0.29	77,77,77,77	0
55	MG	CA	1612	1/1	0.91	0.09	102,102,102,102	0
55	MG	BA	3351	1/1	0.91	0.29	81,81,81,81	0
55	MG	AA	3471	1/1	0.91	0.22	85,85,85,85	0
55	MG	BA	3354	1/1	0.91	0.16	90,90,90,90	0
55	MG	AA	3346	1/1	0.91	0.24	88,88,88,88	0
55	MG	DA	1610	1/1	0.91	0.12	97,97,97,97	0
55	MG	AA	3440	1/1	0.91	0.24	87,87,87,87	0
55	MG	BA	3065	1/1	0.91	0.25	101,101,101,101	0
55	MG	CA	1622	1/1	0.91	0.10	86,86,86,86	0
55	MG	BA	3146	1/1	0.91	0.19	86,86,86,86	0
55	MG	DA	1758	1/1	0.91	0.28	109,109,109,109	0
55	MG	AA	3166	1/1	0.91	0.18	53,53,53,53	0
55	MG	BA	3361	1/1	0.91	0.14	88,88,88,88	0
55	MG	BA	3149	1/1	0.91	0.15	72,72,72,72	0
55	MG	CA	1629	1/1	0.91	0.10	95,95,95,95	0
55	MG	BA	3067	1/1	0.91	0.09	74,74,74,74	0
55	MG	AA	3442	1/1	0.91	0.20	78,78,78,78	0
55	MG	AA	3477	1/1	0.91	0.25	86,86,86,86	0
55	MG	AA	3040	1/1	0.91	0.22	68,68,68,68	0
55	MG	BA	3461	1/1	0.91	0.12	83,83,83,83	0
55	MG	AA	3527	1/1	0.91	0.12	86,86,86,86	0
55	MG	CA	1761	1/1	0.91	0.17	66,66,66,66	0
55	MG	BA	3276	1/1	0.91	0.12	88,88,88,88	0
55	MG	AA	3528	1/1	0.91	0.24	76,76,76,76	0
55	MG	AA	3176	1/1	0.91	0.10	74,74,74,74	0
55	MG	AA	3064	1/1	0.91	0.05	79,79,79,79	0
55	MG	BA	3280	1/1	0.91	0.36	74,74,74,74	0
55	MG	AA	3615	1/1	0.91	0.09	102,102,102,102	0
55	MG	AA	3353	1/1	0.91	0.27	86,86,86,86	0
55	MG	BA	3379	1/1	0.91	0.22	84,84,84,84	0
55	MG	AA	3239	1/1	0.91	0.14	60,60,60,60	0
55	MG	AA	3292	1/1	0.91	0.21	76,76,76,76	0
55	MG	DA	1639	1/1	0.91	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3022	1/1	0.91	0.11	75,75,75,75	0
55	MG	BA	3024	1/1	0.91	0.13	110,110,110,110	0
55	MG	CA	1658	1/1	0.91	0.18	50,50,50,50	0
55	MG	CA	1660	1/1	0.91	0.18	64,64,64,64	0
55	MG	BA	3085	1/1	0.91	0.27	74,74,74,74	0
55	MG	CA	1665	1/1	0.91	0.35	74,74,74,74	0
55	MG	AA	3241	1/1	0.91	0.30	80,80,80,80	0
55	MG	CA	1669	1/1	0.91	0.18	70,70,70,70	0
55	MG	AA	3180	1/1	0.91	0.21	64,64,64,64	0
55	MG	BA	3484	1/1	0.91	0.23	65,65,65,65	0
55	MG	CA	1673	1/1	0.91	0.20	76,76,76,76	0
55	MG	CA	1674	1/1	0.91	0.20	102,102,102,102	0
55	MG	AA	3326	1/1	0.91	0.11	64,64,64,64	0
55	MG	AA	3008	1/1	0.91	0.21	44,44,44,44	0
55	MG	BA	3180	1/1	0.91	0.23	57,57,57,57	0
55	MG	BA	3183	1/1	0.91	0.13	80,80,80,80	0
55	MG	AA	3141	1/1	0.91	0.23	50,50,50,50	0
55	MG	AA	3066	1/1	0.91	0.24	48,48,48,48	0
55	MG	AA	3495	1/1	0.91	0.25	90,90,90,90	0
55	MG	CA	1682	1/1	0.91	0.15	106,106,106,106	0
55	MG	AB	201	1/1	0.91	0.24	96,96,96,96	0
55	MG	AA	3249	1/1	0.91	0.32	76,76,76,76	0
55	MG	AA	3240	1/1	0.92	0.13	80,80,80,80	0
55	MG	BA	3483	1/1	0.92	0.18	34,34,34,34	0
55	MG	AA	3266	1/1	0.92	0.28	49,49,49,49	0
55	MG	CA	1645	1/1	0.92	0.26	60,60,60,60	0
55	MG	AA	3172	1/1	0.92	0.12	94,94,94,94	0
55	MG	AA	3507	1/1	0.92	0.25	99,99,99,99	0
55	MG	BA	3240	1/1	0.92	0.24	72,72,72,72	0
55	MG	CA	1650	1/1	0.92	0.25	73,73,73,73	0
55	MG	AA	3411	1/1	0.92	0.22	85,85,85,85	0
55	MG	AA	3561	1/1	0.92	0.11	82,82,82,82	0
55	MG	AA	3044	1/1	0.92	0.26	52,52,52,52	0
55	MG	BA	3245	1/1	0.92	0.20	72,72,72,72	0
55	MG	BA	3499	1/1	0.92	0.12	78,78,78,78	0
55	MG	AA	3001	1/1	0.92	0.28	44,44,44,44	0
55	MG	BA	3247	1/1	0.92	0.26	74,74,74,74	0
55	MG	BA	3248	1/1	0.92	0.18	54,54,54,54	0
55	MG	BA	3087	1/1	0.92	0.30	80,80,80,80	0
55	MG	AA	3297	1/1	0.92	0.11	69,69,69,69	0
55	MG	CA	1668	1/1	0.92	0.38	79,79,79,79	0
55	MG	BA	3257	1/1	0.92	0.35	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3258	1/1	0.92	0.19	64,64,64,64	0
55	MG	BA	3089	1/1	0.92	0.14	83,83,83,83	0
55	MG	BA	3261	1/1	0.92	0.19	65,65,65,65	0
55	MG	AA	3125	1/1	0.92	0.24	55,55,55,55	0
55	MG	AA	3037	1/1	0.92	0.25	69,69,69,69	0
55	MG	AA	3417	1/1	0.92	0.07	67,67,67,67	0
55	MG	AA	3515	1/1	0.92	0.31	77,77,77,77	0
55	MG	BA	3042	1/1	0.92	0.10	86,86,86,86	0
55	MG	BA	3171	1/1	0.92	0.14	63,63,63,63	0
55	MG	DA	1733	1/1	0.92	0.20	98,98,98,98	0
55	MG	BA	3271	1/1	0.92	0.18	84,84,84,84	0
55	MG	DA	1735	1/1	0.92	0.23	106,106,106,106	0
55	MG	DA	1736	1/1	0.92	0.21	65,65,65,65	0
55	MG	AA	3519	1/1	0.92	0.10	53,53,53,53	0
55	MG	AA	3027	1/1	0.92	0.19	45,45,45,45	0
55	MG	AA	3057	1/1	0.92	0.23	66,66,66,66	0
55	MG	AA	3131	1/1	0.92	0.18	90,90,90,90	0
55	MG	DA	1742	1/1	0.92	0.20	82,82,82,82	0
55	MG	AA	3156	1/1	0.92	0.17	94,94,94,94	0
55	MG	BA	3103	1/1	0.92	0.17	82,82,82,82	0
55	MG	BB	201	1/1	0.92	0.09	90,90,90,90	0
55	MG	BA	3049	1/1	0.92	0.11	86,86,86,86	0
55	MG	BA	3105	1/1	0.92	0.32	81,81,81,81	0
55	MG	BA	3184	1/1	0.92	0.14	76,76,76,76	0
55	MG	CA	1691	1/1	0.92	0.16	56,56,56,56	0
55	MG	BA	3362	1/1	0.92	0.07	71,71,71,71	0
55	MG	AA	3595	1/1	0.92	0.30	79,79,79,79	0
55	MG	CA	1796	1/1	0.92	0.20	82,82,82,82	0
55	MG	CA	1797	1/1	0.92	0.16	93,93,93,93	0
55	MG	AA	3597	1/1	0.92	0.17	91,91,91,91	0
55	MG	AF	301	1/1	0.92	0.14	80,80,80,80	0
55	MG	AA	3306	1/1	0.92	0.21	65,65,65,65	0
55	MG	BA	3289	1/1	0.92	0.19	70,70,70,70	0
55	MG	BA	3448	1/1	0.92	0.10	85,85,85,85	0
55	MG	AA	3163	1/1	0.92	0.12	55,55,55,55	0
55	MG	AA	3455	1/1	0.92	0.25	49,49,49,49	0
55	MG	CA	1806	1/1	0.92	0.10	62,62,62,62	0
55	MG	AA	3530	1/1	0.92	0.13	79,79,79,79	0
55	MG	AA	3058	1/1	0.92	0.20	64,64,64,64	0
55	MG	CA	1813	1/1	0.92	0.10	94,94,94,94	0
55	MG	B3	101	1/1	0.92	0.12	76,76,76,76	0
55	MG	CA	1712	1/1	0.92	0.14	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1601	1/1	0.92	0.16	56,56,56,56	0
55	MG	DA	1772	1/1	0.92	0.17	68,68,68,68	0
55	MG	BA	3297	1/1	0.92	0.13	63,63,63,63	0
55	MG	AA	3013	1/1	0.92	0.13	44,44,44,44	0
55	MG	AA	3533	1/1	0.92	0.12	67,67,67,67	0
55	MG	AA	3534	1/1	0.92	0.17	49,49,49,49	0
55	MG	BA	3458	1/1	0.92	0.09	71,71,71,71	0
55	MG	BA	3302	1/1	0.92	0.20	75,75,75,75	0
55	MG	DA	1665	1/1	0.92	0.26	82,82,82,82	0
55	MG	CA	1722	1/1	0.92	0.21	74,74,74,74	0
55	MG	AA	3311	1/1	0.92	0.20	68,68,68,68	0
55	MG	DA	1785	1/1	0.92	0.17	93,93,93,93	0
55	MG	AA	3494	1/1	0.92	0.21	88,88,88,88	0
55	MG	CA	1827	1/1	0.92	0.10	89,89,89,89	0
55	MG	AA	3016	1/1	0.92	0.16	48,48,48,48	0
55	MG	AA	3234	1/1	0.92	0.12	82,82,82,82	0
55	MG	AA	3167	1/1	0.92	0.26	50,50,50,50	0
55	MG	AA	3544	1/1	0.92	0.22	63,63,63,63	0
55	MG	BA	3310	1/1	0.92	0.17	74,74,74,74	0
55	MG	DA	1797	1/1	0.92	0.22	85,85,85,85	0
55	MG	AA	3285	1/1	0.92	0.23	80,80,80,80	0
55	MG	AA	3168	1/1	0.92	0.25	68,68,68,68	0
55	MG	CA	1732	1/1	0.92	0.18	69,69,69,69	0
55	MG	AA	3169	1/1	0.92	0.17	89,89,89,89	0
55	MG	BA	3394	1/1	0.92	0.26	88,88,88,88	0
55	MG	DA	1685	1/1	0.92	0.33	72,72,72,72	0
55	MG	BA	3314	1/1	0.92	0.16	71,71,71,71	0
55	MG	BA	3223	1/1	0.92	0.20	64,64,64,64	0
55	MG	CA	1634	1/1	0.92	0.20	60,60,60,60	0
55	MG	DS	101	1/1	0.92	0.26	87,87,87,87	0
55	MG	CN	201	1/1	0.92	0.10	78,78,78,78	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	AA	3406	1/1	0.92	0.13	83,83,83,83	0
55	MG	BA	3477	1/1	0.92	0.15	94,94,94,94	0
55	MG	AA	3171	1/1	0.92	0.08	84,84,84,84	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	BA	3481	1/1	0.93	0.18	49,49,49,49	0
55	MG	BA	3230	1/1	0.93	0.16	68,68,68,68	0
55	MG	AA	3246	1/1	0.93	0.27	73,73,73,73	0
55	MG	CA	1642	1/1	0.93	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3145	1/1	0.93	0.23	53,53,53,53	0
55	MG	CA	1744	1/1	0.93	0.29	57,57,57,57	0
55	MG	DA	1707	1/1	0.93	0.15	95,95,95,95	0
55	MG	AA	3214	1/1	0.93	0.30	47,47,47,47	0
55	MG	AA	3215	1/1	0.93	0.16	79,79,79,79	0
55	MG	BA	3491	1/1	0.93	0.08	49,49,49,49	0
55	MG	AA	3086	1/1	0.93	0.32	62,62,62,62	0
55	MG	AA	3565	1/1	0.93	0.26	53,53,53,53	0
55	MG	AA	3569	1/1	0.93	0.18	60,60,60,60	0
55	MG	BA	3497	1/1	0.93	0.19	63,63,63,63	0
55	MG	BA	3411	1/1	0.93	0.29	83,83,83,83	0
55	MG	AA	3116	1/1	0.93	0.24	37,37,37,37	0
55	MG	BA	3244	1/1	0.93	0.21	54,54,54,54	0
55	MG	BA	3153	1/1	0.93	0.28	77,77,77,77	0
55	MG	CA	1656	1/1	0.93	0.26	88,88,88,88	0
55	MG	AA	3476	1/1	0.93	0.23	79,79,79,79	0
55	MG	AA	3220	1/1	0.93	0.17	70,70,70,70	0
55	MG	AA	3577	1/1	0.93	0.09	52,52,52,52	0
55	MG	AA	3026	1/1	0.93	0.08	40,40,40,40	0
55	MG	BA	3253	1/1	0.93	0.23	66,66,66,66	0
55	MG	BA	3255	1/1	0.93	0.23	52,52,52,52	0
55	MG	AA	3101	1/1	0.93	0.13	79,79,79,79	0
55	MG	AA	3344	1/1	0.93	0.21	68,68,68,68	0
55	MG	BA	3515	1/1	0.93	0.15	59,59,59,59	0
55	MG	AA	3314	1/1	0.93	0.22	80,80,80,80	0
55	MG	AA	3186	1/1	0.93	0.12	58,58,58,58	0
55	MG	AA	3379	1/1	0.93	0.23	66,66,66,66	0
55	MG	BA	3262	1/1	0.93	0.06	94,94,94,94	0
55	MG	CA	1772	1/1	0.93	0.07	83,83,83,83	0
55	MG	BA	3167	1/1	0.93	0.22	59,59,59,59	0
55	MG	AA	3133	1/1	0.93	0.22	46,46,46,46	0
55	MG	AA	3090	1/1	0.93	0.18	45,45,45,45	0
55	MG	BA	3046	1/1	0.93	0.18	83,83,83,83	0
55	MG	CA	1777	1/1	0.93	0.16	92,92,92,92	0
55	MG	AA	3190	1/1	0.93	0.09	58,58,58,58	0
55	MG	AA	3596	1/1	0.93	0.19	93,93,93,93	0
55	MG	AE	303	1/1	0.93	0.09	91,91,91,91	0
55	MG	AA	3034	1/1	0.93	0.25	52,52,52,52	0
55	MG	AA	3014	1/1	0.93	0.19	38,38,38,38	0
55	MG	AA	3233	1/1	0.93	0.12	55,55,55,55	0
55	MG	BA	3182	1/1	0.93	0.14	47,47,47,47	0
55	MG	CA	1786	1/1	0.93	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3070	1/1	0.93	0.20	68,68,68,68	0
55	MG	DA	1752	1/1	0.93	0.21	89,89,89,89	0
55	MG	AA	3009	1/1	0.93	0.17	63,63,63,63	0
55	MG	DA	1632	1/1	0.93	0.12	84,84,84,84	0
55	MG	DA	1755	1/1	0.93	0.23	79,79,79,79	0
55	MG	CA	1790	1/1	0.93	0.06	89,89,89,89	0
55	MG	BA	3360	1/1	0.93	0.21	83,83,83,83	0
55	MG	AA	3496	1/1	0.93	0.17	87,87,87,87	0
55	MG	AA	3029	1/1	0.93	0.11	46,46,46,46	0
55	MG	AA	3605	1/1	0.93	0.28	72,72,72,72	0
55	MG	BA	3191	1/1	0.93	0.28	77,77,77,77	0
55	MG	BA	3192	1/1	0.93	0.26	72,72,72,72	0
55	MG	BA	3286	1/1	0.93	0.12	85,85,85,85	0
55	MG	CA	1697	1/1	0.93	0.22	92,92,92,92	0
55	MG	BA	3112	1/1	0.93	0.12	69,69,69,69	0
55	MG	CA	1700	1/1	0.93	0.11	72,72,72,72	0
55	MG	BA	3113	1/1	0.93	0.17	84,84,84,84	0
55	MG	AA	3147	1/1	0.93	0.29	89,89,89,89	0
55	MG	BA	3059	1/1	0.93	0.15	50,50,50,50	0
55	MG	BA	3291	1/1	0.93	0.31	67,67,67,67	0
55	MG	AA	3113	1/1	0.93	0.27	49,49,49,49	0
55	MG	CA	1710	1/1	0.93	0.20	81,81,81,81	0
55	MG	CA	1812	1/1	0.93	0.27	84,84,84,84	0
55	MG	BA	3002	1/1	0.93	0.17	66,66,66,66	0
55	MG	BA	3376	1/1	0.93	0.17	65,65,65,65	0
55	MG	CA	1713	1/1	0.93	0.18	83,83,83,83	0
55	MG	CA	1608	1/1	0.93	0.15	68,68,68,68	0
55	MG	AA	3360	1/1	0.93	0.18	63,63,63,63	0
55	MG	AA	3204	1/1	0.93	0.18	44,44,44,44	0
55	MG	BA	3204	1/1	0.93	0.23	74,74,74,74	0
55	MG	BA	3205	1/1	0.93	0.19	70,70,70,70	0
55	MG	BA	3381	1/1	0.93	0.24	80,80,80,80	0
55	MG	DA	1786	1/1	0.93	0.23	86,86,86,86	0
55	MG	AA	3207	1/1	0.93	0.09	50,50,50,50	0
55	MG	BA	3207	1/1	0.93	0.15	46,46,46,46	0
55	MG	DA	1789	1/1	0.93	0.14	77,77,77,77	0
55	MG	CA	1620	1/1	0.93	0.12	74,74,74,74	0
55	MG	DA	1792	1/1	0.93	0.14	81,81,81,81	0
55	MG	BA	3208	1/1	0.93	0.18	57,57,57,57	0
55	MG	DA	1675	1/1	0.93	0.27	60,60,60,60	0
55	MG	CA	1826	1/1	0.93	0.19	81,81,81,81	0
55	MG	AA	3395	1/1	0.93	0.19	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3552	1/1	0.93	0.28	83,83,83,83	0
55	MG	DA	1679	1/1	0.93	0.29	64,64,64,64	0
55	MG	BA	3014	1/1	0.93	0.17	72,72,72,72	0
55	MG	AA	3004	1/1	0.93	0.19	40,40,40,40	0
55	MG	CA	1626	1/1	0.93	0.13	88,88,88,88	0
55	MG	BA	3071	1/1	0.93	0.13	78,78,78,78	0
55	MG	BA	3132	1/1	0.93	0.17	54,54,54,54	0
55	MG	AA	3430	1/1	0.93	0.07	105,105,105,105	0
55	MG	CA	1631	1/1	0.93	0.07	74,74,74,74	0
55	MG	CA	1836	1/1	0.93	0.10	71,71,71,71	0
55	MG	CA	1837	1/1	0.93	0.20	88,88,88,88	0
55	MG	DA	1691	1/1	0.93	0.25	82,82,82,82	0
55	MG	AA	3332	1/1	0.93	0.10	62,62,62,62	0
55	MG	BA	3137	1/1	0.93	0.19	48,48,48,48	0
55	MG	DC	104	1/1	0.93	0.20	102,102,102,102	0
55	MG	AA	3150	1/1	0.93	0.29	59,59,59,59	0
55	MG	BA	3141	1/1	0.93	0.17	72,72,72,72	0
55	MG	DA	1697	1/1	0.93	0.07	111,111,111,111	0
55	MG	AA	3334	1/1	0.93	0.36	76,76,76,76	0
55	MG	DA	1700	1/1	0.93	0.22	94,94,94,94	0
55	MG	AA	3188	1/1	0.94	0.27	57,57,57,57	0
55	MG	AA	3111	1/1	0.94	0.26	36,36,36,36	0
55	MG	CA	1706	1/1	0.94	0.14	91,91,91,91	0
55	MG	AA	3025	1/1	0.94	0.18	40,40,40,40	0
55	MG	CA	1795	1/1	0.94	0.13	68,68,68,68	0
55	MG	DA	1622	1/1	0.94	0.10	98,98,98,98	0
55	MG	DA	1724	1/1	0.94	0.28	72,72,72,72	0
55	MG	BA	3250	1/1	0.94	0.16	58,58,58,58	0
55	MG	BA	3403	1/1	0.94	0.13	77,77,77,77	0
55	MG	A5	102	1/1	0.94	0.23	83,83,83,83	0
55	MG	AA	3299	1/1	0.94	0.16	79,79,79,79	0
55	MG	BA	3001	1/1	0.94	0.16	64,64,64,64	0
55	MG	BA	3480	1/1	0.94	0.18	56,56,56,56	0
55	MG	AA	3010	1/1	0.94	0.19	47,47,47,47	0
55	MG	AA	3192	1/1	0.94	0.18	63,63,63,63	0
55	MG	AA	3563	1/1	0.94	0.18	52,52,52,52	0
55	MG	BA	3259	1/1	0.94	0.15	54,54,54,54	0
55	MG	CA	1807	1/1	0.94	0.19	64,64,64,64	0
55	MG	AA	3302	1/1	0.94	0.16	104,104,104,104	0
55	MG	DA	1737	1/1	0.94	0.25	74,74,74,74	0
55	MG	AA	3153	1/1	0.94	0.14	48,48,48,48	0
55	MG	CA	1811	1/1	0.94	0.18	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3622	1/1	0.94	0.18	65,65,65,65	0
55	MG	DA	1638	1/1	0.94	0.15	74,74,74,74	0
55	MG	BA	3013	1/1	0.94	0.16	74,74,74,74	0
55	MG	AA	3223	1/1	0.94	0.27	71,71,71,71	0
55	MG	BA	3015	1/1	0.94	0.15	71,71,71,71	0
55	MG	BA	3120	1/1	0.94	0.17	81,81,81,81	0
55	MG	AA	3135	1/1	0.94	0.12	66,66,66,66	0
55	MG	BA	3069	1/1	0.94	0.11	70,70,70,70	0
55	MG	DA	1646	1/1	0.94	0.18	65,65,65,65	0
55	MG	AA	3484	1/1	0.94	0.09	44,44,44,44	0
55	MG	AA	3071	1/1	0.94	0.23	56,56,56,56	0
55	MG	DA	1653	1/1	0.94	0.15	96,96,96,96	0
55	MG	AA	3226	1/1	0.94	0.13	77,77,77,77	0
55	MG	BA	3197	1/1	0.94	0.07	76,76,76,76	0
55	MG	AA	3157	1/1	0.94	0.19	39,39,39,39	0
55	MG	BA	3130	1/1	0.94	0.13	44,44,44,44	0
55	MG	AA	3281	1/1	0.94	0.21	74,74,74,74	0
55	MG	AA	3310	1/1	0.94	0.12	65,65,65,65	0
55	MG	BA	3510	1/1	0.94	0.24	67,67,67,67	0
55	MG	BA	3511	1/1	0.94	0.26	68,68,68,68	0
55	MG	BA	3203	1/1	0.94	0.23	53,53,53,53	0
55	MG	AA	3458	1/1	0.94	0.14	70,70,70,70	0
55	MG	AA	3181	1/1	0.94	0.17	66,66,66,66	0
55	MG	BA	3029	1/1	0.94	0.23	75,75,75,75	0
55	MG	AA	3588	1/1	0.94	0.17	68,68,68,68	0
55	MG	CA	1659	1/1	0.94	0.11	71,71,71,71	0
55	MG	AA	3229	1/1	0.94	0.09	89,89,89,89	0
55	MG	BA	3143	1/1	0.94	0.13	63,63,63,63	0
55	MG	CA	1662	1/1	0.94	0.28	81,81,81,81	0
55	MG	DA	1673	1/1	0.94	0.13	88,88,88,88	0
55	MG	AA	3201	1/1	0.94	0.15	85,85,85,85	0
55	MG	DA	1773	1/1	0.94	0.28	69,69,69,69	0
55	MG	CA	1666	1/1	0.94	0.18	70,70,70,70	0
55	MG	AA	3022	1/1	0.94	0.12	49,49,49,49	0
55	MG	AA	3139	1/1	0.94	0.13	54,54,54,54	0
55	MG	BA	3147	1/1	0.94	0.22	63,63,63,63	0
55	MG	BA	3219	1/1	0.94	0.13	48,48,48,48	0
55	MG	CA	1671	1/1	0.94	0.09	72,72,72,72	0
55	MG	AA	3464	1/1	0.94	0.22	83,83,83,83	0
55	MG	AA	3205	1/1	0.94	0.23	55,55,55,55	0
55	MG	AA	3374	1/1	0.94	0.16	74,74,74,74	0
55	MG	AA	3543	1/1	0.94	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3224	1/1	0.94	0.16	51,51,51,51	0
55	MG	AA	3073	1/1	0.94	0.37	97,97,97,97	0
55	MG	DA	1687	1/1	0.94	0.25	72,72,72,72	0
55	MG	AD	301	1/1	0.94	0.07	99,99,99,99	0
55	MG	BA	3227	1/1	0.94	0.30	50,50,50,50	0
55	MG	BA	3452	1/1	0.94	0.07	96,96,96,96	0
55	MG	AE	301	1/1	0.94	0.14	65,65,65,65	0
55	MG	AA	3436	1/1	0.94	0.17	66,66,66,66	0
55	MG	AA	3054	1/1	0.94	0.24	62,62,62,62	0
55	MG	BA	3097	1/1	0.94	0.11	60,60,60,60	0
55	MG	BA	3309	1/1	0.94	0.23	80,80,80,80	0
55	MG	AA	3210	1/1	0.94	0.18	72,72,72,72	0
55	MG	DA	1799	1/1	0.94	0.18	68,68,68,68	0
55	MG	BA	3237	1/1	0.94	0.16	47,47,47,47	0
55	MG	BE	302	1/1	0.94	0.14	76,76,76,76	0
55	MG	BA	3238	1/1	0.94	0.29	66,66,66,66	0
55	MG	DA	1602	1/1	0.94	0.22	85,85,85,85	0
55	MG	BA	3160	1/1	0.94	0.18	82,82,82,82	0
55	MG	AF	302	1/1	0.94	0.13	93,93,93,93	0
55	MG	BA	3315	1/1	0.94	0.14	91,91,91,91	0
55	MG	AA	3038	1/1	0.94	0.34	80,80,80,80	0
55	MG	AA	3350	1/1	0.94	0.12	90,90,90,90	0
55	MG	DA	1608	1/1	0.94	0.15	92,92,92,92	0
55	MG	BA	3466	1/1	0.94	0.11	73,73,73,73	0
55	MG	AA	3061	1/1	0.94	0.19	79,79,79,79	0
55	MG	DC	102	1/1	0.94	0.18	74,74,74,74	0
55	MG	BA	3165	1/1	0.94	0.18	42,42,42,42	0
55	MG	CA	1611	1/1	0.94	0.15	97,97,97,97	0
55	MG	BA	3323	1/1	0.94	0.27	74,74,74,74	0
55	MG	AA	3555	1/1	0.94	0.18	67,67,67,67	0
55	MG	CA	1702	1/1	0.94	0.09	71,71,71,71	0
55	MG	BA	3325	1/1	0.94	0.29	50,50,50,50	0
55	MG	AA	3093	1/1	0.95	0.26	65,65,65,65	0
55	MG	AA	3545	1/1	0.95	0.15	75,75,75,75	0
55	MG	BA	3178	1/1	0.95	0.19	62,62,62,62	0
55	MG	CA	1657	1/1	0.95	0.18	63,63,63,63	0
55	MG	BA	3026	1/1	0.95	0.21	72,72,72,72	0
55	MG	AA	3238	1/1	0.95	0.24	82,82,82,82	0
55	MG	AA	3112	1/1	0.95	0.34	45,45,45,45	0
55	MG	DA	1645	1/1	0.95	0.19	51,51,51,51	0
55	MG	AA	3015	1/1	0.95	0.20	44,44,44,44	0
55	MG	AA	3011	1/1	0.95	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1651	1/1	0.95	0.17	72,72,72,72	0
55	MG	CA	1663	1/1	0.95	0.09	52,52,52,52	0
55	MG	BA	3382	1/1	0.95	0.18	89,89,89,89	0
55	MG	BA	3185	1/1	0.95	0.24	68,68,68,68	0
55	MG	BB	203	1/1	0.95	0.17	76,76,76,76	0
55	MG	AA	3005	1/1	0.95	0.14	25,25,25,25	0
55	MG	CA	1749	1/1	0.95	0.13	62,62,62,62	0
55	MG	BA	3252	1/1	0.95	0.20	86,86,86,86	0
55	MG	AA	3485	1/1	0.95	0.19	71,71,71,71	0
55	MG	BA	3128	1/1	0.95	0.11	56,56,56,56	0
55	MG	BA	3388	1/1	0.95	0.22	87,87,87,87	0
55	MG	AA	3331	1/1	0.95	0.20	76,76,76,76	0
55	MG	AA	3516	1/1	0.95	0.20	76,76,76,76	0
55	MG	BA	3391	1/1	0.95	0.10	95,95,95,95	0
55	MG	AA	3606	1/1	0.95	0.26	61,61,61,61	0
55	MG	BA	3134	1/1	0.95	0.15	63,63,63,63	0
55	MG	AA	3517	1/1	0.95	0.07	66,66,66,66	0
55	MG	BA	3038	1/1	0.95	0.22	78,78,78,78	0
55	MG	BA	3138	1/1	0.95	0.16	52,52,52,52	0
55	MG	BR	201	1/1	0.95	0.05	77,77,77,77	0
55	MG	AA	3263	1/1	0.95	0.16	51,51,51,51	0
55	MG	AA	3434	1/1	0.95	0.24	44,44,44,44	0
55	MG	AA	3243	1/1	0.95	0.17	51,51,51,51	0
55	MG	B5	101	1/1	0.95	0.18	61,61,61,61	0
55	MG	AO	202	1/1	0.95	0.33	80,80,80,80	0
55	MG	CA	1603	1/1	0.95	0.15	73,73,73,73	0
55	MG	CA	1769	1/1	0.95	0.04	79,79,79,79	0
55	MG	BA	3268	1/1	0.95	0.11	59,59,59,59	0
55	MG	AA	3105	1/1	0.95	0.19	61,61,61,61	0
55	MG	AA	3525	1/1	0.95	0.09	73,73,73,73	0
55	MG	AA	3267	1/1	0.95	0.16	62,62,62,62	0
55	MG	AA	3106	1/1	0.95	0.17	69,69,69,69	0
55	MG	AA	3568	1/1	0.95	0.13	49,49,49,49	0
55	MG	AA	3174	1/1	0.95	0.25	40,40,40,40	0
55	MG	BA	3409	1/1	0.95	0.19	71,71,71,71	0
55	MG	DA	1776	1/1	0.95	0.10	70,70,70,70	0
55	MG	AA	3570	1/1	0.95	0.20	41,41,41,41	0
55	MG	DA	1689	1/1	0.95	0.20	72,72,72,72	0
55	MG	AA	3387	1/1	0.95	0.34	80,80,80,80	0
55	MG	AA	3338	1/1	0.95	0.17	51,51,51,51	0
55	MG	BA	3100	1/1	0.95	0.27	66,66,66,66	0
55	MG	BA	3154	1/1	0.95	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3216	1/1	0.95	0.18	56,56,56,56	0
55	MG	BA	3218	1/1	0.95	0.23	51,51,51,51	0
55	MG	DA	1696	1/1	0.95	0.19	66,66,66,66	0
55	MG	BA	3488	1/1	0.95	0.08	59,59,59,59	0
55	MG	AA	3158	1/1	0.95	0.10	68,68,68,68	0
55	MG	AA	3293	1/1	0.95	0.08	77,77,77,77	0
55	MG	CA	1789	1/1	0.95	0.06	71,71,71,71	0
55	MG	DA	1791	1/1	0.95	0.21	80,80,80,80	0
55	MG	AA	3581	1/1	0.95	0.10	36,36,36,36	0
55	MG	BA	3353	1/1	0.95	0.20	84,84,84,84	0
55	MG	AA	3294	1/1	0.95	0.39	93,93,93,93	0
55	MG	BA	3009	1/1	0.95	0.16	48,48,48,48	0
55	MG	AA	3162	1/1	0.95	0.18	45,45,45,45	0
55	MG	CA	1632	1/1	0.95	0.12	76,76,76,76	0
55	MG	BA	3012	1/1	0.95	0.27	63,63,63,63	0
55	MG	AA	3041	1/1	0.95	0.16	66,66,66,66	0
55	MG	CA	1717	1/1	0.95	0.14	69,69,69,69	0
55	MG	AA	3002	1/1	0.95	0.18	41,41,41,41	0
55	MG	CA	1800	1/1	0.95	0.10	104,104,104,104	0
55	MG	BA	3061	1/1	0.95	0.05	69,69,69,69	0
55	MG	AA	3195	1/1	0.95	0.16	62,62,62,62	0
55	MG	BA	3016	1/1	0.95	0.06	56,56,56,56	0
55	MG	BA	3232	1/1	0.95	0.18	55,55,55,55	0
55	MG	BA	3432	1/1	0.95	0.20	88,88,88,88	0
55	MG	BA	3364	1/1	0.95	0.11	76,76,76,76	0
55	MG	AA	3539	1/1	0.95	0.15	49,49,49,49	0
55	MG	BA	3234	1/1	0.95	0.22	67,67,67,67	0
55	MG	AA	3217	1/1	0.95	0.07	64,64,64,64	0
55	MG	BA	3437	1/1	0.95	0.21	73,73,73,73	0
55	MG	DC	103	1/1	0.95	0.22	78,78,78,78	0
55	MG	BA	3236	1/1	0.95	0.32	41,41,41,41	0
55	MG	DC	105	1/1	0.95	0.22	75,75,75,75	0
55	MG	AA	3591	1/1	0.95	0.13	74,74,74,74	0
55	MG	BA	3173	1/1	0.95	0.24	50,50,50,50	0
55	MG	BA	3517	1/1	0.95	0.15	61,61,61,61	0
56	PAR	CA	1841	42/42	0.95	0.07	40,56,74,83	0
55	MG	AA	3082	1/1	0.95	0.21	50,50,50,50	0
55	MG	AA	3219	1/1	0.95	0.22	81,81,81,81	0
55	MG	AA	3607	1/1	0.96	0.14	44,44,44,44	0
55	MG	AA	3608	1/1	0.96	0.12	41,41,41,41	0
55	MG	AA	3352	1/1	0.96	0.14	52,52,52,52	0
55	MG	BA	3126	1/1	0.96	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3170	1/1	0.96	0.15	41,41,41,41	0
55	MG	BA	3079	1/1	0.96	0.12	82,82,82,82	0
55	MG	AA	3152	1/1	0.96	0.28	58,58,58,58	0
55	MG	CA	1664	1/1	0.96	0.06	47,47,47,47	0
55	MG	BA	3186	1/1	0.96	0.23	52,52,52,52	0
55	MG	AA	3089	1/1	0.96	0.25	64,64,64,64	0
55	MG	BP	201	1/1	0.96	0.08	65,65,65,65	0
55	MG	AA	3572	1/1	0.96	0.27	54,54,54,54	0
55	MG	AA	3573	1/1	0.96	0.17	31,31,31,31	0
55	MG	A1	201	1/1	0.96	0.28	64,64,64,64	0
55	MG	BA	3366	1/1	0.96	0.23	76,76,76,76	0
55	MG	BA	3136	1/1	0.96	0.10	43,43,43,43	0
55	MG	BA	3086	1/1	0.96	0.49	82,82,82,82	0
55	MG	CA	1602	1/1	0.96	0.10	74,74,74,74	0
55	MG	AA	3154	1/1	0.96	0.28	52,52,52,52	0
55	MG	AA	3046	1/1	0.96	0.07	57,57,57,57	0
55	MG	BA	3254	1/1	0.96	0.31	69,69,69,69	0
55	MG	AA	3175	1/1	0.96	0.09	45,45,45,45	0
55	MG	BA	3430	1/1	0.96	0.05	89,89,89,89	0
55	MG	BA	3492	1/1	0.96	0.18	47,47,47,47	0
55	MG	AA	3128	1/1	0.96	0.17	56,56,56,56	0
55	MG	AA	3031	1/1	0.96	0.20	52,52,52,52	0
55	MG	AA	3179	1/1	0.96	0.15	53,53,53,53	0
55	MG	BA	3319	1/1	0.96	0.26	68,68,68,68	0
55	MG	AA	3100	1/1	0.96	0.28	67,67,67,67	0
55	MG	BA	3321	1/1	0.96	0.04	59,59,59,59	0
55	MG	CA	1617	1/1	0.96	0.19	72,72,72,72	0
55	MG	AA	3143	1/1	0.96	0.16	35,35,35,35	0
55	MG	BA	3501	1/1	0.96	0.06	88,88,88,88	0
55	MG	AA	3488	1/1	0.96	0.07	93,93,93,93	0
55	MG	BA	3096	1/1	0.96	0.20	89,89,89,89	0
55	MG	AA	3144	1/1	0.96	0.25	45,45,45,45	0
55	MG	AA	3042	1/1	0.96	0.05	77,77,77,77	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	3589	1/1	0.96	0.12	60,60,60,60	0
55	MG	AA	3549	1/1	0.96	0.34	50,50,50,50	0
55	MG	AA	3550	1/1	0.96	0.22	39,39,39,39	0
55	MG	BA	3011	1/1	0.96	0.22	65,65,65,65	0
55	MG	DA	1647	1/1	0.96	0.10	71,71,71,71	0
55	MG	AA	3551	1/1	0.96	0.23	69,69,69,69	0
55	MG	BA	3514	1/1	0.96	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3593	1/1	0.96	0.32	95,95,95,95	0
55	MG	AA	3146	1/1	0.96	0.17	65,65,65,65	0
55	MG	AA	3206	1/1	0.96	0.09	51,51,51,51	0
55	MG	AA	3012	1/1	0.96	0.17	40,40,40,40	0
55	MG	CA	1707	1/1	0.96	0.23	78,78,78,78	0
55	MG	BA	3017	1/1	0.96	0.19	50,50,50,50	0
55	MG	AA	3523	1/1	0.96	0.12	91,91,91,91	0
55	MG	AA	3208	1/1	0.96	0.12	44,44,44,44	0
55	MG	AA	3323	1/1	0.96	0.07	71,71,71,71	0
55	MG	BA	3166	1/1	0.96	0.16	40,40,40,40	0
55	MG	BA	3400	1/1	0.96	0.20	74,74,74,74	0
55	MG	AA	3069	1/1	0.96	0.11	64,64,64,64	0
55	MG	CA	1646	1/1	0.96	0.17	75,75,75,75	0
55	MG	BA	3168	1/1	0.96	0.14	60,60,60,60	0
55	MG	AA	3035	1/1	0.96	0.13	45,45,45,45	0
55	MG	BA	3023	1/1	0.96	0.26	70,70,70,70	0
55	MG	AA	3036	1/1	0.96	0.06	39,39,39,39	0
55	MG	BB	202	1/1	0.96	0.06	103,103,103,103	0
55	MG	DA	1671	1/1	0.96	0.24	77,77,77,77	0
55	MG	AA	3603	1/1	0.96	0.23	41,41,41,41	0
55	MG	AA	3257	1/1	0.96	0.15	79,79,79,79	0
55	MG	AA	3212	1/1	0.96	0.13	52,52,52,52	0
55	MG	AA	3450	1/1	0.96	0.21	72,72,72,72	0
55	MG	AE	302	1/1	0.96	0.20	45,45,45,45	0
55	MG	DA	1749	1/1	0.96	0.20	101,101,101,101	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	CA	1641	1/1	0.97	0.10	65,65,65,65	0
55	MG	BA	3190	1/1	0.97	0.10	73,73,73,73	0
55	MG	BE	303	1/1	0.97	0.18	57,57,57,57	0
55	MG	BA	3129	1/1	0.97	0.10	41,41,41,41	0
55	MG	AA	3199	1/1	0.97	0.26	46,46,46,46	0
55	MG	AA	3200	1/1	0.97	0.21	71,71,71,71	0
55	MG	BA	3264	1/1	0.97	0.14	59,59,59,59	0
55	MG	DA	1779	1/1	0.97	0.20	91,91,91,91	0
55	MG	BA	3229	1/1	0.97	0.20	50,50,50,50	0
55	MG	AA	3562	1/1	0.97	0.12	82,82,82,82	0
55	MG	A5	101	1/1	0.97	0.11	51,51,51,51	0
55	MG	AB	210	1/1	0.97	0.37	65,65,65,65	0
55	MG	AA	3083	1/1	0.97	0.17	34,34,34,34	0
55	MG	A7	101	1/1	0.97	0.20	60,60,60,60	0
55	MG	AA	3202	1/1	0.97	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3006	1/1	0.97	0.36	46,46,46,46	0
55	MG	BA	3169	1/1	0.97	0.19	56,56,56,56	0
55	MG	BA	3140	1/1	0.97	0.16	42,42,42,42	0
55	MG	CA	1610	1/1	0.97	0.17	54,54,54,54	0
55	MG	AA	3566	1/1	0.97	0.13	27,27,27,27	0
55	MG	AA	3140	1/1	0.97	0.17	67,67,67,67	0
55	MG	CA	1708	1/1	0.97	0.17	45,45,45,45	0
55	MG	BA	3031	1/1	0.97	0.20	60,60,60,60	0
55	MG	AA	3127	1/1	0.97	0.21	53,53,53,53	0
55	MG	AA	3287	1/1	0.97	0.20	69,69,69,69	0
55	MG	AA	3244	1/1	0.97	0.22	45,45,45,45	0
55	MG	CA	1808	1/1	0.97	0.17	67,67,67,67	0
55	MG	BA	3211	1/1	0.97	0.14	57,57,57,57	0
55	MG	AA	3265	1/1	0.97	0.11	95,95,95,95	0
55	MG	BA	3283	1/1	0.97	0.11	43,43,43,43	0
55	MG	BA	3482	1/1	0.97	0.13	65,65,65,65	0
55	MG	DA	1699	1/1	0.97	0.16	68,68,68,68	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	3284	1/1	0.97	0.07	61,61,61,61	0
55	MG	AA	3518	1/1	0.97	0.26	90,90,90,90	0
55	MG	AA	3007	1/1	0.97	0.09	42,42,42,42	0
55	MG	BA	3486	1/1	0.97	0.13	30,30,30,30	0
55	MG	BA	3487	1/1	0.97	0.10	66,66,66,66	0
55	MG	AA	3520	1/1	0.97	0.20	68,68,68,68	0
55	MG	AA	3491	1/1	0.97	0.16	85,85,85,85	0
55	MG	BA	3217	1/1	0.97	0.10	39,39,39,39	0
55	MG	AA	3578	1/1	0.97	0.19	50,50,50,50	0
55	MG	AA	3579	1/1	0.97	0.10	39,39,39,39	0
55	MG	AA	3538	1/1	0.97	0.17	36,36,36,36	0
55	MG	BA	3295	1/1	0.97	0.09	58,58,58,58	0
55	MG	AA	3582	1/1	0.97	0.14	44,44,44,44	0
55	MG	AA	3399	1/1	0.97	0.13	60,60,60,60	0
55	MG	AA	3161	1/1	0.97	0.15	42,42,42,42	0
55	MG	AA	3541	1/1	0.97	0.12	48,48,48,48	0
55	MG	BA	3300	1/1	0.97	0.15	56,56,56,56	0
55	MG	BD	301	1/1	0.97	0.15	39,39,39,39	0
55	MG	BA	3493	1/1	0.98	0.13	39,39,39,39	0
55	MG	DA	1670	1/1	0.98	0.22	49,49,49,49	0
55	MG	AA	3159	1/1	0.98	0.05	28,28,28,28	0
55	MG	BA	3292	1/1	0.98	0.26	51,51,51,51	0
55	MG	CA	1606	1/1	0.98	0.07	94,94,94,94	0

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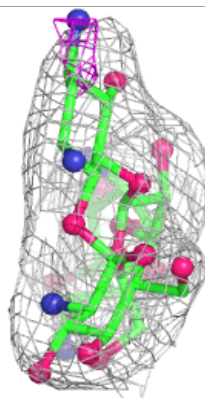
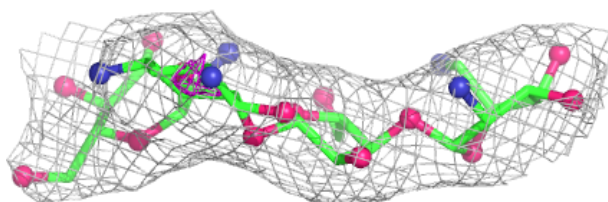
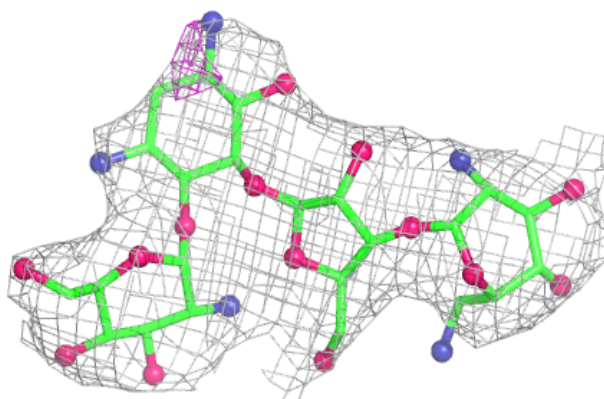
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3080	1/1	0.98	0.11	72,72,72,72	0
55	MG	BA	3322	1/1	0.98	0.16	79,79,79,79	0
55	MG	A7	102	1/1	0.98	0.23	68,68,68,68	0
55	MG	AA	3610	1/1	0.98	0.07	46,46,46,46	0
55	MG	AA	3160	1/1	0.98	0.12	32,32,32,32	0
55	MG	AA	3269	1/1	0.98	0.26	55,55,55,55	0
55	MG	AA	3230	1/1	0.98	0.07	34,34,34,34	0
55	MG	AA	3084	1/1	0.98	0.07	43,43,43,43	0
55	MG	AA	3580	1/1	0.98	0.06	78,78,78,78	0
55	MG	AA	3151	1/1	0.98	0.25	58,58,58,58	0
55	MG	BA	3198	1/1	0.98	0.13	44,44,44,44	0
55	MG	BA	3249	1/1	0.98	0.12	40,40,40,40	0
55	MG	CA	1619	1/1	0.98	0.14	59,59,59,59	0
55	MG	BA	3508	1/1	0.98	0.32	73,73,73,73	0
55	MG	BA	3131	1/1	0.98	0.10	49,49,49,49	0
55	MG	AA	3020	1/1	0.98	0.13	39,39,39,39	0
55	MG	AA	3400	1/1	0.98	0.20	39,39,39,39	0
55	MG	A0	201	1/1	0.98	0.11	62,62,62,62	0
55	MG	AA	3030	1/1	0.98	0.12	45,45,45,45	0
55	MG	BE	301	1/1	0.98	0.14	54,54,54,54	0
55	MG	CA	1627	1/1	0.98	0.13	65,65,65,65	0
55	MG	AA	3021	1/1	0.98	0.15	42,42,42,42	0
55	MG	CA	1699	1/1	0.98	0.09	63,63,63,63	0
55	MG	BA	3181	1/1	0.98	0.09	49,49,49,49	0
55	MG	AA	3138	1/1	0.98	0.23	45,45,45,45	0
55	MG	AA	3088	1/1	0.98	0.09	42,42,42,42	0
55	MG	BA	3285	1/1	0.98	0.06	45,45,45,45	0
55	MG	AA	3571	1/1	0.98	0.10	52,52,52,52	0
55	MG	BA	3209	1/1	0.98	0.16	46,46,46,46	0
55	MG	AA	3213	1/1	0.98	0.26	59,59,59,59	0
55	MG	AA	3018	1/1	0.98	0.20	43,43,43,43	0
55	MG	CA	1780	1/1	0.98	0.22	55,55,55,55	0
55	MG	DA	1744	1/1	0.98	0.27	57,57,57,57	0
55	MG	AA	3053	1/1	0.98	0.45	67,67,67,67	0
55	MG	AA	3178	1/1	0.99	0.06	54,54,54,54	0
55	MG	AA	3567	1/1	0.99	0.14	39,39,39,39	0
55	MG	AA	3110	1/1	0.99	0.03	40,40,40,40	0
57	ZN	DQ	101	1/1	0.99	0.05	118,118,118,118	0

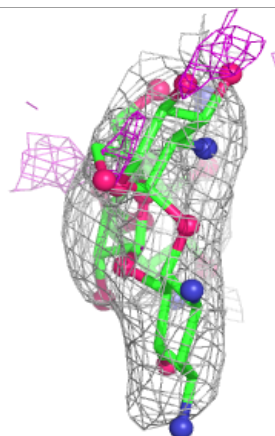
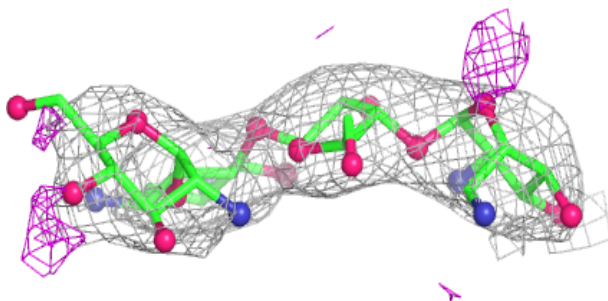
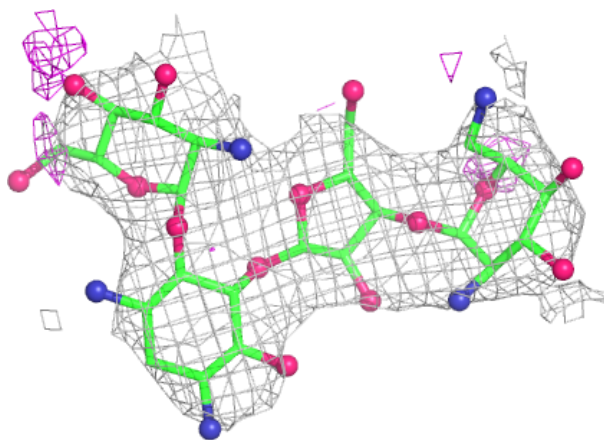
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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