



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 11:50 PM UTC

PDB ID : 4V8B / pdb_00004v8b
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-06
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

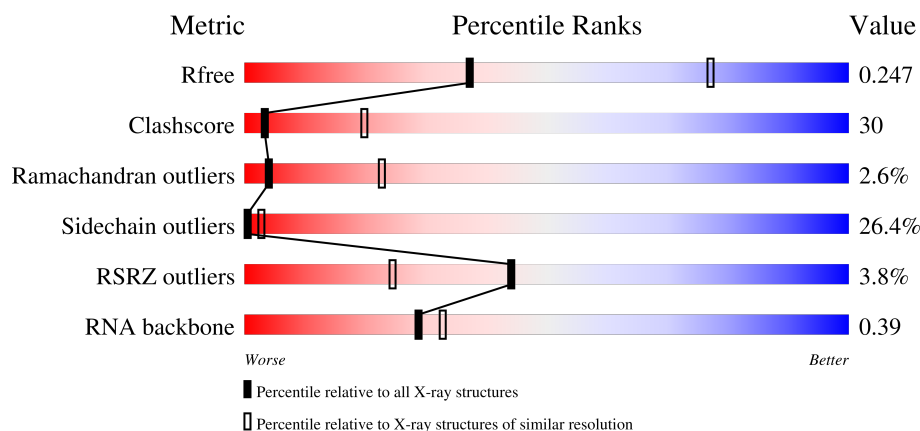
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1506	32% 48% 19%
1	CA	1506	30% 48% 22%
2	AE	256	3% 31% 44% 17% 7%
2	CE	256	32% 39% 21% 7%

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	87	
22	CB	87	
23	AC	77	
23	AD	77	
23	CC	77	
23	CD	77	
24	A1	10	
24	C1	10	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	

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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1643	-	-	-	X
55	MG	AA	1668	-	-	-	X
55	MG	AA	1761	-	-	-	X
55	MG	AA	1819	-	-	-	X
55	MG	AA	1831	-	-	-	X
55	MG	BA	3164	-	-	-	X
55	MG	BA	3317	-	-	-	X
55	MG	BA	3403	-	-	-	X
55	MG	CA	1601	-	-	-	X
55	MG	CA	1622	-	-	-	X
55	MG	CA	1638	-	-	-	X
55	MG	CA	1639	-	-	-	X
55	MG	CA	1684	-	-	-	X
55	MG	CA	1694	-	-	-	X
55	MG	CA	1707	-	-	-	X
55	MG	CA	1713	-	-	-	X
55	MG	DA	3025	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3056	-	-	-	X
55	MG	DA	3073	-	-	-	X
55	MG	DA	3089	-	-	-	X
55	MG	DA	3146	-	-	-	X
55	MG	DA	3302	-	-	-	X
55	MG	DA	3342	-	-	-	X
55	MG	DA	3363	-	-	-	X
55	MG	DA	3381	-	-	-	X
55	MG	DA	3458	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3481	-	-	-	X
55	MG	DA	3491	-	-	-	X
55	MG	DA	3501	-	-	-	X
55	MG	DA	3503	-	-	-	X
55	MG	DA	3507	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
22	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	AD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CD	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
AC	18	C	U	conflict	GB AP012306.1
AD	18	C	U	conflict	GB AP012306.1
CC	18	C	U	conflict	GB AP012306.1
CD	18	C	U	conflict	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
24	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 25 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2912	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
25	DA	2907	Total 62607	C 27866	N 11712	O 20123	P 2906	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	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
DA	168	U	-	insertion	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	A	C	conflict	GB AP008226.1

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	242	Total 242	Mg 242	0	0
55	AG	1	Total 1	Mg 1	0	0
55	AH	1	Total 1	Mg 1	0	0
55	AN	2	Total 2	Mg 2	0	0
55	AQ	1	Total 1	Mg 1	0	0
55	AB	5	Total 5	Mg 5	0	0
55	AC	9	Total 9	Mg 9	0	0
55	AD	1	Total 1	Mg 1	0	0
55	A1	2	Total 2	Mg 2	0	0
55	BA	623	Total 623	Mg 623	0	0
55	BB	17	Total 17	Mg 17	0	0
55	BD	1	Total 1	Mg 1	0	0
55	BE	5	Total 5	Mg 5	0	0
55	BF	3	Total 3	Mg 3	0	0
55	BO	2	Total 2	Mg 2	0	0
55	B0	1	Total 1	Mg 1	0	0
55	B1	1	Total 1	Mg 1	0	0
55	B2	1	Total 1	Mg 1	0	0
55	BU	2	Total 2	Mg 2	0	0
55	B3	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B7	1	Total 1	Mg 1	0	0
55	B8	1	Total 1	Mg 1	0	0
55	CA	207	Total 207	Mg 207	0	0
55	CG	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	CB	3	Total 3	Mg 3	0	0
55	CC	8	Total 8	Mg 8	0	0
55	DA	526	Total 526	Mg 526	0	0
55	DB	14	Total 14	Mg 14	0	0
55	DE	3	Total 3	Mg 3	0	0
55	DP	1	Total 1	Mg 1	0	0
55	DR	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	DU	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0

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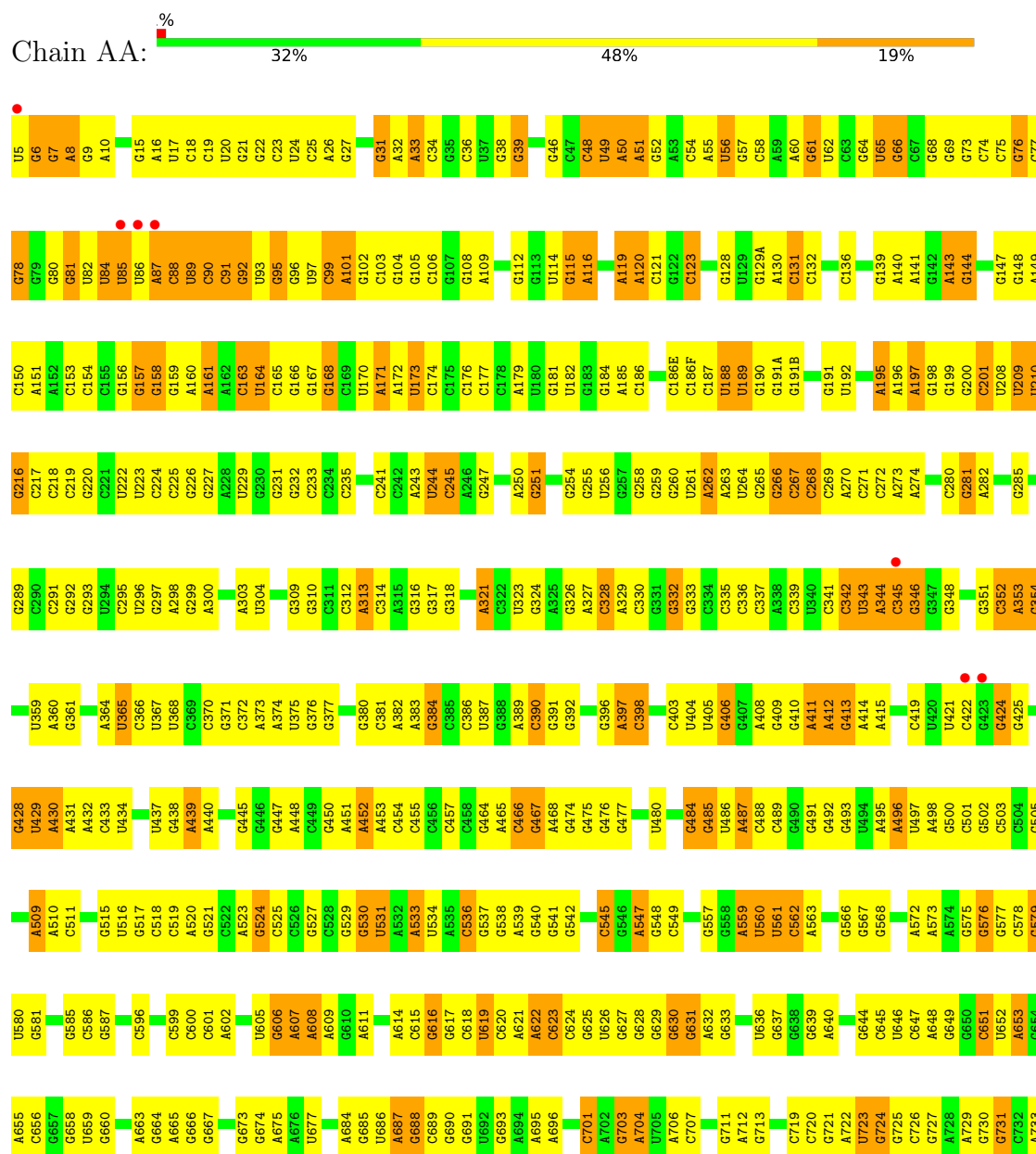
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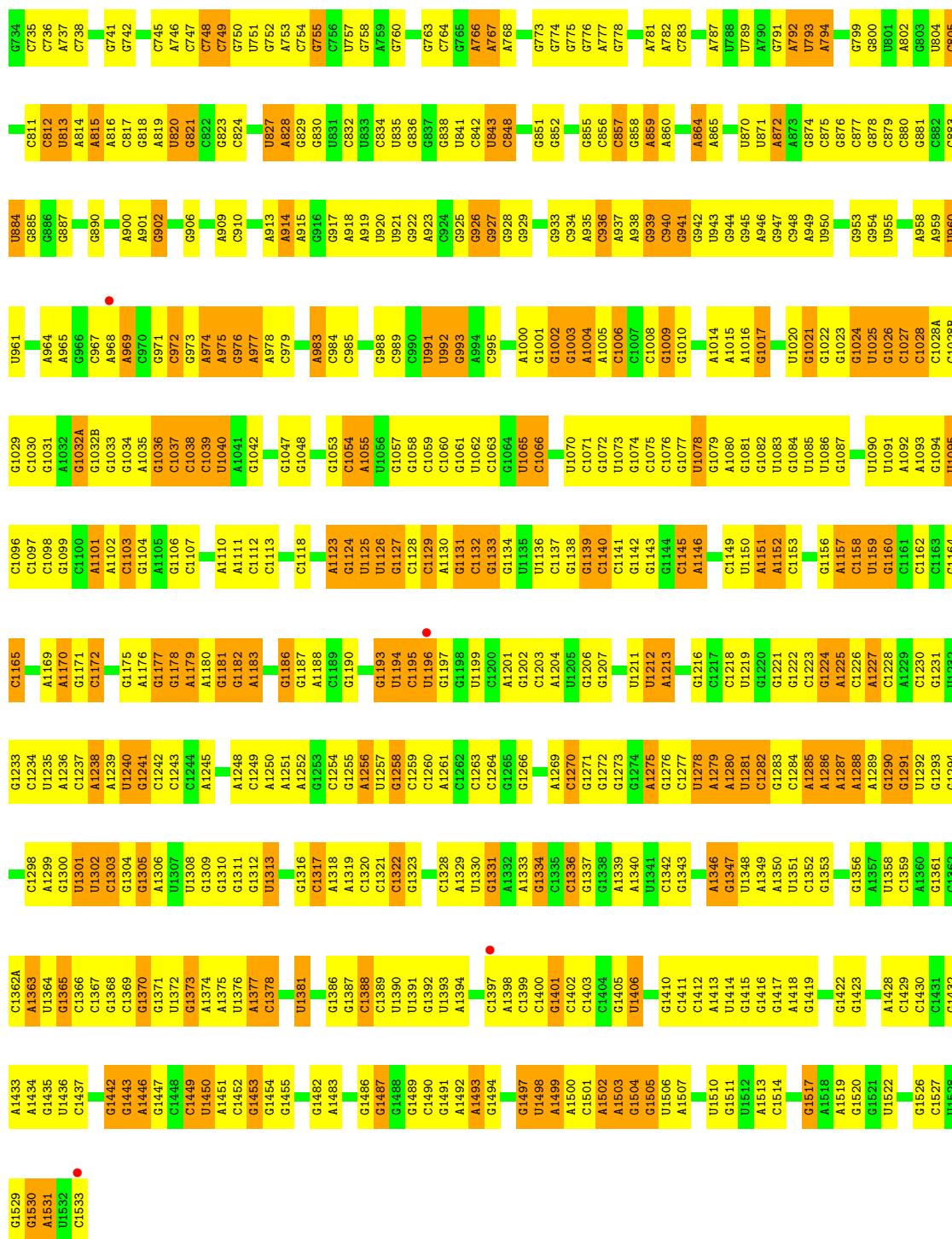
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

3 Residue-property plots

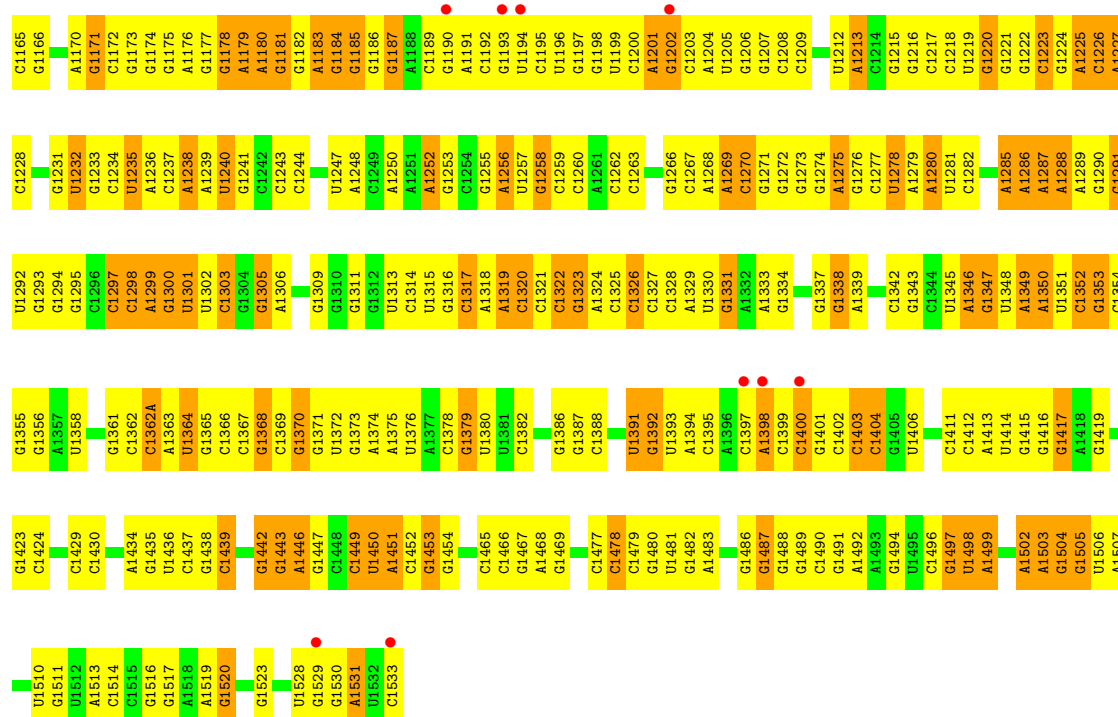
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S ribosomal RNA

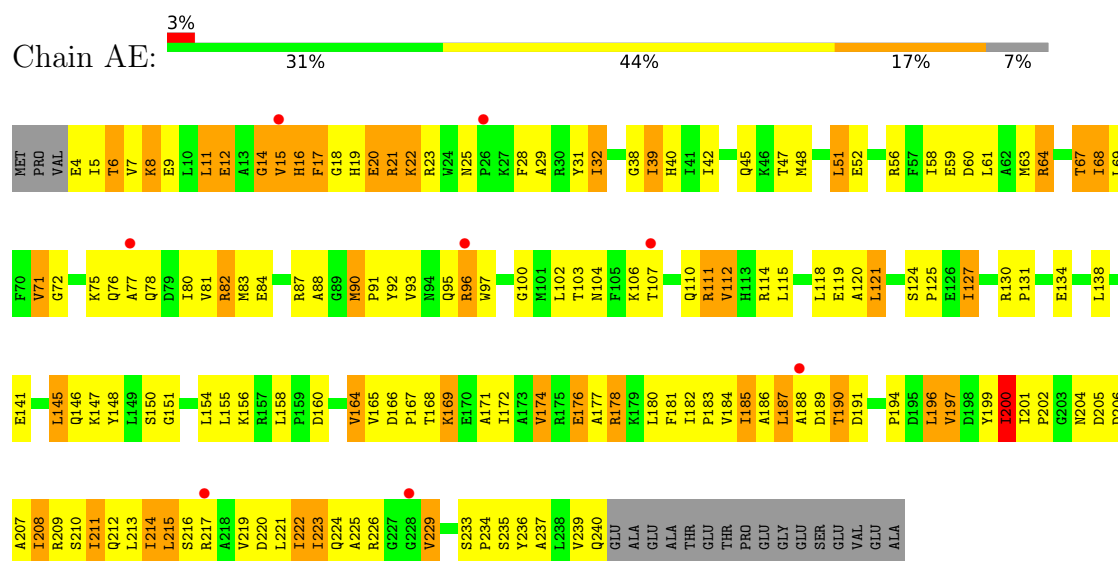




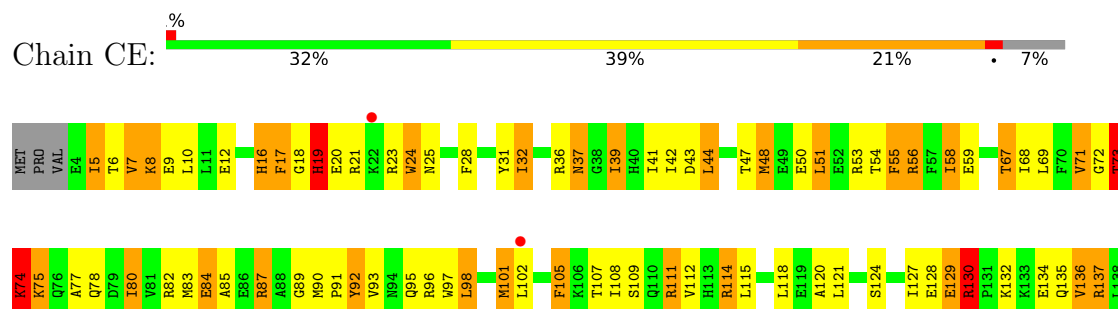
G1104	G1038	U982	U921	U833	U757	G632	G541	G467	C390	C314	C240	G166	G81
A1105	C1039	A983	G922	C834	G758	G683	G542	A468	G391	A315	C241	G167	U82
G1106	U1040	C984	A923	U835	G763	G685	C543	G474	G392	G316	C242	G168	U84
C1107	A1041	C985	G923	G836	G764	U886	G544	C475	A393	G317	C243	C169	U85
G1108	G1042	A986	G926	G837	G765	U887	C545	G476	G394	A321	U243	A170	U86
C1109	C1043	G987	G927	G838	G766	G688	G546	G477	C395	G326	U244	A171	A87
A1110	A1044	C988	G928	U841	A766	G689	A547	A478	G396	A327	C245	A172	C88
C1045	C1045	C989	G929	C842	A767	C689	G548	G479	A397	G328	A246	U173	U89
A1046	A1046	C990	G930	U843	G769	G690	C549	G481	C398	C328	G247	C174	C91
G1047	G1047	U991	C931	C848	G773	G691	G550	A482	U404	A329	G248	G177	G92
G1048	G1048	U992	C932	C849	G774	G692	U551	C483	U405	G332	A250	C178	G93
U1052	G1053	G993	C933	U850	G775	G693	U552	G484	G406	G333	U251	A179	G95
C1054	C1054	A994	G934	C851	G776	A694	A553	G485	U253	G334	U252	U180	
A1055	A1055	C995	A935	G852	G777	A695	C554	U486	G407	C339	G254	G181	A101
U1056	U1056	U996	C936	G853	A777	A696	C555	A487	U340	U340	G255	G182	G102
G1057	G1057	A997	A937	G854	G778	G697	C556	C489	G410	G342	U256	G183	G105
C1058	C1058	C998A	G939	G858	G779	A702	A559	A495	A411	U343	G257	G184	G106
A1059	A1059	U999	C940	A859	A780	G703	U560	A496	G412	U344	G258	A185	
U1125	G1060	G861	G941	A860	G783	U704	U561	U497	A413	A345	G259	C186	
C1061	C1061	U862	U943	C862	G784	U705	C562	A498	G414	G346	U261	C186F	A109
G1062	G1062	U863	G944	U863	G785	G706	A563	G500	U420	G347	A262	C187	G113
C1063	C1063	A864	G945	A864	G786	G707	C564	G501	U421	G348	G265	U187	U114
A1004	A1004	G865	G946	G865	G787	G710	U565	C502	U422	A349	G266	U188	G115
G945	G945	G866	G947	G866	A788	G711	G566	G503	G423	G350	G267	U189	A116
A946	A946	G867	G948	G867	G789	A712	G567	C504	G424	G351	G268	G190	
C1006	C1006	U870	C948	U870	G791	G713	G568	C505	G425	G352	G269	G191A	C121
U1007	U1007	G871	U955	G871	A792	G714	C569	G506	G426	G353	G270	G191B	G122
C1008	C1008	U872	U956	U872	U793	G715	G570	G507	U427	G354	A270	G191C	C123
G1068	G1068	A872	U957	A873	U794	G716	U571	G508	G428	C355	C271	U191D	
U1069	U1069	G873	U958	G873	G795	G720	A572	A509	U429	G356	G272	G126	
G1010	G1010	A874	U959	A874	G796	G721	A573	A510	U430	A356	C273	G191	
U1070	U1070	G875	G953	G875	G797	A722	A574	C511	A430	G357	A273	U192	A130
G1071	G1071	C876	G954	C876	G798	G723	G575	U512	A431	U358	A274	C131	C131
C1072	C1072	U877	U955	U877	G799	G724	G576	C513	A432	U359	G275	C194	C132
U1073	U1073	C878	U956	C878	G800	G725	C514	G514	C433	A360	C276	C194	C132
G1074	G1074	G879	U957	G879	U801	A726	G577	G515	U434	G361	A279	U195	U133
C1075	C1075	U884	U958	U884	A802	A727	G578	U516	U435	G362	C280	A196	A134
U1076	U1076	G885	A958	G885	G803	A728	G579	G517	C436	A363	G281	A197	
G1077	G1077	G886	A959	G886	U804	A729	U580	C518	U437	A364	A282	G198	A141
A1080	A1080	C887	U961	C887	G805	G731	G581	C519	G438	U365	C283	G142	G142
G1081	G1081	U888	C962	U888	C806	G732	U582	A520	A439	C366	C284	C201	A143
C1082	C1082	A889	G963	A889	G807	G733	A583	G521	A440	U367	U287	U208	G144
U1083	U1083	G890	A964	G890	C808	G734	G584	C522	A441	U368	A288	U209	G145
G1084	G1084	A891	A965	A891	C809	G735	G585	G523	C444	C369	G289	U210	G146
U1085	U1085	C892	G966	C892	C810	A736	G586	C524	G445	G372	G216	G217	G147
C1086	C1086	G893	C967	G893	C811	G740	G587	C525	G446	A372	G218	C219	G148
U1088	U1088	A900	C968	A900	G812	G741	G588	G526	G447	A373	G219	C220	C150
G1089	G1089	U901	A969	U901	G813	G742	G589	G527	G448	A374	G221	A151	A151
U1090	U1090	A902	C970	A902	A814	G743	C589	G528	C449	U375	G222	G221	A152
C1091	C1091	G903	G971	G903	A815	A744	G593	G530	G450	G376	A298	G156	G156
U1092	U1092	C904	C972	C904	C817	G745	G594	U531	A451	G380	G299	G226	G157
A1093	A1093	A913	G973	A913	G818	C746	C600	A532	A452	A381	A300	G227	A160
G1094	G1094	U914	A974	U914	G819	C747	C601	A533	A453	G382	G301	A228	A161
U1095	U1095	G915	A975	G915	U820	G748	G604	A534	A454	A383	G302	G230	A162
C1096	C1096	A916	G976	A916	G750	G749	G605	C535	C457	A384	G303	G231	U164
G1097	G1097	G917	A977	G917	G751	U751	G606	C536	C458	G384	G304	G232	C163
U1101	U1101	A918	C979	A918	A753	G752	G607	C537	G464	G388	G309	G233	U164
C1103	C1103	G919	C980	G919	G754	G753	A607	A538	A465	G389	G313	C235	C165
G1104	G1104	U921	U981	U921	C756	G756	A609	G540	C466	A389			

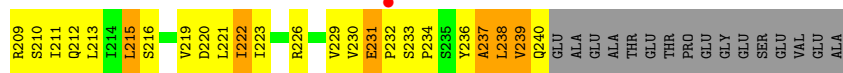


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

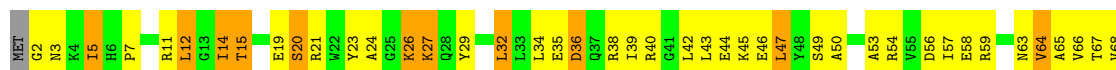


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

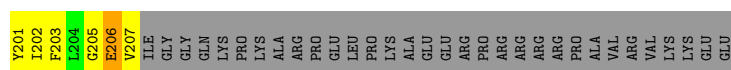
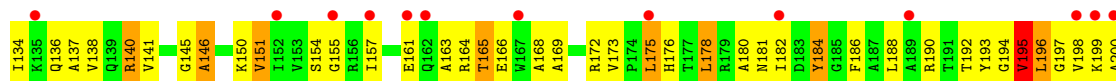
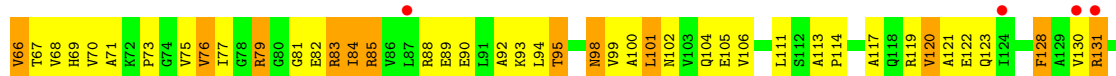
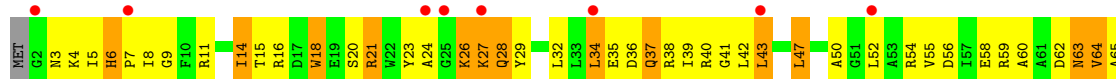




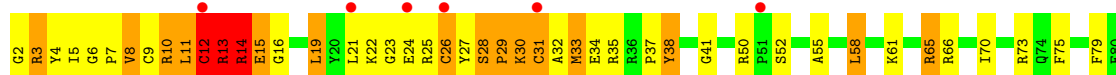
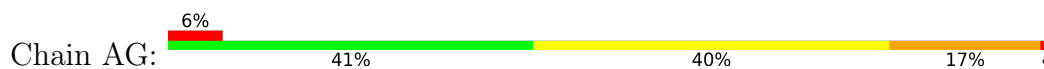
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

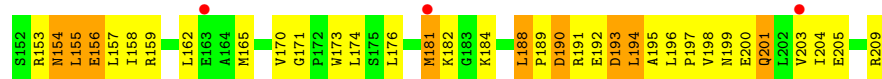


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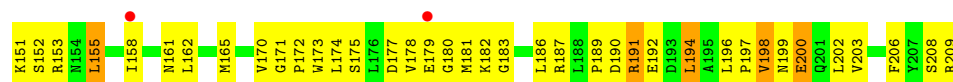
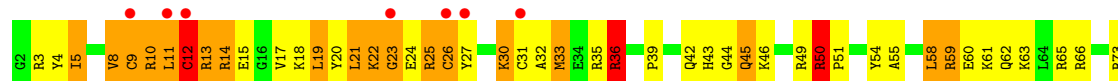


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

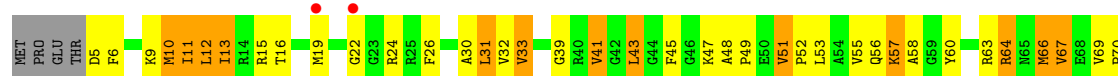




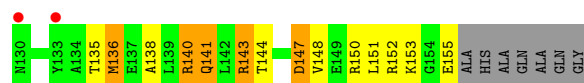
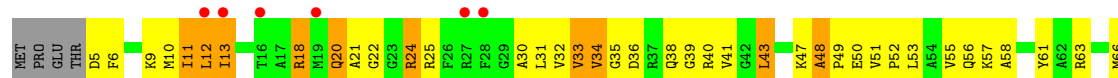
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

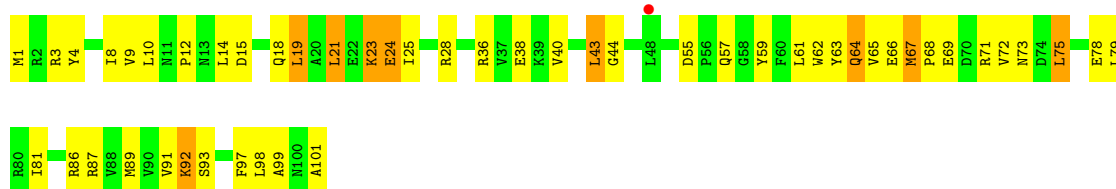


• Molecule 5: 30S RIBOSOMAL PROTEIN S5



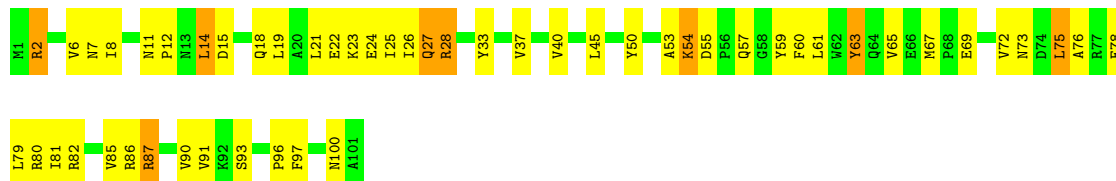
• Molecule 6: 30S RIBOSOMAL PROTEIN S6





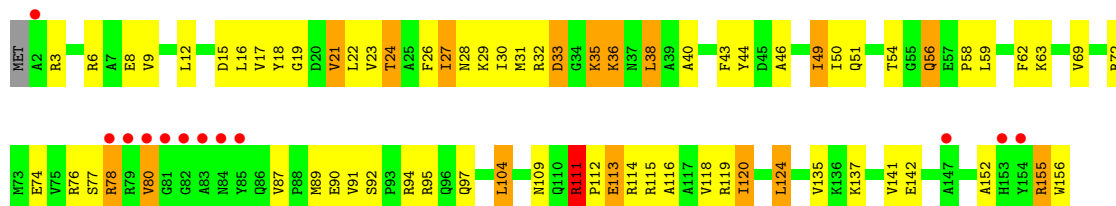
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI: 49% 44% 8%



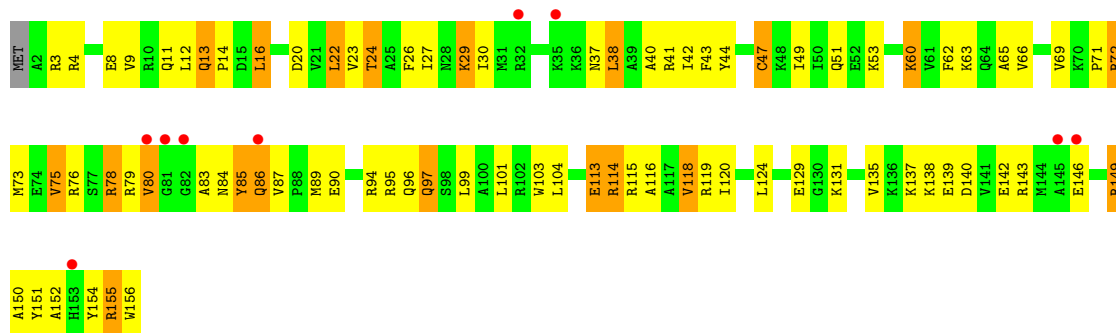
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ: 8% 53% 35% 10% ..



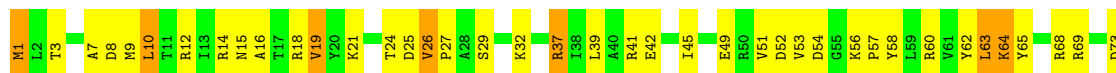
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ: 6% 47% 40% 13% .



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK: 43% 45% 12%





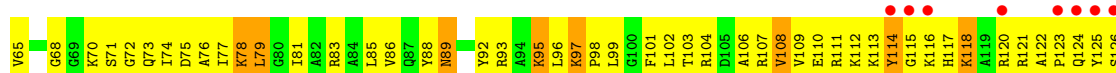
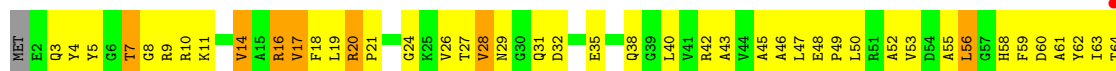
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



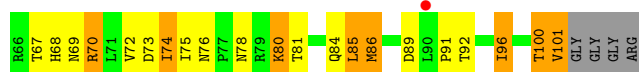
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



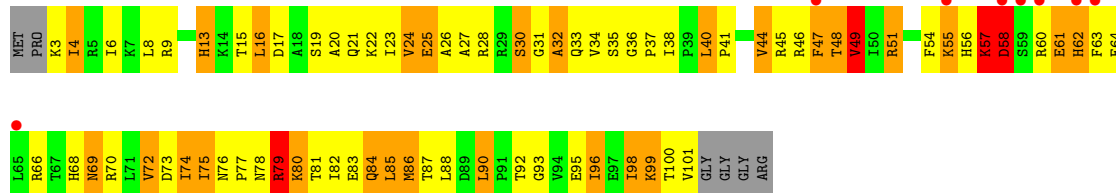
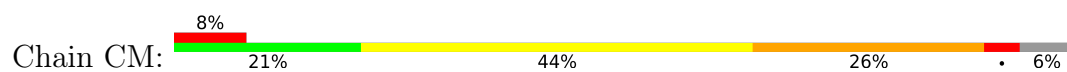
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



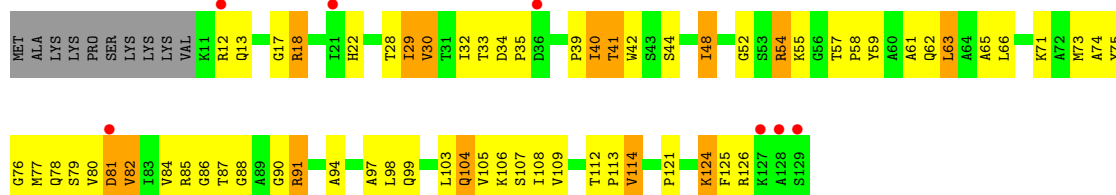
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



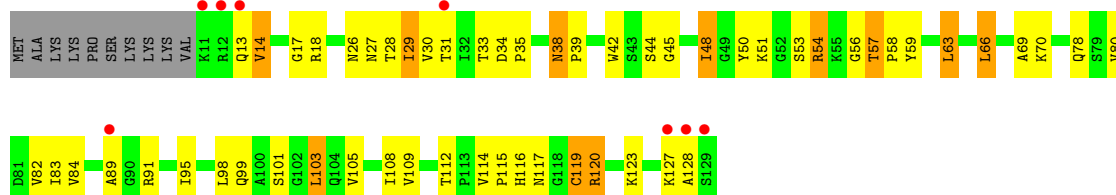
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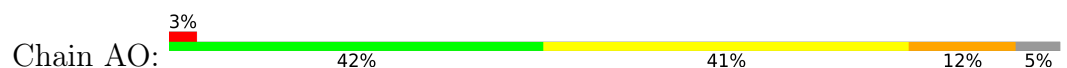
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

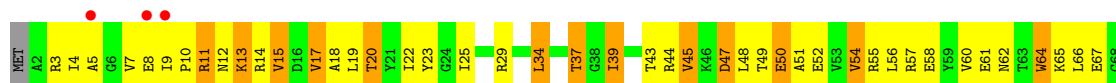


• Molecule 12: 30S RIBOSOMAL PROTEIN S12





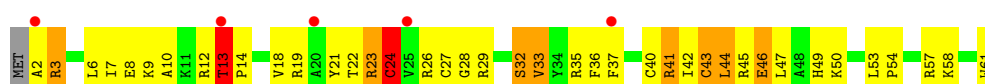
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



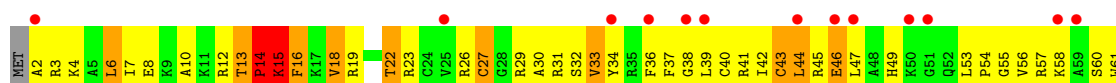
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14



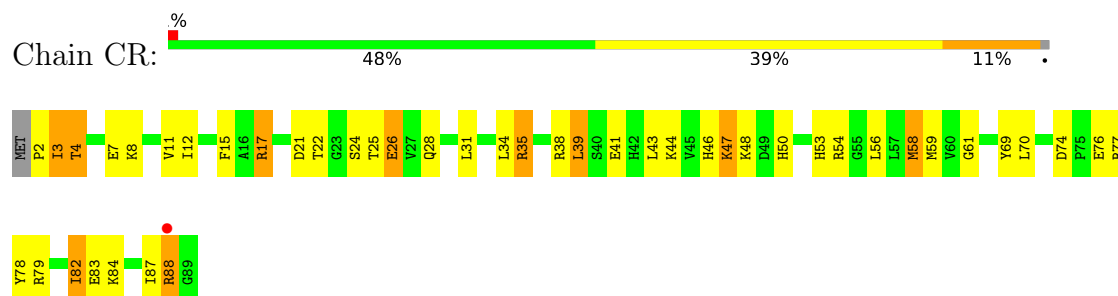
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



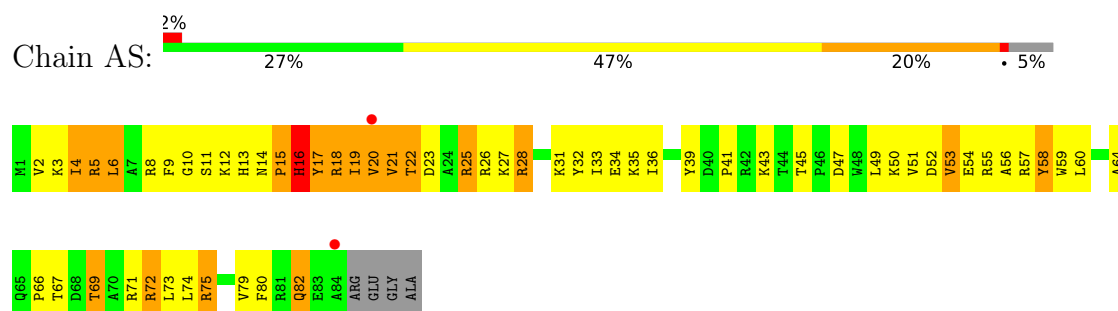
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



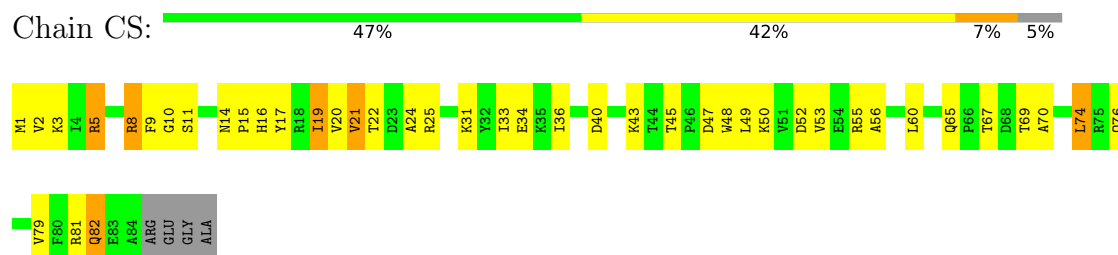
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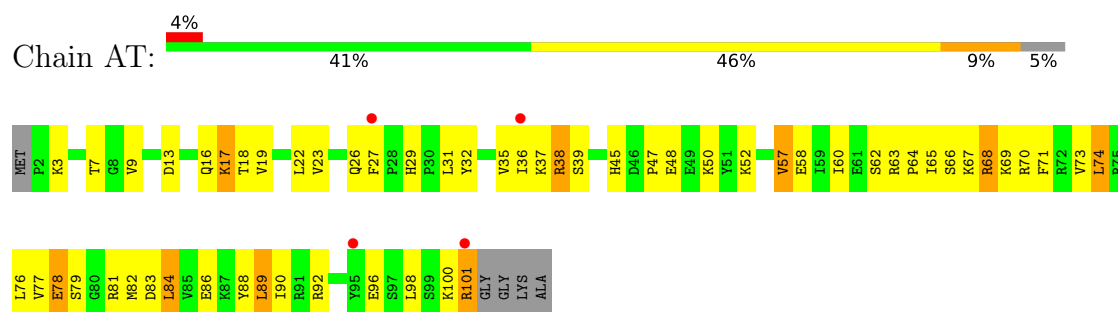
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



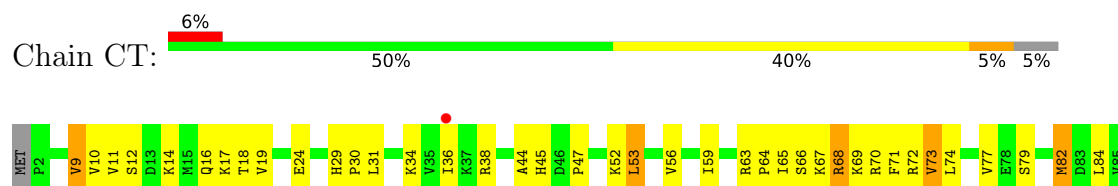
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

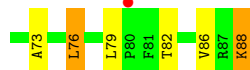
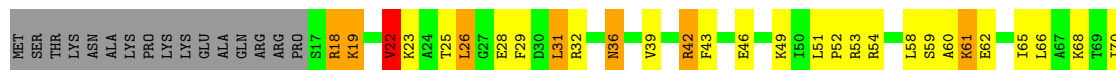


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

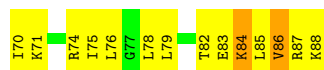
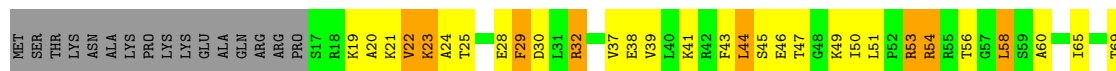




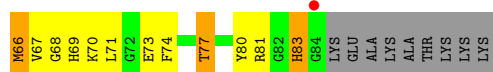
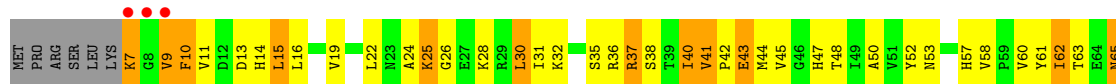
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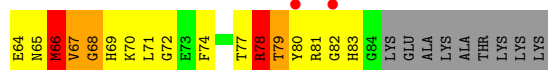
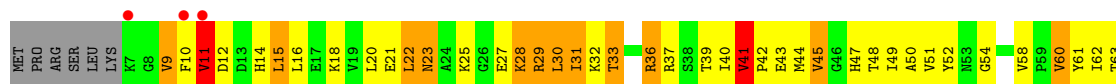
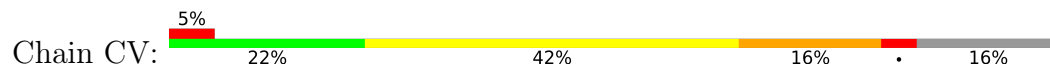
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

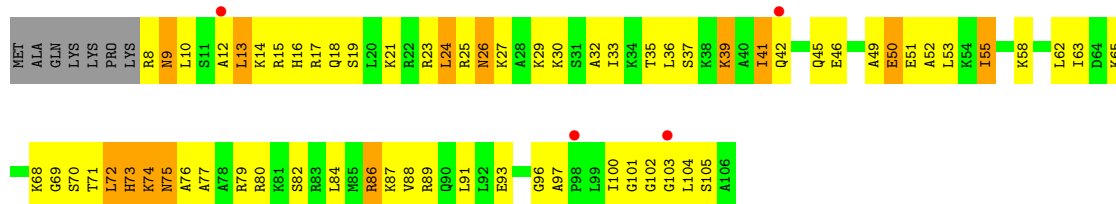


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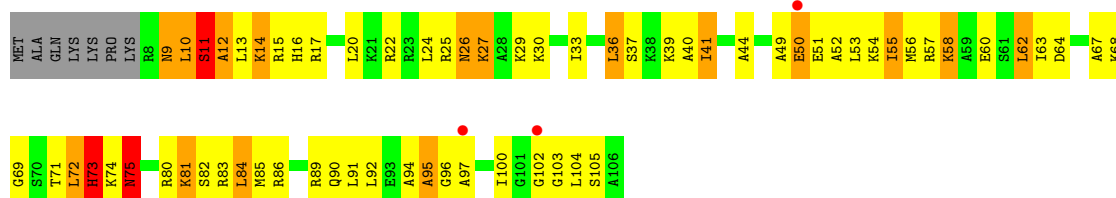


• Molecule 20: 30S RIBOSOMAL PROTEIN S20





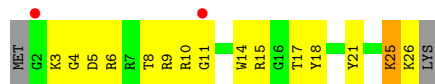
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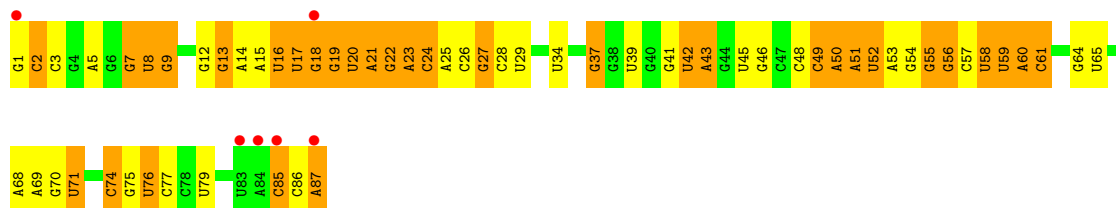
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



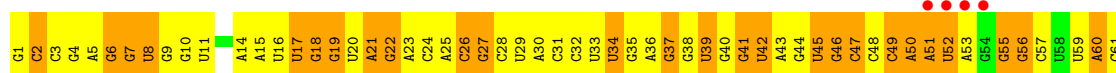
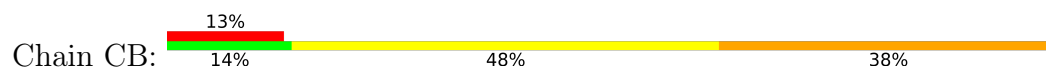
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: TRNA-LEU



• Molecule 22: TRNA-LEU

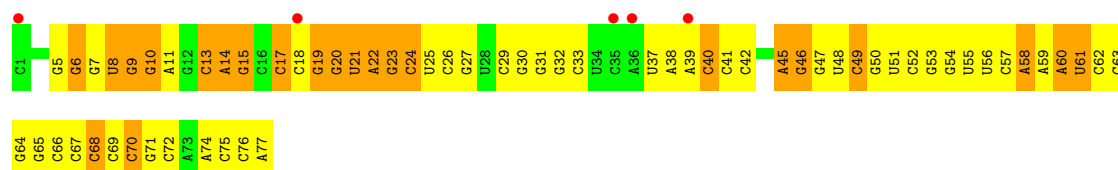
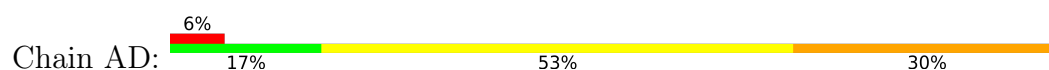




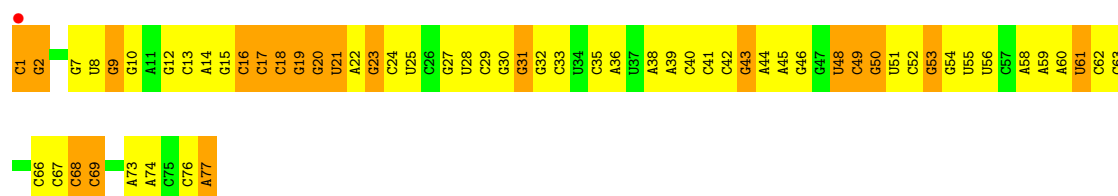
• Molecule 23: TRNA-FMET



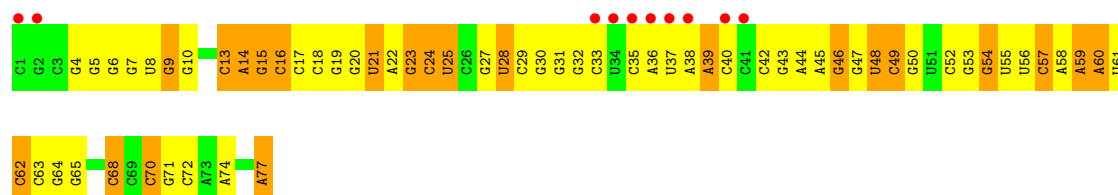
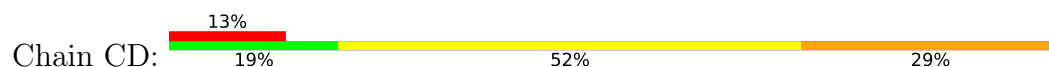
• Molecule 23: TRNA-FMET



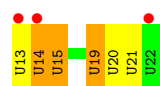
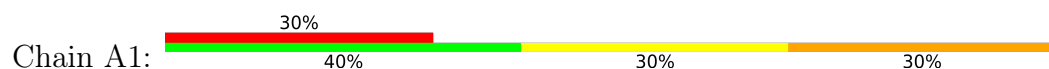
• Molecule 23: TRNA-FMET



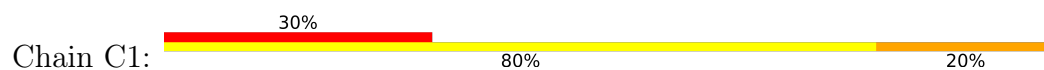
• Molecule 23: TRNA-FMET



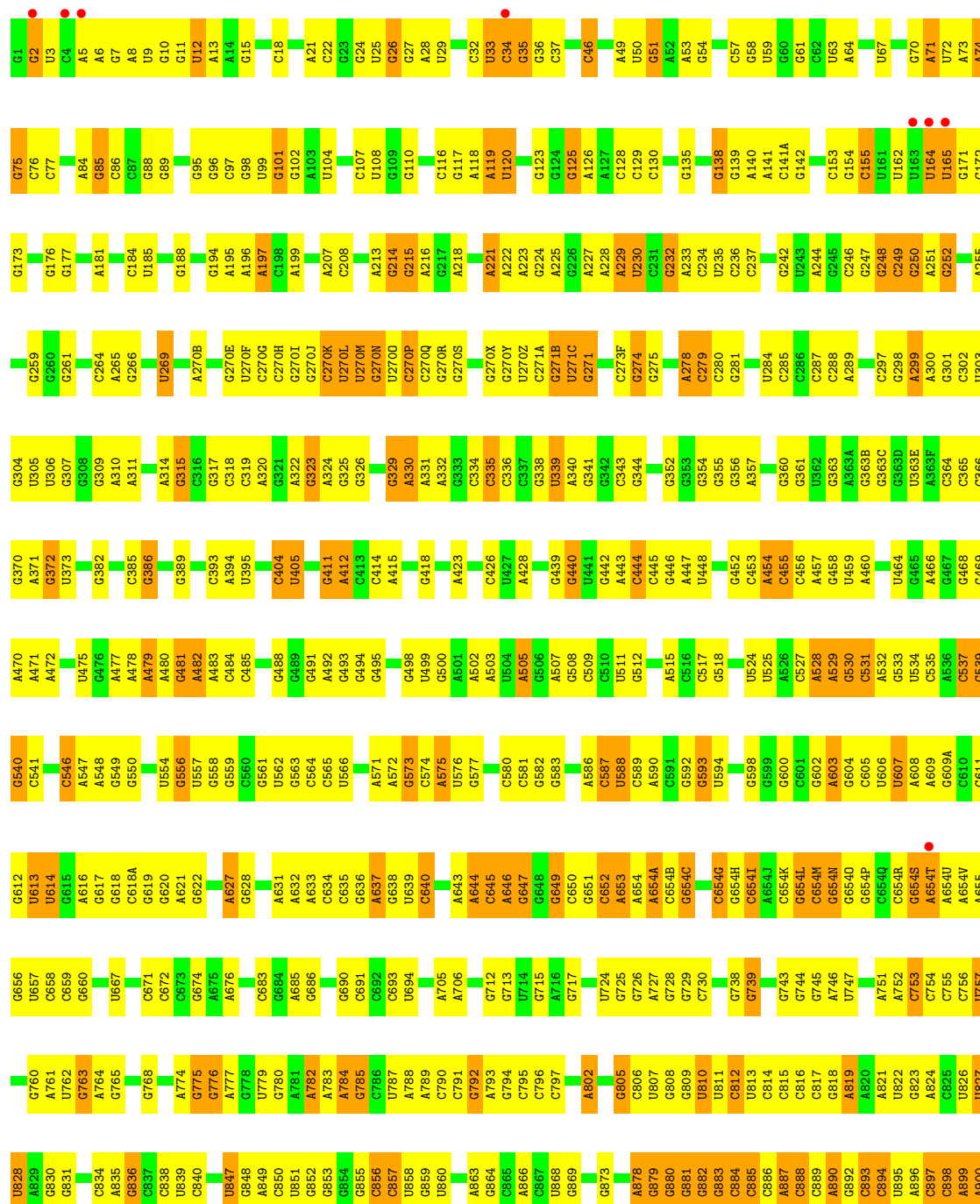
• Molecule 24: MRNA



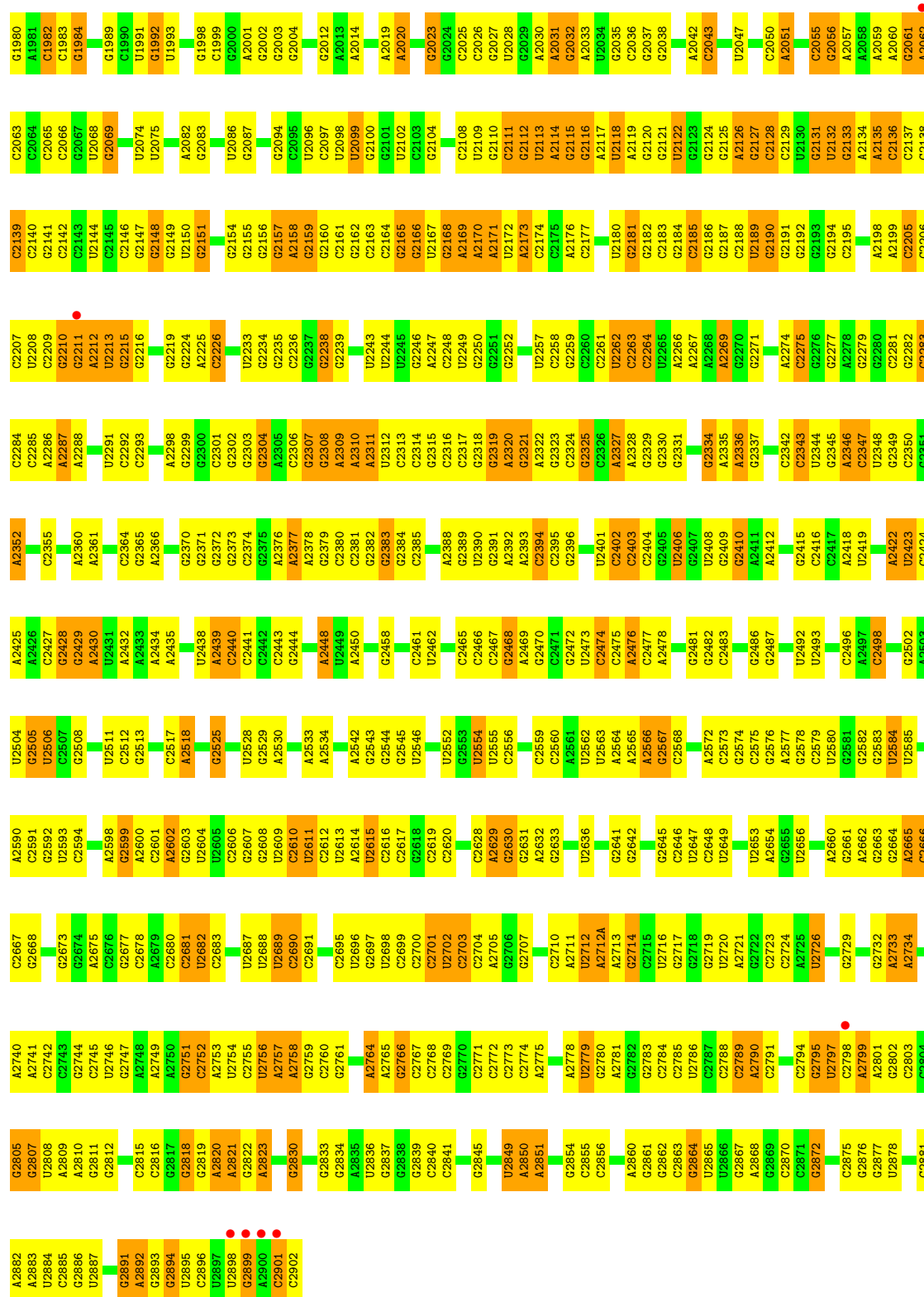
- Molecule 24: MRNA



- Molecule 25: RNA (2912-MER)

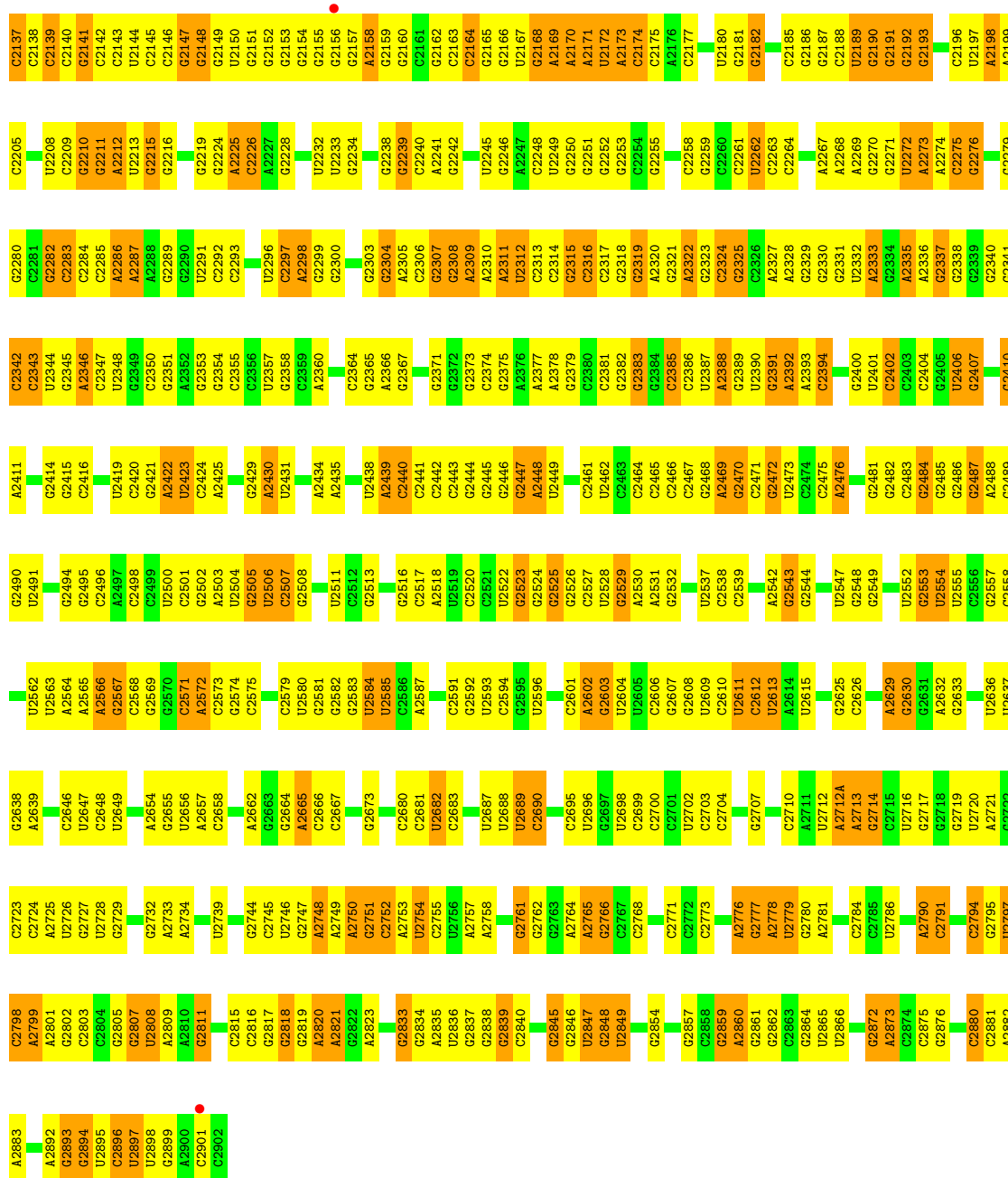


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C1800	G1799	G1718	U1639	A1486	G1417	G1340	U1263	C1180	G1112	A1050	C982	C903
G1801	C1800	G1725	C1640	G1556	C1417	U1341	G1264	C1181	U1113	C1053	C983	C904
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	G1733	G1733	A1652	C1565	U1430	U1352	U1271	A1189	C1123	G1059	A990	A911
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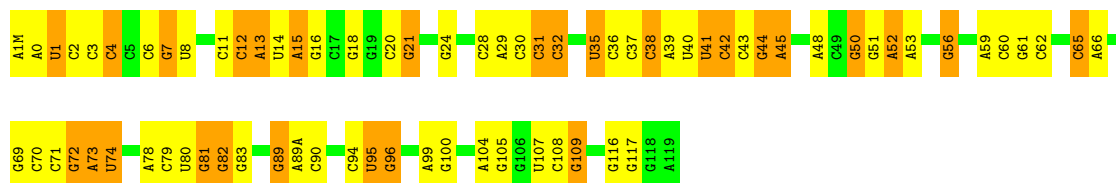
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G1003	C935	C866	G732	G732	A654V	G609A	C546	A470	G372	U305		G176	A91	C20
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C1005	G937	C867	A804	A734	G656	C611	A548	A472	U373	G307	G260	G178	C93	C22
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A1010	U943	A872	G809	G743	G668	A616	U554	A479	U384	G312		C183	U99	C34
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G1024	G959	A887	G825	U757	G681	A633	A571	A497	A401	G329	G270T	U206	C46	C46
G1025	A960	C888	U826	A761	G682	C634	A572	C498	G406	A330	C270U	C115	A49	A49
U1026	G961	C889	C827	U762	G683	C635	G573	U499	U405	A331	G270Y	A213	G51	G51
A1027	C962	G892	U828	G763	G684	G636	C574	G500	C409	A332	U270Z	G214	A52	A52
G1028	U963	C893	A829	G765	G685	A637	A575	A501	C410	G333	C271A	G215	A53	A53
A1029	C964	G894	G830	G766	G686	C640	U576	A502	C414	C334	G271B	A216	G54	G54
U1033	C971	U895	G831	C767	G690		G577	A503	G411	G337	G271C	G217	G55	A55
G1034	G972	A896	U832	U767	G696	A644	A578	U504	C412	G338	G271D	A218	A56	A56
U1035	C973	C897	C833	G768	C697	C645	G579	A505	A413	U339	G271E	A221	C57	C57
G1036	A973	C898	G834	G769	C698	A646	C580	G506	C413	G342	G271F	A222	G58	G58
G1037	G974	A899	A835	G770	A699	G647	C581	A507	A415	G343	G271G	A223	U59	U59
C1038	C974A	A900	G836	G771	C699		G582	A508	G419	G344	G271H	A224	G60	G60
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C1040	C976	C902	C838	U773	G702	G649	U584	C510	C415	G346	C273D	G226	G137A	
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G1042	G978	C904	C840	G775	G704	G651	U585	C511	U421	G348	C273F	A227	G139	G139
C1043	G979	U905	A841	G776	A705	C652	A586	G512	A428	G349	G274	A228	A140	A140
G1044	A980	G906	G842	A777	A706	A653	C587	A513		U360	G275	A229	A141	A141
A1045	G981	U907	G843	G778	A707	A654	U588	A514		G351	A276	A230	G142	G142
A1046	C982	C908	C844	U779	C708	A654A	C599				C277			G68

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C2063		G1906	U1818	C1741	G1559	G1485	G1417	A1337	C1257	A1182	A1111	A1048
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G2133	A1970	A1902		G1723	G1638							
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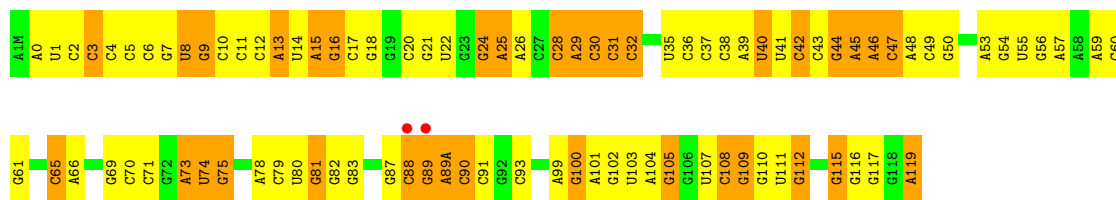


• Molecule 26: 5S RIBOSOMAL RNA

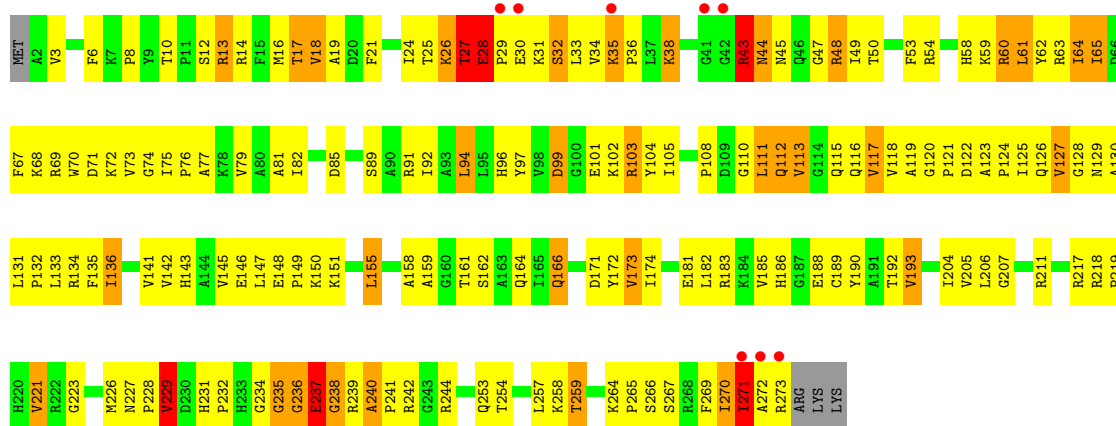
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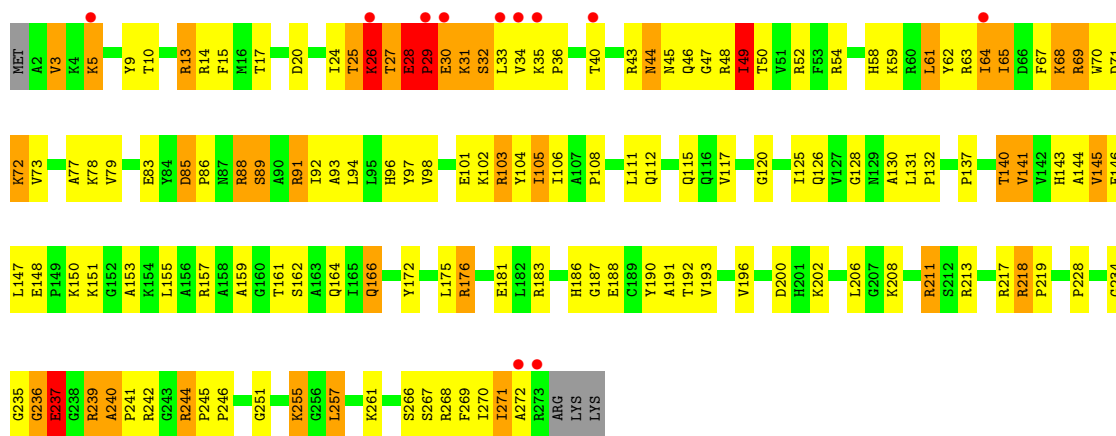
• Molecule 26: 5S RIBOSOMAL RNA



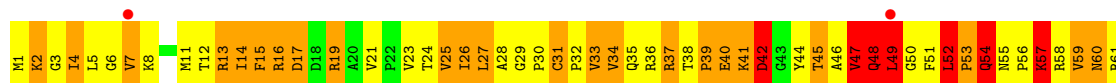
• Molecule 27: 50S ribosomal protein L2

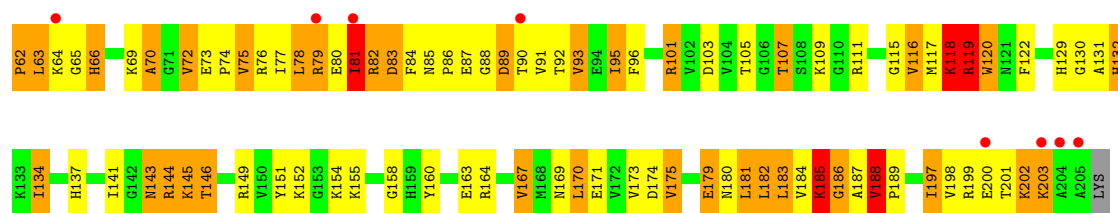


• Molecule 27: 50S ribosomal protein L2

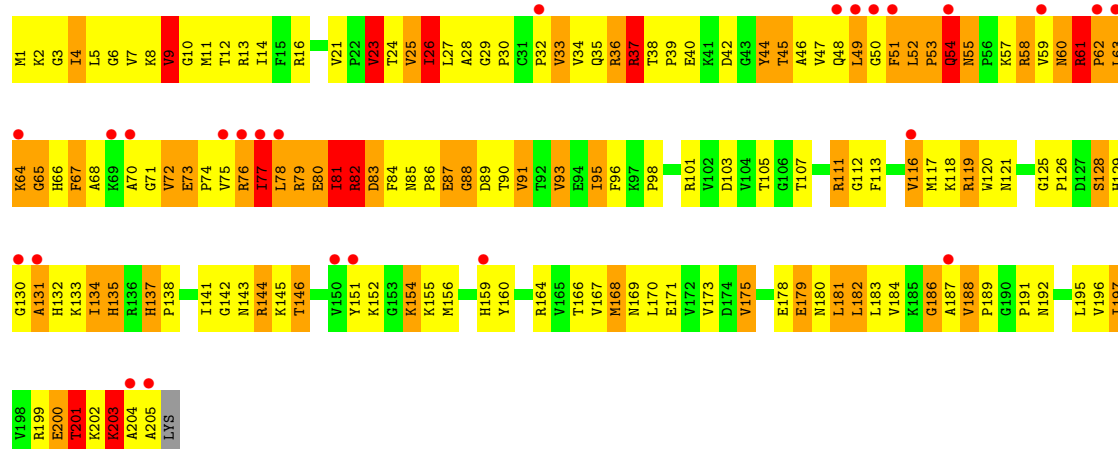


• Molecule 28: 50S ribosomal protein L3

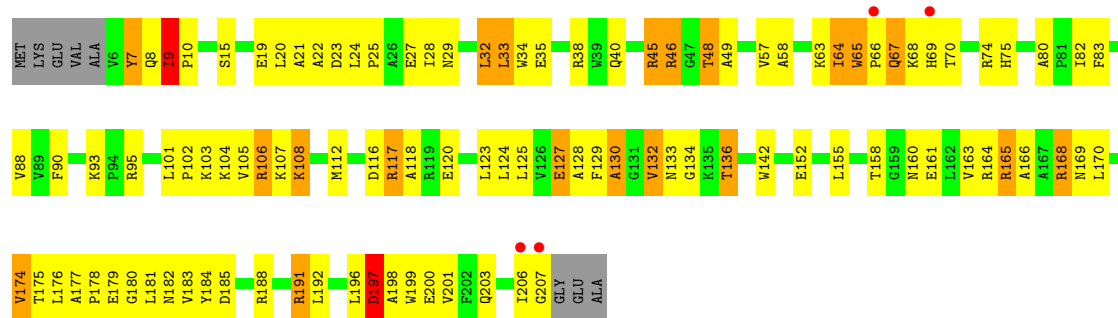




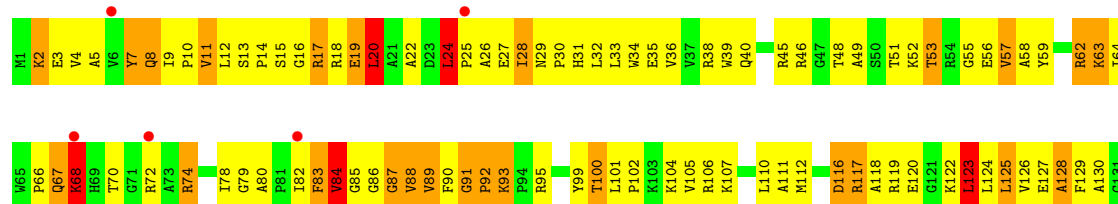
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

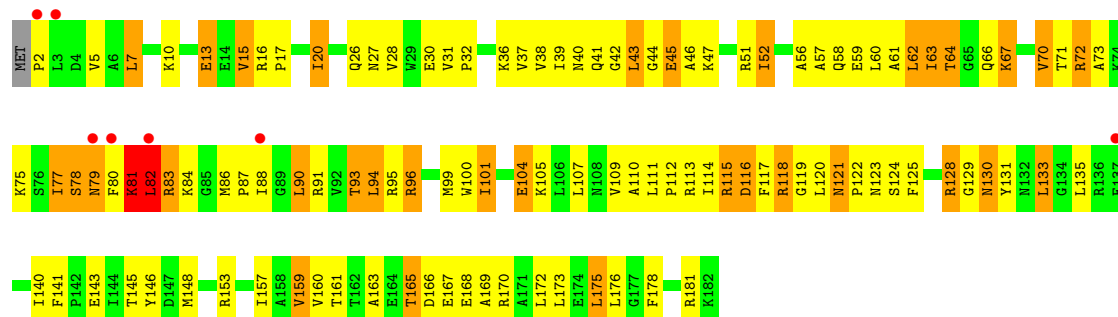


• Molecule 29: 50S ribosomal protein L4

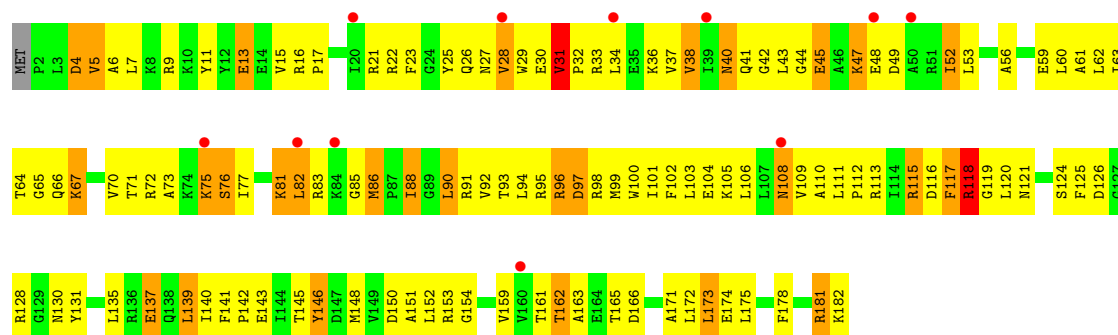




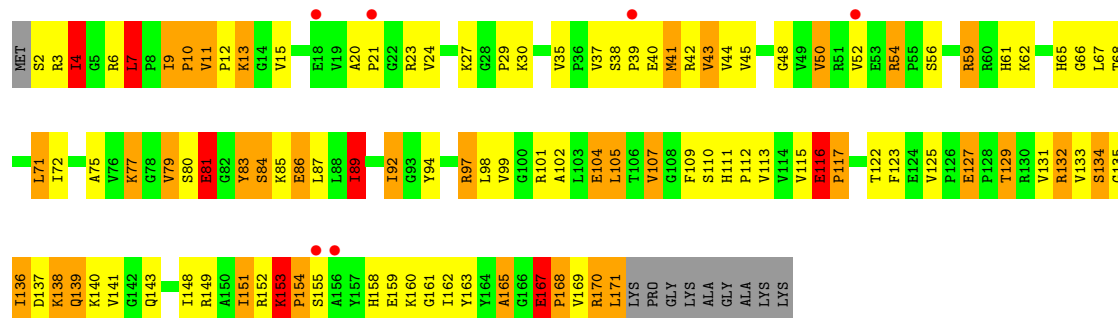
• Molecule 30: 50S ribosomal protein L5



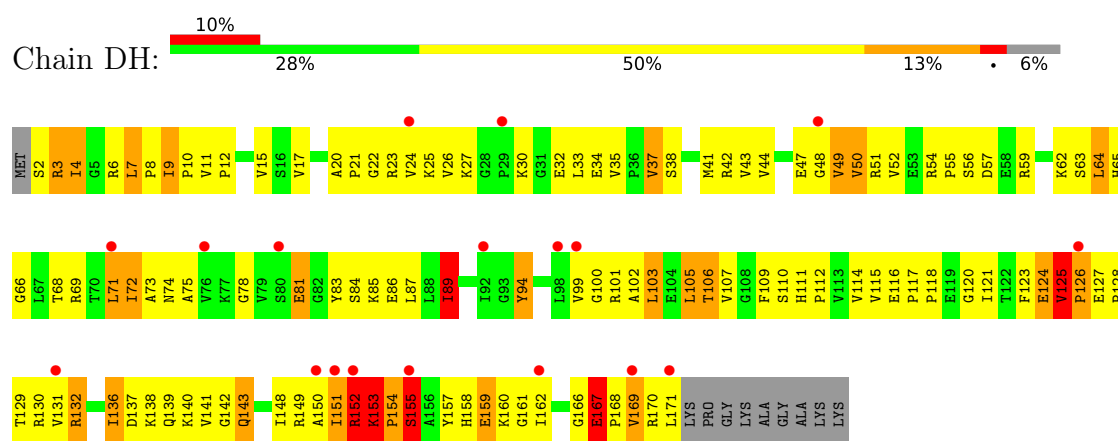
• Molecule 30: 50S ribosomal protein L5



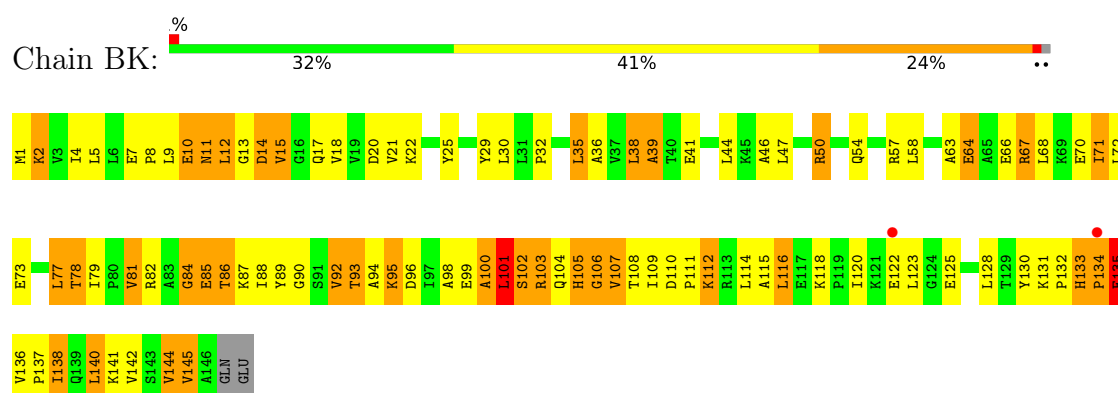
• Molecule 31: 50S ribosomal protein L6



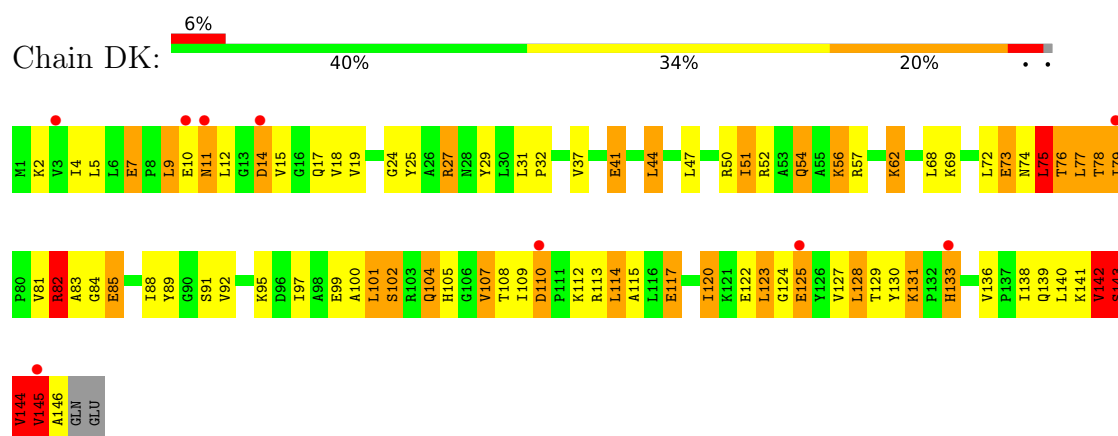
• Molecule 31: 50S ribosomal protein L6



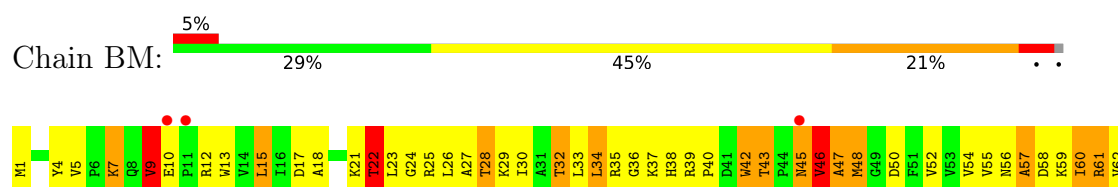
• Molecule 32: 50S ribosomal protein L9

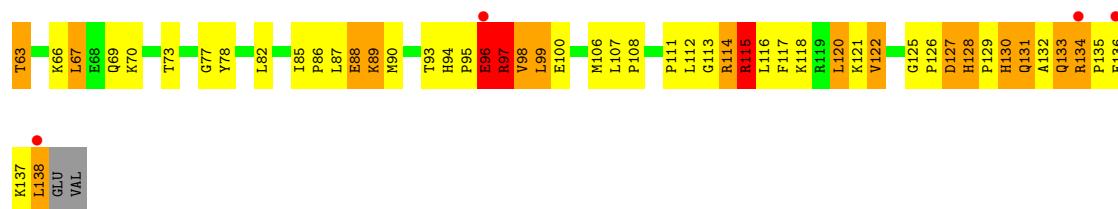


• Molecule 32: 50S ribosomal protein L9

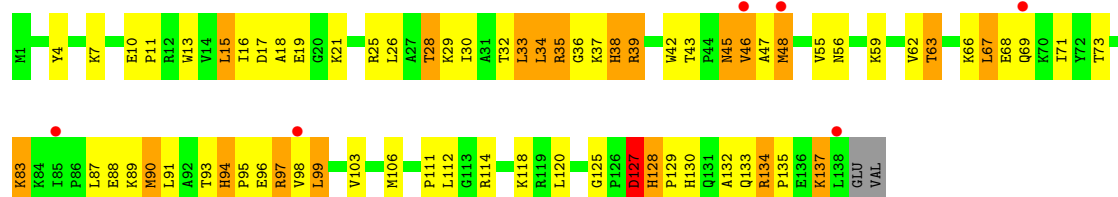


• Molecule 33: 50S ribosomal protein L13

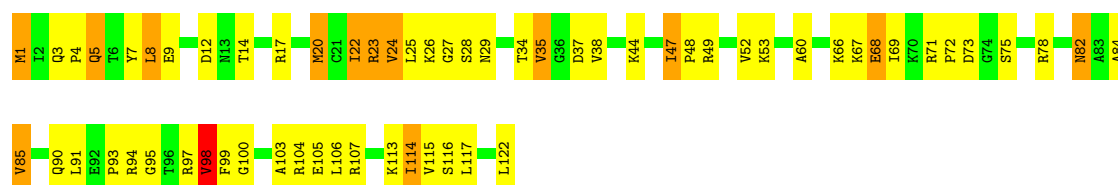




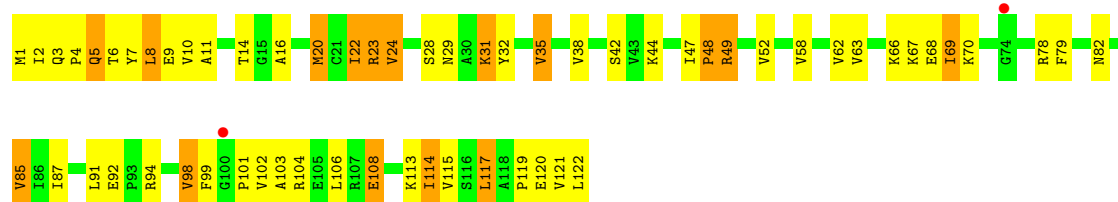
- Molecule 33: 50S ribosomal protein L13



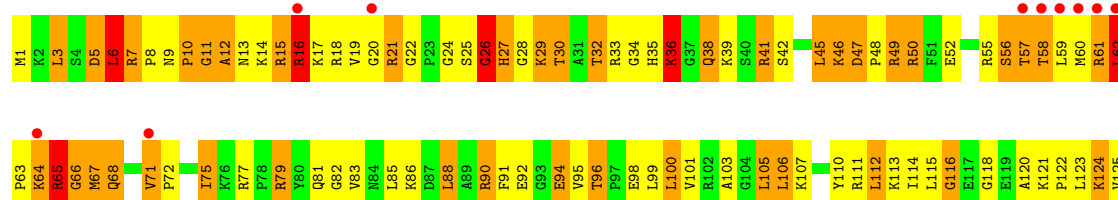
- Molecule 34: 50S ribosomal protein L14



- Molecule 34: 50S ribosomal protein L14

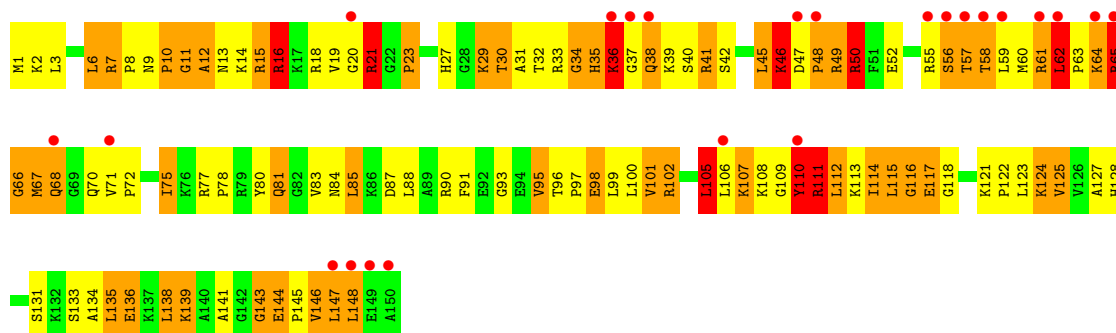
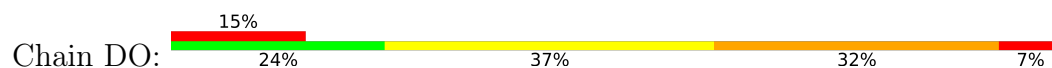


- Molecule 35: 50S ribosomal protein L15

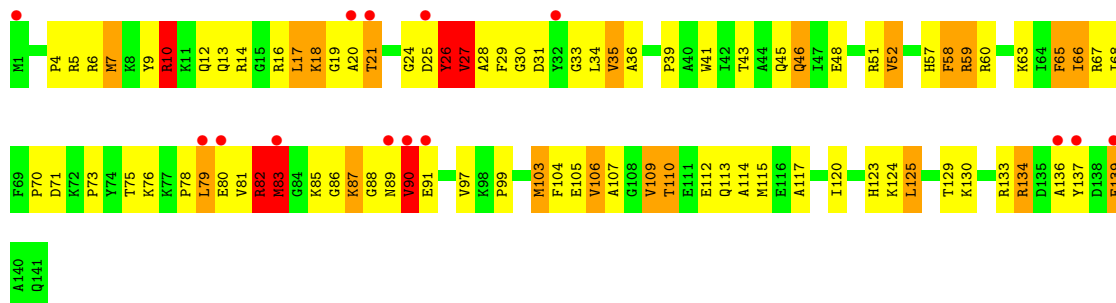




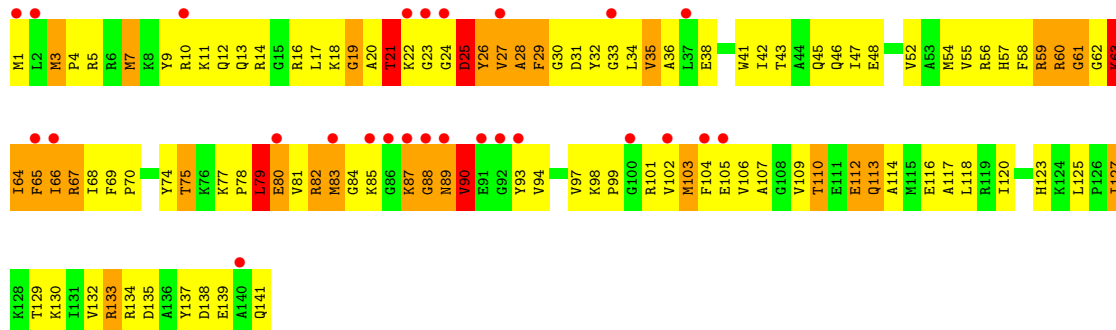
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

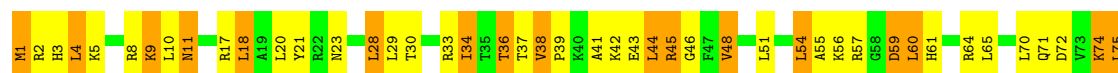


• Molecule 36: 50S ribosomal protein L16

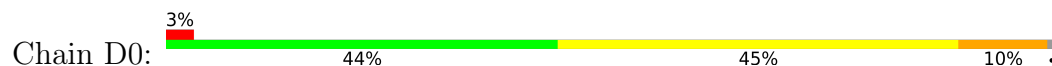


• Molecule 37: 50S ribosomal protein L17

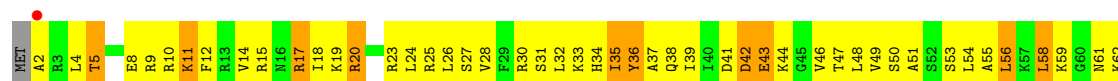




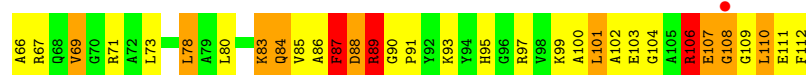
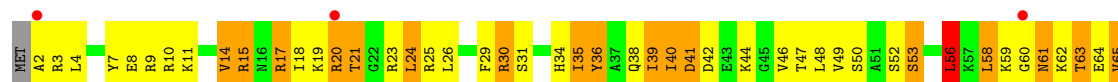
• Molecule 37: 50S ribosomal protein L17



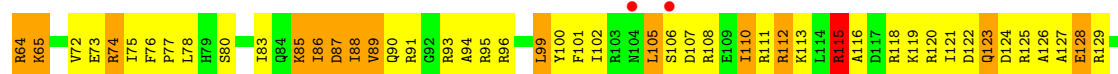
• Molecule 38: 50S ribosomal protein L18

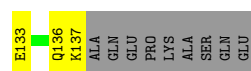


• Molecule 38: 50S ribosomal protein L18

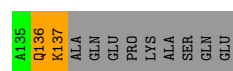
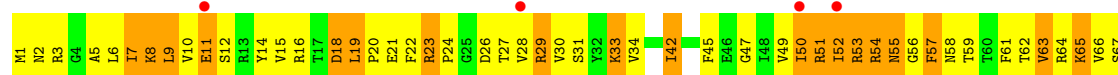


• Molecule 39: 50S ribosomal protein L19

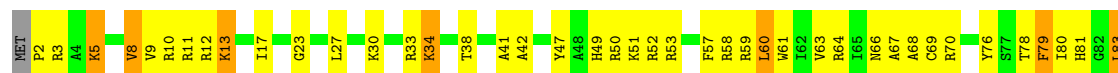




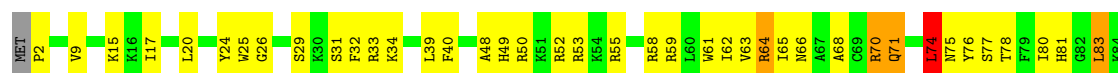
• Molecule 39: 50S ribosomal protein L19



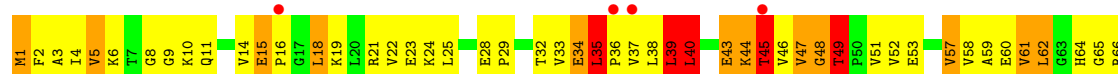
• Molecule 40: 50S ribosomal protein L20



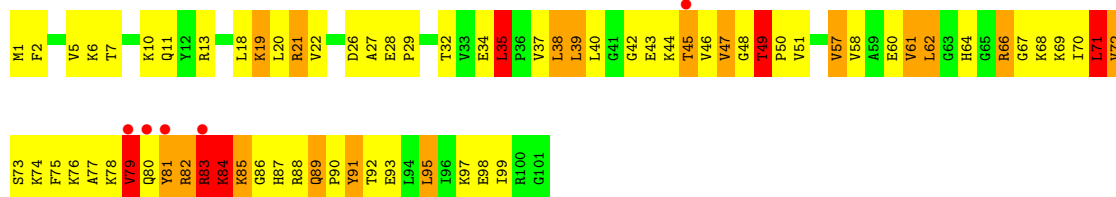
• Molecule 40: 50S ribosomal protein L20



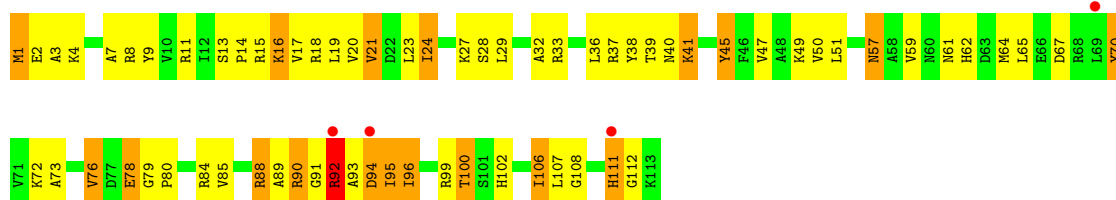
• Molecule 41: 50S ribosomal protein L21



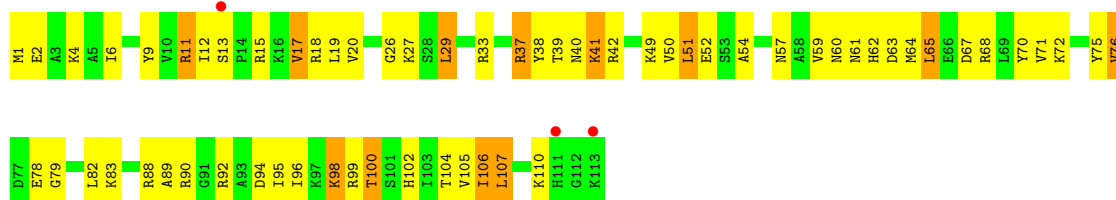
• Molecule 41: 50S ribosomal protein L21



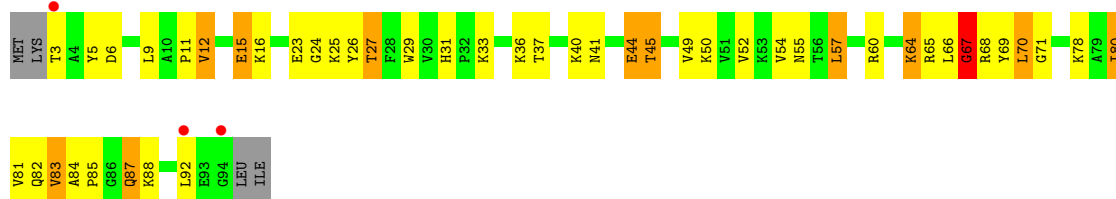
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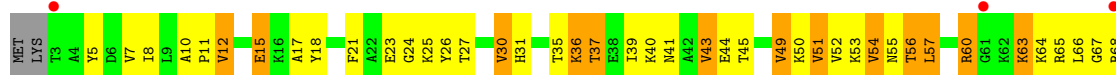
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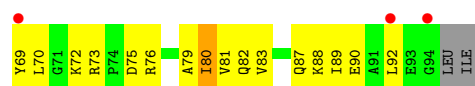


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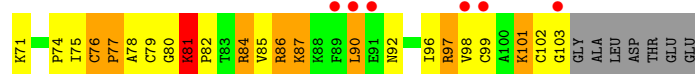
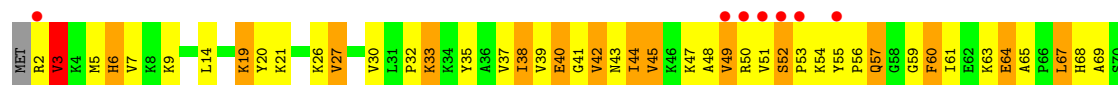


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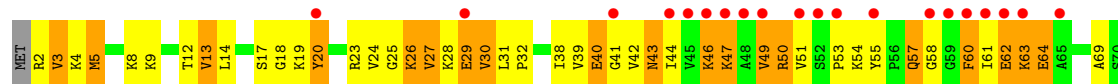
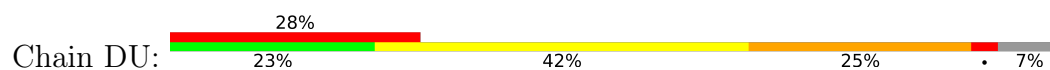




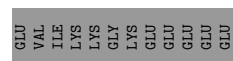
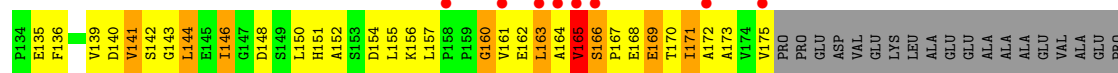
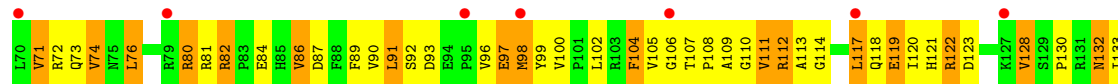
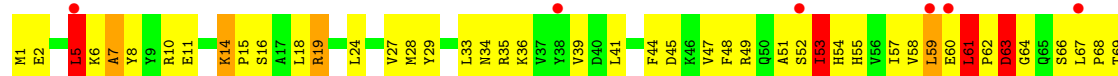
• Molecule 44: 50S ribosomal protein L24



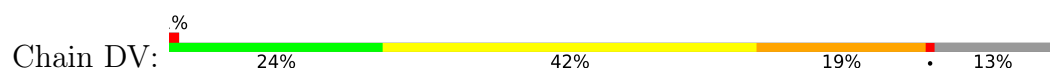
• Molecule 44: 50S ribosomal protein L24

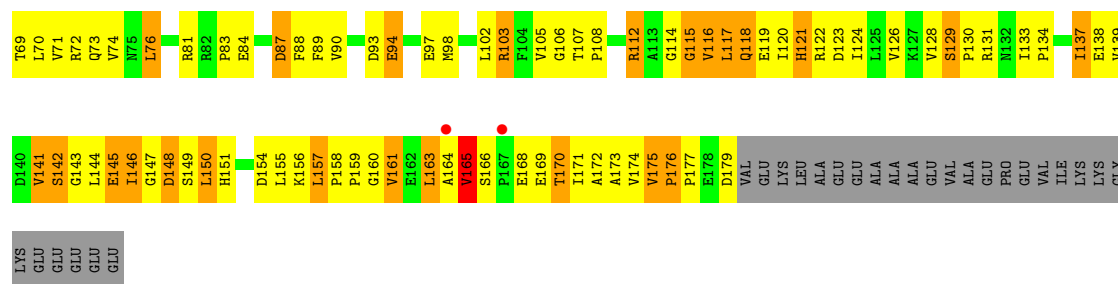


• Molecule 45: 50S ribosomal protein L25

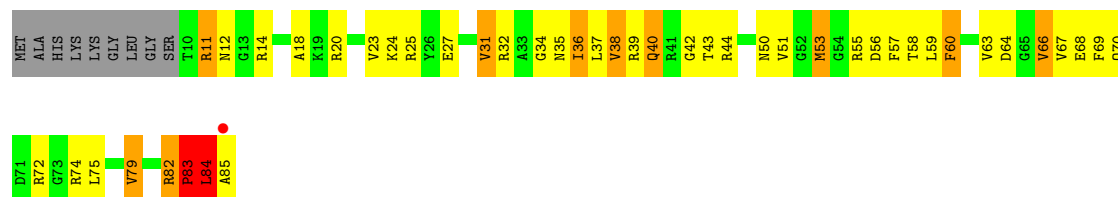


• Molecule 45: 50S ribosomal protein L25

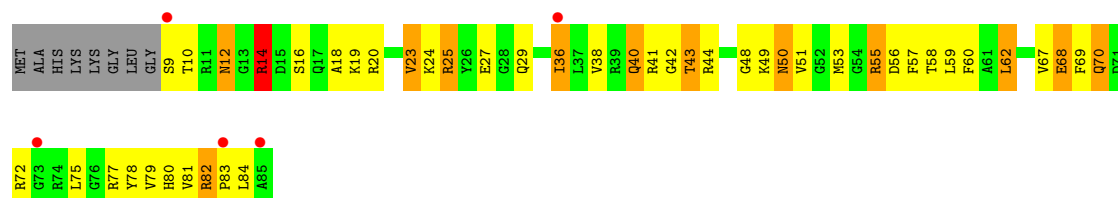




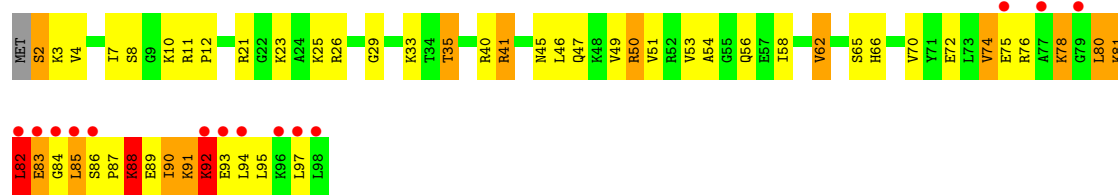
- Molecule 46: 50S ribosomal protein L27



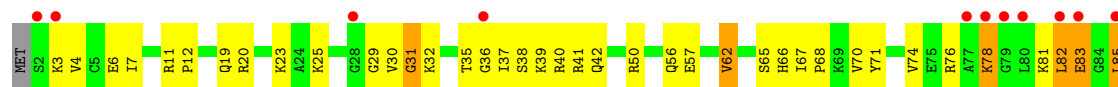
- Molecule 46: 50S ribosomal protein L27

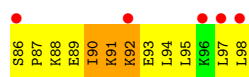


- Molecule 47: 50S ribosomal protein L28

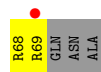
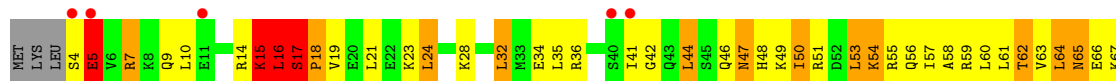


- Molecule 47: 50S ribosomal protein L28

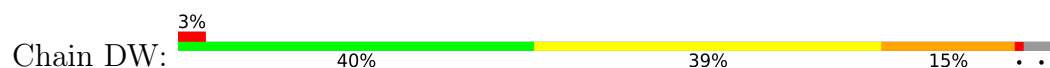




- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29



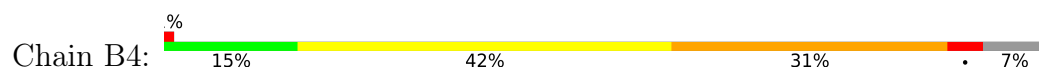
- Molecule 49: 50S ribosomal protein L30



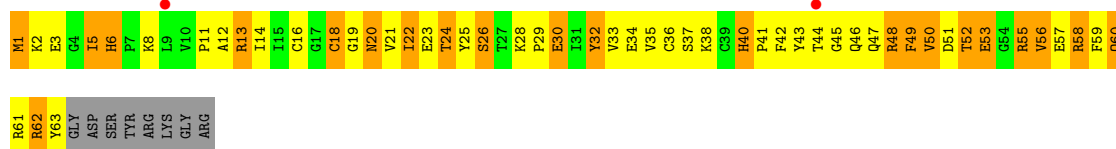
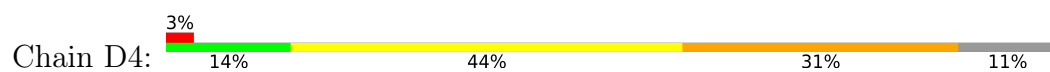
- Molecule 49: 50S ribosomal protein L30



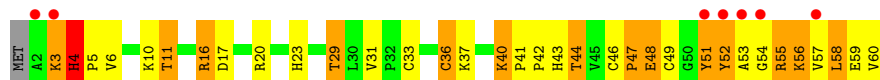
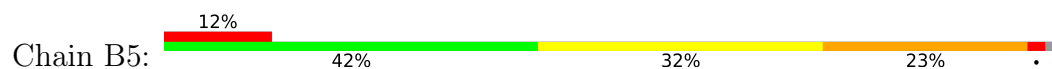
- Molecule 50: 50S ribosomal protein L31



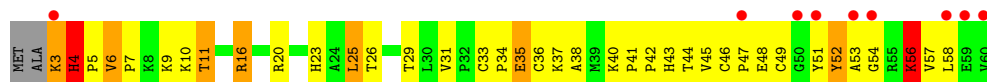
- Molecule 50: 50S ribosomal protein L31



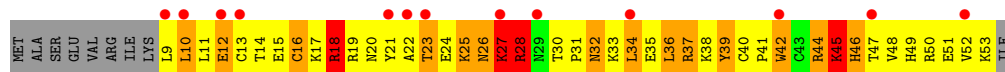
- Molecule 51: 50S ribosomal protein L32



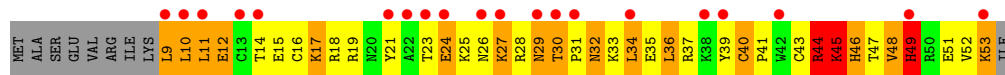
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



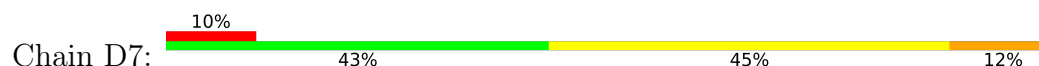
- Molecule 52: 50S ribosomal protein L33

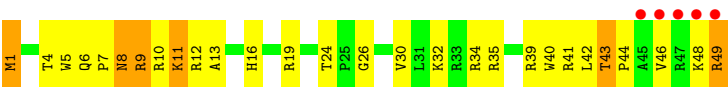


- Molecule 53: 50S ribosomal protein L34

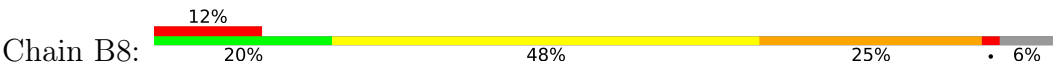


- Molecule 53: 50S ribosomal protein L34



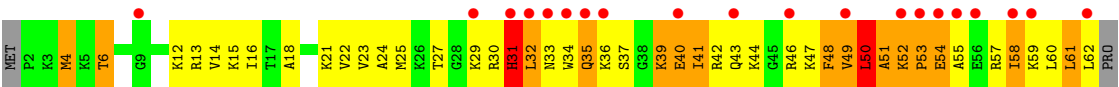
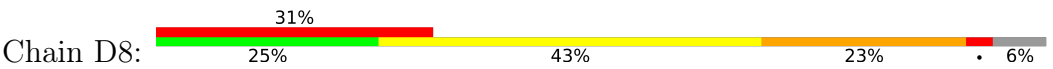


● Molecule 54: 50S ribosomal protein L35



TYR
GLU

● Molecule 54: 50S ribosomal protein L35



TYR
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.211 , 0.272 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.26	0/36234	0.41	0/56554
1	CA	0.24	0/36237	0.40	0/56558
2	AE	0.38	0/1959	0.90	6/2642 (0.2%)
2	CE	0.38	0/1959	0.95	10/2642 (0.4%)
3	AF	0.42	0/1629	0.81	0/2195
3	CF	0.43	0/1636	0.89	4/2205 (0.2%)
4	AG	0.50	1/1733 (0.1%)	1.00	10/2318 (0.4%)
4	CG	0.44	0/1733	0.99	11/2318 (0.5%)
5	AH	0.45	0/1171	0.92	2/1576 (0.1%)
5	CH	0.44	0/1171	0.93	2/1576 (0.1%)
6	AI	0.42	0/856	0.86	2/1154 (0.2%)
6	CI	0.39	0/856	0.82	0/1154
7	AJ	0.39	0/1276	0.87	3/1709 (0.2%)
7	CJ	0.36	0/1276	0.83	1/1709 (0.1%)
8	AK	0.43	0/1136	0.95	2/1527 (0.1%)
8	CK	0.36	0/1136	0.85	2/1527 (0.1%)
9	AL	0.39	0/1029	0.85	0/1379
9	CL	0.38	0/1029	0.90	2/1379 (0.1%)
10	AM	0.43	0/814	0.97	3/1095 (0.3%)
10	CM	0.42	0/814	0.95	4/1095 (0.4%)
11	AN	0.45	0/900	0.93	0/1213
11	CN	0.41	0/900	0.95	3/1213 (0.2%)
12	AO	0.51	0/991	1.08	7/1327 (0.5%)
12	CO	0.46	0/991	0.96	1/1327 (0.1%)
13	AP	0.39	0/938	0.89	4/1258 (0.3%)
13	CP	0.39	0/943	0.88	3/1265 (0.2%)
14	AQ	0.49	0/501	0.96	3/664 (0.5%)
14	CQ	0.35	0/501	0.98	3/664 (0.5%)
15	AR	0.43	0/745	0.88	0/992
15	CR	0.38	0/745	0.79	1/992 (0.1%)
16	AS	0.39	0/721	0.85	1/970 (0.1%)
16	CS	0.42	0/721	0.89	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.42	0/847	0.88	2/1131 (0.2%)
17	CT	0.39	0/847	0.84	1/1131 (0.1%)
18	AU	0.43	0/596	1.00	3/790 (0.4%)
18	CU	0.42	0/596	0.86	0/790
19	AV	0.44	0/638	0.94	1/860 (0.1%)
19	CV	0.44	0/638	1.14	6/860 (0.7%)
20	AW	0.37	0/765	0.86	2/1007 (0.2%)
20	CW	0.42	0/765	1.03	5/1007 (0.5%)
21	AX	0.35	0/221	0.86	1/288 (0.3%)
21	CX	0.36	0/221	0.80	0/288
22	AB	0.60	0/2080	0.52	0/3242
22	CB	0.70	0/2080	0.53	0/3242
23	AC	0.62	0/1835	0.61	0/2859
23	AD	0.35	0/1835	0.39	0/2859
23	CC	0.60	0/1835	0.58	0/2859
23	CD	0.38	0/1835	0.41	0/2859
24	A1	0.84	0/226	0.62	0/348
24	C1	0.87	0/226	0.66	0/348
25	BA	0.33	0/70233	0.45	1/109643 (0.0%)
25	DA	0.29	0/70122	0.43	2/109469 (0.0%)
26	BB	0.28	0/2928	0.42	0/4568
26	DB	0.25	0/2928	0.41	0/4568
27	BD	0.64	1/2165 (0.0%)	1.18	9/2919 (0.3%)
27	DD	0.59	0/2165	1.08	7/2919 (0.2%)
28	BE	0.50	0/1601	1.15	20/2160 (0.9%)
28	DE	0.50	0/1601	1.17	19/2160 (0.9%)
29	BF	0.55	0/1620	1.09	13/2194 (0.6%)
29	DF	0.45	0/1662	1.02	9/2249 (0.4%)
30	BG	0.47	0/1499	0.97	3/2016 (0.1%)
30	DG	0.37	0/1499	0.95	6/2016 (0.3%)
31	BH	0.52	0/1332	1.21	19/1802 (1.1%)
31	DH	0.44	0/1332	1.10	10/1802 (0.6%)
32	BK	0.48	0/1151	1.02	4/1558 (0.3%)
32	DK	0.47	0/1151	1.01	9/1558 (0.6%)
33	BM	0.54	0/1131	1.05	3/1525 (0.2%)
33	DM	0.40	0/1131	0.96	6/1525 (0.4%)
34	BN	0.53	0/943	1.00	4/1269 (0.3%)
34	DN	0.48	0/943	0.89	1/1269 (0.1%)
35	BO	0.52	0/1162	1.22	10/1544 (0.6%)
35	DO	0.45	1/1162 (0.1%)	0.99	8/1544 (0.5%)
36	BP	0.69	1/1143 (0.1%)	1.24	11/1527 (0.7%)
36	DP	0.42	0/1143	0.88	2/1527 (0.1%)
37	B0	0.53	0/982	1.05	5/1312 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	D0	0.48	0/974	0.99	2/1302 (0.2%)
38	BQ	0.51	0/892	0.95	1/1187 (0.1%)
38	DQ	0.40	0/892	0.93	2/1187 (0.2%)
39	BR	0.53	0/1155	1.04	4/1542 (0.3%)
39	DR	0.46	0/1155	0.94	4/1542 (0.3%)
40	B1	0.50	0/982	0.96	2/1306 (0.2%)
40	D1	0.44	0/982	0.92	5/1306 (0.4%)
41	B2	0.55	0/790	1.17	11/1057 (1.0%)
41	D2	0.45	0/790	0.95	5/1057 (0.5%)
42	BS	0.49	0/911	0.93	1/1220 (0.1%)
42	DS	0.53	0/911	0.95	0/1220
43	BT	0.57	0/739	1.00	2/993 (0.2%)
43	DT	0.54	0/739	0.93	1/993 (0.1%)
44	BU	0.60	0/798	1.06	4/1064 (0.4%)
44	DU	0.58	0/798	1.07	5/1064 (0.5%)
45	BV	0.42	0/1427	0.98	6/1935 (0.3%)
45	DV	0.40	0/1460	1.01	9/1982 (0.5%)
46	B3	0.52	0/615	1.00	2/819 (0.2%)
46	D3	0.47	0/621	1.03	3/827 (0.4%)
47	BZ	0.51	0/770	1.00	3/1022 (0.3%)
47	DZ	0.49	0/770	1.01	4/1022 (0.4%)
48	BW	0.57	0/560	1.09	2/741 (0.3%)
48	DW	0.44	0/583	1.03	3/771 (0.4%)
49	BX	0.47	0/474	1.10	3/635 (0.5%)
49	DX	0.42	0/474	0.92	2/635 (0.3%)
50	B4	0.43	0/545	1.08	5/733 (0.7%)
50	D4	0.47	0/527	1.12	4/709 (0.6%)
51	B5	0.57	0/473	1.11	1/639 (0.2%)
51	D5	0.43	0/468	0.97	1/632 (0.2%)
52	B6	0.50	0/396	1.13	3/529 (0.6%)
52	D6	0.47	0/396	1.00	2/529 (0.4%)
53	B7	0.59	0/438	1.00	1/575 (0.2%)
53	D7	0.52	0/438	0.96	2/575 (0.3%)
54	B8	0.64	0/494	1.05	1/649 (0.2%)
54	D8	0.50	0/494	1.02	2/649 (0.3%)
All	All	0.36	4/324027 (0.0%)	0.63	400/485226 (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
2	AE	0	3
2	CE	0	5
3	CF	0	1
4	AG	0	1
8	AK	0	1
10	AM	0	1
12	AO	0	2
14	AQ	0	1
14	CQ	0	2
15	AR	0	1
19	CV	0	1
20	CW	0	1
27	BD	0	6
27	DD	0	3
28	BE	0	1
28	DE	0	6
29	DF	0	2
30	BG	0	1
30	DG	0	1
31	BH	0	2
31	DH	0	2
32	BK	0	3
32	DK	0	4
33	BM	0	1
35	BO	0	4
35	DO	0	3
36	BP	0	3
37	D0	0	2
38	BQ	0	1
38	DQ	0	2
39	BR	0	2
40	B1	0	1
40	D1	0	1
41	B2	0	1
43	BT	0	1
44	DU	0	2
45	BV	0	3
45	DV	0	2
46	B3	0	2
48	BW	0	2
48	DW	0	1
50	B4	0	4
50	D4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
51	B5	0	1
51	D5	0	1
52	B6	0	1
52	D6	0	1
53	B7	0	1
54	B8	0	2
54	D8	0	1
All	All	0	99

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	DO	70	GLN	C-N	6.24	1.40	1.33
4	AG	12	CYS	CB-SG	5.90	2.00	1.81
27	BD	43	ARG	N-CA	5.15	1.52	1.46
36	BP	82	ARG	CA-C	5.05	1.58	1.53

The worst 5 of 400 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	BX	11	SER	CA-C-N	11.86	132.20	119.87
49	BX	11	SER	C-N-CA	11.86	132.20	119.87
28	BE	188	VAL	N-CA-C	11.62	118.62	108.63
45	DV	157	LEU	CA-C-N	11.49	132.22	120.38
45	DV	157	LEU	C-N-CA	11.49	132.22	120.38

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AE	14	GLY	Peptide
2	AE	194	PRO	Peptide
2	AE	71	VAL	Peptide
4	AG	29	PRO	Peptide
8	AK	102	ARG	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	32369	0	16339	1212	1
1	CA	32372	0	16338	1296	1
2	AE	1924	0	1975	161	0
2	CE	1924	0	1975	188	0
3	AF	1605	0	1668	113	0
3	CF	1612	0	1677	151	0
4	AG	1703	0	1764	152	0
4	CG	1703	0	1763	147	1
5	AH	1155	0	1213	81	0
5	CH	1155	0	1213	94	0
6	AI	843	0	857	40	1
6	CI	843	0	857	46	0
7	AJ	1257	0	1296	69	0
7	CJ	1257	0	1296	77	0
8	AK	1116	0	1177	77	0
8	CK	1116	0	1177	69	0
9	AL	1010	0	1037	101	0
9	CL	1010	0	1037	125	0
10	AM	801	0	849	81	0
10	CM	801	0	849	114	0
11	AN	885	0	904	67	0
11	CN	885	0	904	45	0
12	AO	975	0	1062	63	0
12	CO	975	0	1062	78	0
13	AP	928	0	987	72	0
13	CP	933	0	992	111	0
14	AQ	492	0	529	49	0
14	CQ	492	0	531	73	0
15	AR	734	0	771	44	0
15	CR	734	0	771	36	0
16	AS	705	0	725	81	0
16	CS	705	0	725	47	0
17	AT	834	0	904	55	0
17	CT	834	0	904	43	0
18	AU	591	0	662	29	0
18	CU	591	0	662	47	0
19	AV	624	0	636	74	0
19	CV	624	0	636	90	0
20	AW	763	0	859	74	0
20	CW	763	0	861	58	0
21	AX	217	0	234	17	0
21	CX	217	0	234	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AB	1861	0	938	87	0
22	CB	1861	0	938	100	0
23	AC	1643	0	837	74	0
23	AD	1643	0	837	97	0
23	CC	1643	0	837	91	0
23	CD	1643	0	837	108	0
24	A1	205	0	103	12	0
24	C1	205	0	103	10	0
25	BA	62707	0	31613	2108	0
25	DA	62607	0	31565	2107	1
26	BB	2617	0	1328	95	0
26	DB	2617	0	1328	135	0
27	BD	2115	0	2195	246	0
27	DD	2115	0	2195	213	0
28	BE	1568	0	1634	343	0
28	DE	1568	0	1634	261	0
29	BF	1585	0	1632	122	0
29	DF	1627	0	1680	190	0
30	BG	1474	0	1535	177	0
30	DG	1474	0	1535	150	0
31	BH	1307	0	1382	138	0
31	DH	1307	0	1382	156	1
32	BK	1136	0	1223	100	0
32	DK	1136	0	1223	86	0
33	BM	1104	0	1180	148	0
33	DM	1104	0	1180	89	0
34	BN	933	0	996	65	0
34	DN	933	0	996	52	0
35	BO	1145	0	1228	203	0
35	DO	1145	0	1227	244	0
36	BP	1122	0	1179	101	0
36	DP	1122	0	1179	212	0
37	B0	968	0	1033	79	0
37	D0	960	0	1021	60	0
38	BQ	882	0	943	110	0
38	DQ	882	0	943	120	0
39	BR	1141	0	1202	123	0
39	DR	1141	0	1202	131	0
40	B1	964	0	1022	102	0
40	D1	964	0	1022	94	0
41	B2	779	0	852	82	0
41	D2	779	0	852	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BS	900	0	964	72	0
42	DS	900	0	964	43	0
43	BT	725	0	778	55	0
43	DT	725	0	778	76	0
44	BU	785	0	878	78	0
44	DU	785	0	878	103	0
45	BV	1397	0	1430	125	0
45	DV	1428	0	1454	164	0
46	B3	607	0	628	51	0
46	D3	613	0	633	55	0
47	BZ	763	0	848	52	0
47	DZ	763	0	848	47	0
48	BW	558	0	610	46	0
48	DW	581	0	629	49	0
49	BX	469	0	518	35	0
49	DX	469	0	518	23	0
50	B4	533	0	522	86	0
50	D4	515	0	510	86	0
51	B5	459	0	480	53	0
51	D5	454	0	475	44	0
52	B6	389	0	404	83	0
52	D6	389	0	404	86	0
53	B7	430	0	480	30	0
53	D7	430	0	480	36	0
54	B8	488	0	558	114	0
54	D8	488	0	558	117	0
55	A1	2	0	0	0	0
55	AA	242	0	0	0	0
55	AB	5	0	0	0	0
55	AC	9	0	0	0	0
55	AD	1	0	0	0	0
55	AG	1	0	0	0	0
55	AH	1	0	0	0	0
55	AN	2	0	0	0	0
55	AQ	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	1	0	0	0	0
55	B2	1	0	0	0	0
55	B3	1	0	0	0	0
55	B5	1	0	0	0	0
55	B7	1	0	0	0	0
55	B8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BA	623	0	0	0	0
55	BB	17	0	0	0	0
55	BD	1	0	0	0	0
55	BE	5	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BU	2	0	0	0	0
55	CA	207	0	0	0	0
55	CB	3	0	0	0	0
55	CC	8	0	0	0	0
55	CG	2	0	0	0	0
55	CN	1	0	0	0	0
55	CS	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	526	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DR	1	0	0	0	0
55	DU	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299552	0	200910	15102	3

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 30.

The worst 5 of 15102 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)
1:AA:625:G:H4'	16:AS:16:HIS:CD2	1.33	1.61
28:DE:46:ALA:CB	28:DE:82:ARG:HA	1.37	1.55
30:BG:83:ARG:H	30:BG:86:MET:CE	1.24	1.47
47:BZ:85:LEU:C	47:BZ:87:PRO:HD2	1.38	1.45
36:DP:26:TYR:CE1	36:DP:139:GLU:HB2	1.48	1.45

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.90	0.30
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.02	0.18
6:AI:15:ASP:OD2	4:CG:27:TYR:OH[4_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	7	32
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	12	45
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	8	35
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	12	45
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	9	38
5	CH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	AI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	CI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	AJ	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	CJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	AK	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	18	53
8	CK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	AL	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	CL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	AM	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
10	CM	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	14	48
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	7	34
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	4	24
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	6	31
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	7	32
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	32
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	10	40
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	2	15
16	CS	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	AT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	CT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	AU	70/88 (80%)	64 (91%)	5 (7%)	1 (1%)	9	36
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	4	23
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	1	9
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	12	45
21	AX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	CX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	BD	270/276 (98%)	243 (90%)	22 (8%)	5 (2%)	6	30
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	4	23
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0	1
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	0	3
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	2	14
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	4	21
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	21	56
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	11
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1	5
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	5	27
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	1	10
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	8	35
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	50
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	2
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0	0
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	5	26
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	1
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	7	32
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	4	21
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	4	21
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	35
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	48
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	28
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1	4
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	2	16
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	5	26
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	5	26
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	1	10
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	1	7
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	2	14
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	1	8
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	4	22
46	D3	75/85 (88%)	69 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BZ	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	3	18
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	11	43
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	3	19
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8	35
49	BX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	DX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	B4	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	3	19
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	7	34
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	6	31
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	6	31
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	11
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	0	2
53	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
53	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
54	B8	59/65 (91%)	47 (80%)	7 (12%)	5 (8%)	0	3
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	0	1
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	4	23

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AG	13	ARG
4	AG	14	ARG
11	AN	82	VAL
16	AS	17	TYR
18	AU	22	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	
2	AE	205/220 (93%)	149 (73%)	56 (27%)	0	2
2	CE	205/220 (93%)	148 (72%)	57 (28%)	0	2
3	AF	159/188 (85%)	123 (77%)	36 (23%)	1	5
3	CF	160/188 (85%)	120 (75%)	40 (25%)	0	3
4	AG	180/180 (100%)	144 (80%)	36 (20%)	1	7
4	CG	180/180 (100%)	136 (76%)	44 (24%)	1	4
5	AH	116/123 (94%)	82 (71%)	34 (29%)	0	2
5	CH	116/123 (94%)	83 (72%)	33 (28%)	0	2
6	AI	90/90 (100%)	76 (84%)	14 (16%)	2	13
6	CI	90/90 (100%)	72 (80%)	18 (20%)	1	7
7	AJ	126/127 (99%)	101 (80%)	25 (20%)	1	8
7	CJ	126/127 (99%)	84 (67%)	42 (33%)	0	1
8	AK	119/119 (100%)	93 (78%)	26 (22%)	1	6
8	CK	119/119 (100%)	95 (80%)	24 (20%)	1	7
9	AL	98/99 (99%)	68 (69%)	30 (31%)	0	1
9	CL	98/99 (99%)	72 (74%)	26 (26%)	0	3
10	AM	89/92 (97%)	63 (71%)	26 (29%)	0	2
10	CM	89/92 (97%)	53 (60%)	36 (40%)	0	0
11	AN	90/99 (91%)	73 (81%)	17 (19%)	1	9
11	CN	90/99 (91%)	67 (74%)	23 (26%)	0	3
12	AO	104/109 (95%)	83 (80%)	21 (20%)	1	7
12	CO	104/109 (95%)	77 (74%)	27 (26%)	0	3
13	AP	94/101 (93%)	70 (74%)	24 (26%)	0	3
13	CP	94/101 (93%)	72 (77%)	22 (23%)	1	4
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0	1
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	1	7
15	AR	79/80 (99%)	67 (85%)	12 (15%)	3	14
15	CR	79/80 (99%)	65 (82%)	14 (18%)	2	10
16	AS	72/74 (97%)	51 (71%)	21 (29%)	0	2
16	CS	72/74 (97%)	61 (85%)	11 (15%)	3	14
17	AT	95/97 (98%)	81 (85%)	14 (15%)	3	15
17	CT	95/97 (98%)	83 (87%)	12 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	63/77 (82%)	48 (76%)	15 (24%)	1	4
18	CU	63/77 (82%)	46 (73%)	17 (27%)	0	2
19	AV	67/80 (84%)	45 (67%)	22 (33%)	0	1
19	CV	67/80 (84%)	52 (78%)	15 (22%)	1	5
20	AW	76/82 (93%)	55 (72%)	21 (28%)	0	2
20	CW	76/82 (93%)	53 (70%)	23 (30%)	0	1
21	AX	20/22 (91%)	17 (85%)	3 (15%)	3	14
21	CX	20/22 (91%)	19 (95%)	1 (5%)	22	56
27	BD	214/218 (98%)	168 (78%)	46 (22%)	1	6
27	DD	214/218 (98%)	163 (76%)	51 (24%)	1	4
28	BE	165/166 (99%)	111 (67%)	54 (33%)	0	1
28	DE	165/166 (99%)	117 (71%)	48 (29%)	0	2
29	BF	161/166 (97%)	120 (74%)	41 (26%)	0	3
29	DF	165/166 (99%)	120 (73%)	45 (27%)	0	2
30	BG	155/156 (99%)	112 (72%)	43 (28%)	0	2
30	DG	155/156 (99%)	113 (73%)	42 (27%)	0	2
31	BH	142/148 (96%)	98 (69%)	44 (31%)	0	1
31	DH	142/148 (96%)	104 (73%)	38 (27%)	0	2
32	BK	122/124 (98%)	84 (69%)	38 (31%)	0	1
32	DK	122/124 (98%)	79 (65%)	43 (35%)	0	1
33	BM	117/119 (98%)	81 (69%)	36 (31%)	0	1
33	DM	117/119 (98%)	93 (80%)	24 (20%)	1	7
34	BN	100/100 (100%)	81 (81%)	19 (19%)	1	8
34	DN	100/100 (100%)	71 (71%)	29 (29%)	0	2
35	BO	116/116 (100%)	72 (62%)	44 (38%)	0	1
35	DO	116/116 (100%)	72 (62%)	44 (38%)	0	1
36	BP	111/111 (100%)	85 (77%)	26 (23%)	1	4
36	DP	111/111 (100%)	82 (74%)	29 (26%)	0	3
37	B0	101/101 (100%)	75 (74%)	26 (26%)	0	3
37	D0	100/101 (99%)	79 (79%)	21 (21%)	1	6
38	BQ	87/88 (99%)	59 (68%)	28 (32%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DQ	87/88 (99%)	53 (61%)	34 (39%)	0	1
39	BR	120/127 (94%)	82 (68%)	38 (32%)	0	1
39	DR	120/127 (94%)	77 (64%)	43 (36%)	0	1
40	B1	93/94 (99%)	75 (81%)	18 (19%)	1	8
40	D1	93/94 (99%)	77 (83%)	16 (17%)	2	11
41	B2	82/82 (100%)	58 (71%)	24 (29%)	0	2
41	D2	82/82 (100%)	53 (65%)	29 (35%)	0	1
42	BS	92/92 (100%)	64 (70%)	28 (30%)	0	1
42	DS	92/92 (100%)	68 (74%)	24 (26%)	0	3
43	BT	74/78 (95%)	58 (78%)	16 (22%)	1	6
43	DT	74/78 (95%)	58 (78%)	16 (22%)	1	6
44	BU	85/91 (93%)	61 (72%)	24 (28%)	0	2
44	DU	85/91 (93%)	49 (58%)	36 (42%)	0	0
45	BV	154/179 (86%)	115 (75%)	39 (25%)	0	3
45	DV	158/179 (88%)	119 (75%)	39 (25%)	1	4
46	B3	61/67 (91%)	50 (82%)	11 (18%)	2	10
46	D3	62/67 (92%)	44 (71%)	18 (29%)	0	2
47	BZ	82/83 (99%)	61 (74%)	21 (26%)	0	3
47	DZ	82/83 (99%)	62 (76%)	20 (24%)	1	4
48	BW	62/67 (92%)	42 (68%)	20 (32%)	0	1
48	DW	64/67 (96%)	49 (77%)	15 (23%)	1	4
49	BX	51/52 (98%)	42 (82%)	9 (18%)	2	10
49	DX	51/52 (98%)	41 (80%)	10 (20%)	1	8
50	B4	59/63 (94%)	39 (66%)	20 (34%)	0	1
50	D4	57/63 (90%)	37 (65%)	20 (35%)	0	1
51	B5	51/52 (98%)	35 (69%)	16 (31%)	0	1
51	D5	51/52 (98%)	36 (71%)	15 (29%)	0	2
52	B6	44/52 (85%)	26 (59%)	18 (41%)	0	0
52	D6	44/52 (85%)	26 (59%)	18 (41%)	0	0
53	B7	42/42 (100%)	32 (76%)	10 (24%)	1	4
53	D7	42/42 (100%)	31 (74%)	11 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B8	51/55 (93%)	38 (74%)	13 (26%)	0	3
54	D8	51/55 (93%)	37 (72%)	14 (28%)	0	2
All	All	9579/9996 (96%)	7053 (74%)	2526 (26%)	0	3

5 of 2526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	DF	83	PHE
42	DS	106	ILE
30	DG	115	ARG
29	DF	70	THR
35	DO	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 278 such sidechains are listed below:

Mol	Chain	Res	Type
39	DR	90	GLN
41	D2	64	HIS
46	D3	70	GLN
41	B2	11	GLN
40	B1	44	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	377 (25%)	32 (2%)
1	CA	1505/1506 (99%)	410 (27%)	41 (2%)
22	AB	86/87 (98%)	40 (46%)	5 (5%)
22	CB	86/87 (98%)	46 (53%)	2 (2%)
23	AC	77/77 (100%)	23 (29%)	6 (7%)
23	AD	76/77 (98%)	28 (36%)	1 (1%)
23	CC	77/77 (100%)	21 (27%)	5 (6%)
23	CD	76/77 (98%)	26 (34%)	1 (1%)
24	A1	9/10 (90%)	3 (33%)	1 (11%)
24	C1	9/10 (90%)	3 (33%)	0
25	BA	2911/2912 (99%)	715 (24%)	57 (1%)
25	DA	2905/2912 (99%)	766 (26%)	57 (1%)
26	BB	121/122 (99%)	30 (24%)	0
26	DB	121/122 (99%)	39 (32%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9564/9582 (99%)	2527 (26%)	208 (2%)

5 of 2527 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	32	A
1	AA	33	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	353	A
22	CB	21	A
25	DA	2602	A
1	CA	560	U
1	CA	1067	A

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 1700 ligands modelled in this entry, 1700 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	-0.25	11 (0%) 84 66	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.13	22 (1%) 72 49	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.30	8 (3%) 48 27	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.37	3 (1%) 75 53	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.48	8 (3%) 43 24	84, 111, 144, 153	0
3	CF	206/239 (86%)	1.05	25 (12%) 8 5	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.57	13 (6%) 26 13	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.54	9 (4%) 40 21	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.22	3 (1%) 65 41	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.65	9 (5%) 27 14	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.17	1 (0%) 79 59	76, 99, 115, 137	0
6	CI	101/101 (100%)	-0.28	0 100 100	74, 95, 116, 141	0
7	AJ	155/156 (99%)	0.32	12 (7%) 19 10	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.40	9 (5%) 29 15	102, 122, 149, 156	0
8	AK	138/138 (100%)	0.04	0 100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	0.13	1 (0%) 84 66	94, 116, 128, 136	0
9	AL	127/128 (99%)	0.24	8 (6%) 26 13	85, 133, 153, 160	0
9	CL	127/128 (99%)	0.51	11 (8%) 16 8	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.59	9 (9%) 15 8	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.70	8 (8%) 18 9	111, 149, 165, 170	0
11	AN	119/129 (92%)	0.40	7 (5%) 28 14	64, 97, 128, 154	0
11	CN	119/129 (92%)	0.37	8 (6%) 24 12	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.33	4 (3%) 50 29	63, 73, 105, 151	0
12	CO	125/132 (94%)	0.91	15 (12%) 9 5	75, 98, 124, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.49	9 (7%) 19 10	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.55	7 (5%) 27 14	106, 146, 161, 164	0
14	AQ	60/61 (98%)	0.73	5 (8%) 17 9	86, 101, 115, 126	0
14	CQ	60/61 (98%)	1.29	13 (21%) 2 1	118, 132, 146, 153	0
15	AR	88/89 (98%)	0.12	2 (2%) 61 38	72, 93, 114, 117	0
15	CR	88/89 (98%)	0.14	1 (1%) 78 57	73, 104, 127, 133	0
16	AS	84/88 (95%)	0.36	2 (2%) 59 36	90, 107, 133, 165	0
16	CS	84/88 (95%)	0.06	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	0.26	4 (4%) 42 23	82, 100, 118, 130	0
17	CT	100/105 (95%)	0.49	6 (6%) 27 14	82, 102, 125, 137	0
18	AU	72/88 (81%)	0.15	1 (1%) 73 51	78, 99, 132, 159	0
18	CU	72/88 (81%)	-0.11	0 100 100	85, 106, 144, 157	0
19	AV	78/93 (83%)	0.05	4 (5%) 33 17	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.40	5 (6%) 25 13	136, 154, 174, 177	0
20	AW	99/106 (93%)	0.53	4 (4%) 42 23	93, 115, 144, 155	0
20	CW	99/106 (93%)	0.40	3 (3%) 52 30	83, 109, 143, 157	0
21	AX	25/27 (92%)	0.47	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	1.30	2 (8%) 18 9	112, 133, 148, 160	0
22	AB	87/87 (100%)	0.32	6 (6%) 23 12	78, 145, 185, 196	0
22	CB	87/87 (100%)	0.58	11 (12%) 8 5	92, 148, 188, 200	0
23	AC	77/77 (100%)	0.10	2 (2%) 57 34	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.42	5 (6%) 25 13	71, 218, 232, 234	0
23	CC	77/77 (100%)	0.01	1 (1%) 75 53	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.87	10 (12%) 7 4	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.60	3 (30%) 1 1	67, 81, 112, 112	0
24	C1	10/10 (100%)	1.19	3 (30%) 1 1	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.59	17 (0%) 85 69	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.37	11 (0%) 88 76	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.49	0 100 100	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.03	2 (1%) 70 47	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.08	8 (2%) 53 31	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	0.09	11 (4%) 42 23	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.45	10 (4%) 35 18	42, 77, 123, 132	0
28	DE	205/206 (99%)	0.66	25 (12%) 8 5	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.06	4 (1%) 65 41	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.31	6 (2%) 53 31	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.28	7 (3%) 43 24	81, 101, 130, 142	0
30	DG	181/182 (99%)	0.67	11 (6%) 27 14	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.26	6 (3%) 47 27	74, 104, 121, 146	0
31	DH	170/180 (94%)	0.72	18 (10%) 11 6	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.29	2 (1%) 73 51	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.56	9 (6%) 26 14	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.58	7 (5%) 33 17	57, 81, 116, 129	0
33	DM	138/140 (98%)	0.37	6 (4%) 40 21	71, 102, 133, 143	0
34	BN	122/122 (100%)	-0.06	0 100 100	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.35	2 (1%) 70 47	62, 82, 102, 118	0
35	BO	150/150 (100%)	0.51	11 (7%) 21 11	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.86	23 (15%) 5 3	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.62	14 (9%) 13 7	52, 78, 99, 125	0
36	DP	141/141 (100%)	1.19	26 (18%) 3 2	58, 98, 129, 148	0
37	B0	118/118 (100%)	-0.06	1 (0%) 82 64	50, 76, 94, 110	0
37	D0	117/118 (99%)	-0.02	3 (2%) 57 34	50, 74, 97, 113	0
38	BQ	111/112 (99%)	0.16	5 (4%) 38 20	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.55	4 (3%) 46 26	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.50	8 (5%) 29 15	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.60	7 (5%) 33 17	69, 93, 154, 174	0
40	B1	117/118 (99%)	0.02	2 (1%) 69 45	44, 70, 101, 132	0
40	D1	117/118 (99%)	-0.02	0 100 100	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.19	4 (3%) 42 23	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.37	5 (4%) 34 18	58, 115, 133, 142	0
42	BS	113/113 (100%)	0.06	4 (3%) 47 27	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.16	3 (2%) 56 33	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.04	3 (3%)	49	28	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.33	6 (6%)	25	13	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.73	13 (12%)	8	5	67, 92, 142, 159	0
44	DU	102/110 (92%)	1.52	31 (30%)	1	1	82, 109, 160, 176	0
45	BV	175/206 (84%)	0.90	21 (12%)	9	5	80, 117, 179, 183	0
45	DV	179/206 (86%)	0.66	3 (1%)	69	45	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.10	1 (1%)	75	53	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.56	5 (6%)	25	13	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.53	14 (14%)	6	3	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.93	16 (16%)	4	3	54, 77, 126, 148	0
48	BW	66/72 (91%)	0.26	6 (9%)	15	8	55, 73, 90, 120	0
48	DW	69/72 (95%)	0.06	2 (2%)	53	31	77, 100, 130, 167	0
49	BX	59/60 (98%)	0.07	0	100	100	60, 75, 105, 120	0
49	DX	59/60 (98%)	0.07	0	100	100	73, 98, 130, 153	0
50	B4	66/71 (92%)	0.40	1 (1%)	72	49	111, 146, 164, 173	0
50	D4	63/71 (88%)	0.74	2 (3%)	50	29	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.73	7 (11%)	9	5	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.73	9 (15%)	5	3	52, 78, 167, 178	0
52	B6	45/54 (83%)	1.61	13 (28%)	1	1	105, 134, 156, 160	0
52	D6	45/54 (83%)	2.19	20 (44%)	0	1	121, 156, 173, 176	0
53	B7	49/49 (100%)	-0.26	2 (4%)	41	23	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.27	5 (10%)	12	6	44, 54, 112, 131	0
54	B8	61/65 (93%)	0.76	8 (13%)	7	4	51, 64, 81, 102	0
54	D8	61/65 (93%)	1.60	20 (32%)	1	1	65, 79, 94, 123	0
All	All	21104/21634 (97%)	0.08	803 (3%)	44	24	35, 96, 177, 235	0

The worst 5 of 803 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	B5	2	ALA	12.2
9	CL	115	GLY	11.8
28	BE	79	ARG	8.2
30	BG	80	PHE	7.1
9	CL	127	LYS	6.4

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	DA	3441	1/1	0.18	0.17	137,137,137,137	0
55	MG	CA	1644	1/1	0.19	0.33	120,120,120,120	0
55	MG	CA	1753	1/1	0.23	0.25	123,123,123,123	0
55	MG	AA	1761	1/1	0.27	0.41	113,113,113,113	0
55	MG	DA	3315	1/1	0.33	0.20	108,108,108,108	0
55	MG	DB	207	1/1	0.34	0.39	115,115,115,115	0
55	MG	AA	1729	1/1	0.36	0.34	113,113,113,113	0
55	MG	AA	1715	1/1	0.37	0.27	115,115,115,115	0
55	MG	AA	1713	1/1	0.42	0.25	115,115,115,115	0
55	MG	CA	1759	1/1	0.43	0.36	103,103,103,103	0
55	MG	AB	103	1/1	0.45	0.22	111,111,111,111	0
55	MG	BA	3490	1/1	0.46	0.18	166,166,166,166	0
55	MG	DA	3064	1/1	0.48	0.24	101,101,101,101	0
55	MG	BA	3484	1/1	0.48	0.28	117,117,117,117	0
55	MG	CA	1632	1/1	0.49	0.37	95,95,95,95	0
55	MG	DA	3462	1/1	0.49	0.33	107,107,107,107	0
55	MG	CC	107	1/1	0.49	0.17	99,99,99,99	0
55	MG	CA	1719	1/1	0.53	0.26	129,129,129,129	0
55	MG	DA	3491	1/1	0.54	0.52	103,103,103,103	0
55	MG	AA	1731	1/1	0.54	0.27	103,103,103,103	0
55	MG	BA	3075	1/1	0.55	0.32	110,110,110,110	0
55	MG	AA	1700	1/1	0.55	0.24	99,99,99,99	0
55	MG	AA	1710	1/1	0.55	0.31	92,92,92,92	0
55	MG	DA	3273	1/1	0.56	0.24	99,99,99,99	0
55	MG	DA	3508	1/1	0.56	0.36	80,80,80,80	0
55	MG	DA	3405	1/1	0.56	0.34	79,79,79,79	0
55	MG	BA	3580	1/1	0.57	0.15	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1769	1/1	0.57	0.32	104,104,104,104	0
55	MG	BA	3505	1/1	0.58	0.30	96,96,96,96	0
55	MG	DA	3068	1/1	0.58	0.29	91,91,91,91	0
55	MG	AC	106	1/1	0.58	0.36	89,89,89,89	0
55	MG	AA	1638	1/1	0.58	0.31	104,104,104,104	0
55	MG	BA	3495	1/1	0.58	0.24	123,123,123,123	0
55	MG	CA	1659	1/1	0.59	0.23	110,110,110,110	0
55	MG	BA	3379	1/1	0.59	0.39	82,82,82,82	0
55	MG	DA	3487	1/1	0.59	0.25	95,95,95,95	0
55	MG	BB	216	1/1	0.60	0.23	94,94,94,94	0
55	MG	CA	1622	1/1	0.60	0.46	95,95,95,95	0
55	MG	AA	1758	1/1	0.60	0.25	85,85,85,85	0
55	MG	AA	1744	1/1	0.60	0.19	117,117,117,117	0
55	MG	BA	3134	1/1	0.61	0.17	81,81,81,81	0
55	MG	AA	1833	1/1	0.61	0.35	88,88,88,88	0
55	MG	CA	1699	1/1	0.61	0.14	97,97,97,97	0
55	MG	DA	3481	1/1	0.61	0.42	96,96,96,96	0
55	MG	CA	1713	1/1	0.61	0.41	102,102,102,102	0
55	MG	DA	3129	1/1	0.61	0.34	82,82,82,82	0
55	MG	AA	1737	1/1	0.61	0.37	83,83,83,83	0
55	MG	DA	3524	1/1	0.61	0.21	105,105,105,105	0
55	MG	BA	3507	1/1	0.61	0.32	89,89,89,89	0
55	MG	CA	1807	1/1	0.62	0.31	126,126,126,126	0
55	MG	AA	1689	1/1	0.62	0.27	115,115,115,115	0
55	MG	AA	1797	1/1	0.62	0.38	99,99,99,99	0
55	MG	DA	3490	1/1	0.62	0.11	126,126,126,126	0
55	MG	AA	1618	1/1	0.63	0.29	82,82,82,82	0
55	MG	AA	1826	1/1	0.63	0.16	101,101,101,101	0
55	MG	BA	3115	1/1	0.63	0.27	87,87,87,87	0
55	MG	CA	1645	1/1	0.63	0.27	86,86,86,86	0
55	MG	DA	3059	1/1	0.63	0.36	106,106,106,106	0
55	MG	AA	1692	1/1	0.63	0.29	115,115,115,115	0
55	MG	BA	3300	1/1	0.63	0.27	88,88,88,88	0
55	MG	DA	3072	1/1	0.63	0.31	112,112,112,112	0
55	MG	DA	3083	1/1	0.63	0.38	85,85,85,85	0
55	MG	AA	1755	1/1	0.63	0.25	104,104,104,104	0
55	MG	BA	3438	1/1	0.63	0.25	91,91,91,91	0
55	MG	DA	3020	1/1	0.64	0.19	85,85,85,85	0
55	MG	CA	1660	1/1	0.64	0.25	85,85,85,85	0
55	MG	DA	3277	1/1	0.64	0.31	89,89,89,89	0
55	MG	BA	3541	1/1	0.64	0.23	96,96,96,96	0
55	MG	BA	3552	1/1	0.64	0.31	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3519	1/1	0.64	0.34	80,80,80,80	0
55	MG	DA	3007	1/1	0.64	0.21	74,74,74,74	0
55	MG	AA	1640	1/1	0.65	0.35	90,90,90,90	0
55	MG	AA	1728	1/1	0.65	0.19	108,108,108,108	0
55	MG	CA	1704	1/1	0.65	0.29	99,99,99,99	0
55	MG	DA	3429	1/1	0.65	0.32	99,99,99,99	0
55	MG	CA	1707	1/1	0.65	0.45	98,98,98,98	0
55	MG	AA	1711	1/1	0.65	0.26	89,89,89,89	0
55	MG	CA	1714	1/1	0.65	0.20	92,92,92,92	0
55	MG	CA	1717	1/1	0.65	0.28	106,106,106,106	0
55	MG	AA	1708	1/1	0.65	0.35	91,91,91,91	0
55	MG	AA	1828	1/1	0.65	0.30	105,105,105,105	0
55	MG	DA	3503	1/1	0.65	0.45	80,80,80,80	0
55	MG	DA	3120	1/1	0.65	0.30	90,90,90,90	0
55	MG	AA	1831	1/1	0.65	0.50	90,90,90,90	0
55	MG	CA	1774	1/1	0.65	0.25	104,104,104,104	0
55	MG	CA	1727	1/1	0.66	0.36	94,94,94,94	0
55	MG	CA	1747	1/1	0.66	0.33	94,94,94,94	0
55	MG	AA	1832	1/1	0.66	0.32	94,94,94,94	0
55	MG	CA	1601	1/1	0.66	0.55	96,96,96,96	0
55	MG	CA	1770	1/1	0.66	0.33	102,102,102,102	0
55	MG	DA	3151	1/1	0.66	0.30	85,85,85,85	0
55	MG	BA	3500	1/1	0.66	0.21	97,97,97,97	0
55	MG	CA	1638	1/1	0.67	0.48	101,101,101,101	0
55	MG	CA	1757	1/1	0.67	0.28	97,97,97,97	0
55	MG	BA	3420	1/1	0.67	0.24	94,94,94,94	0
55	MG	AH	201	1/1	0.67	0.31	99,99,99,99	0
55	MG	CA	1609	1/1	0.67	0.21	115,115,115,115	0
55	MG	DA	3086	1/1	0.67	0.24	114,114,114,114	0
55	MG	BA	3334	1/1	0.67	0.36	96,96,96,96	0
55	MG	CB	101	1/1	0.67	0.28	101,101,101,101	0
55	MG	CA	1626	1/1	0.67	0.21	93,93,93,93	0
55	MG	CA	1741	1/1	0.67	0.27	106,106,106,106	0
55	MG	DA	3010	1/1	0.67	0.28	97,97,97,97	0
55	MG	AA	1754	1/1	0.67	0.28	95,95,95,95	0
55	MG	DA	3343	1/1	0.68	0.25	95,95,95,95	0
55	MG	DA	3379	1/1	0.68	0.35	85,85,85,85	0
55	MG	DA	3026	1/1	0.68	0.45	95,95,95,95	0
55	MG	BA	3403	1/1	0.68	0.43	93,93,93,93	0
55	MG	DA	3085	1/1	0.68	0.27	91,91,91,91	0
55	MG	AA	1647	1/1	0.68	0.28	88,88,88,88	0
55	MG	AD	101	1/1	0.68	0.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	213	1/1	0.68	0.22	94,94,94,94	0
55	MG	AA	1732	1/1	0.69	0.36	92,92,92,92	0
55	MG	AC	102	1/1	0.69	0.38	93,93,93,93	0
55	MG	BA	3313	1/1	0.69	0.21	88,88,88,88	0
55	MG	AA	1698	1/1	0.69	0.24	72,72,72,72	0
55	MG	AA	1621	1/1	0.69	0.24	108,108,108,108	0
55	MG	AA	1836	1/1	0.69	0.30	79,79,79,79	0
55	MG	CA	1783	1/1	0.69	0.35	100,100,100,100	0
55	MG	CA	1797	1/1	0.69	0.24	87,87,87,87	0
55	MG	CA	1805	1/1	0.69	0.30	94,94,94,94	0
55	MG	AA	1748	1/1	0.69	0.39	84,84,84,84	0
55	MG	DB	211	1/1	0.69	0.27	93,93,93,93	0
55	MG	BA	3509	1/1	0.69	0.29	83,83,83,83	0
55	MG	CA	1662	1/1	0.70	0.28	90,90,90,90	0
55	MG	CA	1689	1/1	0.70	0.28	89,89,89,89	0
55	MG	CA	1748	1/1	0.70	0.25	87,87,87,87	0
55	MG	AA	1782	1/1	0.70	0.09	96,96,96,96	0
55	MG	BA	3391	1/1	0.70	0.34	86,86,86,86	0
55	MG	DA	3377	1/1	0.70	0.20	98,98,98,98	0
55	MG	AB	101	1/1	0.70	0.17	90,90,90,90	0
55	MG	DA	3088	1/1	0.70	0.24	96,96,96,96	0
55	MG	DA	3419	1/1	0.70	0.30	84,84,84,84	0
55	MG	DA	3028	1/1	0.70	0.30	101,101,101,101	0
55	MG	CS	101	1/1	0.70	0.31	87,87,87,87	0
55	MG	DA	3381	1/1	0.71	0.44	99,99,99,99	0
55	MG	DA	3393	1/1	0.71	0.32	69,69,69,69	0
55	MG	CA	1687	1/1	0.71	0.22	89,89,89,89	0
55	MG	BA	3164	1/1	0.71	0.42	86,86,86,86	0
55	MG	BA	3222	1/1	0.71	0.36	89,89,89,89	0
55	MG	BA	3272	1/1	0.71	0.21	94,94,94,94	0
55	MG	AA	1678	1/1	0.71	0.37	74,74,74,74	0
55	MG	BA	3588	1/1	0.71	0.33	83,83,83,83	0
55	MG	BA	3591	1/1	0.71	0.32	64,64,64,64	0
55	MG	BA	3594	1/1	0.71	0.37	79,79,79,79	0
55	MG	CA	1718	1/1	0.71	0.17	92,92,92,92	0
55	MG	BB	209	1/1	0.71	0.33	102,102,102,102	0
55	MG	DA	3350	1/1	0.71	0.28	91,91,91,91	0
55	MG	DA	3357	1/1	0.71	0.27	96,96,96,96	0
55	MG	DA	3371	1/1	0.71	0.34	82,82,82,82	0
55	MG	AA	1693	1/1	0.71	0.22	87,87,87,87	0
55	MG	AA	1714	1/1	0.71	0.28	107,107,107,107	0
55	MG	CA	1778	1/1	0.72	0.31	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	AA	1757	1/1	0.72	0.15	110,110,110,110	0
55	MG	CA	1787	1/1	0.72	0.17	87,87,87,87	0
55	MG	BB	206	1/1	0.72	0.24	86,86,86,86	0
55	MG	CA	1803	1/1	0.72	0.30	96,96,96,96	0
55	MG	AA	1643	1/1	0.72	0.42	85,85,85,85	0
55	MG	AB	105	1/1	0.72	0.21	110,110,110,110	0
55	MG	AA	1760	1/1	0.72	0.27	78,78,78,78	0
55	MG	AC	105	1/1	0.72	0.35	93,93,93,93	0
55	MG	CA	1715	1/1	0.72	0.30	104,104,104,104	0
55	MG	DA	3380	1/1	0.72	0.14	139,139,139,139	0
55	MG	DA	3004	1/1	0.72	0.38	99,99,99,99	0
55	MG	CA	1614	1/1	0.72	0.31	86,86,86,86	0
55	MG	AA	1686	1/1	0.72	0.39	85,85,85,85	0
55	MG	DA	3413	1/1	0.72	0.30	94,94,94,94	0
55	MG	AA	1768	1/1	0.72	0.34	101,101,101,101	0
55	MG	BA	3513	1/1	0.72	0.33	90,90,90,90	0
55	MG	CA	1730	1/1	0.72	0.23	106,106,106,106	0
55	MG	CA	1737	1/1	0.72	0.26	99,99,99,99	0
55	MG	BA	3053	1/1	0.72	0.26	95,95,95,95	0
55	MG	BA	3534	1/1	0.72	0.27	79,79,79,79	0
55	MG	AA	1696	1/1	0.72	0.34	88,88,88,88	0
55	MG	AA	1777	1/1	0.72	0.33	90,90,90,90	0
55	MG	DA	3084	1/1	0.72	0.29	88,88,88,88	0
55	MG	AA	1607	1/1	0.72	0.30	89,89,89,89	0
55	MG	BA	3448	1/1	0.72	0.38	100,100,100,100	0
55	MG	DB	202	1/1	0.72	0.20	98,98,98,98	0
55	MG	CA	1762	1/1	0.72	0.27	96,96,96,96	0
55	MG	CA	1685	1/1	0.72	0.31	93,93,93,93	0
55	MG	BA	3479	1/1	0.72	0.29	82,82,82,82	0
55	MG	BA	3547	1/1	0.73	0.28	77,77,77,77	0
55	MG	CC	108	1/1	0.73	0.22	106,106,106,106	0
55	MG	AA	1639	1/1	0.73	0.37	91,91,91,91	0
55	MG	AA	1772	1/1	0.73	0.30	85,85,85,85	0
55	MG	CA	1658	1/1	0.73	0.39	91,91,91,91	0
55	MG	DA	3304	1/1	0.73	0.28	85,85,85,85	0
55	MG	CA	1694	1/1	0.73	0.41	97,97,97,97	0
55	MG	DA	3337	1/1	0.73	0.22	89,89,89,89	0
55	MG	DA	3024	1/1	0.73	0.38	108,108,108,108	0
55	MG	AA	1735	1/1	0.73	0.24	79,79,79,79	0
55	MG	DA	3437	1/1	0.73	0.27	87,87,87,87	0
55	MG	AA	1781	1/1	0.73	0.38	94,94,94,94	0
55	MG	CA	1735	1/1	0.74	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1796	1/1	0.74	0.25	102,102,102,102	0
55	MG	AA	1753	1/1	0.74	0.21	108,108,108,108	0
55	MG	DA	3073	1/1	0.74	0.49	80,80,80,80	0
55	MG	BA	3441	1/1	0.74	0.10	86,86,86,86	0
55	MG	BB	201	1/1	0.74	0.36	92,92,92,92	0
55	MG	DA	3394	1/1	0.74	0.24	90,90,90,90	0
55	MG	BA	3315	1/1	0.74	0.39	78,78,78,78	0
55	MG	DA	3412	1/1	0.74	0.33	89,89,89,89	0
55	MG	BA	3449	1/1	0.74	0.28	80,80,80,80	0
55	MG	DA	3417	1/1	0.74	0.32	81,81,81,81	0
55	MG	CA	1756	1/1	0.74	0.28	81,81,81,81	0
55	MG	DA	3089	1/1	0.74	0.42	82,82,82,82	0
55	MG	DA	3117	1/1	0.74	0.37	78,78,78,78	0
55	MG	CC	106	1/1	0.74	0.29	96,96,96,96	0
55	MG	AA	1790	1/1	0.74	0.25	98,98,98,98	0
55	MG	DA	3476	1/1	0.74	0.32	107,107,107,107	0
55	MG	DA	3477	1/1	0.74	0.33	89,89,89,89	0
55	MG	BA	3349	1/1	0.74	0.21	97,97,97,97	0
55	MG	AA	1630	1/1	0.74	0.25	101,101,101,101	0
55	MG	CA	1765	1/1	0.74	0.27	101,101,101,101	0
55	MG	DA	3279	1/1	0.74	0.32	84,84,84,84	0
55	MG	CA	1684	1/1	0.74	0.52	85,85,85,85	0
55	MG	CA	1773	1/1	0.74	0.36	92,92,92,92	0
55	MG	DA	3515	1/1	0.74	0.20	82,82,82,82	0
55	MG	DA	3516	1/1	0.74	0.29	105,105,105,105	0
55	MG	AA	1716	1/1	0.74	0.33	92,92,92,92	0
55	MG	BA	3290	1/1	0.74	0.27	97,97,97,97	0
55	MG	AA	1752	1/1	0.74	0.22	78,78,78,78	0
55	MG	CA	1785	1/1	0.74	0.36	105,105,105,105	0
55	MG	DA	3366	1/1	0.74	0.31	83,83,83,83	0
55	MG	DA	3436	1/1	0.75	0.32	98,98,98,98	0
55	MG	BA	3486	1/1	0.75	0.32	80,80,80,80	0
55	MG	CA	1769	1/1	0.75	0.31	105,105,105,105	0
55	MG	DA	3451	1/1	0.75	0.28	75,75,75,75	0
55	MG	DA	3458	1/1	0.75	0.40	92,92,92,92	0
55	MG	AA	1803	1/1	0.75	0.22	91,91,91,91	0
55	MG	CA	1771	1/1	0.75	0.21	76,76,76,76	0
55	MG	CA	1691	1/1	0.75	0.28	78,78,78,78	0
55	MG	BA	3151	1/1	0.75	0.31	83,83,83,83	0
55	MG	DA	3485	1/1	0.75	0.17	81,81,81,81	0
55	MG	CA	1651	1/1	0.75	0.30	90,90,90,90	0
55	MG	CA	1654	1/1	0.75	0.29	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	AA	1702	1/1	0.75	0.26	93,93,93,93	0
55	MG	CA	1710	1/1	0.75	0.29	106,106,106,106	0
55	MG	BA	3397	1/1	0.75	0.22	81,81,81,81	0
55	MG	BA	3467	1/1	0.75	0.30	78,78,78,78	0
55	MG	DA	3269	1/1	0.75	0.38	84,84,84,84	0
55	MG	DA	3040	1/1	0.75	0.18	81,81,81,81	0
55	MG	BA	3477	1/1	0.75	0.37	95,95,95,95	0
55	MG	DA	3061	1/1	0.75	0.27	74,74,74,74	0
55	MG	AA	1738	1/1	0.75	0.27	79,79,79,79	0
55	MG	AA	1834	1/1	0.75	0.33	97,97,97,97	0
55	MG	AA	1813	1/1	0.76	0.24	107,107,107,107	0
55	MG	AA	1822	1/1	0.76	0.18	107,107,107,107	0
55	MG	DA	3093	1/1	0.76	0.19	80,80,80,80	0
55	MG	DA	3025	1/1	0.76	0.48	84,84,84,84	0
55	MG	AA	1720	1/1	0.76	0.20	93,93,93,93	0
55	MG	BA	3215	1/1	0.76	0.31	74,74,74,74	0
55	MG	CA	1667	1/1	0.76	0.13	102,102,102,102	0
55	MG	DA	3208	1/1	0.76	0.35	74,74,74,74	0
55	MG	CA	1627	1/1	0.76	0.24	88,88,88,88	0
55	MG	DA	3500	1/1	0.76	0.22	92,92,92,92	0
55	MG	BA	3354	1/1	0.76	0.16	72,72,72,72	0
55	MG	DA	3507	1/1	0.76	0.45	91,91,91,91	0
55	MG	CA	1633	1/1	0.76	0.31	91,91,91,91	0
55	MG	CA	1723	1/1	0.76	0.16	86,86,86,86	0
55	MG	CA	1725	1/1	0.76	0.28	86,86,86,86	0
55	MG	AA	1614	1/1	0.76	0.26	91,91,91,91	0
55	MG	BA	3086	1/1	0.76	0.20	95,95,95,95	0
55	MG	DB	206	1/1	0.76	0.27	90,90,90,90	0
55	MG	BA	3089	1/1	0.76	0.17	88,88,88,88	0
55	MG	DB	208	1/1	0.76	0.29	90,90,90,90	0
55	MG	AA	1648	1/1	0.76	0.31	78,78,78,78	0
55	MG	BA	3303	1/1	0.76	0.25	72,72,72,72	0
55	MG	DA	3338	1/1	0.77	0.28	86,86,86,86	0
55	MG	BA	3257	1/1	0.77	0.21	64,64,64,64	0
55	MG	CA	1628	1/1	0.77	0.25	101,101,101,101	0
55	MG	DA	3473	1/1	0.77	0.35	96,96,96,96	0
55	MG	CA	1630	1/1	0.77	0.35	91,91,91,91	0
55	MG	AA	1736	1/1	0.77	0.29	90,90,90,90	0
55	MG	AA	1770	1/1	0.77	0.26	102,102,102,102	0
55	MG	DA	3094	1/1	0.77	0.11	94,94,94,94	0
55	MG	BA	3546	1/1	0.77	0.18	87,87,87,87	0
55	MG	DA	3119	1/1	0.77	0.38	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3342	1/1	0.77	0.27	66,66,66,66	0
55	MG	DA	3492	1/1	0.77	0.28	88,88,88,88	0
55	MG	DA	3493	1/1	0.77	0.28	82,82,82,82	0
55	MG	DA	3387	1/1	0.77	0.29	92,92,92,92	0
55	MG	DA	3047	1/1	0.77	0.31	76,76,76,76	0
55	MG	AA	1609	1/1	0.77	0.39	78,78,78,78	0
55	MG	DA	3396	1/1	0.77	0.27	82,82,82,82	0
55	MG	BA	3570	1/1	0.77	0.33	87,87,87,87	0
55	MG	BA	3223	1/1	0.77	0.27	92,92,92,92	0
55	MG	BA	3582	1/1	0.77	0.31	86,86,86,86	0
55	MG	BA	3584	1/1	0.77	0.19	72,72,72,72	0
55	MG	CA	1777	1/1	0.77	0.28	88,88,88,88	0
55	MG	DA	3302	1/1	0.77	0.42	95,95,95,95	0
55	MG	DA	3080	1/1	0.77	0.39	75,75,75,75	0
55	MG	BA	3368	1/1	0.77	0.21	88,88,88,88	0
55	MG	CA	1781	1/1	0.77	0.17	117,117,117,117	0
55	MG	DB	214	1/1	0.77	0.15	96,96,96,96	0
55	MG	BA	3127	1/1	0.78	0.33	53,53,53,53	0
55	MG	BA	3461	1/1	0.78	0.17	91,91,91,91	0
55	MG	DA	3461	1/1	0.78	0.20	84,84,84,84	0
55	MG	DA	3067	1/1	0.78	0.32	94,94,94,94	0
55	MG	BA	3606	1/1	0.78	0.27	77,77,77,77	0
55	MG	DA	3342	1/1	0.78	0.41	82,82,82,82	0
55	MG	CA	1637	1/1	0.78	0.29	79,79,79,79	0
55	MG	DA	3478	1/1	0.78	0.31	80,80,80,80	0
55	MG	BA	3621	1/1	0.78	0.19	63,63,63,63	0
55	MG	DA	3484	1/1	0.78	0.35	83,83,83,83	0
55	MG	CA	1639	1/1	0.78	0.45	95,95,95,95	0
55	MG	BA	3068	1/1	0.78	0.27	75,75,75,75	0
55	MG	CC	104	1/1	0.78	0.27	89,89,89,89	0
55	MG	BB	202	1/1	0.78	0.17	79,79,79,79	0
55	MG	BA	3475	1/1	0.78	0.24	83,83,83,83	0
55	MG	CA	1767	1/1	0.78	0.33	77,77,77,77	0
55	MG	BA	3317	1/1	0.78	0.44	89,89,89,89	0
55	MG	CA	1657	1/1	0.78	0.33	95,95,95,95	0
55	MG	BA	3325	1/1	0.78	0.30	76,76,76,76	0
55	MG	DA	3015	1/1	0.78	0.28	89,89,89,89	0
55	MG	BA	3327	1/1	0.78	0.21	70,70,70,70	0
55	MG	AA	1827	1/1	0.78	0.33	87,87,87,87	0
55	MG	BA	3432	1/1	0.78	0.25	80,80,80,80	0
55	MG	AA	1637	1/1	0.78	0.24	98,98,98,98	0
55	MG	AA	1767	1/1	0.78	0.37	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	3038	1/1	0.78	0.40	97,97,97,97	0
55	MG	CA	1732	1/1	0.78	0.27	109,109,109,109	0
55	MG	DA	3043	1/1	0.78	0.18	82,82,82,82	0
55	MG	BA	3446	1/1	0.78	0.20	92,92,92,92	0
55	MG	AA	1804	1/1	0.78	0.20	74,74,74,74	0
55	MG	CA	1703	1/1	0.79	0.28	94,94,94,94	0
55	MG	BA	3076	1/1	0.79	0.34	68,68,68,68	0
55	MG	DA	3354	1/1	0.79	0.34	73,73,73,73	0
55	MG	AA	1611	1/1	0.79	0.26	92,92,92,92	0
55	MG	DA	3363	1/1	0.79	0.55	79,79,79,79	0
55	MG	BB	203	1/1	0.79	0.35	65,65,65,65	0
55	MG	BA	3219	1/1	0.79	0.34	76,76,76,76	0
55	MG	DA	3375	1/1	0.79	0.28	88,88,88,88	0
55	MG	DA	3146	1/1	0.79	0.42	92,92,92,92	0
55	MG	CA	1661	1/1	0.79	0.27	87,87,87,87	0
55	MG	BB	208	1/1	0.79	0.23	74,74,74,74	0
55	MG	DA	3231	1/1	0.79	0.38	72,72,72,72	0
55	MG	AA	1668	1/1	0.79	0.42	76,76,76,76	0
55	MG	AA	1746	1/1	0.79	0.29	84,84,84,84	0
55	MG	DA	3275	1/1	0.79	0.30	76,76,76,76	0
55	MG	DA	3498	1/1	0.79	0.26	85,85,85,85	0
55	MG	BA	3059	1/1	0.79	0.29	91,91,91,91	0
55	MG	DA	3501	1/1	0.79	0.40	88,88,88,88	0
55	MG	DA	3399	1/1	0.79	0.38	76,76,76,76	0
55	MG	AA	1791	1/1	0.79	0.20	109,109,109,109	0
55	MG	DA	3292	1/1	0.79	0.22	89,89,89,89	0
55	MG	CA	1612	1/1	0.79	0.14	82,82,82,82	0
55	MG	AA	1819	1/1	0.79	0.40	87,87,87,87	0
55	MG	DA	3517	1/1	0.79	0.22	84,84,84,84	0
55	MG	DA	3312	1/1	0.79	0.28	85,85,85,85	0
55	MG	CG	302	1/1	0.79	0.19	101,101,101,101	0
55	MG	BA	3408	1/1	0.79	0.28	87,87,87,87	0
55	MG	DA	3090	1/1	0.79	0.35	86,86,86,86	0
55	MG	DA	3340	1/1	0.79	0.20	85,85,85,85	0
55	MG	DA	3445	1/1	0.79	0.27	78,78,78,78	0
55	MG	DA	3449	1/1	0.79	0.20	87,87,87,87	0
55	MG	CA	1625	1/1	0.79	0.29	90,90,90,90	0
55	MG	BA	3321	1/1	0.80	0.29	77,77,77,77	0
55	MG	DA	3289	1/1	0.80	0.28	90,90,90,90	0
55	MG	AA	1677	1/1	0.80	0.31	87,87,87,87	0
55	MG	AA	1817	1/1	0.80	0.29	85,85,85,85	0
55	MG	AA	1615	1/1	0.80	0.30	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1740	1/1	0.80	0.11	75,75,75,75	0
55	MG	BA	3623	1/1	0.80	0.29	60,60,60,60	0
55	MG	DA	3333	1/1	0.80	0.34	87,87,87,87	0
55	MG	CG	301	1/1	0.80	0.29	83,83,83,83	0
55	MG	CA	1693	1/1	0.80	0.41	76,76,76,76	0
55	MG	BA	3514	1/1	0.80	0.23	71,71,71,71	0
55	MG	CA	1696	1/1	0.80	0.36	91,91,91,91	0
55	MG	CA	1635	1/1	0.80	0.37	86,86,86,86	0
55	MG	BA	3345	1/1	0.80	0.50	73,73,73,73	0
55	MG	CA	1761	1/1	0.80	0.43	92,92,92,92	0
55	MG	AA	1684	1/1	0.80	0.22	90,90,90,90	0
55	MG	DA	3358	1/1	0.80	0.36	88,88,88,88	0
55	MG	CA	1763	1/1	0.80	0.27	91,91,91,91	0
55	MG	DA	3091	1/1	0.80	0.27	92,92,92,92	0
55	MG	DA	3005	1/1	0.80	0.34	77,77,77,77	0
55	MG	AA	1725	1/1	0.80	0.22	82,82,82,82	0
55	MG	BA	3145	1/1	0.80	0.35	74,74,74,74	0
55	MG	BA	3292	1/1	0.80	0.39	85,85,85,85	0
55	MG	BB	211	1/1	0.80	0.21	92,92,92,92	0
55	MG	DA	3502	1/1	0.80	0.36	97,97,97,97	0
55	MG	DA	3128	1/1	0.80	0.30	77,77,77,77	0
55	MG	AA	1674	1/1	0.80	0.29	98,98,98,98	0
55	MG	AA	1749	1/1	0.80	0.19	81,81,81,81	0
55	MG	BA	3573	1/1	0.80	0.26	83,83,83,83	0
55	MG	BA	3203	1/1	0.80	0.26	85,85,85,85	0
55	MG	BA	3204	1/1	0.80	0.31	78,78,78,78	0
55	MG	DA	3518	1/1	0.80	0.34	83,83,83,83	0
55	MG	DA	3259	1/1	0.80	0.18	72,72,72,72	0
55	MG	BA	3210	1/1	0.80	0.17	74,74,74,74	0
55	MG	CA	1624	1/1	0.80	0.27	88,88,88,88	0
55	MG	CA	1729	1/1	0.80	0.29	77,77,77,77	0
55	MG	DA	3276	1/1	0.80	0.39	68,68,68,68	0
55	MG	DA	3056	1/1	0.80	0.41	81,81,81,81	0
55	MG	DA	3430	1/1	0.80	0.24	62,62,62,62	0
55	MG	DA	3434	1/1	0.80	0.08	74,74,74,74	0
55	MG	AA	1807	1/1	0.81	0.54	98,98,98,98	0
55	MG	CA	1702	1/1	0.81	0.31	78,78,78,78	0
55	MG	BA	3414	1/1	0.81	0.13	72,72,72,72	0
55	MG	AA	1730	1/1	0.81	0.13	78,78,78,78	0
55	MG	DA	3435	1/1	0.81	0.16	72,72,72,72	0
55	MG	AA	1679	1/1	0.81	0.29	86,86,86,86	0
55	MG	BA	3496	1/1	0.81	0.27	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	3283	1/1	0.81	0.18	61,61,61,61	0
55	MG	AA	1794	1/1	0.81	0.30	84,84,84,84	0
55	MG	BA	3613	1/1	0.81	0.46	93,93,93,93	0
55	MG	CA	1780	1/1	0.81	0.37	88,88,88,88	0
55	MG	BA	3361	1/1	0.81	0.23	64,64,64,64	0
55	MG	DA	3309	1/1	0.81	0.23	94,94,94,94	0
55	MG	BA	3444	1/1	0.81	0.28	78,78,78,78	0
55	MG	AA	1616	1/1	0.81	0.21	94,94,94,94	0
55	MG	DA	3319	1/1	0.81	0.33	74,74,74,74	0
55	MG	CA	1786	1/1	0.81	0.27	73,73,73,73	0
55	MG	DA	3336	1/1	0.81	0.30	87,87,87,87	0
55	MG	BA	3447	1/1	0.81	0.27	71,71,71,71	0
55	MG	BA	3324	1/1	0.81	0.33	73,73,73,73	0
55	MG	BA	3385	1/1	0.81	0.14	87,87,87,87	0
55	MG	BA	3521	1/1	0.81	0.36	79,79,79,79	0
55	MG	BA	3524	1/1	0.81	0.21	66,66,66,66	0
55	MG	BA	3527	1/1	0.81	0.27	93,93,93,93	0
55	MG	BB	214	1/1	0.81	0.16	86,86,86,86	0
55	MG	BA	3530	1/1	0.81	0.24	81,81,81,81	0
55	MG	B8	101	1/1	0.81	0.35	97,97,97,97	0
55	MG	CA	1663	1/1	0.81	0.34	81,81,81,81	0
55	MG	BA	3458	1/1	0.81	0.17	82,82,82,82	0
55	MG	CA	1677	1/1	0.81	0.31	73,73,73,73	0
55	MG	AA	1625	1/1	0.81	0.20	57,57,57,57	0
55	MG	CA	1755	1/1	0.81	0.47	92,92,92,92	0
55	MG	BA	3394	1/1	0.81	0.20	81,81,81,81	0
55	MG	BA	3470	1/1	0.81	0.26	88,88,88,88	0
55	MG	CA	1616	1/1	0.81	0.27	88,88,88,88	0
55	MG	DA	3136	1/1	0.81	0.30	76,76,76,76	0
55	MG	BA	3472	1/1	0.81	0.33	89,89,89,89	0
55	MG	AA	1786	1/1	0.81	0.19	86,86,86,86	0
55	MG	DA	3185	1/1	0.81	0.26	74,74,74,74	0
55	MG	BA	3399	1/1	0.81	0.35	90,90,90,90	0
55	MG	AQ	101	1/1	0.81	0.17	88,88,88,88	0
55	MG	DA	3237	1/1	0.81	0.25	83,83,83,83	0
55	MG	DB	209	1/1	0.81	0.18	92,92,92,92	0
55	MG	CA	1766	1/1	0.81	0.33	85,85,85,85	0
55	MG	DA	3415	1/1	0.81	0.40	96,96,96,96	0
55	MG	DA	3268	1/1	0.81	0.32	69,69,69,69	0
55	MG	CC	105	1/1	0.82	0.36	82,82,82,82	0
55	MG	DA	3403	1/1	0.82	0.27	76,76,76,76	0
55	MG	BA	3116	1/1	0.82	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3406	1/1	0.82	0.26	86,86,86,86	0
55	MG	DA	3410	1/1	0.82	0.30	78,78,78,78	0
55	MG	BA	3518	1/1	0.82	0.23	70,70,70,70	0
55	MG	CA	1744	1/1	0.82	0.34	79,79,79,79	0
55	MG	AA	1706	1/1	0.82	0.34	74,74,74,74	0
55	MG	BA	3278	1/1	0.82	0.32	81,81,81,81	0
55	MG	BA	3360	1/1	0.82	0.16	84,84,84,84	0
55	MG	DA	3236	1/1	0.82	0.12	55,55,55,55	0
55	MG	BA	3525	1/1	0.82	0.26	77,77,77,77	0
55	MG	DA	3014	1/1	0.82	0.36	74,74,74,74	0
55	MG	BA	3454	1/1	0.82	0.24	92,92,92,92	0
55	MG	DA	3018	1/1	0.82	0.28	77,77,77,77	0
55	MG	BB	217	1/1	0.82	0.20	98,98,98,98	0
55	MG	AA	1690	1/1	0.82	0.31	96,96,96,96	0
55	MG	BA	3362	1/1	0.82	0.09	48,48,48,48	0
55	MG	BA	3291	1/1	0.82	0.24	72,72,72,72	0
55	MG	CA	1610	1/1	0.82	0.27	97,97,97,97	0
55	MG	DA	3282	1/1	0.82	0.18	69,69,69,69	0
55	MG	DA	3459	1/1	0.82	0.22	86,86,86,86	0
55	MG	DA	3036	1/1	0.82	0.25	99,99,99,99	0
55	MG	CA	1611	1/1	0.82	0.38	93,93,93,93	0
55	MG	AA	1824	1/1	0.82	0.34	86,86,86,86	0
55	MG	DA	3041	1/1	0.82	0.34	86,86,86,86	0
55	MG	AA	1681	1/1	0.82	0.36	80,80,80,80	0
55	MG	BA	3548	1/1	0.82	0.43	76,76,76,76	0
55	MG	CA	1617	1/1	0.82	0.26	93,93,93,93	0
55	MG	DA	3057	1/1	0.82	0.25	83,83,83,83	0
55	MG	AA	1685	1/1	0.82	0.28	88,88,88,88	0
55	MG	DA	3327	1/1	0.82	0.19	61,61,61,61	0
55	MG	BA	3563	1/1	0.82	0.23	82,82,82,82	0
55	MG	DA	3335	1/1	0.82	0.22	61,61,61,61	0
55	MG	DA	3063	1/1	0.82	0.47	75,75,75,75	0
55	MG	AB	102	1/1	0.82	0.23	86,86,86,86	0
55	MG	AA	1743	1/1	0.82	0.20	107,107,107,107	0
55	MG	BA	3085	1/1	0.82	0.15	73,73,73,73	0
55	MG	CA	1708	1/1	0.82	0.20	97,97,97,97	0
55	MG	BA	3400	1/1	0.82	0.42	80,80,80,80	0
55	MG	CA	1629	1/1	0.82	0.19	98,98,98,98	0
55	MG	BA	3489	1/1	0.82	0.18	70,70,70,70	0
55	MG	BA	3585	1/1	0.82	0.26	60,60,60,60	0
55	MG	DA	3509	1/1	0.82	0.22	64,64,64,64	0
55	MG	AA	1695	1/1	0.82	0.29	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	3087	1/1	0.82	0.33	77,77,77,77	0
55	MG	AA	1727	1/1	0.82	0.36	87,87,87,87	0
55	MG	BA	3498	1/1	0.82	0.22	85,85,85,85	0
55	MG	DA	3519	1/1	0.82	0.29	85,85,85,85	0
55	MG	CA	1724	1/1	0.82	0.28	84,84,84,84	0
55	MG	CA	1806	1/1	0.82	0.38	96,96,96,96	0
55	MG	DA	3092	1/1	0.82	0.20	68,68,68,68	0
55	MG	AA	1818	1/1	0.82	0.45	76,76,76,76	0
55	MG	CA	1640	1/1	0.82	0.30	81,81,81,81	0
55	MG	BA	3330	1/1	0.82	0.30	79,79,79,79	0
55	MG	BA	3239	1/1	0.82	0.21	74,74,74,74	0
55	MG	BA	3341	1/1	0.82	0.22	81,81,81,81	0
55	MG	BA	3247	1/1	0.82	0.30	70,70,70,70	0
55	MG	CA	1604	1/1	0.83	0.24	81,81,81,81	0
55	MG	BA	3473	1/1	0.83	0.27	76,76,76,76	0
55	MG	BA	3358	1/1	0.83	0.28	74,74,74,74	0
55	MG	AA	1739	1/1	0.83	0.08	93,93,93,93	0
55	MG	DA	3341	1/1	0.83	0.33	84,84,84,84	0
55	MG	BA	3586	1/1	0.83	0.29	63,63,63,63	0
55	MG	BA	3340	1/1	0.83	0.23	77,77,77,77	0
55	MG	BA	3481	1/1	0.83	0.33	69,69,69,69	0
55	MG	DA	3467	1/1	0.83	0.25	61,61,61,61	0
55	MG	DA	3353	1/1	0.83	0.35	93,93,93,93	0
55	MG	CA	1782	1/1	0.83	0.38	93,93,93,93	0
55	MG	CA	1664	1/1	0.83	0.36	99,99,99,99	0
55	MG	BA	3445	1/1	0.83	0.24	79,79,79,79	0
55	MG	DA	3479	1/1	0.83	0.17	99,99,99,99	0
55	MG	DA	3197	1/1	0.83	0.32	70,70,70,70	0
55	MG	DA	3207	1/1	0.83	0.33	66,66,66,66	0
55	MG	BA	3060	1/1	0.83	0.20	64,64,64,64	0
55	MG	DA	3486	1/1	0.83	0.14	68,68,68,68	0
55	MG	BA	3366	1/1	0.83	0.43	94,94,94,94	0
55	MG	BA	3618	1/1	0.83	0.33	73,73,73,73	0
55	MG	DA	3049	1/1	0.83	0.27	74,74,74,74	0
55	MG	BA	3619	1/1	0.83	0.41	69,69,69,69	0
55	MG	BA	3529	1/1	0.83	0.29	68,68,68,68	0
55	MG	DA	3497	1/1	0.83	0.17	74,74,74,74	0
55	MG	BA	3404	1/1	0.83	0.11	60,60,60,60	0
55	MG	BA	3493	1/1	0.83	0.32	63,63,63,63	0
55	MG	CA	1751	1/1	0.83	0.32	94,94,94,94	0
55	MG	BA	3537	1/1	0.83	0.30	89,89,89,89	0
55	MG	BA	3406	1/1	0.83	0.29	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3401	1/1	0.83	0.20	71,71,71,71	0
55	MG	DA	3402	1/1	0.83	0.29	101,101,101,101	0
55	MG	BA	3301	1/1	0.83	0.27	76,76,76,76	0
55	MG	DA	3511	1/1	0.83	0.32	76,76,76,76	0
55	MG	AA	1620	1/1	0.83	0.21	66,66,66,66	0
55	MG	CB	103	1/1	0.83	0.20	103,103,103,103	0
55	MG	CC	101	1/1	0.83	0.18	92,92,92,92	0
55	MG	BA	3419	1/1	0.83	0.31	85,85,85,85	0
55	MG	DA	3297	1/1	0.83	0.20	83,83,83,83	0
55	MG	AA	1756	1/1	0.83	0.16	69,69,69,69	0
55	MG	CA	1706	1/1	0.83	0.30	87,87,87,87	0
55	MG	BA	3506	1/1	0.83	0.29	78,78,78,78	0
55	MG	BA	3431	1/1	0.83	0.34	88,88,88,88	0
55	MG	BA	3571	1/1	0.83	0.26	92,92,92,92	0
55	MG	BO	202	1/1	0.83	0.17	37,37,37,37	0
55	MG	CA	1768	1/1	0.83	0.20	84,84,84,84	0
55	MG	AA	1683	1/1	0.83	0.20	87,87,87,87	0
55	MG	BA	3511	1/1	0.83	0.18	89,89,89,89	0
55	MG	DE	302	1/1	0.83	0.27	65,65,65,65	0
55	MG	BA	3265	1/1	0.84	0.35	60,60,60,60	0
55	MG	DA	3039	1/1	0.84	0.21	85,85,85,85	0
55	MG	BE	305	1/1	0.84	0.27	71,71,71,71	0
55	MG	BO	201	1/1	0.84	0.32	62,62,62,62	0
55	MG	BA	3143	1/1	0.84	0.55	72,72,72,72	0
55	MG	BA	3072	1/1	0.84	0.23	77,77,77,77	0
55	MG	DA	3427	1/1	0.84	0.25	76,76,76,76	0
55	MG	BA	3577	1/1	0.84	0.22	73,73,73,73	0
55	MG	BA	3455	1/1	0.84	0.15	76,76,76,76	0
55	MG	CA	1606	1/1	0.84	0.30	87,87,87,87	0
55	MG	DA	3058	1/1	0.84	0.21	76,76,76,76	0
55	MG	CA	1607	1/1	0.84	0.44	85,85,85,85	0
55	MG	CA	1788	1/1	0.84	0.29	84,84,84,84	0
55	MG	CA	1791	1/1	0.84	0.25	79,79,79,79	0
55	MG	DA	3442	1/1	0.84	0.23	91,91,91,91	0
55	MG	CA	1608	1/1	0.84	0.34	81,81,81,81	0
55	MG	DA	3448	1/1	0.84	0.41	79,79,79,79	0
55	MG	DA	3303	1/1	0.84	0.31	70,70,70,70	0
55	MG	DA	3066	1/1	0.84	0.26	65,65,65,65	0
55	MG	DA	3454	1/1	0.84	0.28	92,92,92,92	0
55	MG	DA	3308	1/1	0.84	0.29	97,97,97,97	0
55	MG	BA	3510	1/1	0.84	0.22	108,108,108,108	0
55	MG	CA	1800	1/1	0.84	0.18	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	CA	1801	1/1	0.84	0.20	89,89,89,89	0
55	MG	BA	3282	1/1	0.84	0.10	83,83,83,83	0
55	MG	DA	3075	1/1	0.84	0.34	79,79,79,79	0
55	MG	DA	3475	1/1	0.84	0.30	88,88,88,88	0
55	MG	AA	1814	1/1	0.84	0.32	83,83,83,83	0
55	MG	DA	3082	1/1	0.84	0.23	91,91,91,91	0
55	MG	AA	1682	1/1	0.84	0.22	91,91,91,91	0
55	MG	CA	1742	1/1	0.84	0.21	97,97,97,97	0
55	MG	CA	1743	1/1	0.84	0.38	80,80,80,80	0
55	MG	DA	3483	1/1	0.84	0.19	90,90,90,90	0
55	MG	AA	1734	1/1	0.84	0.14	96,96,96,96	0
55	MG	BA	3293	1/1	0.84	0.23	65,65,65,65	0
55	MG	BA	3412	1/1	0.84	0.24	78,78,78,78	0
55	MG	CA	1749	1/1	0.84	0.24	89,89,89,89	0
55	MG	DA	3345	1/1	0.84	0.28	64,64,64,64	0
55	MG	DA	3349	1/1	0.84	0.21	63,63,63,63	0
55	MG	BA	3295	1/1	0.84	0.30	81,81,81,81	0
55	MG	BA	3417	1/1	0.84	0.23	99,99,99,99	0
55	MG	AA	1747	1/1	0.84	0.41	88,88,88,88	0
55	MG	AA	1787	1/1	0.84	0.35	96,96,96,96	0
55	MG	AA	1776	1/1	0.84	0.24	82,82,82,82	0
55	MG	CA	1698	1/1	0.84	0.11	107,107,107,107	0
55	MG	DA	3364	1/1	0.84	0.20	71,71,71,71	0
55	MG	CA	1760	1/1	0.84	0.25	91,91,91,91	0
55	MG	DA	3505	1/1	0.84	0.34	81,81,81,81	0
55	MG	DA	3369	1/1	0.84	0.22	74,74,74,74	0
55	MG	BA	3110	1/1	0.84	0.28	59,59,59,59	0
55	MG	BA	3437	1/1	0.84	0.28	67,67,67,67	0
55	MG	DA	3376	1/1	0.84	0.42	82,82,82,82	0
55	MG	BA	3065	1/1	0.84	0.27	91,91,91,91	0
55	MG	DA	3139	1/1	0.84	0.26	80,80,80,80	0
55	MG	BA	3367	1/1	0.84	0.23	82,82,82,82	0
55	MG	AA	1724	1/1	0.84	0.28	84,84,84,84	0
55	MG	BA	3069	1/1	0.84	0.31	77,77,77,77	0
55	MG	DA	3193	1/1	0.84	0.31	63,63,63,63	0
55	MG	BA	3133	1/1	0.84	0.23	66,66,66,66	0
55	MG	CA	1709	1/1	0.84	0.39	108,108,108,108	0
55	MG	DA	3398	1/1	0.84	0.28	74,74,74,74	0
55	MG	BA	3071	1/1	0.84	0.24	70,70,70,70	0
55	MG	DA	3228	1/1	0.84	0.28	44,44,44,44	0
55	MG	CA	1712	1/1	0.84	0.38	86,86,86,86	0
55	MG	BA	3566	1/1	0.84	0.28	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	BA	3568	1/1	0.84	0.32	83,83,83,83	0
55	MG	DA	3249	1/1	0.84	0.30	72,72,72,72	0
55	MG	DA	3281	1/1	0.85	0.51	76,76,76,76	0
55	MG	BA	3104	1/1	0.85	0.16	57,57,57,57	0
55	MG	CA	1784	1/1	0.85	0.23	81,81,81,81	0
55	MG	BA	3411	1/1	0.85	0.28	68,68,68,68	0
55	MG	DA	3290	1/1	0.85	0.26	79,79,79,79	0
55	MG	BA	3106	1/1	0.85	0.25	75,75,75,75	0
55	MG	DA	3432	1/1	0.85	0.25	69,69,69,69	0
55	MG	BA	3533	1/1	0.85	0.32	72,72,72,72	0
55	MG	BA	3476	1/1	0.85	0.23	81,81,81,81	0
55	MG	CA	1790	1/1	0.85	0.20	110,110,110,110	0
55	MG	AA	1661	1/1	0.85	0.22	48,48,48,48	0
55	MG	DA	3440	1/1	0.85	0.16	86,86,86,86	0
55	MG	BB	215	1/1	0.85	0.25	82,82,82,82	0
55	MG	BA	3478	1/1	0.85	0.27	63,63,63,63	0
55	MG	DA	3443	1/1	0.85	0.28	80,80,80,80	0
55	MG	BA	3415	1/1	0.85	0.29	84,84,84,84	0
55	MG	DA	3313	1/1	0.85	0.26	85,85,85,85	0
55	MG	CA	1740	1/1	0.85	0.20	68,68,68,68	0
55	MG	BE	304	1/1	0.85	0.19	80,80,80,80	0
55	MG	DA	3453	1/1	0.85	0.17	66,66,66,66	0
55	MG	DA	3322	1/1	0.85	0.32	70,70,70,70	0
55	MG	AA	1742	1/1	0.85	0.24	78,78,78,78	0
55	MG	DA	3330	1/1	0.85	0.22	81,81,81,81	0
55	MG	DA	3332	1/1	0.85	0.21	76,76,76,76	0
55	MG	AA	1789	1/1	0.85	0.31	74,74,74,74	0
55	MG	DA	3466	1/1	0.85	0.38	78,78,78,78	0
55	MG	BA	3551	1/1	0.85	0.27	87,87,87,87	0
55	MG	DA	3468	1/1	0.85	0.23	92,92,92,92	0
55	MG	DA	3469	1/1	0.85	0.38	80,80,80,80	0
55	MG	CA	1745	1/1	0.85	0.21	91,91,91,91	0
55	MG	BA	3485	1/1	0.85	0.24	80,80,80,80	0
55	MG	AA	1751	1/1	0.85	0.26	98,98,98,98	0
55	MG	BA	3487	1/1	0.85	0.15	94,94,94,94	0
55	MG	BA	3364	1/1	0.85	0.21	82,82,82,82	0
55	MG	CA	1752	1/1	0.85	0.18	70,70,70,70	0
55	MG	AA	1703	1/1	0.85	0.34	92,92,92,92	0
55	MG	BA	3073	1/1	0.85	0.27	82,82,82,82	0
55	MG	AA	1649	1/1	0.85	0.22	79,79,79,79	0
55	MG	BA	3369	1/1	0.85	0.29	73,73,73,73	0
55	MG	CA	1758	1/1	0.85	0.37	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	3002	1/1	0.85	0.50	93,93,93,93	0
55	MG	BA	3371	1/1	0.85	0.32	70,70,70,70	0
55	MG	AA	1733	1/1	0.85	0.37	71,71,71,71	0
55	MG	BA	3328	1/1	0.85	0.40	69,69,69,69	0
55	MG	DA	3138	1/1	0.85	0.24	70,70,70,70	0
55	MG	BA	3146	1/1	0.85	0.27	59,59,59,59	0
55	MG	DA	3367	1/1	0.85	0.31	82,82,82,82	0
55	MG	BA	3393	1/1	0.85	0.30	81,81,81,81	0
55	MG	CA	1764	1/1	0.85	0.43	72,72,72,72	0
55	MG	DA	3153	1/1	0.85	0.21	70,70,70,70	0
55	MG	AA	1801	1/1	0.85	0.43	84,84,84,84	0
55	MG	DA	3019	1/1	0.85	0.60	90,90,90,90	0
55	MG	BA	3339	1/1	0.85	0.31	88,88,88,88	0
55	MG	AA	1840	1/1	0.85	0.44	87,87,87,87	0
55	MG	BA	3595	1/1	0.85	0.18	65,65,65,65	0
55	MG	DA	3383	1/1	0.85	0.38	87,87,87,87	0
55	MG	DA	3513	1/1	0.85	0.26	67,67,67,67	0
55	MG	DA	3212	1/1	0.85	0.35	48,48,48,48	0
55	MG	BA	3600	1/1	0.85	0.24	66,66,66,66	0
55	MG	AA	1823	1/1	0.85	0.30	77,77,77,77	0
55	MG	AA	1672	1/1	0.85	0.26	87,87,87,87	0
55	MG	DA	3397	1/1	0.85	0.18	60,60,60,60	0
55	MG	CA	1772	1/1	0.85	0.32	72,72,72,72	0
55	MG	DA	3525	1/1	0.85	0.25	79,79,79,79	0
55	MG	BA	3615	1/1	0.85	0.34	81,81,81,81	0
55	MG	BA	3464	1/1	0.85	0.30	77,77,77,77	0
55	MG	BA	3466	1/1	0.85	0.30	97,97,97,97	0
55	MG	DA	3042	1/1	0.85	0.23	81,81,81,81	0
55	MG	BA	3094	1/1	0.85	0.33	78,78,78,78	0
55	MG	DB	210	1/1	0.85	0.34	71,71,71,71	0
55	MG	DA	3045	1/1	0.85	0.35	94,94,94,94	0
55	MG	BA	3523	1/1	0.85	0.50	70,70,70,70	0
55	MG	BA	3468	1/1	0.85	0.26	77,77,77,77	0
55	MG	BA	3348	1/1	0.85	0.21	61,61,61,61	0
55	MG	D1	201	1/1	0.85	0.37	71,71,71,71	0
55	MG	DU	201	1/1	0.85	0.16	72,72,72,72	0
55	MG	CA	1681	1/1	0.86	0.26	72,72,72,72	0
55	MG	DA	3263	1/1	0.86	0.68	82,82,82,82	0
55	MG	AA	1775	1/1	0.86	0.11	79,79,79,79	0
55	MG	DA	3414	1/1	0.86	0.37	85,85,85,85	0
55	MG	BF	303	1/1	0.86	0.32	66,66,66,66	0
55	MG	DA	3270	1/1	0.86	0.21	83,83,83,83	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	0.86	0.28	80,80,80,80	0
55	MG	DA	3422	1/1	0.86	0.32	84,84,84,84	0
55	MG	BA	3396	1/1	0.86	0.17	82,82,82,82	0
55	MG	BU	202	1/1	0.86	0.09	55,55,55,55	0
55	MG	BA	3191	1/1	0.86	0.19	81,81,81,81	0
55	MG	BA	3316	1/1	0.86	0.39	69,69,69,69	0
55	MG	CA	1603	1/1	0.86	0.40	77,77,77,77	0
55	MG	BA	3555	1/1	0.86	0.14	38,38,38,38	0
55	MG	AC	103	1/1	0.86	0.28	66,66,66,66	0
55	MG	BA	3565	1/1	0.86	0.29	77,77,77,77	0
55	MG	BA	3084	1/1	0.86	0.40	82,82,82,82	0
55	MG	AA	1613	1/1	0.86	0.13	85,85,85,85	0
55	MG	AA	1765	1/1	0.86	0.24	84,84,84,84	0
55	MG	AC	108	1/1	0.86	0.28	85,85,85,85	0
55	MG	AC	109	1/1	0.86	0.27	82,82,82,82	0
55	MG	DA	3065	1/1	0.86	0.26	74,74,74,74	0
55	MG	AA	1666	1/1	0.86	0.37	62,62,62,62	0
55	MG	BA	3225	1/1	0.86	0.19	65,65,65,65	0
55	MG	BA	3337	1/1	0.86	0.22	72,72,72,72	0
55	MG	CA	1618	1/1	0.86	0.26	93,93,93,93	0
55	MG	BA	3226	1/1	0.86	0.21	50,50,50,50	0
55	MG	BA	3238	1/1	0.86	0.33	41,41,41,41	0
55	MG	DA	3320	1/1	0.86	0.14	76,76,76,76	0
55	MG	CA	1716	1/1	0.86	0.21	79,79,79,79	0
55	MG	AA	1635	1/1	0.86	0.30	86,86,86,86	0
55	MG	BA	3426	1/1	0.86	0.45	85,85,85,85	0
55	MG	BA	3246	1/1	0.86	0.30	68,68,68,68	0
55	MG	CA	1720	1/1	0.86	0.42	102,102,102,102	0
55	MG	BA	3105	1/1	0.86	0.23	75,75,75,75	0
55	MG	BA	3054	1/1	0.86	0.26	80,80,80,80	0
55	MG	BA	3598	1/1	0.86	0.11	77,77,77,77	0
55	MG	BA	3055	1/1	0.86	0.35	57,57,57,57	0
55	MG	BA	3266	1/1	0.86	0.33	77,77,77,77	0
55	MG	AA	1721	1/1	0.86	0.25	77,77,77,77	0
55	MG	BA	3276	1/1	0.86	0.23	74,74,74,74	0
55	MG	AA	1655	1/1	0.86	0.40	88,88,88,88	0
55	MG	DA	3344	1/1	0.86	0.27	95,95,95,95	0
55	MG	DA	3096	1/1	0.86	0.36	53,53,53,53	0
55	MG	DA	3112	1/1	0.86	0.10	81,81,81,81	0
55	MG	CA	1736	1/1	0.86	0.35	79,79,79,79	0
55	MG	BA	3062	1/1	0.86	0.25	56,56,56,56	0
55	MG	BA	3363	1/1	0.86	0.36	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	DA	3355	1/1	0.86	0.38	77,77,77,77	0
55	MG	DA	3356	1/1	0.86	0.24	67,67,67,67	0
55	MG	DA	3494	1/1	0.86	0.14	75,75,75,75	0
55	MG	BA	3132	1/1	0.86	0.26	71,71,71,71	0
55	MG	AA	1805	1/1	0.86	0.32	65,65,65,65	0
55	MG	DA	3499	1/1	0.86	0.22	61,61,61,61	0
55	MG	DA	3362	1/1	0.86	0.25	53,53,53,53	0
55	MG	CA	1648	1/1	0.86	0.24	65,65,65,65	0
55	MG	AA	1825	1/1	0.86	0.13	93,93,93,93	0
55	MG	BA	3140	1/1	0.86	0.17	58,58,58,58	0
55	MG	DA	3140	1/1	0.86	0.21	78,78,78,78	0
55	MG	CA	1655	1/1	0.86	0.35	87,87,87,87	0
55	MG	CA	1656	1/1	0.86	0.25	92,92,92,92	0
55	MG	AA	1656	1/1	0.86	0.35	87,87,87,87	0
55	MG	DA	3162	1/1	0.86	0.28	66,66,66,66	0
55	MG	DA	3179	1/1	0.86	0.25	70,70,70,70	0
55	MG	BB	207	1/1	0.86	0.19	83,83,83,83	0
55	MG	BA	3462	1/1	0.86	0.27	87,87,87,87	0
55	MG	AA	1810	1/1	0.86	0.31	67,67,67,67	0
55	MG	AB	104	1/1	0.86	0.23	82,82,82,82	0
55	MG	BA	3532	1/1	0.86	0.33	85,85,85,85	0
55	MG	DA	3521	1/1	0.86	0.26	69,69,69,69	0
55	MG	DA	3209	1/1	0.86	0.31	66,66,66,66	0
55	MG	BA	3381	1/1	0.86	0.46	90,90,90,90	0
55	MG	DA	3395	1/1	0.86	0.37	69,69,69,69	0
55	MG	DA	3222	1/1	0.86	0.32	60,60,60,60	0
55	MG	DA	3224	1/1	0.86	0.34	66,66,66,66	0
55	MG	AA	1812	1/1	0.86	0.28	73,73,73,73	0
55	MG	DA	3230	1/1	0.86	0.16	59,59,59,59	0
55	MG	BA	3304	1/1	0.86	0.22	56,56,56,56	0
55	MG	CA	1668	1/1	0.86	0.24	79,79,79,79	0
55	MG	BA	3309	1/1	0.86	0.23	68,68,68,68	0
55	MG	DA	3242	1/1	0.86	0.34	63,63,63,63	0
55	MG	CA	1680	1/1	0.86	0.35	68,68,68,68	0
55	MG	DA	3407	1/1	0.86	0.33	73,73,73,73	0
55	MG	D1	202	1/1	0.86	0.19	89,89,89,89	0
55	MG	DA	3409	1/1	0.86	0.24	76,76,76,76	0
55	MG	DA	3447	1/1	0.87	0.20	82,82,82,82	0
55	MG	BA	3384	1/1	0.87	0.26	73,73,73,73	0
55	MG	DA	3044	1/1	0.87	0.23	73,73,73,73	0
55	MG	BA	3604	1/1	0.87	0.16	61,61,61,61	0
55	MG	CA	1678	1/1	0.87	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3048	1/1	0.87	0.48	75,75,75,75	0
55	MG	DA	3456	1/1	0.87	0.49	83,83,83,83	0
55	MG	BA	3049	1/1	0.87	0.35	68,68,68,68	0
55	MG	BA	3607	1/1	0.87	0.24	96,96,96,96	0
55	MG	CA	1682	1/1	0.87	0.23	86,86,86,86	0
55	MG	BA	3480	1/1	0.87	0.34	50,50,50,50	0
55	MG	DA	3464	1/1	0.87	0.28	98,98,98,98	0
55	MG	CA	1798	1/1	0.87	0.23	85,85,85,85	0
55	MG	BA	3387	1/1	0.87	0.32	73,73,73,73	0
55	MG	CA	1686	1/1	0.87	0.42	73,73,73,73	0
55	MG	CA	1802	1/1	0.87	0.34	74,74,74,74	0
55	MG	DA	3471	1/1	0.87	0.26	80,80,80,80	0
55	MG	BA	3388	1/1	0.87	0.33	88,88,88,88	0
55	MG	BA	3535	1/1	0.87	0.27	80,80,80,80	0
55	MG	DA	3251	1/1	0.87	0.25	74,74,74,74	0
55	MG	DA	3253	1/1	0.87	0.17	87,87,87,87	0
55	MG	DA	3254	1/1	0.87	0.32	50,50,50,50	0
55	MG	AA	1820	1/1	0.87	0.31	75,75,75,75	0
55	MG	CA	1692	1/1	0.87	0.34	82,82,82,82	0
55	MG	DA	3264	1/1	0.87	0.44	59,59,59,59	0
55	MG	DA	3070	1/1	0.87	0.23	78,78,78,78	0
55	MG	AA	1624	1/1	0.87	0.22	79,79,79,79	0
55	MG	BA	3156	1/1	0.87	0.20	40,40,40,40	0
55	MG	DA	3271	1/1	0.87	0.36	58,58,58,58	0
55	MG	CA	1754	1/1	0.87	0.28	86,86,86,86	0
55	MG	DA	3390	1/1	0.87	0.29	75,75,75,75	0
55	MG	BA	3242	1/1	0.87	0.24	50,50,50,50	0
55	MG	AA	1793	1/1	0.87	0.24	73,73,73,73	0
55	MG	BA	3550	1/1	0.87	0.17	93,93,93,93	0
55	MG	BA	3166	1/1	0.87	0.34	72,72,72,72	0
55	MG	BA	3248	1/1	0.87	0.23	53,53,53,53	0
55	MG	BA	3402	1/1	0.87	0.26	91,91,91,91	0
55	MG	BA	3457	1/1	0.87	0.46	88,88,88,88	0
55	MG	DA	3400	1/1	0.87	0.30	89,89,89,89	0
55	MG	BA	3254	1/1	0.87	0.20	43,43,43,43	0
55	MG	BA	3460	1/1	0.87	0.16	83,83,83,83	0
55	MG	BA	3314	1/1	0.87	0.30	64,64,64,64	0
55	MG	DA	3506	1/1	0.87	0.22	78,78,78,78	0
55	MG	AA	1726	1/1	0.87	0.28	81,81,81,81	0
55	MG	DA	3298	1/1	0.87	0.30	77,77,77,77	0
55	MG	DA	3300	1/1	0.87	0.21	81,81,81,81	0
55	MG	CA	1711	1/1	0.87	0.38	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	3463	1/1	0.87	0.12	72,72,72,72	0
55	MG	BA	3118	1/1	0.87	0.27	61,61,61,61	0
55	MG	AC	107	1/1	0.87	0.24	94,94,94,94	0
55	MG	BA	3206	1/1	0.87	0.30	75,75,75,75	0
55	MG	BA	3273	1/1	0.87	0.33	94,94,94,94	0
55	MG	DA	3416	1/1	0.87	0.27	59,59,59,59	0
55	MG	BA	3583	1/1	0.87	0.10	86,86,86,86	0
55	MG	DA	3125	1/1	0.87	0.31	45,45,45,45	0
55	MG	BA	3275	1/1	0.87	0.22	73,73,73,73	0
55	MG	AA	1612	1/1	0.87	0.13	91,91,91,91	0
55	MG	DB	205	1/1	0.87	0.24	69,69,69,69	0
55	MG	AA	1809	1/1	0.87	0.28	63,63,63,63	0
55	MG	BA	3522	1/1	0.87	0.36	82,82,82,82	0
55	MG	DA	3031	1/1	0.87	0.26	72,72,72,72	0
55	MG	DA	3034	1/1	0.87	0.24	62,62,62,62	0
55	MG	AA	1636	1/1	0.87	0.33	87,87,87,87	0
55	MG	DA	3148	1/1	0.87	0.34	75,75,75,75	0
55	MG	DA	3150	1/1	0.87	0.29	68,68,68,68	0
55	MG	BA	3592	1/1	0.87	0.30	89,89,89,89	0
55	MG	BA	3422	1/1	0.87	0.26	78,78,78,78	0
55	MG	BA	3005	1/1	0.87	0.30	43,43,43,43	0
55	MG	CA	1665	1/1	0.87	0.21	83,83,83,83	0
55	MG	BA	3032	1/1	0.87	0.50	49,49,49,49	0
55	MG	AA	1779	1/1	0.88	0.35	72,72,72,72	0
55	MG	DA	3123	1/1	0.88	0.28	83,83,83,83	0
55	MG	DA	3124	1/1	0.88	0.32	54,54,54,54	0
55	MG	DA	3008	1/1	0.88	0.23	70,70,70,70	0
55	MG	CA	1690	1/1	0.88	0.27	68,68,68,68	0
55	MG	BA	3351	1/1	0.88	0.49	78,78,78,78	0
55	MG	BA	3593	1/1	0.88	0.21	80,80,80,80	0
55	MG	AA	1835	1/1	0.88	0.26	87,87,87,87	0
55	MG	AA	1633	1/1	0.88	0.31	74,74,74,74	0
55	MG	AA	1651	1/1	0.88	0.42	71,71,71,71	0
55	MG	DA	3143	1/1	0.88	0.24	58,58,58,58	0
55	MG	DA	3022	1/1	0.88	0.33	60,60,60,60	0
55	MG	AA	1675	1/1	0.88	0.23	80,80,80,80	0
55	MG	BA	3603	1/1	0.88	0.22	63,63,63,63	0
55	MG	AA	1665	1/1	0.88	0.48	70,70,70,70	0
55	MG	DA	3455	1/1	0.88	0.20	69,69,69,69	0
55	MG	AA	1654	1/1	0.88	0.32	75,75,75,75	0
55	MG	DA	3156	1/1	0.88	0.34	48,48,48,48	0
55	MG	BA	3311	1/1	0.88	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3611	1/1	0.88	0.29	87,87,87,87	0
55	MG	DA	3347	1/1	0.88	0.09	75,75,75,75	0
55	MG	DA	3183	1/1	0.88	0.29	57,57,57,57	0
55	MG	BA	3137	1/1	0.88	0.27	47,47,47,47	0
55	MG	BA	3019	1/1	0.88	0.33	66,66,66,66	0
55	MG	BA	3026	1/1	0.88	0.20	47,47,47,47	0
55	MG	BA	3080	1/1	0.88	0.14	91,91,91,91	0
55	MG	DA	3470	1/1	0.88	0.18	80,80,80,80	0
55	MG	BA	3540	1/1	0.88	0.18	61,61,61,61	0
55	MG	CA	1775	1/1	0.88	0.28	72,72,72,72	0
55	MG	BA	3622	1/1	0.88	0.23	59,59,59,59	0
55	MG	DA	3361	1/1	0.88	0.41	79,79,79,79	0
55	MG	DA	3218	1/1	0.88	0.29	62,62,62,62	0
55	MG	BA	3031	1/1	0.88	0.19	33,33,33,33	0
55	MG	BA	3482	1/1	0.88	0.20	57,57,57,57	0
55	MG	BA	3433	1/1	0.88	0.18	70,70,70,70	0
55	MG	BA	3375	1/1	0.88	0.20	50,50,50,50	0
55	MG	DA	3368	1/1	0.88	0.42	73,73,73,73	0
55	MG	BA	3378	1/1	0.88	0.44	76,76,76,76	0
55	MG	AA	1687	1/1	0.88	0.33	72,72,72,72	0
55	MG	CA	1646	1/1	0.88	0.30	76,76,76,76	0
55	MG	BA	3038	1/1	0.88	0.22	56,56,56,56	0
55	MG	DA	3248	1/1	0.88	0.36	75,75,75,75	0
55	MG	CA	1722	1/1	0.88	0.36	75,75,75,75	0
55	MG	BA	3268	1/1	0.88	0.40	67,67,67,67	0
55	MG	DA	3062	1/1	0.88	0.16	72,72,72,72	0
55	MG	DA	3496	1/1	0.88	0.24	83,83,83,83	0
55	MG	BA	3558	1/1	0.88	0.11	63,63,63,63	0
55	MG	DA	3386	1/1	0.88	0.31	61,61,61,61	0
55	MG	BA	3559	1/1	0.88	0.19	81,81,81,81	0
55	MG	BA	3562	1/1	0.88	0.28	79,79,79,79	0
55	MG	BA	3044	1/1	0.88	0.26	62,62,62,62	0
55	MG	DA	3266	1/1	0.88	0.31	55,55,55,55	0
55	MG	BA	3088	1/1	0.88	0.11	77,77,77,77	0
55	MG	CA	1731	1/1	0.88	0.49	72,72,72,72	0
55	MG	BD	301	1/1	0.88	0.29	85,85,85,85	0
55	MG	CA	1734	1/1	0.88	0.28	93,93,93,93	0
55	MG	DA	3272	1/1	0.88	0.14	64,64,64,64	0
55	MG	BE	301	1/1	0.88	0.27	59,59,59,59	0
55	MG	AA	1626	1/1	0.88	0.21	69,69,69,69	0
55	MG	DA	3078	1/1	0.88	0.31	89,89,89,89	0
55	MG	AA	1670	1/1	0.88	0.30	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3392	1/1	0.88	0.31	70,70,70,70	0
55	MG	BA	3101	1/1	0.88	0.35	63,63,63,63	0
55	MG	AA	1718	1/1	0.88	0.27	82,82,82,82	0
55	MG	BA	3286	1/1	0.88	0.26	66,66,66,66	0
55	MG	B3	101	1/1	0.88	0.45	71,71,71,71	0
55	MG	DA	3522	1/1	0.88	0.16	78,78,78,78	0
55	MG	DA	3523	1/1	0.88	0.33	81,81,81,81	0
55	MG	DA	3411	1/1	0.88	0.11	70,70,70,70	0
55	MG	CB	102	1/1	0.88	0.16	87,87,87,87	0
55	MG	CA	1673	1/1	0.88	0.21	64,64,64,64	0
55	MG	DA	3295	1/1	0.88	0.32	50,50,50,50	0
55	MG	BA	3579	1/1	0.88	0.19	92,92,92,92	0
55	MG	BA	3459	1/1	0.88	0.36	70,70,70,70	0
55	MG	BA	3287	1/1	0.88	0.31	62,62,62,62	0
55	MG	AC	101	1/1	0.88	0.22	53,53,53,53	0
55	MG	CA	1605	1/1	0.88	0.42	76,76,76,76	0
55	MG	DA	3425	1/1	0.88	0.23	81,81,81,81	0
55	MG	DB	212	1/1	0.88	0.14	88,88,88,88	0
55	MG	DA	3426	1/1	0.88	0.25	58,58,58,58	0
55	MG	BA	3343	1/1	0.88	0.24	60,60,60,60	0
55	MG	DA	3428	1/1	0.88	0.33	84,84,84,84	0
55	MG	AA	1795	1/1	0.88	0.22	73,73,73,73	0
55	MG	AA	1778	1/1	0.88	0.19	106,106,106,106	0
55	MG	BA	3465	1/1	0.88	0.23	93,93,93,93	0
55	MG	CA	1642	1/1	0.89	0.22	91,91,91,91	0
55	MG	DA	3293	1/1	0.89	0.31	75,75,75,75	0
55	MG	BA	3323	1/1	0.89	0.28	66,66,66,66	0
55	MG	BA	3160	1/1	0.89	0.30	42,42,42,42	0
55	MG	BA	3528	1/1	0.89	0.31	76,76,76,76	0
55	MG	CA	1647	1/1	0.89	0.34	61,61,61,61	0
55	MG	DA	3301	1/1	0.89	0.25	63,63,63,63	0
55	MG	BA	3016	1/1	0.89	0.35	39,39,39,39	0
55	MG	AA	1694	1/1	0.89	0.24	91,91,91,91	0
55	MG	CA	1653	1/1	0.89	0.14	77,77,77,77	0
55	MG	DA	3307	1/1	0.89	0.26	77,77,77,77	0
55	MG	DA	3438	1/1	0.89	0.20	87,87,87,87	0
55	MG	BA	3185	1/1	0.89	0.31	76,76,76,76	0
55	MG	BA	3109	1/1	0.89	0.21	70,70,70,70	0
55	MG	DA	3310	1/1	0.89	0.34	71,71,71,71	0
55	MG	DA	3113	1/1	0.89	0.28	43,43,43,43	0
55	MG	CA	1739	1/1	0.89	0.46	75,75,75,75	0
55	MG	DA	3118	1/1	0.89	0.29	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3333	1/1	0.89	0.33	80,80,80,80	0
55	MG	AA	1604	1/1	0.89	0.25	67,67,67,67	0
55	MG	DA	3450	1/1	0.89	0.24	88,88,88,88	0
55	MG	BA	3536	1/1	0.89	0.24	73,73,73,73	0
55	MG	DA	3452	1/1	0.89	0.20	83,83,83,83	0
55	MG	DA	3326	1/1	0.89	0.27	70,70,70,70	0
55	MG	BA	3335	1/1	0.89	0.25	58,58,58,58	0
55	MG	BA	3112	1/1	0.89	0.21	77,77,77,77	0
55	MG	DA	3331	1/1	0.89	0.33	50,50,50,50	0
55	MG	DA	3127	1/1	0.89	0.38	74,74,74,74	0
55	MG	BA	3277	1/1	0.89	0.39	86,86,86,86	0
55	MG	AA	1774	1/1	0.89	0.16	91,91,91,91	0
55	MG	DA	3131	1/1	0.89	0.30	79,79,79,79	0
55	MG	AA	1653	1/1	0.89	0.39	81,81,81,81	0
55	MG	BA	3285	1/1	0.89	0.29	72,72,72,72	0
55	MG	BA	3211	1/1	0.89	0.30	39,39,39,39	0
55	MG	DA	3011	1/1	0.89	0.13	65,65,65,65	0
55	MG	AA	1610	1/1	0.89	0.30	51,51,51,51	0
55	MG	BA	3289	1/1	0.89	0.36	60,60,60,60	0
55	MG	BA	3553	1/1	0.89	0.20	78,78,78,78	0
55	MG	CA	1675	1/1	0.89	0.28	62,62,62,62	0
55	MG	BA	3413	1/1	0.89	0.33	78,78,78,78	0
55	MG	BA	3078	1/1	0.89	0.31	65,65,65,65	0
55	MG	DA	3155	1/1	0.89	0.24	46,46,46,46	0
55	MG	BA	3128	1/1	0.89	0.34	46,46,46,46	0
55	MG	BA	3561	1/1	0.89	0.19	74,74,74,74	0
55	MG	DA	3165	1/1	0.89	0.50	65,65,65,65	0
55	MG	DA	3482	1/1	0.89	0.23	81,81,81,81	0
55	MG	BA	3416	1/1	0.89	0.19	87,87,87,87	0
55	MG	AA	1764	1/1	0.89	0.16	79,79,79,79	0
55	MG	DA	3029	1/1	0.89	0.32	79,79,79,79	0
55	MG	DA	3192	1/1	0.89	0.29	62,62,62,62	0
55	MG	BA	3418	1/1	0.89	0.28	78,78,78,78	0
55	MG	DA	3194	1/1	0.89	0.32	73,73,73,73	0
55	MG	BA	3357	1/1	0.89	0.36	81,81,81,81	0
55	MG	DA	3365	1/1	0.89	0.36	58,58,58,58	0
55	MG	AA	1816	1/1	0.89	0.23	81,81,81,81	0
55	MG	DA	3037	1/1	0.89	0.30	98,98,98,98	0
55	MG	CA	1688	1/1	0.89	0.30	71,71,71,71	0
55	MG	CA	1602	1/1	0.89	0.28	80,80,80,80	0
55	MG	BA	3569	1/1	0.89	0.34	85,85,85,85	0
55	MG	DA	3373	1/1	0.89	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1617	1/1	0.89	0.31	69,69,69,69	0
55	MG	BA	3423	1/1	0.89	0.28	61,61,61,61	0
55	MG	DA	3227	1/1	0.89	0.46	50,50,50,50	0
55	MG	DA	3378	1/1	0.89	0.32	63,63,63,63	0
55	MG	BA	3424	1/1	0.89	0.38	72,72,72,72	0
55	MG	BA	3574	1/1	0.89	0.34	78,78,78,78	0
55	MG	BA	3575	1/1	0.89	0.24	71,71,71,71	0
55	MG	BA	3425	1/1	0.89	0.39	91,91,91,91	0
55	MG	BA	3227	1/1	0.89	0.34	91,91,91,91	0
55	MG	BA	3232	1/1	0.89	0.18	72,72,72,72	0
55	MG	DA	3246	1/1	0.89	0.34	53,53,53,53	0
55	MG	AA	1766	1/1	0.89	0.14	79,79,79,79	0
55	MG	AA	1628	1/1	0.89	0.43	69,69,69,69	0
55	MG	BA	3435	1/1	0.89	0.20	65,65,65,65	0
55	MG	BA	3501	1/1	0.89	0.18	55,55,55,55	0
55	MG	BA	3142	1/1	0.89	0.24	51,51,51,51	0
55	MG	BA	3310	1/1	0.89	0.23	57,57,57,57	0
55	MG	AA	1802	1/1	0.89	0.31	85,85,85,85	0
55	MG	BA	3442	1/1	0.89	0.24	76,76,76,76	0
55	MG	BA	3312	1/1	0.89	0.28	57,57,57,57	0
55	MG	AA	1650	1/1	0.89	0.32	71,71,71,71	0
55	MG	BA	3512	1/1	0.89	0.24	69,69,69,69	0
55	MG	AA	1785	1/1	0.89	0.30	96,96,96,96	0
55	MG	BA	3376	1/1	0.89	0.28	73,73,73,73	0
55	MG	AA	1662	1/1	0.89	0.40	81,81,81,81	0
55	MG	BA	3256	1/1	0.89	0.30	61,61,61,61	0
55	MG	DA	3274	1/1	0.89	0.27	87,87,87,87	0
55	MG	DA	3074	1/1	0.89	0.19	70,70,70,70	0
55	MG	BA	3010	1/1	0.89	0.29	46,46,46,46	0
55	MG	CA	1799	1/1	0.89	0.23	96,96,96,96	0
55	MG	BA	3318	1/1	0.89	0.41	75,75,75,75	0
55	MG	DA	3081	1/1	0.89	0.32	64,64,64,64	0
55	MG	BA	3609	1/1	0.89	0.37	70,70,70,70	0
55	MG	BA	3456	1/1	0.89	0.32	78,78,78,78	0
55	MG	BA	3258	1/1	0.89	0.23	45,45,45,45	0
55	MG	CA	1804	1/1	0.89	0.24	75,75,75,75	0
55	MG	CA	1779	1/1	0.90	0.22	72,72,72,72	0
55	MG	BA	3195	1/1	0.90	0.38	47,47,47,47	0
55	MG	AA	1657	1/1	0.90	0.26	50,50,50,50	0
55	MG	BA	3557	1/1	0.90	0.25	77,77,77,77	0
55	MG	BB	204	1/1	0.90	0.28	78,78,78,78	0
55	MG	CA	1641	1/1	0.90	0.30	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	DA	3196	1/1	0.90	0.29	50,50,50,50	0
55	MG	BA	3014	1/1	0.90	0.30	53,53,53,53	0
55	MG	DA	3051	1/1	0.90	0.27	85,85,85,85	0
55	MG	BA	3332	1/1	0.90	0.18	61,61,61,61	0
55	MG	BA	3560	1/1	0.90	0.33	78,78,78,78	0
55	MG	BA	3499	1/1	0.90	0.26	68,68,68,68	0
55	MG	CA	1789	1/1	0.90	0.33	71,71,71,71	0
55	MG	DA	3351	1/1	0.90	0.20	79,79,79,79	0
55	MG	BA	3205	1/1	0.90	0.16	80,80,80,80	0
55	MG	AA	1688	1/1	0.90	0.25	72,72,72,72	0
55	MG	CA	1795	1/1	0.90	0.21	76,76,76,76	0
55	MG	BA	3131	1/1	0.90	0.23	59,59,59,59	0
55	MG	AA	1762	1/1	0.90	0.22	80,80,80,80	0
55	MG	BA	3067	1/1	0.90	0.15	48,48,48,48	0
55	MG	DA	3234	1/1	0.90	0.26	52,52,52,52	0
55	MG	AA	1667	1/1	0.90	0.27	68,68,68,68	0
55	MG	BA	3221	1/1	0.90	0.29	60,60,60,60	0
55	MG	DA	3239	1/1	0.90	0.22	45,45,45,45	0
55	MG	BE	302	1/1	0.90	0.21	56,56,56,56	0
55	MG	BA	3136	1/1	0.90	0.12	74,74,74,74	0
55	MG	BA	3098	1/1	0.90	0.14	48,48,48,48	0
55	MG	AA	1606	1/1	0.90	0.12	91,91,91,91	0
55	MG	BA	3405	1/1	0.90	0.30	56,56,56,56	0
55	MG	BA	3517	1/1	0.90	0.38	70,70,70,70	0
55	MG	DA	3372	1/1	0.90	0.27	65,65,65,65	0
55	MG	DA	3480	1/1	0.90	0.20	63,63,63,63	0
55	MG	B2	201	1/1	0.90	0.31	85,85,85,85	0
55	MG	BA	3102	1/1	0.90	0.23	66,66,66,66	0
55	MG	AA	1601	1/1	0.90	0.28	56,56,56,56	0
55	MG	B7	101	1/1	0.90	0.31	67,67,67,67	0
55	MG	BA	3581	1/1	0.90	0.32	69,69,69,69	0
55	MG	CA	1670	1/1	0.90	0.36	56,56,56,56	0
55	MG	BA	3229	1/1	0.90	0.10	50,50,50,50	0
55	MG	AA	1605	1/1	0.90	0.29	82,82,82,82	0
55	MG	DA	3382	1/1	0.90	0.33	78,78,78,78	0
55	MG	AA	1680	1/1	0.90	0.25	80,80,80,80	0
55	MG	BA	3149	1/1	0.90	0.26	80,80,80,80	0
55	MG	BA	3108	1/1	0.90	0.29	86,86,86,86	0
55	MG	CA	1750	1/1	0.90	0.32	79,79,79,79	0
55	MG	BA	3305	1/1	0.90	0.37	70,70,70,70	0
55	MG	DA	3001	1/1	0.90	0.27	67,67,67,67	0
55	MG	BA	3244	1/1	0.90	0.21	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	DA	3103	1/1	0.90	0.29	50,50,50,50	0
55	MG	CA	1683	1/1	0.90	0.35	87,87,87,87	0
55	MG	BA	3152	1/1	0.90	0.32	40,40,40,40	0
55	MG	DA	3116	1/1	0.90	0.26	74,74,74,74	0
55	MG	AA	1808	1/1	0.90	0.34	76,76,76,76	0
55	MG	BA	3531	1/1	0.90	0.13	53,53,53,53	0
55	MG	DA	3291	1/1	0.90	0.35	65,65,65,65	0
55	MG	BA	3001	1/1	0.90	0.32	47,47,47,47	0
55	MG	BA	3252	1/1	0.90	0.26	67,67,67,67	0
55	MG	DA	3510	1/1	0.90	0.27	85,85,85,85	0
55	MG	BA	3253	1/1	0.90	0.16	51,51,51,51	0
55	MG	AA	1759	1/1	0.90	0.21	77,77,77,77	0
55	MG	DA	3514	1/1	0.90	0.29	59,59,59,59	0
55	MG	BA	3370	1/1	0.90	0.26	56,56,56,56	0
55	MG	BA	3114	1/1	0.90	0.18	74,74,74,74	0
55	MG	CA	1621	1/1	0.90	0.30	66,66,66,66	0
55	MG	BA	3168	1/1	0.90	0.25	49,49,49,49	0
55	MG	DA	3023	1/1	0.90	0.21	57,57,57,57	0
55	MG	CA	1695	1/1	0.90	0.44	87,87,87,87	0
55	MG	DA	3305	1/1	0.90	0.28	77,77,77,77	0
55	MG	BA	3170	1/1	0.90	0.36	55,55,55,55	0
55	MG	CA	1697	1/1	0.90	0.29	65,65,65,65	0
55	MG	BA	3543	1/1	0.90	0.28	80,80,80,80	0
55	MG	DA	3526	1/1	0.90	0.31	68,68,68,68	0
55	MG	BA	3008	1/1	0.90	0.29	37,37,37,37	0
55	MG	DA	3311	1/1	0.90	0.30	73,73,73,73	0
55	MG	BA	3187	1/1	0.90	0.44	73,73,73,73	0
55	MG	DA	3032	1/1	0.90	0.14	76,76,76,76	0
55	MG	BA	3617	1/1	0.90	0.40	71,71,71,71	0
55	MG	BA	3380	1/1	0.90	0.17	65,65,65,65	0
55	MG	BA	3549	1/1	0.90	0.25	68,68,68,68	0
55	MG	DA	3154	1/1	0.90	0.27	69,69,69,69	0
55	MG	BA	3057	1/1	0.90	0.10	70,70,70,70	0
55	MG	BA	3439	1/1	0.90	0.31	71,71,71,71	0
55	MG	BA	3269	1/1	0.90	0.28	61,61,61,61	0
55	MG	CA	1636	1/1	0.90	0.28	78,78,78,78	0
55	MG	DR	201	1/1	0.90	0.12	71,71,71,71	0
55	MG	DA	3167	1/1	0.90	0.31	70,70,70,70	0
55	MG	DA	3439	1/1	0.90	0.15	62,62,62,62	0
55	MG	DA	3168	1/1	0.90	0.23	49,49,49,49	0
55	MG	DA	3316	1/1	0.91	0.25	61,61,61,61	0
55	MG	CA	1793	1/1	0.91	0.30	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1634	1/1	0.91	0.27	62,62,62,62	0
55	MG	BA	3587	1/1	0.91	0.17	64,64,64,64	0
55	MG	DA	3172	1/1	0.91	0.27	88,88,88,88	0
55	MG	DA	3173	1/1	0.91	0.18	60,60,60,60	0
55	MG	DA	3175	1/1	0.91	0.38	83,83,83,83	0
55	MG	DA	3052	1/1	0.91	0.40	71,71,71,71	0
55	MG	DA	3181	1/1	0.91	0.32	50,50,50,50	0
55	MG	DA	3053	1/1	0.91	0.35	62,62,62,62	0
55	MG	DA	3334	1/1	0.91	0.14	68,68,68,68	0
55	MG	AA	1705	1/1	0.91	0.28	83,83,83,83	0
55	MG	DA	3186	1/1	0.91	0.23	60,60,60,60	0
55	MG	BA	3297	1/1	0.91	0.21	58,58,58,58	0
55	MG	BA	3299	1/1	0.91	0.37	89,89,89,89	0
55	MG	DA	3339	1/1	0.91	0.34	66,66,66,66	0
55	MG	CA	1666	1/1	0.91	0.28	71,71,71,71	0
55	MG	BA	3111	1/1	0.91	0.26	59,59,59,59	0
55	MG	BA	3359	1/1	0.91	0.33	79,79,79,79	0
55	MG	DA	3205	1/1	0.91	0.24	67,67,67,67	0
55	MG	CA	1669	1/1	0.91	0.10	60,60,60,60	0
55	MG	BA	3240	1/1	0.91	0.42	88,88,88,88	0
55	MG	DA	3346	1/1	0.91	0.32	75,75,75,75	0
55	MG	AA	1773	1/1	0.91	0.24	87,87,87,87	0
55	MG	DA	3348	1/1	0.91	0.37	73,73,73,73	0
55	MG	BA	3030	1/1	0.91	0.33	44,44,44,44	0
55	MG	DA	3214	1/1	0.91	0.18	40,40,40,40	0
55	MG	BA	3245	1/1	0.91	0.41	49,49,49,49	0
55	MG	DA	3352	1/1	0.91	0.28	64,64,64,64	0
55	MG	BA	3308	1/1	0.91	0.23	61,61,61,61	0
55	MG	BA	3167	1/1	0.91	0.32	73,73,73,73	0
55	MG	DA	3225	1/1	0.91	0.40	73,73,73,73	0
55	MG	AA	1642	1/1	0.91	0.47	72,72,72,72	0
55	MG	BA	3169	1/1	0.91	0.39	63,63,63,63	0
55	MG	AA	1631	1/1	0.91	0.17	66,66,66,66	0
55	MG	BA	3176	1/1	0.91	0.30	48,48,48,48	0
55	MG	DA	3232	1/1	0.91	0.29	44,44,44,44	0
55	MG	BA	3614	1/1	0.91	0.12	69,69,69,69	0
55	MG	CC	102	1/1	0.91	0.27	73,73,73,73	0
55	MG	CA	1619	1/1	0.91	0.25	61,61,61,61	0
55	MG	BA	3182	1/1	0.91	0.15	43,43,43,43	0
55	MG	BA	3616	1/1	0.91	0.18	58,58,58,58	0
55	MG	BA	3033	1/1	0.91	0.24	38,38,38,38	0
55	MG	BA	3120	1/1	0.91	0.23	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	DA	3370	1/1	0.91	0.13	67,67,67,67	0
55	MG	BA	3492	1/1	0.91	0.36	77,77,77,77	0
55	MG	DA	3087	1/1	0.91	0.29	63,63,63,63	0
55	MG	BA	3122	1/1	0.91	0.17	37,37,37,37	0
55	MG	DA	3003	1/1	0.91	0.18	64,64,64,64	0
55	MG	BA	3494	1/1	0.91	0.43	76,76,76,76	0
55	MG	BA	3193	1/1	0.91	0.32	85,85,85,85	0
55	MG	BA	3035	1/1	0.91	0.17	37,37,37,37	0
55	MG	DA	3265	1/1	0.91	0.23	50,50,50,50	0
55	MG	BA	3267	1/1	0.91	0.16	61,61,61,61	0
55	MG	DA	3267	1/1	0.91	0.24	64,64,64,64	0
55	MG	BA	3200	1/1	0.91	0.27	62,62,62,62	0
55	MG	CA	1634	1/1	0.91	0.35	77,77,77,77	0
55	MG	DA	3384	1/1	0.91	0.31	65,65,65,65	0
55	MG	DA	3012	1/1	0.91	0.37	66,66,66,66	0
55	MG	DA	3504	1/1	0.91	0.23	65,65,65,65	0
55	MG	DA	3106	1/1	0.91	0.27	48,48,48,48	0
55	MG	DA	3389	1/1	0.91	0.32	64,64,64,64	0
55	MG	DA	3107	1/1	0.91	0.24	53,53,53,53	0
55	MG	DA	3391	1/1	0.91	0.16	78,78,78,78	0
55	MG	DA	3110	1/1	0.91	0.29	58,58,58,58	0
55	MG	AA	1709	1/1	0.91	0.24	70,70,70,70	0
55	MG	CA	1700	1/1	0.91	0.33	77,77,77,77	0
55	MG	DA	3017	1/1	0.91	0.29	75,75,75,75	0
55	MG	AA	1645	1/1	0.91	0.33	50,50,50,50	0
55	MG	BA	3048	1/1	0.91	0.35	77,77,77,77	0
55	MG	AA	1815	1/1	0.91	0.45	84,84,84,84	0
55	MG	CA	1705	1/1	0.91	0.32	80,80,80,80	0
55	MG	AA	1796	1/1	0.91	0.22	75,75,75,75	0
55	MG	BA	3135	1/1	0.91	0.36	72,72,72,72	0
55	MG	BB	212	1/1	0.91	0.29	81,81,81,81	0
55	MG	AA	1658	1/1	0.91	0.31	49,49,49,49	0
55	MG	DA	3027	1/1	0.91	0.15	77,77,77,77	0
55	MG	BA	3281	1/1	0.91	0.33	72,72,72,72	0
55	MG	BA	3336	1/1	0.91	0.33	66,66,66,66	0
55	MG	AA	1712	1/1	0.91	0.28	78,78,78,78	0
55	MG	BA	3338	1/1	0.91	0.16	71,71,71,71	0
55	MG	BA	3516	1/1	0.91	0.34	78,78,78,78	0
55	MG	CA	1649	1/1	0.91	0.21	64,64,64,64	0
55	MG	AA	1837	1/1	0.91	0.26	73,73,73,73	0
55	MG	CA	1652	1/1	0.91	0.27	71,71,71,71	0
55	MG	AA	1839	1/1	0.91	0.30	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	1669	1/1	0.91	0.33	68,68,68,68	0
55	MG	AA	1841	1/1	0.91	0.27	59,59,59,59	0
55	MG	AA	1660	1/1	0.91	0.33	53,53,53,53	0
55	MG	BA	3407	1/1	0.91	0.09	59,59,59,59	0
55	MG	AA	1741	1/1	0.91	0.26	67,67,67,67	0
55	MG	AA	1603	1/1	0.91	0.25	63,63,63,63	0
55	MG	DA	3158	1/1	0.91	0.34	44,44,44,44	0
55	MG	BA	3526	1/1	0.91	0.29	86,86,86,86	0
55	MG	DA	3314	1/1	0.91	0.32	76,76,76,76	0
55	MG	DA	3164	1/1	0.91	0.35	47,47,47,47	0
55	MG	D3	101	1/1	0.91	0.30	66,66,66,66	0
55	MG	BA	3503	1/1	0.92	0.18	65,65,65,65	0
55	MG	AA	1788	1/1	0.92	0.41	77,77,77,77	0
55	MG	DA	3016	1/1	0.92	0.33	78,78,78,78	0
55	MG	DA	3226	1/1	0.92	0.30	62,62,62,62	0
55	MG	AA	1632	1/1	0.92	0.21	67,67,67,67	0
55	MG	DA	3446	1/1	0.92	0.35	75,75,75,75	0
55	MG	AA	1602	1/1	0.92	0.20	79,79,79,79	0
55	MG	DA	3095	1/1	0.92	0.25	49,49,49,49	0
55	MG	BA	3070	1/1	0.92	0.12	63,63,63,63	0
55	MG	DA	3100	1/1	0.92	0.28	44,44,44,44	0
55	MG	BA	3003	1/1	0.92	0.27	47,47,47,47	0
55	MG	DA	3104	1/1	0.92	0.27	43,43,43,43	0
55	MG	BA	3153	1/1	0.92	0.27	52,52,52,52	0
55	MG	AA	1780	1/1	0.92	0.17	86,86,86,86	0
55	MG	DA	3108	1/1	0.92	0.21	54,54,54,54	0
55	MG	DA	3244	1/1	0.92	0.38	71,71,71,71	0
55	MG	BA	3006	1/1	0.92	0.24	38,38,38,38	0
55	MG	DA	3247	1/1	0.92	0.16	87,87,87,87	0
55	MG	BA	3235	1/1	0.92	0.28	54,54,54,54	0
55	MG	BA	3113	1/1	0.92	0.32	57,57,57,57	0
55	MG	BA	3578	1/1	0.92	0.34	81,81,81,81	0
55	MG	DA	3465	1/1	0.92	0.24	74,74,74,74	0
55	MG	DA	3359	1/1	0.92	0.31	76,76,76,76	0
55	MG	AA	1704	1/1	0.92	0.10	83,83,83,83	0
55	MG	BF	302	1/1	0.92	0.11	72,72,72,72	0
55	MG	DA	3030	1/1	0.92	0.23	74,74,74,74	0
55	MG	DA	3262	1/1	0.92	0.39	48,48,48,48	0
55	MG	AA	1697	1/1	0.92	0.23	84,84,84,84	0
55	MG	DA	3472	1/1	0.92	0.37	71,71,71,71	0
55	MG	BA	3051	1/1	0.92	0.21	74,74,74,74	0
55	MG	BA	3117	1/1	0.92	0.38	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3350	1/1	0.92	0.25	55,55,55,55	0
55	MG	BA	3052	1/1	0.92	0.17	64,64,64,64	0
55	MG	BA	3174	1/1	0.92	0.49	71,71,71,71	0
55	MG	AA	1629	1/1	0.92	0.17	86,86,86,86	0
55	MG	BA	3181	1/1	0.92	0.24	39,39,39,39	0
55	MG	BA	3469	1/1	0.92	0.21	60,60,60,60	0
55	MG	BA	3249	1/1	0.92	0.13	30,30,30,30	0
55	MG	BA	3471	1/1	0.92	0.24	72,72,72,72	0
55	MG	BA	3251	1/1	0.92	0.34	68,68,68,68	0
55	MG	AA	1723	1/1	0.92	0.34	84,84,84,84	0
55	MG	DA	3145	1/1	0.92	0.34	60,60,60,60	0
55	MG	CA	1733	1/1	0.92	0.36	69,69,69,69	0
55	MG	DA	3488	1/1	0.92	0.25	86,86,86,86	0
55	MG	BA	3184	1/1	0.92	0.12	39,39,39,39	0
55	MG	BA	3126	1/1	0.92	0.33	46,46,46,46	0
55	MG	AN	202	1/1	0.92	0.19	82,82,82,82	0
55	MG	BA	3601	1/1	0.92	0.25	85,85,85,85	0
55	MG	DA	3284	1/1	0.92	0.25	56,56,56,56	0
55	MG	DA	3285	1/1	0.92	0.19	50,50,50,50	0
55	MG	DA	3286	1/1	0.92	0.08	47,47,47,47	0
55	MG	BA	3188	1/1	0.92	0.28	60,60,60,60	0
55	MG	BA	3421	1/1	0.92	0.24	62,62,62,62	0
55	MG	BA	3056	1/1	0.92	0.18	54,54,54,54	0
55	MG	DA	3157	1/1	0.92	0.31	47,47,47,47	0
55	MG	BA	3129	1/1	0.92	0.34	52,52,52,52	0
55	MG	CA	1679	1/1	0.92	0.38	85,85,85,85	0
55	MG	CA	1615	1/1	0.92	0.22	81,81,81,81	0
55	MG	BA	3020	1/1	0.92	0.34	41,41,41,41	0
55	MG	DA	3166	1/1	0.92	0.31	58,58,58,58	0
55	MG	BA	3058	1/1	0.92	0.17	62,62,62,62	0
55	MG	BA	3320	1/1	0.92	0.23	62,62,62,62	0
55	MG	BA	3429	1/1	0.92	0.09	75,75,75,75	0
55	MG	CA	1620	1/1	0.92	0.34	64,64,64,64	0
55	MG	BA	3430	1/1	0.92	0.16	57,57,57,57	0
55	MG	BA	3372	1/1	0.92	0.16	73,73,73,73	0
55	MG	BA	3090	1/1	0.92	0.36	49,49,49,49	0
55	MG	BA	3021	1/1	0.92	0.30	41,41,41,41	0
55	MG	DA	3184	1/1	0.92	0.42	61,61,61,61	0
55	MG	BA	3096	1/1	0.92	0.32	56,56,56,56	0
55	MG	BA	3620	1/1	0.92	0.29	68,68,68,68	0
55	MG	DA	3189	1/1	0.92	0.26	41,41,41,41	0
55	MG	BA	3097	1/1	0.92	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3024	1/1	0.92	0.21	27,27,27,27	0
55	MG	BA	3556	1/1	0.92	0.30	58,58,58,58	0
55	MG	DA	3318	1/1	0.92	0.18	63,63,63,63	0
55	MG	CA	1631	1/1	0.92	0.12	81,81,81,81	0
55	MG	DA	3421	1/1	0.92	0.21	62,62,62,62	0
55	MG	DB	201	1/1	0.92	0.32	81,81,81,81	0
55	MG	AA	1646	1/1	0.92	0.23	67,67,67,67	0
55	MG	DA	3424	1/1	0.92	0.32	70,70,70,70	0
55	MG	DA	3204	1/1	0.92	0.23	51,51,51,51	0
55	MG	BA	3440	1/1	0.92	0.35	74,74,74,74	0
55	MG	AA	1821	1/1	0.92	0.30	75,75,75,75	0
55	MG	DA	3328	1/1	0.92	0.21	47,47,47,47	0
55	MG	BA	3331	1/1	0.92	0.19	65,65,65,65	0
55	MG	BA	3386	1/1	0.92	0.28	59,59,59,59	0
55	MG	DA	3431	1/1	0.92	0.38	91,91,91,91	0
55	MG	DA	3210	1/1	0.92	0.28	63,63,63,63	0
55	MG	DA	3433	1/1	0.92	0.37	57,57,57,57	0
55	MG	DE	301	1/1	0.92	0.22	41,41,41,41	0
55	MG	CA	1701	1/1	0.92	0.40	88,88,88,88	0
55	MG	BA	3066	1/1	0.92	0.29	62,62,62,62	0
55	MG	DA	3216	1/1	0.92	0.15	49,49,49,49	0
55	MG	DA	3013	1/1	0.92	0.37	56,56,56,56	0
55	MG	DA	3220	1/1	0.92	0.30	66,66,66,66	0
55	MG	DA	3221	1/1	0.92	0.45	63,63,63,63	0
56	ZN	AQ	102	1/1	0.92	0.15	122,122,122,122	0
55	MG	DA	3109	1/1	0.93	0.22	65,65,65,65	0
55	MG	DA	3235	1/1	0.93	0.26	48,48,48,48	0
55	MG	BA	3095	1/1	0.93	0.24	37,37,37,37	0
55	MG	DA	3021	1/1	0.93	0.24	51,51,51,51	0
55	MG	AA	1784	1/1	0.93	0.39	66,66,66,66	0
55	MG	AA	1771	1/1	0.93	0.07	70,70,70,70	0
55	MG	BA	3050	1/1	0.93	0.24	39,39,39,39	0
55	MG	BA	3234	1/1	0.93	0.35	86,86,86,86	0
55	MG	BA	3294	1/1	0.93	0.27	72,72,72,72	0
55	MG	AA	1644	1/1	0.93	0.13	62,62,62,62	0
55	MG	DA	3457	1/1	0.93	0.33	65,65,65,65	0
55	MG	DA	3121	1/1	0.93	0.19	64,64,64,64	0
55	MG	BA	3296	1/1	0.93	0.25	53,53,53,53	0
55	MG	DA	3460	1/1	0.93	0.37	72,72,72,72	0
55	MG	BA	3236	1/1	0.93	0.30	52,52,52,52	0
55	MG	A1	101	1/1	0.93	0.15	66,66,66,66	0
55	MG	BA	3483	1/1	0.93	0.25	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3173	1/1	0.93	0.33	52,52,52,52	0
55	MG	BA	3023	1/1	0.93	0.23	45,45,45,45	0
55	MG	A1	102	1/1	0.93	0.30	86,86,86,86	0
55	MG	DA	3134	1/1	0.93	0.23	72,72,72,72	0
55	MG	BA	3180	1/1	0.93	0.24	37,37,37,37	0
55	MG	DA	3137	1/1	0.93	0.23	82,82,82,82	0
55	MG	BA	3365	1/1	0.93	0.16	50,50,50,50	0
55	MG	CA	1643	1/1	0.93	0.28	82,82,82,82	0
55	MG	BA	3428	1/1	0.93	0.32	68,68,68,68	0
55	MG	DA	3474	1/1	0.93	0.30	83,83,83,83	0
55	MG	AA	1699	1/1	0.93	0.19	64,64,64,64	0
55	MG	BA	3028	1/1	0.93	0.33	46,46,46,46	0
55	MG	AA	1619	1/1	0.93	0.24	63,63,63,63	0
55	MG	BA	3081	1/1	0.93	0.29	75,75,75,75	0
55	MG	BA	3082	1/1	0.93	0.32	64,64,64,64	0
55	MG	DA	3046	1/1	0.93	0.20	65,65,65,65	0
55	MG	CA	1650	1/1	0.93	0.21	102,102,102,102	0
55	MG	AA	1829	1/1	0.93	0.35	77,77,77,77	0
55	MG	CA	1794	1/1	0.93	0.28	74,74,74,74	0
55	MG	CA	1721	1/1	0.93	0.24	80,80,80,80	0
55	MG	BA	3189	1/1	0.93	0.31	49,49,49,49	0
55	MG	BA	3567	1/1	0.93	0.31	80,80,80,80	0
55	MG	DA	3385	1/1	0.93	0.39	62,62,62,62	0
55	MG	DA	3160	1/1	0.93	0.20	49,49,49,49	0
55	MG	BA	3374	1/1	0.93	0.34	71,71,71,71	0
55	MG	DA	3388	1/1	0.93	0.18	74,74,74,74	0
55	MG	DA	3288	1/1	0.93	0.22	47,47,47,47	0
55	MG	BA	3190	1/1	0.93	0.23	63,63,63,63	0
55	MG	BA	3502	1/1	0.93	0.21	67,67,67,67	0
55	MG	CA	1728	1/1	0.93	0.33	69,69,69,69	0
55	MG	DA	3060	1/1	0.93	0.38	73,73,73,73	0
55	MG	AA	1799	1/1	0.93	0.34	78,78,78,78	0
55	MG	DA	3169	1/1	0.93	0.23	69,69,69,69	0
55	MG	BA	3572	1/1	0.93	0.25	87,87,87,87	0
55	MG	BA	3144	1/1	0.93	0.23	48,48,48,48	0
55	MG	AA	1664	1/1	0.93	0.10	45,45,45,45	0
55	MG	DA	3176	1/1	0.93	0.33	65,65,65,65	0
55	MG	BA	3197	1/1	0.93	0.38	46,46,46,46	0
55	MG	BA	3319	1/1	0.93	0.25	65,65,65,65	0
55	MG	AA	1622	1/1	0.93	0.23	76,76,76,76	0
55	MG	BA	3147	1/1	0.93	0.12	55,55,55,55	0
55	MG	BA	3148	1/1	0.93	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3063	1/1	0.93	0.07	43,43,43,43	0
55	MG	DA	3187	1/1	0.93	0.22	42,42,42,42	0
55	MG	BA	3453	1/1	0.93	0.34	60,60,60,60	0
55	MG	DA	3512	1/1	0.93	0.33	75,75,75,75	0
55	MG	BA	3515	1/1	0.93	0.22	72,72,72,72	0
55	MG	BA	3150	1/1	0.93	0.27	36,36,36,36	0
55	MG	BA	3270	1/1	0.93	0.09	76,76,76,76	0
55	MG	CC	103	1/1	0.93	0.36	72,72,72,72	0
55	MG	CA	1672	1/1	0.93	0.29	75,75,75,75	0
55	MG	DA	3198	1/1	0.93	0.21	47,47,47,47	0
55	MG	DA	3317	1/1	0.93	0.16	81,81,81,81	0
55	MG	DA	3418	1/1	0.93	0.35	78,78,78,78	0
55	MG	DA	3202	1/1	0.93	0.29	47,47,47,47	0
55	MG	BA	3208	1/1	0.93	0.06	45,45,45,45	0
55	MG	BA	3209	1/1	0.93	0.25	39,39,39,39	0
55	MG	BA	3520	1/1	0.93	0.29	44,44,44,44	0
55	MG	DA	3324	1/1	0.93	0.29	78,78,78,78	0
55	MG	BA	3590	1/1	0.93	0.27	63,63,63,63	0
55	MG	AA	1783	1/1	0.93	0.42	67,67,67,67	0
55	MG	BA	3395	1/1	0.93	0.14	72,72,72,72	0
55	MG	BA	3015	1/1	0.93	0.20	38,38,38,38	0
55	MG	BA	3119	1/1	0.93	0.24	62,62,62,62	0
55	MG	DA	3215	1/1	0.93	0.24	42,42,42,42	0
55	MG	BA	3398	1/1	0.93	0.29	70,70,70,70	0
55	MG	BA	3218	1/1	0.93	0.26	48,48,48,48	0
55	MG	BA	3279	1/1	0.93	0.13	70,70,70,70	0
55	MG	BA	3154	1/1	0.93	0.21	55,55,55,55	0
55	MG	BA	3602	1/1	0.93	0.26	67,67,67,67	0
55	MG	BA	3155	1/1	0.93	0.08	45,45,45,45	0
55	MG	BA	3283	1/1	0.93	0.25	49,49,49,49	0
55	MG	BA	3284	1/1	0.93	0.34	56,56,56,56	0
55	MG	DE	303	1/1	0.93	0.32	56,56,56,56	0
55	MG	BA	3045	1/1	0.93	0.25	45,45,45,45	0
55	MG	CA	1623	1/1	0.93	0.15	90,90,90,90	0
55	MG	DA	3229	1/1	0.93	0.40	62,62,62,62	0
55	MG	BA	3121	1/1	0.93	0.25	57,57,57,57	0
55	MG	BA	3163	1/1	0.93	0.38	50,50,50,50	0
55	MG	BA	3288	1/1	0.93	0.33	76,76,76,76	0
55	MG	DA	3245	1/1	0.94	0.35	60,60,60,60	0
55	MG	DA	3142	1/1	0.94	0.27	40,40,40,40	0
55	MG	AA	1811	1/1	0.94	0.33	67,67,67,67	0
55	MG	BA	3022	1/1	0.94	0.27	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3002	1/1	0.94	0.26	43,43,43,43	0
55	MG	DA	3250	1/1	0.94	0.29	63,63,63,63	0
55	MG	DA	3147	1/1	0.94	0.26	53,53,53,53	0
55	MG	BA	3373	1/1	0.94	0.30	64,64,64,64	0
55	MG	DA	3149	1/1	0.94	0.35	57,57,57,57	0
55	MG	DA	3255	1/1	0.94	0.20	75,75,75,75	0
55	MG	DA	3256	1/1	0.94	0.23	49,49,49,49	0
55	MG	DA	3257	1/1	0.94	0.19	49,49,49,49	0
55	MG	DA	3360	1/1	0.94	0.19	65,65,65,65	0
55	MG	BA	3326	1/1	0.94	0.23	52,52,52,52	0
55	MG	DA	3463	1/1	0.94	0.16	73,73,73,73	0
55	MG	DA	3261	1/1	0.94	0.27	58,58,58,58	0
55	MG	BA	3237	1/1	0.94	0.36	57,57,57,57	0
55	MG	AA	1830	1/1	0.94	0.30	73,73,73,73	0
55	MG	BA	3130	1/1	0.94	0.29	44,44,44,44	0
55	MG	BA	3427	1/1	0.94	0.26	65,65,65,65	0
55	MG	DA	3069	1/1	0.94	0.32	60,60,60,60	0
55	MG	BA	3025	1/1	0.94	0.23	42,42,42,42	0
55	MG	DA	3071	1/1	0.94	0.19	81,81,81,81	0
55	MG	BA	3194	1/1	0.94	0.28	68,68,68,68	0
55	MG	DA	3006	1/1	0.94	0.23	71,71,71,71	0
55	MG	BA	3159	1/1	0.94	0.29	58,58,58,58	0
55	MG	AG	301	1/1	0.94	0.38	81,81,81,81	0
55	MG	DA	3076	1/1	0.94	0.25	86,86,86,86	0
55	MG	DA	3077	1/1	0.94	0.10	64,64,64,64	0
55	MG	BA	3161	1/1	0.94	0.10	56,56,56,56	0
55	MG	BA	3201	1/1	0.94	0.45	66,66,66,66	0
55	MG	DA	3170	1/1	0.94	0.41	68,68,68,68	0
55	MG	BA	3589	1/1	0.94	0.18	41,41,41,41	0
55	MG	DA	3280	1/1	0.94	0.30	46,46,46,46	0
55	MG	BA	3434	1/1	0.94	0.34	75,75,75,75	0
55	MG	BA	3202	1/1	0.94	0.22	51,51,51,51	0
55	MG	BA	3162	1/1	0.94	0.29	45,45,45,45	0
55	MG	DA	3177	1/1	0.94	0.30	74,74,74,74	0
55	MG	DA	3178	1/1	0.94	0.31	59,59,59,59	0
55	MG	BA	3539	1/1	0.94	0.12	74,74,74,74	0
55	MG	AA	1659	1/1	0.94	0.32	69,69,69,69	0
55	MG	BA	3029	1/1	0.94	0.28	35,35,35,35	0
55	MG	BA	3597	1/1	0.94	0.26	79,79,79,79	0
55	MG	BA	3542	1/1	0.94	0.28	72,72,72,72	0
55	MG	BA	3599	1/1	0.94	0.32	69,69,69,69	0
55	MG	BA	3007	1/1	0.94	0.41	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3294	1/1	0.94	0.19	64,64,64,64	0
55	MG	BA	3544	1/1	0.94	0.23	72,72,72,72	0
55	MG	DA	3296	1/1	0.94	0.39	51,51,51,51	0
55	MG	DA	3190	1/1	0.94	0.32	61,61,61,61	0
55	MG	DA	3191	1/1	0.94	0.26	46,46,46,46	0
55	MG	BA	3545	1/1	0.94	0.18	69,69,69,69	0
55	MG	AA	1745	1/1	0.94	0.41	67,67,67,67	0
55	MG	BA	3255	1/1	0.94	0.23	46,46,46,46	0
55	MG	DA	3195	1/1	0.94	0.32	70,70,70,70	0
55	MG	DA	3404	1/1	0.94	0.13	61,61,61,61	0
55	MG	BA	3443	1/1	0.94	0.21	77,77,77,77	0
55	MG	DA	3098	1/1	0.94	0.15	68,68,68,68	0
55	MG	AA	1627	1/1	0.94	0.27	53,53,53,53	0
55	MG	DA	3102	1/1	0.94	0.20	51,51,51,51	0
55	MG	BA	3346	1/1	0.94	0.16	51,51,51,51	0
55	MG	BA	3610	1/1	0.94	0.34	61,61,61,61	0
55	MG	DA	3105	1/1	0.94	0.20	45,45,45,45	0
55	MG	CA	1792	1/1	0.94	0.31	70,70,70,70	0
55	MG	BA	3302	1/1	0.94	0.24	26,26,26,26	0
55	MG	DA	3033	1/1	0.94	0.17	62,62,62,62	0
55	MG	DA	3211	1/1	0.94	0.25	42,42,42,42	0
55	MG	AA	1806	1/1	0.94	0.22	81,81,81,81	0
55	MG	DA	3213	1/1	0.94	0.24	41,41,41,41	0
55	MG	DA	3520	1/1	0.94	0.34	76,76,76,76	0
55	MG	BA	3034	1/1	0.94	0.22	41,41,41,41	0
55	MG	BA	3401	1/1	0.94	0.23	62,62,62,62	0
55	MG	BA	3259	1/1	0.94	0.13	40,40,40,40	0
55	MG	DA	3217	1/1	0.94	0.26	55,55,55,55	0
55	MG	BA	3260	1/1	0.94	0.25	47,47,47,47	0
55	MG	DA	3325	1/1	0.94	0.34	73,73,73,73	0
55	MG	AA	1652	1/1	0.94	0.34	81,81,81,81	0
55	MG	BA	3217	1/1	0.94	0.18	52,52,52,52	0
55	MG	AA	1800	1/1	0.94	0.38	82,82,82,82	0
55	MG	DA	3223	1/1	0.94	0.24	52,52,52,52	0
55	MG	BA	3040	1/1	0.94	0.31	54,54,54,54	0
55	MG	BA	3177	1/1	0.94	0.28	57,57,57,57	0
55	MG	BA	3409	1/1	0.94	0.13	68,68,68,68	0
55	MG	CA	1746	1/1	0.94	0.37	57,57,57,57	0
55	MG	BA	3564	1/1	0.94	0.28	84,84,84,84	0
55	MG	BA	3179	1/1	0.94	0.36	64,64,64,64	0
55	MG	BA	3017	1/1	0.94	0.23	25,25,25,25	0
55	MG	DA	3050	1/1	0.94	0.33	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	DA	3130	1/1	0.94	0.13	60,60,60,60	0
55	MG	DA	3233	1/1	0.94	0.33	52,52,52,52	0
55	MG	BA	3018	1/1	0.94	0.26	54,54,54,54	0
55	MG	AA	1722	1/1	0.94	0.35	68,68,68,68	0
55	MG	BA	3183	1/1	0.94	0.14	47,47,47,47	0
55	MG	AA	1717	1/1	0.94	0.32	74,74,74,74	0
55	MG	BA	3125	1/1	0.94	0.42	52,52,52,52	0
55	MG	BB	210	1/1	0.94	0.34	64,64,64,64	0
55	MG	BA	3233	1/1	0.94	0.22	48,48,48,48	0
56	ZN	CG	303	1/1	0.94	0.21	118,118,118,118	0
55	MG	BA	3165	1/1	0.95	0.36	61,61,61,61	0
55	MG	BA	3141	1/1	0.95	0.26	35,35,35,35	0
55	MG	BA	3383	1/1	0.95	0.20	71,71,71,71	0
55	MG	DA	3392	1/1	0.95	0.35	68,68,68,68	0
55	MG	CA	1613	1/1	0.95	0.20	68,68,68,68	0
55	MG	BA	3307	1/1	0.95	0.31	39,39,39,39	0
55	MG	BA	3199	1/1	0.95	0.22	49,49,49,49	0
55	MG	AA	1691	1/1	0.95	0.34	50,50,50,50	0
55	MG	CA	1726	1/1	0.95	0.48	75,75,75,75	0
55	MG	BA	3344	1/1	0.95	0.25	55,55,55,55	0
55	MG	DA	3240	1/1	0.95	0.29	42,42,42,42	0
55	MG	DA	3163	1/1	0.95	0.40	62,62,62,62	0
55	MG	BA	3004	1/1	0.95	0.27	35,35,35,35	0
55	MG	BA	3389	1/1	0.95	0.17	59,59,59,59	0
55	MG	CA	1674	1/1	0.95	0.10	70,70,70,70	0
55	MG	AA	1798	1/1	0.95	0.16	58,58,58,58	0
55	MG	CA	1676	1/1	0.95	0.38	55,55,55,55	0
55	MG	AA	1641	1/1	0.95	0.19	57,57,57,57	0
55	MG	AA	1792	1/1	0.95	0.11	55,55,55,55	0
55	MG	DA	3408	1/1	0.95	0.08	73,73,73,73	0
55	MG	DA	3171	1/1	0.95	0.31	63,63,63,63	0
55	MG	DA	3489	1/1	0.95	0.10	71,71,71,71	0
55	MG	DA	3252	1/1	0.95	0.26	64,64,64,64	0
55	MG	AA	1676	1/1	0.95	0.24	70,70,70,70	0
55	MG	BA	3436	1/1	0.95	0.19	59,59,59,59	0
55	MG	DA	3174	1/1	0.95	0.27	44,44,44,44	0
55	MG	BA	3175	1/1	0.95	0.10	69,69,69,69	0
55	MG	DA	3097	1/1	0.95	0.19	52,52,52,52	0
55	MG	DA	3258	1/1	0.95	0.13	37,37,37,37	0
55	MG	CA	1738	1/1	0.95	0.32	63,63,63,63	0
55	MG	DA	3099	1/1	0.95	0.14	40,40,40,40	0
55	MG	DA	3035	1/1	0.95	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3420	1/1	0.95	0.18	67,67,67,67	0
55	MG	DA	3180	1/1	0.95	0.29	52,52,52,52	0
55	MG	BB	205	1/1	0.95	0.26	74,74,74,74	0
55	MG	DA	3423	1/1	0.95	0.39	75,75,75,75	0
55	MG	BA	3576	1/1	0.95	0.24	74,74,74,74	0
55	MG	BA	3352	1/1	0.95	0.29	76,76,76,76	0
55	MG	BA	3353	1/1	0.95	0.29	52,52,52,52	0
55	MG	BA	3207	1/1	0.95	0.30	41,41,41,41	0
55	MG	BA	3356	1/1	0.95	0.33	70,70,70,70	0
55	MG	DA	3188	1/1	0.95	0.47	56,56,56,56	0
55	MG	BA	3037	1/1	0.95	0.20	44,44,44,44	0
55	MG	BA	3009	1/1	0.95	0.17	36,36,36,36	0
55	MG	BA	3039	1/1	0.95	0.21	42,42,42,42	0
55	MG	BA	3250	1/1	0.95	0.19	60,60,60,60	0
55	MG	AA	1623	1/1	0.95	0.36	65,65,65,65	0
55	MG	DA	3114	1/1	0.95	0.41	54,54,54,54	0
55	MG	DA	3115	1/1	0.95	0.26	49,49,49,49	0
55	MG	BA	3538	1/1	0.95	0.36	66,66,66,66	0
55	MG	BA	3322	1/1	0.95	0.37	64,64,64,64	0
55	MG	CN	201	1/1	0.95	0.15	74,74,74,74	0
55	MG	BA	3061	1/1	0.95	0.44	61,61,61,61	0
55	MG	DA	3203	1/1	0.95	0.14	48,48,48,48	0
55	MG	BA	3041	1/1	0.95	0.23	46,46,46,46	0
55	MG	BA	3451	1/1	0.95	0.31	65,65,65,65	0
55	MG	DA	3444	1/1	0.95	0.10	73,73,73,73	0
55	MG	BA	3497	1/1	0.95	0.28	71,71,71,71	0
55	MG	BA	3013	1/1	0.95	0.29	34,34,34,34	0
55	MG	AN	201	1/1	0.95	0.16	68,68,68,68	0
55	MG	DB	203	1/1	0.95	0.25	66,66,66,66	0
55	MG	BA	3047	1/1	0.95	0.35	74,74,74,74	0
55	MG	BA	3186	1/1	0.95	0.21	36,36,36,36	0
55	MG	BA	3329	1/1	0.95	0.29	65,65,65,65	0
55	MG	BU	201	1/1	0.95	0.21	81,81,81,81	0
55	MG	BA	3158	1/1	0.95	0.14	41,41,41,41	0
55	MG	BA	3504	1/1	0.95	0.22	45,45,45,45	0
55	MG	B5	101	1/1	0.95	0.17	45,45,45,45	0
55	MG	BA	3027	1/1	0.95	0.28	36,36,36,36	0
55	MG	AA	1663	1/1	0.95	0.10	47,47,47,47	0
55	MG	BA	3262	1/1	0.95	0.36	33,33,33,33	0
55	MG	BA	3554	1/1	0.95	0.28	45,45,45,45	0
55	MG	BA	3508	1/1	0.95	0.31	59,59,59,59	0
55	MG	BA	3605	1/1	0.95	0.34	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3263	1/1	0.95	0.43	54,54,54,54	0
55	MG	BA	3091	1/1	0.95	0.25	35,35,35,35	0
55	MG	DA	3306	1/1	0.95	0.33	65,65,65,65	0
55	MG	BA	3138	1/1	0.95	0.41	46,46,46,46	0
55	MG	BA	3139	1/1	0.95	0.24	35,35,35,35	0
55	MG	D5	2001	1/1	0.95	0.23	46,46,46,46	0
55	MG	AA	1701	1/1	0.95	0.17	70,70,70,70	0
55	MG	CA	1776	1/1	0.95	0.34	71,71,71,71	0
55	MG	BF	301	1/1	0.96	0.07	73,73,73,73	0
55	MG	BA	3224	1/1	0.96	0.11	55,55,55,55	0
55	MG	DA	3141	1/1	0.96	0.30	38,38,38,38	0
55	MG	BA	3100	1/1	0.96	0.25	42,42,42,42	0
55	MG	DA	3495	1/1	0.96	0.14	63,63,63,63	0
55	MG	BA	3064	1/1	0.96	0.10	49,49,49,49	0
55	MG	DA	3144	1/1	0.96	0.24	60,60,60,60	0
55	MG	DA	3200	1/1	0.96	0.29	44,44,44,44	0
55	MG	DA	3201	1/1	0.96	0.12	47,47,47,47	0
55	MG	DA	3260	1/1	0.96	0.35	41,41,41,41	0
55	MG	BA	3612	1/1	0.96	0.36	66,66,66,66	0
55	MG	DA	3321	1/1	0.96	0.41	66,66,66,66	0
55	MG	DA	3009	1/1	0.96	0.25	68,68,68,68	0
55	MG	CA	1671	1/1	0.96	0.31	49,49,49,49	0
55	MG	B0	201	1/1	0.96	0.20	51,51,51,51	0
55	MG	BA	3124	1/1	0.96	0.39	45,45,45,45	0
55	MG	DA	3055	1/1	0.96	0.44	68,68,68,68	0
55	MG	AA	1608	1/1	0.96	0.18	64,64,64,64	0
55	MG	DA	3152	1/1	0.96	0.13	67,67,67,67	0
55	MG	BA	3261	1/1	0.96	0.36	52,52,52,52	0
55	MG	BA	3230	1/1	0.96	0.44	56,56,56,56	0
55	MG	BA	3198	1/1	0.96	0.09	45,45,45,45	0
55	MG	BA	3172	1/1	0.96	0.17	34,34,34,34	0
55	MG	BA	3103	1/1	0.96	0.29	52,52,52,52	0
55	MG	BA	3083	1/1	0.96	0.10	62,62,62,62	0
55	MG	AC	104	1/1	0.96	0.24	56,56,56,56	0
55	MG	AA	1719	1/1	0.96	0.21	79,79,79,79	0
55	MG	BA	3107	1/1	0.96	0.26	36,36,36,36	0
55	MG	DA	3278	1/1	0.96	0.28	42,42,42,42	0
55	MG	BA	3271	1/1	0.96	0.07	35,35,35,35	0
55	MG	DA	3111	1/1	0.96	0.17	52,52,52,52	0
55	MG	AA	1763	1/1	0.96	0.31	53,53,53,53	0
55	MG	BA	3306	1/1	0.96	0.21	67,67,67,67	0
55	MG	BA	3042	1/1	0.96	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3274	1/1	0.96	0.15	46,46,46,46	0
55	MG	BA	3043	1/1	0.96	0.11	32,32,32,32	0
55	MG	BA	3011	1/1	0.96	0.19	42,42,42,42	0
55	MG	DA	3287	1/1	0.96	0.36	65,65,65,65	0
55	MG	BA	3012	1/1	0.96	0.20	45,45,45,45	0
55	MG	DB	204	1/1	0.96	0.25	82,82,82,82	0
55	MG	BA	3488	1/1	0.96	0.24	80,80,80,80	0
55	MG	BA	3046	1/1	0.96	0.22	39,39,39,39	0
55	MG	BA	3092	1/1	0.96	0.25	32,32,32,32	0
55	MG	DA	3122	1/1	0.96	0.32	46,46,46,46	0
55	MG	BA	3347	1/1	0.96	0.30	68,68,68,68	0
55	MG	BB	213	1/1	0.96	0.29	66,66,66,66	0
55	MG	DA	3079	1/1	0.96	0.29	54,54,54,54	0
55	MG	DA	3126	1/1	0.96	0.11	41,41,41,41	0
55	MG	DA	3238	1/1	0.96	0.31	60,60,60,60	0
55	MG	BA	3280	1/1	0.96	0.30	50,50,50,50	0
55	MG	BA	3213	1/1	0.96	0.37	49,49,49,49	0
55	MG	DA	3241	1/1	0.96	0.23	46,46,46,46	0
55	MG	BA	3093	1/1	0.96	0.18	57,57,57,57	0
55	MG	AA	1673	1/1	0.96	0.29	78,78,78,78	0
55	MG	AA	1671	1/1	0.96	0.14	67,67,67,67	0
55	MG	DA	3132	1/1	0.96	0.14	53,53,53,53	0
55	MG	AA	1838	1/1	0.96	0.21	61,61,61,61	0
55	MG	DA	3135	1/1	0.96	0.19	49,49,49,49	0
55	MG	BA	3079	1/1	0.96	0.31	55,55,55,55	0
56	ZN	AG	302	1/1	0.96	0.23	95,95,95,95	0
55	MG	AA	1750	1/1	0.96	0.36	62,62,62,62	0
55	MG	BA	3192	1/1	0.96	0.16	34,34,34,34	0
55	MG	DA	3159	1/1	0.97	0.12	37,37,37,37	0
55	MG	DA	3299	1/1	0.97	0.15	38,38,38,38	0
55	MG	BA	3220	1/1	0.97	0.21	44,44,44,44	0
55	MG	BA	3450	1/1	0.97	0.08	54,54,54,54	0
55	MG	DA	3243	1/1	0.97	0.30	79,79,79,79	0
55	MG	BA	3231	1/1	0.97	0.36	73,73,73,73	0
55	MG	BA	3452	1/1	0.97	0.24	41,41,41,41	0
55	MG	BA	3074	1/1	0.97	0.29	49,49,49,49	0
55	MG	AA	1707	1/1	0.97	0.31	50,50,50,50	0
55	MG	DA	3219	1/1	0.97	0.14	70,70,70,70	0
55	MG	BA	3390	1/1	0.97	0.30	60,60,60,60	0
55	MG	BA	3214	1/1	0.97	0.27	67,67,67,67	0
55	MG	AA	1842	1/1	0.97	0.27	59,59,59,59	0
55	MG	DA	3374	1/1	0.97	0.32	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3054	1/1	0.97	0.22	58,58,58,58	0
55	MG	BA	3377	1/1	0.97	0.41	62,62,62,62	0
55	MG	BA	3298	1/1	0.97	0.26	65,65,65,65	0
55	MG	DA	3101	1/1	0.97	0.18	43,43,43,43	0
55	MG	DA	3199	1/1	0.97	0.26	61,61,61,61	0
55	MG	BE	303	1/1	0.97	0.28	44,44,44,44	0
55	MG	BA	3410	1/1	0.97	0.30	62,62,62,62	0
55	MG	BA	3216	1/1	0.97	0.17	33,33,33,33	0
55	MG	BA	3608	1/1	0.97	0.23	39,39,39,39	0
55	MG	BA	3196	1/1	0.97	0.15	33,33,33,33	0
55	MG	BA	3123	1/1	0.97	0.11	51,51,51,51	0
55	MG	DA	3206	1/1	0.97	0.42	65,65,65,65	0
55	MG	DA	3323	1/1	0.97	0.09	42,42,42,42	0
55	MG	BA	3228	1/1	0.97	0.51	72,72,72,72	0
55	MG	BA	3099	1/1	0.97	0.37	67,67,67,67	0
55	MG	DA	3182	1/1	0.97	0.37	44,44,44,44	0
55	MG	BA	3241	1/1	0.97	0.27	60,60,60,60	0
55	MG	B1	201	1/1	0.97	0.21	47,47,47,47	0
55	MG	BA	3077	1/1	0.98	0.20	54,54,54,54	0
55	MG	DA	3329	1/1	0.98	0.15	44,44,44,44	0
55	MG	DA	3161	1/1	0.98	0.19	45,45,45,45	0
55	MG	BA	3596	1/1	0.98	0.29	55,55,55,55	0
55	MG	BA	3171	1/1	0.98	0.33	61,61,61,61	0
55	MG	BA	3036	1/1	0.98	0.29	44,44,44,44	0
55	MG	DP	201	1/1	0.98	0.25	65,65,65,65	0
55	MG	BA	3212	1/1	0.98	0.32	43,43,43,43	0
55	MG	BA	3264	1/1	0.98	0.08	30,30,30,30	0
55	MG	BA	3243	1/1	0.98	0.31	48,48,48,48	0
55	MG	BA	3491	1/1	0.98	0.34	42,42,42,42	0
55	MG	BA	3157	1/1	0.98	0.37	45,45,45,45	0
55	MG	BA	3382	1/1	0.98	0.26	43,43,43,43	0
55	MG	BA	3355	1/1	0.98	0.31	46,46,46,46	0
55	MG	BA	3178	1/1	0.98	0.20	36,36,36,36	0
55	MG	DA	3133	1/1	0.98	0.23	42,42,42,42	0
56	ZN	CQ	101	1/1	0.98	0.05	120,120,120,120	0

6.5 Other polymers

There are no such residues in this entry.