



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 07:57 pm GMT

PDB ID : 4V8C  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex with paromomycin).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-07  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

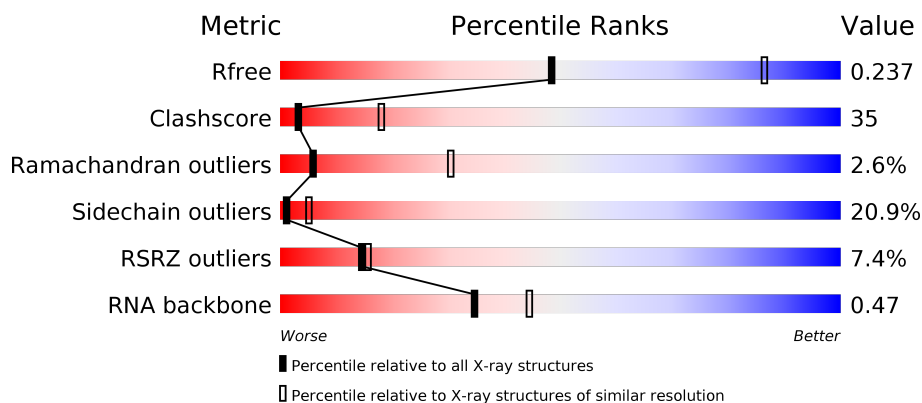
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)
RNA backbone	2636	1009 (3.74-2.86)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	<div> <div>28%</div> <div>50%</div> <div>20%</div> <div>•</div> </div>
1	BA	2912	<div> <div>27%</div> <div>51%</div> <div>20%</div> <div>•</div> </div>
2	AB	122	<div> <div>32%</div> <div>48%</div> <div>18%</div> <div>•</div> </div>
2	BB	122	<div> <div>25%</div> <div>56%</div> <div>19%</div> <div>•</div> </div>

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


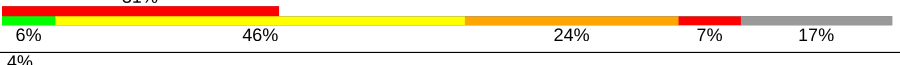

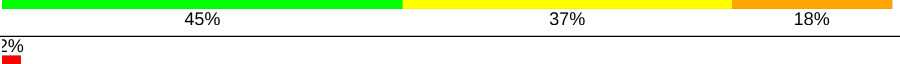
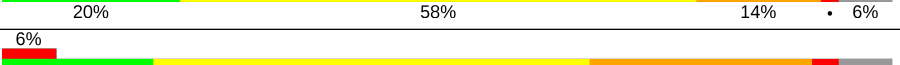
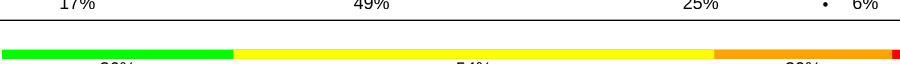
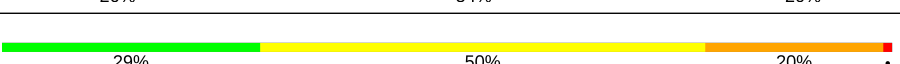
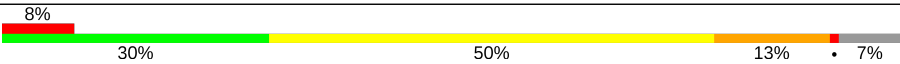
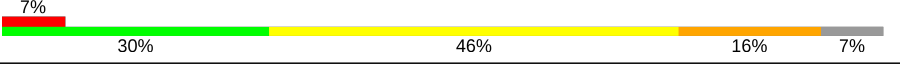
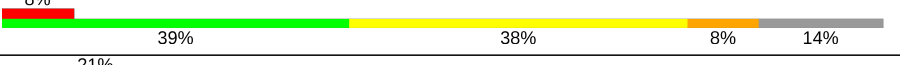
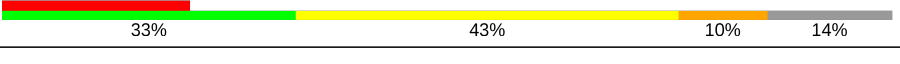
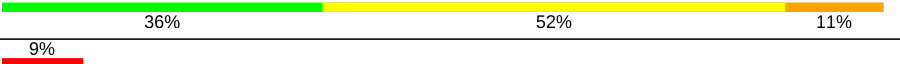

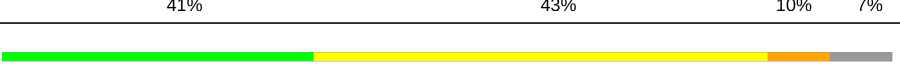
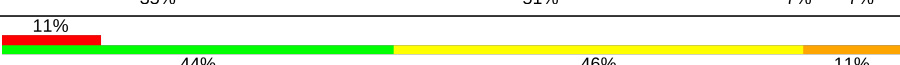
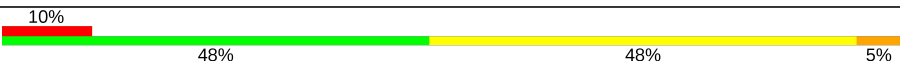

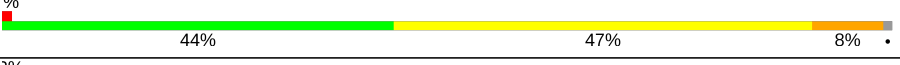


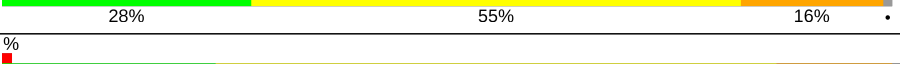
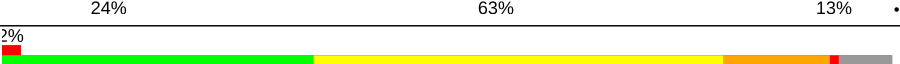



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Mol	Chain	Length	Quality of chain
15	BR	146	
16	A1	118	
16	B1	118	
17	A2	101	
17	B2	101	
18	AS	113	
18	BS	113	
19	AT	96	
19	BT	96	
20	AU	110	
20	BU	110	
21	AV	206	
21	BV	206	
22	A3	85	
22	B3	85	
23	AZ	98	
23	BZ	98	
24	AW	72	
24	BW	72	
25	AX	60	
25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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	A3	101	-	-	-	X
55	MG	A5	102	-	-	-	X
55	MG	A6	101	-	-	-	X
55	MG	AA	3039	-	-	-	X
55	MG	AA	3053	-	-	-	X
55	MG	AA	3060	-	-	-	X
55	MG	AA	3067	-	-	-	X
55	MG	AA	3073	-	-	-	X
55	MG	AA	3075	-	-	-	X
55	MG	AA	3077	-	-	-	X
55	MG	AA	3078	-	-	-	X
55	MG	AA	3080	-	-	-	X
55	MG	AA	3093	-	-	-	X
55	MG	AA	3097	-	-	-	X
55	MG	AA	3108	-	-	-	X
55	MG	AA	3118	-	-	-	X
55	MG	AA	3121	-	-	-	X
55	MG	AA	3132	-	-	-	X
55	MG	AA	3148	-	-	-	X
55	MG	AA	3156	-	-	-	X
55	MG	AA	3182	-	-	-	X
55	MG	AA	3185	-	-	-	X
55	MG	AA	3193	-	-	-	X
55	MG	AA	3224	-	-	-	X
55	MG	AA	3225	-	-	-	X
55	MG	AA	3231	-	-	-	X
55	MG	AA	3235	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3236	-	-	-	X
55	MG	AA	3249	-	-	-	X
55	MG	AA	3258	-	-	-	X
55	MG	AA	3260	-	-	-	X
55	MG	AA	3261	-	-	-	X
55	MG	AA	3264	-	-	-	X
55	MG	AA	3268	-	-	-	X
55	MG	AA	3278	-	-	-	X
55	MG	AA	3286	-	-	-	X
55	MG	AA	3291	-	-	-	X
55	MG	AA	3294	-	-	-	X
55	MG	AA	3295	-	-	-	X
55	MG	AA	3302	-	-	-	X
55	MG	AA	3307	-	-	-	X
55	MG	AA	3309	-	-	-	X
55	MG	AA	3334	-	-	-	X
55	MG	AA	3335	-	-	-	X
55	MG	AA	3353	-	-	-	X
55	MG	AA	3356	-	-	-	X
55	MG	AA	3357	-	-	-	X
55	MG	AA	3358	-	-	-	X
55	MG	AA	3359	-	-	-	X
55	MG	AA	3361	-	-	-	X
55	MG	AA	3363	-	-	-	X
55	MG	AA	3366	-	-	-	X
55	MG	AA	3367	-	-	-	X
55	MG	AA	3369	-	-	-	X
55	MG	AA	3371	-	-	-	X
55	MG	AA	3373	-	-	-	X
55	MG	AA	3374	-	-	-	X
55	MG	AA	3375	-	-	-	X
55	MG	AA	3376	-	-	-	X
55	MG	AA	3377	-	-	-	X
55	MG	AA	3381	-	-	-	X
55	MG	AA	3382	-	-	-	X
55	MG	AA	3384	-	-	-	X
55	MG	AA	3385	-	-	-	X
55	MG	AA	3390	-	-	-	X
55	MG	AA	3391	-	-	-	X
55	MG	AA	3392	-	-	-	X
55	MG	AA	3393	-	-	-	X
55	MG	AA	3395	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3396	-	-	-	X
55	MG	AA	3397	-	-	-	X
55	MG	AA	3402	-	-	-	X
55	MG	AA	3407	-	-	-	X
55	MG	AA	3409	-	-	-	X
55	MG	AA	3416	-	-	-	X
55	MG	AA	3419	-	-	-	X
55	MG	AA	3421	-	-	-	X
55	MG	AA	3426	-	-	-	X
55	MG	AA	3435	-	-	-	X
55	MG	AA	3437	-	-	-	X
55	MG	AA	3438	-	-	-	X
55	MG	AA	3439	-	-	-	X
55	MG	AA	3441	-	-	-	X
55	MG	AA	3452	-	-	-	X
55	MG	AA	3456	-	-	-	X
55	MG	AA	3463	-	-	-	X
55	MG	AA	3466	-	-	-	X
55	MG	AA	3469	-	-	-	X
55	MG	AA	3480	-	-	-	X
55	MG	AA	3490	-	-	-	X
55	MG	AA	3497	-	-	-	X
55	MG	AA	3498	-	-	-	X
55	MG	AA	3499	-	-	-	X
55	MG	AA	3501	-	-	-	X
55	MG	AA	3502	-	-	-	X
55	MG	AA	3522	-	-	-	X
55	MG	AA	3524	-	-	-	X
55	MG	AA	3527	-	-	-	X
55	MG	AA	3536	-	-	-	X
55	MG	AA	3556	-	-	-	X
55	MG	AA	3557	-	-	-	X
55	MG	AA	3583	-	-	-	X
55	MG	AA	3593	-	-	-	X
55	MG	AA	3594	-	-	-	X
55	MG	AA	3604	-	-	-	X
55	MG	AA	3612	-	-	-	X
55	MG	AA	3626	-	-	-	X
55	MG	AB	204	-	-	-	X
55	MG	AB	209	-	-	-	X
55	MG	AB	212	-	-	-	X
55	MG	BA	3003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3024	-	-	-	X
55	MG	BA	3041	-	-	-	X
55	MG	BA	3044	-	-	-	X
55	MG	BA	3065	-	-	-	X
55	MG	BA	3067	-	-	-	X
55	MG	BA	3073	-	-	-	X
55	MG	BA	3108	-	-	-	X
55	MG	BA	3121	-	-	-	X
55	MG	BA	3125	-	-	-	X
55	MG	BA	3185	-	-	-	X
55	MG	BA	3191	-	-	-	X
55	MG	BA	3226	-	-	-	X
55	MG	BA	3235	-	-	-	X
55	MG	BA	3266	-	-	-	X
55	MG	BA	3289	-	-	-	X
55	MG	BA	3350	-	-	-	X
55	MG	BA	3355	-	-	-	X
55	MG	BA	3374	-	-	-	X
55	MG	BA	3383	-	-	-	X
55	MG	BA	3387	-	-	-	X
55	MG	BA	3390	-	-	-	X
55	MG	BA	3394	-	-	-	X
55	MG	BA	3398	-	-	-	X
55	MG	BA	3410	-	-	-	X
55	MG	BA	3413	-	-	-	X
55	MG	BA	3423	-	-	-	X
55	MG	BA	3424	-	-	-	X
55	MG	BA	3444	-	-	-	X
55	MG	BA	3454	-	-	-	X
55	MG	BA	3472	-	-	-	X
55	MG	BA	3474	-	-	-	X
55	MG	BB	208	-	-	-	X
55	MG	BB	213	-	-	-	X
55	MG	BR	202	-	-	-	X
55	MG	C1	101	-	-	-	X
55	MG	CA	1617	-	-	-	X
55	MG	CA	1639	-	-	-	X
55	MG	CA	1653	-	-	-	X
55	MG	CA	1662	-	-	-	X
55	MG	CA	1694	-	-	-	X
55	MG	CA	1704	-	-	-	X
55	MG	CA	1709	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	1714	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1734	-	-	-	X
55	MG	CA	1735	-	-	-	X
55	MG	CA	1757	-	-	-	X
55	MG	CA	1758	-	-	-	X
55	MG	CA	1766	-	-	-	X
55	MG	CA	1774	-	-	-	X
55	MG	CA	1776	-	-	-	X
55	MG	CA	1778	-	-	-	X
55	MG	CA	1782	-	-	-	X
55	MG	CA	1783	-	-	-	X
55	MG	CA	1798	-	-	-	X
55	MG	CA	1803	-	-	-	X
55	MG	CA	1813	-	-	-	X
55	MG	CC	107	-	-	-	X
55	MG	CG	301	-	-	-	X
55	MG	DA	1613	-	-	-	X
55	MG	DA	1661	-	-	-	X
55	MG	DA	1678	-	-	-	X
55	MG	DA	1682	-	-	-	X
55	MG	DA	1683	-	-	-	X
55	MG	DA	1698	-	-	-	X
55	MG	DA	1708	-	-	-	X
55	MG	DA	1710	-	-	-	X
55	MG	DA	1711	-	-	-	X
55	MG	DA	1712	-	-	-	X
55	MG	DA	1719	-	-	-	X
55	MG	DA	1748	-	-	-	X
55	MG	DA	1758	-	-	-	X
55	MG	DA	1759	-	-	-	X
55	MG	DA	1760	-	-	-	X
55	MG	DA	1764	-	-	-	X
55	MG	DA	1766	-	-	-	X
55	MG	DA	1777	-	-	-	X
55	MG	DA	1791	-	-	-	X
55	MG	DA	1794	-	-	-	X
55	MG	DA	1802	-	-	-	X
55	MG	DA	1803	-	-	-	X
55	MG	DC	107	-	-	-	X
55	MG	DS	101	-	-	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (2912-MER).

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 54 is a RNA chain called MRNA.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	528	Total Mg 528 528	0	0
55	CA	240	Total Mg 240 240	0	0
55	AB	17	Total Mg 17 17	0	0
55	A6	1	Total Mg 1 1	0	0
55	BE	3	Total Mg 3 3	0	0
55	B1	1	Total Mg 1 1	0	0
55	C1	1	Total Mg 1 1	0	0
55	CD	1	Total Mg 1 1	0	0
55	BP	1	Total Mg 1 1	0	0
55	CN	2	Total Mg 2 2	0	0
55	A2	1	Total Mg 1 1	0	0
55	DC	8	Total Mg 8 8	0	0
55	B5	1	Total Mg 1 1	0	0
55	BB	15	Total Mg 15 15	0	0
55	AE	4	Total Mg 4 4	0	0
55	DG	2	Total Mg 2 2	0	0
55	AA	626	Total Mg 626 626	0	0
55	CQ	2	Total Mg 2 2	0	0
55	A5	2	Total Mg 2 2	0	0
55	CG	2	Total Mg 2 2	0	0
55	A1	1	Total Mg 1 1	0	0
55	AD	1	Total Mg 1 1	0	0

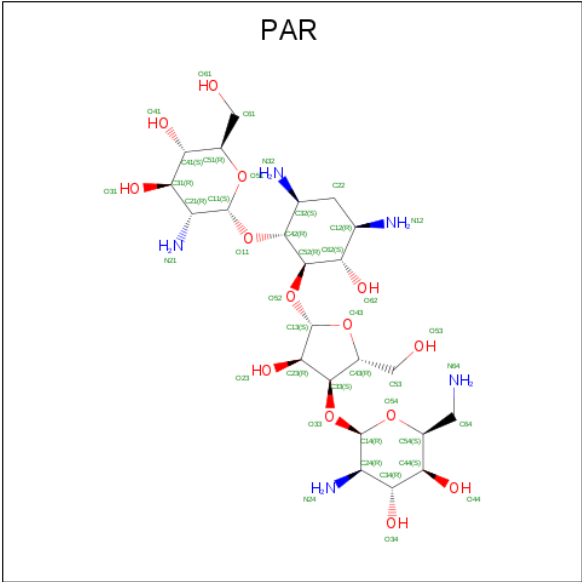
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CT	1	Total 1	Mg 1	0	0
55	DH	1	Total 1	Mg 1	0	0
55	CC	7	Total 7	Mg 7	0	0
55	DS	1	Total 1	Mg 1	0	0
55	B3	1	Total 1	Mg 1	0	0
55	BR	2	Total 2	Mg 2	0	0
55	AZ	1	Total 1	Mg 1	0	0
55	DA	204	Total 204	Mg 204	0	0
55	AU	1	Total 1	Mg 1	0	0
55	A0	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	A7	2	Total 2	Mg 2	0	0
55	BD	1	Total 1	Mg 1	0	0
55	AO	3	Total 3	Mg 3	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	3	Total 3	Mg 3	0	0
55	DB	2	Total 2	Mg 2	0	0

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





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

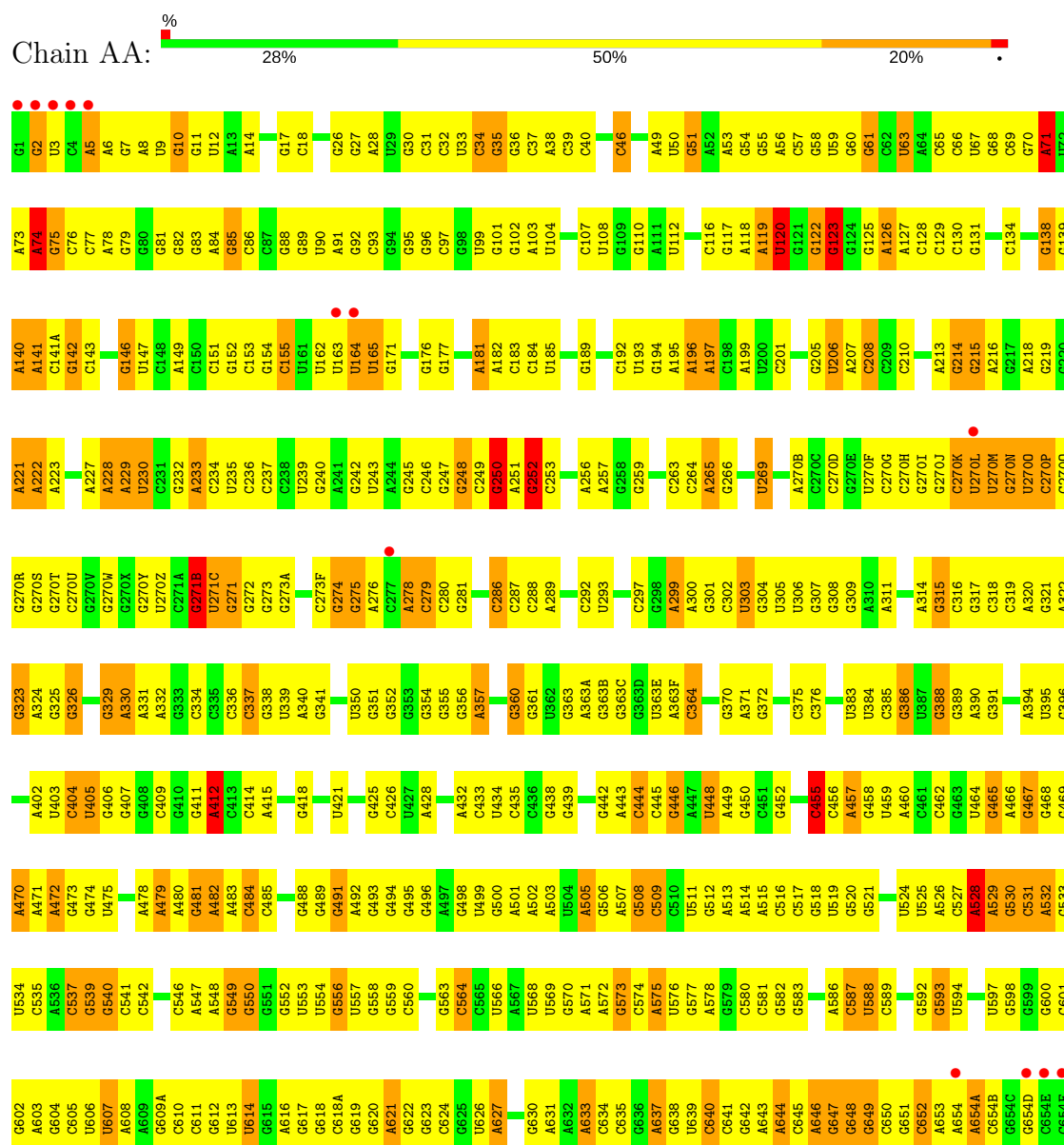
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 3 Residue-property plots

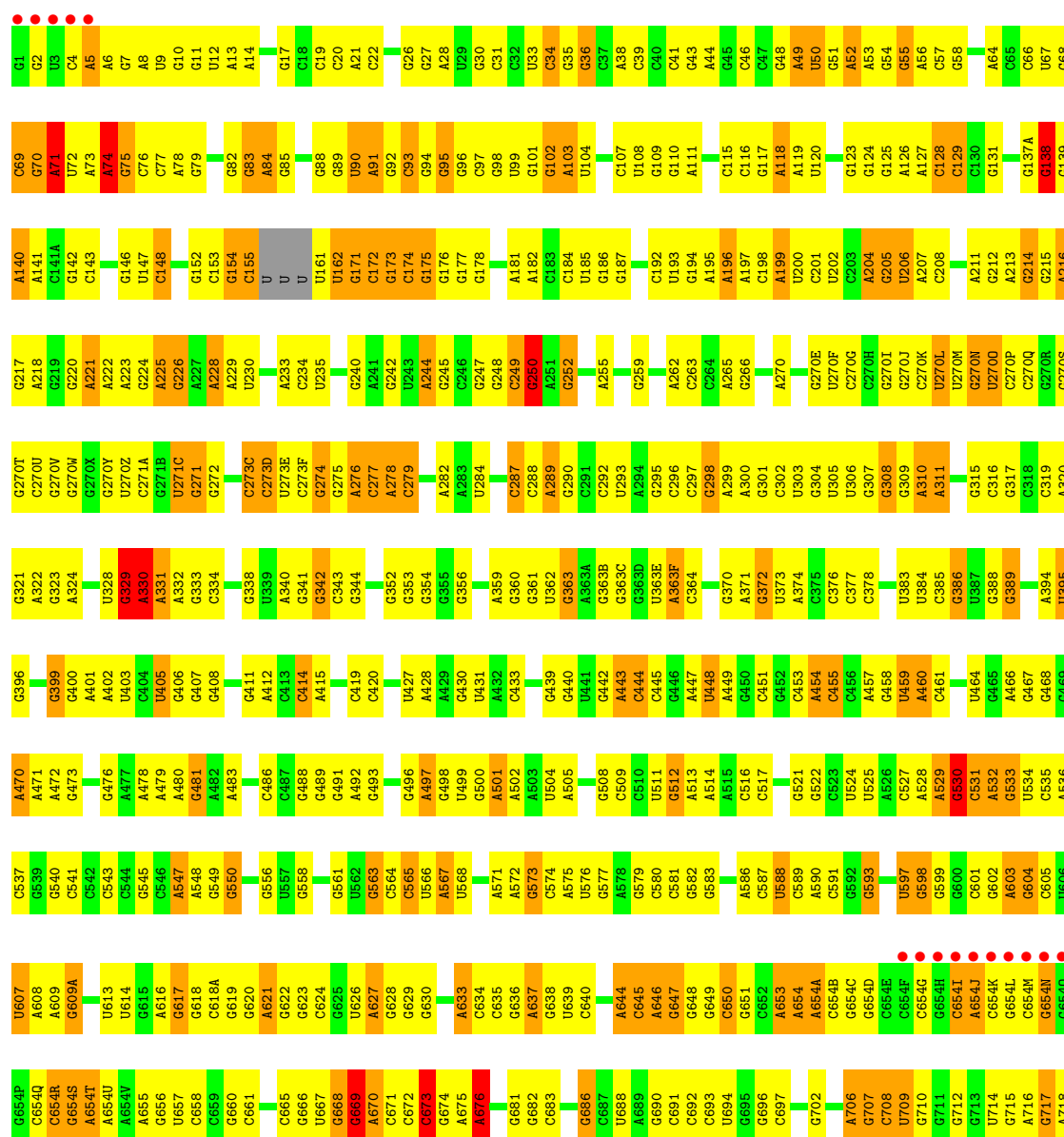
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: RNA (2912-MER)



A1586	A1587	G1525	G1461	A1395	U1326	C1251	C1180	G1117	A1054	C986	A917	U851	G707	C654G
A1588	G1526	G1527	C1462	U1397	C1327	G1252	C1181	G1118	G1055	G987	A918	G852	C708	C654H
C1589	G1528	G1529	C1463	U1398	C1328	A1253	G1182	C1119	A1056	A988	G919	G853	C709	C654I
U1590	A1529	A1529	G1464	C1399	U1329	C1257	G1184	G1122	U1058	A990	U922	G855	G710	A654J
U1591	G1530	G1531	G1465	G1400	C1330	G1257	C1185	G1122	G1059	C991	C923	C856	G715	C654K
C1592	C1531	C1532	C1467	G1401	A1331	C1258	G1186	G1122	U1060	C992	C924	C857	A716	C654L
G1593	C1533	C1534	C1468	C1402	G1332	G1259	G1187	G1125	U1061	G994	C925	U858	G717	C654M
G1594	C1535	G1534	A1469	C1403	A1336	G1260	U1188	A1126	G1062	C995	A926	G795	A718	C654N
A1595	U1535	U1535	G1470	U1405	C1337	C1261	A1189	A1127	U1063	C996	G928	G859	G719	C654O
A1597	U1536	U1536	A1471	U1406	G1338	A1262	G1190	A1128	C1064	A996	G929	A861	C720	C654P
C1598	C1537	C1538	C1472	C1407	G1339	G1263	G1191	A1129	U1065	G997	U930	G862	C721	C654Q
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G1606	G1538	G1539	G1475	C1409	U1341	A1265	G1193	G1131	A1067	U999	G932	C864	G728	C654S
C1607	G1540	G1540	C1476	G1410	U1342	G1266	A1194	A1132	G1068	A1000	A933	C865	G729	A654T
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A1616	C1548	C1548	G1487	G1488	G1355	G1276	G1206	A1142A	C1079	C1013	G955	G881	A746	C664
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C1648	G1568	G1568	A1507	G1441	U1379	G1303	G1232	U1165	A1098	G1037	C971	A901	G771	C692
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C1662	C1585	C1585	G1521	G1459	U1393	A1322	G1250	C1179	G1113			C850	C786	





G1651	A1449	C1513	A1384	U1313	A1247	A1177	G1112	G1051	A988	U922	A861	G799	C719
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	G1461		A1396	C1324	C1257	U1189	G1126	G1062	U999	G934	A872	U810	C731
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C1670	A1469	U1532	U1406	G1333	G1266	G1200	G1135	A1070	C1007	U944	G880	C818	C752
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	A1477	U1540	G1413	G1343	A1274	C1208	A1142A		G1015	G953	C888	U828	A761
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G1697	C1492	G1554	C1428	A1359	G1290	G1226	G1157	G1093	C903	G842	G843	G842	U779
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U2786	C2787	C2788	C2789	C2790	C2791	C2794	C2795	C2796	C2797	C2798	C2799	A2801	C2802	C2803	C2804	C2805	C2807	U2808	A2809	A2810	C2811	A2812	C2813	C2814	C2815	C2816	C2817	C2818	A2749	C2819	C2820	A2821	C2822	A2823	C2824	C2825	G2833	G2834	U2835	G2836	G2837	G2838	G2839	C2840	C2841	G2842	G2843	G2844	G2845	G2846	U2847	G2848	U2849	A2850	A2851	G2854	C2855	C2856	
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• Molecule 2: 5S RIBOSOMAL RNA



• Molecule 2: 5S RIBOSOMAL RNA

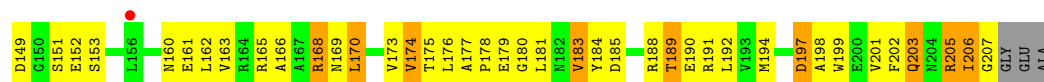


• Molecule 3: 50S ribosomal protein L2

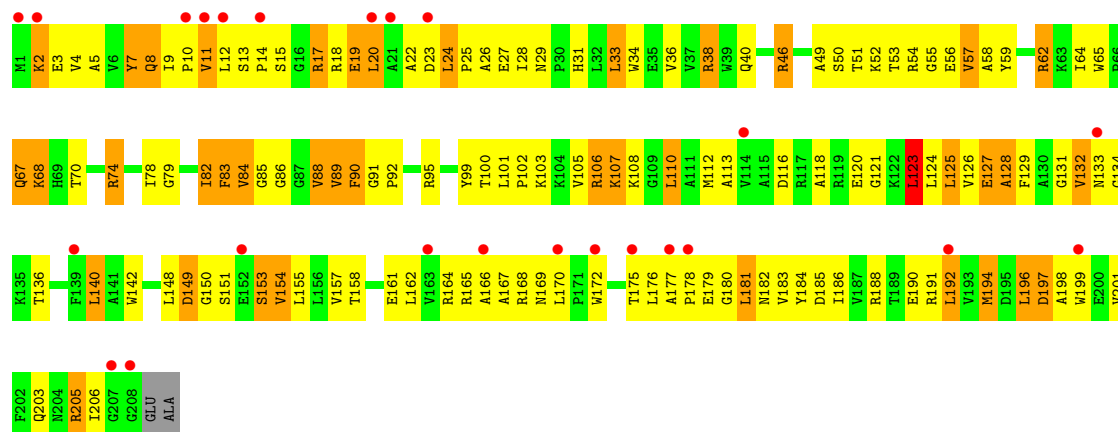




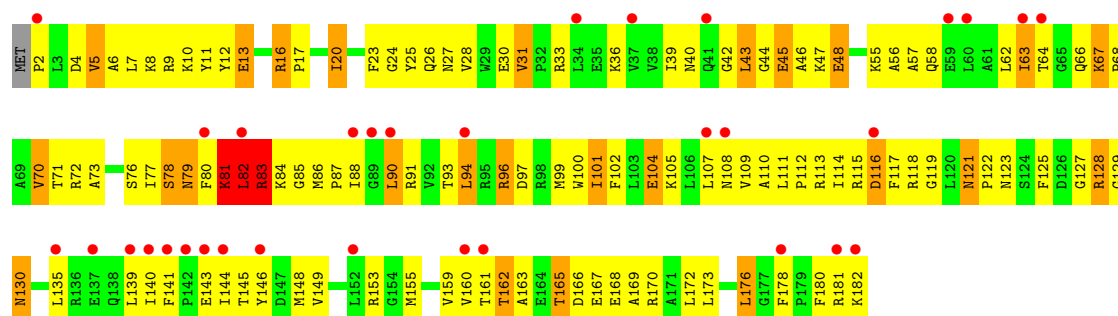




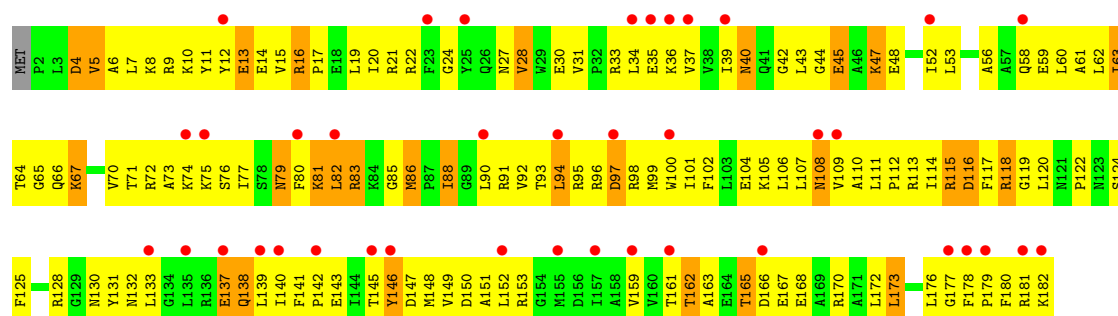
• Molecule 5: 50S ribosomal protein L4



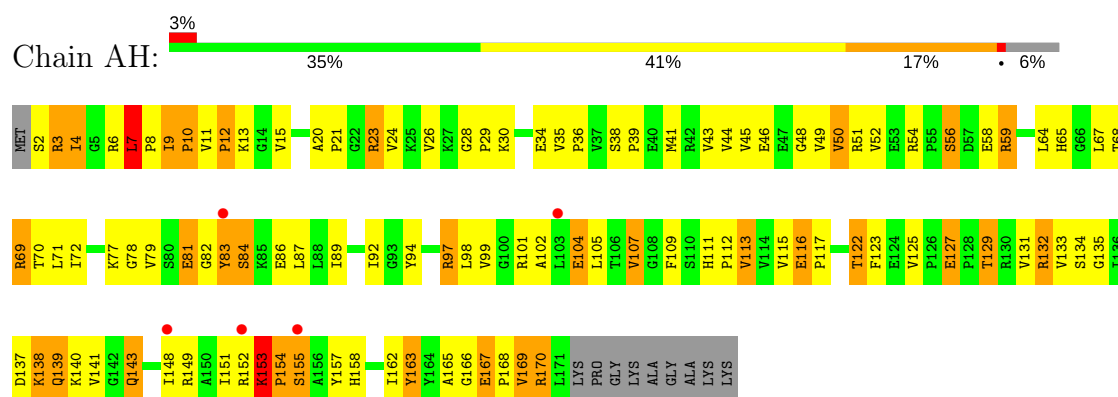
• Molecule 6: 50S ribosomal protein L5



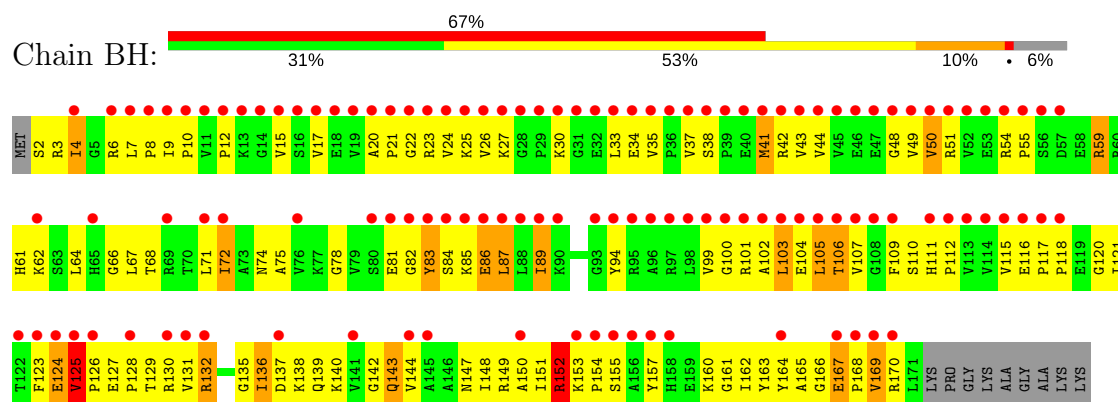
• Molecule 6: 50S ribosomal protein L5



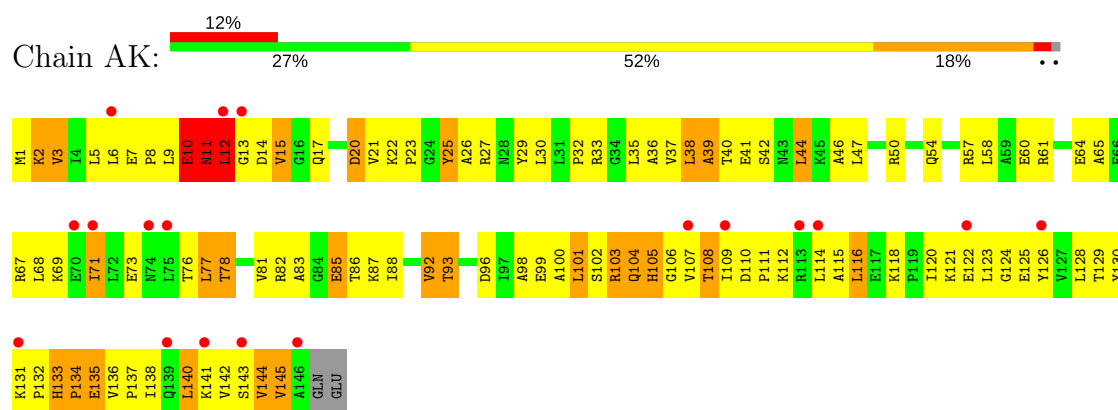
• Molecule 7: 50S ribosomal protein L6



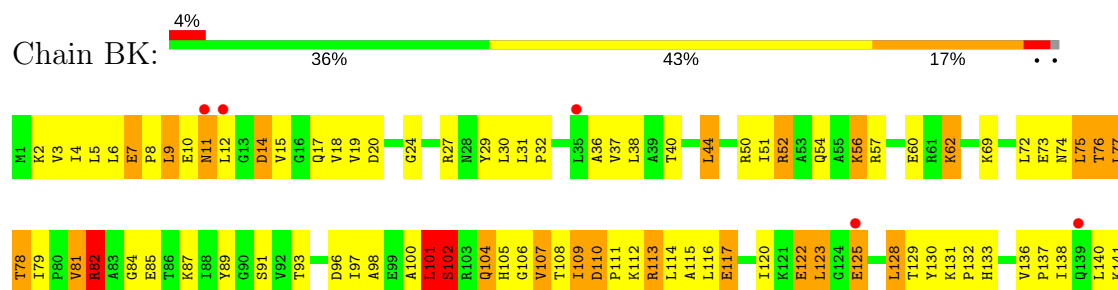
• Molecule 7: 50S ribosomal protein L6

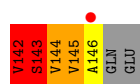


• Molecule 8: 50S ribosomal protein L9

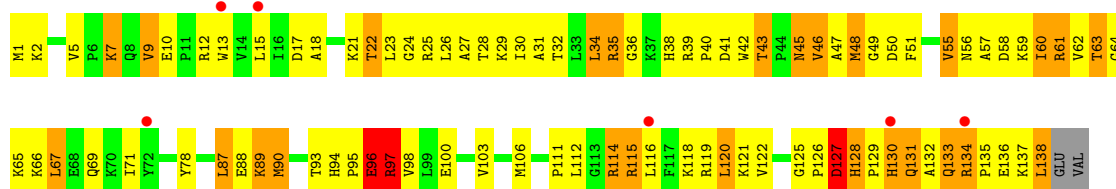


• Molecule 8: 50S ribosomal protein L9

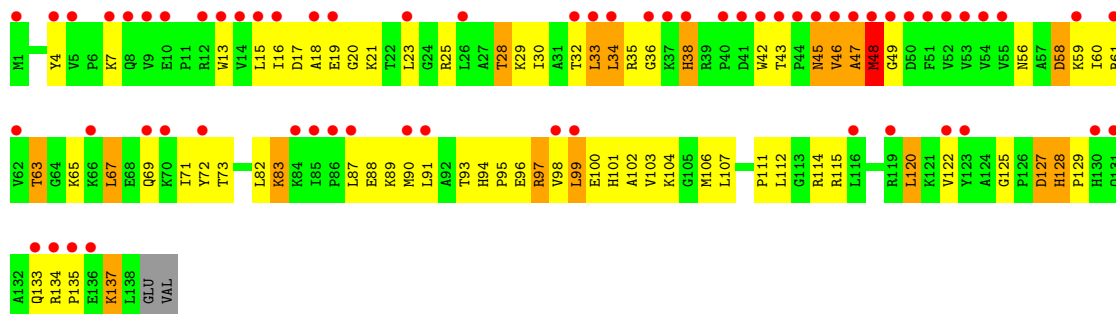




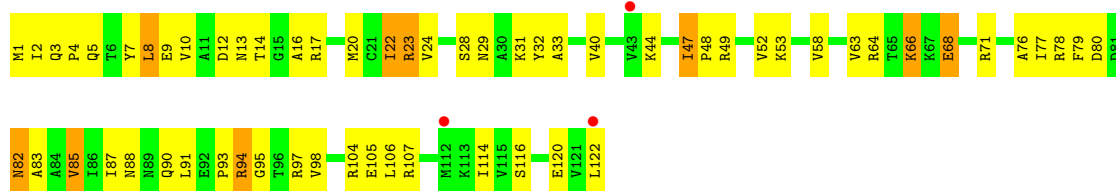
• Molecule 9: 50S ribosomal protein L13



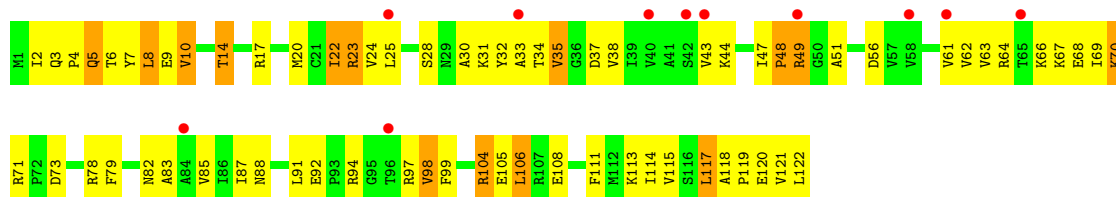
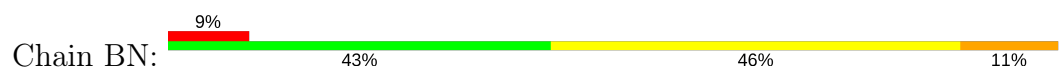
• Molecule 9: 50S ribosomal protein L13



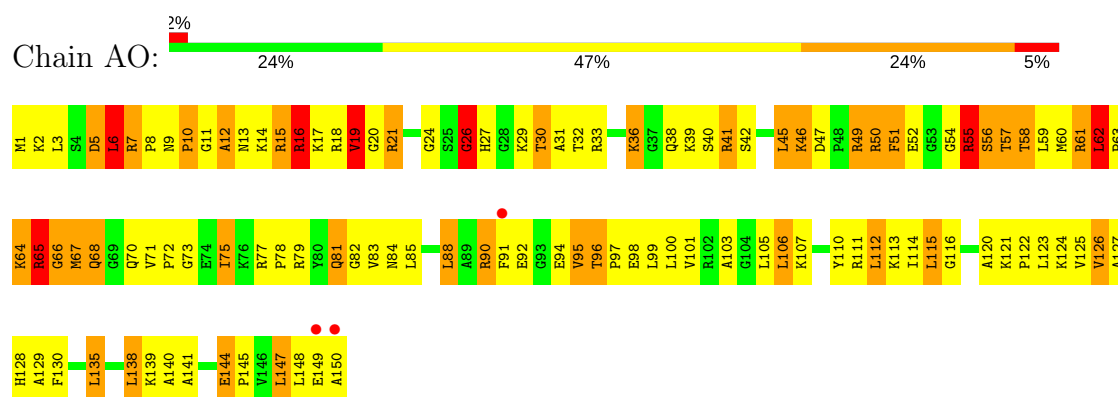
• Molecule 10: 50S ribosomal protein L14



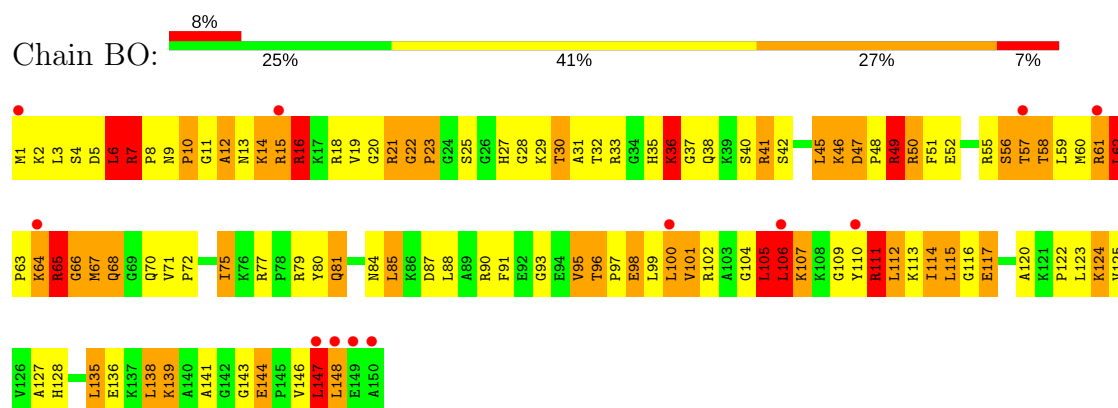
• Molecule 10: 50S ribosomal protein L14



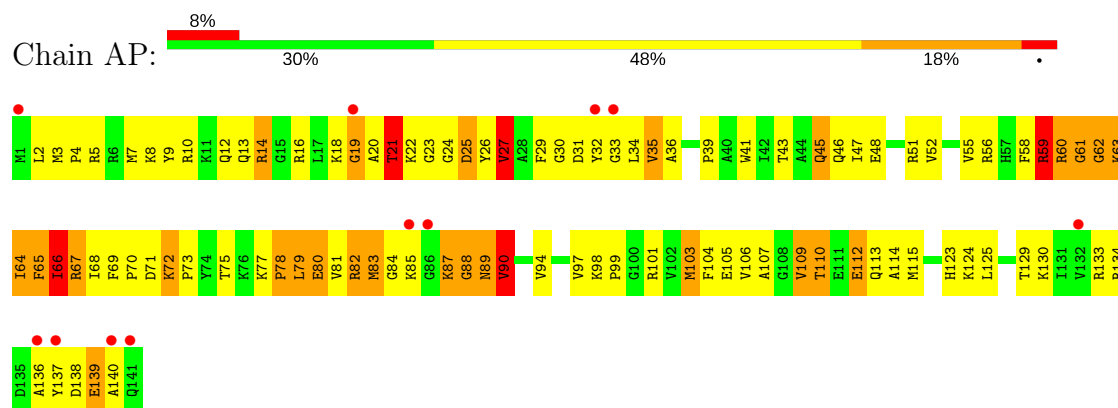
• Molecule 11: 50S ribosomal protein L15



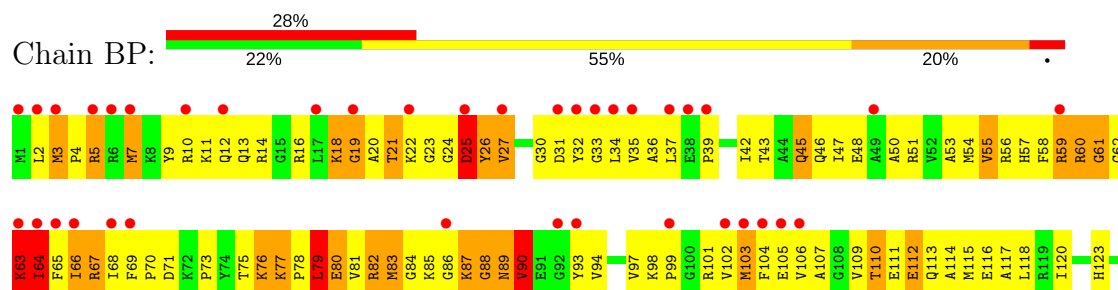
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

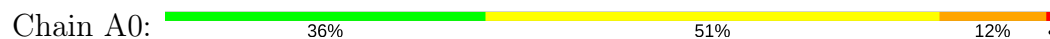


• Molecule 12: 50S ribosomal protein L16





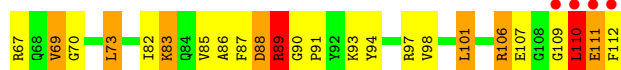
- Molecule 13: 50S ribosomal protein L17



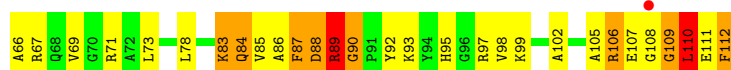
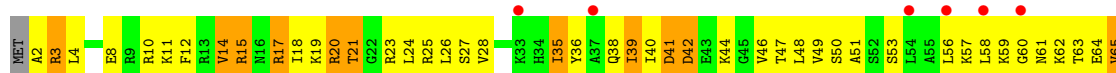
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

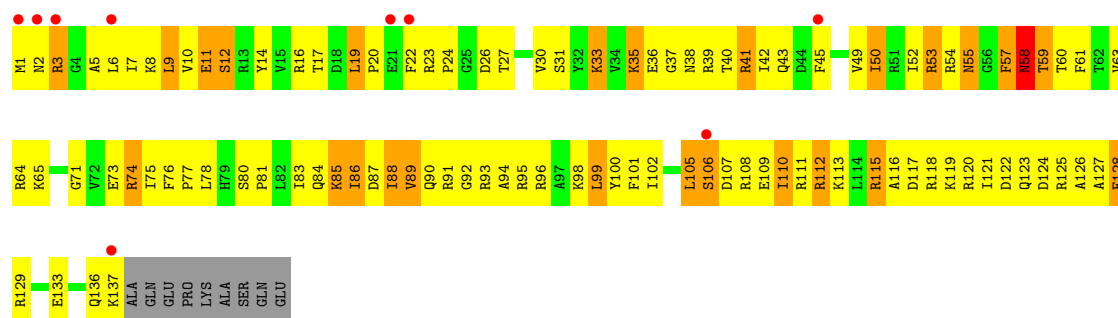


- Molecule 14: 50S ribosomal protein L18

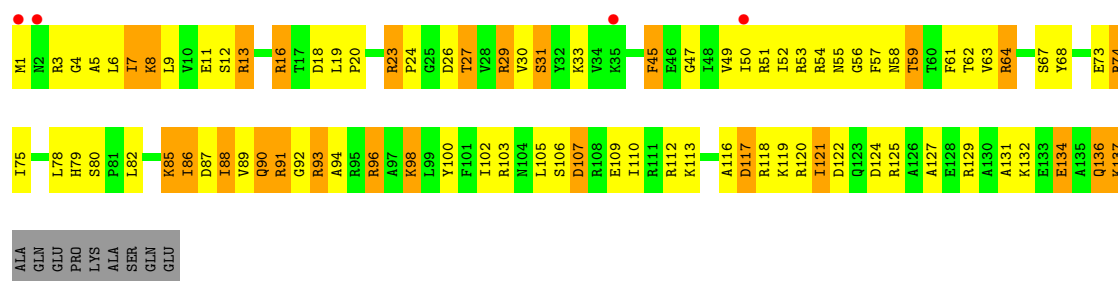


- Molecule 15: 50S ribosomal protein L19

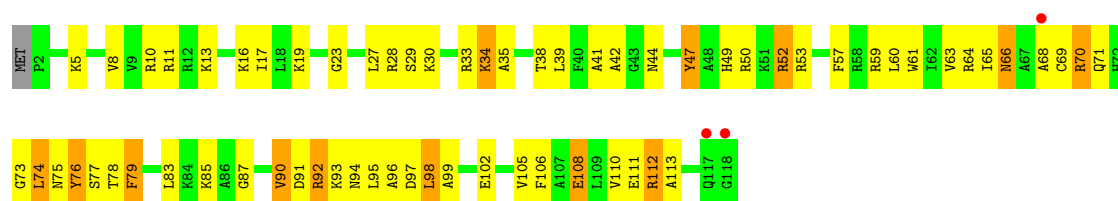
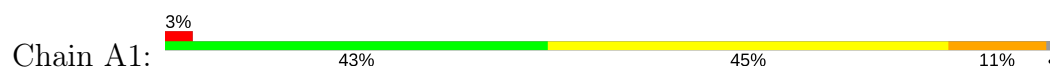




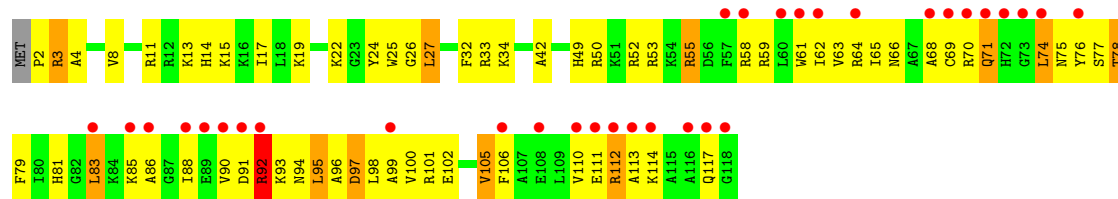
- Molecule 15: 50S ribosomal protein L19



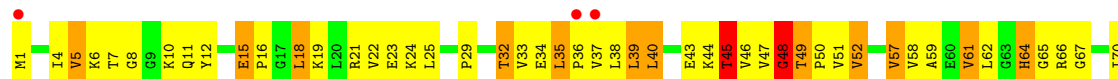
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20

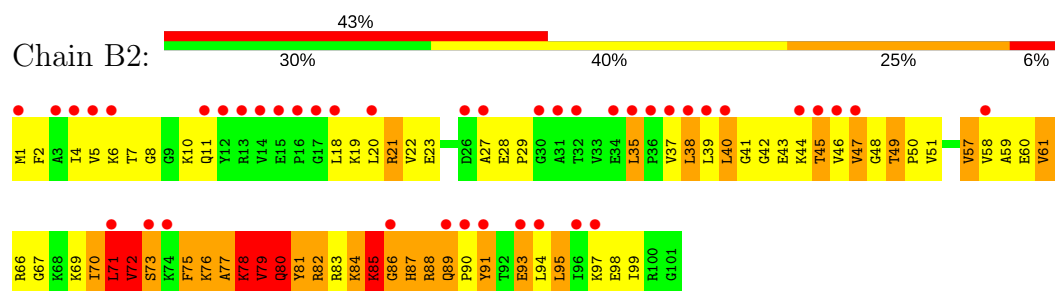


- Molecule 17: 50S ribosomal protein L21

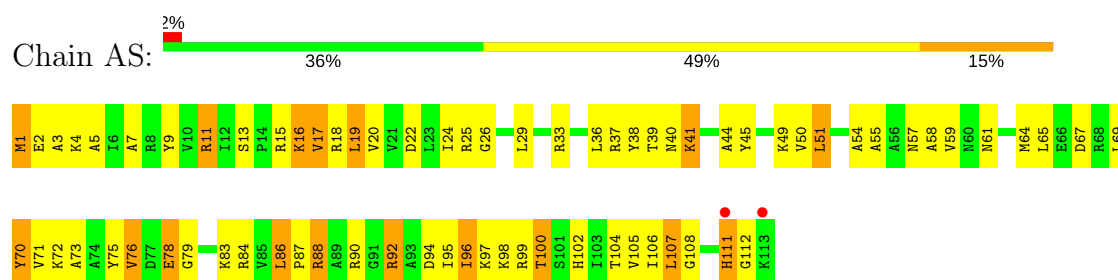




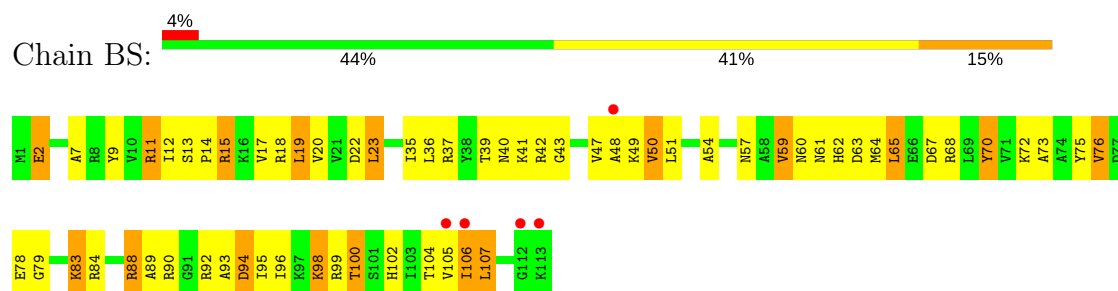
• Molecule 17: 50S ribosomal protein L21



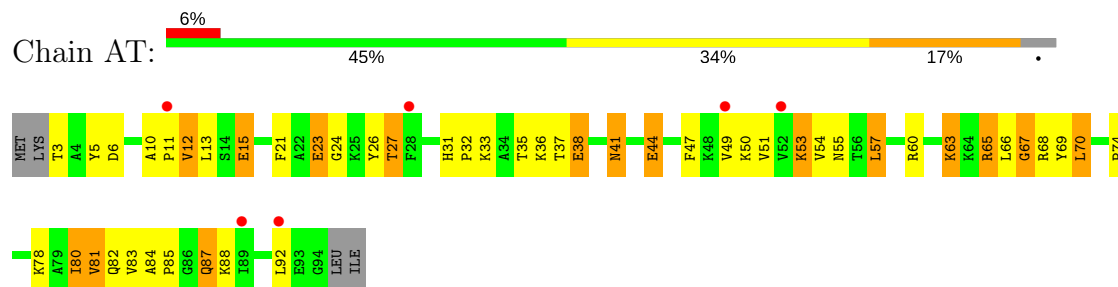
• Molecule 18: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L22



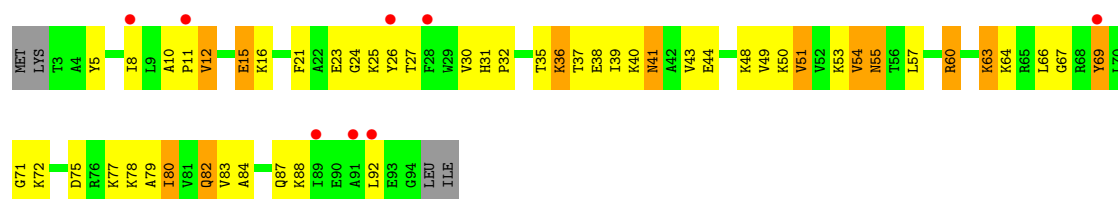
• Molecule 19: 50S ribosomal protein L23



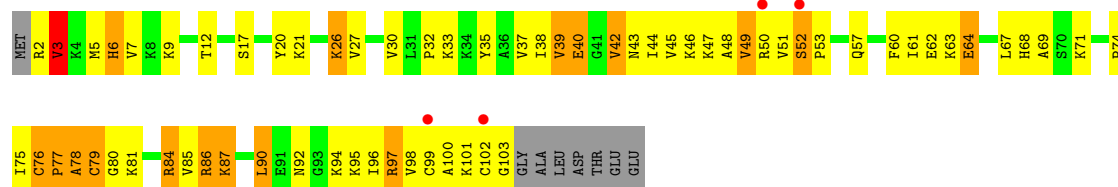
• Molecule 19: 50S ribosomal protein L23



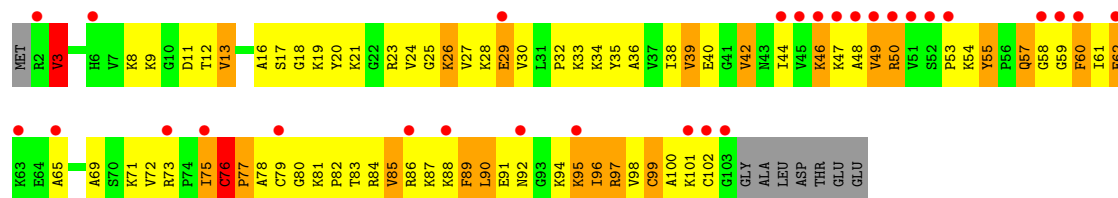




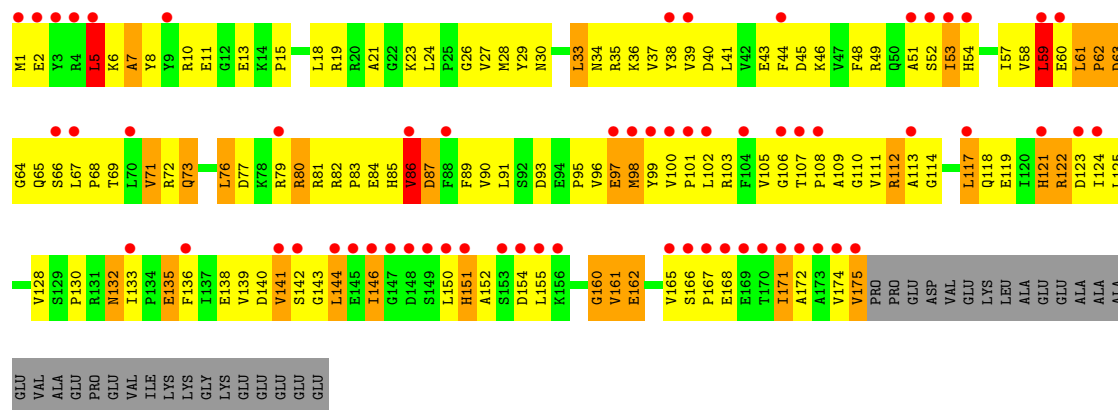
• Molecule 20: 50S ribosomal protein L24



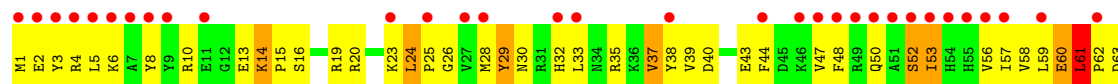
• Molecule 20: 50S ribosomal protein L24

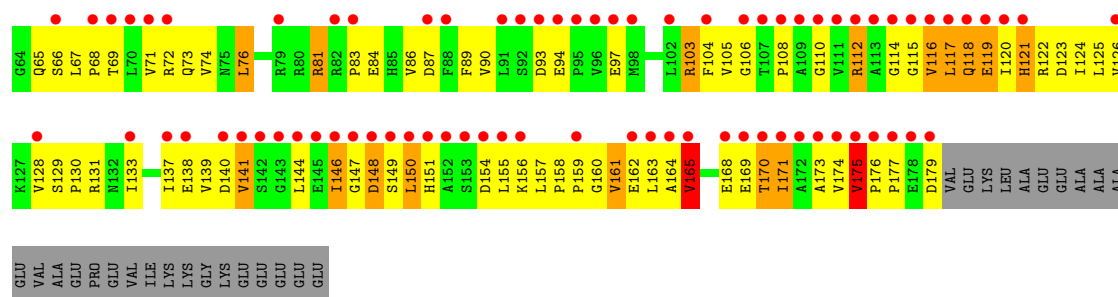


• Molecule 21: 50S ribosomal protein L25

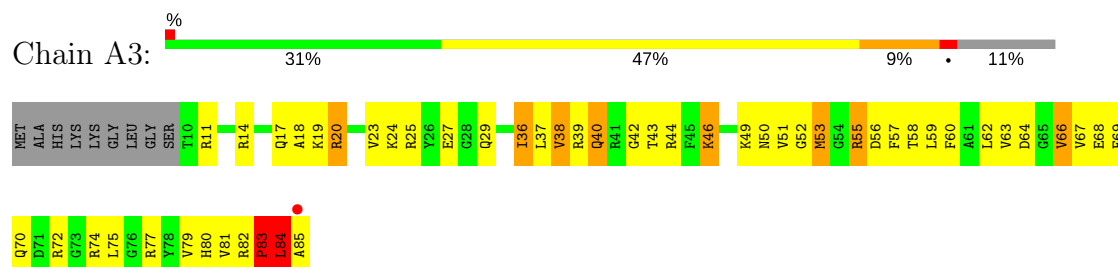


• Molecule 21: 50S ribosomal protein L25

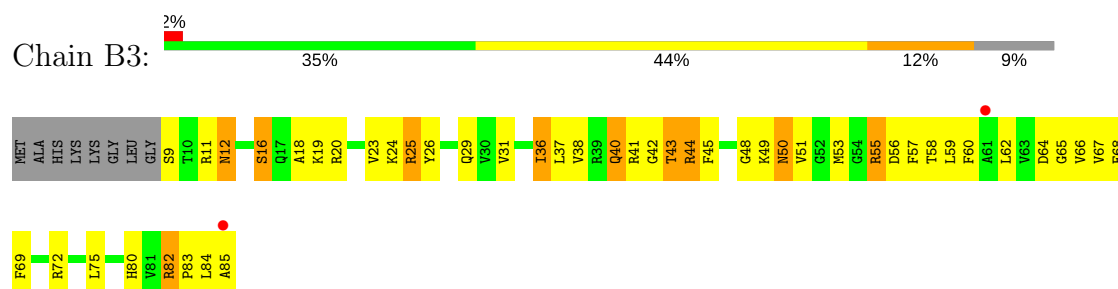




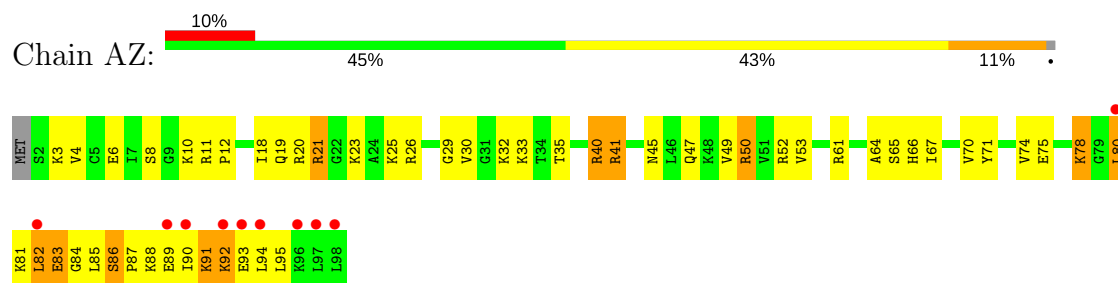
• Molecule 22: 50S ribosomal protein L27



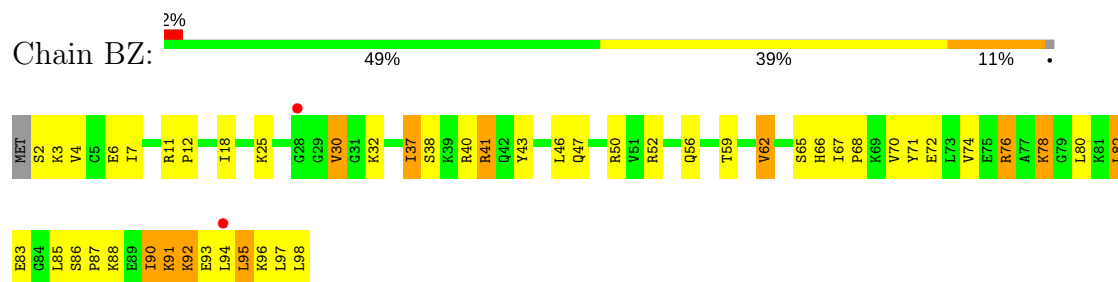
• Molecule 22: 50S ribosomal protein L27



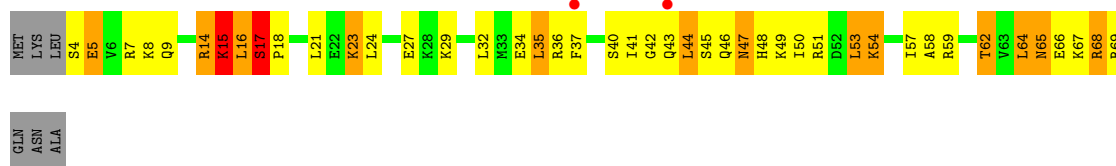
• Molecule 23: 50S ribosomal protein L28



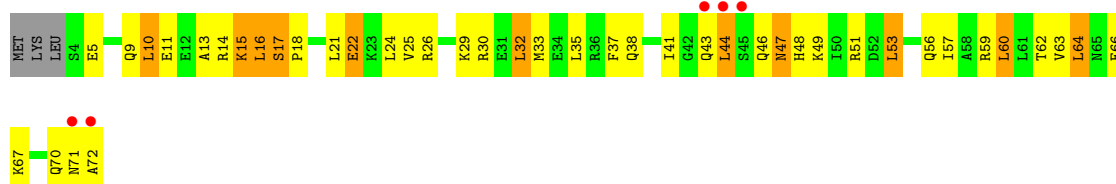
• Molecule 23: 50S ribosomal protein L28



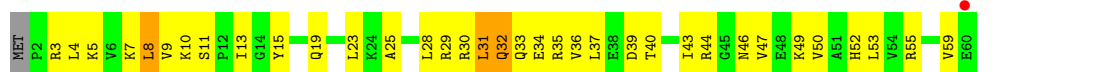

## • Molecule 24: 50S ribosomal protein L29

Chain AW: 


## • Molecule 24: 50S ribosomal protein L29

Chain BW: 

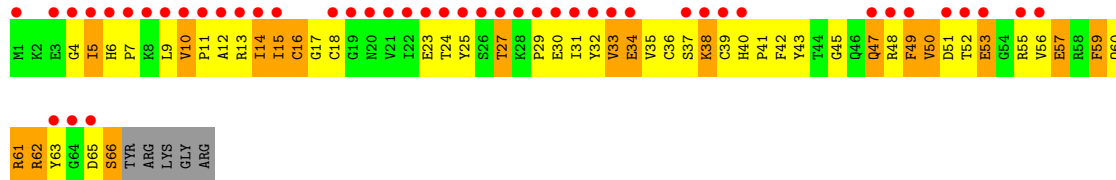

## • Molecule 25: 50S ribosomal protein L30

Chain AX: 


## • Molecule 25: 50S ribosomal protein L30

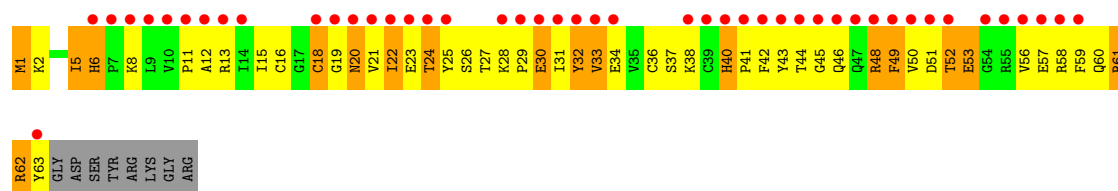
Chain BX: 

## • Molecule 26: 50S ribosomal protein L31

Chain A4: 

## • Molecule 26: 50S ribosomal protein L31

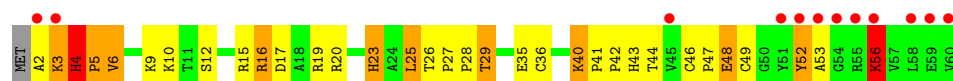
Chain B4: 



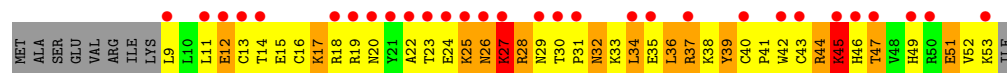
- Molecule 27: 50S ribosomal protein L32



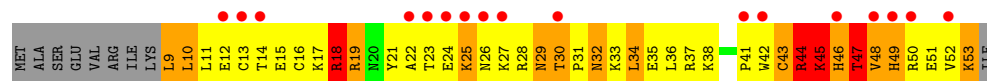
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



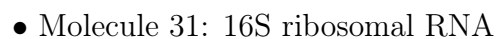
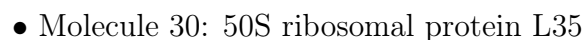
- Molecule 29: 50S ribosomal protein L34

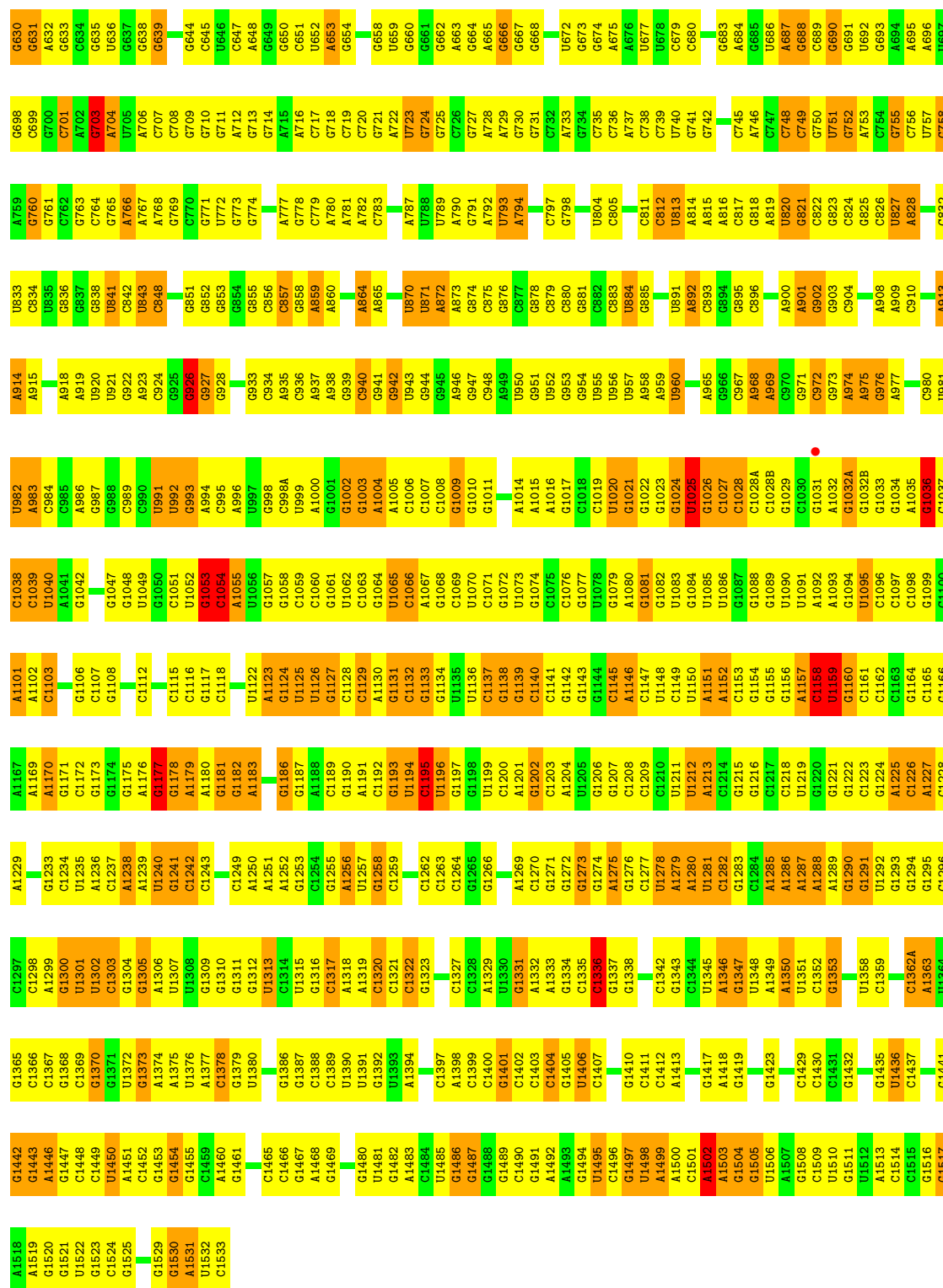


- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



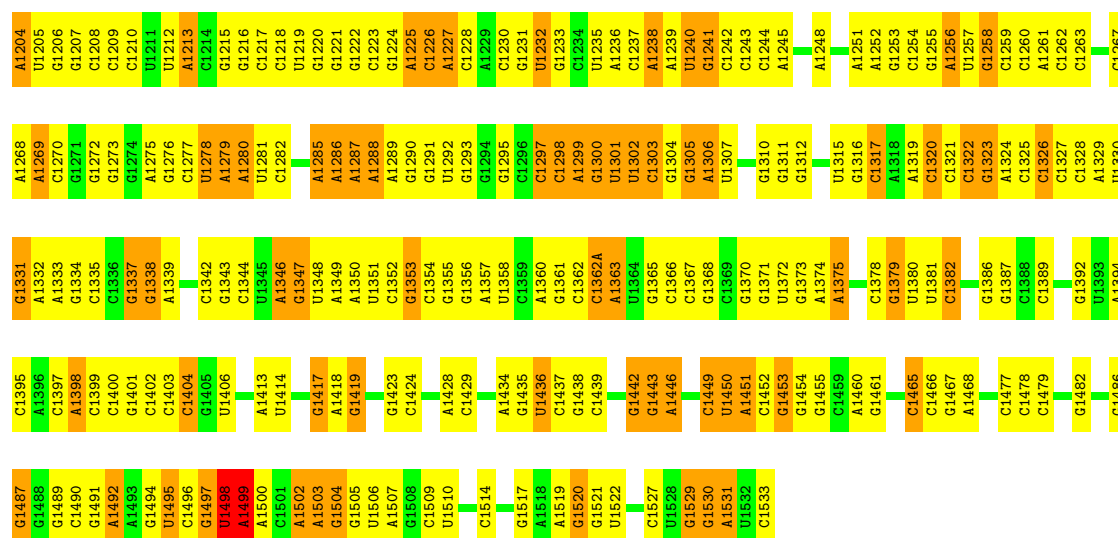


• Molecule 31: 16S ribosomal RNA

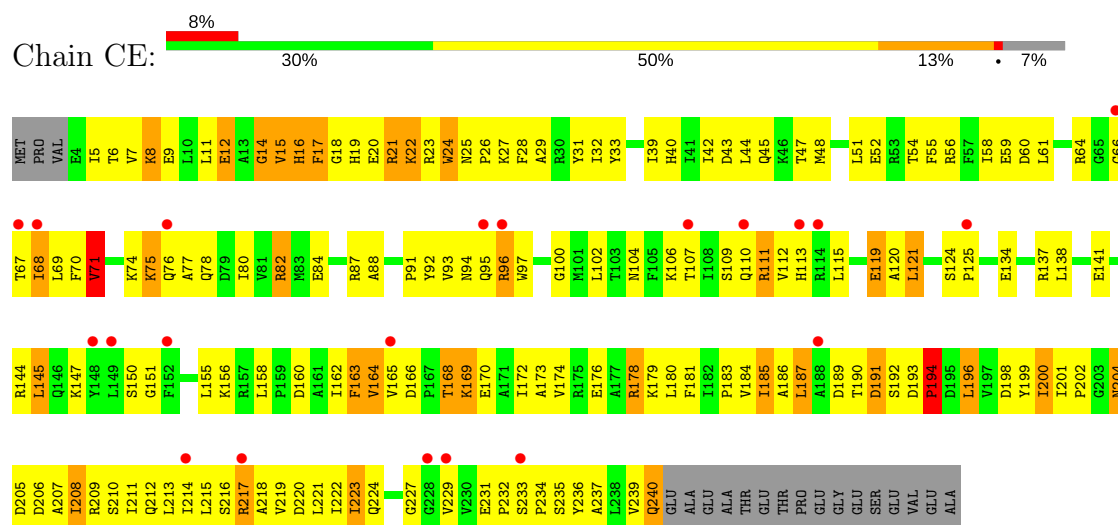
Chain DA: 29% 50% 20%



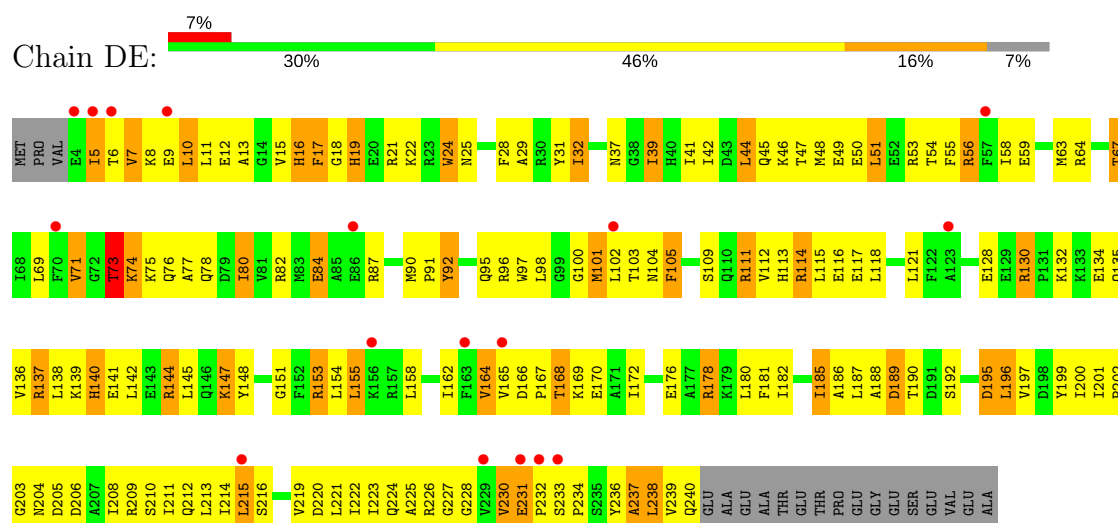
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G1141	A1081	U1020	C961	G894	A815		G668	G593	G528	G445	A374	G300	U222	G155	G80
G1142	G1021	G1021	C962	G895	A816	G745	U669		C528		U375	G301	U223	G156	G81
G1143	G1082	G1022	G963	C896	C817	A746		C596	G529	A448	G376	G302	C224	G157	G82
G1144	G1083	G1023	G964	C897	G818	G747	G673		G530	A449			C225		U84
G1145	G1084	G1024	A965	G898	A819	G748	G674	C600	G531	A450	C379	G309		A160	U85
A1146	U1085	U1025	G966	C899	G820	G749		C601	A532	A451			U229	A161	U86
C1147	G967	G1026	G821	A900	C822	G750	U677		A533	A452	A382	C312	G230	A162	U87
U1148	A968	C1027	A968	A901	G823	U751		G604	U534	A453	A383	A313	G231	A163	C88
C1149	A969	G1028	A969	G902	G824	G752	C680	U605	A535		G384			U164	U89
U1150	C970	C1028A	C970	A907	C824	A753		G606	C536	A457		G316	C235	G165	C90
A1151	U1089	U1028B	C971	A908	G825	G754	U686	A607		A458				G166	C91
A1152	C972	G1029	C972	A909	C826	G755	A887	A608	A539	A459	C379	C320	C241	G167	G92
C1153	G973	C1030	A973	A909	U827	G756	G688	A609	G540	A460		A321	C242	G168	U93
G1154	A1093	G1031	G974	C910	U828	U757	G689		G541	A461	A382		U229	A161	U86
G1155	G1094	A1032	A975	C910	G829	G758	G690	C612	G542	A462	A383		G230	A162	C88
G1156	U1095	G1032A	G976	A913	G830	A759	G691	C613	G543	A463	G391		C243	U164	U89
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C1161	A1101	G1036	U981	U921	G837	G764	A695	C618		A468			C248	C169	G95
C1162	A1102	C1037	U982	G922	G838	G765		G619	G550	A469			C249	U170	
C1163	C1103	C1038	A983	A923	G838	A766	G703	C620	U551	A470			C250	U173	A101
	G1104	C1039	C984	C924	U841	A767	A704	A621	U552	A471			G251	C174	G105
A1170		A1040	C985	G925	C842	A768		A622	U553	A472			G252	C175	G106
C1171	G1106	A1041	U986	G926	U843	G769	C707	C623	C554	A483			G253	C176	G107
C1172	C1107	G1042	G987	G927	C948	G770	G708	C624	C555	C484			G254	C177	G108
G1173	G1108	G1043	G988	G928	C949	G771	G709	G625	C556	A485			G255	C178	G109
G1174	C1109	C1044	C989	G929	U850	U772	G710	U626	G557	A486			G256	C179	G110
C1175	A1110	G1045	C990	C930	G851	G773	G711	G627	G558	A487			G257	U180	G111
A1176	A1111	A1046	U991	C931	G852	G774	A712	G628	A959	A488			G258	C186	G112
C1177	C1112	G1047	U992	G932	G853	G775	G713	G629	U560	A489			G259	C187	G113
A1179	A1179	G1048	G993	G933	G854	G776	G714	G630	U561	A490			G260	C188	G114
C1114	C1114		A994	C934	G855	A777	A715	G631	C562	G490			G261	C189	G115
C1115	C1115	G1051	C995	A935	C856	G778	A716	A632	A563				G262	U188	G116
C1116	C1116	U1052	A996	C936	C857	G779		A633	C564	G493			G263	U189	G117
G1182	G1117	G1053	U997	A937	G858	A780	C719	C634		A494			G264	G190	G118
A1183	C1118	C1054	C998	A938	A859	A781	G720	G635	G567	A495			G265	G191A	G119
G1184	C1119	A1055	C998A	G939	A860	A782	G721	U636	G568	A496			G266	G191B	G120
G1185	G1120	U1056	U999	G940	G861		A722		C569	A497			G267	G191C	G121
G1186	U1121	G1057	A1000	G941	C862	A787	U723	C647	G570	A498			G268	A130	G129A
G1187	U1122	G1058	G1001	G942	U863	U788	G724	A648	U571	G500			G269	C131	A130
A1188	A1123	C1059	G1002	U943	U863	U789	G725	G649	A572	G502			G270	C132	A131
C1189	G1124	G1060	G1003	G944	G869	A790	G726	G650	A573	G503			G271	U192	C132
G1190	U1125	G1061	A1004	G945	U870	G791	G727	C651	A574	C504			G272	U193	C133
A1191	U1126	U1062	A1005	A946	U871	A792	A728	U652	G575	G505			G273	C194	A134
C1192	G1127	C1063	C1006	G947	A872	U793	A729	A653	G576				G274	A196	G142
G1193	C1128	G1064	C1007	C948	A873	A794	G730	G654	G577	A509			G275	A197	G143
U1194	C1129	U1065	G1008	A949	G874		G731	A655		A510			G276	G198	A144
C1195	A1130	C1066	G1009	U950		G799	C732	C656	U580	C511			G277	C201	G145
U1196	G1131	A1067	G1010	G951	C877	G800	A733	G657	G581	U512			G278	U208	G146
G1197	C1132	G1068	G1011	U952	G878	U801	G734		U582	C513			G279	U209	G147
G1198	G1133	C1069	U1012	G953	C879	A802	C735	G660	A583				G280	U210	G148
U1199	G1134	U1070	G1013	G954	C879	G803	G736	G661	G584	U516			G281	U219	G149
C1200	U1135	C1071	U955	U955	C883	U804	A737	G662		G517			G282	C216	A149
A1201	U1136	U1072	U956	U957	U884		C738	A663	G587	C518			G283	C217	C150
C1202	C1137	U1073	U957		G885	C811	C739	G664		C519			G284	C218	C151
C1203	G1138		G1017	A958		C812	U740	A665	C590	A520			G285	C219	A152



### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

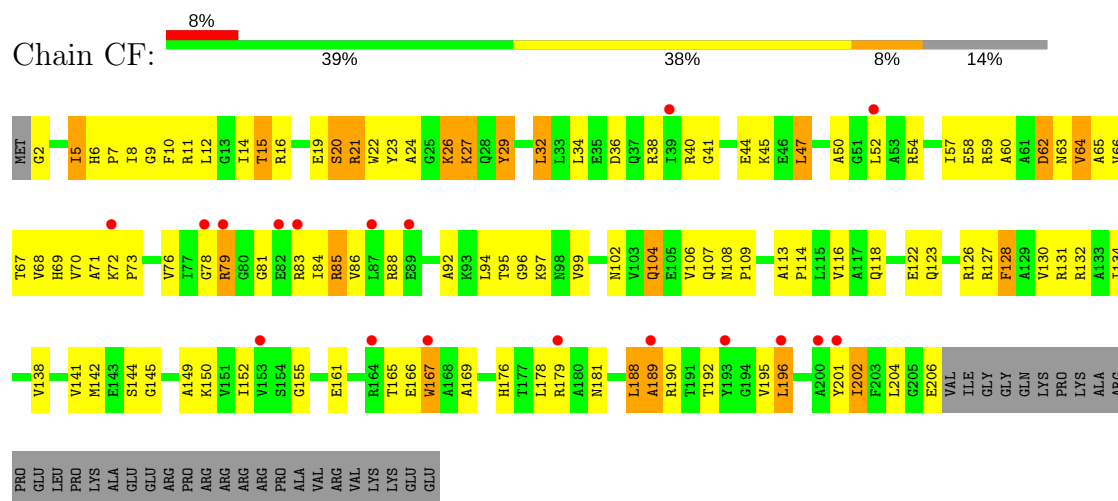


### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

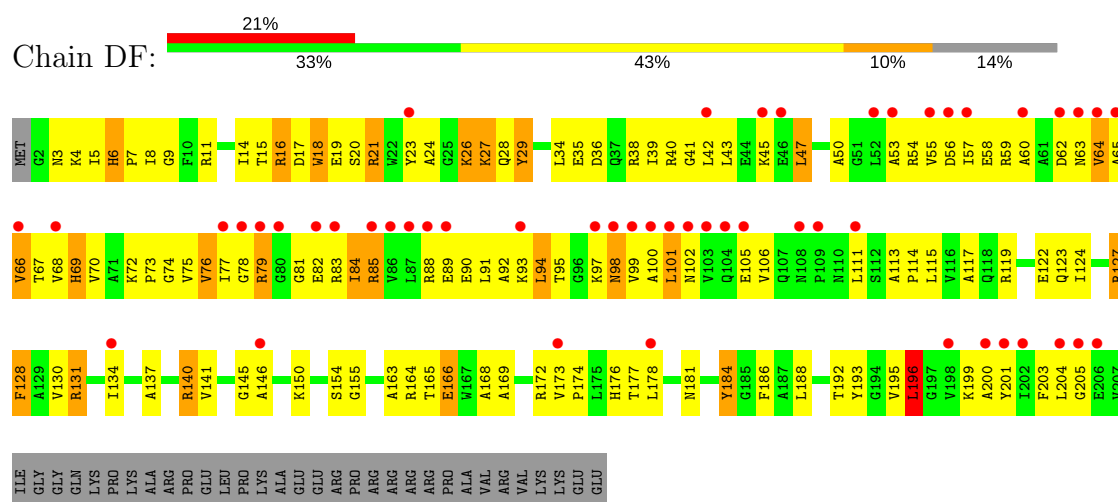




• Molecule 33: 30S RIBOSOMAL PROTEIN S3



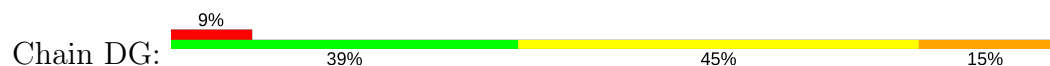
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

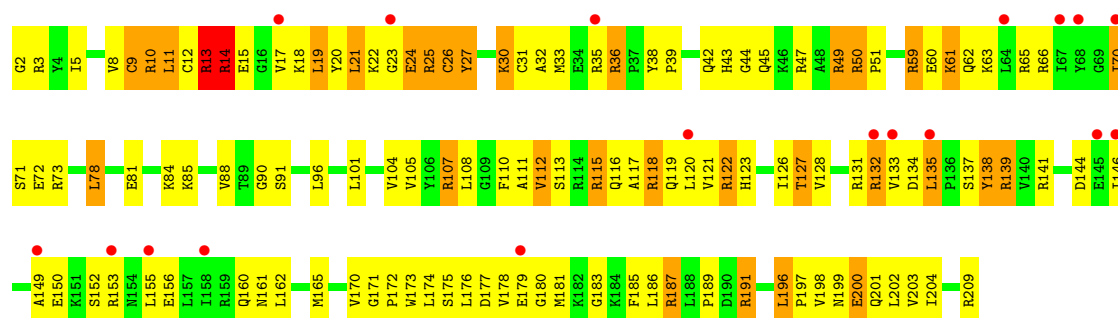


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

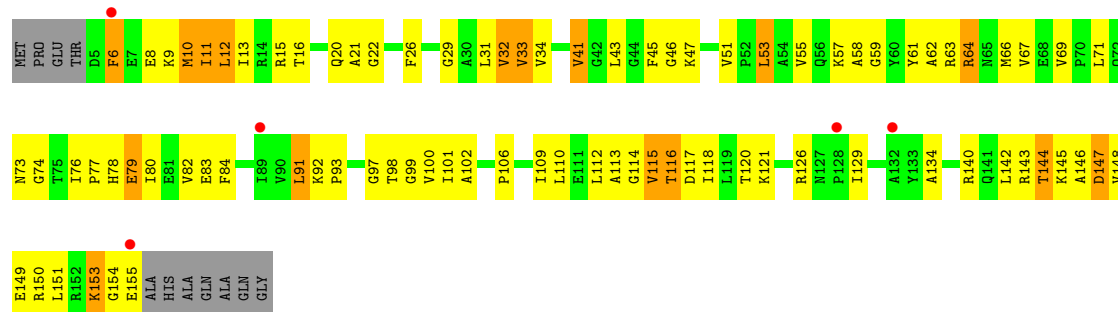
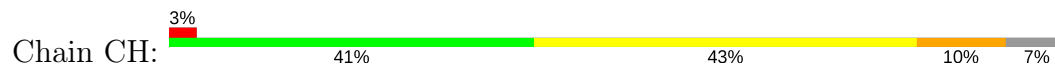


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

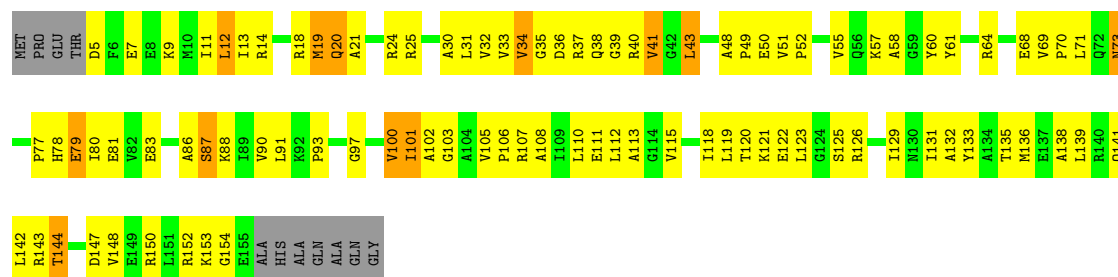




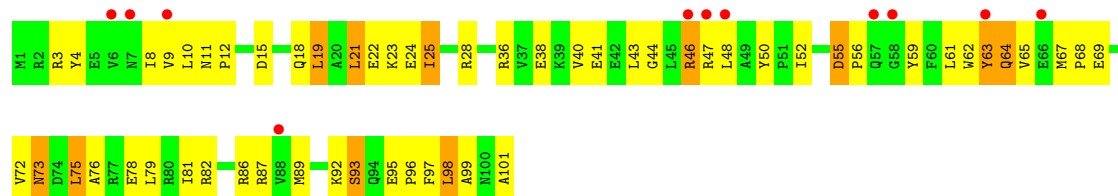
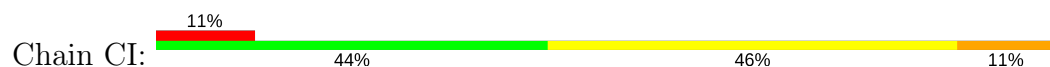
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



• Molecule 35: 30S RIBOSOMAL PROTEIN S5

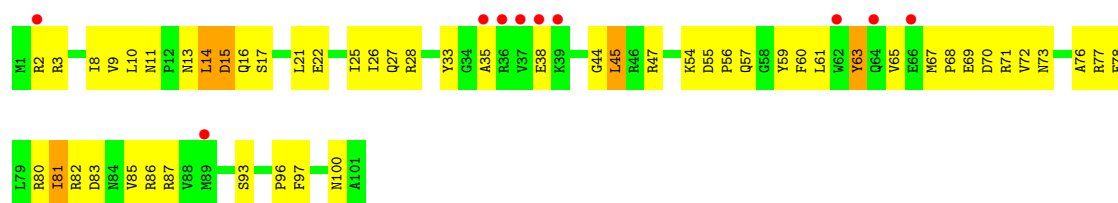


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

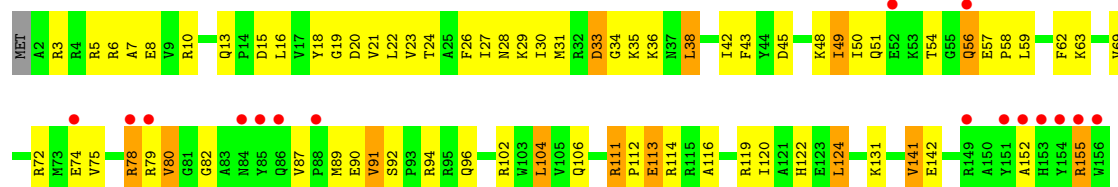


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

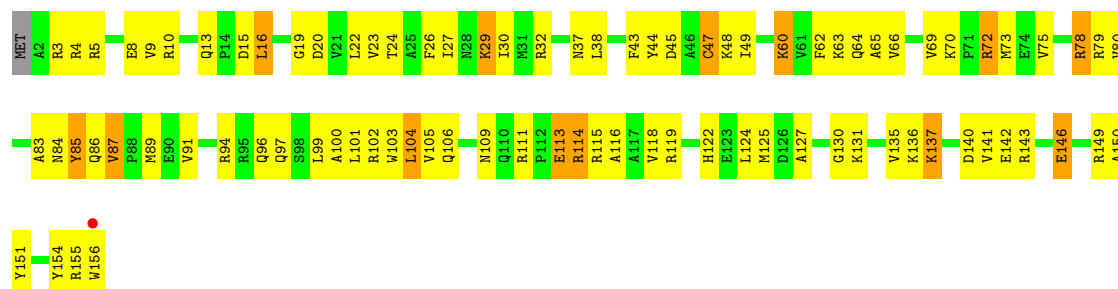
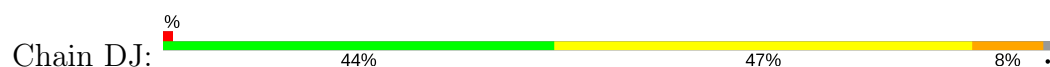




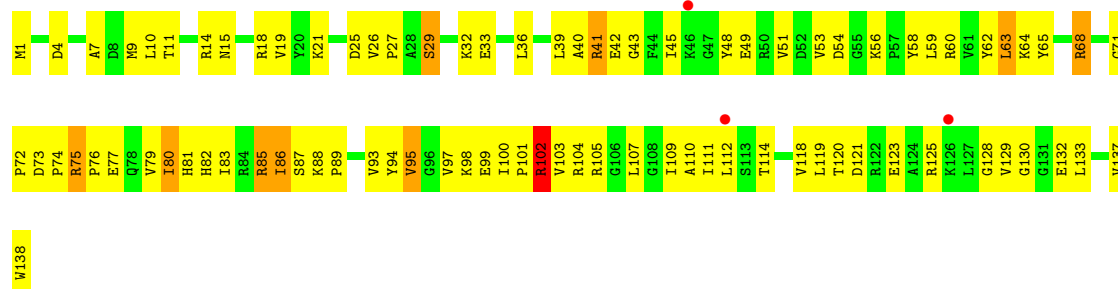
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

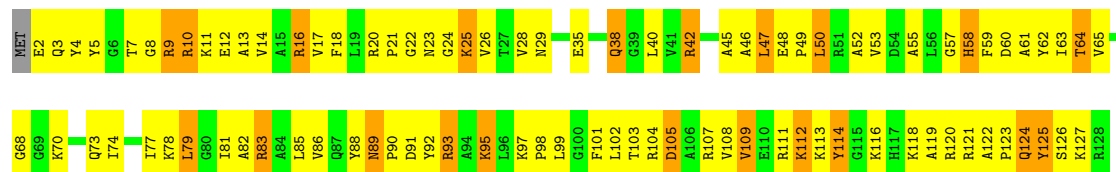


• Molecule 38: 30S RIBOSOMAL PROTEIN S8

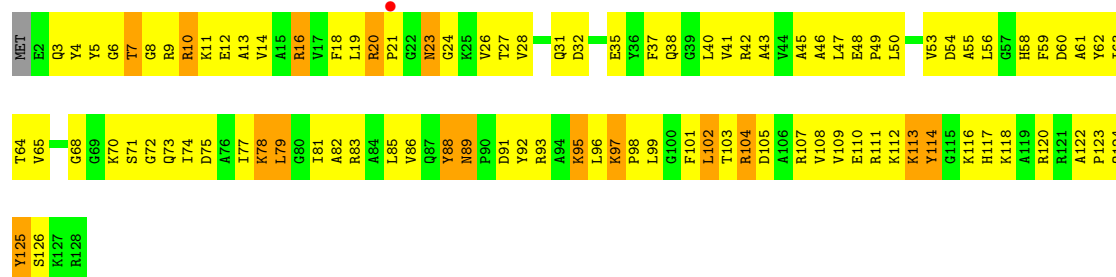




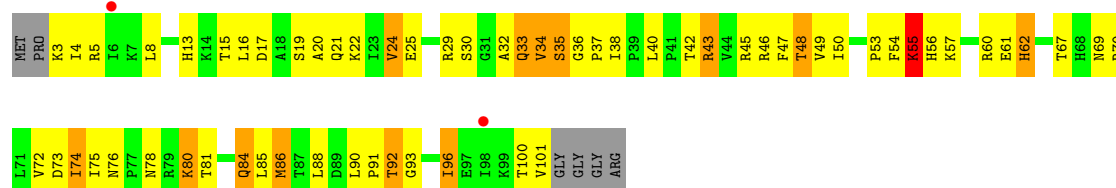
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



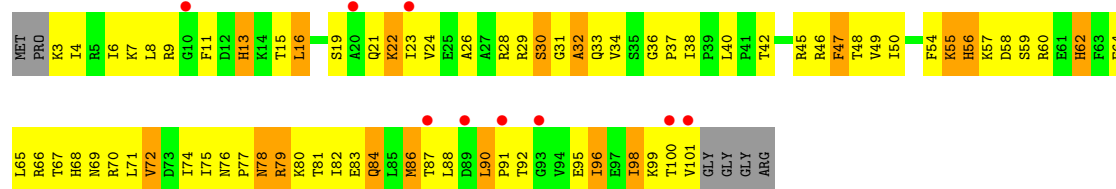
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



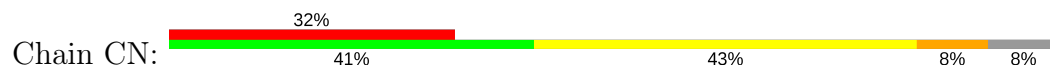
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

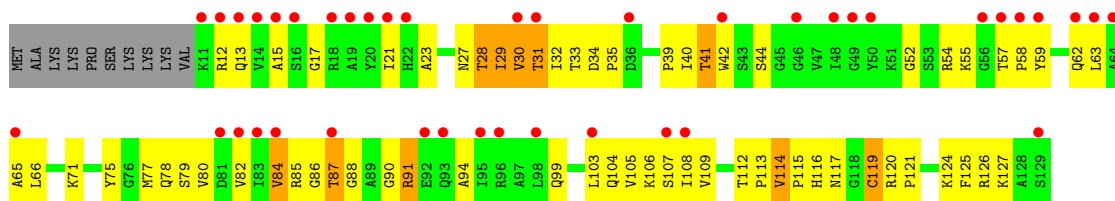


• Molecule 40: 30S RIBOSOMAL PROTEIN S10

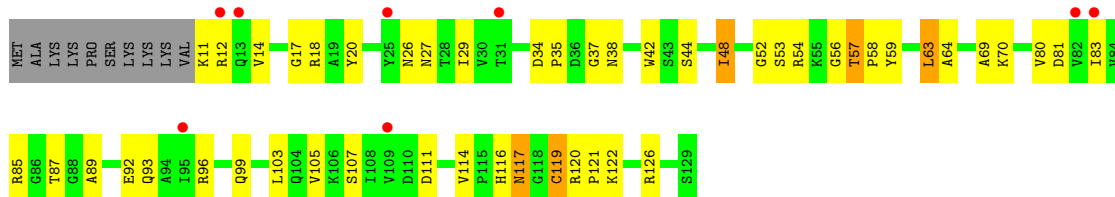


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

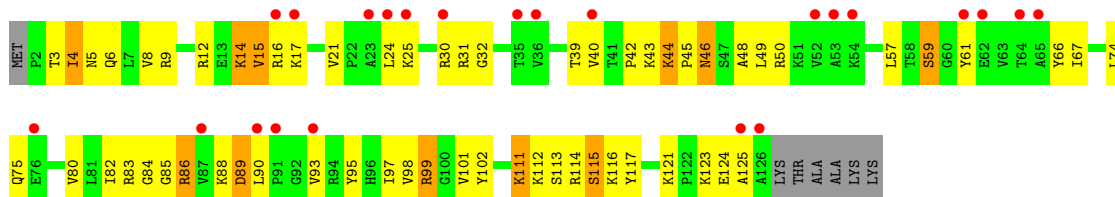




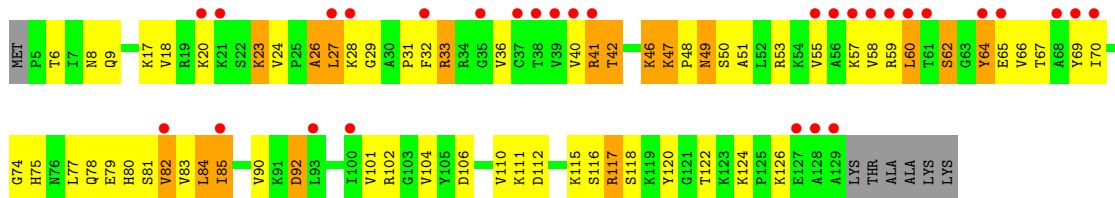
## • Molecule 41: 30S RIBOSOMAL PROTEIN S11



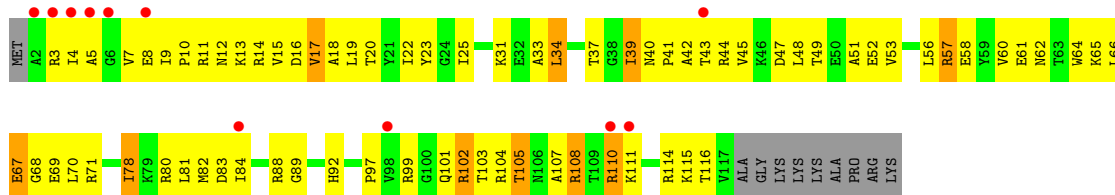
## • Molecule 42: 30S RIBOSOMAL PROTEIN S12



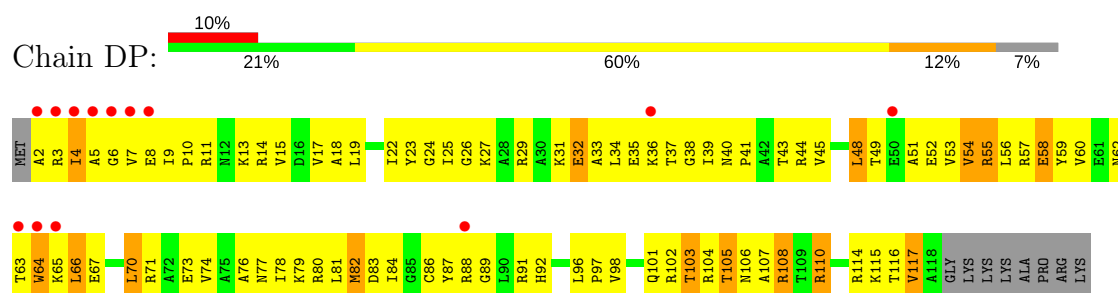
## • Molecule 42: 30S RIBOSOMAL PROTEIN S12



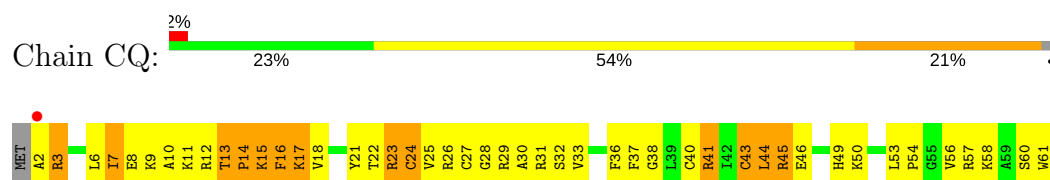
## • Molecule 43: 30S RIBOSOMAL PROTEIN S13



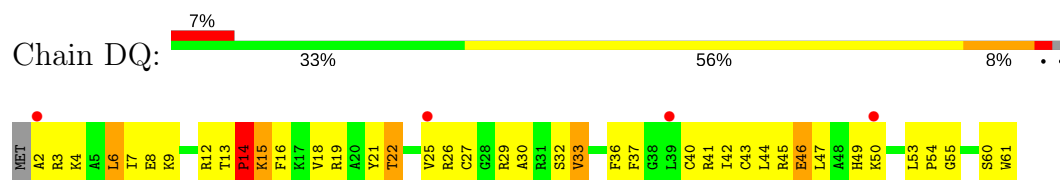
## • Molecule 43: 30S RIBOSOMAL PROTEIN S13



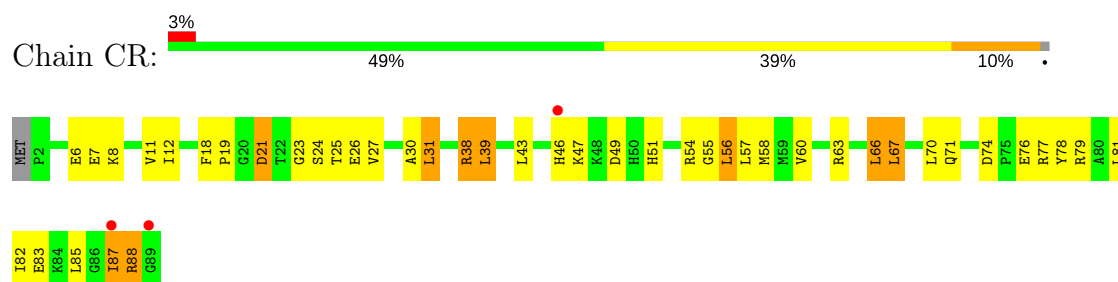
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



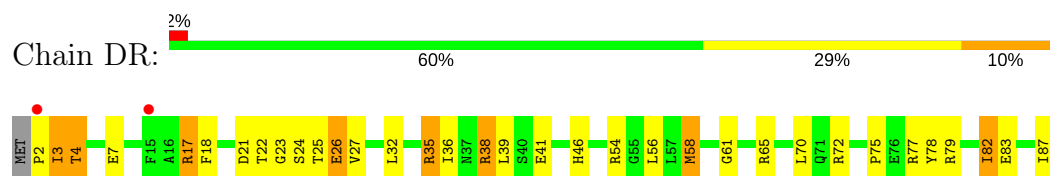
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



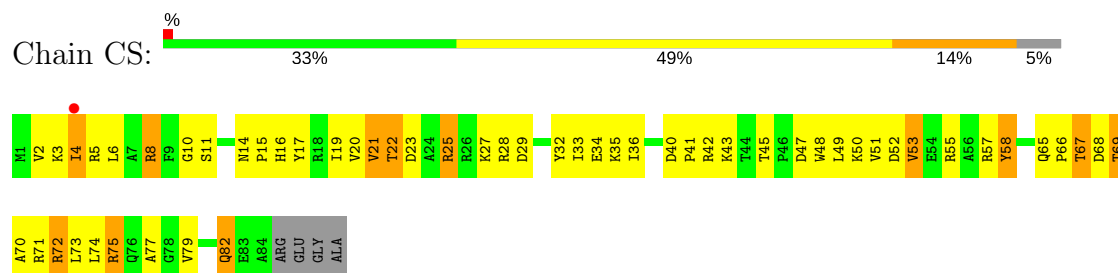
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



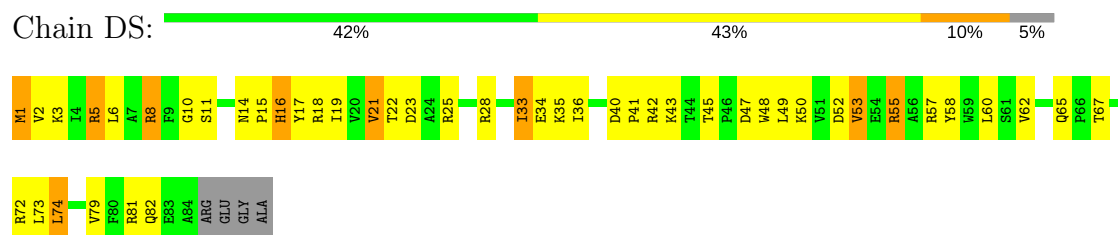
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



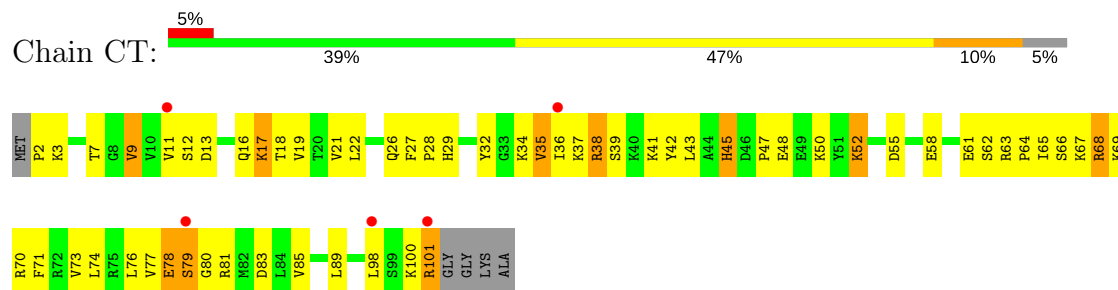
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



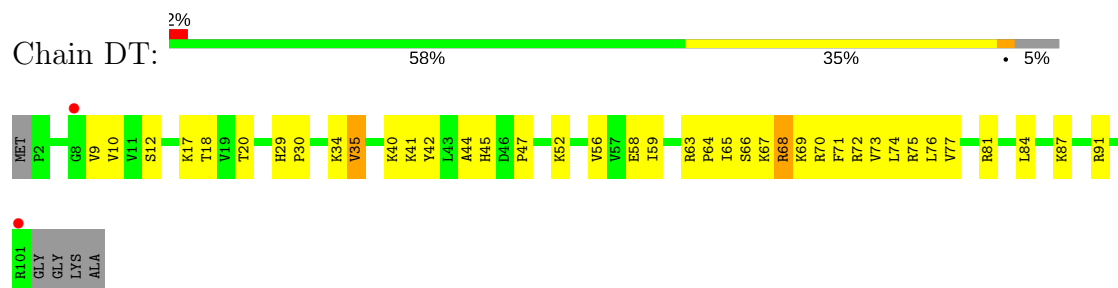
- Molecule 46: 30S RIBOSOMAL PROTEIN S16



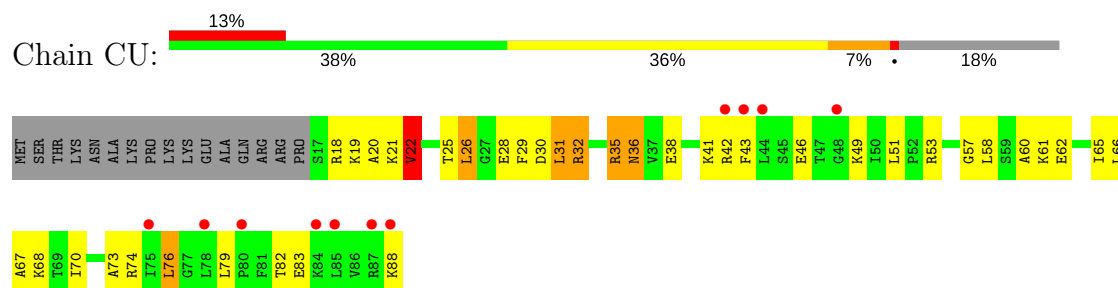
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



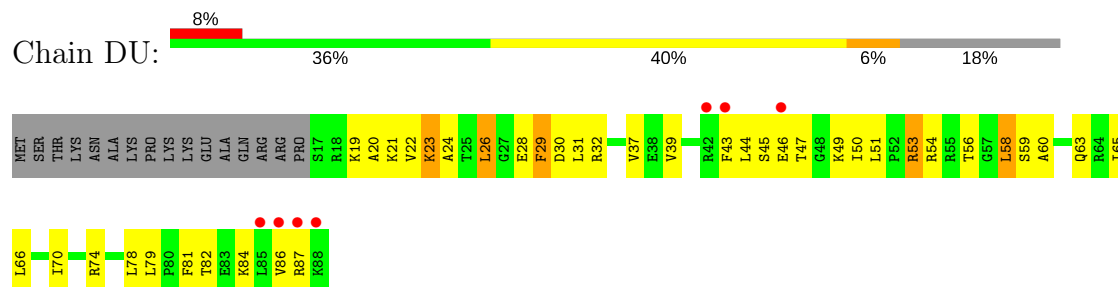
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



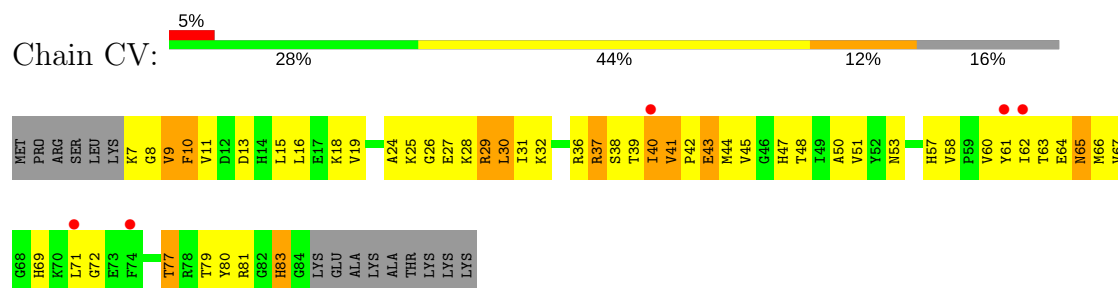
- Molecule 48: 30S RIBOSOMAL PROTEIN S18



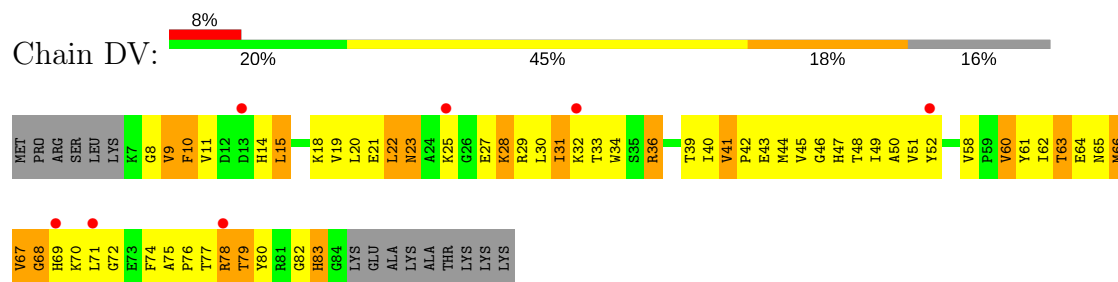
- Molecule 48: 30S RIBOSOMAL PROTEIN S18



- Molecule 49: 30S RIBOSOMAL PROTEIN S19



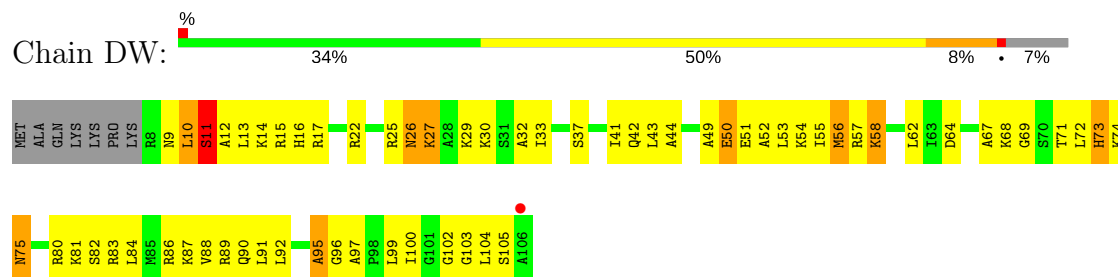
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



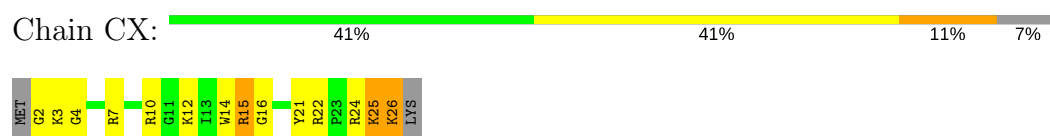
- Molecule 50: 30S RIBOSOMAL PROTEIN S20



- Molecule 50: 30S RIBOSOMAL PROTEIN S20



- Molecule 51: 30S RIBOSOMAL PROTEIN THX



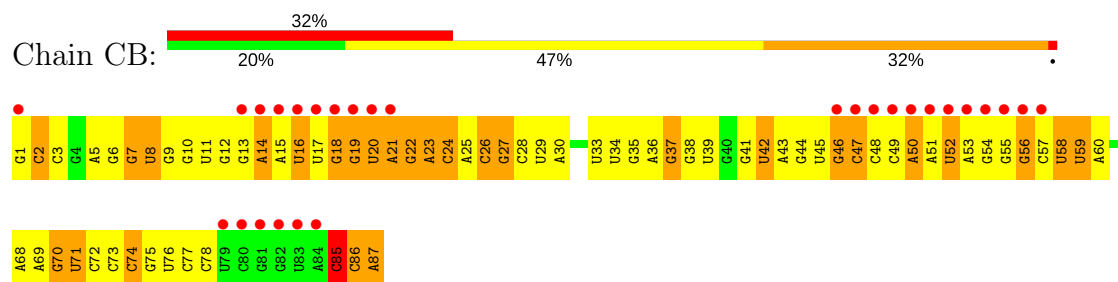
- Molecule 51: 30S RIBOSOMAL PROTEIN THX



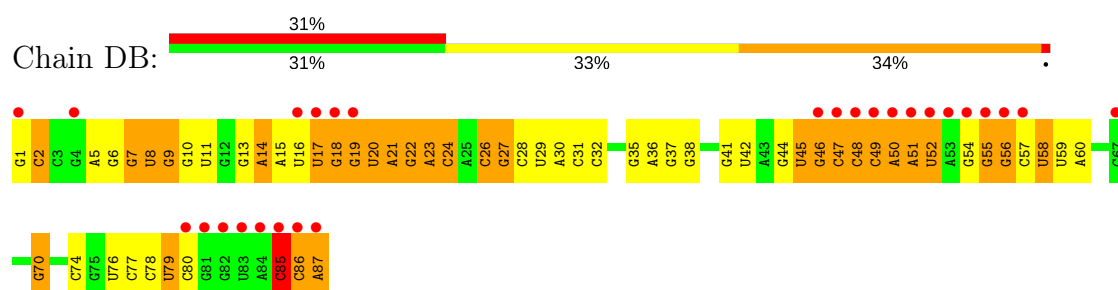




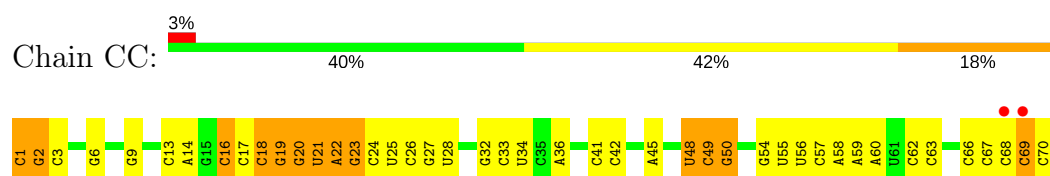
- Molecule 52: TRNA-LEU



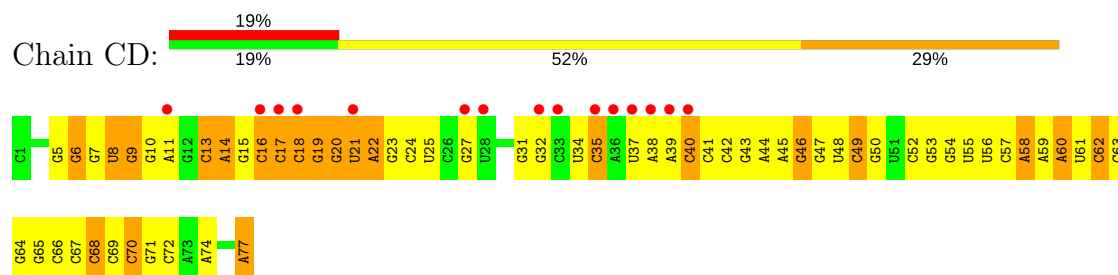
- Molecule 52: TRNA-LEU



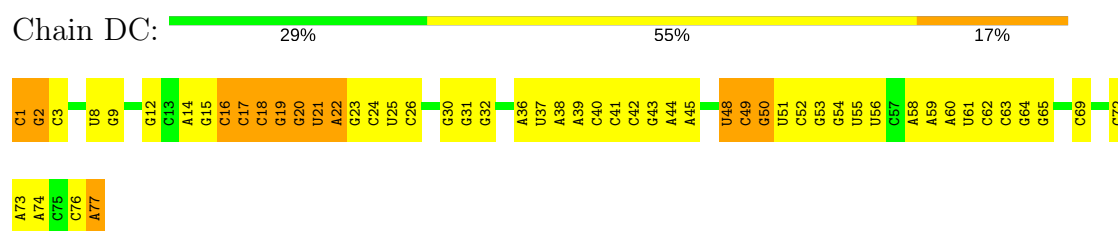
- Molecule 53: TRNA-FMET



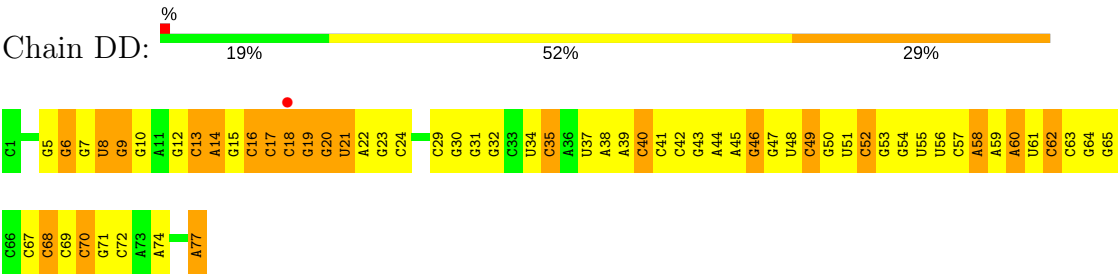
- Molecule 53: TRNA-FMET



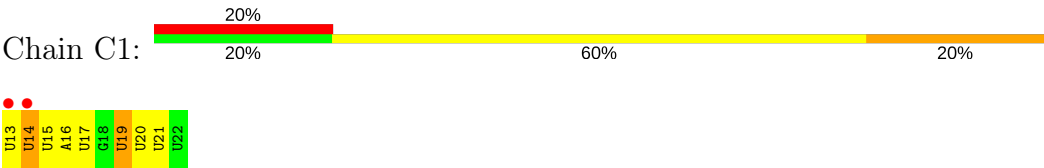
- Molecule 53: TRNA-FMET



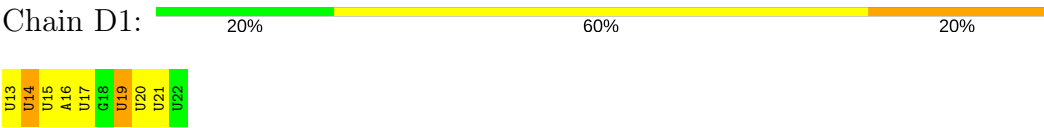
- Molecule 53: TRNA-FMET



• Molecule 54: MRNA



• Molecule 54: MRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.43Å 448.15Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.73 – 3.30 224.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (189.73-3.30) 95.4 (224.07-3.30)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, $R_{free}$	0.199 , 0.237 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 87.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	299682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	122	ASP	Peptide
3	AD	236	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	28	GLU	Peptide
3	AD	47	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 17558 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BO:62:LEU:CD1	30:B8:30:ARG:HH11	1.03	1.63
11:BO:71:VAL:CG1	11:BO:72:PRO:HD3	1.32	1.59
4:AE:23:VAL:HG12	4:AE:185:LYS:CA	1.33	1.59
1:BA:2015:A:C1'	27:B5:2:ALA:HA	1.42	1.48
4:BE:51:PHE:CG	4:BE:52:LEU:HB3	1.45	1.47

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:276:A:OP2	31:DA:86:U:O2'[3_555]	1.96	0.24
7:BH:100:GLY:O	31:CA:85:U:O2'[3_545]	2.02	0.18
36:CI:15:ASP:OD2	34:DG:27:TYR:OH[4_555]	2.06	0.14
7:BH:132:ARG:O	31:CA:84:U:N3[3_545]	2.18	0.02
17:A2:51:VAL:N	27:A5:60:VAL:O[4_465]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/276 (98%)	244 (90%)	20 (7%)	6 (2%)	7	34
3	BD	270/276 (98%)	246 (91%)	15 (6%)	9 (3%)	4	25
4	AE	203/206 (98%)	149 (73%)	37 (18%)	17 (8%)	1	6
4	BE	203/206 (98%)	149 (73%)	34 (17%)	20 (10%)	1	4
5	AF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
5	BF	206/210 (98%)	172 (84%)	29 (14%)	5 (2%)	6	32
6	AG	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	3	21
6	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	27	61
7	AH	168/180 (93%)	135 (80%)	25 (15%)	8 (5%)	2	17
7	BH	168/180 (93%)	129 (77%)	37 (22%)	2 (1%)	14	47
8	AK	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	2	13
8	BK	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	8	35
9	AM	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	3	18
9	BM	136/140 (97%)	120 (88%)	12 (9%)	4 (3%)	5	28
10	AN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	BN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	21	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AO	148/150 (99%)	101 (68%)	31 (21%)	16 (11%)	0	3
11	BO	148/150 (99%)	95 (64%)	32 (22%)	21 (14%)	0	1
12	AP	139/141 (99%)	101 (73%)	19 (14%)	19 (14%)	0	1
12	BP	139/141 (99%)	88 (63%)	34 (24%)	17 (12%)	0	2
13	A0	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	19	53
13	B0	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	AQ	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	9	39
14	BQ	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	4	23
15	AR	135/146 (92%)	111 (82%)	22 (16%)	2 (2%)	11	42
15	BR	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
16	A1	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	19	53
16	B1	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	19	53
17	A2	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	5	27
17	B2	99/101 (98%)	73 (74%)	13 (13%)	13 (13%)	0	2
18	AS	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	19	53
18	BS	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
19	AT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	7	34
19	BT	90/96 (94%)	81 (90%)	8 (9%)	1 (1%)	16	50
20	AU	100/110 (91%)	84 (84%)	10 (10%)	6 (6%)	2	12
20	BU	100/110 (91%)	67 (67%)	27 (27%)	6 (6%)	2	12
21	AV	173/206 (84%)	131 (76%)	35 (20%)	7 (4%)	3	21
21	BV	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	3	18
22	A3	74/85 (87%)	68 (92%)	4 (5%)	2 (3%)	5	29
22	B3	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	AZ	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	4	26
23	BZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	16	50
24	AW	64/72 (89%)	60 (94%)	1 (2%)	3 (5%)	2	17
24	BW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	11	42
25	AX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	BX	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	A4	64/71 (90%)	42 (66%)	20 (31%)	2 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B4	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	4	25
27	A5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	9	39
27	B5	57/60 (95%)	48 (84%)	6 (10%)	3 (5%)	2	14
28	A6	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	17
28	B6	43/54 (80%)	26 (60%)	11 (26%)	6 (14%)	0	1
29	A7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	B7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	A8	59/65 (91%)	54 (92%)	4 (7%)	1 (2%)	10	40
30	B8	59/65 (91%)	42 (71%)	10 (17%)	7 (12%)	0	2
32	CE	235/256 (92%)	190 (81%)	44 (19%)	1 (0%)	36	69
32	DE	235/256 (92%)	186 (79%)	45 (19%)	4 (2%)	10	40
33	CF	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
33	DF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	17	51
34	CG	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	31	65
34	DG	206/208 (99%)	177 (86%)	28 (14%)	1 (0%)	31	65
35	CH	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	24	59
35	DH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
36	DI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
37	CJ	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
37	DJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
38	CK	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	24	59
38	DK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	CL	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
39	DL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	CM	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
40	DM	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	8	35
41	CN	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
41	DN	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
42	CO	123/132 (93%)	108 (88%)	13 (11%)	2 (2%)	11	41
42	DO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	11	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	CP	114/126 (90%)	90 (79%)	24 (21%)	0	100	100
43	DP	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	19	53
44	CQ	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	4	25
44	DQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	10	40
45	CR	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
45	DR	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
46	CS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
46	DS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	CT	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	8	37
47	DT	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
48	CU	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	12	43
48	DU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	CV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	6	30
49	DV	76/93 (82%)	58 (76%)	13 (17%)	5 (7%)	1	10
50	CW	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	17	51
50	DW	97/106 (92%)	81 (84%)	15 (16%)	1 (1%)	17	51
51	CX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
51	DX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
All	All	11336/12052 (94%)	9645 (85%)	1396 (12%)	295 (3%)	6	30

5 of 295 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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



analysed, and the total number of residues.

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	CH	116/123 (94%)	94 (81%)	22 (19%)	1	7
35	DH	116/123 (94%)	97 (84%)	19 (16%)	2	12
36	CI	90/90 (100%)	78 (87%)	12 (13%)	4	19
36	DI	90/90 (100%)	78 (87%)	12 (13%)	4	19
37	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	11
37	DJ	126/127 (99%)	100 (79%)	26 (21%)	1	5
38	CK	119/119 (100%)	106 (89%)	13 (11%)	7	27
38	DK	119/119 (100%)	102 (86%)	17 (14%)	3	17
39	CL	98/99 (99%)	69 (70%)	29 (30%)	0	1
39	DL	98/99 (99%)	72 (74%)	26 (26%)	0	2
40	CM	89/92 (97%)	69 (78%)	20 (22%)	1	3
40	DM	89/92 (97%)	65 (73%)	24 (27%)	0	2
41	CN	90/99 (91%)	77 (86%)	13 (14%)	3	17
41	DN	90/99 (91%)	79 (88%)	11 (12%)	5	23
42	CO	104/109 (95%)	88 (85%)	16 (15%)	3	14
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	8
43	CP	94/101 (93%)	76 (81%)	18 (19%)	1	7
43	DP	94/101 (93%)	77 (82%)	17 (18%)	2	9
44	CQ	49/50 (98%)	34 (69%)	15 (31%)	0	1
44	DQ	49/50 (98%)	37 (76%)	12 (24%)	1	2
45	CR	79/80 (99%)	69 (87%)	10 (13%)	5	21
45	DR	79/80 (99%)	68 (86%)	11 (14%)	4	18
46	CS	72/74 (97%)	58 (81%)	14 (19%)	1	7
46	DS	72/74 (97%)	58 (81%)	14 (19%)	1	7
47	CT	95/97 (98%)	83 (87%)	12 (13%)	5	21
47	DT	95/97 (98%)	88 (93%)	7 (7%)	15	44
48	CU	63/77 (82%)	51 (81%)	12 (19%)	1	7
48	DU	63/77 (82%)	50 (79%)	13 (21%)	1	5
49	CV	67/80 (84%)	50 (75%)	17 (25%)	0	2
49	DV	67/80 (84%)	53 (79%)	14 (21%)	1	5
50	CW	76/82 (93%)	64 (84%)	12 (16%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	DW	76/82 (93%)	62 (82%)	14 (18%)	2	8
51	CX	20/22 (91%)	15 (75%)	5 (25%)	0	2
51	DX	20/22 (91%)	18 (90%)	2 (10%)	8	30
All	All	9579/9996 (96%)	7581 (79%)	1998 (21%)	1	5

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

Mol	Chain	Res	Type
11	BO	101	VAL
20	BU	96	ILE
40	DM	30	SER
12	BP	83	MET
15	BR	134	GLU

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

Mol	Chain	Res	Type
16	B1	49	HIS
23	BZ	66	HIS
40	DM	13	HIS
17	B2	64	HIS
19	BT	82	GLN

### 5.3.3 RNA ⓘ

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

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

5 of 2329 RNA backbone outliers are listed below:

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

5 of 206 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2282	G
31	CA	428	G
31	DA	1305	G
1	BA	2422	A
1	BA	2893	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PAR	CA	1841	-	44,45,45	0.53	0	62,67,67	1.39	9 (14%)
56	PAR	DA	1805	-	44,45,45	0.56	0	62,67,67	1.70	17 (27%)

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

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

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	1805	PAR	C13-O52-C52	-4.28	107.28	117.97
56	CA	1841	PAR	C41-C31-C21	-3.60	104.72	111.03
56	DA	1805	PAR	C11-O11-C42	-3.36	109.58	117.97
56	DA	1805	PAR	C14-O33-C33	-3.07	110.29	117.97
56	CA	1841	PAR	C11-O11-C42	-2.75	111.10	117.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	2912/2912 (100%)	-0.06	43 (1%) 73 71	50, 81, 215, 247	0
1	BA	2909/2912 (99%)	-0.16	40 (1%) 75 74	60, 95, 235, 249	0
2	AB	122/122 (100%)	-0.28	1 (0%) 86 86	81, 105, 124, 182	0
2	BB	122/122 (100%)	-0.36	2 (1%) 72 70	98, 133, 156, 203	0
3	AD	272/276 (98%)	0.73	12 (4%) 34 34	47, 72, 94, 112	0
3	BD	272/276 (98%)	0.53	14 (5%) 28 27	56, 82, 103, 138	0
4	AE	205/206 (99%)	0.87	38 (18%) 1 1	55, 91, 137, 149	0
4	BE	205/206 (99%)	1.01	36 (17%) 1 1	66, 104, 153, 172	0
5	AF	202/210 (96%)	0.05	2 (0%) 82 82	52, 84, 123, 137	0
5	BF	208/210 (99%)	0.78	24 (11%) 5 4	64, 108, 166, 191	0
6	AG	181/182 (99%)	1.15	32 (17%) 1 1	95, 115, 143, 157	0
6	BG	181/182 (99%)	1.18	39 (21%) 1 1	125, 148, 169, 176	0
7	AH	170/180 (94%)	0.25	5 (2%) 51 51	89, 119, 138, 160	0
7	BH	170/180 (94%)	3.45	120 (70%) 0 0	161, 203, 224, 232	0
8	AK	146/148 (98%)	0.68	18 (12%) 4 4	85, 134, 151, 157	0
8	BK	146/148 (98%)	0.35	6 (4%) 37 36	91, 134, 158, 167	0
9	AM	138/140 (98%)	0.30	6 (4%) 35 35	70, 95, 131, 144	0
9	BM	138/140 (98%)	1.87	63 (45%) 0 0	86, 118, 148, 158	0
10	AN	122/122 (100%)	0.61	3 (2%) 57 55	63, 82, 98, 111	0
10	BN	122/122 (100%)	0.89	11 (9%) 9 10	76, 98, 117, 133	0
11	AO	150/150 (100%)	0.25	3 (2%) 65 64	45, 90, 122, 167	0
11	BO	150/150 (100%)	0.58	12 (8%) 12 13	44, 101, 149, 186	0
12	AP	141/141 (100%)	0.71	11 (7%) 13 13	58, 91, 116, 142	0
12	BP	141/141 (100%)	1.57	40 (28%) 0 0	58, 107, 142, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	A0	118/118 (100%)	0.07	0	100 100	64, 90, 109, 123	0
13	B0	117/118 (99%)	0.12	1 (0%)	84 84	68, 90, 113, 128	0
14	AQ	111/112 (99%)	0.76	12 (10%)	6 6	83, 103, 126, 142	0
14	BQ	111/112 (99%)	0.38	7 (6%)	20 20	95, 132, 156, 175	0
15	AR	137/146 (93%)	0.64	9 (6%)	18 19	75, 97, 147, 178	0
15	BR	137/146 (93%)	0.37	4 (2%)	51 51	86, 107, 167, 187	0
16	A1	117/118 (99%)	-0.15	3 (2%)	56 54	61, 84, 116, 145	0
16	B1	117/118 (99%)	1.43	33 (28%)	0 0	71, 106, 146, 165	0
17	A2	101/101 (100%)	0.17	3 (2%)	50 50	61, 105, 126, 145	0
17	B2	101/101 (100%)	2.01	43 (42%)	0 0	73, 131, 148, 158	0
18	AS	113/113 (100%)	-0.09	2 (1%)	68 67	55, 80, 111, 163	0
18	BS	113/113 (100%)	0.55	5 (4%)	34 34	69, 84, 121, 162	0
19	AT	92/96 (95%)	0.58	6 (6%)	19 19	63, 78, 102, 118	0
19	BT	92/96 (95%)	0.73	8 (8%)	10 11	78, 96, 119, 134	0
20	AU	102/110 (92%)	0.20	4 (3%)	39 38	82, 107, 157, 172	0
20	BU	102/110 (92%)	1.49	29 (28%)	0 0	97, 123, 176, 191	0
21	AV	175/206 (84%)	1.52	63 (36%)	0 0	93, 133, 193, 198	0
21	BV	179/206 (86%)	2.94	108 (60%)	0 0	128, 166, 212, 218	0
22	A3	76/85 (89%)	0.22	1 (1%)	77 77	65, 84, 98, 137	0
22	B3	77/85 (90%)	0.35	2 (2%)	56 54	79, 101, 122, 155	0
23	AZ	97/98 (98%)	0.78	10 (10%)	6 6	61, 81, 137, 165	0
23	BZ	97/98 (98%)	0.31	2 (2%)	63 62	69, 91, 141, 162	0
24	AW	66/72 (91%)	0.09	2 (3%)	50 50	69, 87, 106, 137	0
24	BW	69/72 (95%)	0.66	5 (7%)	15 17	90, 114, 148, 183	0
25	AX	59/60 (98%)	-0.04	1 (1%)	70 68	73, 90, 120, 135	0
25	BX	59/60 (98%)	1.36	12 (20%)	1 1	86, 114, 146, 166	0
26	A4	66/71 (92%)	3.36	46 (69%)	0 0	127, 161, 179, 187	0
26	B4	63/71 (88%)	3.59	46 (73%)	0 0	154, 190, 200, 207	0
27	A5	59/60 (98%)	0.48	7 (11%)	4 4	55, 95, 180, 185	0
27	B5	59/60 (98%)	1.09	12 (20%)	1 1	65, 94, 181, 192	0
28	A6	45/54 (83%)	3.26	30 (66%)	0 0	122, 152, 173, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	B6	45/54 (83%)	1.84	17 (37%) 0 0	141, 173, 188, 192	0
29	A7	49/49 (100%)	0.04	2 (4%) 37 36	50, 60, 106, 137	0
29	B7	49/49 (100%)	0.42	4 (8%) 11 12	60, 69, 129, 148	0
30	A8	61/65 (93%)	0.37	1 (1%) 72 70	64, 78, 95, 120	0
30	B8	61/65 (93%)	0.91	4 (6%) 18 19	78, 95, 110, 142	0
31	CA	1506/1506 (100%)	-0.36	6 (0%) 92 92	64, 112, 193, 248	0
31	DA	1506/1506 (100%)	-0.39	5 (0%) 93 94	76, 122, 195, 248	0
32	CE	237/256 (92%)	0.52	21 (8%) 9 10	115, 149, 188, 198	0
32	DE	237/256 (92%)	0.24	17 (7%) 15 17	127, 165, 200, 215	0
33	CF	205/239 (85%)	0.63	18 (8%) 10 11	98, 124, 158, 166	0
33	DF	206/239 (86%)	1.11	51 (24%) 0 0	128, 151, 180, 188	0
34	CG	208/208 (100%)	-0.10	0 100 100	95, 119, 143, 154	0
34	DG	208/208 (100%)	0.71	18 (8%) 10 11	91, 116, 137, 151	0
35	CH	151/162 (93%)	0.39	5 (3%) 46 45	87, 109, 132, 166	0
35	DH	151/162 (93%)	-0.04	0 100 100	104, 125, 148, 169	0
36	CI	101/101 (100%)	0.86	11 (10%) 5 5	89, 112, 130, 153	0
36	DI	101/101 (100%)	0.65	10 (9%) 7 7	87, 109, 130, 156	0
37	CJ	155/156 (99%)	0.65	16 (10%) 6 6	111, 128, 158, 167	0
37	DJ	155/156 (99%)	-0.15	1 (0%) 89 89	116, 136, 164, 170	0
38	CK	138/138 (100%)	0.11	3 (2%) 62 61	95, 116, 130, 137	0
38	DK	138/138 (100%)	-0.25	0 100 100	109, 129, 143, 151	0
39	CL	127/128 (99%)	-0.27	0 100 100	99, 147, 167, 173	0
39	DL	127/128 (99%)	-0.50	1 (0%) 86 86	120, 158, 174, 178	0
40	CM	99/105 (94%)	-0.12	2 (2%) 65 64	93, 146, 176, 179	0
40	DM	99/105 (94%)	0.36	9 (9%) 9 10	127, 164, 180, 185	0
41	CN	119/129 (92%)	1.78	41 (34%) 0 0	79, 110, 142, 169	0
41	DN	119/129 (92%)	0.56	8 (6%) 18 18	90, 116, 148, 172	0
42	CO	125/132 (94%)	1.05	23 (18%) 1 1	76, 87, 119, 164	0
42	DO	125/132 (94%)	1.26	30 (24%) 0 0	88, 112, 137, 175	0
43	CP	116/126 (92%)	0.59	11 (9%) 8 9	98, 132, 151, 160	0
43	DP	117/126 (92%)	0.80	13 (11%) 5 5	117, 160, 174, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	CQ	60/61 (98%)	0.03	1 (1%) 70 68	95, 115, 129, 139	0
44	DQ	60/61 (98%)	0.35	4 (6%) 18 18	129, 146, 159, 166	0
45	CR	88/89 (98%)	0.19	3 (3%) 45 44	86, 108, 129, 133	0
45	DR	88/89 (98%)	0.18	2 (2%) 60 59	85, 118, 142, 148	0
46	CS	84/88 (95%)	0.16	1 (1%) 79 78	104, 121, 148, 179	0
46	DS	84/88 (95%)	0.12	0 100 100	94, 111, 134, 166	0
47	CT	100/105 (95%)	0.15	5 (5%) 29 28	94, 115, 132, 146	0
47	DT	100/105 (95%)	0.20	2 (2%) 65 64	95, 117, 141, 155	0
48	CU	72/88 (81%)	0.93	11 (15%) 2 2	91, 112, 146, 173	0
48	DU	72/88 (81%)	0.61	7 (9%) 8 8	97, 120, 156, 173	0
49	CV	78/93 (83%)	0.61	5 (6%) 19 20	112, 136, 151, 158	0
49	DV	78/93 (83%)	0.79	7 (8%) 9 10	150, 167, 187, 191	0
50	CW	99/106 (93%)	-0.17	0 100 100	106, 130, 158, 169	0
50	DW	99/106 (93%)	-0.18	1 (1%) 82 82	97, 124, 158, 172	0
51	CX	25/27 (92%)	-0.24	0 100 100	101, 124, 142, 160	0
51	DX	25/27 (92%)	-0.10	0 100 100	126, 149, 163, 175	0
52	CB	87/87 (100%)	1.55	28 (32%) 0 0	91, 155, 201, 213	2 (2%)
52	DB	87/87 (100%)	1.45	27 (31%) 0 0	97, 156, 203, 216	2 (2%)
53	CC	77/77 (100%)	0.32	2 (2%) 56 54	82, 118, 149, 164	0
53	CD	77/77 (100%)	0.72	15 (19%) 1 1	86, 232, 246, 248	0
53	DC	77/77 (100%)	-0.31	0 100 100	87, 120, 153, 167	0
53	DD	77/77 (100%)	-0.48	1 (1%) 77 77	91, 234, 245, 249	0
54	C1	10/10 (100%)	1.27	2 (20%) 1 1	85, 102, 117, 131	0
54	D1	10/10 (100%)	-0.14	0 100 100	88, 109, 119, 137	0
All	All	21107/21634 (97%)	0.30	1569 (7%) 14 16	44, 110, 191, 249	4 (0%)

The worst 5 of 1569 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	654(J)	A	13.7
21	BV	179	ASP	13.6
1	AA	654(K)	C	11.7
41	CN	11	LYS	11.7
7	BH	29	PRO	11.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	BA	3420	1/1	-0.36	0.18	136,136,136,136	0
55	MG	CA	1704	1/1	-0.20	0.42	113,113,113,113	0
55	MG	AA	3224	1/1	-0.03	0.45	93,93,93,93	0
55	MG	CA	1728	1/1	0.02	0.37	117,117,117,117	0
55	MG	CA	1694	1/1	0.13	0.60	104,104,104,104	0
55	MG	CA	1693	1/1	0.17	0.37	102,102,102,102	0
55	MG	BA	3024	1/1	0.18	1.02	110,110,110,110	0
55	MG	BA	3471	1/1	0.21	0.38	96,96,96,96	0
55	MG	DA	1703	1/1	0.22	0.37	115,115,115,115	0
55	MG	BA	3371	1/1	0.23	0.16	129,129,129,129	0
55	MG	AA	3385	1/1	0.23	0.54	88,88,88,88	0
55	MG	BA	3406	1/1	0.24	0.30	97,97,97,97	0
55	MG	CA	1720	1/1	0.25	0.27	102,102,102,102	0
55	MG	CA	1653	1/1	0.25	0.41	91,91,91,91	0
55	MG	CA	1714	1/1	0.25	0.47	118,118,118,118	0
55	MG	DA	1713	1/1	0.26	0.36	111,111,111,111	0
55	MG	BB	212	1/1	0.27	0.31	104,104,104,104	0
55	MG	CA	1621	1/1	0.27	0.38	107,107,107,107	0
55	MG	DA	1802	1/1	0.28	0.47	102,102,102,102	0
55	MG	CA	1774	1/1	0.28	0.43	97,97,97,97	0
55	MG	BA	3078	1/1	0.28	0.23	95,95,95,95	0
55	MG	BA	3329	1/1	0.29	0.17	66,66,66,66	0
55	MG	AA	3433	1/1	0.29	0.12	152,152,152,152	0
55	MG	BA	3116	1/1	0.30	0.22	107,107,107,107	0
55	MG	DA	1719	1/1	0.30	0.56	112,112,112,112	0
55	MG	DA	1641	1/1	0.31	0.31	95,95,95,95	0
55	MG	BB	208	1/1	0.31	0.42	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3279	1/1	0.32	0.32	89,89,89,89	0
55	MG	CB	102	1/1	0.32	0.33	106,106,106,106	0
55	MG	AA	3413	1/1	0.33	0.40	109,109,109,109	0
55	MG	BA	3383	1/1	0.33	0.49	95,95,95,95	0
55	MG	CA	1637	1/1	0.34	0.32	106,106,106,106	0
55	MG	AA	3382	1/1	0.34	0.50	102,102,102,102	0
55	MG	AA	3393	1/1	0.35	0.57	98,98,98,98	0
55	MG	BA	3027	1/1	0.36	0.24	107,107,107,107	0
55	MG	BA	3472	1/1	0.36	0.44	83,83,83,83	0
55	MG	AA	3482	1/1	0.36	0.32	96,96,96,96	0
55	MG	BA	3465	1/1	0.36	0.34	97,97,97,97	0
55	MG	AA	3193	1/1	0.37	0.69	96,96,96,96	0
55	MG	AA	3466	1/1	0.37	0.48	100,100,100,100	0
55	MG	AA	3407	1/1	0.38	0.48	110,110,110,110	0
55	MG	BA	3463	1/1	0.38	0.29	114,114,114,114	0
55	MG	DA	1793	1/1	0.39	0.38	108,108,108,108	0
55	MG	BA	3422	1/1	0.39	0.36	102,102,102,102	0
55	MG	BA	3344	1/1	0.39	0.35	101,101,101,101	0
55	MG	BA	3095	1/1	0.40	0.38	112,112,112,112	0
55	MG	AA	3564	1/1	0.40	0.34	76,76,76,76	0
55	MG	AA	3347	1/1	0.40	0.33	92,92,92,92	0
55	MG	DA	1784	1/1	0.40	0.34	103,103,103,103	0
55	MG	AA	3416	1/1	0.41	0.45	95,95,95,95	0
55	MG	BA	3395	1/1	0.41	0.21	89,89,89,89	0
55	MG	CA	1773	1/1	0.41	0.36	101,101,101,101	0
55	MG	CA	1783	1/1	0.41	0.86	106,106,106,106	0
55	MG	AB	204	1/1	0.42	0.56	96,96,96,96	0
55	MG	AA	3409	1/1	0.43	0.54	104,104,104,104	0
55	MG	AA	3320	1/1	0.43	0.32	103,103,103,103	0
55	MG	BA	3399	1/1	0.44	0.26	104,104,104,104	0
55	MG	AA	3370	1/1	0.44	0.22	106,106,106,106	0
55	MG	BA	3507	1/1	0.45	0.34	102,102,102,102	0
55	MG	CA	1679	1/1	0.45	0.35	101,101,101,101	0
55	MG	DA	1625	1/1	0.45	0.22	105,105,105,105	0
55	MG	DA	1663	1/1	0.45	0.26	103,103,103,103	0
55	MG	BA	3277	1/1	0.46	0.30	109,109,109,109	0
55	MG	CA	1718	1/1	0.46	0.39	93,93,93,93	0
55	MG	BA	3303	1/1	0.46	0.37	89,89,89,89	0
55	MG	BA	3301	1/1	0.46	0.32	106,106,106,106	0
55	MG	CA	1768	1/1	0.46	0.33	105,105,105,105	0
55	MG	AA	3132	1/1	0.46	0.57	106,106,106,106	0
55	MG	BA	3468	1/1	0.47	0.28	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	3612	1/1	0.47	0.69	92,92,92,92	0
55	MG	BA	3051	1/1	0.47	0.33	90,90,90,90	0
55	MG	DA	1801	1/1	0.48	0.32	90,90,90,90	0
55	MG	AA	3537	1/1	0.48	0.30	105,105,105,105	0
55	MG	CA	1823	1/1	0.48	0.14	110,110,110,110	0
55	MG	AA	3456	1/1	0.48	0.41	91,91,91,91	0
55	MG	DA	1794	1/1	0.48	0.43	91,91,91,91	0
55	MG	BA	3367	1/1	0.49	0.39	91,91,91,91	0
55	MG	AA	3626	1/1	0.49	0.62	96,96,96,96	0
55	MG	DA	1795	1/1	0.49	0.32	101,101,101,101	0
55	MG	AA	3325	1/1	0.49	0.37	100,100,100,100	0
55	MG	AA	3522	1/1	0.50	0.55	97,97,97,97	0
55	MG	AA	3080	1/1	0.50	0.57	104,104,104,104	0
55	MG	BA	3407	1/1	0.50	0.14	96,96,96,96	0
55	MG	DA	1664	1/1	0.50	0.20	97,97,97,97	0
55	MG	CA	1672	1/1	0.50	0.26	106,106,106,106	0
55	MG	BA	3336	1/1	0.50	0.34	97,97,97,97	0
55	MG	AA	3366	1/1	0.50	0.55	92,92,92,92	0
55	MG	CG	301	1/1	0.50	0.49	94,94,94,94	0
55	MG	CA	1758	1/1	0.50	0.40	97,97,97,97	0
55	MG	CA	1803	1/1	0.51	0.66	94,94,94,94	0
55	MG	BA	3521	1/1	0.51	0.33	79,79,79,79	0
55	MG	CC	107	1/1	0.51	0.43	93,93,93,93	0
55	MG	AA	3304	1/1	0.51	0.32	90,90,90,90	0
55	MG	DA	1774	1/1	0.51	0.33	103,103,103,103	0
55	MG	DA	1804	1/1	0.51	0.34	123,123,123,123	0
55	MG	AA	3524	1/1	0.51	0.41	94,94,94,94	0
55	MG	CA	1832	1/1	0.51	0.25	106,106,106,106	0
55	MG	CA	1745	1/1	0.51	0.37	95,95,95,95	0
55	MG	CA	1767	1/1	0.52	0.27	120,120,120,120	0
55	MG	BA	3104	1/1	0.52	0.35	115,115,115,115	0
55	MG	BA	3164	1/1	0.52	0.21	99,99,99,99	0
55	MG	AA	3498	1/1	0.52	0.50	95,95,95,95	0
55	MG	AA	3073	1/1	0.52	0.57	97,97,97,97	0
55	MG	CA	1776	1/1	0.52	0.49	79,79,79,79	0
55	MG	BA	3193	1/1	0.53	0.34	102,102,102,102	0
55	MG	CA	1613	1/1	0.53	0.17	94,94,94,94	0
55	MG	BA	3098	1/1	0.53	0.25	106,106,106,106	0
55	MG	AA	3501	1/1	0.54	0.44	99,99,99,99	0
55	MG	AA	3156	1/1	0.54	0.46	94,94,94,94	0
55	MG	AA	3430	1/1	0.54	0.28	105,105,105,105	0
55	MG	CA	1727	1/1	0.54	0.27	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1770	1/1	0.54	0.32	90,90,90,90	0
55	MG	AA	3148	1/1	0.54	0.59	83,83,83,83	0
55	MG	BA	3003	1/1	0.54	0.50	99,99,99,99	0
55	MG	AA	3441	1/1	0.54	0.59	101,101,101,101	0
55	MG	AA	3273	1/1	0.54	0.29	101,101,101,101	0
55	MG	CB	104	1/1	0.54	0.35	101,101,101,101	0
55	MG	AA	3446	1/1	0.55	0.40	93,93,93,93	0
55	MG	AA	3107	1/1	0.55	0.31	69,69,69,69	0
55	MG	DC	107	1/1	0.55	0.41	105,105,105,105	0
55	MG	BA	3416	1/1	0.55	0.31	103,103,103,103	0
55	MG	AA	3301	1/1	0.55	0.30	85,85,85,85	0
55	MG	DA	1787	1/1	0.55	0.37	114,114,114,114	0
55	MG	AA	3425	1/1	0.55	0.33	94,94,94,94	0
55	MG	DA	1624	1/1	0.55	0.25	95,95,95,95	0
55	MG	CA	1831	1/1	0.55	0.33	105,105,105,105	0
55	MG	CA	1757	1/1	0.55	0.43	92,92,92,92	0
55	MG	BA	3151	1/1	0.56	0.27	96,96,96,96	0
55	MG	BA	3413	1/1	0.56	0.53	94,94,94,94	0
55	MG	AA	3604	1/1	0.56	0.46	93,93,93,93	0
55	MG	BA	3423	1/1	0.56	0.42	91,91,91,91	0
55	MG	AA	3286	1/1	0.57	0.46	86,86,86,86	0
55	MG	AA	3319	1/1	0.57	0.33	94,94,94,94	0
55	MG	CA	1753	1/1	0.57	0.24	107,107,107,107	0
55	MG	BA	3527	1/1	0.57	0.31	97,97,97,97	0
55	MG	BB	214	1/1	0.57	0.34	99,99,99,99	0
55	MG	CA	1710	1/1	0.57	0.35	81,81,81,81	0
55	MG	CA	1716	1/1	0.57	0.30	117,117,117,117	0
55	MG	BB	207	1/1	0.57	0.34	116,116,116,116	0
55	MG	CA	1821	1/1	0.57	0.38	94,94,94,94	0
55	MG	AA	3397	1/1	0.57	0.46	95,95,95,95	0
55	MG	AB	214	1/1	0.57	0.39	102,102,102,102	0
55	MG	BA	3478	1/1	0.57	0.39	92,92,92,92	0
55	MG	AA	3354	1/1	0.57	0.38	84,84,84,84	0
55	MG	BA	3398	1/1	0.58	0.55	96,96,96,96	0
55	MG	BA	3174	1/1	0.58	0.32	82,82,82,82	0
55	MG	CA	1611	1/1	0.58	0.21	97,97,97,97	0
55	MG	AA	3308	1/1	0.58	0.23	96,96,96,96	0
55	MG	BA	3520	1/1	0.58	0.32	101,101,101,101	0
55	MG	BA	3375	1/1	0.58	0.30	75,75,75,75	0
55	MG	CA	1724	1/1	0.58	0.22	97,97,97,97	0
55	MG	BA	3500	1/1	0.58	0.20	104,104,104,104	0
55	MG	AA	3402	1/1	0.58	0.46	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1758	1/1	0.59	0.46	109,109,109,109	0
55	MG	DA	1757	1/1	0.59	0.32	104,104,104,104	0
55	MG	BA	3332	1/1	0.59	0.23	100,100,100,100	0
55	MG	AA	3391	1/1	0.59	0.43	106,106,106,106	0
55	MG	BA	3447	1/1	0.59	0.30	100,100,100,100	0
55	MG	BA	3290	1/1	0.59	0.21	82,82,82,82	0
55	MG	AA	3075	1/1	0.59	0.61	85,85,85,85	0
55	MG	BA	3334	1/1	0.59	0.14	103,103,103,103	0
55	MG	CA	1706	1/1	0.59	0.34	91,91,91,91	0
55	MG	BB	210	1/1	0.59	0.38	96,96,96,96	0
55	MG	DA	1768	1/1	0.59	0.13	82,82,82,82	0
55	MG	AA	3235	1/1	0.59	0.46	84,84,84,84	0
55	MG	CA	1635	1/1	0.59	0.28	100,100,100,100	0
55	MG	AA	3277	1/1	0.59	0.32	82,82,82,82	0
55	MG	CN	202	1/1	0.60	0.32	99,99,99,99	0
55	MG	CA	1828	1/1	0.60	0.23	98,98,98,98	0
55	MG	AB	212	1/1	0.60	0.45	94,94,94,94	0
55	MG	BA	3459	1/1	0.60	0.22	115,115,115,115	0
55	MG	BA	3312	1/1	0.60	0.33	98,98,98,98	0
55	MG	BA	3424	1/1	0.60	0.64	86,86,86,86	0
55	MG	DA	1710	1/1	0.60	0.49	100,100,100,100	0
55	MG	BA	3475	1/1	0.60	0.32	90,90,90,90	0
55	MG	AA	3278	1/1	0.60	0.71	100,100,100,100	0
55	MG	AA	3265	1/1	0.60	0.23	95,95,95,95	0
55	MG	BA	3393	1/1	0.60	0.10	84,84,84,84	0
55	MG	DA	1785	1/1	0.61	0.30	93,93,93,93	0
55	MG	CA	1827	1/1	0.61	0.29	89,89,89,89	0
55	MG	CA	1809	1/1	0.61	0.39	79,79,79,79	0
55	MG	BA	3379	1/1	0.61	0.32	84,84,84,84	0
55	MG	DA	1629	1/1	0.61	0.20	92,92,92,92	0
55	MG	CA	1760	1/1	0.61	0.20	91,91,91,91	0
55	MG	BA	3041	1/1	0.61	0.48	104,104,104,104	0
55	MG	AA	3394	1/1	0.62	0.36	99,99,99,99	0
55	MG	BA	3449	1/1	0.62	0.29	109,109,109,109	0
55	MG	AA	3437	1/1	0.62	0.47	122,122,122,122	0
55	MG	BR	202	1/1	0.62	0.83	105,105,105,105	0
55	MG	BA	3067	1/1	0.62	0.42	74,74,74,74	0
55	MG	CA	1788	1/1	0.62	0.15	105,105,105,105	0
55	MG	BA	3090	1/1	0.62	0.33	109,109,109,109	0
55	MG	CA	1725	1/1	0.62	0.31	98,98,98,98	0
55	MG	C1	101	1/1	0.62	0.50	98,98,98,98	0
55	MG	BA	3397	1/1	0.62	0.32	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	CA	1800	1/1	0.62	0.17	104,104,104,104	0
55	MG	AA	3359	1/1	0.62	0.41	84,84,84,84	0
55	MG	BA	3363	1/1	0.62	0.23	88,88,88,88	0
55	MG	BA	3318	1/1	0.62	0.32	89,89,89,89	0
55	MG	BA	3037	1/1	0.63	0.26	75,75,75,75	0
55	MG	BA	3004	1/1	0.63	0.27	105,105,105,105	0
55	MG	DA	1763	1/1	0.63	0.28	89,89,89,89	0
55	MG	BA	3033	1/1	0.63	0.25	94,94,94,94	0
55	MG	CA	1819	1/1	0.63	0.21	109,109,109,109	0
55	MG	AA	3253	1/1	0.63	0.30	81,81,81,81	0
55	MG	AA	3367	1/1	0.63	0.52	87,87,87,87	0
55	MG	BA	3294	1/1	0.63	0.28	98,98,98,98	0
55	MG	DA	1777	1/1	0.63	0.40	87,87,87,87	0
55	MG	BA	3461	1/1	0.63	0.19	83,83,83,83	0
55	MG	BA	3175	1/1	0.63	0.22	100,100,100,100	0
55	MG	AA	3335	1/1	0.63	0.65	91,91,91,91	0
55	MG	BA	3081	1/1	0.63	0.21	91,91,91,91	0
55	MG	CA	1804	1/1	0.63	0.39	107,107,107,107	0
55	MG	AA	3435	1/1	0.63	0.45	78,78,78,78	0
55	MG	BA	3299	1/1	0.64	0.21	82,82,82,82	0
55	MG	CA	1775	1/1	0.64	0.27	113,113,113,113	0
55	MG	AA	3420	1/1	0.64	0.31	88,88,88,88	0
55	MG	BA	3454	1/1	0.64	0.42	105,105,105,105	0
55	MG	CA	1628	1/1	0.64	0.40	85,85,85,85	0
55	MG	AA	3556	1/1	0.64	0.49	96,96,96,96	0
55	MG	CA	1797	1/1	0.64	0.19	93,93,93,93	0
55	MG	AA	3372	1/1	0.64	0.28	87,87,87,87	0
55	MG	BA	3008	1/1	0.64	0.31	89,89,89,89	0
55	MG	CA	1711	1/1	0.64	0.30	98,98,98,98	0
55	MG	BA	3404	1/1	0.64	0.21	101,101,101,101	0
55	MG	AA	3118	1/1	0.64	0.41	87,87,87,87	0
55	MG	AA	3357	1/1	0.64	0.57	99,99,99,99	0
55	MG	DA	1754	1/1	0.64	0.25	98,98,98,98	0
55	MG	AE	303	1/1	0.64	0.37	91,91,91,91	0
55	MG	DA	1759	1/1	0.65	0.42	108,108,108,108	0
55	MG	DA	1749	1/1	0.65	0.25	101,101,101,101	0
55	MG	DA	1740	1/1	0.65	0.17	113,113,113,113	0
55	MG	AA	3469	1/1	0.65	0.49	103,103,103,103	0
55	MG	DA	1714	1/1	0.65	0.29	105,105,105,105	0
55	MG	AA	3492	1/1	0.65	0.32	94,94,94,94	0
55	MG	AA	3620	1/1	0.65	0.34	115,115,115,115	0
55	MG	AA	3169	1/1	0.65	0.35	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	BA	3226	1/1	0.65	0.45	82,82,82,82	0
55	MG	CA	1759	1/1	0.65	0.36	117,117,117,117	0
55	MG	AA	3362	1/1	0.65	0.36	89,89,89,89	0
55	MG	BA	3170	1/1	0.65	0.24	96,96,96,96	0
55	MG	BA	3101	1/1	0.65	0.25	94,94,94,94	0
55	MG	DA	1764	1/1	0.65	0.41	85,85,85,85	0
55	MG	CA	1615	1/1	0.65	0.32	104,104,104,104	0
55	MG	CA	1701	1/1	0.65	0.15	105,105,105,105	0
55	MG	DA	1682	1/1	0.65	0.47	96,96,96,96	0
55	MG	BA	3282	1/1	0.66	0.30	93,93,93,93	0
55	MG	AA	3443	1/1	0.66	0.34	90,90,90,90	0
55	MG	AA	3486	1/1	0.66	0.34	90,90,90,90	0
55	MG	BA	3392	1/1	0.66	0.21	85,85,85,85	0
55	MG	BA	3401	1/1	0.66	0.21	100,100,100,100	0
55	MG	BA	3429	1/1	0.66	0.16	95,95,95,95	0
55	MG	A6	101	1/1	0.66	0.50	111,111,111,111	0
55	MG	DA	1800	1/1	0.66	0.33	99,99,99,99	0
55	MG	AA	3445	1/1	0.66	0.30	95,95,95,95	0
55	MG	CA	1689	1/1	0.66	0.22	115,115,115,115	0
55	MG	CA	1640	1/1	0.66	0.35	85,85,85,85	0
55	MG	AA	3261	1/1	0.66	0.52	85,85,85,85	0
55	MG	AA	3097	1/1	0.66	0.59	106,106,106,106	0
55	MG	AA	3509	1/1	0.66	0.31	95,95,95,95	0
55	MG	BA	3384	1/1	0.66	0.35	92,92,92,92	0
55	MG	BA	3513	1/1	0.67	0.23	104,104,104,104	0
55	MG	DA	1611	1/1	0.67	0.38	100,100,100,100	0
55	MG	BA	3457	1/1	0.67	0.24	99,99,99,99	0
55	MG	BA	3469	1/1	0.67	0.35	92,92,92,92	0
55	MG	BA	3073	1/1	0.67	0.41	99,99,99,99	0
55	MG	DA	1760	1/1	0.67	0.45	100,100,100,100	0
55	MG	BA	3467	1/1	0.67	0.40	93,93,93,93	0
55	MG	BA	3056	1/1	0.67	0.25	96,96,96,96	0
55	MG	AA	3384	1/1	0.67	0.56	87,87,87,87	0
55	MG	DA	1688	1/1	0.67	0.27	99,99,99,99	0
55	MG	AA	3395	1/1	0.67	0.51	80,80,80,80	0
55	MG	AA	3236	1/1	0.67	0.57	96,96,96,96	0
55	MG	AE	304	1/1	0.67	0.13	87,87,87,87	0
55	MG	BA	3474	1/1	0.67	0.41	88,88,88,88	0
55	MG	AA	3560	1/1	0.67	0.35	87,87,87,87	0
55	MG	AA	3259	1/1	0.67	0.29	81,81,81,81	0
55	MG	BA	3339	1/1	0.67	0.20	90,90,90,90	0
55	MG	BA	3235	1/1	0.68	0.44	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	3270	1/1	0.68	0.30	69,69,69,69	0
55	MG	AA	3480	1/1	0.68	0.55	86,86,86,86	0
55	MG	DA	1747	1/1	0.68	0.30	105,105,105,105	0
55	MG	AA	3340	1/1	0.68	0.38	83,83,83,83	0
55	MG	BA	3121	1/1	0.68	0.45	99,99,99,99	0
55	MG	CA	1629	1/1	0.68	0.15	95,95,95,95	0
55	MG	DA	1711	1/1	0.68	0.41	89,89,89,89	0
55	MG	CA	1681	1/1	0.68	0.35	80,80,80,80	0
55	MG	AA	3361	1/1	0.68	0.54	93,93,93,93	0
55	MG	BA	3331	1/1	0.68	0.20	101,101,101,101	0
55	MG	DA	1618	1/1	0.68	0.31	104,104,104,104	0
55	MG	BA	3063	1/1	0.68	0.30	89,89,89,89	0
55	MG	BA	3050	1/1	0.68	0.24	103,103,103,103	0
55	MG	CA	1662	1/1	0.68	0.42	81,81,81,81	0
55	MG	BA	3394	1/1	0.68	0.43	88,88,88,88	0
55	MG	AA	3182	1/1	0.68	0.47	88,88,88,88	0
55	MG	BA	3453	1/1	0.68	0.24	93,93,93,93	0
55	MG	AA	3185	1/1	0.68	0.60	88,88,88,88	0
55	MG	DA	1613	1/1	0.68	0.42	88,88,88,88	0
55	MG	AA	3060	1/1	0.68	0.43	84,84,84,84	0
55	MG	CA	1719	1/1	0.68	0.35	85,85,85,85	0
55	MG	BB	215	1/1	0.69	0.17	101,101,101,101	0
55	MG	AA	3249	1/1	0.69	0.41	76,76,76,76	0
55	MG	BA	3444	1/1	0.69	0.50	96,96,96,96	0
55	MG	AA	3525	1/1	0.69	0.17	73,73,73,73	0
55	MG	BA	3287	1/1	0.69	0.35	87,87,87,87	0
55	MG	AA	3341	1/1	0.69	0.26	95,95,95,95	0
55	MG	BA	3441	1/1	0.69	0.34	93,93,93,93	0
55	MG	BA	3293	1/1	0.69	0.22	96,96,96,96	0
55	MG	CA	1722	1/1	0.69	0.41	74,74,74,74	0
55	MG	AB	208	1/1	0.69	0.34	92,92,92,92	0
55	MG	AA	3120	1/1	0.69	0.32	86,86,86,86	0
55	MG	CA	1813	1/1	0.69	0.58	94,94,94,94	0
55	MG	BA	3345	1/1	0.69	0.19	87,87,87,87	0
55	MG	BA	3105	1/1	0.69	0.24	81,81,81,81	0
55	MG	CA	1647	1/1	0.69	0.21	92,92,92,92	0
55	MG	AA	3392	1/1	0.69	0.50	93,93,93,93	0
55	MG	AA	3374	1/1	0.69	0.41	74,74,74,74	0
55	MG	BA	3068	1/1	0.69	0.27	93,93,93,93	0
55	MG	AF	302	1/1	0.69	0.33	93,93,93,93	0
55	MG	BA	3464	1/1	0.70	0.33	104,104,104,104	0
55	MG	AA	3275	1/1	0.70	0.40	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3369	1/1	0.70	0.53	93,93,93,93	0
55	MG	AA	3461	1/1	0.70	0.39	105,105,105,105	0
55	MG	AA	3077	1/1	0.70	0.49	103,103,103,103	0
55	MG	CA	1806	1/1	0.70	0.17	62,62,62,62	0
55	MG	AB	202	1/1	0.70	0.23	92,92,92,92	0
55	MG	CA	1752	1/1	0.70	0.15	96,96,96,96	0
55	MG	AA	3475	1/1	0.70	0.27	102,102,102,102	0
55	MG	AA	3053	1/1	0.70	0.58	67,67,67,67	0
55	MG	AA	3497	1/1	0.70	0.61	95,95,95,95	0
55	MG	AA	3307	1/1	0.70	0.45	76,76,76,76	0
55	MG	DA	1718	1/1	0.70	0.21	132,132,132,132	0
55	MG	BA	3380	1/1	0.70	0.23	78,78,78,78	0
55	MG	DA	1702	1/1	0.70	0.36	99,99,99,99	0
55	MG	DA	1615	1/1	0.70	0.32	96,96,96,96	0
55	MG	BA	3313	1/1	0.71	0.20	106,106,106,106	0
55	MG	DA	1607	1/1	0.71	0.32	92,92,92,92	0
55	MG	CB	101	1/1	0.71	0.32	108,108,108,108	0
55	MG	BA	3387	1/1	0.71	0.48	107,107,107,107	0
55	MG	BA	3378	1/1	0.71	0.20	78,78,78,78	0
55	MG	AA	3419	1/1	0.71	0.57	89,89,89,89	0
55	MG	AA	3426	1/1	0.71	0.44	80,80,80,80	0
55	MG	CA	1735	1/1	0.71	0.46	101,101,101,101	0
55	MG	AA	3490	1/1	0.71	0.58	97,97,97,97	0
55	MG	CA	1816	1/1	0.71	0.20	95,95,95,95	0
55	MG	AA	3527	1/1	0.71	0.43	86,86,86,86	0
55	MG	DA	1770	1/1	0.71	0.35	95,95,95,95	0
55	MG	CA	1787	1/1	0.71	0.29	100,100,100,100	0
55	MG	CA	1715	1/1	0.71	0.26	115,115,115,115	0
55	MG	BA	3191	1/1	0.71	0.43	77,77,77,77	0
55	MG	BA	3370	1/1	0.71	0.22	98,98,98,98	0
55	MG	AA	3363	1/1	0.71	0.43	95,95,95,95	0
55	MG	DA	1746	1/1	0.71	0.25	104,104,104,104	0
55	MG	A3	101	1/1	0.71	0.42	74,74,74,74	0
55	MG	DA	1791	1/1	0.71	0.45	80,80,80,80	0
55	MG	CA	1778	1/1	0.71	0.43	95,95,95,95	0
55	MG	DA	1717	1/1	0.71	0.19	103,103,103,103	0
55	MG	AA	3390	1/1	0.71	0.40	109,109,109,109	0
55	MG	BA	3045	1/1	0.71	0.26	88,88,88,88	0
55	MG	AA	3583	1/1	0.72	0.56	103,103,103,103	0
55	MG	AA	3479	1/1	0.72	0.21	94,94,94,94	0
55	MG	DA	1683	1/1	0.72	0.56	80,80,80,80	0
55	MG	AA	3513	1/1	0.72	0.36	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	AA	3464	1/1	0.72	0.32	83,83,83,83	0
55	MG	BA	3448	1/1	0.72	0.22	85,85,85,85	0
55	MG	CG	302	1/1	0.72	0.17	122,122,122,122	0
55	MG	BA	3064	1/1	0.72	0.24	103,103,103,103	0
55	MG	CQ	102	1/1	0.72	0.25	97,97,97,97	0
55	MG	DA	1708	1/1	0.72	0.59	102,102,102,102	0
55	MG	DA	1789	1/1	0.72	0.22	77,77,77,77	0
55	MG	BA	3297	1/1	0.72	0.12	63,63,63,63	0
55	MG	AA	3067	1/1	0.72	0.52	108,108,108,108	0
55	MG	AA	3373	1/1	0.72	0.44	106,106,106,106	0
55	MG	AA	3309	1/1	0.72	0.70	90,90,90,90	0
55	MG	DA	1642	1/1	0.72	0.25	110,110,110,110	0
55	MG	BA	3114	1/1	0.72	0.29	103,103,103,103	0
55	MG	BA	3421	1/1	0.72	0.14	102,102,102,102	0
55	MG	CA	1815	1/1	0.72	0.27	91,91,91,91	0
55	MG	BA	3077	1/1	0.72	0.24	101,101,101,101	0
55	MG	BA	3039	1/1	0.72	0.32	85,85,85,85	0
55	MG	CC	101	1/1	0.72	0.30	108,108,108,108	0
55	MG	DA	1745	1/1	0.72	0.24	106,106,106,106	0
55	MG	AA	3316	1/1	0.72	0.18	83,83,83,83	0
55	MG	AA	3108	1/1	0.72	0.49	66,66,66,66	0
55	MG	DA	1778	1/1	0.72	0.25	118,118,118,118	0
55	MG	AA	3601	1/1	0.72	0.23	86,86,86,86	0
55	MG	AA	3410	1/1	0.73	0.40	95,95,95,95	0
55	MG	AA	3532	1/1	0.73	0.31	88,88,88,88	0
55	MG	AA	3332	1/1	0.73	0.15	62,62,62,62	0
55	MG	DA	1798	1/1	0.73	0.22	92,92,92,92	0
55	MG	BA	3382	1/1	0.73	0.24	89,89,89,89	0
55	MG	DA	1623	1/1	0.73	0.38	96,96,96,96	0
55	MG	DA	1748	1/1	0.73	0.50	91,91,91,91	0
55	MG	DC	104	1/1	0.73	0.21	102,102,102,102	0
55	MG	DA	1722	1/1	0.73	0.28	106,106,106,106	0
55	MG	BA	3057	1/1	0.73	0.20	97,97,97,97	0
55	MG	AA	3096	1/1	0.73	0.32	89,89,89,89	0
55	MG	BA	3065	1/1	0.73	0.44	101,101,101,101	0
55	MG	BA	3477	1/1	0.73	0.25	94,94,94,94	0
55	MG	AA	3104	1/1	0.73	0.34	80,80,80,80	0
55	MG	BA	3432	1/1	0.73	0.35	88,88,88,88	0
55	MG	BA	3410	1/1	0.73	0.43	94,94,94,94	0
55	MG	AA	3280	1/1	0.73	0.34	94,94,94,94	0
55	MG	DA	1606	1/1	0.73	0.29	95,95,95,95	0
55	MG	DA	1712	1/1	0.73	0.43	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3264	1/1	0.73	0.54	80,80,80,80	0
55	MG	CA	1661	1/1	0.73	0.17	52,52,52,52	0
55	MG	CA	1765	1/1	0.73	0.25	109,109,109,109	0
55	MG	AA	3381	1/1	0.73	0.71	90,90,90,90	0
55	MG	CA	1709	1/1	0.74	0.46	96,96,96,96	0
55	MG	BA	3296	1/1	0.74	0.25	76,76,76,76	0
55	MG	BA	3350	1/1	0.74	0.51	77,77,77,77	0
55	MG	BA	3089	1/1	0.74	0.27	83,83,83,83	0
55	MG	CA	1764	1/1	0.74	0.20	92,92,92,92	0
55	MG	CA	1685	1/1	0.74	0.27	103,103,103,103	0
55	MG	BA	3091	1/1	0.74	0.37	86,86,86,86	0
55	MG	AA	3442	1/1	0.74	0.37	78,78,78,78	0
55	MG	AA	3302	1/1	0.74	0.41	104,104,104,104	0
55	MG	AA	3172	1/1	0.74	0.30	94,94,94,94	0
55	MG	CA	1766	1/1	0.74	0.53	108,108,108,108	0
55	MG	BA	3278	1/1	0.74	0.32	92,92,92,92	0
55	MG	BA	3112	1/1	0.74	0.12	69,69,69,69	0
55	MG	BA	3070	1/1	0.74	0.28	81,81,81,81	0
55	MG	BA	3355	1/1	0.74	0.43	87,87,87,87	0
55	MG	BA	3435	1/1	0.74	0.16	108,108,108,108	0
55	MG	BA	3099	1/1	0.74	0.20	98,98,98,98	0
55	MG	AA	3093	1/1	0.74	0.52	65,65,65,65	0
55	MG	BB	206	1/1	0.75	0.12	102,102,102,102	0
55	MG	CA	1612	1/1	0.75	0.23	102,102,102,102	0
55	MG	BA	3204	1/1	0.75	0.30	74,74,74,74	0
55	MG	AA	3256	1/1	0.75	0.39	66,66,66,66	0
55	MG	DA	1661	1/1	0.75	0.50	98,98,98,98	0
55	MG	CA	1790	1/1	0.75	0.26	89,89,89,89	0
55	MG	DA	1636	1/1	0.75	0.24	103,103,103,103	0
55	MG	BA	3402	1/1	0.75	0.32	95,95,95,95	0
55	MG	BA	3519	1/1	0.75	0.24	107,107,107,107	0
55	MG	BA	3368	1/1	0.75	0.30	106,106,106,106	0
55	MG	BA	3526	1/1	0.75	0.26	92,92,92,92	0
55	MG	AA	3439	1/1	0.75	0.40	97,97,97,97	0
55	MG	CA	1652	1/1	0.75	0.30	93,93,93,93	0
55	MG	BA	3034	1/1	0.75	0.28	81,81,81,81	0
55	MG	BA	3442	1/1	0.75	0.37	91,91,91,91	0
55	MG	AA	3376	1/1	0.75	0.62	85,85,85,85	0
55	MG	DA	1720	1/1	0.75	0.32	96,96,96,96	0
55	MG	AA	3421	1/1	0.75	0.56	94,94,94,94	0
55	MG	BA	3044	1/1	0.75	0.48	104,104,104,104	0
55	MG	BA	3374	1/1	0.75	0.52	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3595	1/1	0.75	0.36	79,79,79,79	0
55	MG	AA	3593	1/1	0.75	0.50	95,95,95,95	0
55	MG	AA	3396	1/1	0.75	0.55	104,104,104,104	0
55	MG	AA	3121	1/1	0.75	0.71	90,90,90,90	0
55	MG	AA	3291	1/1	0.76	0.45	68,68,68,68	0
55	MG	AA	3171	1/1	0.76	0.33	84,84,84,84	0
55	MG	AA	3375	1/1	0.76	0.43	88,88,88,88	0
55	MG	BA	3327	1/1	0.76	0.28	91,91,91,91	0
55	MG	BA	3311	1/1	0.76	0.22	82,82,82,82	0
55	MG	DA	1602	1/1	0.76	0.33	85,85,85,85	0
55	MG	AA	3499	1/1	0.76	0.67	93,93,93,93	0
55	MG	AA	3258	1/1	0.76	0.42	92,92,92,92	0
55	MG	BA	3262	1/1	0.76	0.21	94,94,94,94	0
55	MG	CA	1677	1/1	0.76	0.25	90,90,90,90	0
55	MG	DA	1655	1/1	0.76	0.33	96,96,96,96	0
55	MG	BA	3426	1/1	0.76	0.39	87,87,87,87	0
55	MG	BA	3391	1/1	0.76	0.29	95,95,95,95	0
55	MG	BA	3305	1/1	0.76	0.33	76,76,76,76	0
55	MG	CA	1683	1/1	0.76	0.32	104,104,104,104	0
55	MG	AA	3231	1/1	0.76	0.53	106,106,106,106	0
55	MG	BA	3117	1/1	0.76	0.39	91,91,91,91	0
55	MG	BA	3163	1/1	0.76	0.21	84,84,84,84	0
55	MG	CA	1616	1/1	0.76	0.24	103,103,103,103	0
55	MG	BA	3046	1/1	0.76	0.34	83,83,83,83	0
55	MG	BA	3304	1/1	0.76	0.33	91,91,91,91	0
55	MG	BA	3266	1/1	0.76	0.48	91,91,91,91	0
55	MG	CA	1633	1/1	0.76	0.30	83,83,83,83	0
55	MG	AA	3242	1/1	0.76	0.23	93,93,93,93	0
55	MG	DS	101	1/1	0.76	0.48	87,87,87,87	0
55	MG	DG	302	1/1	0.76	0.08	112,112,112,112	0
55	MG	AA	3418	1/1	0.76	0.30	91,91,91,91	0
55	MG	AA	3334	1/1	0.76	0.70	76,76,76,76	0
55	MG	AA	3078	1/1	0.77	0.64	88,88,88,88	0
55	MG	AA	3126	1/1	0.77	0.24	83,83,83,83	0
55	MG	DA	1769	1/1	0.77	0.34	79,79,79,79	0
55	MG	BA	3390	1/1	0.77	0.46	77,77,77,77	0
55	MG	CA	1623	1/1	0.77	0.30	73,73,73,73	0
55	MG	DA	1660	1/1	0.77	0.24	102,102,102,102	0
55	MG	BA	3035	1/1	0.77	0.25	103,103,103,103	0
55	MG	AA	3463	1/1	0.77	0.42	90,90,90,90	0
55	MG	AA	3039	1/1	0.77	0.67	82,82,82,82	0
55	MG	DA	1725	1/1	0.77	0.39	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3415	1/1	0.77	0.30	109,109,109,109	0
55	MG	DA	1698	1/1	0.77	0.48	103,103,103,103	0
55	MG	BA	3111	1/1	0.77	0.20	82,82,82,82	0
55	MG	BA	3165	1/1	0.77	0.34	42,42,42,42	0
55	MG	BA	3466	1/1	0.77	0.14	73,73,73,73	0
55	MG	CA	1834	1/1	0.77	0.33	90,90,90,90	0
55	MG	BA	3337	1/1	0.77	0.34	100,100,100,100	0
55	MG	AA	3353	1/1	0.77	0.52	86,86,86,86	0
55	MG	AA	3423	1/1	0.77	0.20	74,74,74,74	0
55	MG	AA	3616	1/1	0.77	0.30	95,95,95,95	0
55	MG	AA	3260	1/1	0.77	0.55	91,91,91,91	0
55	MG	AA	3094	1/1	0.77	0.35	62,62,62,62	0
55	MG	DA	1627	1/1	0.77	0.13	105,105,105,105	0
55	MG	AA	3365	1/1	0.77	0.38	74,74,74,74	0
55	MG	BB	213	1/1	0.77	0.45	97,97,97,97	0
55	MG	BA	3289	1/1	0.77	0.43	70,70,70,70	0
55	MG	AA	3493	1/1	0.77	0.33	92,92,92,92	0
55	MG	AA	3294	1/1	0.77	0.76	93,93,93,93	0
55	MG	CA	1729	1/1	0.77	0.35	94,94,94,94	0
55	MG	AA	3358	1/1	0.77	0.68	89,89,89,89	0
55	MG	CA	1799	1/1	0.77	0.38	95,95,95,95	0
55	MG	BA	3357	1/1	0.77	0.39	71,71,71,71	0
55	MG	AA	3173	1/1	0.78	0.34	67,67,67,67	0
55	MG	BA	3088	1/1	0.78	0.20	94,94,94,94	0
55	MG	BA	3043	1/1	0.78	0.22	108,108,108,108	0
55	MG	BA	3040	1/1	0.78	0.20	94,94,94,94	0
55	MG	BA	3427	1/1	0.78	0.33	100,100,100,100	0
55	MG	BA	3107	1/1	0.78	0.23	89,89,89,89	0
55	MG	BA	3108	1/1	0.78	0.40	99,99,99,99	0
55	MG	AA	3377	1/1	0.78	0.55	94,94,94,94	0
55	MG	CA	1798	1/1	0.78	0.40	82,82,82,82	0
55	MG	BA	3436	1/1	0.78	0.28	94,94,94,94	0
55	MG	CA	1808	1/1	0.78	0.26	67,67,67,67	0
55	MG	CA	1782	1/1	0.78	0.55	94,94,94,94	0
55	MG	BA	3119	1/1	0.78	0.20	79,79,79,79	0
55	MG	CA	1617	1/1	0.78	0.51	72,72,72,72	0
55	MG	CD	101	1/1	0.78	0.19	105,105,105,105	0
55	MG	CA	1817	1/1	0.78	0.27	85,85,85,85	0
55	MG	AA	3364	1/1	0.78	0.34	69,69,69,69	0
55	MG	BA	3389	1/1	0.78	0.17	96,96,96,96	0
55	MG	BA	3356	1/1	0.78	0.19	84,84,84,84	0
55	MG	AA	3557	1/1	0.78	0.49	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3076	1/1	0.78	0.37	91,91,91,91	0
55	MG	AA	3217	1/1	0.78	0.17	64,64,64,64	0
55	MG	AA	3268	1/1	0.78	0.49	85,85,85,85	0
55	MG	CA	1805	1/1	0.78	0.37	75,75,75,75	0
55	MG	CB	105	1/1	0.78	0.12	113,113,113,113	0
55	MG	BA	3256	1/1	0.78	0.35	102,102,102,102	0
55	MG	BB	209	1/1	0.78	0.31	95,95,95,95	0
55	MG	AA	3356	1/1	0.78	0.54	86,86,86,86	0
55	MG	CA	1748	1/1	0.78	0.38	87,87,87,87	0
55	MG	BA	3270	1/1	0.78	0.28	81,81,81,81	0
55	MG	CA	1738	1/1	0.78	0.31	103,103,103,103	0
55	MG	DA	1686	1/1	0.78	0.34	97,97,97,97	0
55	MG	AB	209	1/1	0.79	0.50	108,108,108,108	0
55	MG	AA	3536	1/1	0.79	0.47	92,92,92,92	0
55	MG	AA	3452	1/1	0.79	0.43	76,76,76,76	0
55	MG	BA	3125	1/1	0.79	1.04	104,104,104,104	0
55	MG	CA	1743	1/1	0.79	0.16	112,112,112,112	0
55	MG	AA	3295	1/1	0.79	0.66	102,102,102,102	0
55	MG	CA	1639	1/1	0.79	0.42	86,86,86,86	0
55	MG	DA	1639	1/1	0.79	0.33	78,78,78,78	0
55	MG	AA	3438	1/1	0.79	0.45	90,90,90,90	0
55	MG	AA	3064	1/1	0.79	0.12	79,79,79,79	0
55	MG	BA	3476	1/1	0.79	0.18	68,68,68,68	0
55	MG	BA	3361	1/1	0.79	0.15	88,88,88,88	0
55	MG	AA	3310	1/1	0.79	0.26	65,65,65,65	0
55	MG	BA	3185	1/1	0.79	0.41	68,68,68,68	0
55	MG	BA	3019	1/1	0.79	0.24	100,100,100,100	0
55	MG	DA	1803	1/1	0.79	0.49	100,100,100,100	0
55	MG	CA	1737	1/1	0.79	0.26	92,92,92,92	0
55	MG	DA	1788	1/1	0.79	0.39	90,90,90,90	0
55	MG	CA	1723	1/1	0.79	0.39	106,106,106,106	0
55	MG	CA	1833	1/1	0.79	0.14	95,95,95,95	0
55	MG	DA	1678	1/1	0.79	0.46	86,86,86,86	0
55	MG	BA	3353	1/1	0.79	0.22	84,84,84,84	0
55	MG	AA	3502	1/1	0.79	0.65	96,96,96,96	0
55	MG	AA	3467	1/1	0.79	0.38	87,87,87,87	0
55	MG	AF	301	1/1	0.79	0.20	80,80,80,80	0
55	MG	AA	3225	1/1	0.79	0.44	95,95,95,95	0
55	MG	AA	3371	1/1	0.79	0.43	89,89,89,89	0
55	MG	DA	1684	1/1	0.79	0.25	92,92,92,92	0
55	MG	BA	3092	1/1	0.79	0.24	95,95,95,95	0
55	MG	CA	1726	1/1	0.79	0.26	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3094	1/1	0.79	0.23	79,79,79,79	0
55	MG	BR	201	1/1	0.79	0.24	77,77,77,77	0
55	MG	A5	102	1/1	0.79	0.42	83,83,83,83	0
55	MG	DA	1631	1/1	0.79	0.20	102,102,102,102	0
55	MG	DA	1766	1/1	0.79	0.53	116,116,116,116	0
55	MG	DA	1765	1/1	0.79	0.20	93,93,93,93	0
55	MG	BA	3093	1/1	0.79	0.17	78,78,78,78	0
55	MG	AA	3518	1/1	0.79	0.36	90,90,90,90	0
55	MG	BA	3074	1/1	0.80	0.20	83,83,83,83	0
55	MG	BA	3445	1/1	0.80	0.23	95,95,95,95	0
55	MG	DA	1767	1/1	0.80	0.40	113,113,113,113	0
55	MG	AA	3594	1/1	0.80	0.56	105,105,105,105	0
55	MG	AA	3099	1/1	0.80	0.46	64,64,64,64	0
55	MG	AA	3523	1/1	0.80	0.21	91,91,91,91	0
55	MG	DA	1635	1/1	0.80	0.29	79,79,79,79	0
55	MG	AA	3473	1/1	0.80	0.46	77,77,77,77	0
55	MG	DA	1626	1/1	0.80	0.34	104,104,104,104	0
55	MG	BA	3258	1/1	0.80	0.34	64,64,64,64	0
55	MG	CA	1736	1/1	0.80	0.26	88,88,88,88	0
55	MG	AA	3494	1/1	0.80	0.37	88,88,88,88	0
55	MG	BA	3124	1/1	0.80	0.39	102,102,102,102	0
55	MG	CA	1690	1/1	0.80	0.40	102,102,102,102	0
55	MG	AZ	101	1/1	0.80	0.30	77,77,77,77	0
55	MG	DH	201	1/1	0.80	0.18	105,105,105,105	0
55	MG	BA	3298	1/1	0.80	0.15	61,61,61,61	0
55	MG	CA	1687	1/1	0.80	0.29	78,78,78,78	0
55	MG	BA	3498	1/1	0.80	0.15	99,99,99,99	0
55	MG	DA	1608	1/1	0.80	0.24	92,92,92,92	0
55	MG	CA	1734	1/1	0.80	0.51	86,86,86,86	0
55	MG	CA	1644	1/1	0.80	0.21	84,84,84,84	0
55	MG	AA	3350	1/1	0.80	0.24	90,90,90,90	0
55	MG	DA	1633	1/1	0.80	0.32	88,88,88,88	0
55	MG	AA	3542	1/1	0.80	0.37	93,93,93,93	0
55	MG	BA	3348	1/1	0.80	0.32	98,98,98,98	0
55	MG	AA	3163	1/1	0.80	0.31	55,55,55,55	0
55	MG	AA	3055	1/1	0.80	0.35	67,67,67,67	0
55	MG	BA	3047	1/1	0.80	0.18	80,80,80,80	0
55	MG	AA	3227	1/1	0.80	0.62	90,90,90,90	0
55	MG	AA	3276	1/1	0.81	0.53	78,78,78,78	0
55	MG	AA	3201	1/1	0.81	0.34	85,85,85,85	0
55	MG	BA	3153	1/1	0.81	0.39	77,77,77,77	0
55	MG	AA	3489	1/1	0.81	0.66	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3503	1/1	0.81	0.47	81,81,81,81	0
55	MG	CA	1630	1/1	0.81	0.28	112,112,112,112	0
55	MG	AA	3237	1/1	0.81	0.45	83,83,83,83	0
55	MG	BA	3326	1/1	0.81	0.23	84,84,84,84	0
55	MG	BA	3433	1/1	0.81	0.24	88,88,88,88	0
55	MG	AA	3328	1/1	0.81	0.39	82,82,82,82	0
55	MG	AA	3500	1/1	0.81	0.39	103,103,103,103	0
55	MG	AA	3109	1/1	0.81	0.37	53,53,53,53	0
55	MG	DA	1743	1/1	0.81	0.24	94,94,94,94	0
55	MG	AA	3184	1/1	0.81	0.39	94,94,94,94	0
55	MG	AA	3250	1/1	0.81	0.33	99,99,99,99	0
55	MG	AA	3207	1/1	0.81	0.21	50,50,50,50	0
55	MG	AA	3515	1/1	0.81	0.37	77,77,77,77	0
55	MG	AB	211	1/1	0.81	0.53	100,100,100,100	0
55	MG	BA	3188	1/1	0.81	0.30	85,85,85,85	0
55	MG	BA	3109	1/1	0.81	0.16	75,75,75,75	0
55	MG	CA	1739	1/1	0.81	0.56	86,86,86,86	0
55	MG	BA	3195	1/1	0.81	0.40	94,94,94,94	0
55	MG	BA	3346	1/1	0.81	0.40	99,99,99,99	0
55	MG	BA	3058	1/1	0.81	0.35	89,89,89,89	0
55	MG	BA	3505	1/1	0.81	0.29	94,94,94,94	0
55	MG	AA	3429	1/1	0.81	0.44	90,90,90,90	0
55	MG	BA	3376	1/1	0.81	0.33	65,65,65,65	0
55	MG	AA	3215	1/1	0.81	0.32	79,79,79,79	0
55	MG	DA	1614	1/1	0.81	0.54	93,93,93,93	0
55	MG	CA	1656	1/1	0.81	0.52	88,88,88,88	0
55	MG	BA	3405	1/1	0.81	0.23	87,87,87,87	0
55	MG	BA	3341	1/1	0.81	0.43	82,82,82,82	0
55	MG	BA	3273	1/1	0.81	0.34	102,102,102,102	0
55	MG	AA	3206	1/1	0.81	0.16	51,51,51,51	0
55	MG	DC	108	1/1	0.81	0.17	102,102,102,102	0
55	MG	BA	3260	1/1	0.81	0.14	82,82,82,82	0
55	MG	AA	3042	1/1	0.81	0.18	77,77,77,77	0
55	MG	BA	3446	1/1	0.81	0.32	98,98,98,98	0
55	MG	AA	3468	1/1	0.82	0.29	95,95,95,95	0
55	MG	AA	3624	1/1	0.82	0.32	111,111,111,111	0
55	MG	A2	201	1/1	0.82	0.50	101,101,101,101	0
55	MG	AA	3451	1/1	0.82	0.38	76,76,76,76	0
55	MG	AA	3292	1/1	0.82	0.39	76,76,76,76	0
55	MG	BA	3362	1/1	0.82	0.14	71,71,71,71	0
55	MG	AA	3510	1/1	0.82	0.53	84,84,84,84	0
55	MG	BA	3209	1/1	0.82	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3113	1/1	0.82	0.12	84,84,84,84	0
55	MG	BA	3120	1/1	0.82	0.18	81,81,81,81	0
55	MG	AB	216	1/1	0.82	0.34	106,106,106,106	0
55	MG	CA	1668	1/1	0.82	0.53	79,79,79,79	0
55	MG	AA	3251	1/1	0.82	0.34	68,68,68,68	0
55	MG	AA	3511	1/1	0.82	0.70	98,98,98,98	0
55	MG	AA	3531	1/1	0.82	0.45	96,96,96,96	0
55	MG	BA	3055	1/1	0.82	0.30	99,99,99,99	0
55	MG	BA	3460	1/1	0.82	0.17	101,101,101,101	0
55	MG	CA	1771	1/1	0.82	0.22	102,102,102,102	0
55	MG	AA	3038	1/1	0.82	0.55	80,80,80,80	0
55	MG	AA	3440	1/1	0.82	0.42	87,87,87,87	0
55	MG	BA	3495	1/1	0.82	0.29	81,81,81,81	0
55	MG	AA	3241	1/1	0.82	0.67	80,80,80,80	0
55	MG	AA	3323	1/1	0.82	0.26	71,71,71,71	0
55	MG	AA	3554	1/1	0.82	0.46	74,74,74,74	0
55	MG	BE	302	1/1	0.82	0.15	76,76,76,76	0
55	MG	CA	1649	1/1	0.82	0.29	86,86,86,86	0
55	MG	BA	3499	1/1	0.82	0.15	78,78,78,78	0
55	MG	BA	3032	1/1	0.82	0.36	110,110,110,110	0
55	MG	AA	3589	1/1	0.82	0.38	60,60,60,60	0
55	MG	DA	1779	1/1	0.82	0.34	91,91,91,91	0
55	MG	BA	3026	1/1	0.82	0.30	72,72,72,72	0
55	MG	DA	1637	1/1	0.82	0.30	97,97,97,97	0
55	MG	AA	3428	1/1	0.82	0.23	120,120,120,120	0
55	MG	AA	3415	1/1	0.82	0.47	87,87,87,87	0
55	MG	BA	3021	1/1	0.82	0.35	105,105,105,105	0
55	MG	CA	1646	1/1	0.82	0.37	75,75,75,75	0
55	MG	DA	1771	1/1	0.82	0.29	114,114,114,114	0
55	MG	BA	3411	1/1	0.82	0.35	83,83,83,83	0
55	MG	BA	3122	1/1	0.82	0.33	95,95,95,95	0
55	MG	CA	1762	1/1	0.82	0.14	89,89,89,89	0
55	MG	AA	3346	1/1	0.82	0.42	88,88,88,88	0
55	MG	CA	1730	1/1	0.83	0.28	107,107,107,107	0
55	MG	AD	301	1/1	0.83	0.29	99,99,99,99	0
55	MG	CA	1659	1/1	0.83	0.30	71,71,71,71	0
55	MG	BA	3172	1/1	0.83	0.31	85,85,85,85	0
55	MG	CA	1822	1/1	0.83	0.14	105,105,105,105	0
55	MG	BA	3455	1/1	0.83	0.17	92,92,92,92	0
55	MG	CA	1794	1/1	0.83	0.13	106,106,106,106	0
55	MG	DA	1709	1/1	0.83	0.28	109,109,109,109	0
55	MG	AA	3048	1/1	0.83	0.31	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3502	1/1	0.83	0.19	91,91,91,91	0
55	MG	BA	3031	1/1	0.83	0.32	60,60,60,60	0
55	MG	AA	3289	1/1	0.83	0.55	84,84,84,84	0
55	MG	BA	3202	1/1	0.83	0.23	69,69,69,69	0
55	MG	AA	3444	1/1	0.83	0.33	58,58,58,58	0
55	MG	AA	3512	1/1	0.83	0.14	97,97,97,97	0
55	MG	AA	3559	1/1	0.83	0.33	83,83,83,83	0
55	MG	BA	3030	1/1	0.83	0.20	99,99,99,99	0
55	MG	DA	1730	1/1	0.83	0.42	102,102,102,102	0
55	MG	AA	3398	1/1	0.83	0.36	73,73,73,73	0
55	MG	DA	1772	1/1	0.83	0.32	68,68,68,68	0
55	MG	AA	3408	1/1	0.83	0.38	83,83,83,83	0
55	MG	AA	3411	1/1	0.83	0.50	85,85,85,85	0
55	MG	AA	3158	1/1	0.83	0.34	68,68,68,68	0
55	MG	BA	3118	1/1	0.83	0.26	110,110,110,110	0
55	MG	CA	1761	1/1	0.83	0.42	66,66,66,66	0
55	MG	DA	1776	1/1	0.83	0.27	70,70,70,70	0
55	MG	CA	1750	1/1	0.83	0.51	104,104,104,104	0
55	MG	BA	3320	1/1	0.83	0.28	77,77,77,77	0
55	MG	AA	3561	1/1	0.83	0.24	82,82,82,82	0
55	MG	AA	3615	1/1	0.83	0.33	102,102,102,102	0
55	MG	AA	3238	1/1	0.83	0.52	82,82,82,82	0
55	MG	BA	3524	1/1	0.83	0.46	105,105,105,105	0
55	MG	AA	3336	1/1	0.83	0.25	82,82,82,82	0
55	MG	CA	1810	1/1	0.83	0.35	108,108,108,108	0
55	MG	CC	102	1/1	0.83	0.29	69,69,69,69	0
55	MG	CA	1826	1/1	0.83	0.28	81,81,81,81	0
55	MG	AA	3198	1/1	0.83	0.65	74,74,74,74	0
55	MG	DA	1773	1/1	0.83	0.47	69,69,69,69	0
55	MG	AA	3507	1/1	0.83	0.48	99,99,99,99	0
55	MG	BA	3366	1/1	0.83	0.25	76,76,76,76	0
55	MG	AA	3331	1/1	0.83	0.46	76,76,76,76	0
55	MG	BA	3434	1/1	0.83	0.16	90,90,90,90	0
55	MG	DA	1601	1/1	0.83	0.16	107,107,107,107	0
55	MG	BA	3479	1/1	0.83	0.35	95,95,95,95	0
55	MG	CA	1755	1/1	0.84	0.26	81,81,81,81	0
55	MG	BA	3386	1/1	0.84	0.23	81,81,81,81	0
55	MG	CA	1814	1/1	0.84	0.28	86,86,86,86	0
55	MG	DA	1671	1/1	0.84	0.40	77,77,77,77	0
55	MG	DA	1603	1/1	0.84	0.44	89,89,89,89	0
55	MG	AA	3613	1/1	0.84	0.31	76,76,76,76	0
55	MG	AA	3625	1/1	0.84	0.28	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	BA	3079	1/1	0.84	0.18	82,82,82,82	0
55	MG	CA	1829	1/1	0.84	0.22	102,102,102,102	0
55	MG	AA	3313	1/1	0.84	0.45	70,70,70,70	0
55	MG	BA	3343	1/1	0.84	0.24	75,75,75,75	0
55	MG	BA	3247	1/1	0.84	0.33	74,74,74,74	0
55	MG	AO	203	1/1	0.84	0.34	43,43,43,43	0
55	MG	DA	1621	1/1	0.84	0.46	99,99,99,99	0
55	MG	CA	1698	1/1	0.84	0.26	89,89,89,89	0
55	MG	CT	201	1/1	0.84	0.32	102,102,102,102	0
55	MG	AA	3618	1/1	0.84	0.54	97,97,97,97	0
55	MG	AA	3448	1/1	0.84	0.38	106,106,106,106	0
55	MG	AA	3317	1/1	0.84	0.41	85,85,85,85	0
55	MG	CA	1812	1/1	0.84	0.20	84,84,84,84	0
55	MG	BA	3020	1/1	0.84	0.26	76,76,76,76	0
55	MG	CA	1703	1/1	0.84	0.16	103,103,103,103	0
55	MG	BA	3330	1/1	0.84	0.39	91,91,91,91	0
55	MG	AA	3131	1/1	0.84	0.20	90,90,90,90	0
55	MG	BA	3212	1/1	0.84	0.49	70,70,70,70	0
55	MG	BA	3438	1/1	0.84	0.23	88,88,88,88	0
55	MG	AA	3588	1/1	0.84	0.47	68,68,68,68	0
55	MG	AA	3465	1/1	0.84	0.32	71,71,71,71	0
55	MG	AA	3412	1/1	0.84	0.36	110,110,110,110	0
55	MG	DG	301	1/1	0.84	0.34	94,94,94,94	0
55	MG	CA	1655	1/1	0.84	0.52	95,95,95,95	0
55	MG	BA	3162	1/1	0.84	0.15	92,92,92,92	0
55	MG	AA	3272	1/1	0.84	0.37	65,65,65,65	0
55	MG	CA	1626	1/1	0.84	0.33	88,88,88,88	0
55	MG	CA	1731	1/1	0.84	0.35	98,98,98,98	0
55	MG	BA	3335	1/1	0.84	0.13	100,100,100,100	0
55	MG	AA	3605	1/1	0.84	0.58	72,72,72,72	0
55	MG	AA	3470	1/1	0.84	0.52	96,96,96,96	0
55	MG	BA	3506	1/1	0.85	0.20	74,74,74,74	0
55	MG	DA	1775	1/1	0.85	0.41	102,102,102,102	0
55	MG	AA	3223	1/1	0.85	0.30	71,71,71,71	0
55	MG	BA	3473	1/1	0.85	0.25	78,78,78,78	0
55	MG	DA	1677	1/1	0.85	0.24	82,82,82,82	0
55	MG	BA	3359	1/1	0.85	0.46	98,98,98,98	0
55	MG	AA	3329	1/1	0.85	0.16	94,94,94,94	0
55	MG	BA	3443	1/1	0.85	0.23	92,92,92,92	0
55	MG	BA	3106	1/1	0.85	0.06	85,85,85,85	0
55	MG	BA	3110	1/1	0.85	0.37	92,92,92,92	0
55	MG	CA	1747	1/1	0.85	0.43	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	BB	201	1/1	0.85	0.24	90,90,90,90	0
55	MG	DA	1781	1/1	0.85	0.13	87,87,87,87	0
55	MG	BA	3084	1/1	0.85	0.15	99,99,99,99	0
55	MG	AA	3495	1/1	0.85	0.60	90,90,90,90	0
55	MG	AA	3189	1/1	0.85	0.38	90,90,90,90	0
55	MG	BA	3085	1/1	0.85	0.34	74,74,74,74	0
55	MG	CA	1784	1/1	0.85	0.46	101,101,101,101	0
55	MG	BA	3369	1/1	0.85	0.35	69,69,69,69	0
55	MG	BA	3075	1/1	0.85	0.17	99,99,99,99	0
55	MG	DA	1640	1/1	0.85	0.17	101,101,101,101	0
55	MG	AA	3496	1/1	0.85	0.49	87,87,87,87	0
55	MG	BA	3510	1/1	0.85	0.26	67,67,67,67	0
55	MG	BA	3333	1/1	0.85	0.27	73,73,73,73	0
55	MG	AA	3587	1/1	0.85	0.55	77,77,77,77	0
55	MG	CA	1688	1/1	0.85	0.23	77,77,77,77	0
55	MG	CA	1707	1/1	0.85	0.38	78,78,78,78	0
55	MG	BA	3338	1/1	0.85	0.38	71,71,71,71	0
55	MG	AA	3274	1/1	0.85	0.42	72,72,72,72	0
55	MG	AA	3263	1/1	0.85	0.28	51,51,51,51	0
55	MG	AA	3303	1/1	0.85	0.39	95,95,95,95	0
55	MG	AA	3386	1/1	0.85	0.17	74,74,74,74	0
55	MG	AA	3404	1/1	0.85	0.29	95,95,95,95	0
55	MG	CB	103	1/1	0.85	0.21	110,110,110,110	0
55	MG	AA	3296	1/1	0.85	0.53	72,72,72,72	0
55	MG	BA	3528	1/1	0.85	0.20	98,98,98,98	0
55	MG	AA	3622	1/1	0.85	0.53	65,65,65,65	0
55	MG	DA	1700	1/1	0.85	0.41	94,94,94,94	0
55	MG	DC	106	1/1	0.85	0.15	111,111,111,111	0
55	MG	AA	3599	1/1	0.85	0.32	87,87,87,87	0
55	MG	AA	3424	1/1	0.85	0.48	54,54,54,54	0
55	MG	DA	1762	1/1	0.85	0.21	109,109,109,109	0
55	MG	BA	3086	1/1	0.86	0.38	82,82,82,82	0
55	MG	AA	3562	1/1	0.86	0.30	82,82,82,82	0
55	MG	AA	3602	1/1	0.86	0.19	59,59,59,59	0
55	MG	BA	3308	1/1	0.86	0.22	108,108,108,108	0
55	MG	DA	1662	1/1	0.86	0.45	78,78,78,78	0
55	MG	BA	3322	1/1	0.86	0.22	79,79,79,79	0
55	MG	AA	3194	1/1	0.86	0.49	102,102,102,102	0
55	MG	DA	1628	1/1	0.86	0.42	97,97,97,97	0
55	MG	CA	1793	1/1	0.86	0.15	96,96,96,96	0
55	MG	DA	1695	1/1	0.86	0.43	88,88,88,88	0
55	MG	AA	3338	1/1	0.86	0.47	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3488	1/1	0.86	0.25	93,93,93,93	0
55	MG	B3	101	1/1	0.86	0.21	76,76,76,76	0
55	MG	CA	1791	1/1	0.86	0.17	97,97,97,97	0
55	MG	AA	3360	1/1	0.86	0.36	63,63,63,63	0
55	MG	BA	3269	1/1	0.86	0.30	58,58,58,58	0
55	MG	BA	3259	1/1	0.86	0.35	54,54,54,54	0
55	MG	BA	3396	1/1	0.86	0.35	91,91,91,91	0
55	MG	DA	1685	1/1	0.86	0.43	72,72,72,72	0
55	MG	DA	1693	1/1	0.86	0.40	93,93,93,93	0
55	MG	AA	3547	1/1	0.86	0.20	45,45,45,45	0
55	MG	BA	3354	1/1	0.86	0.30	90,90,90,90	0
55	MG	DA	1756	1/1	0.86	0.46	106,106,106,106	0
55	MG	BA	3360	1/1	0.86	0.32	83,83,83,83	0
55	MG	AA	3344	1/1	0.86	0.46	68,68,68,68	0
55	MG	DA	1739	1/1	0.86	0.15	113,113,113,113	0
55	MG	BA	3281	1/1	0.86	0.32	92,92,92,92	0
55	MG	AA	3183	1/1	0.86	0.32	93,93,93,93	0
55	MG	BA	3205	1/1	0.86	0.24	70,70,70,70	0
55	MG	BA	3347	1/1	0.86	0.23	85,85,85,85	0
55	MG	BA	3061	1/1	0.86	0.13	69,69,69,69	0
55	MG	BA	3439	1/1	0.86	0.23	103,103,103,103	0
55	MG	DA	1707	1/1	0.86	0.25	95,95,95,95	0
55	MG	AB	206	1/1	0.86	0.48	93,93,93,93	0
55	MG	DA	1753	1/1	0.86	0.51	87,87,87,87	0
55	MG	BA	3373	1/1	0.86	0.39	88,88,88,88	0
55	MG	AA	3348	1/1	0.86	0.25	94,94,94,94	0
55	MG	DA	1797	1/1	0.86	0.35	85,85,85,85	0
55	MG	CA	1717	1/1	0.86	0.22	69,69,69,69	0
55	MG	BA	3525	1/1	0.86	0.36	98,98,98,98	0
55	MG	BA	3302	1/1	0.86	0.36	75,75,75,75	0
55	MG	CA	1824	1/1	0.86	0.14	94,94,94,94	0
55	MG	AA	3252	1/1	0.86	0.49	94,94,94,94	0
55	MG	AA	3254	1/1	0.86	0.63	85,85,85,85	0
55	MG	BB	204	1/1	0.86	0.32	90,90,90,90	0
55	MG	AA	3305	1/1	0.86	0.36	80,80,80,80	0
55	MG	BA	3201	1/1	0.86	0.22	94,94,94,94	0
55	MG	AA	3079	1/1	0.87	0.23	92,92,92,92	0
55	MG	BA	3115	1/1	0.87	0.28	79,79,79,79	0
55	MG	AA	3378	1/1	0.87	0.53	84,84,84,84	0
55	MG	BA	3351	1/1	0.87	0.47	81,81,81,81	0
55	MG	BA	3450	1/1	0.87	0.31	99,99,99,99	0
55	MG	AA	3619	1/1	0.87	0.50	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3580	1/1	0.87	0.30	78,78,78,78	0
55	MG	BA	3072	1/1	0.87	0.27	104,104,104,104	0
55	MG	AA	3190	1/1	0.87	0.24	58,58,58,58	0
55	MG	CN	201	1/1	0.87	0.09	78,78,78,78	0
55	MG	AA	3056	1/1	0.87	0.65	98,98,98,98	0
55	MG	AA	3271	1/1	0.87	0.36	92,92,92,92	0
55	MG	AA	3245	1/1	0.87	0.41	75,75,75,75	0
55	MG	DA	1630	1/1	0.87	0.26	102,102,102,102	0
55	MG	AA	3290	1/1	0.87	0.42	72,72,72,72	0
55	MG	CA	1695	1/1	0.87	0.36	90,90,90,90	0
55	MG	BA	3487	1/1	0.87	0.19	66,66,66,66	0
55	MG	AA	3552	1/1	0.87	0.35	83,83,83,83	0
55	MG	A7	101	1/1	0.87	0.38	60,60,60,60	0
55	MG	BA	3381	1/1	0.87	0.36	80,80,80,80	0
55	MG	CA	1741	1/1	0.87	0.24	80,80,80,80	0
55	MG	CA	1756	1/1	0.87	0.13	113,113,113,113	0
55	MG	BA	3176	1/1	0.87	0.20	79,79,79,79	0
55	MG	BA	3364	1/1	0.87	0.22	76,76,76,76	0
55	MG	BA	3203	1/1	0.87	0.39	53,53,53,53	0
55	MG	BA	3025	1/1	0.87	0.13	80,80,80,80	0
55	MG	BA	3321	1/1	0.87	0.11	59,59,59,59	0
55	MG	AA	3449	1/1	0.87	0.26	63,63,63,63	0
55	MG	CA	1676	1/1	0.87	0.29	76,76,76,76	0
55	MG	BA	3342	1/1	0.87	0.17	80,80,80,80	0
55	MG	AA	3611	1/1	0.87	0.26	100,100,100,100	0
55	MG	BA	3414	1/1	0.87	0.18	92,92,92,92	0
55	MG	AA	3453	1/1	0.87	0.30	95,95,95,95	0
55	MG	AA	3063	1/1	0.87	0.30	85,85,85,85	0
55	MG	AA	3197	1/1	0.87	0.40	74,74,74,74	0
55	MG	BA	3358	1/1	0.87	0.51	85,85,85,85	0
55	MG	BA	3189	1/1	0.87	0.32	61,61,61,61	0
55	MG	BA	3310	1/1	0.87	0.24	74,74,74,74	0
55	MG	DC	101	1/1	0.87	0.12	95,95,95,95	0
55	MG	AB	213	1/1	0.87	0.54	73,73,73,73	0
55	MG	BA	3408	1/1	0.87	0.42	88,88,88,88	0
55	MG	CA	1712	1/1	0.87	0.28	92,92,92,92	0
55	MG	BA	3005	1/1	0.87	0.29	70,70,70,70	0
55	MG	AA	3221	1/1	0.87	0.41	47,47,47,47	0
55	MG	AA	3155	1/1	0.87	0.45	71,71,71,71	0
55	MG	CA	1733	1/1	0.87	0.18	107,107,107,107	0
55	MG	AA	3322	1/1	0.87	0.53	68,68,68,68	0
55	MG	BA	3252	1/1	0.87	0.31	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1669	1/1	0.87	0.46	68,68,68,68	0
55	MG	AA	3519	1/1	0.87	0.16	53,53,53,53	0
55	MG	BA	3522	1/1	0.87	0.43	84,84,84,84	0
55	MG	AA	3176	1/1	0.87	0.22	74,74,74,74	0
55	MG	AA	3483	1/1	0.88	0.16	87,87,87,87	0
55	MG	BB	203	1/1	0.88	0.29	76,76,76,76	0
55	MG	DA	1728	1/1	0.88	0.32	112,112,112,112	0
55	MG	CA	1675	1/1	0.88	0.24	97,97,97,97	0
55	MG	BA	3494	1/1	0.88	0.33	88,88,88,88	0
55	MG	BA	3223	1/1	0.88	0.27	64,64,64,64	0
55	MG	BA	3023	1/1	0.88	0.39	70,70,70,70	0
55	MG	AA	3091	1/1	0.88	0.43	78,78,78,78	0
55	MG	CA	1779	1/1	0.88	0.13	113,113,113,113	0
55	MG	BA	3249	1/1	0.88	0.21	40,40,40,40	0
55	MG	BA	3207	1/1	0.88	0.29	46,46,46,46	0
55	MG	AA	3572	1/1	0.88	0.49	54,54,54,54	0
55	MG	DA	1799	1/1	0.88	0.37	68,68,68,68	0
55	MG	BA	3234	1/1	0.88	0.30	67,67,67,67	0
55	MG	AA	3529	1/1	0.88	0.28	68,68,68,68	0
55	MG	AA	3521	1/1	0.88	0.45	75,75,75,75	0
55	MG	BA	3470	1/1	0.88	0.28	81,81,81,81	0
55	MG	BA	3316	1/1	0.88	0.26	67,67,67,67	0
55	MG	AA	3135	1/1	0.88	0.30	66,66,66,66	0
55	MG	BA	3150	1/1	0.88	0.40	96,96,96,96	0
55	MG	AA	3582	1/1	0.88	0.31	44,44,44,44	0
55	MG	CA	1818	1/1	0.88	0.25	89,89,89,89	0
55	MG	CA	1795	1/1	0.88	0.30	68,68,68,68	0
55	MG	DA	1783	1/1	0.88	0.33	86,86,86,86	0
55	MG	DB	102	1/1	0.88	0.11	107,107,107,107	0
55	MG	AA	3485	1/1	0.88	0.52	71,71,71,71	0
55	MG	CA	1625	1/1	0.88	0.18	71,71,71,71	0
55	MG	AA	3414	1/1	0.88	0.48	94,94,94,94	0
55	MG	BA	3508	1/1	0.88	0.34	73,73,73,73	0
55	MG	CA	1670	1/1	0.88	0.29	70,70,70,70	0
55	MG	AA	3342	1/1	0.88	0.49	70,70,70,70	0
55	MG	AA	3458	1/1	0.88	0.26	70,70,70,70	0
55	MG	AA	3405	1/1	0.88	0.72	90,90,90,90	0
55	MG	AA	3102	1/1	0.88	0.33	90,90,90,90	0
55	MG	AB	217	1/1	0.88	0.40	110,110,110,110	0
55	MG	DA	1727	1/1	0.88	0.36	86,86,86,86	0
55	MG	AA	3491	1/1	0.88	0.45	85,85,85,85	0
55	MG	AA	3297	1/1	0.88	0.38	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3323	1/1	0.88	0.55	74,74,74,74	0
55	MG	AA	3337	1/1	0.88	0.45	99,99,99,99	0
55	MG	BA	3504	1/1	0.88	0.15	117,117,117,117	0
55	MG	BA	3069	1/1	0.88	0.14	70,70,70,70	0
55	MG	BA	3096	1/1	0.88	0.19	89,89,89,89	0
55	MG	DA	1680	1/1	0.88	0.35	81,81,81,81	0
55	MG	BA	3309	1/1	0.88	0.30	80,80,80,80	0
55	MG	CA	1684	1/1	0.88	0.31	101,101,101,101	0
55	MG	AA	3388	1/1	0.88	0.51	85,85,85,85	0
55	MG	BA	3198	1/1	0.88	0.26	44,44,44,44	0
55	MG	DA	1716	1/1	0.88	0.42	105,105,105,105	0
55	MG	BA	3083	1/1	0.88	0.21	92,92,92,92	0
55	MG	BA	3306	1/1	0.89	0.25	86,86,86,86	0
55	MG	AA	3432	1/1	0.89	0.42	87,87,87,87	0
55	MG	AA	3505	1/1	0.89	0.57	85,85,85,85	0
55	MG	BA	3049	1/1	0.89	0.23	86,86,86,86	0
55	MG	BA	3419	1/1	0.89	0.13	99,99,99,99	0
55	MG	AA	3349	1/1	0.89	0.44	84,84,84,84	0
55	MG	AE	301	1/1	0.89	0.15	65,65,65,65	0
55	MG	AA	3553	1/1	0.89	0.35	87,87,87,87	0
55	MG	AA	3558	1/1	0.89	0.33	89,89,89,89	0
55	MG	CQ	101	1/1	0.89	0.18	102,102,102,102	0
55	MG	CA	1686	1/1	0.89	0.37	86,86,86,86	0
55	MG	CA	1802	1/1	0.89	0.23	77,77,77,77	0
55	MG	BA	3029	1/1	0.89	0.39	75,75,75,75	0
55	MG	DA	1699	1/1	0.89	0.40	68,68,68,68	0
55	MG	CA	1692	1/1	0.89	0.11	127,127,127,127	0
55	MG	CA	1721	1/1	0.89	0.28	89,89,89,89	0
55	MG	DA	1738	1/1	0.89	0.37	85,85,85,85	0
55	MG	AA	3009	1/1	0.89	0.33	63,63,63,63	0
55	MG	CA	1754	1/1	0.89	0.39	114,114,114,114	0
55	MG	DA	1651	1/1	0.89	0.27	72,72,72,72	0
55	MG	DA	1659	1/1	0.89	0.12	80,80,80,80	0
55	MG	DA	1750	1/1	0.89	0.19	84,84,84,84	0
55	MG	BA	3048	1/1	0.89	0.17	74,74,74,74	0
55	MG	BA	3291	1/1	0.89	0.26	67,67,67,67	0
55	MG	BA	3246	1/1	0.89	0.14	99,99,99,99	0
55	MG	AA	3170	1/1	0.89	0.17	41,41,41,41	0
55	MG	CA	1838	1/1	0.89	0.14	103,103,103,103	0
55	MG	AA	3200	1/1	0.89	0.35	71,71,71,71	0
55	MG	BA	3161	1/1	0.89	0.30	89,89,89,89	0
55	MG	BA	3340	1/1	0.89	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3122	1/1	0.89	0.20	84,84,84,84	0
55	MG	BA	3462	1/1	0.89	0.11	123,123,123,123	0
55	MG	AA	3315	1/1	0.89	0.48	70,70,70,70	0
55	MG	AA	3072	1/1	0.89	0.12	101,101,101,101	0
55	MG	AA	3585	1/1	0.89	0.61	91,91,91,91	0
55	MG	AA	3255	1/1	0.89	0.44	88,88,88,88	0
55	MG	AA	3134	1/1	0.89	0.36	79,79,79,79	0
55	MG	CA	1671	1/1	0.89	0.26	72,72,72,72	0
55	MG	AA	3351	1/1	0.89	0.37	82,82,82,82	0
55	MG	DA	1790	1/1	0.89	0.48	100,100,100,100	0
55	MG	AA	3609	1/1	0.89	0.28	62,62,62,62	0
55	MG	DA	1604	1/1	0.89	0.27	92,92,92,92	0
55	MG	AA	3065	1/1	0.89	0.42	88,88,88,88	0
55	MG	BA	3451	1/1	0.89	0.24	89,89,89,89	0
55	MG	BA	3523	1/1	0.89	0.43	84,84,84,84	0
55	MG	AA	3222	1/1	0.89	0.46	54,54,54,54	0
55	MG	BA	3103	1/1	0.89	0.19	82,82,82,82	0
55	MG	CA	1663	1/1	0.89	0.24	52,52,52,52	0
55	MG	AA	3234	1/1	0.89	0.38	82,82,82,82	0
55	MG	DA	1619	1/1	0.89	0.33	77,77,77,77	0
55	MG	AA	3211	1/1	0.89	0.32	58,58,58,58	0
55	MG	AA	3454	1/1	0.89	0.56	94,94,94,94	0
55	MG	BA	3233	1/1	0.89	0.36	74,74,74,74	0
55	MG	AA	3555	1/1	0.89	0.19	67,67,67,67	0
55	MG	AO	202	1/1	0.89	0.60	80,80,80,80	0
55	MG	AA	3089	1/1	0.89	0.54	64,64,64,64	0
55	MG	BA	3512	1/1	0.89	0.26	75,75,75,75	0
55	MG	AA	3196	1/1	0.89	0.21	61,61,61,61	0
55	MG	BA	3257	1/1	0.89	0.56	86,86,86,86	0
55	MG	AA	3298	1/1	0.89	0.59	73,73,73,73	0
55	MG	CA	1697	1/1	0.89	0.76	92,92,92,92	0
55	MG	CC	104	1/1	0.90	0.18	97,97,97,97	0
55	MG	DA	1694	1/1	0.90	0.60	84,84,84,84	0
55	MG	BA	3263	1/1	0.90	0.24	84,84,84,84	0
55	MG	AA	3481	1/1	0.90	0.15	112,112,112,112	0
55	MG	AA	3186	1/1	0.90	0.21	58,58,58,58	0
55	MG	AF	303	1/1	0.90	0.33	69,69,69,69	0
55	MG	BA	3042	1/1	0.90	0.16	86,86,86,86	0
55	MG	AA	3422	1/1	0.90	0.47	106,106,106,106	0
55	MG	AA	3208	1/1	0.90	0.23	44,44,44,44	0
55	MG	AA	3031	1/1	0.90	0.43	52,52,52,52	0
55	MG	AA	3596	1/1	0.90	0.49	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3349	1/1	0.90	0.28	93,93,93,93	0
55	MG	CA	1691	1/1	0.90	0.34	56,56,56,56	0
55	MG	AA	3526	1/1	0.90	0.42	90,90,90,90	0
55	MG	AA	3299	1/1	0.90	0.34	79,79,79,79	0
55	MG	BA	3213	1/1	0.90	0.26	75,75,75,75	0
55	MG	BA	3038	1/1	0.90	0.27	78,78,78,78	0
55	MG	CA	1839	1/1	0.90	0.21	68,68,68,68	0
55	MG	BA	3377	1/1	0.90	0.31	81,81,81,81	0
55	MG	DA	1726	1/1	0.90	0.50	79,79,79,79	0
55	MG	AA	3478	1/1	0.90	0.30	75,75,75,75	0
55	MG	DA	1751	1/1	0.90	0.35	124,124,124,124	0
55	MG	BB	205	1/1	0.90	0.21	86,86,86,86	0
55	MG	CA	1666	1/1	0.90	0.20	70,70,70,70	0
55	MG	BA	3267	1/1	0.90	0.23	62,62,62,62	0
55	MG	AA	3345	1/1	0.90	0.58	93,93,93,93	0
55	MG	BA	3431	1/1	0.90	0.25	84,84,84,84	0
55	MG	AA	3262	1/1	0.90	0.29	33,33,33,33	0
55	MG	BA	3240	1/1	0.90	0.33	72,72,72,72	0
55	MG	AA	3508	1/1	0.90	0.37	101,101,101,101	0
55	MG	AA	3088	1/1	0.90	0.22	42,42,42,42	0
55	MG	DA	1697	1/1	0.90	0.17	111,111,111,111	0
55	MG	CA	1785	1/1	0.90	0.57	89,89,89,89	0
55	MG	AA	3548	1/1	0.90	0.30	54,54,54,54	0
55	MG	CA	1769	1/1	0.90	0.09	79,79,79,79	0
55	MG	BA	3516	1/1	0.90	0.14	73,73,73,73	0
55	MG	DA	1650	1/1	0.90	0.47	95,95,95,95	0
55	MG	DA	1761	1/1	0.90	0.40	84,84,84,84	0
55	MG	AA	3062	1/1	0.90	0.37	86,86,86,86	0
55	MG	DA	1782	1/1	0.90	0.36	94,94,94,94	0
55	MG	AA	3050	1/1	0.90	0.76	108,108,108,108	0
55	MG	BA	3458	1/1	0.90	0.24	71,71,71,71	0
55	MG	AA	3592	1/1	0.90	0.35	76,76,76,76	0
55	MG	CA	1665	1/1	0.90	0.53	74,74,74,74	0
55	MG	DA	1731	1/1	0.90	0.43	70,70,70,70	0
55	MG	CA	1830	1/1	0.90	0.33	94,94,94,94	0
55	MG	BA	3192	1/1	0.90	0.35	72,72,72,72	0
55	MG	AA	3140	1/1	0.90	0.38	67,67,67,67	0
55	MG	BA	3372	1/1	0.90	0.38	105,105,105,105	0
55	MG	DA	1741	1/1	0.90	0.37	93,93,93,93	0
55	MG	AA	3293	1/1	0.90	0.20	77,77,77,77	0
55	MG	AA	3218	1/1	0.90	0.40	73,73,73,73	0
55	MG	AA	3333	1/1	0.90	0.47	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3245	1/1	0.90	0.19	72,72,72,72	0
55	MG	DA	1734	1/1	0.90	0.31	88,88,88,88	0
55	MG	CA	1742	1/1	0.90	0.13	115,115,115,115	0
55	MG	AA	3487	1/1	0.90	0.08	77,77,77,77	0
55	MG	AA	3598	1/1	0.90	0.29	87,87,87,87	0
55	MG	AA	3105	1/1	0.90	0.42	61,61,61,61	0
55	MG	BA	3243	1/1	0.90	0.26	65,65,65,65	0
55	MG	BA	3503	1/1	0.90	0.13	69,69,69,69	0
55	MG	DA	1735	1/1	0.90	0.38	106,106,106,106	0
55	MG	AA	3543	1/1	0.90	0.45	46,46,46,46	0
55	MG	BA	3007	1/1	0.90	0.07	83,83,83,83	0
55	MG	AA	3586	1/1	0.90	0.14	53,53,53,53	0
55	MG	BE	301	1/1	0.90	0.26	54,54,54,54	0
55	MG	BA	3509	1/1	0.90	0.34	73,73,73,73	0
55	MG	AA	3623	1/1	0.91	0.29	74,74,74,74	0
55	MG	CC	103	1/1	0.91	0.38	104,104,104,104	0
55	MG	AA	3506	1/1	0.91	0.20	80,80,80,80	0
55	MG	CA	1624	1/1	0.91	0.19	97,97,97,97	0
55	MG	BA	3254	1/1	0.91	0.46	69,69,69,69	0
55	MG	DA	1792	1/1	0.91	0.22	81,81,81,81	0
55	MG	DA	1752	1/1	0.91	0.37	89,89,89,89	0
55	MG	AA	3355	1/1	0.91	0.36	94,94,94,94	0
55	MG	BA	3054	1/1	0.91	0.17	81,81,81,81	0
55	MG	AU	201	1/1	0.91	0.23	85,85,85,85	0
55	MG	CA	1705	1/1	0.91	0.16	95,95,95,95	0
55	MG	DA	1687	1/1	0.91	0.39	72,72,72,72	0
55	MG	AA	3311	1/1	0.91	0.57	68,68,68,68	0
55	MG	AA	3431	1/1	0.91	0.31	89,89,89,89	0
55	MG	AA	3379	1/1	0.91	0.30	66,66,66,66	0
55	MG	BA	3199	1/1	0.91	0.37	76,76,76,76	0
55	MG	AA	3380	1/1	0.91	0.20	96,96,96,96	0
55	MG	AB	201	1/1	0.91	0.67	96,96,96,96	0
55	MG	AA	3214	1/1	0.91	0.44	47,47,47,47	0
55	MG	AA	3545	1/1	0.91	0.36	75,75,75,75	0
55	MG	AA	3300	1/1	0.91	0.44	81,81,81,81	0
55	MG	DA	1736	1/1	0.91	0.48	65,65,65,65	0
55	MG	AO	201	1/1	0.91	0.43	65,65,65,65	0
55	MG	AA	3092	1/1	0.91	0.31	71,71,71,71	0
55	MG	AA	3165	1/1	0.91	0.45	82,82,82,82	0
55	MG	DA	1605	1/1	0.91	0.43	82,82,82,82	0
55	MG	AA	3069	1/1	0.91	0.28	64,64,64,64	0
55	MG	AB	205	1/1	0.91	0.38	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	DA	1645	1/1	0.91	0.34	51,51,51,51	0
55	MG	AA	3191	1/1	0.91	0.17	95,95,95,95	0
55	MG	AA	3071	1/1	0.91	0.48	56,56,56,56	0
55	MG	DB	101	1/1	0.91	0.21	103,103,103,103	0
55	MG	AA	3145	1/1	0.91	0.63	91,91,91,91	0
55	MG	AA	3210	1/1	0.91	0.43	72,72,72,72	0
55	MG	AA	3399	1/1	0.91	0.30	60,60,60,60	0
55	MG	AA	3447	1/1	0.91	0.59	75,75,75,75	0
55	MG	AA	3103	1/1	0.91	0.39	97,97,97,97	0
55	MG	BA	3036	1/1	0.91	0.44	85,85,85,85	0
55	MG	BA	3177	1/1	0.91	0.27	75,75,75,75	0
55	MG	AA	3540	1/1	0.91	0.41	63,63,63,63	0
55	MG	BA	3190	1/1	0.91	0.23	73,73,73,73	0
55	MG	AA	3533	1/1	0.91	0.20	67,67,67,67	0
55	MG	AA	3474	1/1	0.91	0.34	65,65,65,65	0
55	MG	AA	3043	1/1	0.91	0.37	108,108,108,108	0
55	MG	AA	3240	1/1	0.91	0.32	80,80,80,80	0
55	MG	CA	1608	1/1	0.91	0.22	68,68,68,68	0
55	MG	AA	3287	1/1	0.91	0.28	69,69,69,69	0
55	MG	CA	1837	1/1	0.91	0.25	88,88,88,88	0
55	MG	DA	1681	1/1	0.91	0.22	106,106,106,106	0
55	MG	BA	3196	1/1	0.91	0.32	84,84,84,84	0
55	MG	BA	3187	1/1	0.91	0.37	65,65,65,65	0
55	MG	BA	3066	1/1	0.91	0.21	86,86,86,86	0
55	MG	AA	3188	1/1	0.91	0.51	57,57,57,57	0
55	MG	DA	1634	1/1	0.91	0.24	77,77,77,77	0
55	MG	AA	3406	1/1	0.91	0.41	83,83,83,83	0
55	MG	AA	3100	1/1	0.91	0.52	67,67,67,67	0
55	MG	BA	3388	1/1	0.91	0.32	87,87,87,87	0
55	MG	AA	3212	1/1	0.92	0.34	52,52,52,52	0
55	MG	AA	3081	1/1	0.92	0.56	51,51,51,51	0
55	MG	BA	3155	1/1	0.92	0.30	87,87,87,87	0
55	MG	AA	3164	1/1	0.92	0.25	95,95,95,95	0
55	MG	AA	3199	1/1	0.92	0.48	46,46,46,46	0
55	MG	CA	1751	1/1	0.92	0.23	78,78,78,78	0
55	MG	A5	101	1/1	0.92	0.21	51,51,51,51	0
55	MG	AA	3219	1/1	0.92	0.41	81,81,81,81	0
55	MG	AA	3146	1/1	0.92	0.41	65,65,65,65	0
55	MG	DA	1780	1/1	0.92	0.45	107,107,107,107	0
55	MG	BA	3307	1/1	0.92	0.35	106,106,106,106	0
55	MG	AA	3195	1/1	0.92	0.21	62,62,62,62	0
55	MG	AA	3216	1/1	0.92	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3383	1/1	0.92	0.29	85,85,85,85	0
55	MG	BA	3087	1/1	0.92	0.41	80,80,80,80	0
55	MG	DA	1732	1/1	0.92	0.39	94,94,94,94	0
55	MG	AA	3117	1/1	0.92	0.31	54,54,54,54	0
55	MG	DA	1668	1/1	0.92	0.16	73,73,73,73	0
55	MG	AA	3504	1/1	0.92	0.41	80,80,80,80	0
55	MG	BA	3015	1/1	0.92	0.20	71,71,71,71	0
55	MG	BA	3480	1/1	0.92	0.23	56,56,56,56	0
55	MG	AA	3326	1/1	0.92	0.31	64,64,64,64	0
55	MG	AA	3603	1/1	0.92	0.43	41,41,41,41	0
55	MG	BA	3271	1/1	0.92	0.32	84,84,84,84	0
55	MG	DA	1679	1/1	0.92	0.33	64,64,64,64	0
55	MG	BA	3142	1/1	0.92	0.23	70,70,70,70	0
55	MG	AA	3014	1/1	0.92	0.29	38,38,38,38	0
55	MG	BA	3228	1/1	0.92	0.35	74,74,74,74	0
55	MG	DA	1755	1/1	0.92	0.47	79,79,79,79	0
55	MG	CA	1614	1/1	0.92	0.32	101,101,101,101	0
55	MG	BA	3496	1/1	0.92	0.35	96,96,96,96	0
55	MG	DA	1666	1/1	0.92	0.35	115,115,115,115	0
55	MG	AA	3129	1/1	0.92	0.45	73,73,73,73	0
55	MG	CA	1636	1/1	0.92	0.29	91,91,91,91	0
55	MG	AA	3136	1/1	0.92	0.14	61,61,61,61	0
55	MG	BA	3518	1/1	0.92	0.42	74,74,74,74	0
55	MG	DA	1667	1/1	0.92	0.27	82,82,82,82	0
55	MG	BA	3452	1/1	0.92	0.14	96,96,96,96	0
55	MG	DA	1733	1/1	0.92	0.35	98,98,98,98	0
55	MG	BA	3180	1/1	0.92	0.29	57,57,57,57	0
55	MG	BA	3147	1/1	0.92	0.23	63,63,63,63	0
55	MG	BA	3440	1/1	0.92	0.23	80,80,80,80	0
55	MG	AA	3187	1/1	0.92	0.46	87,87,87,87	0
55	MG	CA	1713	1/1	0.92	0.29	83,83,83,83	0
55	MG	BP	201	1/1	0.92	0.18	65,65,65,65	0
55	MG	DA	1786	1/1	0.92	0.38	86,86,86,86	0
55	MG	DA	1616	1/1	0.92	0.35	100,100,100,100	0
55	MG	DA	1737	1/1	0.92	0.35	74,74,74,74	0
55	MG	CA	1674	1/1	0.92	0.33	102,102,102,102	0
55	MG	DA	1665	1/1	0.92	0.37	82,82,82,82	0
55	MG	BA	3013	1/1	0.92	0.26	74,74,74,74	0
55	MG	BA	3128	1/1	0.92	0.23	56,56,56,56	0
55	MG	AA	3128	1/1	0.92	0.38	56,56,56,56	0
55	MG	BA	3102	1/1	0.92	0.11	86,86,86,86	0
55	MG	BA	3315	1/1	0.92	0.17	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	3138	1/1	0.92	0.41	45,45,45,45	0
55	MG	BB	202	1/1	0.92	0.14	103,103,103,103	0
55	MG	AA	3269	1/1	0.92	0.50	55,55,55,55	0
55	MG	BA	3284	1/1	0.93	0.12	61,61,61,61	0
55	MG	CA	1638	1/1	0.93	0.42	108,108,108,108	0
55	MG	CA	1780	1/1	0.93	0.34	55,55,55,55	0
55	MG	CA	1669	1/1	0.93	0.23	70,70,70,70	0
55	MG	BA	3082	1/1	0.93	0.37	76,76,76,76	0
55	MG	AA	3387	1/1	0.93	0.64	80,80,80,80	0
55	MG	AA	3246	1/1	0.93	0.52	73,73,73,73	0
55	MG	AA	3314	1/1	0.93	0.52	80,80,80,80	0
55	MG	AA	3535	1/1	0.93	0.16	103,103,103,103	0
55	MG	AA	3180	1/1	0.93	0.52	64,64,64,64	0
55	MG	DA	1691	1/1	0.93	0.48	82,82,82,82	0
55	MG	BA	3130	1/1	0.93	0.24	44,44,44,44	0
55	MG	BA	3144	1/1	0.93	0.50	95,95,95,95	0
55	MG	AA	3228	1/1	0.93	0.46	79,79,79,79	0
55	MG	AA	3162	1/1	0.93	0.30	45,45,45,45	0
55	MG	DA	1620	1/1	0.93	0.30	85,85,85,85	0
55	MG	BA	3279	1/1	0.93	0.34	73,73,73,73	0
55	MG	BA	3178	1/1	0.93	0.27	62,62,62,62	0
55	MG	CA	1789	1/1	0.93	0.07	71,71,71,71	0
55	MG	AA	3149	1/1	0.93	0.37	57,57,57,57	0
55	MG	CA	1772	1/1	0.93	0.21	83,83,83,83	0
55	MG	DA	1692	1/1	0.93	0.40	81,81,81,81	0
55	MG	AA	3119	1/1	0.93	0.38	75,75,75,75	0
55	MG	AA	3147	1/1	0.93	0.54	89,89,89,89	0
55	MG	AA	3281	1/1	0.93	0.45	74,74,74,74	0
55	MG	DA	1632	1/1	0.93	0.17	84,84,84,84	0
55	MG	CA	1680	1/1	0.93	0.31	79,79,79,79	0
55	MG	DA	1744	1/1	0.93	0.40	57,57,57,57	0
55	MG	BA	3206	1/1	0.93	0.26	98,98,98,98	0
55	MG	A7	102	1/1	0.93	0.46	68,68,68,68	0
55	MG	CA	1643	1/1	0.93	0.39	91,91,91,91	0
55	MG	BA	3214	1/1	0.93	0.27	77,77,77,77	0
55	MG	CA	1696	1/1	0.93	0.39	90,90,90,90	0
55	MG	BA	3148	1/1	0.93	0.23	91,91,91,91	0
55	MG	CA	1648	1/1	0.93	0.40	79,79,79,79	0
55	MG	BA	3220	1/1	0.93	0.32	40,40,40,40	0
55	MG	AA	3417	1/1	0.93	0.28	67,67,67,67	0
55	MG	AA	3232	1/1	0.93	0.66	104,104,104,104	0
55	MG	CA	1811	1/1	0.93	0.33	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3330	1/1	0.93	0.34	60,60,60,60	0
55	MG	BA	3018	1/1	0.93	0.29	83,83,83,83	0
55	MG	AA	3459	1/1	0.93	0.28	81,81,81,81	0
55	MG	BA	3385	1/1	0.93	0.18	97,97,97,97	0
55	MG	BA	3146	1/1	0.93	0.24	86,86,86,86	0
55	MG	AA	3457	1/1	0.93	0.56	64,64,64,64	0
55	MG	B1	201	1/1	0.93	0.23	82,82,82,82	0
55	MG	DA	1701	1/1	0.93	0.52	80,80,80,80	0
55	MG	BA	3253	1/1	0.93	0.42	66,66,66,66	0
55	MG	BA	3250	1/1	0.93	0.24	58,58,58,58	0
55	MG	AA	3472	1/1	0.93	0.67	80,80,80,80	0
55	MG	AA	3045	1/1	0.93	0.49	54,54,54,54	0
55	MG	CA	1700	1/1	0.93	0.09	72,72,72,72	0
55	MG	CA	1740	1/1	0.93	0.38	72,72,72,72	0
55	MG	BA	3251	1/1	0.93	0.24	81,81,81,81	0
55	MG	CA	1732	1/1	0.93	0.33	69,69,69,69	0
55	MG	CA	1654	1/1	0.93	0.38	75,75,75,75	0
55	MG	AA	3059	1/1	0.93	0.42	80,80,80,80	0
55	MG	AA	3150	1/1	0.93	0.54	59,59,59,59	0
55	MG	AA	3248	1/1	0.93	0.51	74,74,74,74	0
55	MG	BA	3238	1/1	0.93	0.26	66,66,66,66	0
55	MG	BA	3183	1/1	0.93	0.19	80,80,80,80	0
55	MG	DA	1657	1/1	0.93	0.46	95,95,95,95	0
55	MG	AA	3544	1/1	0.93	0.37	63,63,63,63	0
55	MG	CA	1609	1/1	0.93	0.43	78,78,78,78	0
55	MG	AA	3530	1/1	0.93	0.39	79,79,79,79	0
55	MG	BA	3317	1/1	0.93	0.32	91,91,91,91	0
55	MG	AA	3229	1/1	0.93	0.20	89,89,89,89	0
55	MG	AA	3086	1/1	0.93	0.57	62,62,62,62	0
55	MG	AB	215	1/1	0.93	0.39	93,93,93,93	0
55	MG	CA	1820	1/1	0.93	0.43	88,88,88,88	0
55	MG	AA	3159	1/1	0.93	0.07	28,28,28,28	0
55	MG	CA	1807	1/1	0.93	0.38	64,64,64,64	0
55	MG	AA	3575	1/1	0.93	0.39	42,42,42,42	0
55	MG	AA	3239	1/1	0.94	0.45	60,60,60,60	0
55	MG	BA	3186	1/1	0.94	0.28	52,52,52,52	0
55	MG	AA	3157	1/1	0.94	0.45	39,39,39,39	0
55	MG	AA	3563	1/1	0.94	0.40	52,52,52,52	0
55	MG	AA	3032	1/1	0.94	0.32	65,65,65,65	0
55	MG	DA	1696	1/1	0.94	0.32	66,66,66,66	0
55	MG	AA	3403	1/1	0.94	0.28	91,91,91,91	0
55	MG	AA	3033	1/1	0.94	0.33	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3569	1/1	0.94	0.31	60,60,60,60	0
55	MG	AA	3282	1/1	0.94	0.39	78,78,78,78	0
55	MG	BA	3365	1/1	0.94	0.38	90,90,90,90	0
55	MG	AA	3167	1/1	0.94	0.38	50,50,50,50	0
55	MG	CA	1746	1/1	0.94	0.25	98,98,98,98	0
55	MG	CA	1622	1/1	0.94	0.15	86,86,86,86	0
55	MG	BA	3160	1/1	0.94	0.30	82,82,82,82	0
55	MG	DA	1715	1/1	0.94	0.31	92,92,92,92	0
55	MG	AA	3389	1/1	0.94	0.55	72,72,72,72	0
55	MG	BA	3173	1/1	0.94	0.39	50,50,50,50	0
55	MG	BA	3511	1/1	0.94	0.21	68,68,68,68	0
55	MG	BA	3501	1/1	0.94	0.16	88,88,88,88	0
55	MG	BA	3071	1/1	0.94	0.29	78,78,78,78	0
55	MG	BA	3437	1/1	0.94	0.35	73,73,73,73	0
55	MG	AA	3244	1/1	0.94	0.44	45,45,45,45	0
55	MG	BA	3456	1/1	0.94	0.23	88,88,88,88	0
55	MG	DA	1729	1/1	0.94	0.46	84,84,84,84	0
55	MG	CA	1678	1/1	0.94	0.29	69,69,69,69	0
55	MG	AA	3054	1/1	0.94	0.29	62,62,62,62	0
55	MG	BA	3224	1/1	0.94	0.26	51,51,51,51	0
55	MG	CA	1673	1/1	0.94	0.40	76,76,76,76	0
55	MG	CA	1781	1/1	0.94	0.38	62,62,62,62	0
55	MG	AA	3546	1/1	0.94	0.25	74,74,74,74	0
55	MG	AA	3181	1/1	0.94	0.39	66,66,66,66	0
55	MG	CA	1801	1/1	0.94	0.24	84,84,84,84	0
55	MG	AA	3152	1/1	0.94	0.54	58,58,58,58	0
55	MG	AA	3226	1/1	0.94	0.30	77,77,77,77	0
55	MG	CA	1744	1/1	0.94	0.46	57,57,57,57	0
55	MG	BA	3272	1/1	0.94	0.38	81,81,81,81	0
55	MG	AA	3013	1/1	0.94	0.34	44,44,44,44	0
55	MG	AA	3460	1/1	0.94	0.26	106,106,106,106	0
56	PAR	DA	1805	42/42	0.94	0.21	46,59,73,84	0
55	MG	BA	3417	1/1	0.94	0.14	88,88,88,88	0
55	MG	BA	3514	1/1	0.94	0.34	51,51,51,51	0
55	MG	CA	1631	1/1	0.94	0.21	74,74,74,74	0
55	MG	AA	3621	1/1	0.94	0.46	91,91,91,91	0
55	MG	AA	3076	1/1	0.94	0.38	82,82,82,82	0
55	MG	DA	1675	1/1	0.94	0.39	60,60,60,60	0
55	MG	AA	3051	1/1	0.94	0.33	71,71,71,71	0
55	MG	AA	3058	1/1	0.94	0.29	64,64,64,64	0
55	MG	CA	1651	1/1	0.94	0.38	75,75,75,75	0
55	MG	AA	3179	1/1	0.94	0.29	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	AA	3168	1/1	0.94	0.31	68,68,68,68	0
55	MG	CA	1602	1/1	0.94	0.17	74,74,74,74	0
55	MG	BA	3274	1/1	0.94	0.19	90,90,90,90	0
55	MG	AA	3114	1/1	0.94	0.50	56,56,56,56	0
55	MG	CA	1606	1/1	0.94	0.07	94,94,94,94	0
55	MG	AA	3570	1/1	0.94	0.39	41,41,41,41	0
55	MG	BA	3425	1/1	0.94	0.49	85,85,85,85	0
55	MG	AA	3047	1/1	0.94	0.26	60,60,60,60	0
55	MG	DA	1674	1/1	0.94	0.27	76,76,76,76	0
55	MG	BA	3143	1/1	0.94	0.21	63,63,63,63	0
55	MG	CA	1835	1/1	0.94	0.16	87,87,87,87	0
55	MG	BA	3022	1/1	0.94	0.23	75,75,75,75	0
55	MG	DA	1796	1/1	0.94	0.25	97,97,97,97	0
55	MG	BA	3418	1/1	0.94	0.17	73,73,73,73	0
55	MG	BA	3493	1/1	0.94	0.27	39,39,39,39	0
55	MG	BA	3194	1/1	0.94	0.38	70,70,70,70	0
55	MG	AA	3514	1/1	0.94	0.36	67,67,67,67	0
55	MG	CA	1699	1/1	0.94	0.11	63,63,63,63	0
55	MG	AA	3401	1/1	0.94	0.49	93,93,93,93	0
55	MG	BA	3491	1/1	0.94	0.10	49,49,49,49	0
55	MG	BA	3184	1/1	0.94	0.14	76,76,76,76	0
55	MG	BA	3171	1/1	0.94	0.24	63,63,63,63	0
55	MG	CA	1632	1/1	0.94	0.21	76,76,76,76	0
55	MG	AB	207	1/1	0.94	0.20	103,103,103,103	0
55	MG	AA	3520	1/1	0.94	0.27	68,68,68,68	0
55	MG	CA	1792	1/1	0.94	0.31	81,81,81,81	0
55	MG	AA	3324	1/1	0.94	0.24	92,92,92,92	0
55	MG	AA	3617	1/1	0.94	0.46	92,92,92,92	0
55	MG	CA	1618	1/1	0.94	0.28	94,94,94,94	0
55	MG	BA	3276	1/1	0.94	0.14	88,88,88,88	0
55	MG	AA	3517	1/1	0.94	0.20	66,66,66,66	0
55	MG	AA	3584	1/1	0.94	0.15	63,63,63,63	0
55	MG	BA	3292	1/1	0.94	0.36	51,51,51,51	0
55	MG	AA	3087	1/1	0.94	0.45	76,76,76,76	0
55	MG	DA	1610	1/1	0.94	0.24	97,97,97,97	0
55	MG	AA	3321	1/1	0.94	0.33	65,65,65,65	0
55	MG	BA	3152	1/1	0.94	0.19	73,73,73,73	0
55	MG	AA	3144	1/1	0.95	0.47	45,45,45,45	0
55	MG	BE	303	1/1	0.95	0.23	57,57,57,57	0
55	MG	AA	3471	1/1	0.95	0.45	85,85,85,85	0
55	MG	BA	3328	1/1	0.95	0.14	61,61,61,61	0
55	MG	DC	103	1/1	0.95	0.33	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	1704	1/1	0.95	0.49	87,87,87,87	0
55	MG	BA	3139	1/1	0.95	0.19	58,58,58,58	0
55	MG	AA	3578	1/1	0.95	0.39	50,50,50,50	0
55	MG	BA	3300	1/1	0.95	0.38	56,56,56,56	0
55	MG	AA	3085	1/1	0.95	0.41	34,34,34,34	0
55	MG	CA	1786	1/1	0.95	0.08	74,74,74,74	0
55	MG	CA	1840	1/1	0.95	0.32	69,69,69,69	0
55	MG	AB	203	1/1	0.95	0.42	69,69,69,69	0
55	MG	CA	1682	1/1	0.95	0.16	106,106,106,106	0
55	MG	AA	3052	1/1	0.95	0.29	73,73,73,73	0
55	MG	DA	1622	1/1	0.95	0.13	98,98,98,98	0
55	MG	A1	201	1/1	0.95	0.37	64,64,64,64	0
55	MG	DA	1644	1/1	0.95	0.31	82,82,82,82	0
55	MG	BA	3028	1/1	0.95	0.50	85,85,85,85	0
55	MG	AA	3137	1/1	0.95	0.12	51,51,51,51	0
55	MG	AA	3285	1/1	0.95	0.52	80,80,80,80	0
56	PAR	CA	1841	42/42	0.95	0.30	40,56,74,83	0
55	MG	AA	3011	1/1	0.95	0.37	37,37,37,37	0
55	MG	CA	1645	1/1	0.95	0.42	60,60,60,60	0
55	MG	AA	3037	1/1	0.95	0.35	69,69,69,69	0
55	MG	CA	1749	1/1	0.95	0.32	62,62,62,62	0
55	MG	DA	1646	1/1	0.95	0.27	65,65,65,65	0
55	MG	BA	3126	1/1	0.95	0.21	51,51,51,51	0
55	MG	BA	3265	1/1	0.95	0.46	86,86,86,86	0
55	MG	DA	1658	1/1	0.95	0.21	113,113,113,113	0
55	MG	DA	1670	1/1	0.95	0.36	49,49,49,49	0
55	MG	AA	3550	1/1	0.95	0.52	39,39,39,39	0
55	MG	BA	3006	1/1	0.95	0.09	47,47,47,47	0
55	MG	BA	3400	1/1	0.95	0.28	74,74,74,74	0
55	MG	CA	1763	1/1	0.95	0.44	81,81,81,81	0
55	MG	AA	3288	1/1	0.95	0.62	90,90,90,90	0
55	MG	AA	3066	1/1	0.95	0.53	48,48,48,48	0
55	MG	BA	3483	1/1	0.95	0.32	34,34,34,34	0
55	MG	BA	3325	1/1	0.95	0.42	50,50,50,50	0
55	MG	BA	3136	1/1	0.95	0.23	43,43,43,43	0
55	MG	CA	1708	1/1	0.95	0.42	45,45,45,45	0
55	MG	AA	3339	1/1	0.95	0.35	85,85,85,85	0
55	MG	BA	3230	1/1	0.95	0.19	68,68,68,68	0
55	MG	CA	1610	1/1	0.95	0.32	54,54,54,54	0
55	MG	AA	3090	1/1	0.95	0.30	45,45,45,45	0
55	MG	AA	3002	1/1	0.95	0.43	41,41,41,41	0
55	MG	BA	3428	1/1	0.95	0.11	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	BA	3280	1/1	0.95	0.35	74,74,74,74	0
55	MG	AA	3036	1/1	0.95	0.21	39,39,39,39	0
55	MG	DA	1612	1/1	0.95	0.14	73,73,73,73	0
55	MG	BA	3242	1/1	0.95	0.35	62,62,62,62	0
55	MG	AA	3044	1/1	0.95	0.41	52,52,52,52	0
55	MG	AA	3041	1/1	0.95	0.33	66,66,66,66	0
55	MG	AA	3528	1/1	0.95	0.49	76,76,76,76	0
55	MG	BA	3319	1/1	0.95	0.43	68,68,68,68	0
55	MG	BA	3149	1/1	0.95	0.23	72,72,72,72	0
55	MG	AA	3551	1/1	0.95	0.31	69,69,69,69	0
55	MG	BA	3244	1/1	0.95	0.34	54,54,54,54	0
55	MG	AA	3257	1/1	0.95	0.42	79,79,79,79	0
55	MG	BA	3261	1/1	0.95	0.37	65,65,65,65	0
55	MG	AA	3581	1/1	0.95	0.12	36,36,36,36	0
55	MG	AA	3590	1/1	0.95	0.31	81,81,81,81	0
55	MG	BA	3060	1/1	0.95	0.17	51,51,51,51	0
55	MG	AA	3040	1/1	0.95	0.31	68,68,68,68	0
55	MG	DA	1690	1/1	0.95	0.41	92,92,92,92	0
55	MG	BA	3080	1/1	0.95	0.20	72,72,72,72	0
55	MG	AA	3106	1/1	0.95	0.35	69,69,69,69	0
55	MG	AA	3312	1/1	0.95	0.46	76,76,76,76	0
55	MG	AA	3477	1/1	0.95	0.60	86,86,86,86	0
55	MG	BB	211	1/1	0.95	0.31	71,71,71,71	0
55	MG	BA	3053	1/1	0.95	0.36	65,65,65,65	0
55	MG	A0	201	1/1	0.95	0.21	62,62,62,62	0
55	MG	BA	3197	1/1	0.95	0.11	76,76,76,76	0
55	MG	BA	3314	1/1	0.95	0.29	71,71,71,71	0
55	MG	AA	3143	1/1	0.95	0.38	35,35,35,35	0
55	MG	BA	3157	1/1	0.95	0.42	93,93,93,93	0
55	MG	AA	3213	1/1	0.95	0.46	59,59,59,59	0
55	MG	BA	3486	1/1	0.95	0.24	30,30,30,30	0
55	MG	BA	3129	1/1	0.95	0.24	41,41,41,41	0
55	MG	CC	106	1/1	0.95	0.21	92,92,92,92	0
55	MG	BA	3181	1/1	0.95	0.15	49,49,49,49	0
55	MG	AA	3343	1/1	0.95	0.35	74,74,74,74	0
55	MG	AA	3243	1/1	0.95	0.39	51,51,51,51	0
55	MG	DA	1656	1/1	0.95	0.37	99,99,99,99	0
55	MG	AA	3591	1/1	0.95	0.18	74,74,74,74	0
55	MG	AA	3318	1/1	0.96	0.29	92,92,92,92	0
55	MG	CA	1650	1/1	0.96	0.40	73,73,73,73	0
55	MG	AA	3068	1/1	0.96	0.36	72,72,72,72	0
55	MG	BA	3283	1/1	0.96	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3577	1/1	0.96	0.19	52,52,52,52	0
55	MG	BA	3166	1/1	0.96	0.32	40,40,40,40	0
55	MG	BA	3484	1/1	0.96	0.25	65,65,65,65	0
55	MG	AA	3573	1/1	0.96	0.34	31,31,31,31	0
55	MG	BA	3182	1/1	0.96	0.17	47,47,47,47	0
55	MG	BA	3430	1/1	0.96	0.08	89,89,89,89	0
55	MG	CA	1627	1/1	0.96	0.25	65,65,65,65	0
55	MG	AA	3095	1/1	0.96	0.29	89,89,89,89	0
55	MG	AA	3142	1/1	0.96	0.22	71,71,71,71	0
55	MG	AA	3057	1/1	0.96	0.41	66,66,66,66	0
55	MG	AA	3209	1/1	0.96	0.37	81,81,81,81	0
55	MG	BA	3324	1/1	0.96	0.38	75,75,75,75	0
55	MG	DA	1706	1/1	0.96	0.61	90,90,90,90	0
55	MG	AA	3202	1/1	0.96	0.29	46,46,46,46	0
55	MG	AA	3484	1/1	0.96	0.21	44,44,44,44	0
55	MG	AA	3161	1/1	0.96	0.33	42,42,42,42	0
55	MG	AA	3034	1/1	0.96	0.40	52,52,52,52	0
55	MG	DA	1643	1/1	0.96	0.39	81,81,81,81	0
55	MG	AA	3166	1/1	0.96	0.38	53,53,53,53	0
55	MG	BA	3403	1/1	0.96	0.19	77,77,77,77	0
55	MG	DA	1742	1/1	0.96	0.26	82,82,82,82	0
55	MG	BA	3200	1/1	0.96	0.38	65,65,65,65	0
55	MG	BA	3097	1/1	0.96	0.25	60,60,60,60	0
55	MG	AA	3247	1/1	0.96	0.42	74,74,74,74	0
55	MG	AA	3534	1/1	0.96	0.43	49,49,49,49	0
55	MG	CA	1836	1/1	0.96	0.26	71,71,71,71	0
55	MG	CA	1601	1/1	0.96	0.19	56,56,56,56	0
55	MG	BA	3492	1/1	0.96	0.28	47,47,47,47	0
55	MG	BA	3352	1/1	0.96	0.42	102,102,102,102	0
55	MG	BA	3137	1/1	0.96	0.30	48,48,48,48	0
55	MG	AA	3175	1/1	0.96	0.20	45,45,45,45	0
55	MG	AA	3123	1/1	0.96	0.42	52,52,52,52	0
55	MG	AA	3124	1/1	0.96	0.51	47,47,47,47	0
55	MG	AA	3006	1/1	0.96	0.54	46,46,46,46	0
55	MG	BA	3123	1/1	0.96	0.13	77,77,77,77	0
55	MG	AA	3567	1/1	0.96	0.25	39,39,39,39	0
55	MG	CA	1702	1/1	0.96	0.09	71,71,71,71	0
55	MG	AA	3115	1/1	0.96	0.55	70,70,70,70	0
55	MG	AA	3010	1/1	0.96	0.39	47,47,47,47	0
55	MG	AA	3177	1/1	0.96	0.46	46,46,46,46	0
55	MG	AA	3001	1/1	0.96	0.45	44,44,44,44	0
55	MG	BA	3208	1/1	0.96	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3220	1/1	0.96	0.41	70,70,70,70	0
55	MG	BA	3159	1/1	0.96	0.23	83,83,83,83	0
55	MG	AA	3074	1/1	0.96	0.51	68,68,68,68	0
55	MG	DA	1721	1/1	0.96	0.36	71,71,71,71	0
55	MG	BA	3409	1/1	0.96	0.30	71,71,71,71	0
55	MG	AA	3606	1/1	0.96	0.53	61,61,61,61	0
55	MG	AA	3111	1/1	0.96	0.51	36,36,36,36	0
55	MG	DC	105	1/1	0.96	0.38	75,75,75,75	0
55	MG	AA	3267	1/1	0.96	0.36	62,62,62,62	0
55	MG	AA	3597	1/1	0.96	0.17	91,91,91,91	0
55	MG	BA	3229	1/1	0.96	0.32	50,50,50,50	0
55	MG	AA	3434	1/1	0.96	0.50	44,44,44,44	0
55	MG	AA	3005	1/1	0.96	0.30	25,25,25,25	0
55	MG	BA	3497	1/1	0.96	0.23	63,63,63,63	0
55	MG	AA	3266	1/1	0.96	0.47	49,49,49,49	0
55	MG	AA	3061	1/1	0.96	0.26	79,79,79,79	0
55	MG	AA	3015	1/1	0.96	0.40	44,44,44,44	0
55	MG	BA	3222	1/1	0.96	0.18	54,54,54,54	0
55	MG	BA	3219	1/1	0.96	0.25	48,48,48,48	0
55	MG	BA	3231	1/1	0.96	0.24	47,47,47,47	0
55	MG	DA	1676	1/1	0.96	0.43	82,82,82,82	0
55	MG	BA	3100	1/1	0.96	0.24	66,66,66,66	0
55	MG	AA	3600	1/1	0.96	0.45	74,74,74,74	0
55	MG	AA	3028	1/1	0.96	0.38	54,54,54,54	0
55	MG	B5	101	1/1	0.96	0.20	61,61,61,61	0
55	MG	BA	3275	1/1	0.96	0.38	52,52,52,52	0
55	MG	CA	1657	1/1	0.96	0.32	63,63,63,63	0
55	MG	BA	3217	1/1	0.96	0.30	39,39,39,39	0
55	MG	AA	3020	1/1	0.96	0.24	39,39,39,39	0
55	MG	BA	3288	1/1	0.96	0.22	98,98,98,98	0
55	MG	AA	3574	1/1	0.96	0.34	54,54,54,54	0
55	MG	AA	3151	1/1	0.96	0.45	58,58,58,58	0
55	MG	AA	3029	1/1	0.96	0.20	46,46,46,46	0
55	MG	BA	3141	1/1	0.96	0.23	72,72,72,72	0
55	MG	CA	1607	1/1	0.96	0.41	93,93,93,93	0
55	MG	BA	3158	1/1	0.96	0.21	70,70,70,70	0
55	MG	CA	1825	1/1	0.96	0.07	114,114,114,114	0
55	MG	BA	3052	1/1	0.96	0.29	58,58,58,58	0
55	MG	AA	3284	1/1	0.96	0.43	81,81,81,81	0
55	MG	BA	3014	1/1	0.96	0.26	72,72,72,72	0
55	MG	BA	3481	1/1	0.96	0.26	49,49,49,49	0
55	MG	BA	3001	1/1	0.96	0.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3236	1/1	0.96	0.43	41,41,41,41	0
55	MG	CA	1620	1/1	0.96	0.19	74,74,74,74	0
55	MG	AA	3368	1/1	0.96	0.48	90,90,90,90	0
55	MG	AA	3049	1/1	0.96	0.36	80,80,80,80	0
55	MG	DA	1672	1/1	0.96	0.32	63,63,63,63	0
55	MG	AA	3283	1/1	0.96	0.38	91,91,91,91	0
55	MG	AA	3571	1/1	0.96	0.19	52,52,52,52	0
55	MG	BA	3059	1/1	0.96	0.26	50,50,50,50	0
55	MG	BA	3154	1/1	0.96	0.14	46,46,46,46	0
55	MG	AA	3462	1/1	0.97	0.33	85,85,85,85	0
55	MG	AA	3127	1/1	0.97	0.37	53,53,53,53	0
55	MG	BA	3485	1/1	0.97	0.28	46,46,46,46	0
55	MG	BA	3012	1/1	0.97	0.32	63,63,63,63	0
55	MG	AA	3178	1/1	0.97	0.17	54,54,54,54	0
55	MG	CC	105	1/1	0.97	0.22	105,105,105,105	0
55	MG	AA	3614	1/1	0.97	0.55	78,78,78,78	0
55	MG	AA	3450	1/1	0.97	0.46	72,72,72,72	0
55	MG	AA	3153	1/1	0.97	0.26	48,48,48,48	0
55	MG	CA	1667	1/1	0.97	0.27	77,77,77,77	0
55	MG	BD	301	1/1	0.97	0.20	39,39,39,39	0
55	MG	DA	1653	1/1	0.97	0.24	96,96,96,96	0
55	MG	AA	3018	1/1	0.97	0.36	43,43,43,43	0
55	MG	BA	3002	1/1	0.97	0.22	66,66,66,66	0
55	MG	AA	3008	1/1	0.97	0.37	44,44,44,44	0
55	MG	AA	3476	1/1	0.97	0.63	79,79,79,79	0
55	MG	AA	3566	1/1	0.97	0.29	27,27,27,27	0
55	MG	AA	3025	1/1	0.97	0.39	40,40,40,40	0
55	MG	CA	1664	1/1	0.97	0.13	47,47,47,47	0
55	MG	BA	3140	1/1	0.97	0.26	42,42,42,42	0
55	MG	AA	3021	1/1	0.97	0.30	42,42,42,42	0
55	MG	AA	3101	1/1	0.97	0.32	79,79,79,79	0
55	MG	BA	3133	1/1	0.97	0.22	50,50,50,50	0
55	MG	AA	3230	1/1	0.97	0.10	34,34,34,34	0
55	MG	AA	3541	1/1	0.97	0.24	48,48,48,48	0
55	MG	BA	3016	1/1	0.97	0.07	56,56,56,56	0
55	MG	DA	1652	1/1	0.97	0.17	85,85,85,85	0
55	MG	BA	3515	1/1	0.97	0.21	59,59,59,59	0
55	MG	AA	3568	1/1	0.97	0.24	49,49,49,49	0
55	MG	BA	3517	1/1	0.97	0.21	61,61,61,61	0
55	MG	AA	3098	1/1	0.97	0.40	81,81,81,81	0
55	MG	BA	3167	1/1	0.97	0.29	59,59,59,59	0
55	MG	AE	302	1/1	0.97	0.41	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3489	1/1	0.97	0.40	68,68,68,68	0
55	MG	CA	1796	1/1	0.97	0.44	82,82,82,82	0
55	MG	BA	3255	1/1	0.97	0.37	52,52,52,52	0
55	MG	BA	3227	1/1	0.97	0.37	50,50,50,50	0
55	MG	CA	1604	1/1	0.97	0.34	77,77,77,77	0
55	MG	AA	3608	1/1	0.97	0.27	41,41,41,41	0
55	MG	BA	3017	1/1	0.97	0.34	50,50,50,50	0
55	MG	DA	1724	1/1	0.97	0.45	72,72,72,72	0
55	MG	AA	3083	1/1	0.97	0.39	34,34,34,34	0
55	MG	BA	3011	1/1	0.97	0.29	65,65,65,65	0
55	MG	CA	1658	1/1	0.97	0.43	50,50,50,50	0
55	MG	AA	3516	1/1	0.97	0.31	76,76,76,76	0
55	MG	AA	3084	1/1	0.97	0.26	43,43,43,43	0
55	MG	DA	1638	1/1	0.97	0.25	74,74,74,74	0
55	MG	DA	1648	1/1	0.97	0.10	69,69,69,69	0
55	MG	AA	3116	1/1	0.97	0.47	37,37,37,37	0
55	MG	AA	3233	1/1	0.97	0.30	55,55,55,55	0
55	MG	AA	3070	1/1	0.97	0.31	68,68,68,68	0
55	MG	BA	3295	1/1	0.97	0.17	58,58,58,58	0
55	MG	AA	3113	1/1	0.97	0.50	49,49,49,49	0
55	MG	BA	3062	1/1	0.97	0.26	110,110,110,110	0
55	MG	DA	1617	1/1	0.97	0.28	102,102,102,102	0
55	MG	AB	210	1/1	0.97	0.38	65,65,65,65	0
55	MG	AA	3204	1/1	0.97	0.31	44,44,44,44	0
55	MG	AA	3019	1/1	0.97	0.29	55,55,55,55	0
55	MG	DA	1705	1/1	0.97	0.35	97,97,97,97	0
55	MG	AA	3174	1/1	0.97	0.41	40,40,40,40	0
55	MG	DA	1673	1/1	0.97	0.12	88,88,88,88	0
55	MG	AA	3400	1/1	0.97	0.47	39,39,39,39	0
55	MG	BA	3135	1/1	0.97	0.33	52,52,52,52	0
55	MG	BA	3248	1/1	0.97	0.22	54,54,54,54	0
57	ZN	DQ	101	1/1	0.97	0.17	118,118,118,118	0
55	MG	AA	3352	1/1	0.97	0.35	52,52,52,52	0
55	MG	BA	3218	1/1	0.97	0.35	51,51,51,51	0
55	MG	AA	3205	1/1	0.97	0.35	55,55,55,55	0
55	MG	AA	3133	1/1	0.97	0.51	46,46,46,46	0
55	MG	AA	3192	1/1	0.97	0.35	63,63,63,63	0
55	MG	DC	102	1/1	0.97	0.16	74,74,74,74	0
55	MG	DA	1723	1/1	0.97	0.32	83,83,83,83	0
55	MG	AA	3607	1/1	0.97	0.36	44,44,44,44	0
55	MG	AA	3427	1/1	0.97	0.38	82,82,82,82	0
55	MG	BA	3490	1/1	0.97	0.25	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3179	1/1	0.97	0.34	61,61,61,61	0
55	MG	AA	3082	1/1	0.97	0.38	50,50,50,50	0
55	MG	AA	3306	1/1	0.97	0.40	65,65,65,65	0
55	MG	BA	3239	1/1	0.97	0.24	80,80,80,80	0
55	MG	CA	1777	1/1	0.97	0.35	92,92,92,92	0
55	MG	CA	1605	1/1	0.97	0.27	86,86,86,86	0
55	MG	AA	3046	1/1	0.98	0.14	57,57,57,57	0
55	MG	BA	3127	1/1	0.98	0.38	55,55,55,55	0
55	MG	DA	1654	1/1	0.98	0.41	92,92,92,92	0
55	MG	BA	3169	1/1	0.98	0.25	56,56,56,56	0
55	MG	CA	1619	1/1	0.98	0.26	59,59,59,59	0
55	MG	AA	3026	1/1	0.98	0.24	40,40,40,40	0
55	MG	BA	3412	1/1	0.98	0.41	50,50,50,50	0
55	MG	AA	3565	1/1	0.98	0.37	53,53,53,53	0
55	MG	AA	3112	1/1	0.98	0.59	45,45,45,45	0
55	MG	AA	3141	1/1	0.98	0.35	50,50,50,50	0
55	MG	BA	3264	1/1	0.98	0.25	59,59,59,59	0
55	MG	BA	3211	1/1	0.98	0.25	57,57,57,57	0
55	MG	BA	3221	1/1	0.98	0.25	37,37,37,37	0
55	MG	AA	3154	1/1	0.98	0.44	52,52,52,52	0
55	MG	BA	3285	1/1	0.98	0.19	45,45,45,45	0
55	MG	AA	3576	1/1	0.98	0.47	46,46,46,46	0
55	MG	BA	3168	1/1	0.98	0.21	60,60,60,60	0
55	MG	BA	3225	1/1	0.98	0.20	78,78,78,78	0
55	MG	AA	3130	1/1	0.98	0.22	67,67,67,67	0
55	MG	BA	3488	1/1	0.98	0.14	59,59,59,59	0
55	MG	AA	3539	1/1	0.98	0.30	49,49,49,49	0
55	MG	BA	3131	1/1	0.98	0.17	49,49,49,49	0
55	MG	AA	3022	1/1	0.98	0.27	49,49,49,49	0
55	MG	CA	1642	1/1	0.98	0.32	69,69,69,69	0
55	MG	AA	3023	1/1	0.98	0.55	56,56,56,56	0
55	MG	DA	1609	1/1	0.98	0.23	116,116,116,116	0
57	ZN	CG	303	1/1	0.98	0.34	95,95,95,95	0
55	MG	AA	3160	1/1	0.98	0.30	32,32,32,32	0
55	MG	BA	3009	1/1	0.98	0.25	48,48,48,48	0
55	MG	DA	1689	1/1	0.98	0.33	72,72,72,72	0
55	MG	AA	3024	1/1	0.98	0.39	45,45,45,45	0
55	MG	AA	3538	1/1	0.98	0.32	36,36,36,36	0
55	MG	BA	3156	1/1	0.98	0.40	87,87,87,87	0
55	MG	CA	1660	1/1	0.98	0.38	64,64,64,64	0
55	MG	BA	3237	1/1	0.98	0.21	47,47,47,47	0
55	MG	BA	3210	1/1	0.98	0.37	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3145	1/1	0.98	0.36	53,53,53,53	0
55	MG	AA	3549	1/1	0.98	0.54	50,50,50,50	0
55	MG	AA	3579	1/1	0.98	0.29	39,39,39,39	0
55	MG	BA	3138	1/1	0.98	0.30	52,52,52,52	0
55	MG	AA	3455	1/1	0.98	0.46	49,49,49,49	0
55	MG	CA	1603	1/1	0.98	0.20	73,73,73,73	0
55	MG	AA	3030	1/1	0.98	0.31	45,45,45,45	0
55	MG	AA	3139	1/1	0.98	0.29	54,54,54,54	0
55	MG	AA	3203	1/1	0.98	0.47	65,65,65,65	0
55	MG	BA	3482	1/1	0.98	0.19	65,65,65,65	0
55	MG	AA	3016	1/1	0.98	0.31	48,48,48,48	0
55	MG	BA	3010	1/1	0.98	0.24	68,68,68,68	0
55	MG	AA	3327	1/1	0.98	0.52	84,84,84,84	0
55	MG	BA	3286	1/1	0.98	0.24	85,85,85,85	0
55	MG	AA	3017	1/1	0.98	0.47	64,64,64,64	0
55	MG	AA	3436	1/1	0.98	0.46	66,66,66,66	0
55	MG	AA	3003	1/1	0.98	0.48	64,64,64,64	0
55	MG	BA	3134	1/1	0.98	0.28	63,63,63,63	0
55	MG	AA	3125	1/1	0.98	0.42	55,55,55,55	0
55	MG	BA	3241	1/1	0.98	0.36	52,52,52,52	0
55	MG	AA	3004	1/1	0.98	0.39	40,40,40,40	0
55	MG	CA	1634	1/1	0.99	0.32	60,60,60,60	0
55	MG	CA	1641	1/1	0.99	0.23	65,65,65,65	0
55	MG	AA	3007	1/1	0.99	0.28	42,42,42,42	0
55	MG	AA	3035	1/1	0.99	0.30	45,45,45,45	0
57	ZN	CQ	103	1/1	0.99	0.13	144,144,144,144	0
55	MG	BA	3232	1/1	0.99	0.27	55,55,55,55	0
55	MG	BA	3216	1/1	0.99	0.28	56,56,56,56	0
55	MG	AA	3027	1/1	0.99	0.36	45,45,45,45	0
55	MG	BA	3268	1/1	0.99	0.15	59,59,59,59	0
55	MG	AA	3012	1/1	0.99	0.38	40,40,40,40	0
55	MG	DA	1649	1/1	0.99	0.29	93,93,93,93	0
55	MG	DA	1647	1/1	0.99	0.18	71,71,71,71	0
57	ZN	DG	303	1/1	0.99	0.29	134,134,134,134	0
55	MG	BA	3215	1/1	0.99	0.32	66,66,66,66	0
55	MG	AA	3610	1/1	0.99	0.19	46,46,46,46	0
55	MG	AA	3110	1/1	0.99	0.16	40,40,40,40	0
55	MG	BA	3132	1/1	0.99	0.25	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.