



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 08:43 am BST

PDB ID : 4V5D
Title : Structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, paromomycin, acylated A- and P-site tRNAs, and E-site tRNA.
Authors : Voorhees, R.M.; Weixlbaumer, A.; Loakes, D.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-03-24
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

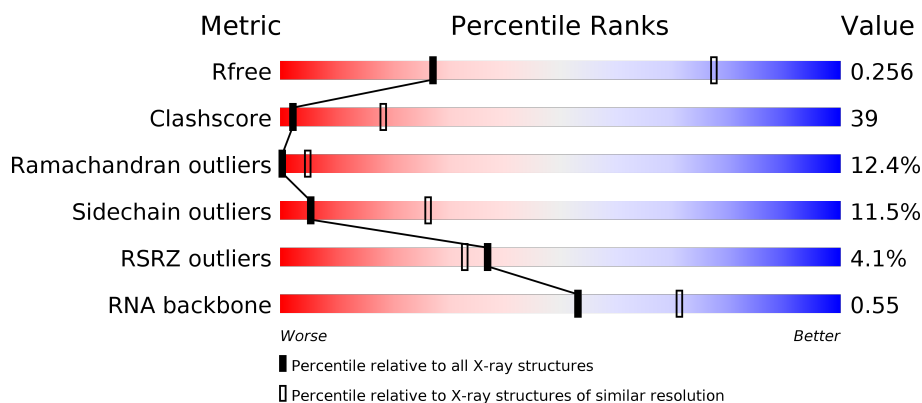
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>2%</div> <div>27%</div> <div>60%</div> <div>11%</div> <div>..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>26%</div> <div>61%</div> <div>11%</div> <div>..</div> </div>
2	AB	256	<div> <div>3%</div> <div>17%</div> <div>58%</div> <div>14%</div> <div>• 8%</div> </div>
2	CB	256	<div> <div>2%</div> <div>17%</div> <div>58%</div> <div>14%</div> <div>• 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AY	77	
22	CV	77	
22	CY	77	
23	AW	76	
23	CW	76	
24	AX	11	
24	CX	11	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2822	
35	DA	2822	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BN	140	
44	DN	140	
45	BO	122	
45	DO	122	
46	BP	150	
46	DP	150	
47	BQ	141	
47	DQ	141	
48	BR	118	
48	DR	118	
49	BS	112	
49	DS	112	
50	BT	146	
50	DT	146	
51	BU	118	
51	DU	118	

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Mol	Chain	Length	Quality of chain
52	BV	101	
52	DV	101	
53	BW	113	
53	DW	113	
54	BX	96	
54	DX	96	
55	BY	110	
55	DY	110	
56	BZ	206	
56	DZ	206	

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
57	MG	AA	1603	-	-	-	X
57	MG	AA	1616	-	-	-	X
57	MG	AA	1622	-	-	-	X
57	MG	AA	1625	-	-	-	X
57	MG	AA	1641	-	-	-	X
57	MG	AA	1646	-	-	-	X
57	MG	AA	1651	-	-	-	X
57	MG	AA	1653	-	-	-	X
57	MG	AA	1657	-	-	-	X
57	MG	AA	1661	-	-	-	X
57	MG	AA	1666	-	-	-	X
57	MG	AA	1667	-	-	-	X
57	MG	AA	1672	-	-	-	X
57	MG	AA	1673	-	-	-	X
57	MG	AA	1679	-	-	-	X
57	MG	AA	1681	-	-	-	X
57	MG	AA	1689	-	-	-	X
57	MG	AA	1700	-	-	-	X
57	MG	AA	1701	-	-	-	X
57	MG	AA	1702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1706	-	-	-	X
57	MG	AA	1715	-	-	-	X
57	MG	AA	1721	-	-	-	X
57	MG	AA	1727	-	-	-	X
57	MG	AA	1732	-	-	-	X
57	MG	AA	1733	-	-	-	X
57	MG	AA	1734	-	-	-	X
57	MG	AA	1737	-	-	-	X
57	MG	AA	1741	-	-	-	X
57	MG	AA	1743	-	-	-	X
57	MG	AA	1744	-	-	-	X
57	MG	AA	1751	-	-	-	X
57	MG	AA	1757	-	-	-	X
57	MG	AA	1761	-	-	-	X
57	MG	AA	1769	-	-	-	X
57	MG	AA	1795	-	-	-	X
57	MG	AA	1796	-	-	-	X
57	MG	AA	1798	-	-	-	X
57	MG	AD	301	-	-	-	X
57	MG	AG	201	-	-	-	X
57	MG	AV	103	-	-	-	X
57	MG	AV	104	-	-	-	X
57	MG	AW	105	-	-	-	X
57	MG	AW	107	-	-	-	X
57	MG	BA	3006	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3067	-	-	-	X
57	MG	BA	3101	-	-	-	X
57	MG	BA	3138	-	-	-	X
57	MG	BA	3151	-	-	-	X
57	MG	BA	3152	-	-	-	X
57	MG	BA	3155	-	-	-	X
57	MG	BA	3158	-	-	-	X
57	MG	BA	3160	-	-	-	X
57	MG	BA	3177	-	-	-	X
57	MG	BA	3179	-	-	-	X
57	MG	BA	3195	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3223	-	-	-	X
57	MG	BA	3225	-	-	-	X
57	MG	BA	3230	-	-	-	X
57	MG	BA	3235	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3237	-	-	-	X
57	MG	BA	3241	-	-	-	X
57	MG	BA	3267	-	-	-	X
57	MG	BA	3270	-	-	-	X
57	MG	BA	3295	-	-	-	X
57	MG	BA	3297	-	-	-	X
57	MG	BA	3324	-	-	-	X
57	MG	BA	3327	-	-	-	X
57	MG	BA	3331	-	-	-	X
57	MG	BA	3339	-	-	-	X
57	MG	BA	3340	-	-	-	X
57	MG	BA	3345	-	-	-	X
57	MG	BA	3349	-	-	-	X
57	MG	BA	3353	-	-	-	X
57	MG	BA	3371	-	-	-	X
57	MG	BA	3373	-	-	-	X
57	MG	BA	3376	-	-	-	X
57	MG	BA	3383	-	-	-	X
57	MG	BA	3399	-	-	-	X
57	MG	BA	3419	-	-	-	X
57	MG	BB	214	-	-	-	X
57	MG	BN	201	-	-	-	X
57	MG	BU	201	-	-	-	X
57	MG	CA	1602	-	-	-	X
57	MG	CA	1609	-	-	-	X
57	MG	CA	1613	-	-	-	X
57	MG	CA	1617	-	-	-	X
57	MG	CA	1622	-	-	-	X
57	MG	CA	1623	-	-	-	X
57	MG	CA	1625	-	-	-	X
57	MG	CA	1640	-	-	-	X
57	MG	CA	1644	-	-	-	X
57	MG	CA	1645	-	-	-	X
57	MG	CA	1647	-	-	-	X
57	MG	CA	1649	-	-	-	X
57	MG	CA	1652	-	-	-	X
57	MG	CA	1654	-	-	-	X
57	MG	CA	1655	-	-	-	X
57	MG	CA	1656	-	-	-	X
57	MG	CA	1666	-	-	-	X
57	MG	CA	1668	-	-	-	X
57	MG	CA	1673	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	CA	1674	-	-	-	X
57	MG	CA	1676	-	-	-	X
57	MG	CA	1678	-	-	-	X
57	MG	CA	1680	-	-	-	X
57	MG	CA	1682	-	-	-	X
57	MG	CA	1683	-	-	-	X
57	MG	CA	1688	-	-	-	X
57	MG	CA	1690	-	-	-	X
57	MG	CA	1701	-	-	-	X
57	MG	CA	1706	-	-	-	X
57	MG	CA	1716	-	-	-	X
57	MG	CA	1721	-	-	-	X
57	MG	CA	1726	-	-	-	X
57	MG	CA	1727	-	-	-	X
57	MG	CA	1728	-	-	-	X
57	MG	CA	1735	-	-	-	X
57	MG	CA	1739	-	-	-	X
57	MG	CA	1745	-	-	-	X
57	MG	CA	1746	-	-	-	X
57	MG	CA	1754	-	-	-	X
57	MG	CA	1759	-	-	-	X
57	MG	CA	1761	-	-	-	X
57	MG	CA	1771	-	-	-	X
57	MG	CA	1780	-	-	-	X
57	MG	CA	1795	-	-	-	X
57	MG	CL	201	-	-	-	X
57	MG	D7	101	-	-	-	X
57	MG	D7	102	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3006	-	-	-	X
57	MG	DA	3032	-	-	-	X
57	MG	DA	3049	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3090	-	-	-	X
57	MG	DA	3106	-	-	-	X
57	MG	DA	3108	-	-	-	X
57	MG	DA	3111	-	-	-	X
57	MG	DA	3122	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3136	-	-	-	X
57	MG	DA	3139	-	-	-	X
57	MG	DA	3152	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3153	-	-	-	X
57	MG	DA	3157	-	-	-	X
57	MG	DA	3160	-	-	-	X
57	MG	DA	3166	-	-	-	X
57	MG	DA	3170	-	-	-	X
57	MG	DA	3188	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3197	-	-	-	X
57	MG	DA	3202	-	-	-	X
57	MG	DA	3210	-	-	-	X
57	MG	DA	3222	-	-	-	X
57	MG	DA	3227	-	-	-	X
57	MG	DA	3229	-	-	-	X
57	MG	DA	3239	-	-	-	X
57	MG	DA	3243	-	-	-	X
57	MG	DA	3246	-	-	-	X
57	MG	DA	3260	-	-	-	X
57	MG	DA	3262	-	-	-	X
57	MG	DA	3276	-	-	-	X
57	MG	DA	3279	-	-	-	X
57	MG	DA	3289	-	-	-	X
57	MG	DA	3290	-	-	-	X
57	MG	DA	3296	-	-	-	X
57	MG	DA	3299	-	-	-	X
57	MG	DA	3304	-	-	-	X
57	MG	DA	3307	-	-	-	X
57	MG	DA	3319	-	-	-	X
57	MG	DA	3321	-	-	-	X
57	MG	DA	3324	-	-	-	X
57	MG	DA	3328	-	-	-	X
57	MG	DA	3340	-	-	-	X
57	MG	DA	3353	-	-	-	X
57	MG	DA	3358	-	-	-	X
57	MG	DA	3367	-	-	-	X
57	MG	DA	3369	-	-	-	X
57	MG	DA	3370	-	-	-	X
57	MG	DA	3372	-	-	-	X
57	MG	DA	3379	-	-	-	X
57	MG	DA	3389	-	-	-	X
57	MG	DA	3392	-	-	-	X
57	MG	DA	3393	-	-	-	X
57	MG	DA	3405	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DB	203	-	-	-	X
57	MG	DB	213	-	-	-	X
57	MG	DF	302	-	-	-	X
57	MG	DN	201	-	-	-	X
57	MG	DX	102	-	-	-	X
57	MG	DX	103	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 296042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P AND A-SITE PHE-TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	AY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			
24	CX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
29	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1140	689	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
42	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
43	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
44	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
45	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
46	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
48	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
49	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
50	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
51	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
52	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
53	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
54	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
55	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
56	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	422	Total	Mg	0	0
			422	422		
57	CA	199	Total	Mg	0	0
			199	199		
57	DF	2	Total	Mg	0	0
			2	2		
57	CV	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D2	3	Total 3	Mg 3	0	0
57	BE	1	Total 1	Mg 1	0	0
57	AW	8	Total 8	Mg 8	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	1	Total 1	Mg 1	0	0
57	AX	2	Total 2	Mg 2	0	0
57	CN	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DC	1	Total 1	Mg 1	0	0
57	DD	2	Total 2	Mg 2	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	14	Total 14	Mg 14	0	0
57	DO	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	AV	5	Total 5	Mg 5	0	0
57	BX	2	Total 2	Mg 2	0	0
57	B2	2	Total 2	Mg 2	0	0
57	AA	198	Total 198	Mg 198	0	0
57	D7	2	Total 2	Mg 2	0	0
57	CX	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DV	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	AD	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	AI	1	Total 1	Mg 1	0	0
57	DS	1	Total 1	Mg 1	0	0
57	DE	1	Total 1	Mg 1	0	0
57	DX	3	Total 3	Mg 3	0	0
57	DA	421	Total 421	Mg 421	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	BV	1	Total 1	Mg 1	0	0
57	AG	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	1	Total 1	Mg 1	0	0
57	CI	1	Total 1	Mg 1	0	0
57	CW	7	Total 7	Mg 7	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	B0	1	Total 1	Mg 1	0	0
57	CE	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	CL	1	Total Mg 1 1	0	0
57	DB	13	Total Mg 13 13	0	0

-
- The chemical structure of PAR (Pantetheine) is a complex molecule consisting of a central pyrimidine ring substituted with a ribose moiety, a phosphate group, and a pantoic acid moiety. The structure is shown with various atoms labeled with their element symbols and atomic numbers (e.g., C13(30), O13(3), N24). The molecule is a derivative of pantoic acid, which is a key component of the coenzyme NAD(P)⁺.

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CN	1	Total Zn 1 1	0	0
59	AN	1	Total Zn 1 1	0	0
59	B9	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0
59	CD	1	Total Zn 1 1	0	0

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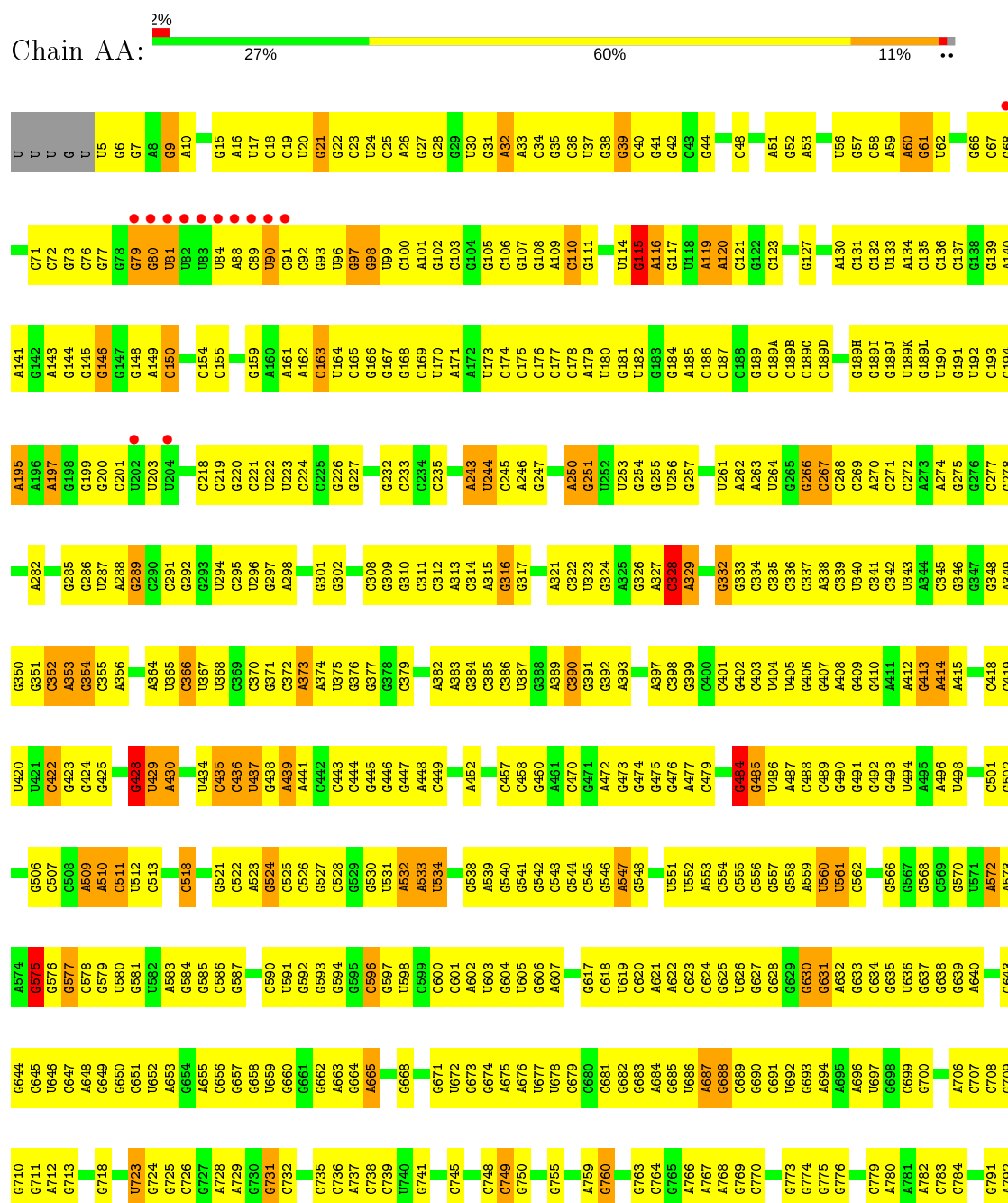
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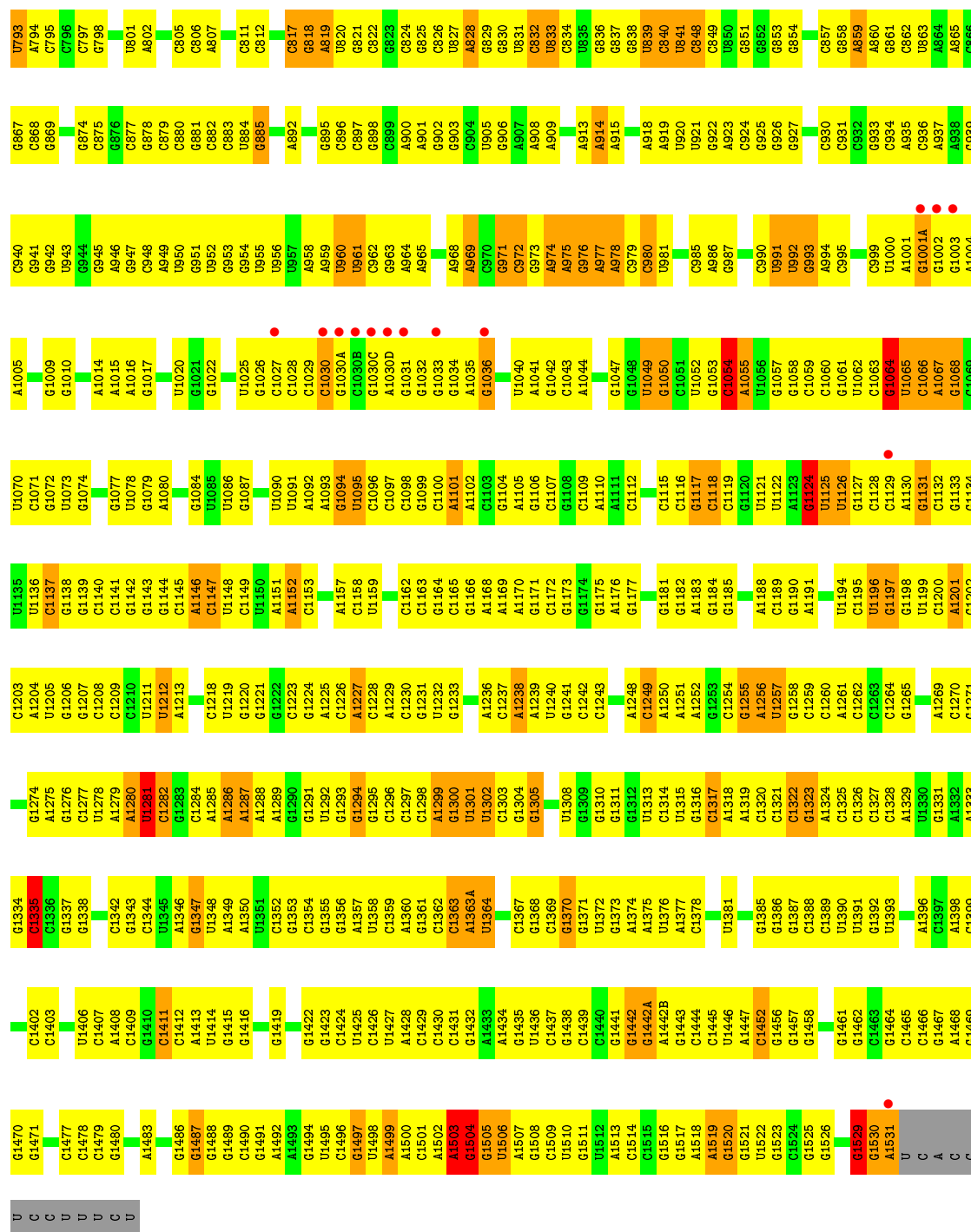
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

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.

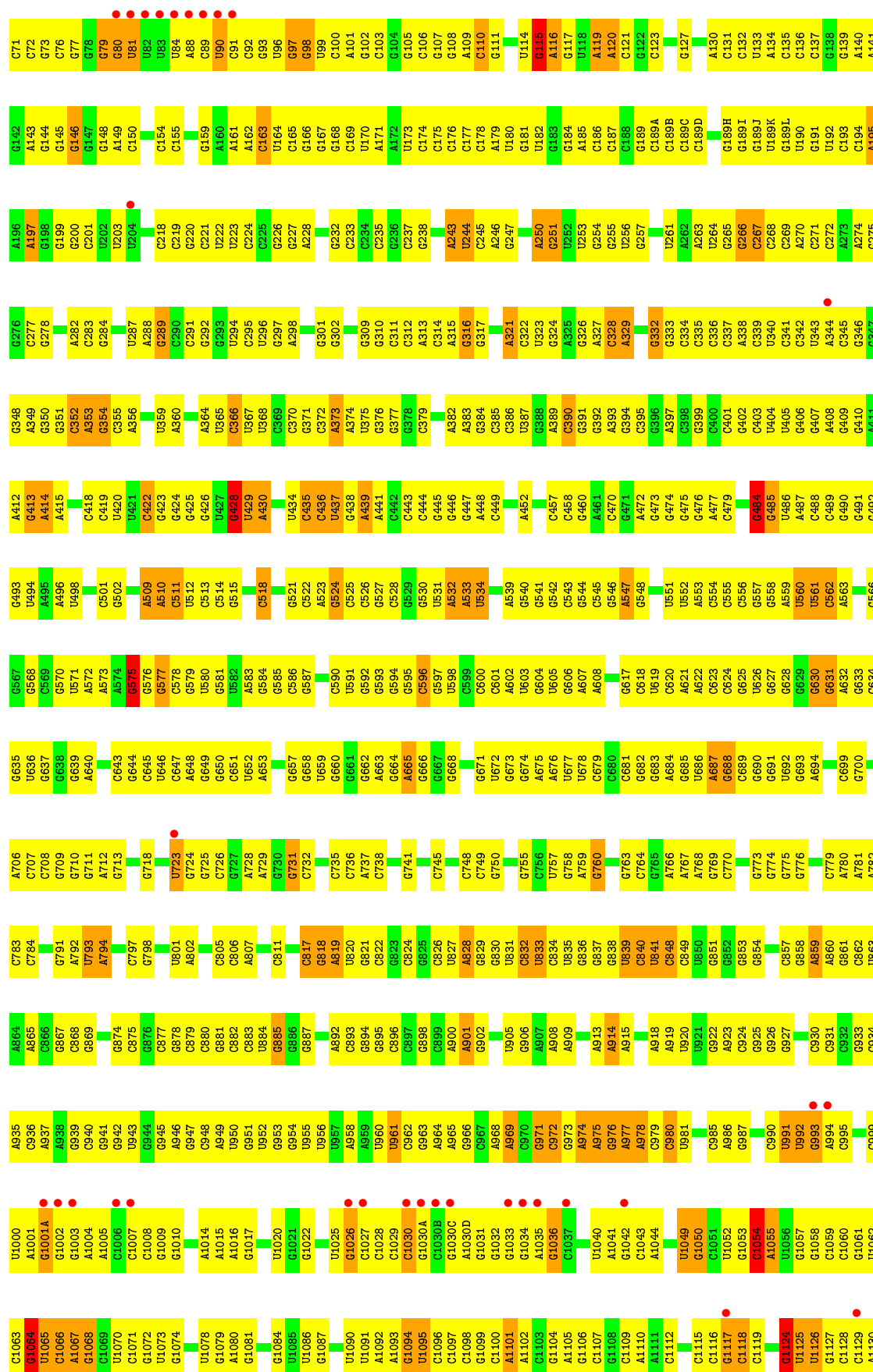
- Molecule 1: 16S ribosomal RNA



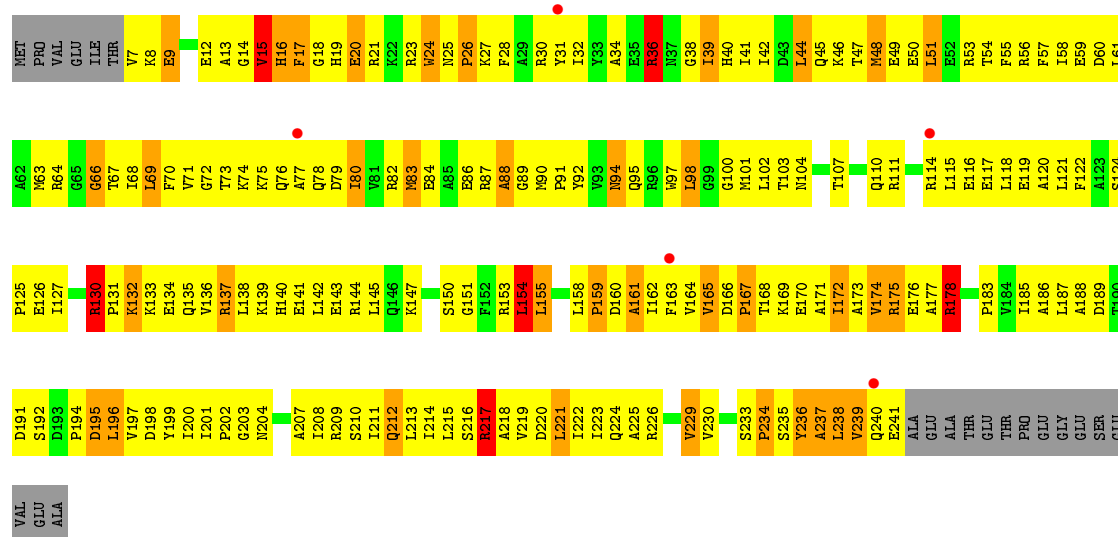


• Molecule 1: 16S ribosomal RNA



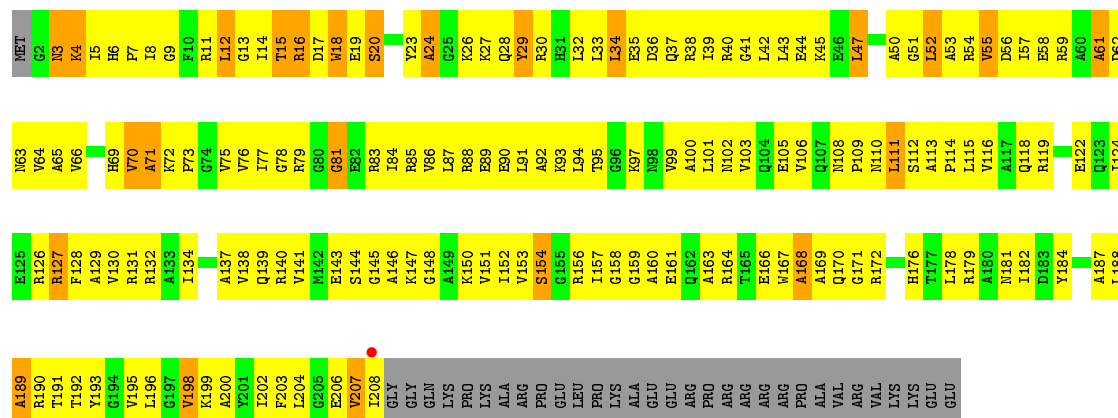






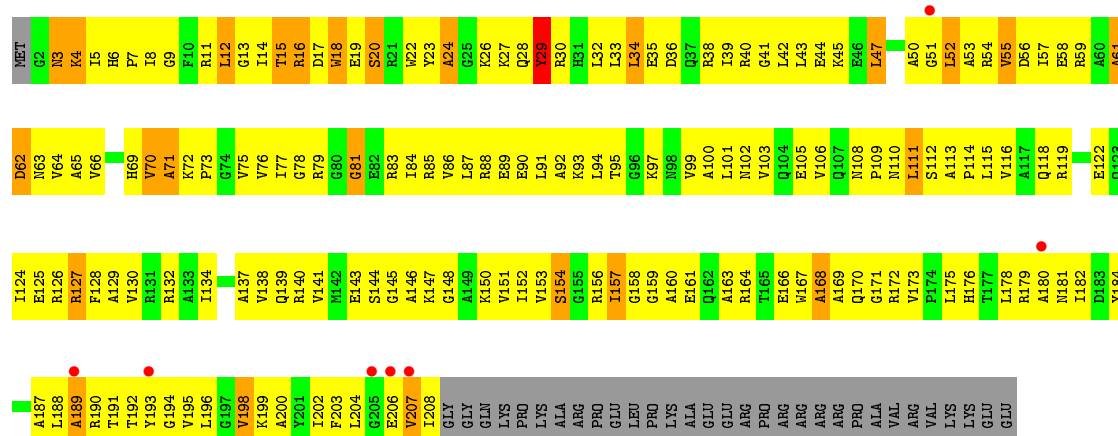
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 18% 58% 10% 13%

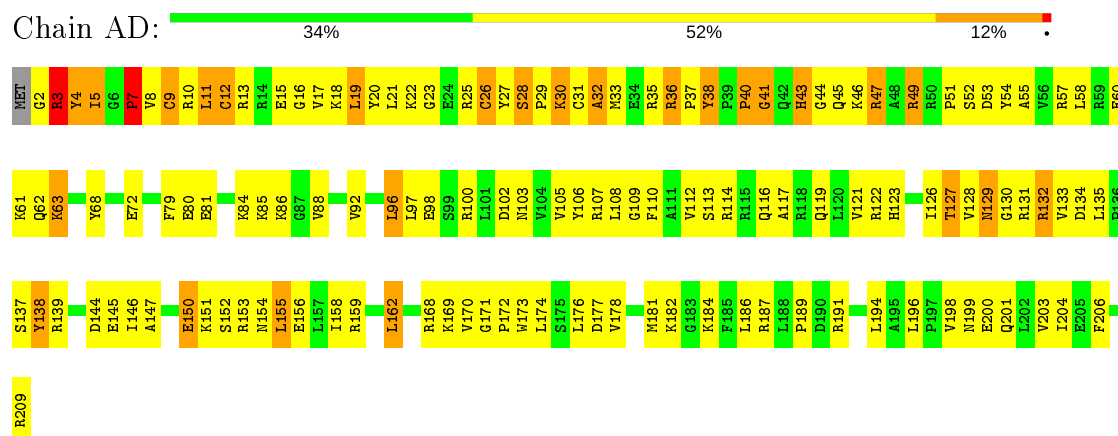


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

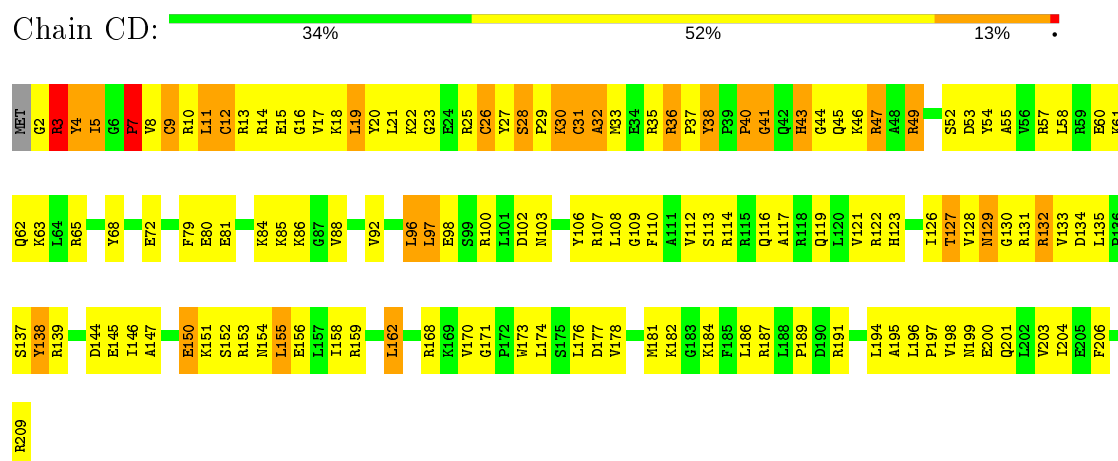
Chain CC: 3% 17% 59% 10% 13%



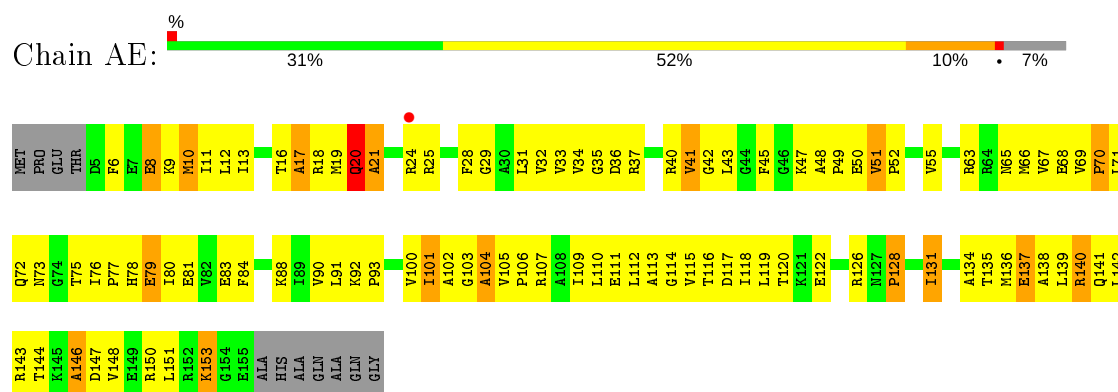
● Molecule 4: 30S RIBOSOMAL PROTEIN S4



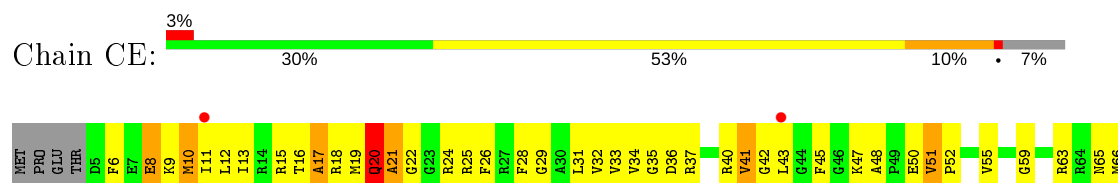
● Molecule 4: 30S RIBOSOMAL PROTEIN S4

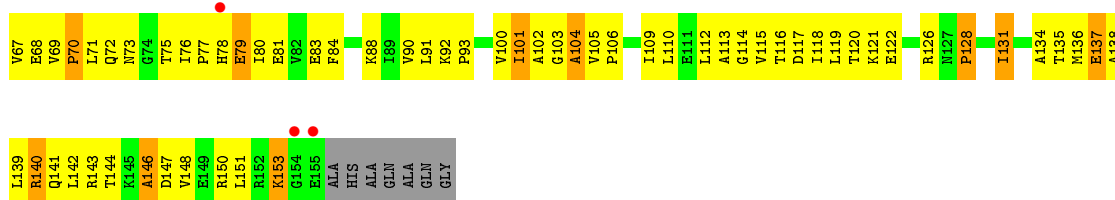


● Molecule 5: 30S RIBOSOMAL PROTEIN S5

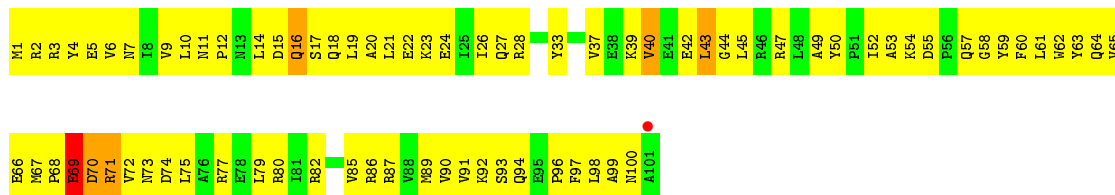


● Molecule 5: 30S RIBOSOMAL PROTEIN S5

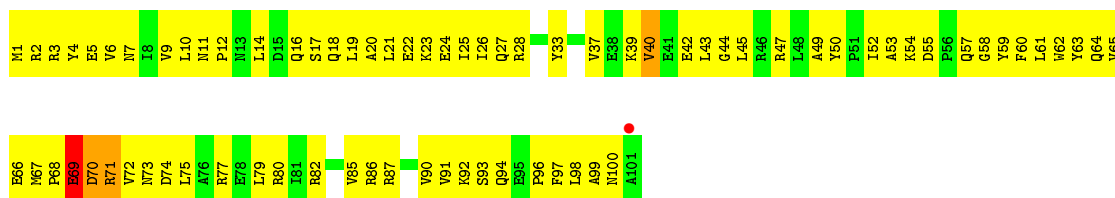




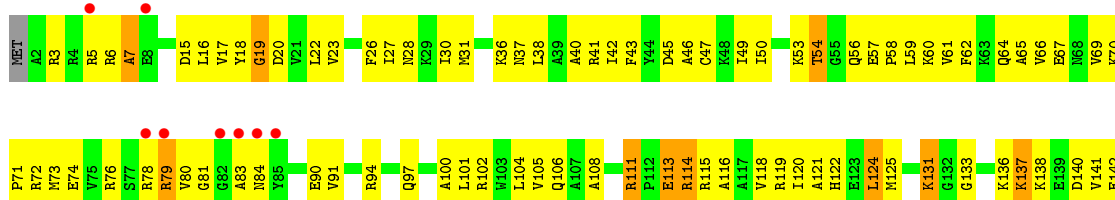
● Molecule 6: 30S RIBOSOMAL PROTEIN S6



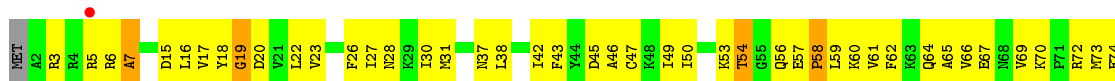
● Molecule 6: 30S RIBOSOMAL PROTEIN S6

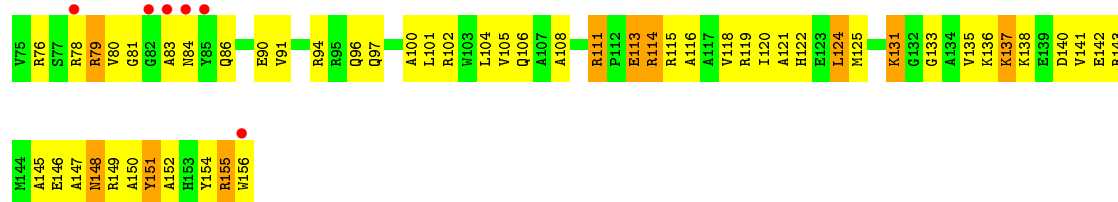


● Molecule 7: 30S RIBOSOMAL PROTEIN S7

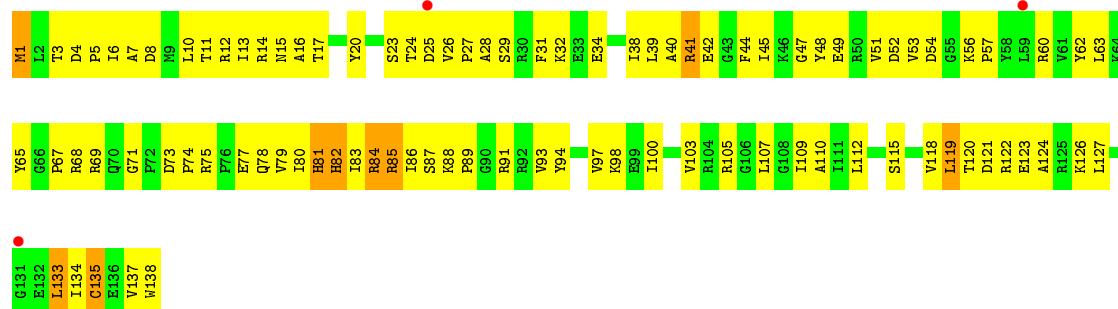


● Molecule 7: 30S RIBOSOMAL PROTEIN S7

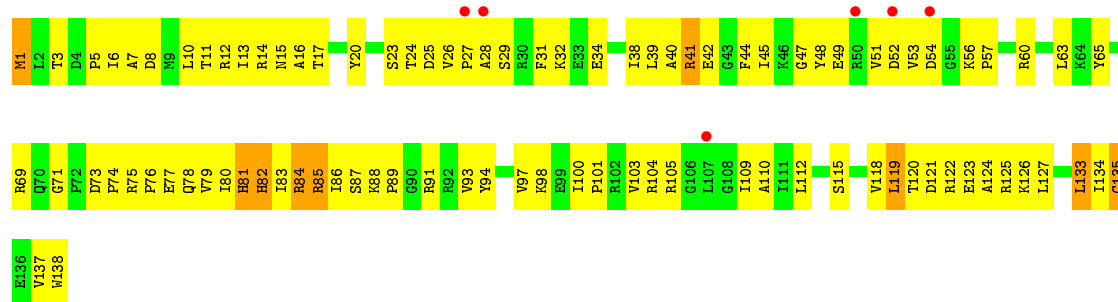




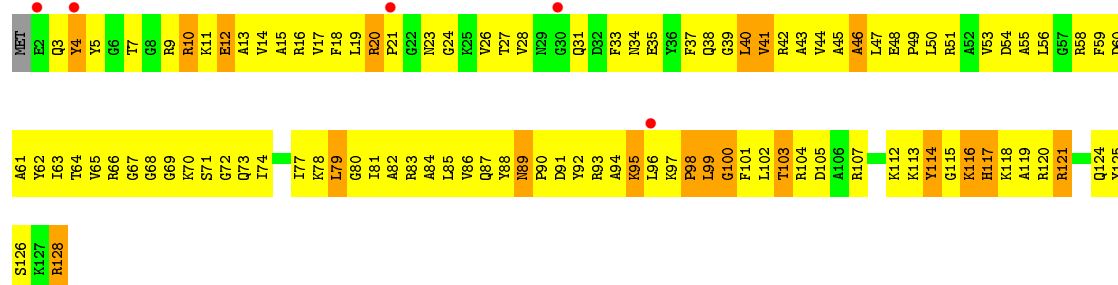
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



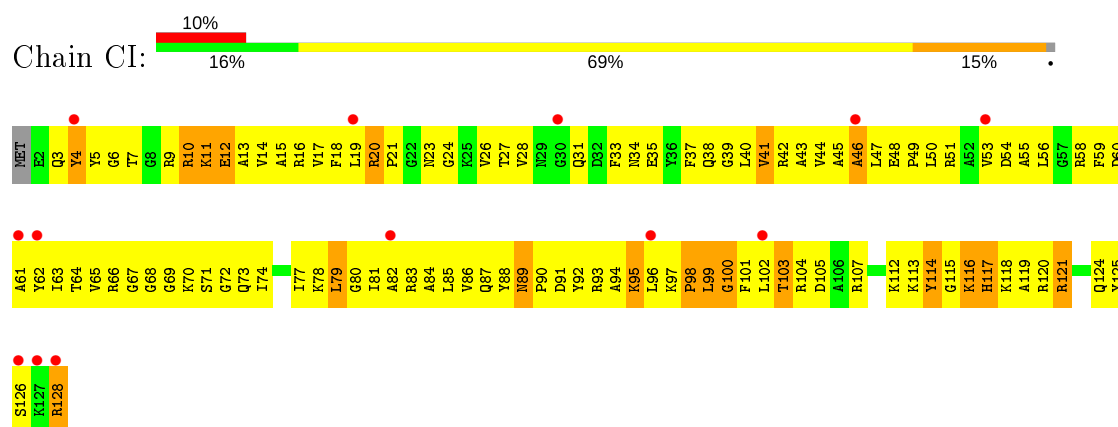
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



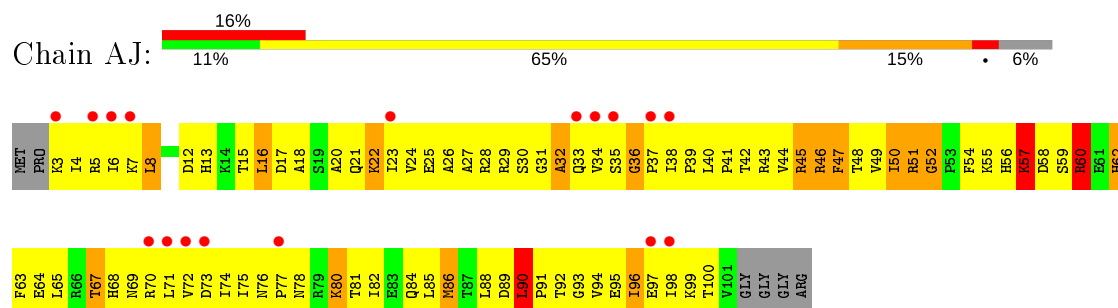
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



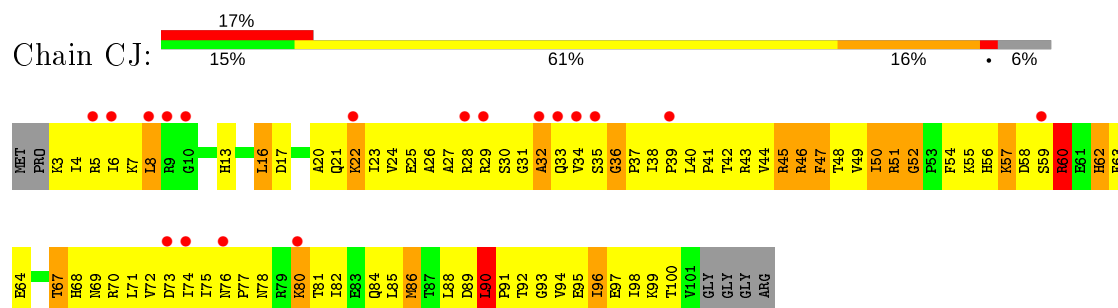
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



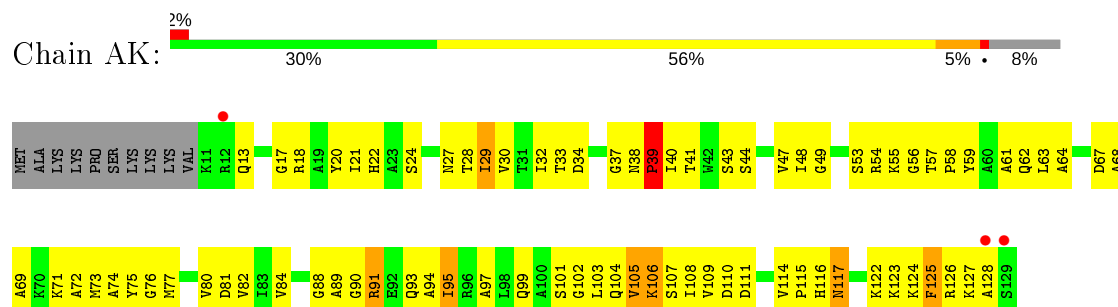
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

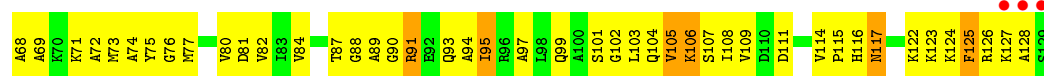


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

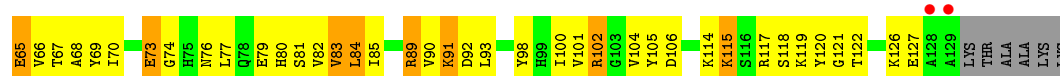


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

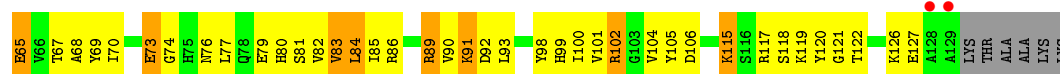
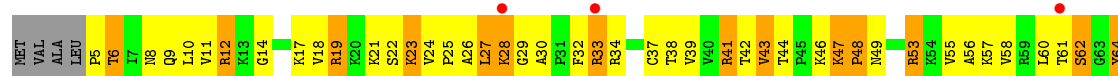




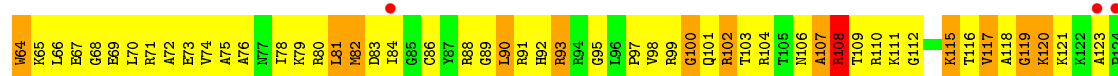
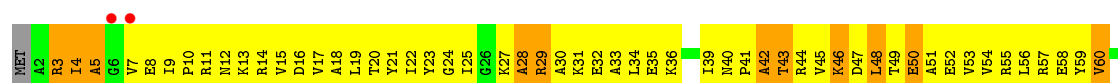
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



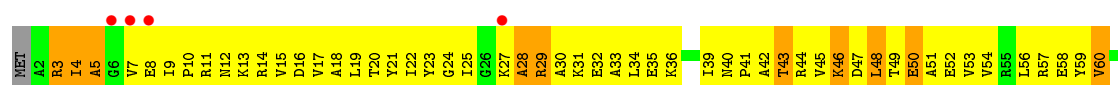
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

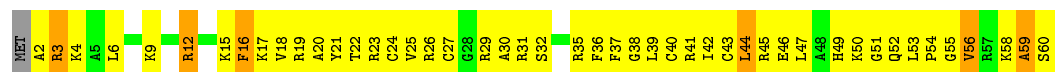


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

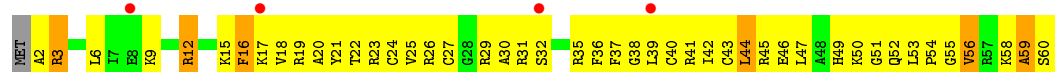




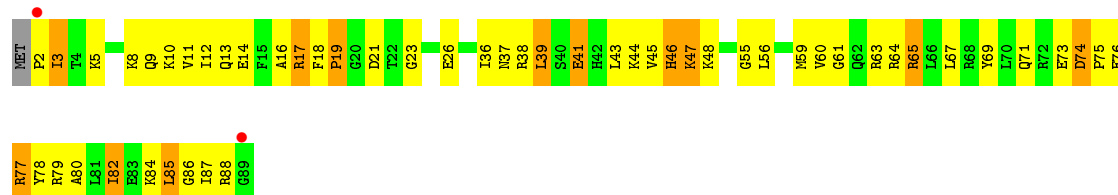
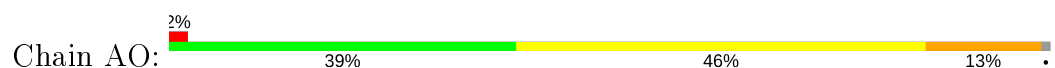
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



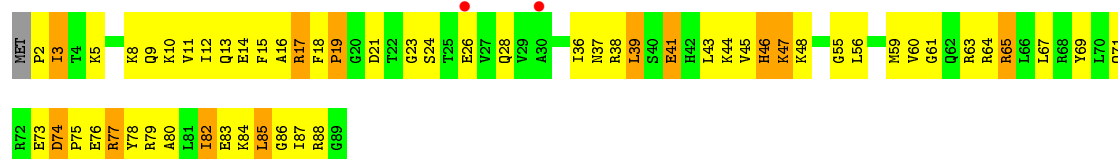
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



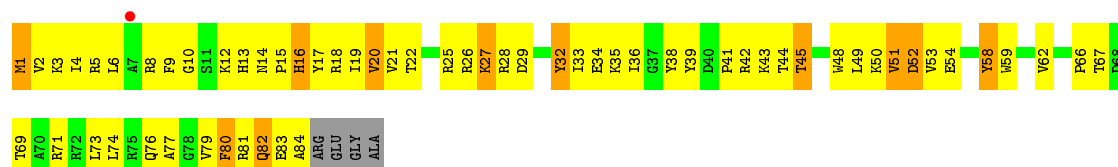
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



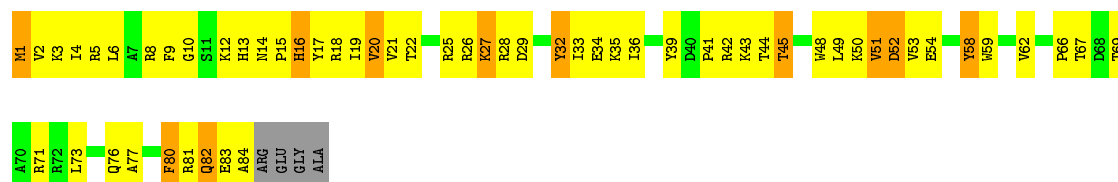
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



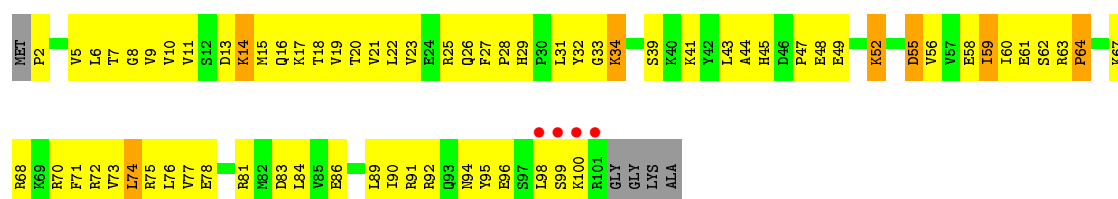
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



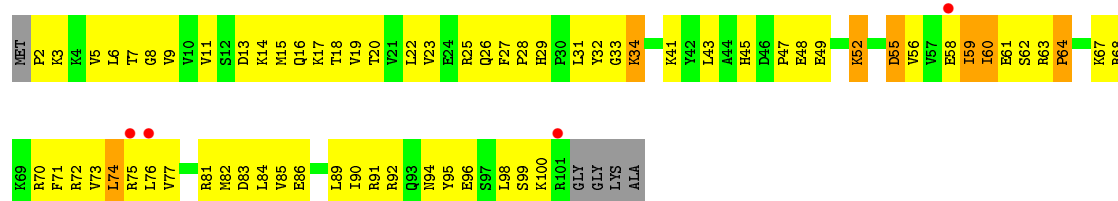
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 

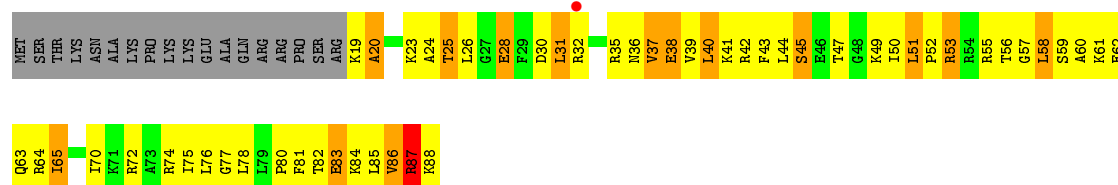

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 

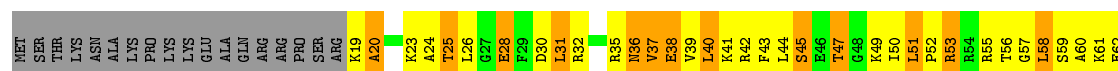

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

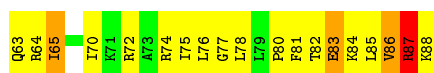
Chain CQ: 

- Molecule 18: 30S RIBOSOMAL PROTEIN S18

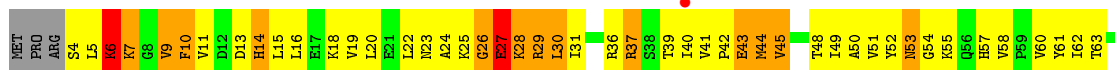
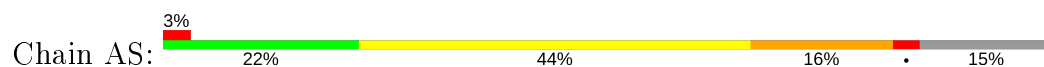
Chain AR: 

- Molecule 18: 30S RIBOSOMAL PROTEIN S18

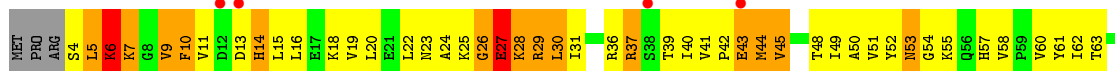
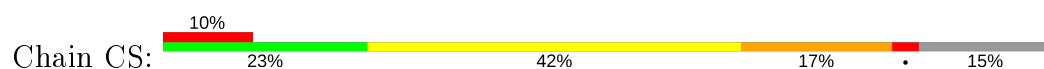
Chain CR: 



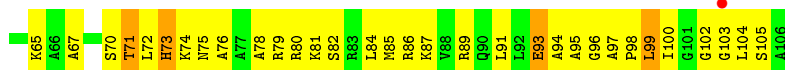
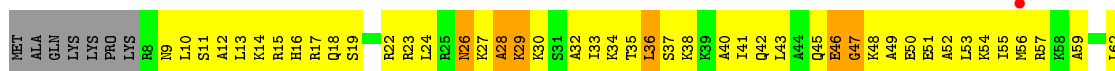
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



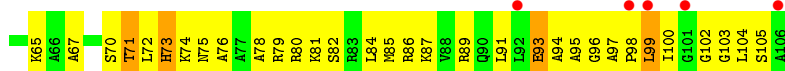
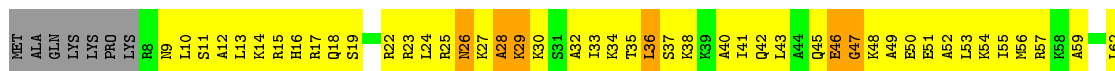
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

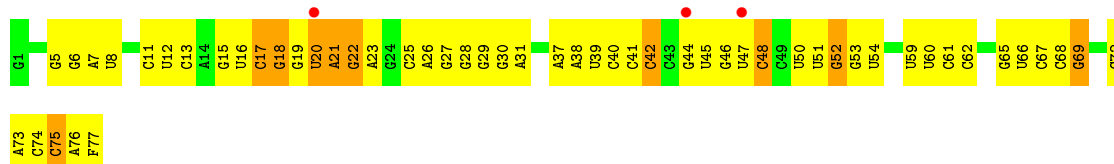


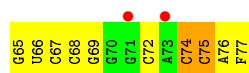


- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 22: P AND A-SITE PHE-TRNA PHE

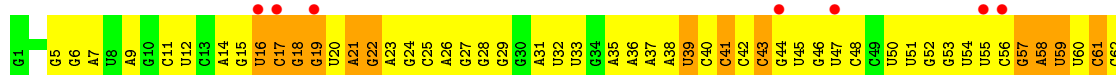




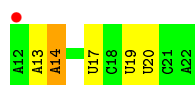
- Molecule 23: E-SITE TRNA PHE



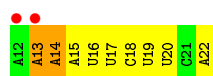
- Molecule 23: E-SITE TRNA PHE



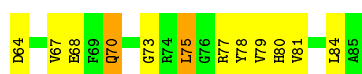
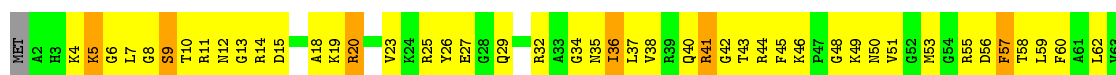
- Molecule 24: MRNA



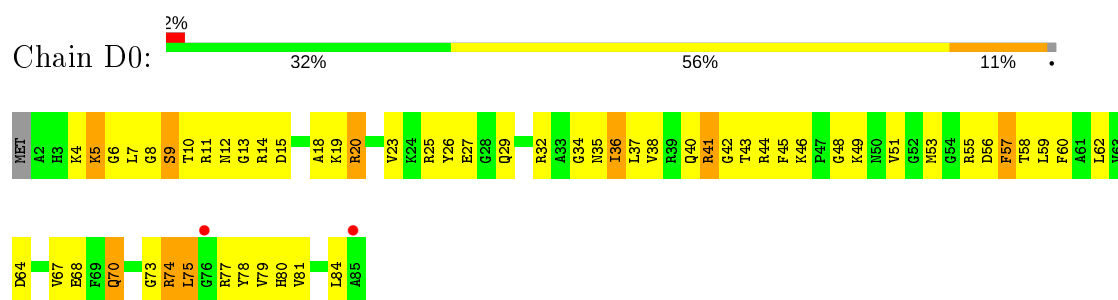
- Molecule 24: MRNA



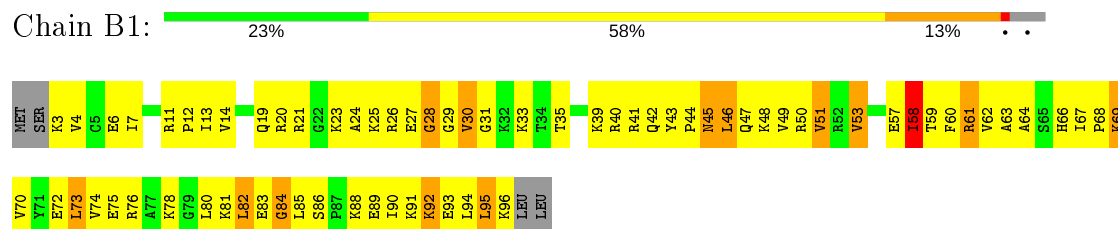
- Molecule 25: 50S RIBOSOMAL PROTEIN L27



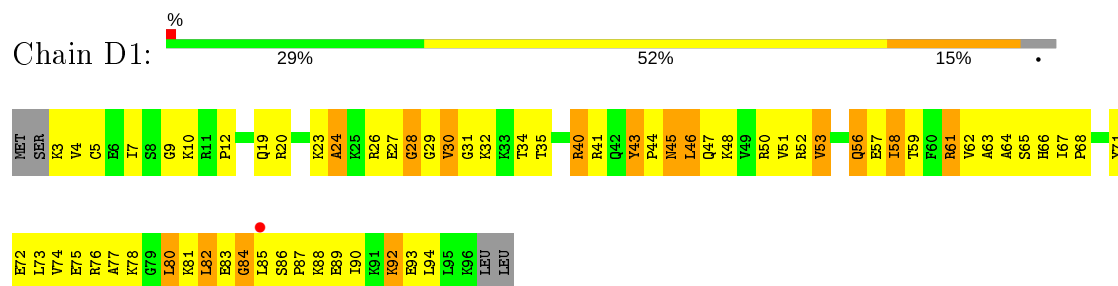
- Molecule 25: 50S RIBOSOMAL PROTEIN L27



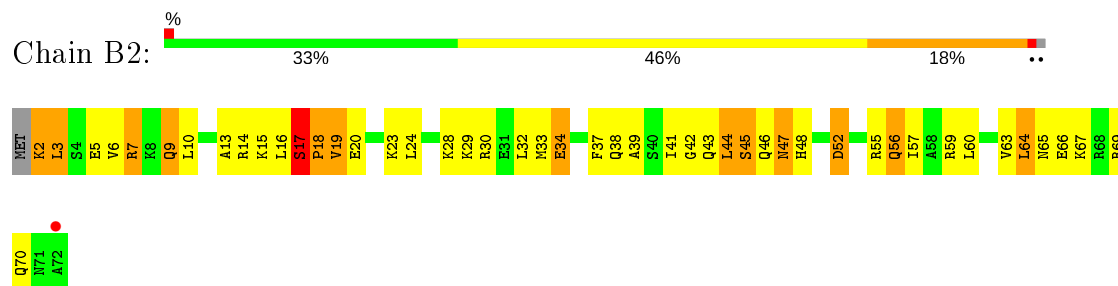
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



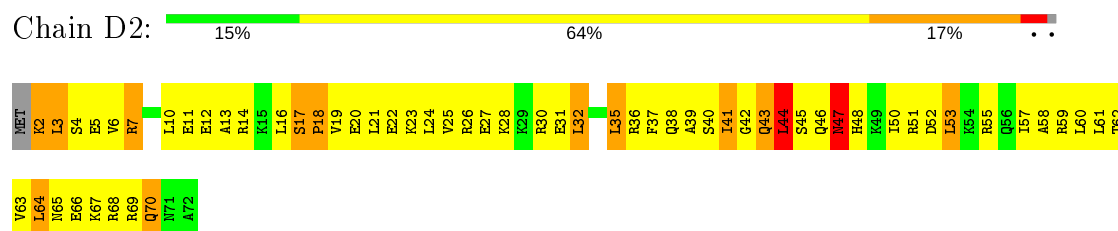
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



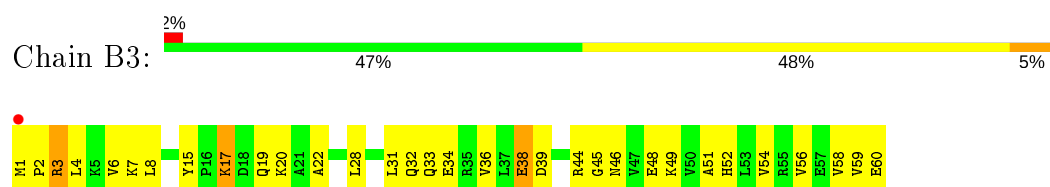
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



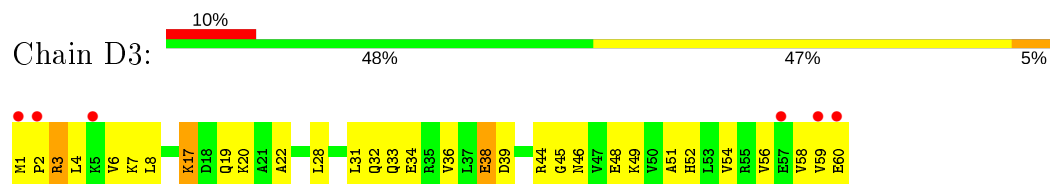
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



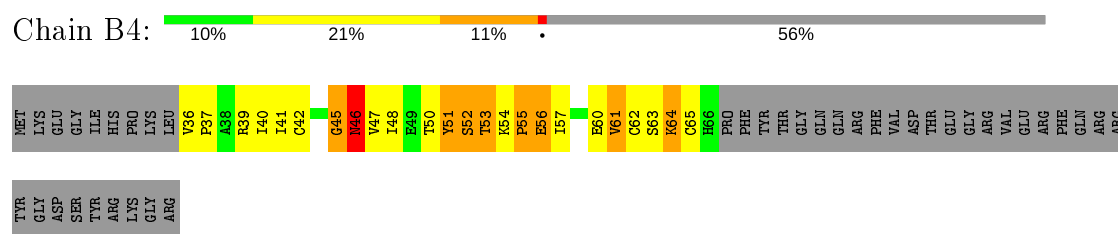
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



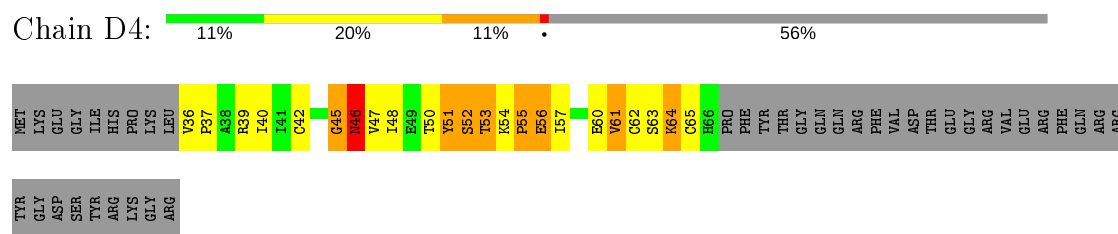
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



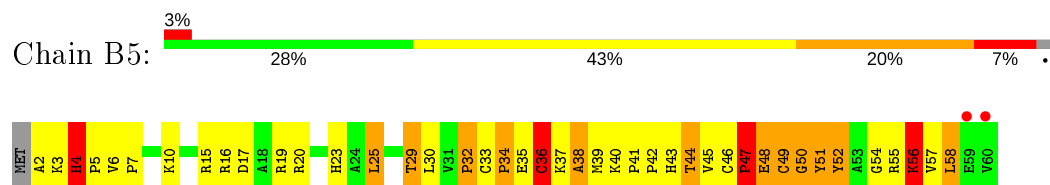
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



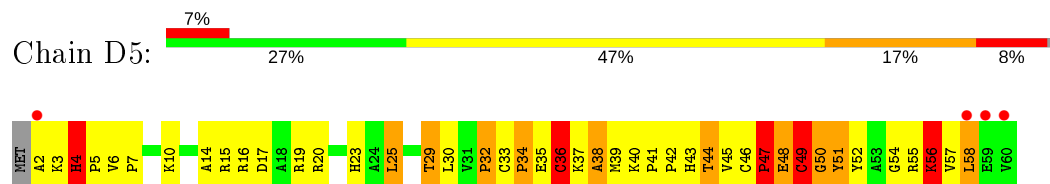
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

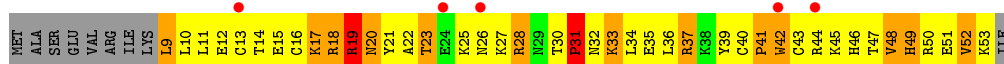


- Molecule 30: 50S RIBOSOMAL PROTEIN L32

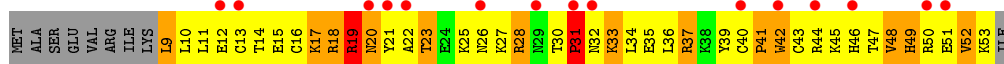


- Molecule 31: 50S RIBOSOMAL PROTEIN L33





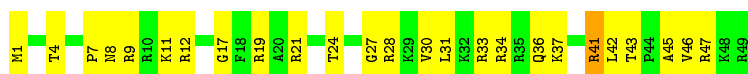
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



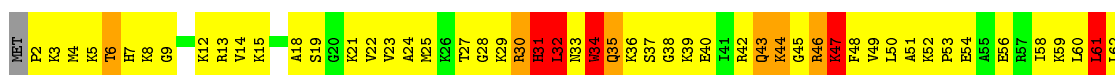
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



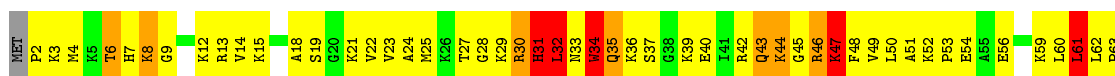
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



• Molecule 33: 50S RIBOSOMAL PROTEIN L35



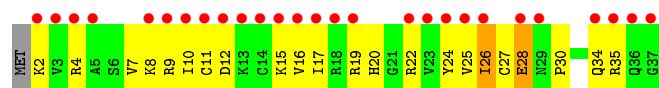
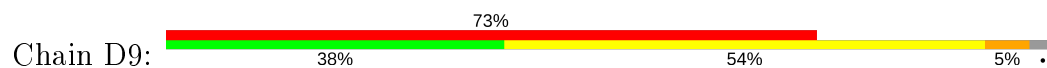
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



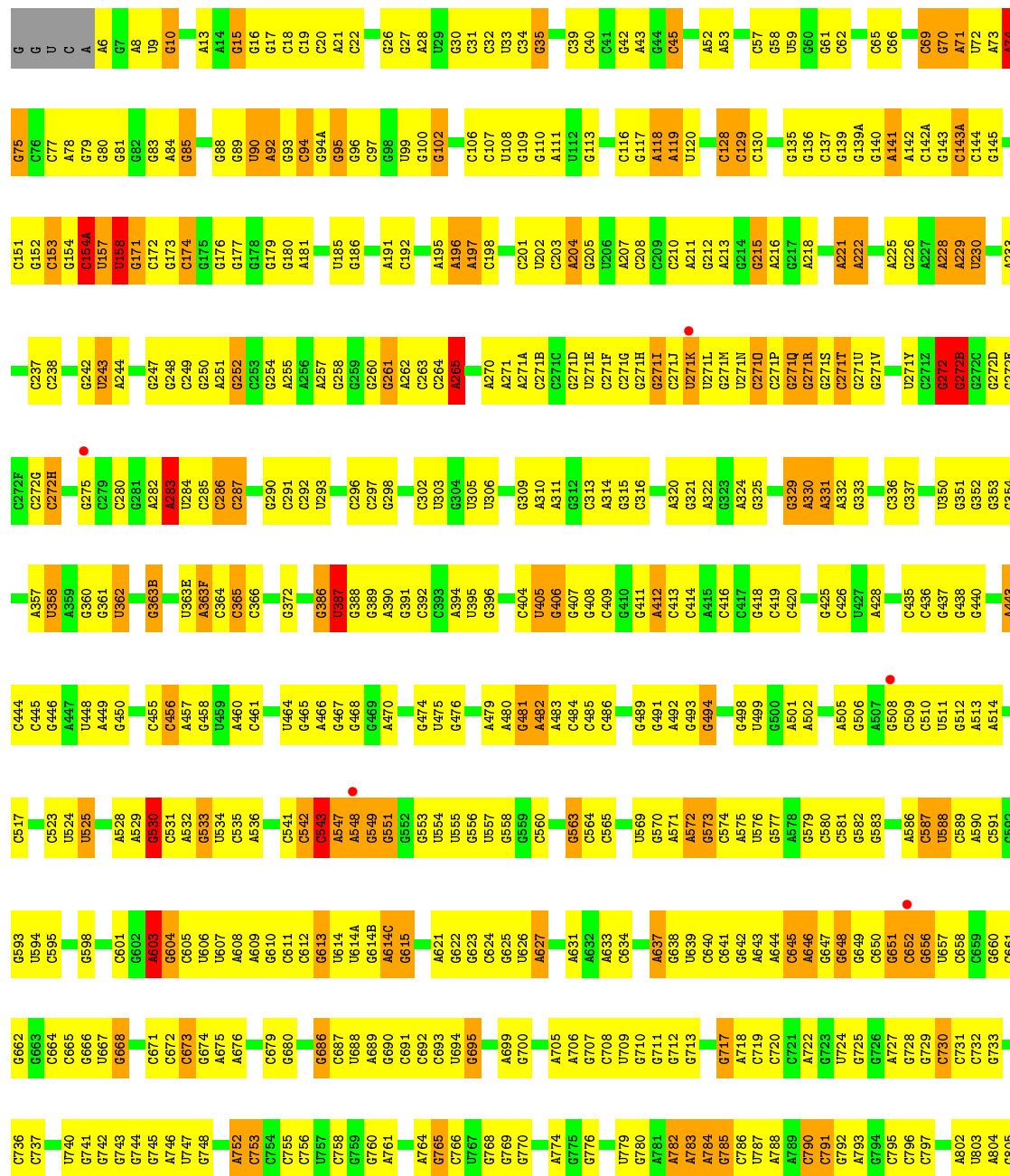
• Molecule 34: 50S RIBOSOMAL PROTEIN L36



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

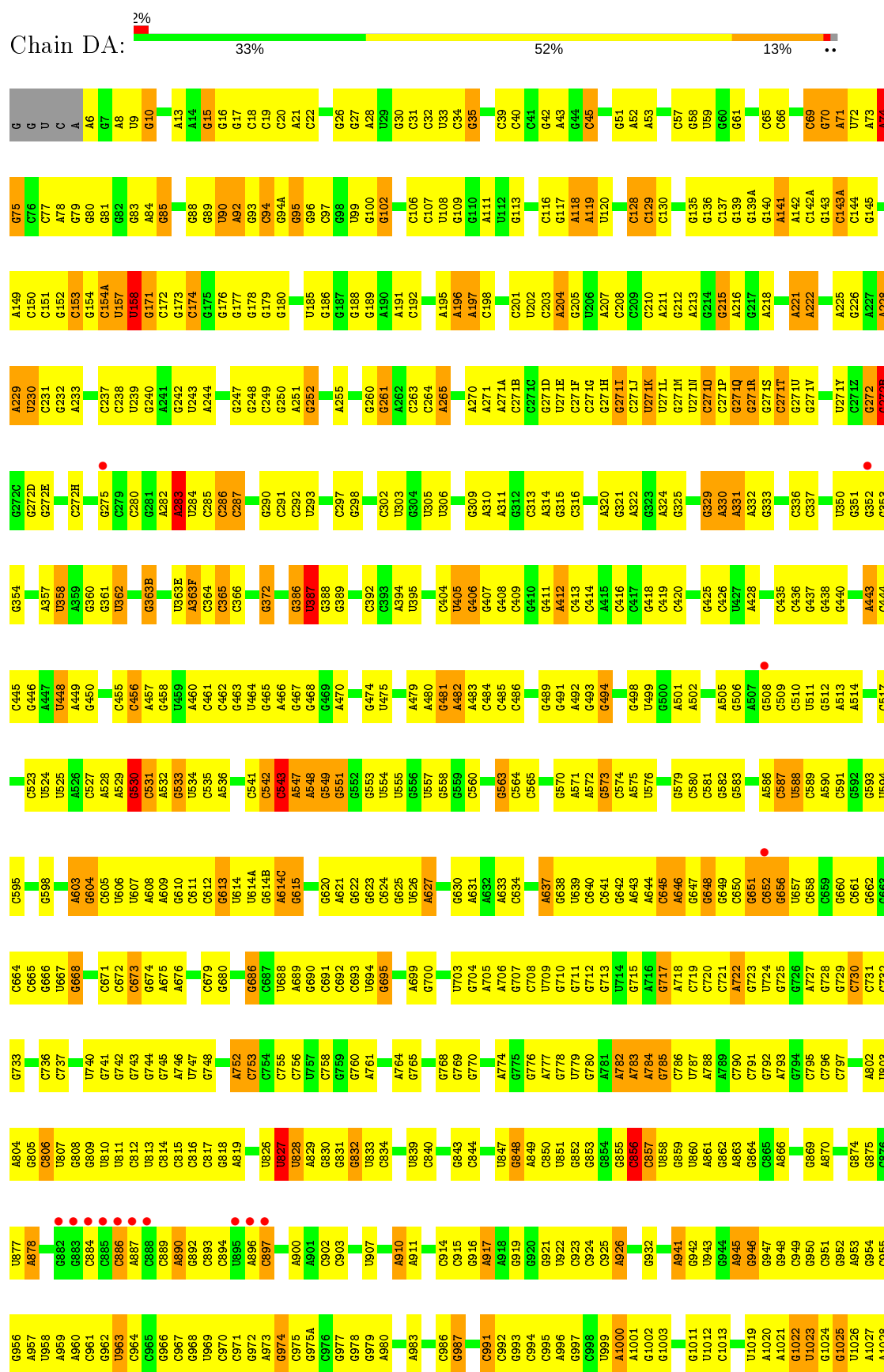


• Molecule 35: 23S RIBOSOMAL RNA



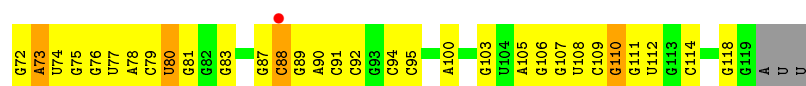
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C1844	G1776	C1687	C1608	U1518	C1451	A1378	G1303	G1224	G1153	U1034	C961	G881	G808
G1845	U1777	U1688	A1607	G1519	C1452	A1379	C1309	G1227	G1154	U1035	C962	G882	G809
G1846	U1778	A1689	A1609	G1520	U1453	G1380	G1310	G1227	A1155	G1036	U963	G883	U810
A1847	U1779	A1690	A1610	G1525	G1455	C1384	G1311	G1231	A1156	C1037	C964	G884	U811
A1848	C1781	C1691	C1611	G1526	G1456	A1385	U1312	G1232	G1157	C1038	C967	G885	C812
U1851	G1782	U1692	C1612	G1527	A1457	G1386	U1313	G1233	C1158	C1039	C968	G886	U813
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A1853	A1784	G1697	C1615	A1528A	A1460	G1388	G1315	G1235	G1163	G1042	C970	C888	C815
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G1855	G1699	G1699	C1617	G1461	U1396	U1396	A1317	U1241	U1165	G1044	G972	G892	C817
C1856	A1700	C1618	A1618	C1464	G1401	G1401	C1318	A1241	C1166	A1045	A973	C893	G818
G1857	C1788	C1788	C1626	C1532	C1402	G1402	G1319	A1242	U1167	A1046	C975	C894	A819
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A1859	G1790	C1630	C1543	C1468	C1404	C1404	A1321	G1244	G1169	A1048	C976	U827	U827
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A1889	G1748	G1573	G1573	C1493	C1429	C1429	G1357	U1281	G1192	A1128	G1002	G853	G853
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G1896	C1751	U1578	U1578	A1495	U1431	U1431	G1359	A1272	G1195	G1132	C1004	C856	C856
G1897	G1752	A1579	A1579	A1496	A1434	A1434	G1363	U1287	G1201	U1133	C1005	C857	C857
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A1901	U1757	C1584	C1584	U1502	U1438	U1438	G1367	C1290	A1204	G1138	G1014	A861	A861
C1902	G1758	A1586	A1586	U1503	U1439	U1439	G1368	U1291	G1205	G1139	G1015	G862	G862
G1903	C1827	U1587	U1587	C1504	G1440	G1440	A1359	C1292	G1215	U1019	G945	G863	G863
G1906	G1762	C1588	C1588	C1505	G1441	G1441	G1369	U1287	G1216	A1140	A1020	G864	G864
G1907	G1763	C1589	C1589	C1506	G1442	G1442	G1370	U1287	A1210	U1141	A1021	C865	C865
C1908	G1764	U1590	U1590	C1507	G1443	G1443	G1371	U1289	U1211	U1142	G1022	A866	A866
C1909	C1765	A1591	A1591	C1508	G1444	G1444	G1372	C1290	G1212	A1143	U1023	C951	C951
G1910	U1766	C1592	C1592	C1509	A1445	A1445	A1365	C1291	G1213	A1144	G1024	G869	G869
U1911	C1767	U1593	U1593	A1509A	C1446	C1446	G1366	U1292	G1214	G1145	G1025	A870	A870
A1912	U1768	G1594	G1594	U1510	C1447	C1447	A1373	C1293	G1215	C1146	A1026	G874	G874
A1913	C1771	G1598	G1598	C1511	G1448	G1448	G1374	C1293	A1220	C1147	A1027	G875	G875
C1914	G1772	C1599	C1599	G1515	A1449	A1449	C1375	U1300	G1221	C1147	A1028	G876	G876
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- Molecule 35: 23S RIBOSOMAL RNA

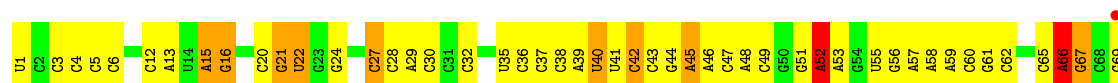


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G2061	G1984	G1910	U1834	G1765	G1674	G1594	A1509A	G1442	A1365	U1292	A1220	C1150	U1033
A2062	G1985	A1911	G1835	U1766	C1675	G1595	A1509B	G1443	A1366	C1293	C1221	C1151	G1034
C2063	A1986	A1912	C1836	C1767	A1676	C1598	G1510	G1444	G1368	U1294	C1221A	G1152	U1035
C2064	G1987	A1913	C1837	C1768	A1677	C1599	G1511	A1445	G1369	C1295	C1222	C1153	G1036
C2065	G1988	C1914	C1838	G1771	G1678	C1599	C1445A	C1445A	A1373	G1299	C1224	C1154	G1037
C2066	C1989	U1915	G1839	C1772	U1679	C1600	G1518	G1446	A1374	U1299	G1227	A1155	C1038
U2068	C1990	A1916	G1842	U1772	U1680	C1601	G1519	G1447	G1374	U1300	G1227	A1156	U1039
G2069	G1991	U1917	C1843	A1773	G1681	G1602	G1520	A1448	C1375	A1301	G1227	A1157	C1040
G2070	G1992	A1918	C1844	C1774	G1682	U1603	G1521	A1449	C1376	A1302	G1227	C1158	G1041
A2071	U1993	G1845	G1844	U1775	C1685	C1607	G1525	G1450	G1377	G1309	G1231	C1158	G1042
G2072	G1997	G1845	G1845	G1776	C1686	A1608	G1526	C1450A	A1378	G1310	G1232	C1161	C1043
C2073	G1998	G1846	G1846	U1777	C1686	A1608	G1527	G1451	A1379	G1310	C1233	C1162	G1044
G2079	G1999	A1847	A1848	U1778	U1687	A1609	A1528	A1452	G1380	G1311	C1234	G1163	G1045
U2080	G2000	U1851	G1852	A1780	U1688	A1610	G1529	U1453	U1312	U1312	U1235	G1164	A1046
G2081	G2001	G1853	G1853	G1781	A1689	C1612	G1530	A1384	G1385	C1314	U1240	U1165	G1047
G2082	C2008	G1854	G1854	G1782	C1691	G1613	C1531	G1459	C1386	G1315	A1241	C1166	G1048
G2083	G2009	A1854	A1854	A1783	U1692	A1614	C1532	A1460	A1395	U1317	A1242	U1167	C1049
G2086	G2010	G1855	G1855	A1784	G1696	C1615	G1533	A1461	U1396	A1318	G1244	G1168	A1050
G2087	U2011	G1856	G1856	A1786	G1697	A1616	C1543	C1464	U1396	G1319	G1245	G1170	G1051
G2088	G2012	G1857	G1857	A1787	A1698	A1617	A1544	C1464	U1396	G1320	A1246	G1171	C1052
G2089	A2013	G1858	G1858	G1788	G1699	A1618	C1547	C1467	G1401	C1321	A1247	G1173	C1053
G2090	A2014	A1859	A1859	A1789	A1700	G1626	C1548	C1468	C1402	A1321	G1248	A1174	A1106
U2091	U2015	G1860	G1860	C1790	G1700	U1629	C1549	A1469	C1403	C1327	G1251	G1175	G1107
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U2099	U2022	G1865	G1865	U1796	C1711	C1638	G1556	G1474	C1408	G1333	C1257	C1180	U1113
G2100	G2023	C1866	C1866	C1797	C1712	U1639	A1558	G1478	C1409	C1334	G1258	C1181	G1114
G2101	G2024	A1876	A1876	U1713	U1713	C1640	A1559	G1479	G1410	U1335	G1259	G1191	G1115
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G2103	C2026	C1878	C1878	G1715	G1715	G1642	C1565	U1481	A1412	G1337	C1261	G1193	A1127
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C2108	G2032	G1882	C1882	G1721	G1721	C1648	G1568	G1485	C1417	U1340	G1264	U1188	C1124
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A2114	G2037	A1888	A1888	C1743	C1743	C1656	G1573	A1490	G1424	G1347	A1269	A1194	G1131
G2115	G2038	A1890	A1890	G1744	C1744	C1657	C1574	G1491	G1425	G1348	C1270	G1195	A1132
G2116	C2039	G1897	G1897	G1747	U1747	U1659	U1578	A1494	A1427	C1350	A1272	C1201	U1133
A2117	A2042	G1898	G1898	G1747A	G1747A	C1660	A1580	A1495	G1428	C1351	A1275	G1202	C1135
U2118	C2043	U1899	U1899	G1748	G1748	G1661	G1581	A1496	G1429	U1352	G1278	G1203	G1136
U2122	A2051	A1900	A1900	C1751	C1751	C1662	G1582	U1497	C1430	A1353	A1279	U1204	G1137
G2123	G2052	G1901	G1901	G1752	G1752	C1663	A1583	C1498	U1431	G1354	G1279	G1205	G1138
G2124	C1902	A1902	A1902	G1753	G1753	A1665	A1586	C1501	A1434	G1355	G1281	C1208	C1139
G2125	C2055	G1903	G1903	G1754	G1754	G1666	A1587	C1502	G1485	G1356	G1281	G1209	U1141
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G2127	A2057	A1828	A1828	G1756	G1756	A1668	C1589	C1504	C1437	G1358	A1287	U1211	A1142A
C2128	A2058	A1929	A1929	A1762	A1762	C1670	U1590	C1505	A1439	A1359	U1288	G1212	A1144
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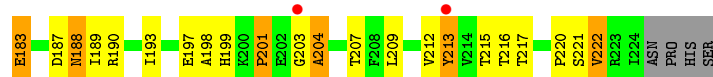
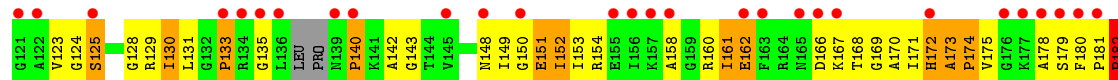
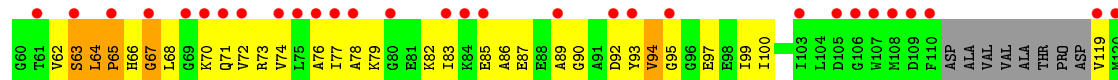
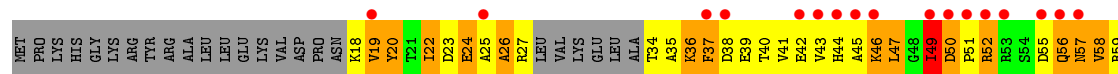




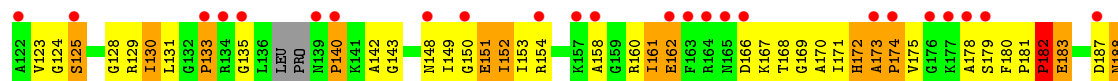
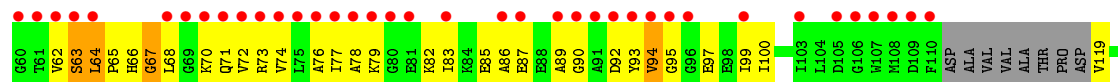
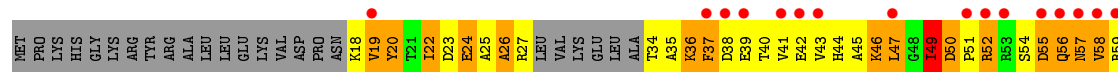
• Molecule 36: 5S RIBOSOMAL RNA



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

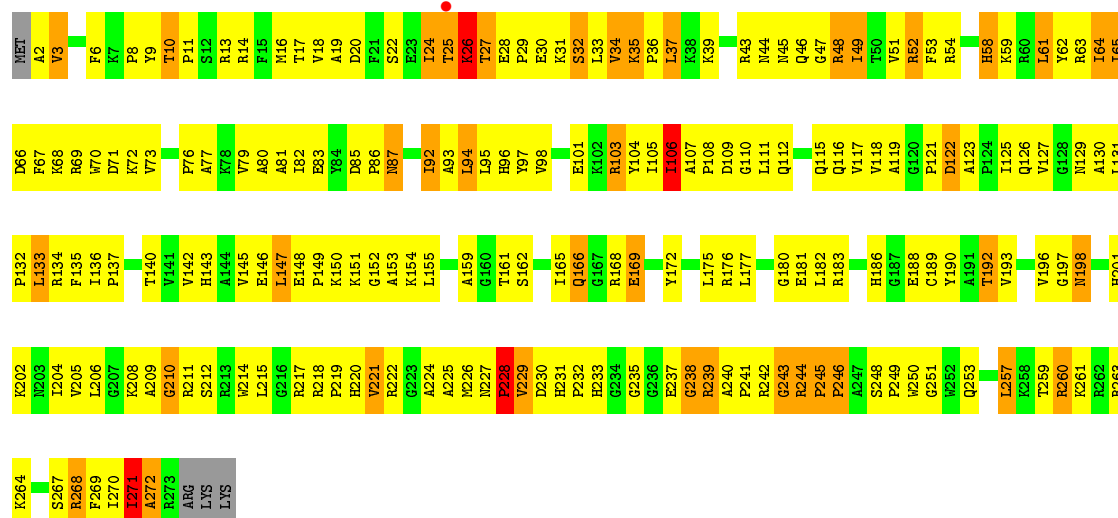


• Molecule 37: 50S RIBOSOMAL PROTEIN L1



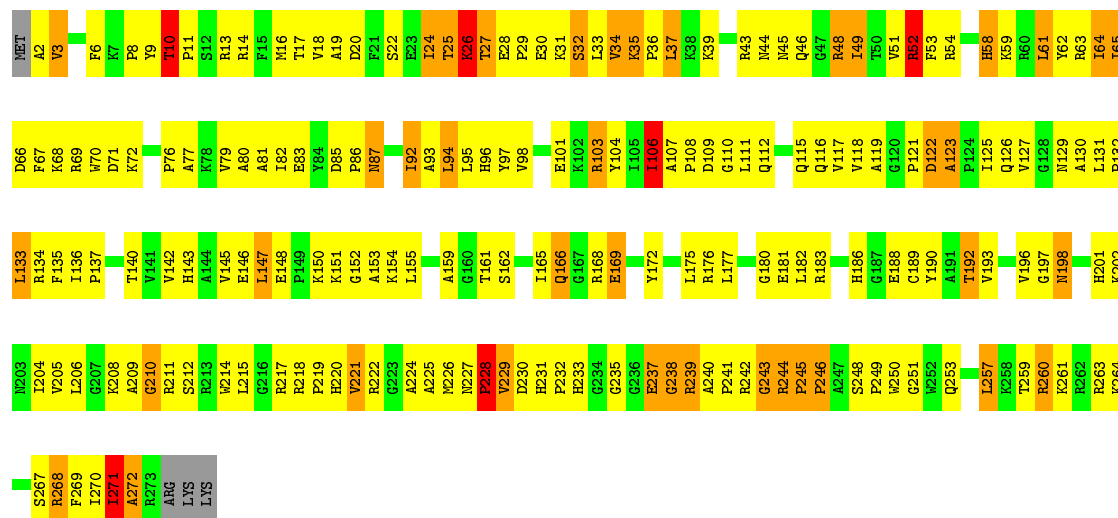
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:  27% 56% 14% ..



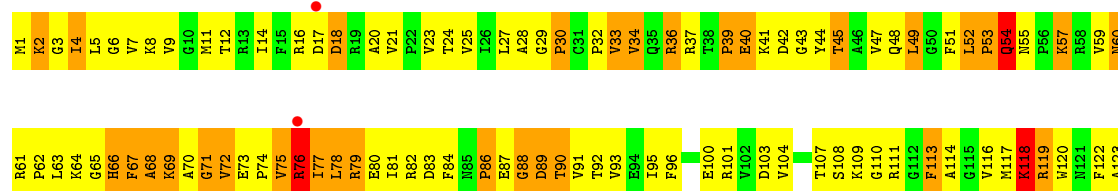
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

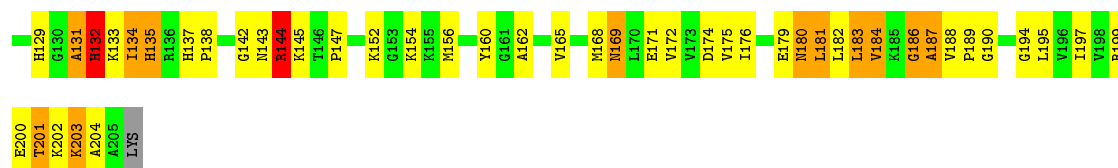
Chain DD:  28% 54% 14% ..



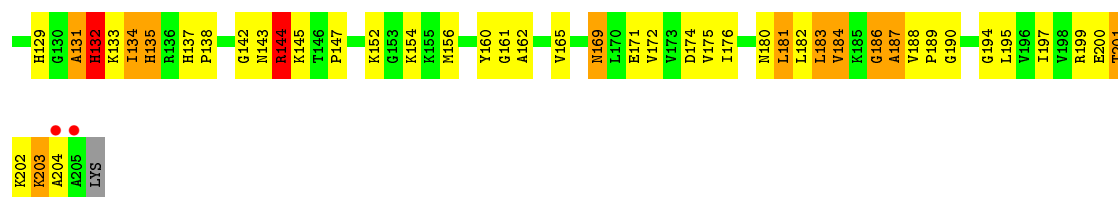
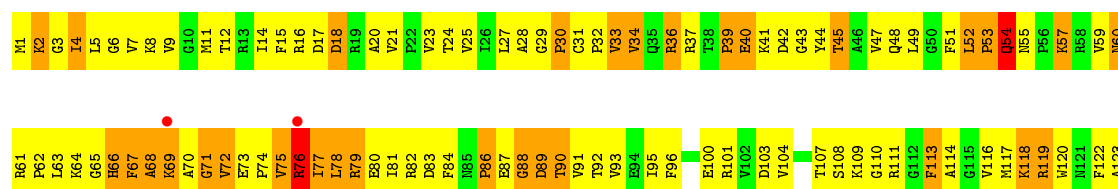
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:  29% 47% 21% .

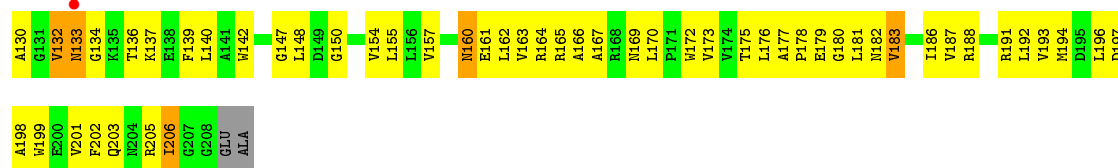
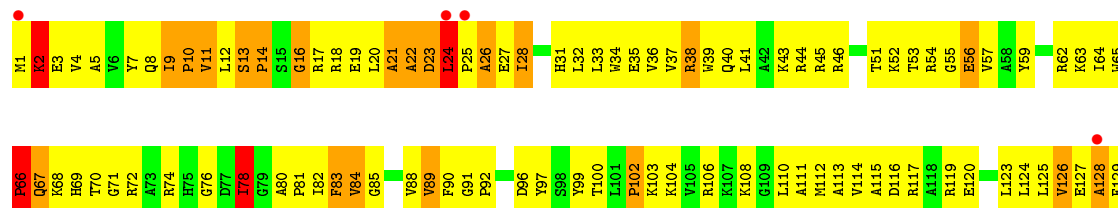




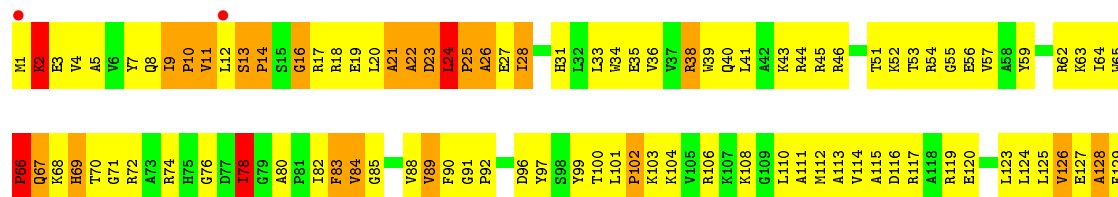
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

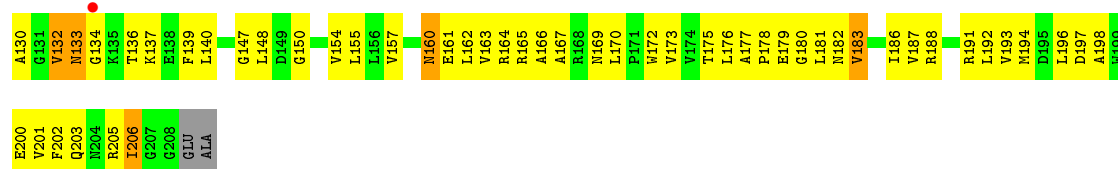


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

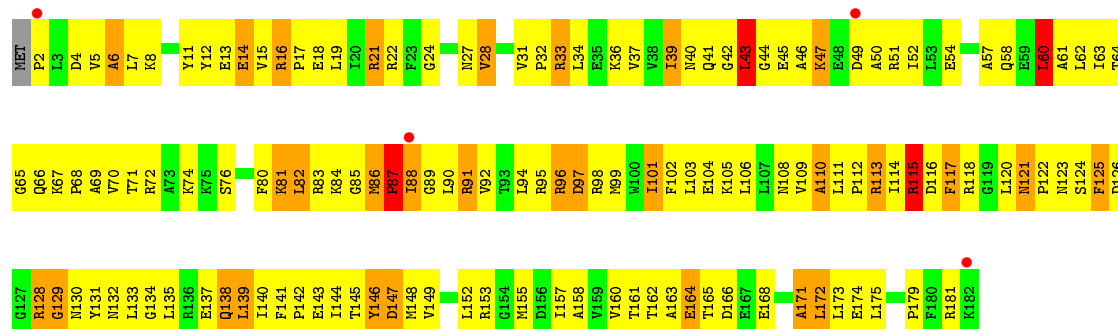


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

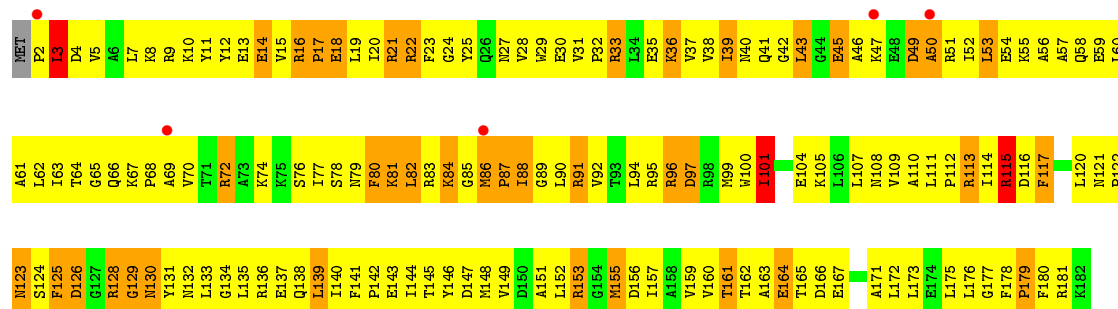
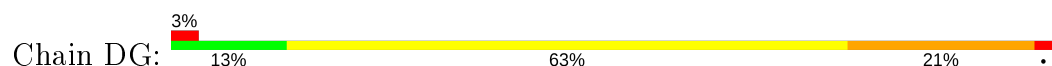




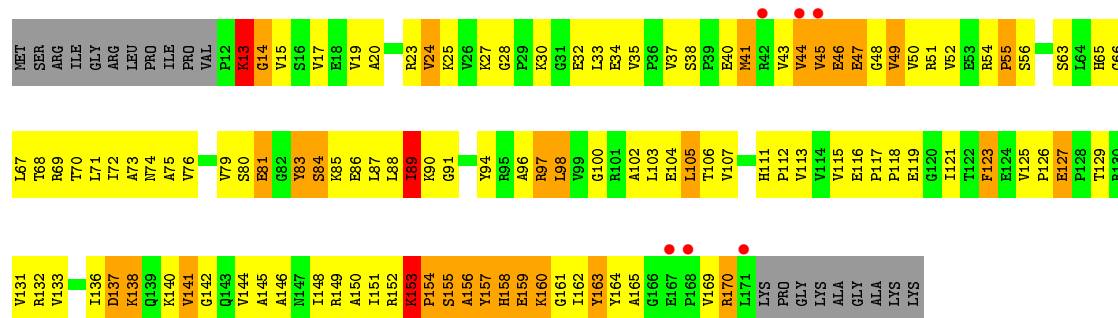
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



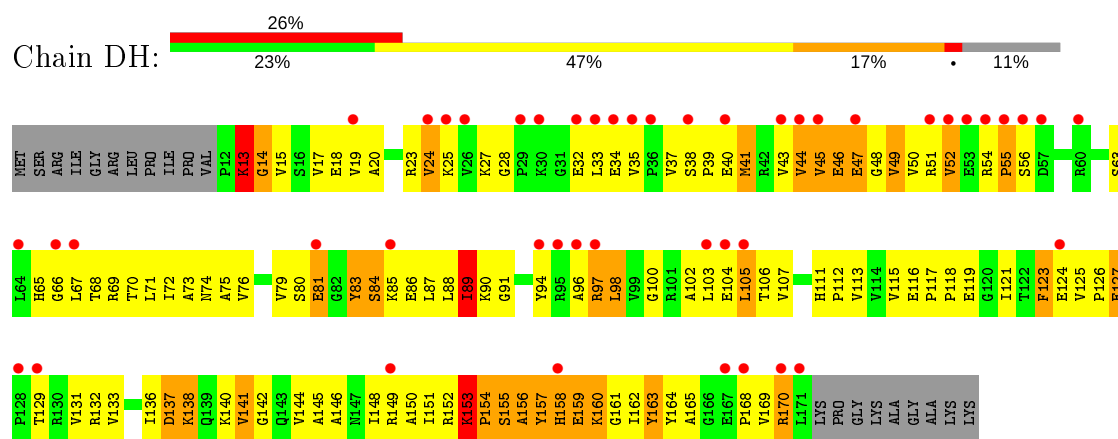
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



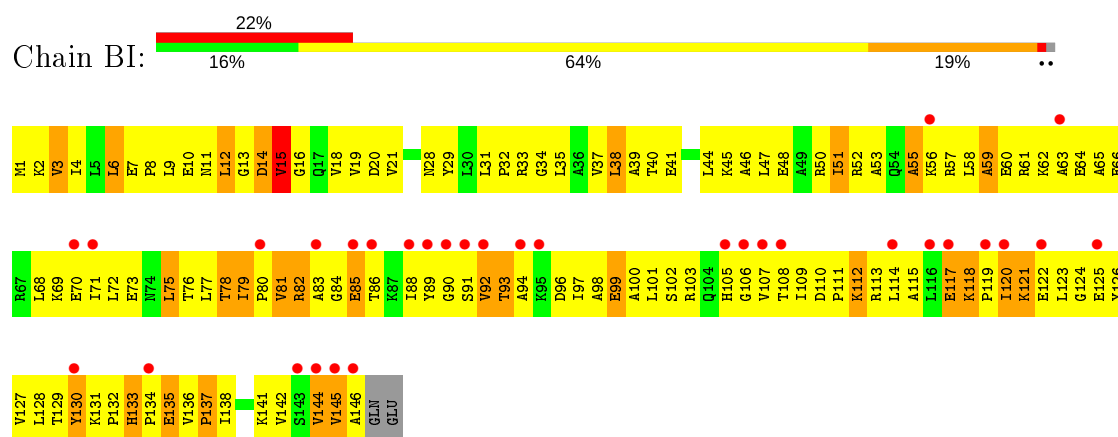
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



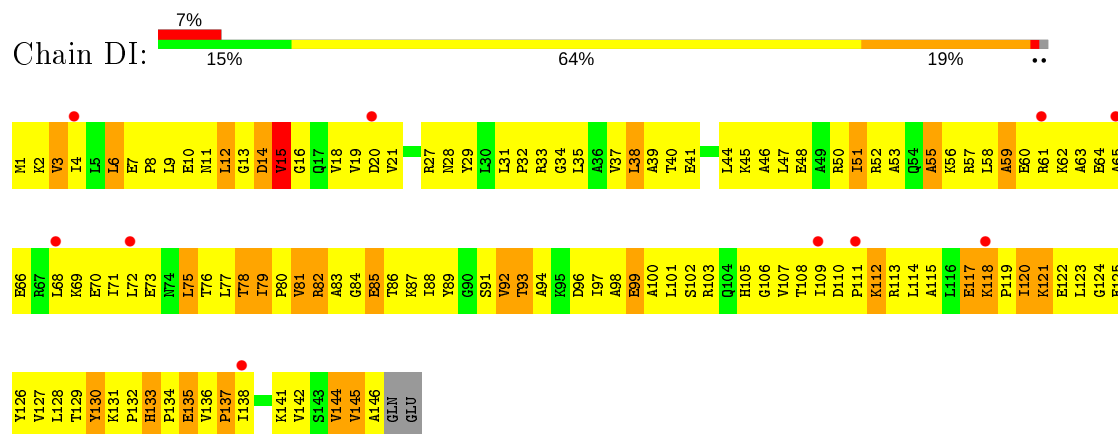
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



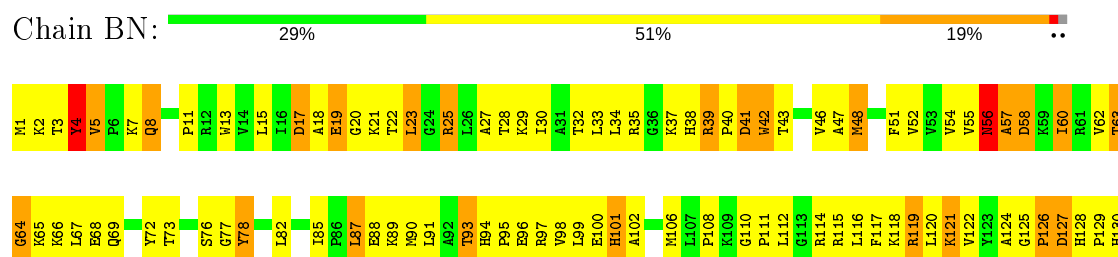
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

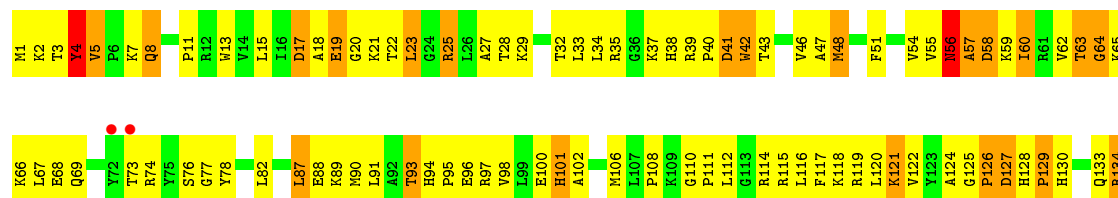


• Molecule 44: 50S RIBOSOMAL PROTEIN L13

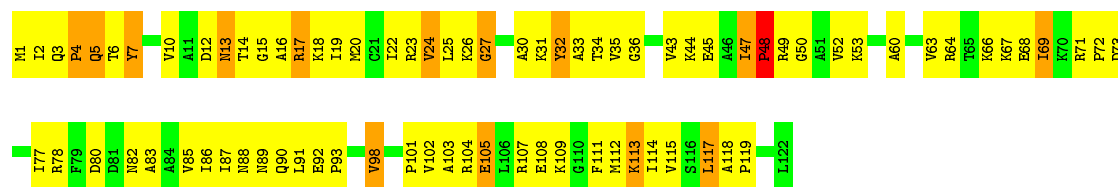




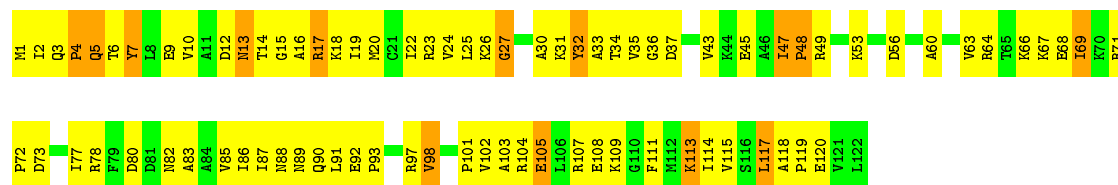
• Molecule 44: 50S RIBOSOMAL PROTEIN L13



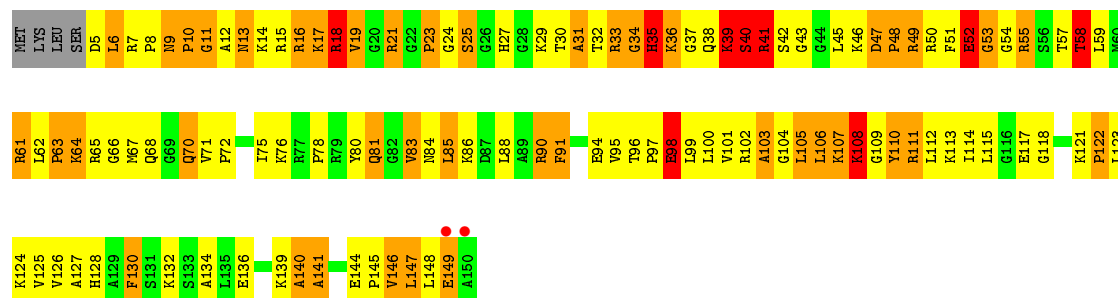
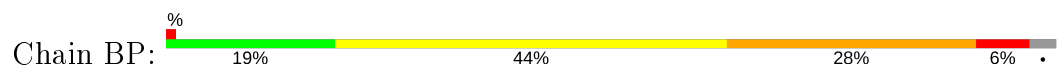
• Molecule 45: 50S RIBOSOMAL PROTEIN L14



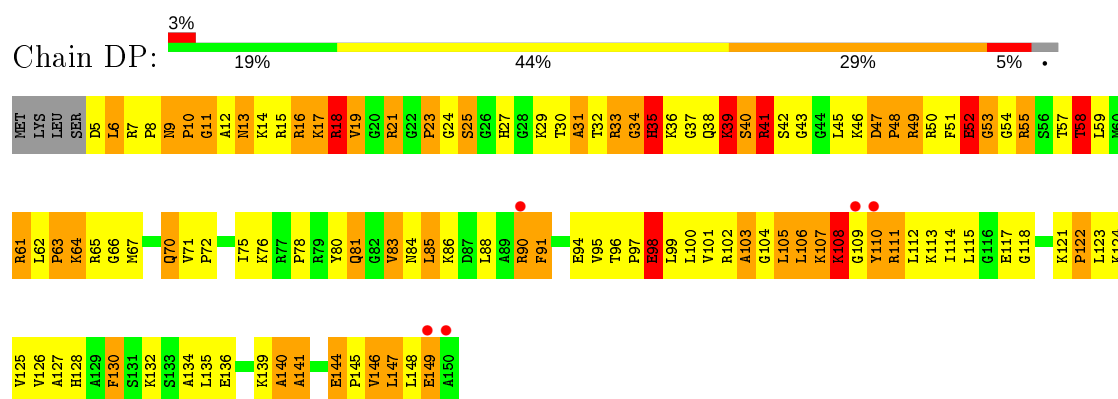
• Molecule 45: 50S RIBOSOMAL PROTEIN L14



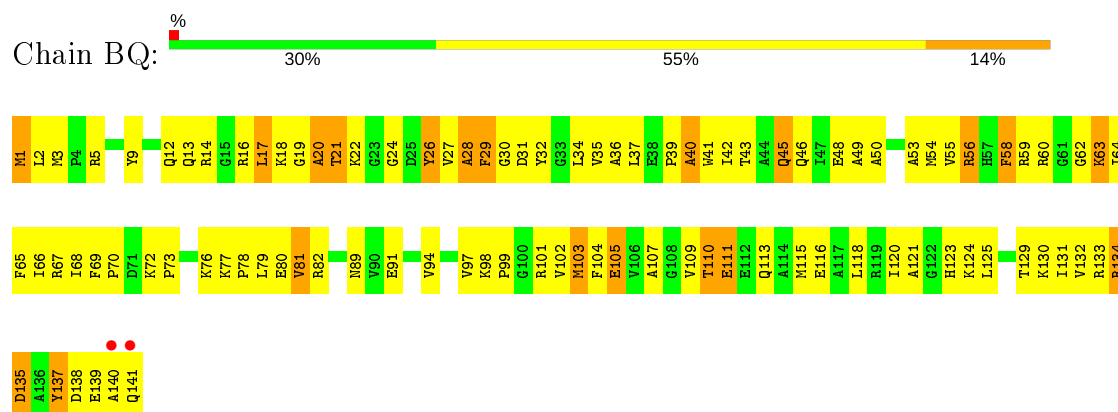
• Molecule 46: 50S RIBOSOMAL PROTEIN L15



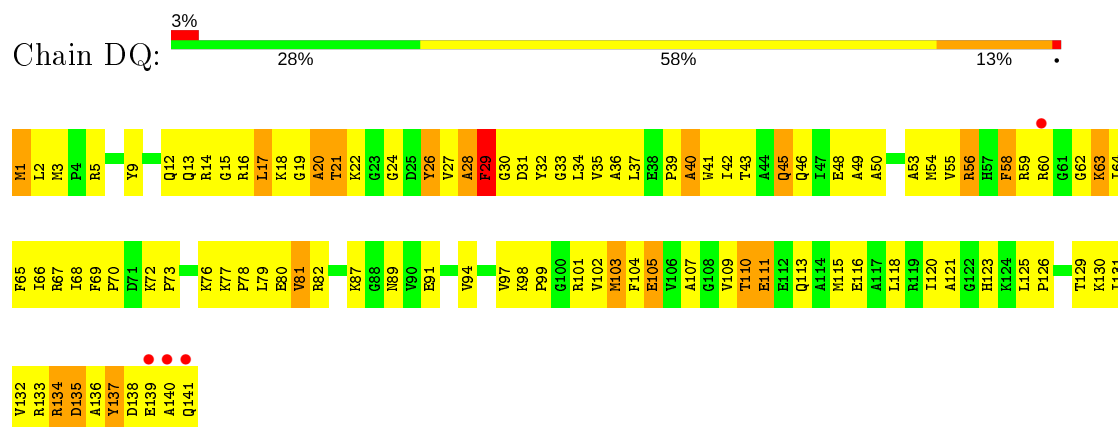
• Molecule 46: 50S RIBOSOMAL PROTEIN L15



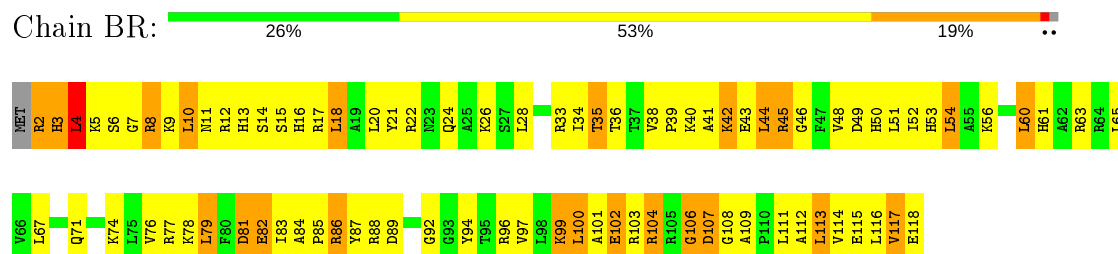
• Molecule 47: 50S RIBOSOMAL PROTEIN L16



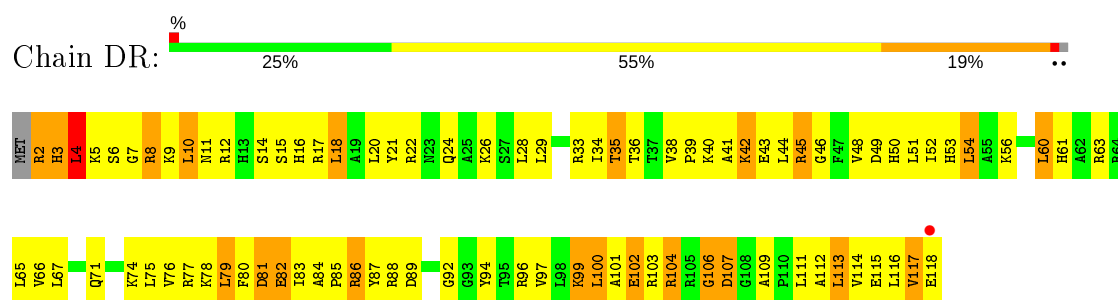
• Molecule 47: 50S RIBOSOMAL PROTEIN L16



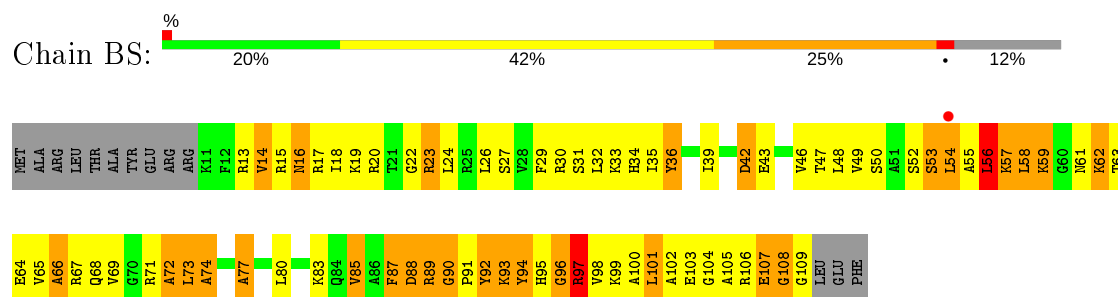
• Molecule 48: 50S RIBOSOMAL PROTEIN L17



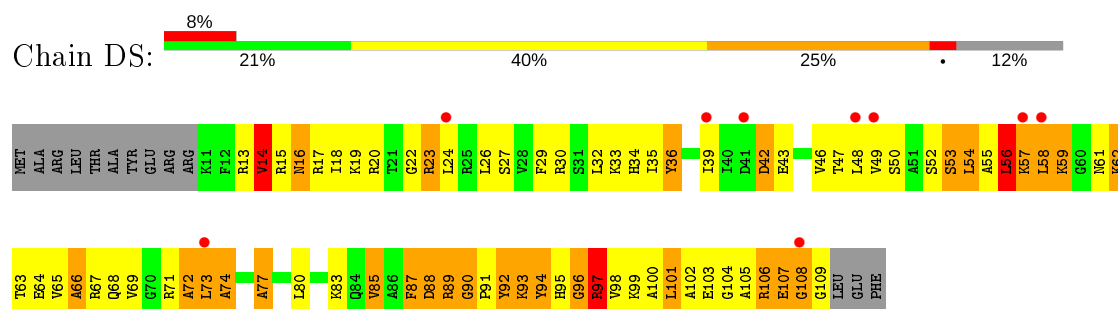
• Molecule 48: 50S RIBOSOMAL PROTEIN L17



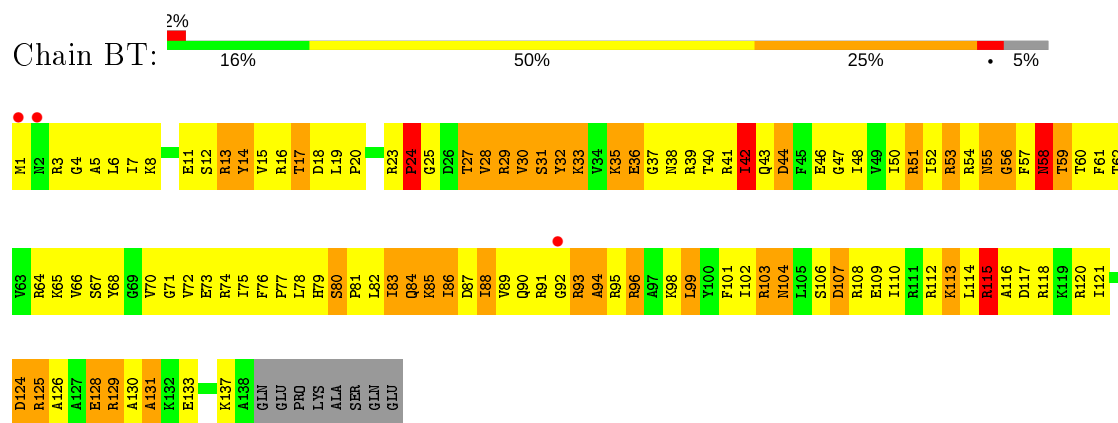
• Molecule 49: 50S RIBOSOMAL PROTEIN L18



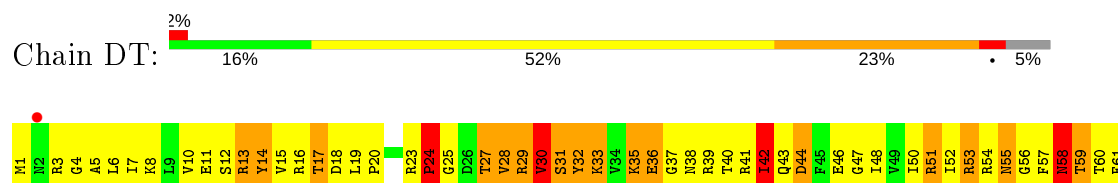
• Molecule 49: 50S RIBOSOMAL PROTEIN L18

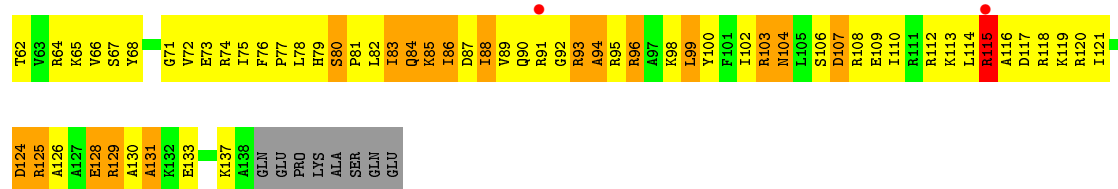


• Molecule 50: 50S RIBOSOMAL PROTEIN L19

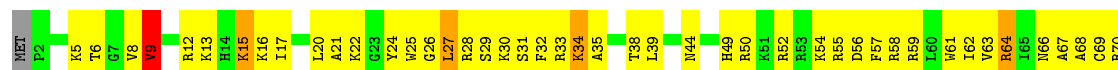


• Molecule 50: 50S RIBOSOMAL PROTEIN L19

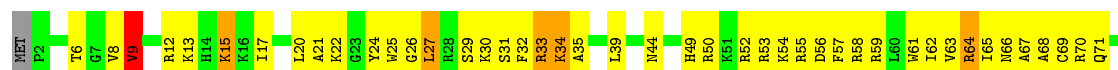




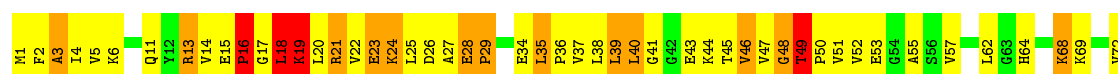
• Molecule 51: 50S RIBOSOMAL PROTEIN L20



• Molecule 51: 50S RIBOSOMAL PROTEIN L20



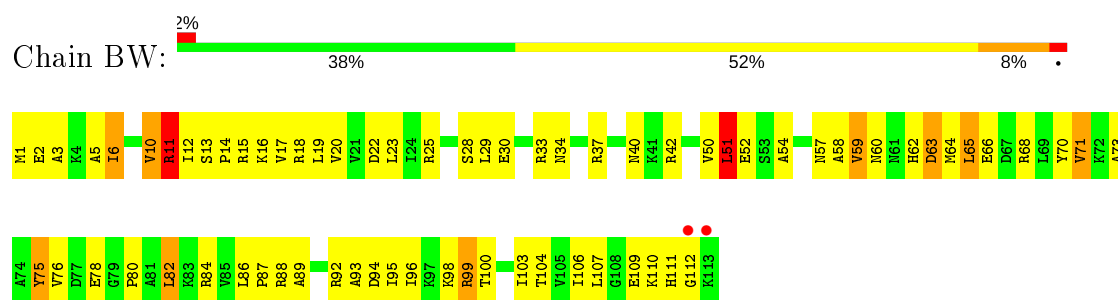
• Molecule 52: 50S RIBOSOMAL PROTEIN L21



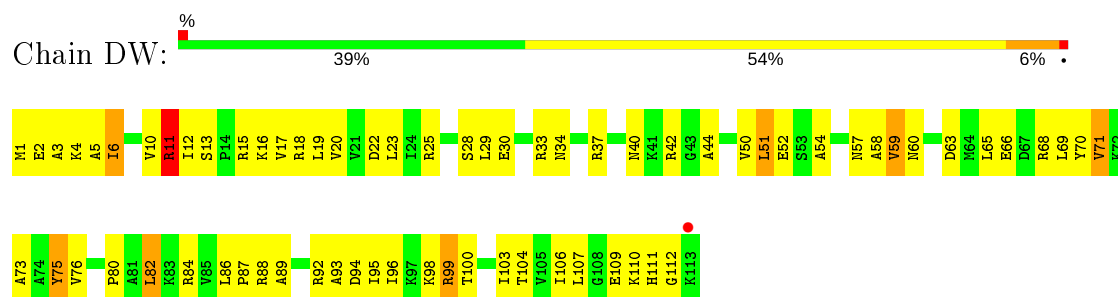
• Molecule 52: 50S RIBOSOMAL PROTEIN L21



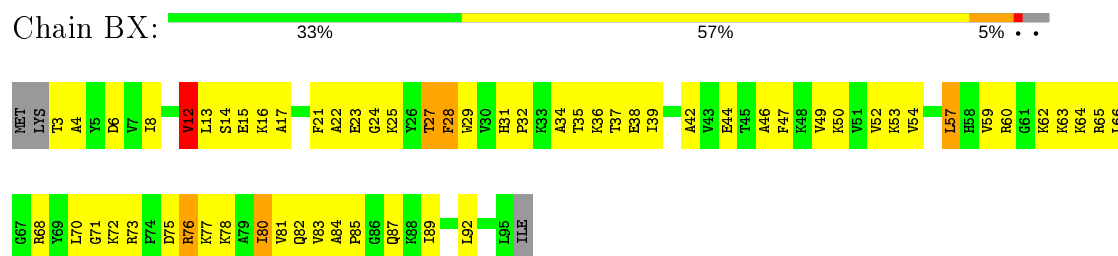
• Molecule 53: 50S RIBOSOMAL PROTEIN L22



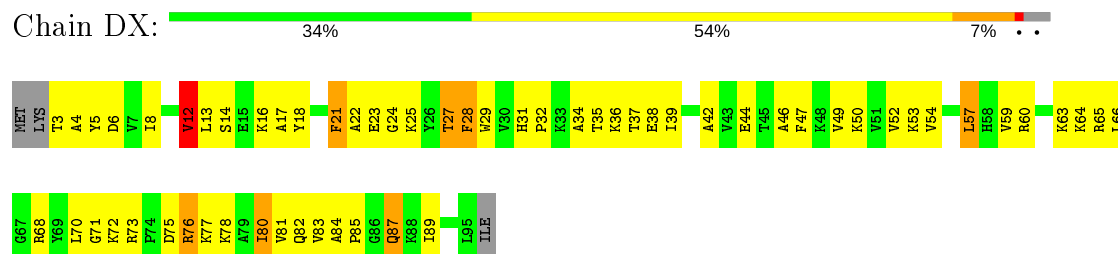
• Molecule 53: 50S RIBOSOMAL PROTEIN L22



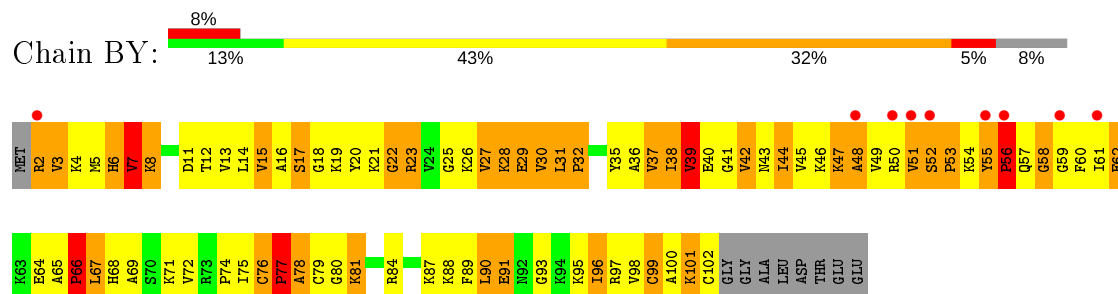
• Molecule 54: 50S RIBOSOMAL PROTEIN L23



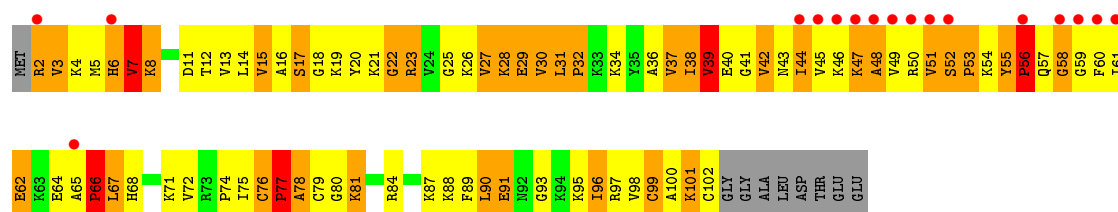
• Molecule 54: 50S RIBOSOMAL PROTEIN L23



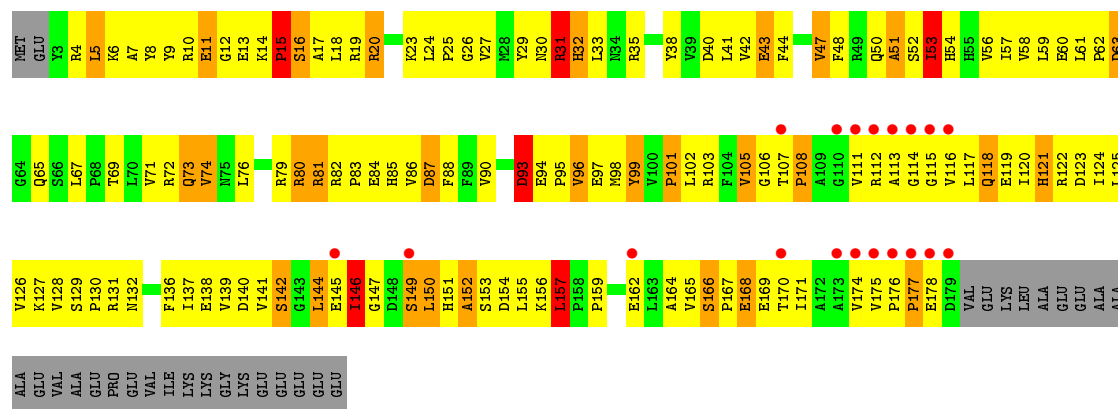
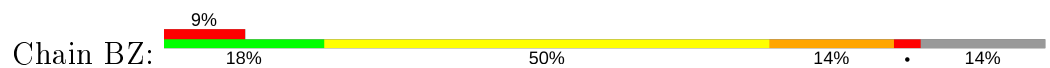
• Molecule 55: 50S RIBOSOMAL PROTEIN L24



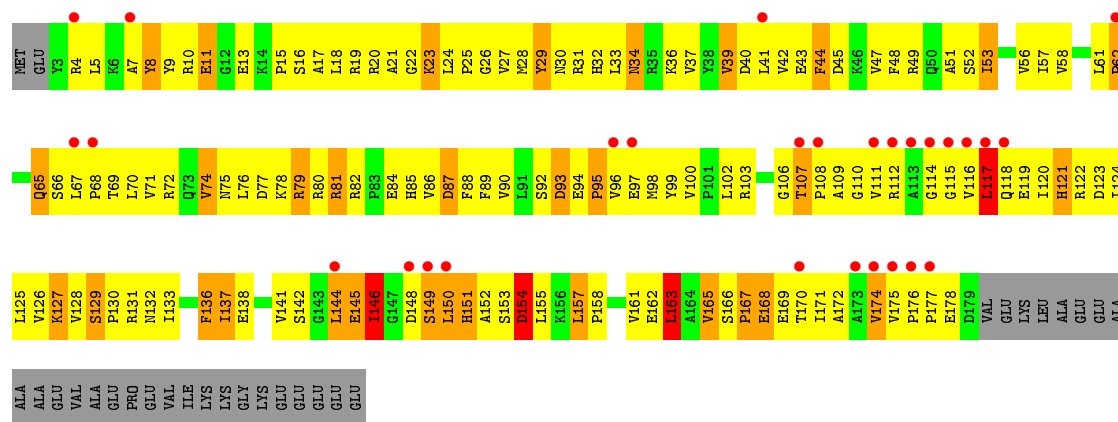
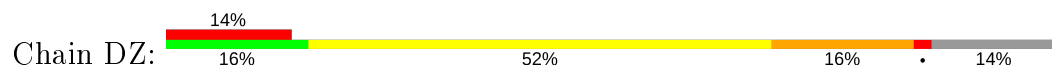
• Molecule 55: 50S RIBOSOMAL PROTEIN L24



• Molecule 56: 50S RIBOSOMAL PROTEIN L25



• Molecule 56: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.86Å 450.46Å 628.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.50) 97.2 (49.74-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.256 0.210 , 0.256	Depositor DCC
R_{free} test set	36181 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296042	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 8AN, PHA

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	0.42	0/36190	0.70	16/56486 (0.0%)
1	CA	0.40	0/36190	0.69	14/56486 (0.0%)
2	AB	0.33	0/1936	0.60	0/2611
2	CB	0.32	0/1936	0.60	0/2611
3	AC	0.34	0/1637	0.60	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.36	0/1733	0.64	0/2318
4	CD	0.36	0/1733	0.64	0/2318
5	AE	0.36	0/1163	0.64	0/1566
5	CE	0.35	0/1163	0.64	0/1566
6	AF	0.36	0/856	0.66	0/1154
6	CF	0.35	0/856	0.66	0/1154
7	AG	0.32	0/1276	0.57	0/1709
7	CG	0.31	0/1276	0.57	0/1709
8	AH	0.31	0/1136	0.63	0/1527
8	CH	0.30	0/1136	0.62	0/1527
9	AI	0.32	0/1027	0.59	0/1372
9	CI	0.32	0/1027	0.59	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.35	0/808	0.64	0/1087
11	AK	0.35	0/900	0.62	0/1213
11	CK	0.33	0/900	0.61	0/1213
12	AL	0.39	0/987	0.70	0/1322
12	CL	0.37	0/987	0.68	0/1322
13	AM	0.34	0/996	0.66	0/1329
13	CM	0.33	0/996	0.66	0/1329
14	AN	0.36	0/501	0.62	0/664
14	CN	0.33	0/501	0.61	0/664
15	AO	0.35	0/745	0.59	0/992
15	CO	0.33	0/745	0.58	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.61	0/1119
17	CQ	0.37	0/837	0.62	0/1119
18	AR	0.36	0/579	0.60	0/768
18	CR	0.36	0/579	0.60	0/768
19	AS	0.38	0/643	0.63	0/867
19	CS	0.36	0/643	0.62	0/867
20	AT	0.30	0/765	0.59	0/1007
20	CT	0.30	0/765	0.58	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.45	0/213	0.60	0/279
22	AV	0.44	0/1784	0.75	0/2780
22	AY	0.47	0/1784	0.74	0/2780
22	CV	0.40	0/1784	0.71	0/2780
22	CY	0.41	0/1784	0.73	0/2780
23	AW	0.43	0/1809	0.71	0/2819
23	CW	0.42	0/1809	0.71	0/2819
24	AX	0.48	0/253	0.72	0/391
24	CX	0.42	0/253	0.73	1/391 (0.3%)
25	B0	0.44	0/671	0.71	0/892
25	D0	0.41	0/671	0.69	0/892
26	B1	0.48	0/739	0.85	0/983
26	D1	0.46	0/739	0.72	0/983
27	B2	0.43	0/600	0.73	0/793
27	D2	0.39	0/600	0.65	0/793
28	B3	0.43	0/473	0.68	0/636
28	D3	0.37	0/473	0.64	0/636
29	B4	0.46	0/229	0.68	0/311
29	D4	0.44	0/229	0.67	0/311
30	B5	0.62	0/473	0.96	0/639
30	D5	0.49	0/473	0.92	0/639
31	B6	0.57	0/387	0.76	0/517
31	D6	0.51	0/387	0.75	0/517
32	B7	0.52	0/427	0.67	0/563
32	D7	0.48	0/427	0.65	0/563
33	B8	0.59	0/516	0.89	2/681 (0.3%)
33	D8	0.51	0/516	0.88	2/681 (0.3%)
34	B9	0.33	0/302	0.54	0/397
34	D9	0.29	0/302	0.53	0/397
35	BA	0.59	5/67716 (0.0%)	0.76	38/105718 (0.0%)
35	DA	0.48	4/67716 (0.0%)	0.74	31/105718 (0.0%)
36	BB	0.50	0/2853	0.75	1/4451 (0.0%)
36	DB	0.42	0/2853	0.74	1/4451 (0.0%)
37	BC	0.37	0/1143	0.68	5/1552 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.37	0/1145	0.69	6/1556 (0.4%)
38	BD	0.51	0/2155	0.80	1/2907 (0.0%)
38	DD	0.47	0/2155	0.79	1/2907 (0.0%)
39	BE	0.47	0/1597	0.80	1/2155 (0.0%)
39	DE	0.41	0/1597	0.77	0/2155
40	BF	0.46	0/1659	0.71	0/2246
40	DF	0.42	0/1659	0.69	0/2246
41	BG	0.40	0/1498	0.77	2/2013 (0.1%)
41	DG	0.38	0/1498	0.71	1/2013 (0.0%)
42	BH	0.44	0/1246	0.77	0/1684
42	DH	0.37	0/1246	0.74	0/1684
43	BI	0.36	0/1147	0.65	0/1553
43	DI	0.35	0/1147	0.63	0/1553
44	BN	0.45	0/1132	0.75	0/1527
44	DN	0.38	0/1132	0.72	0/1527
45	BO	0.44	0/943	0.68	0/1269
45	DO	0.37	0/943	0.67	0/1269
46	BP	0.51	0/1131	1.01	5/1504 (0.3%)
46	DP	0.45	0/1131	0.98	5/1504 (0.3%)
47	BQ	0.45	0/1143	0.69	0/1527
47	DQ	0.40	0/1143	0.67	0/1527
48	BR	0.44	0/974	0.79	2/1302 (0.2%)
48	DR	0.39	0/974	0.76	1/1302 (0.1%)
49	BS	0.48	0/779	0.83	1/1038 (0.1%)
49	DS	0.42	0/779	0.79	2/1038 (0.2%)
50	BT	0.44	0/1156	0.79	1/1544 (0.1%)
50	DT	0.41	0/1156	0.78	1/1544 (0.1%)
51	BU	0.52	0/975	0.79	2/1297 (0.2%)
51	DU	0.42	0/975	0.74	2/1297 (0.2%)
52	BV	0.46	0/790	0.77	1/1057 (0.1%)
52	DV	0.38	0/790	0.74	1/1057 (0.1%)
53	BW	0.49	0/907	0.78	1/1216 (0.1%)
53	DW	0.42	0/907	0.75	0/1216
54	BX	0.48	0/740	0.73	1/995 (0.1%)
54	DX	0.44	0/740	0.71	1/995 (0.1%)
55	BY	0.56	0/789	0.85	0/1053
55	DY	0.49	0/789	0.83	0/1053
56	BZ	0.42	0/1436	0.72	0/1951
56	DZ	0.36	0/1436	0.65	0/1951
All	All	0.47	9/320004 (0.0%)	0.72	150/478610 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	10
1	CA	0	8
23	AW	0	2
35	BA	4	39
35	DA	3	33
36	BB	0	3
36	DB	0	3
All	All	7	98

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	652	C	C3'-O3'	8.01	1.53	1.42
35	DA	652	C	C3'-O3'	7.44	1.52	1.42
35	BA	652	C	O3'-P	6.31	1.68	1.61
35	DA	652	C	O3'-P	5.91	1.68	1.61
35	BA	652	C	O5'-C5'	5.67	1.53	1.44

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BP	52	GLU	N-CA-C	9.63	137.00	111.00
46	DP	52	GLU	N-CA-C	9.54	136.76	111.00
35	BA	283	A	C2'-C3'-O3'	9.40	130.18	109.50
35	BA	1799	G	C2'-C3'-O3'	9.35	130.07	109.50
35	DA	1799	G	C2'-C3'-O3'	9.28	129.91	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	283	A	C3'
35	BA	1378	A	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'
35	DA	283	A	C3'

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	484	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	Sidechain
1	AA	9	G	Sidechain

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	32329	0	16315	1280	0
1	CA	32329	0	16312	1275	0
2	AB	1901	0	1951	273	0
2	CB	1901	0	1951	273	0
3	AC	1613	0	1677	245	0
3	CC	1613	0	1677	250	0
4	AD	1703	0	1762	166	0
4	CD	1703	0	1763	166	0
5	AE	1147	0	1207	137	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	97	0
6	CF	843	0	857	91	0
7	AG	1257	0	1296	117	0
7	CG	1257	0	1296	113	0
8	AH	1116	0	1177	127	0
8	CH	1116	0	1177	127	0
9	AI	1011	0	1041	170	0
9	CI	1011	0	1041	167	0
10	AJ	795	0	840	175	0
10	CJ	795	0	840	177	0
11	AK	885	0	904	103	0
11	CK	885	0	904	98	0
12	AL	971	0	1057	130	0
12	CL	971	0	1057	126	0
13	AM	988	0	1056	173	0
13	CM	988	0	1056	168	0
14	AN	492	0	529	74	0
14	CN	492	0	529	75	0
15	AO	734	0	771	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	77	0
16	AP	701	0	720	82	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	92	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	82	0
18	CR	574	0	644	86	0
19	AS	630	0	652	105	0
19	CS	630	0	652	96	0
20	AT	763	0	861	102	0
20	CT	763	0	861	102	0
21	AU	209	0	221	17	0
21	CU	209	0	221	19	0
22	AV	1630	0	831	65	0
22	AY	1630	0	831	84	0
22	CV	1630	0	831	78	0
22	CY	1630	0	831	71	0
23	AW	1619	0	822	93	0
23	CW	1619	0	821	94	0
24	AX	227	0	119	7	0
24	CX	227	0	118	10	0
25	B0	662	0	688	81	0
25	D0	662	0	688	81	0
26	B1	732	0	808	95	0
26	D1	732	0	808	88	0
27	B2	598	0	653	59	0
27	D2	598	0	653	86	0
28	B3	468	0	523	31	0
28	D3	468	0	523	30	0
29	B4	226	0	229	43	0
29	D4	226	0	229	35	0
30	B5	459	0	480	86	0
30	D5	459	0	480	86	0
31	B6	381	0	390	106	0
31	D6	381	0	390	105	0
32	B7	419	0	467	30	0
32	D7	419	0	467	30	0
33	B8	508	0	576	100	0
33	D8	508	0	576	98	0
34	B9	299	0	325	29	0
34	D9	299	0	325	31	0
35	BA	60459	0	30474	2060	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	60459	0	30478	2070	0
36	BB	2551	0	1294	105	0
36	DB	2551	0	1294	89	0
37	BC	1140	0	863	123	0
37	DC	1142	0	865	126	0
38	BD	2105	0	2182	327	0
38	DD	2105	0	2182	319	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	245	0
40	BF	1624	0	1677	211	0
40	DF	1624	0	1677	207	0
41	BG	1474	0	1534	253	0
41	DG	1474	0	1534	269	0
42	BH	1223	0	1282	173	0
42	DH	1223	0	1282	173	0
43	BI	1132	0	1218	196	0
43	DI	1132	0	1218	198	0
44	BN	1105	0	1180	138	0
44	DN	1105	0	1180	138	0
45	BO	933	0	996	121	0
45	DO	933	0	996	123	0
46	BP	1114	0	1187	280	0
46	DP	1114	0	1187	278	0
47	BQ	1122	0	1179	169	0
47	DQ	1122	0	1179	166	0
48	BR	960	0	1021	139	0
48	DR	960	0	1021	140	0
49	BS	771	0	832	152	0
49	DS	771	0	832	143	0
50	BT	1142	0	1202	241	0
50	DT	1142	0	1202	228	0
51	BU	958	0	1015	156	0
51	DU	958	0	1015	154	0
52	BV	779	0	852	159	0
52	DV	779	0	852	162	0
53	BW	896	0	953	90	0
53	DW	896	0	953	85	0
54	BX	726	0	778	87	0
54	DX	726	0	778	86	0
55	BY	776	0	870	184	0
55	DY	776	0	870	193	0
56	BZ	1404	0	1432	232	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DZ	1404	0	1432	232	0
57	AA	198	0	0	0	0
57	AD	1	0	0	0	0
57	AE	1	0	0	0	0
57	AG	1	0	0	0	0
57	AI	1	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AV	5	0	0	0	0
57	AW	8	0	0	0	0
57	AX	2	0	0	0	0
57	B0	1	0	0	0	0
57	B1	1	0	0	0	0
57	B2	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	422	0	0	0	0
57	BB	14	0	0	0	0
57	BD	2	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	1	0
57	BV	1	0	0	0	0
57	BX	2	0	0	0	0
57	CA	199	0	0	0	0
57	CE	1	0	0	0	0
57	CI	1	0	0	0	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CV	5	0	0	0	0
57	CW	7	0	0	0	0
57	CX	3	0	0	0	0
57	D1	1	0	0	0	0
57	D2	3	0	0	0	0
57	D5	2	0	0	0	0
57	D7	2	0	0	0	0
57	DA	421	0	0	0	0
57	DB	13	0	0	0	0
57	DC	1	0	0	0	0
57	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DE	1	0	0	0	0
57	DF	2	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DS	1	0	0	0	0
57	DV	1	0	0	0	0
57	DX	3	0	0	0	0
58	AA	42	0	45	2	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D9	1	0	0	0	0
All	All	296042	0	199734	19172	0

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 39.

The worst 5 of 19172 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)
54:BX:63:LYS:HE3	54:BX:72:LYS:HE3	1.23	1.21
56:DZ:53:ILE:HG23	56:DZ:71:VAL:HG23	1.21	1.18
46:DP:59:LEU:HA	46:DP:61:ARG:CZ	1.73	1.18
53:BW:1:MET:HE2	53:BW:2:GLU:H	1.06	1.17
35:BA:2334:G:H21	49:BS:18:ILE:HD11	1.09	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	138 (59%)	63 (27%)	32 (14%)	0	4
2	CB	233/256 (91%)	138 (59%)	62 (27%)	33 (14%)	0	3
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	0	7
3	CC	205/239 (86%)	128 (62%)	56 (27%)	21 (10%)	0	7
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	9
4	CD	206/209 (99%)	150 (73%)	38 (18%)	18 (9%)	1	9
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	1	11
5	CE	149/162 (92%)	115 (77%)	22 (15%)	12 (8%)	1	9
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	19
6	CF	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	2	19
7	AG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	3	25
7	CG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	3	25
8	AH	136/138 (99%)	107 (79%)	25 (18%)	4 (3%)	4	31
8	CH	136/138 (99%)	108 (79%)	24 (18%)	4 (3%)	4	31
9	AI	121/128 (94%)	85 (70%)	23 (19%)	13 (11%)	0	6
9	CI	121/128 (94%)	83 (69%)	26 (22%)	12 (10%)	0	7
10	AJ	97/105 (92%)	62 (64%)	25 (26%)	10 (10%)	0	7
10	CJ	97/105 (92%)	63 (65%)	24 (25%)	10 (10%)	0	7
11	AK	117/129 (91%)	86 (74%)	26 (22%)	5 (4%)	2	22
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	2	22
12	AL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	6
12	CL	123/135 (91%)	83 (68%)	26 (21%)	14 (11%)	0	6
13	AM	117/126 (93%)	67 (57%)	30 (26%)	20 (17%)	0	2
13	CM	117/126 (93%)	67 (57%)	31 (26%)	19 (16%)	0	2
14	AN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	3
14	CN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	3
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	0	8
15	CO	86/89 (97%)	57 (66%)	21 (24%)	8 (9%)	0	8
16	AP	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	6	35
16	CP	82/88 (93%)	59 (72%)	21 (26%)	2 (2%)	6	35
17	AQ	98/105 (93%)	74 (76%)	20 (20%)	4 (4%)	3	23
17	CQ	98/105 (93%)	76 (78%)	19 (19%)	3 (3%)	4	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	41 (60%)	14 (21%)	13 (19%)	0	2
18	CR	68/88 (77%)	41 (60%)	13 (19%)	14 (21%)	0	1
19	AS	77/93 (83%)	49 (64%)	16 (21%)	12 (16%)	0	2
19	CS	77/93 (83%)	49 (64%)	15 (20%)	13 (17%)	0	2
20	AT	97/106 (92%)	69 (71%)	18 (19%)	10 (10%)	0	7
20	CT	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	0	7
21	AU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	9
21	CU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	9
25	B0	82/85 (96%)	65 (79%)	14 (17%)	3 (4%)	3	26
25	D0	82/85 (96%)	61 (74%)	17 (21%)	4 (5%)	2	19
26	B1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	0	6
26	D1	92/98 (94%)	66 (72%)	18 (20%)	8 (9%)	1	9
27	B2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	0	7
27	D2	69/72 (96%)	37 (54%)	23 (33%)	9 (13%)	0	4
28	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	18
28	D3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	18
29	B4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
29	D4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
30	B5	57/60 (95%)	38 (67%)	8 (14%)	11 (19%)	0	2
30	D5	57/60 (95%)	39 (68%)	6 (10%)	12 (21%)	0	1
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
31	D6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	3
33	D8	62/65 (95%)	43 (69%)	10 (16%)	9 (14%)	0	3
34	B9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
34	D9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
37	BC	183/229 (80%)	81 (44%)	47 (26%)	55 (30%)	0	0
37	DC	183/229 (80%)	82 (45%)	47 (26%)	54 (30%)	0	0
38	BD	270/276 (98%)	208 (77%)	38 (14%)	24 (9%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	205 (76%)	38 (14%)	27 (10%)	0	7
39	BE	203/206 (98%)	130 (64%)	40 (20%)	33 (16%)	0	2
39	DE	203/206 (98%)	127 (63%)	44 (22%)	32 (16%)	0	2
40	BF	206/210 (98%)	142 (69%)	35 (17%)	29 (14%)	0	3
40	DF	206/210 (98%)	143 (69%)	35 (17%)	28 (14%)	0	4
41	BG	177/182 (97%)	107 (60%)	50 (28%)	20 (11%)	0	6
41	DG	177/182 (97%)	108 (61%)	45 (25%)	24 (14%)	0	4
42	BH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	2
42	DH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	2
43	BI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	3
43	DI	144/148 (97%)	85 (59%)	37 (26%)	22 (15%)	0	3
44	BN	137/140 (98%)	90 (66%)	30 (22%)	17 (12%)	0	5
44	DN	137/140 (98%)	91 (66%)	29 (21%)	17 (12%)	0	5
45	BO	120/122 (98%)	91 (76%)	21 (18%)	8 (7%)	1	13
45	DO	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	13
46	BP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
46	DP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
47	BQ	139/141 (99%)	107 (77%)	24 (17%)	8 (6%)	1	16
47	DQ	139/141 (99%)	106 (76%)	23 (16%)	10 (7%)	1	11
48	BR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	5
48	DR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	5
49	BS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	0
49	DS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	0
50	BT	136/146 (93%)	82 (60%)	26 (19%)	28 (21%)	0	1
50	DT	136/146 (93%)	81 (60%)	27 (20%)	28 (21%)	0	1
51	BU	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	1	15
51	DU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	10
52	BV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	3
52	DV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	3
53	BW	111/113 (98%)	87 (78%)	15 (14%)	9 (8%)	1	9
53	DW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BX	91/96 (95%)	74 (81%)	14 (15%)	3 (3%)	4	28
54	DX	91/96 (95%)	74 (81%)	13 (14%)	4 (4%)	2	21
55	BY	99/110 (90%)	37 (37%)	30 (30%)	32 (32%)	0	0
55	DY	99/110 (90%)	35 (35%)	32 (32%)	32 (32%)	0	0
56	BZ	175/206 (85%)	113 (65%)	38 (22%)	24 (14%)	0	4
56	DZ	175/206 (85%)	103 (59%)	45 (26%)	27 (15%)	0	3
All	All	11670/12592 (93%)	7783 (67%)	2440 (21%)	1447 (12%)	0	5

5 of 1447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	88	ALA
2	AB	154	LEU
2	AB	165	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	181 (90%)	21 (10%)	7	31
2	CB	202/220 (92%)	181 (90%)	21 (10%)	7	31
3	AC	160/188 (85%)	152 (95%)	8 (5%)	24	58
3	CC	160/188 (85%)	151 (94%)	9 (6%)	21	54
4	AD	180/181 (99%)	161 (89%)	19 (11%)	6	30
4	CD	180/181 (99%)	159 (88%)	21 (12%)	5	26
5	AE	115/123 (94%)	106 (92%)	9 (8%)	12	42
5	CE	115/123 (94%)	107 (93%)	8 (7%)	15	46
6	AF	90/90 (100%)	85 (94%)	5 (6%)	21	54
6	CF	90/90 (100%)	85 (94%)	5 (6%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	118 (94%)	8 (6%)	18	51
7	CG	126/127 (99%)	117 (93%)	9 (7%)	14	46
8	AH	119/119 (100%)	111 (93%)	8 (7%)	16	48
8	CH	119/119 (100%)	111 (93%)	8 (7%)	16	48
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	32
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	32
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	3	20
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	23
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	48
11	CK	90/99 (91%)	84 (93%)	6 (7%)	16	48
12	AL	104/111 (94%)	93 (89%)	11 (11%)	6	30
12	CL	104/111 (94%)	92 (88%)	12 (12%)	5	26
13	AM	99/101 (98%)	90 (91%)	9 (9%)	9	36
13	CM	99/101 (98%)	90 (91%)	9 (9%)	9	36
14	AN	49/50 (98%)	46 (94%)	3 (6%)	18	51
14	CN	49/50 (98%)	46 (94%)	3 (6%)	18	51
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	26
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	26
16	AP	72/74 (97%)	61 (85%)	11 (15%)	2	17
16	CP	72/74 (97%)	61 (85%)	11 (15%)	2	17
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	22	55
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	22	55
18	AR	61/77 (79%)	53 (87%)	8 (13%)	4	21
18	CR	61/77 (79%)	52 (85%)	9 (15%)	3	17
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	21
19	CS	69/80 (86%)	60 (87%)	9 (13%)	4	21
20	AT	76/82 (93%)	71 (93%)	5 (7%)	16	49
20	CT	76/82 (93%)	71 (93%)	5 (7%)	16	49
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	55
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	55
25	B0	66/67 (98%)	59 (89%)	7 (11%)	6	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	6	30
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	12
26	D1	78/83 (94%)	66 (85%)	12 (15%)	2	16
27	B2	66/67 (98%)	57 (86%)	9 (14%)	3	20
27	D2	66/67 (98%)	57 (86%)	9 (14%)	3	20
28	B3	51/52 (98%)	49 (96%)	2 (4%)	32	64
28	D3	51/52 (98%)	49 (96%)	2 (4%)	32	64
29	B4	27/63 (43%)	23 (85%)	4 (15%)	3	17
29	D4	27/63 (43%)	23 (85%)	4 (15%)	3	17
30	B5	51/52 (98%)	42 (82%)	9 (18%)	2	10
30	D5	51/52 (98%)	41 (80%)	10 (20%)	1	7
31	B6	43/52 (83%)	34 (79%)	9 (21%)	1	6
31	D6	43/52 (83%)	34 (79%)	9 (21%)	1	6
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	23
32	D7	41/42 (98%)	36 (88%)	5 (12%)	5	23
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	6
33	D8	53/55 (96%)	42 (79%)	11 (21%)	1	6
34	B9	33/34 (97%)	30 (91%)	3 (9%)	9	36
34	D9	33/34 (97%)	30 (91%)	3 (9%)	9	36
37	BC	61/181 (34%)	53 (87%)	8 (13%)	4	21
37	DC	61/181 (34%)	53 (87%)	8 (13%)	4	21
38	BD	213/218 (98%)	183 (86%)	30 (14%)	3	19
38	DD	213/218 (98%)	183 (86%)	30 (14%)	3	19
39	BE	165/166 (99%)	142 (86%)	23 (14%)	3	20
39	DE	165/166 (99%)	143 (87%)	22 (13%)	4	21
40	BF	165/166 (99%)	150 (91%)	15 (9%)	9	36
40	DF	165/166 (99%)	151 (92%)	14 (8%)	10	39
41	BG	155/156 (99%)	133 (86%)	22 (14%)	3	19
41	DG	155/156 (99%)	129 (83%)	26 (17%)	2	12
42	BH	132/148 (89%)	119 (90%)	13 (10%)	8	33
42	DH	132/148 (89%)	119 (90%)	13 (10%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	113 (93%)	9 (7%)	13	44
43	DI	122/124 (98%)	113 (93%)	9 (7%)	13	44
44	BN	117/119 (98%)	98 (84%)	19 (16%)	2	14
44	DN	117/119 (98%)	100 (86%)	17 (14%)	3	18
45	BO	100/100 (100%)	90 (90%)	10 (10%)	7	32
45	DO	100/100 (100%)	92 (92%)	8 (8%)	12	41
46	BP	112/116 (97%)	92 (82%)	20 (18%)	2	9
46	DP	112/116 (97%)	93 (83%)	19 (17%)	2	12
47	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	17
47	DQ	111/111 (100%)	94 (85%)	17 (15%)	2	17
48	BR	100/101 (99%)	88 (88%)	12 (12%)	5	24
48	DR	100/101 (99%)	88 (88%)	12 (12%)	5	24
49	BS	77/88 (88%)	68 (88%)	9 (12%)	5	26
49	DS	77/88 (88%)	67 (87%)	10 (13%)	4	21
50	BT	120/127 (94%)	101 (84%)	19 (16%)	2	15
50	DT	120/127 (94%)	101 (84%)	19 (16%)	2	15
51	BU	92/94 (98%)	80 (87%)	12 (13%)	4	21
51	DU	92/94 (98%)	80 (87%)	12 (13%)	4	21
52	BV	82/82 (100%)	68 (83%)	14 (17%)	2	12
52	DV	82/82 (100%)	69 (84%)	13 (16%)	2	14
53	BW	91/92 (99%)	83 (91%)	8 (9%)	10	38
53	DW	91/92 (99%)	83 (91%)	8 (9%)	10	38
54	BX	74/78 (95%)	67 (90%)	7 (10%)	8	34
54	DX	74/78 (95%)	67 (90%)	7 (10%)	8	34
55	BY	84/91 (92%)	70 (83%)	14 (17%)	2	12
55	DY	84/91 (92%)	70 (83%)	14 (17%)	2	12
56	BZ	155/179 (87%)	133 (86%)	22 (14%)	3	19
56	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	16
All	All	9654/10432 (92%)	8547 (88%)	1107 (12%)	5	26

5 of 1107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BV	99	ILE
7	CG	113	GLU
50	DT	99	LEU
54	BX	80	ILE
2	CB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
53	BW	62	HIS
6	CF	100	ASN
48	DR	53	HIS
54	BX	55	ASN
3	CC	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	215 (14%)	29 (1%)
1	CA	1503/1522 (98%)	216 (14%)	29 (1%)
22	AV	74/77 (96%)	15 (20%)	0
22	AY	74/77 (96%)	20 (27%)	1 (1%)
22	CV	74/77 (96%)	19 (25%)	1 (1%)
22	CY	74/77 (96%)	20 (27%)	1 (1%)
23	AW	75/76 (98%)	13 (17%)	0
23	CW	75/76 (98%)	15 (20%)	0
24	AX	10/11 (90%)	1 (10%)	0
24	CX	10/11 (90%)	2 (20%)	0
35	BA	2806/2822 (99%)	516 (18%)	55 (1%)
35	DA	2806/2822 (99%)	515 (18%)	53 (1%)
36	BB	118/122 (96%)	13 (11%)	1 (0%)
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9320/9414 (99%)	1593 (17%)	171 (1%)

5 of 1593 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	48	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2481	G
1	CA	366	C
35	DA	2172	U
35	BA	2610	C
1	CA	30	U

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
22	PHA	CY	77	22	10,11,11	1.08	0	10,13,13	0.40	0
22	8AN	AY	76	35,22	19,24,25	1.11	1 (5%)	13,35,38	0.95	1 (7%)
22	8AN	CV	76	57,22	19,24,25	1.09	2 (10%)	13,35,38	1.09	2 (15%)
22	8AN	AV	76	57,22	19,24,25	1.03	1 (5%)	13,35,38	1.12	2 (15%)
22	PHA	AV	77	22	10,11,11	0.64	0	10,13,13	0.42	0
22	PHA	CV	77	22	10,11,11	0.65	0	10,13,13	0.36	0
22	8AN	CY	76	35,22	19,24,25	0.94	1 (5%)	13,35,38	0.89	1 (7%)
22	PHA	AY	77	22	10,11,11	0.66	0	10,13,13	0.61	0

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
22	PHA	CY	77	22	-	2/5/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	8AN	AY	76	35,22	-	0/3/25/26	0/3/3/3
22	8AN	CV	76	57,22	-	1/3/25/26	0/3/3/3
22	8AN	AV	76	57,22	-	1/3/25/26	0/3/3/3
22	PHA	AV	77	22	-	0/5/6/6	0/1/1/1
22	PHA	CV	77	22	-	0/5/6/6	0/1/1/1
22	8AN	CY	76	35,22	-	0/3/25/26	0/3/3/3
22	PHA	AY	77	22	-	3/5/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AY	76	8AN	C3'-N3'	-3.68	1.41	1.47
22	AV	76	8AN	C3'-N3'	-3.62	1.41	1.47
22	CV	76	8AN	C3'-N3'	-3.44	1.42	1.47
22	CY	76	8AN	C3'-N3'	-2.77	1.43	1.47
22	CV	76	8AN	C2-N3	2.34	1.35	1.32

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AY	76	8AN	C5-C6-N6	2.54	124.20	120.35
22	AV	76	8AN	C5-C6-N6	2.41	124.02	120.35
22	CV	76	8AN	C5-C6-N6	2.39	123.99	120.35
22	CY	76	8AN	C5-C6-N6	2.35	123.93	120.35
22	AV	76	8AN	O4'-C4'-C3'	2.23	107.35	104.15

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CY	77	PHA	C-CA-CB-CG
22	CV	76	8AN	C4'-C5'-O5'-P
22	AV	76	8AN	C4'-C5'-O5'-P
22	AY	77	PHA	O-C-CA-CB
22	CY	77	PHA	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	CY	77	PHA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AY	76	8AN	3	0
22	CV	76	8AN	2	0
22	AV	76	8AN	1	0
22	AV	77	PHA	1	0
22	CV	77	PHA	2	0
22	CY	76	8AN	2	0
22	AY	77	PHA	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1354 ligands modelled in this entry, 1352 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
58	PAR	AA	1799	-	45,45,45	2.09	14 (31%)	64,67,67	1.39	8 (12%)
58	PAR	CA	1800	-	45,45,45	1.83	11 (24%)	64,67,67	1.30	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	1799	-	-	4/18/94/94	0/4/4/4
58	PAR	CA	1800	-	-	4/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	1799	PAR	C64-C54	5.92	1.60	1.52
58	CA	1800	PAR	C64-C54	5.41	1.59	1.52
58	AA	1799	PAR	C31-C21	5.15	1.60	1.53
58	AA	1799	PAR	C11-C21	4.33	1.60	1.52
58	CA	1800	PAR	O54-C14	3.59	1.51	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	1799	PAR	O33-C14-C24	3.94	115.00	108.22
58	AA	1799	PAR	O11-C11-C21	3.87	114.89	108.22
58	AA	1799	PAR	O54-C54-C64	3.86	113.19	106.01
58	CA	1800	PAR	O54-C54-C64	3.80	113.09	106.01
58	CA	1800	PAR	C14-O54-C54	3.72	120.99	113.69

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1799	PAR	O43-C43-C53-O53
58	AA	1799	PAR	C44-C54-C64-N64
58	CA	1800	PAR	O43-C43-C53-O53
58	AA	1799	PAR	C33-C43-C53-O53
58	CA	1800	PAR	C33-C43-C53-O53

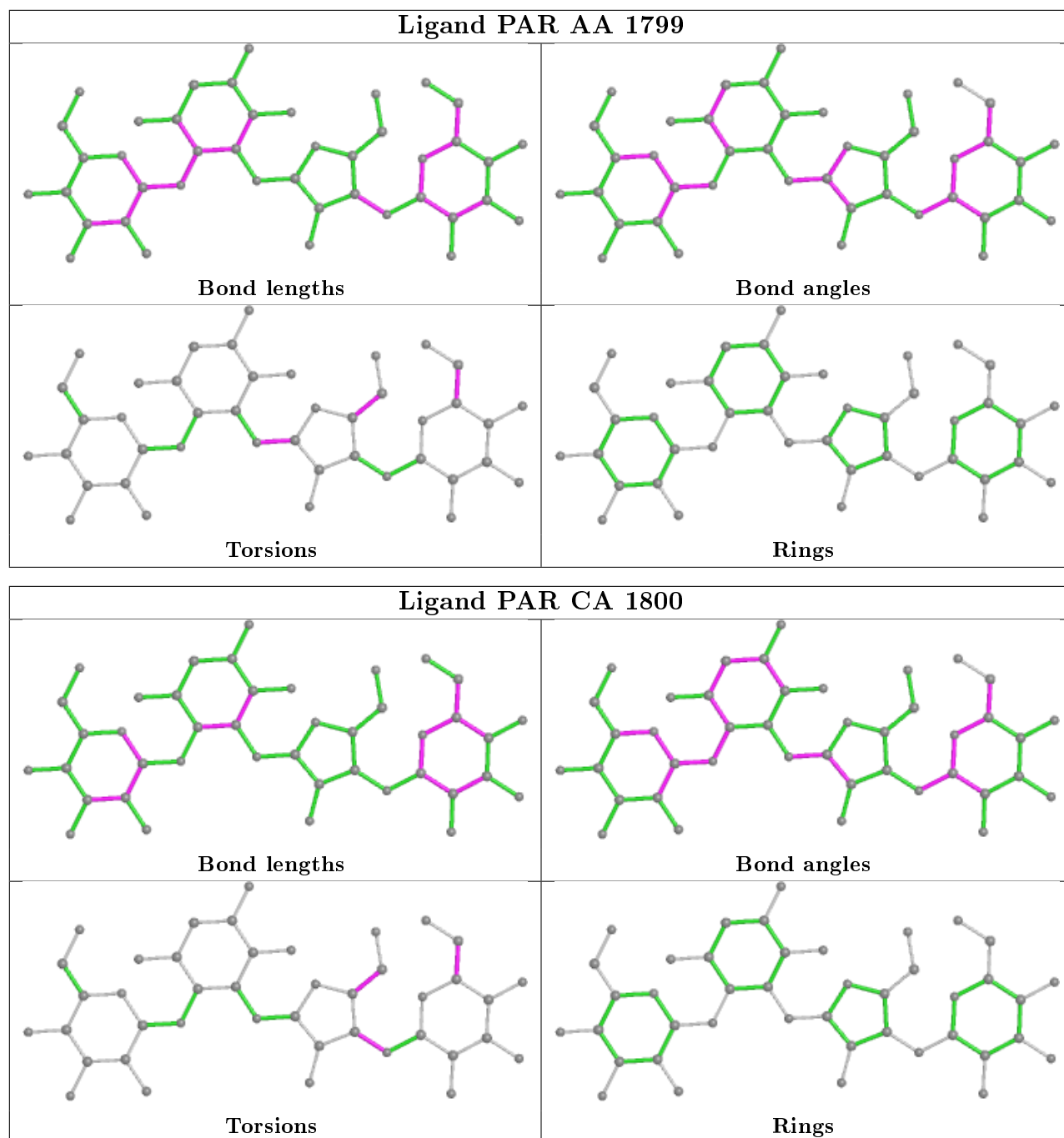
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AA	1799	PAR	2	0
58	CA	1800	PAR	2	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
9	AI	2
9	CI	2
41	DG	1
41	BG	1
31	D6	1
31	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	4.60
1	B6	46:HIS	C	47:THR	N	4.59
1	BG	112:PRO	C	113:ARG	N	3.80
1	DG	112:PRO	C	113:ARG	N	3.77
1	CM	69:GLU	C	70:LEU	N	3.15

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.05	27 (1%) 68 62	47, 104, 183, 200	0
1	CA	1504/1522 (98%)	0.07	35 (2%) 60 54	69, 117, 189, 200	0
2	AB	235/256 (91%)	0.04	7 (2%) 50 44	73, 131, 181, 200	0
2	CB	235/256 (91%)	0.18	5 (2%) 63 58	85, 154, 189, 200	0
3	AC	207/239 (86%)	-0.05	1 (0%) 91 88	71, 116, 160, 200	0
3	CC	207/239 (86%)	0.20	7 (3%) 45 40	87, 139, 180, 200	0
4	AD	208/209 (99%)	-0.25	0 100 100	60, 110, 153, 185	0
4	CD	208/209 (99%)	-0.35	0 100 100	58, 101, 142, 181	0
5	AE	151/162 (93%)	-0.18	1 (0%) 87 83	52, 101, 144, 174	0
5	CE	151/162 (93%)	0.19	5 (3%) 46 41	66, 119, 168, 200	0
6	AF	101/101 (100%)	-0.36	1 (0%) 82 77	56, 96, 142, 181	0
6	CF	101/101 (100%)	-0.26	1 (0%) 82 77	51, 107, 147, 196	0
7	AG	155/156 (99%)	0.09	9 (5%) 23 20	65, 117, 166, 200	0
7	CG	155/156 (99%)	0.18	7 (4%) 33 29	80, 129, 161, 182	0
8	AH	138/138 (100%)	-0.06	3 (2%) 62 56	62, 106, 140, 174	0
8	CH	138/138 (100%)	0.22	6 (4%) 35 31	82, 122, 160, 195	0
9	AI	127/128 (99%)	0.22	5 (3%) 39 35	79, 136, 176, 200	0
9	CI	127/128 (99%)	0.51	13 (10%) 6 7	96, 145, 188, 200	0
10	AJ	99/105 (94%)	0.64	17 (17%) 1 1	65, 140, 184, 200	0
10	CJ	99/105 (94%)	0.78	18 (18%) 1 1	70, 153, 195, 200	0
11	AK	119/129 (92%)	-0.01	3 (2%) 57 51	62, 99, 159, 198	0
11	CK	119/129 (92%)	-0.16	4 (3%) 45 40	74, 111, 155, 184	0
12	AL	125/135 (92%)	-0.14	2 (1%) 72 66	51, 91, 144, 190	0
12	CL	125/135 (92%)	0.27	5 (4%) 38 33	59, 113, 161, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.15	7 (5%) 24 22	75, 120, 163, 200	0
13	CM	125/126 (99%)	0.63	14 (11%) 5 6	77, 137, 184, 200	0
14	AN	60/61 (98%)	-0.28	0 100 100	50, 109, 147, 200	0
14	CN	60/61 (98%)	0.56	4 (6%) 17 16	89, 135, 183, 200	0
15	AO	88/89 (98%)	-0.19	2 (2%) 60 54	55, 100, 144, 162	0
15	CO	88/89 (98%)	-0.01	2 (2%) 60 54	69, 108, 154, 182	0
16	AP	84/88 (95%)	0.19	1 (1%) 79 73	78, 107, 147, 184	0
16	CP	84/88 (95%)	0.16	0 100 100	61, 100, 150, 179	0
17	AQ	100/105 (95%)	0.01	4 (4%) 38 33	82, 109, 150, 181	0
17	CQ	100/105 (95%)	0.10	4 (4%) 38 33	71, 115, 153, 167	0
18	AR	70/88 (79%)	-0.17	1 (1%) 75 69	59, 96, 139, 169	0
18	CR	70/88 (79%)	0.10	0 100 100	66, 111, 152, 173	0
19	AS	79/93 (84%)	0.38	3 (3%) 40 36	82, 122, 176, 200	0
19	CS	79/93 (84%)	0.80	9 (11%) 5 6	91, 145, 188, 200	0
20	AT	99/106 (93%)	0.14	2 (2%) 65 60	77, 120, 170, 195	0
20	CT	99/106 (93%)	0.19	5 (5%) 28 25	67, 116, 174, 200	0
21	AU	25/27 (92%)	1.08	5 (20%) 1 1	80, 119, 154, 178	0
21	CU	25/27 (92%)	1.72	10 (40%) 0 0	79, 141, 171, 185	0
22	AV	75/77 (97%)	0.17	3 (4%) 38 33	55, 121, 158, 197	0
22	AY	75/77 (97%)	0.76	8 (10%) 6 6	49, 162, 196, 200	0
22	CV	75/77 (97%)	0.03	1 (1%) 77 71	64, 144, 178, 192	0
22	CY	75/77 (97%)	1.16	11 (14%) 2 3	84, 181, 199, 200	0
23	AW	76/76 (100%)	0.57	9 (11%) 4 5	99, 173, 199, 200	0
23	CW	76/76 (100%)	0.58	7 (9%) 9 9	117, 178, 200, 200	0
24	AX	11/11 (100%)	0.52	1 (9%) 9 9	68, 116, 146, 168	0
24	CX	11/11 (100%)	0.78	2 (18%) 1 1	87, 126, 158, 159	0
25	B0	84/85 (98%)	-0.25	0 100 100	30, 62, 111, 143	0
25	D0	84/85 (98%)	0.25	2 (2%) 59 53	58, 106, 148, 178	0
26	B1	94/98 (95%)	-0.18	0 100 100	37, 68, 129, 162	0
26	D1	94/98 (95%)	-0.05	1 (1%) 80 75	38, 79, 131, 166	0
27	B2	71/72 (98%)	-0.27	1 (1%) 75 69	40, 80, 141, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.24	0 100 100	62, 97, 150, 182	0
28	B3	60/60 (100%)	-0.25	1 (1%) 70 64	31, 67, 112, 190	0
28	D3	60/60 (100%)	0.92	6 (10%) 7 8	65, 124, 163, 200	0
29	B4	31/71 (43%)	-0.29	0 100 100	67, 132, 172, 182	0
29	D4	31/71 (43%)	-0.32	0 100 100	105, 142, 184, 197	0
30	B5	59/60 (98%)	-0.30	2 (3%) 45 40	37, 60, 164, 200	0
30	D5	59/60 (98%)	-0.08	4 (6%) 17 16	52, 88, 175, 191	0
31	B6	45/54 (83%)	0.90	5 (11%) 5 6	57, 113, 166, 174	0
31	D6	45/54 (83%)	1.64	15 (33%) 0 0	92, 138, 175, 200	0
32	B7	49/49 (100%)	-0.32	0 100 100	25, 53, 112, 194	0
32	D7	49/49 (100%)	-0.07	0 100 100	41, 67, 119, 181	0
33	B8	64/65 (98%)	-0.08	1 (1%) 72 66	25, 69, 131, 198	0
33	D8	64/65 (98%)	0.08	0 100 100	45, 92, 149, 183	0
34	B9	36/37 (97%)	1.61	11 (30%) 0 0	70, 99, 142, 153	0
34	D9	36/37 (97%)	3.26	27 (75%) 0 0	120, 159, 194, 200	0
35	BA	2807/2822 (99%)	-0.06	49 (1%) 70 64	35, 64, 176, 200	0
35	DA	2807/2822 (99%)	0.02	61 (2%) 62 56	44, 93, 186, 200	0
36	BB	119/122 (97%)	-0.32	1 (0%) 86 81	57, 81, 135, 179	0
36	DB	119/122 (97%)	-0.05	2 (1%) 70 64	90, 129, 183, 197	0
37	BC	191/229 (83%)	2.00	77 (40%) 0 0	115, 175, 200, 200	0
37	DC	191/229 (83%)	1.74	80 (41%) 0 0	113, 172, 200, 200	0
38	BD	272/276 (98%)	-0.40	1 (0%) 92 90	33, 62, 106, 186	0
38	DD	272/276 (98%)	-0.29	0 100 100	40, 76, 114, 158	0
39	BE	205/206 (99%)	-0.22	2 (0%) 82 77	28, 65, 151, 200	0
39	DE	205/206 (99%)	0.14	4 (1%) 65 60	53, 105, 162, 193	0
40	BF	208/210 (99%)	-0.42	5 (2%) 59 53	26, 65, 154, 194	0
40	DF	208/210 (99%)	-0.24	3 (1%) 75 69	41, 91, 166, 200	0
41	BG	181/182 (99%)	-0.14	4 (2%) 62 56	57, 99, 158, 197	0
41	DG	181/182 (99%)	0.09	5 (2%) 53 47	78, 120, 160, 182	0
42	BH	160/180 (88%)	-0.00	6 (3%) 40 36	44, 94, 160, 199	0
42	DH	160/180 (88%)	1.40	46 (28%) 0 0	107, 169, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.94	32 (21%) 0 0	48, 154, 200, 200	0
43	DI	146/148 (98%)	0.37	10 (6%) 17 16	74, 126, 175, 200	0
44	BN	139/140 (99%)	-0.45	0 100 100	33, 68, 138, 187	0
44	DN	139/140 (99%)	0.28	2 (1%) 75 69	75, 116, 173, 200	0
45	BO	122/122 (100%)	-0.40	0 100 100	30, 69, 107, 139	0
45	DO	122/122 (100%)	-0.19	0 100 100	59, 105, 137, 157	0
46	BP	146/150 (97%)	-0.07	2 (1%) 75 69	25, 84, 158, 188	0
46	DP	146/150 (97%)	0.16	5 (3%) 45 40	51, 108, 169, 200	0
47	BQ	141/141 (100%)	-0.33	2 (1%) 75 69	41, 69, 130, 200	0
47	DQ	141/141 (100%)	0.04	4 (2%) 53 47	66, 115, 166, 200	0
48	BR	117/118 (99%)	-0.39	0 100 100	21, 62, 114, 165	0
48	DR	117/118 (99%)	-0.16	1 (0%) 84 79	37, 89, 131, 173	0
49	BS	99/112 (88%)	-0.00	1 (1%) 82 77	43, 83, 138, 181	0
49	DS	99/112 (88%)	0.54	9 (9%) 9 9	80, 128, 179, 200	0
50	BT	138/146 (94%)	-0.32	3 (2%) 62 56	40, 86, 164, 195	0
50	DT	138/146 (94%)	-0.05	3 (2%) 62 56	74, 116, 173, 200	0
51	BU	117/118 (99%)	-0.58	1 (0%) 84 79	23, 55, 106, 158	0
51	DU	117/118 (99%)	-0.15	4 (3%) 45 40	56, 101, 167, 200	0
52	BV	101/101 (100%)	-0.32	0 100 100	29, 76, 135, 200	0
52	DV	101/101 (100%)	0.46	5 (4%) 28 25	55, 135, 177, 200	0
53	BW	113/113 (100%)	-0.32	2 (1%) 68 62	26, 55, 122, 200	0
53	DW	113/113 (100%)	-0.19	1 (0%) 84 79	50, 80, 140, 194	0
54	BX	93/96 (96%)	-0.53	0 100 100	41, 66, 106, 157	0
54	DX	93/96 (96%)	-0.26	0 100 100	42, 86, 118, 150	0
55	BY	101/110 (91%)	0.29	9 (8%) 9 10	42, 88, 178, 200	0
55	DY	101/110 (91%)	0.77	17 (16%) 1 2	49, 107, 181, 200	0
56	BZ	177/206 (85%)	0.19	19 (10%) 6 6	40, 107, 185, 200	0
56	DZ	177/206 (85%)	0.89	28 (15%) 2 2	96, 152, 198, 200	0
All	All	21244/22006 (96%)	0.07	879 (4%) 37 33	21, 102, 183, 200	0

The worst 5 of 879 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	179	SER	14.1
1	CA	83	U	13.3
56	DZ	112	ARG	11.6
35	BA	888	C	10.7
37	BC	51	PRO	10.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PHA	CV	77	11/11	0.87	0.28	121,125,131,132	0
22	PHA	AV	77	11/11	0.90	0.37	121,125,131,132	0
22	PHA	CY	77	11/11	0.92	0.39	42,44,48,152	0
22	8AN	CY	76	22/23	0.94	0.24	29,48,67,71	0
22	8AN	CV	76	22/23	0.95	0.18	12,58,100,116	0
22	8AN	AV	76	22/23	0.97	0.22	12,58,100,116	0
22	8AN	AY	76	22/23	0.97	0.24	29,48,67,71	0
22	PHA	AY	77	11/11	0.97	0.39	42,44,47,48	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	AL	202	1/1	-0.37	0.33	165,165,165,165	0
57	MG	CA	1673	1/1	-0.07	0.63	128,128,128,128	1
57	MG	AA	1672	1/1	-0.07	0.98	125,125,125,125	1
57	MG	BA	3101	1/1	0.07	0.77	72,72,72,72	1
57	MG	CV	104	1/1	0.11	0.40	163,163,163,163	0
57	MG	CA	1602	1/1	0.12	0.75	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3235	1/1	0.13	0.61	156,156,156,156	0
57	MG	CA	1721	1/1	0.17	0.46	97,97,97,97	0
57	MG	AA	1737	1/1	0.21	1.75	136,136,136,136	0
57	MG	DA	3128	1/1	0.21	1.31	73,73,73,73	1
57	MG	AW	108	1/1	0.22	0.23	82,82,82,82	1
57	MG	CA	1640	1/1	0.22	0.92	121,121,121,121	0
57	MG	AA	1733	1/1	0.23	0.87	141,141,141,141	0
57	MG	AA	1761	1/1	0.24	0.91	122,122,122,122	0
57	MG	AV	104	1/1	0.24	0.41	127,127,127,127	0
57	MG	BA	3177	1/1	0.27	0.40	112,112,112,112	0
57	MG	AA	1657	1/1	0.28	0.56	121,121,121,121	0
57	MG	AA	1783	1/1	0.29	0.34	105,105,105,105	0
57	MG	DX	102	1/1	0.29	1.07	126,126,126,126	0
57	MG	CA	1649	1/1	0.30	0.41	95,95,95,95	0
57	MG	AA	1757	1/1	0.31	0.85	87,87,87,87	1
57	MG	AA	1603	1/1	0.32	0.70	84,84,84,84	0
57	MG	DA	3369	1/1	0.32	0.41	112,112,112,112	0
57	MG	AW	102	1/1	0.33	0.21	135,135,135,135	0
57	MG	BA	3339	1/1	0.35	0.61	125,125,125,125	1
57	MG	AA	1622	1/1	0.37	0.55	135,135,135,135	0
57	MG	DA	3152	1/1	0.38	0.81	82,82,82,82	0
57	MG	AA	1661	1/1	0.38	0.57	84,84,84,84	0
57	MG	CA	1726	1/1	0.38	0.57	104,104,104,104	1
57	MG	AA	1701	1/1	0.40	0.77	92,92,92,92	0
57	MG	CA	1745	1/1	0.40	0.87	115,115,115,115	0
57	MG	CA	1644	1/1	0.40	0.45	102,102,102,102	0
57	MG	CA	1728	1/1	0.40	0.64	101,101,101,101	0
57	MG	BA	3196	1/1	0.40	0.58	130,130,130,130	1
57	MG	CA	1688	1/1	0.41	0.68	15,15,15,15	1
57	MG	DA	3279	1/1	0.43	0.93	49,49,49,49	1
57	MG	AA	1667	1/1	0.43	0.49	72,72,72,72	0
57	MG	DB	203	1/1	0.44	0.96	33,33,33,33	1
57	MG	BA	3312	1/1	0.45	0.36	102,102,102,102	0
57	MG	AA	1741	1/1	0.45	0.73	124,124,124,124	0
57	MG	CW	107	1/1	0.46	0.21	113,113,113,113	1
57	MG	BA	3251	1/1	0.46	0.37	136,136,136,136	1
57	MG	CA	1680	1/1	0.46	1.13	94,94,94,94	0
57	MG	CA	1683	1/1	0.47	0.48	110,110,110,110	0
57	MG	DA	3392	1/1	0.48	0.62	107,107,107,107	0
57	MG	BA	3420	1/1	0.48	0.12	78,78,78,78	0
57	MG	DA	3192	1/1	0.48	0.63	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3293	1/1	0.49	0.24	74,74,74,74	0
57	MG	AA	1798	1/1	0.49	0.56	90,90,90,90	0
57	MG	BA	3270	1/1	0.49	0.45	76,76,76,76	0
57	MG	DX	103	1/1	0.50	0.49	102,102,102,102	0
57	MG	CA	1746	1/1	0.50	0.46	91,91,91,91	0
57	MG	CA	1701	1/1	0.50	0.99	93,93,93,93	0
57	MG	DA	3247	1/1	0.50	0.20	61,61,61,61	0
57	MG	BB	214	1/1	0.51	0.59	75,75,75,75	1
57	MG	DA	3157	1/1	0.51	0.62	79,79,79,79	0
57	MG	AA	1743	1/1	0.51	0.61	86,86,86,86	0
57	MG	AA	1744	1/1	0.52	0.55	84,84,84,84	0
57	MG	AA	1776	1/1	0.52	0.28	103,103,103,103	0
57	MG	AA	1651	1/1	0.53	0.68	70,70,70,70	0
57	MG	DA	3228	1/1	0.53	0.28	83,83,83,83	0
57	MG	CA	1761	1/1	0.54	0.61	74,74,74,74	0
57	MG	CA	1625	1/1	0.55	0.42	96,96,96,96	0
57	MG	DA	3405	1/1	0.55	0.65	53,53,53,53	1
57	MG	AD	301	1/1	0.55	0.45	155,155,155,155	0
57	MG	BA	3158	1/1	0.56	0.72	55,55,55,55	0
57	MG	BA	3373	1/1	0.56	0.61	83,83,83,83	1
57	MG	CA	1771	1/1	0.56	0.76	98,98,98,98	0
57	MG	BA	3327	1/1	0.56	0.85	67,67,67,67	0
57	MG	AG	201	1/1	0.57	0.44	80,80,80,80	0
57	MG	DA	3072	1/1	0.57	0.48	94,94,94,94	0
57	MG	DA	3300	1/1	0.57	0.29	95,95,95,95	0
57	MG	DA	3353	1/1	0.57	0.59	107,107,107,107	0
57	MG	AA	1704	1/1	0.57	0.29	103,103,103,103	0
57	MG	CA	1629	1/1	0.58	0.22	59,59,59,59	0
57	MG	AA	1641	1/1	0.58	0.69	83,83,83,83	0
57	MG	DA	3196	1/1	0.58	0.29	96,96,96,96	0
57	MG	DA	3197	1/1	0.59	0.59	106,106,106,106	0
57	MG	BA	3417	1/1	0.59	0.11	72,72,72,72	0
57	MG	DA	3399	1/1	0.59	0.29	119,119,119,119	0
57	MG	DA	3202	1/1	0.59	1.02	73,73,73,73	0
57	MG	DA	3108	1/1	0.60	0.86	83,83,83,83	0
57	MG	DA	3289	1/1	0.60	1.13	74,74,74,74	0
57	MG	BA	3371	1/1	0.60	0.71	101,101,101,101	0
57	MG	DA	3370	1/1	0.60	0.47	92,92,92,92	0
57	MG	DA	3264	1/1	0.60	0.13	96,96,96,96	0
57	MG	CA	1713	1/1	0.60	0.17	73,73,73,73	0
57	MG	DF	302	1/1	0.60	0.57	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AW	107	1/1	0.60	0.40	101,101,101,101	0
57	MG	DA	3246	1/1	0.60	0.48	97,97,97,97	0
57	MG	CA	1655	1/1	0.61	0.56	94,94,94,94	1
57	MG	CA	1705	1/1	0.61	0.40	150,150,150,150	0
57	MG	DA	3276	1/1	0.61	0.76	115,115,115,115	0
57	MG	BA	3279	1/1	0.61	0.29	53,53,53,53	0
57	MG	AA	1738	1/1	0.61	0.36	55,55,55,55	1
57	MG	BA	3349	1/1	0.61	0.70	94,94,94,94	1
57	MG	DA	3032	1/1	0.61	0.52	66,66,66,66	0
57	MG	DA	3136	1/1	0.61	0.89	63,63,63,63	0
57	MG	AA	1749	1/1	0.62	0.38	100,100,100,100	1
57	MG	AA	1796	1/1	0.62	0.56	121,121,121,121	0
57	MG	CA	1668	1/1	0.62	0.98	99,99,99,99	0
57	MG	DA	3106	1/1	0.63	0.45	78,78,78,78	0
57	MG	CA	1754	1/1	0.63	0.53	105,105,105,105	1
57	MG	DA	3414	1/1	0.63	0.40	84,84,84,84	0
57	MG	CA	1793	1/1	0.63	0.33	100,100,100,100	1
57	MG	CA	1727	1/1	0.63	0.83	139,139,139,139	0
57	MG	CA	1739	1/1	0.63	0.49	128,128,128,128	0
57	MG	BA	3416	1/1	0.64	0.30	93,93,93,93	0
57	MG	BA	3342	1/1	0.64	0.29	84,84,84,84	0
57	MG	DA	3321	1/1	0.64	0.62	126,126,126,126	0
57	MG	BA	3331	1/1	0.64	0.43	65,65,65,65	1
57	MG	D7	101	1/1	0.65	0.41	73,73,73,73	0
57	MG	DA	3284	1/1	0.65	0.38	74,74,74,74	0
57	MG	DA	3419	1/1	0.65	0.11	115,115,115,115	0
57	MG	BA	3160	1/1	0.65	0.46	74,74,74,74	0
57	MG	CA	1674	1/1	0.65	0.47	63,63,63,63	1
57	MG	DA	3324	1/1	0.65	0.48	64,64,64,64	1
57	MG	AA	1677	1/1	0.65	0.29	89,89,89,89	0
57	MG	DA	3042	1/1	0.65	0.30	89,89,89,89	0
57	MG	DA	3372	1/1	0.65	0.44	120,120,120,120	1
57	MG	DA	3340	1/1	0.65	0.59	98,98,98,98	1
57	MG	CA	1656	1/1	0.65	0.54	120,120,120,120	0
57	MG	AA	1769	1/1	0.65	0.52	80,80,80,80	0
57	MG	DA	3415	1/1	0.65	0.31	96,96,96,96	0
57	MG	BA	3138	1/1	0.66	1.02	124,124,124,124	0
57	MG	DA	3367	1/1	0.66	0.51	108,108,108,108	0
57	MG	DA	3281	1/1	0.66	0.23	52,52,52,52	0
57	MG	BA	3186	1/1	0.66	0.28	144,144,144,144	0
57	MG	BA	3179	1/1	0.66	1.56	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1706	1/1	0.66	0.70	80,80,80,80	0
57	MG	DA	3331	1/1	0.66	0.32	155,155,155,155	1
57	MG	BA	3383	1/1	0.66	1.01	101,101,101,101	0
57	MG	BA	3254	1/1	0.66	0.19	44,44,44,44	0
57	MG	DS	201	1/1	0.67	0.26	74,74,74,74	1
57	MG	CA	1623	1/1	0.67	0.50	71,71,71,71	0
57	MG	AA	1764	1/1	0.67	0.34	64,64,64,64	0
57	MG	BA	3237	1/1	0.67	0.58	74,74,74,74	0
57	MG	DA	3296	1/1	0.67	0.57	138,138,138,138	0
57	MG	CA	1795	1/1	0.67	0.59	78,78,78,78	0
57	MG	DA	3153	1/1	0.67	0.43	60,60,60,60	1
57	MG	DA	3311	1/1	0.67	0.16	65,65,65,65	1
57	MG	BA	3310	1/1	0.67	0.19	102,102,102,102	1
57	MG	AA	1653	1/1	0.67	0.91	82,82,82,82	0
57	MG	CL	201	1/1	0.68	0.74	91,91,91,91	0
57	MG	BA	3155	1/1	0.68	0.85	116,116,116,116	0
57	MG	BA	3419	1/1	0.68	1.19	90,90,90,90	1
57	MG	AA	1763	1/1	0.68	0.18	62,62,62,62	0
57	MG	BA	3311	1/1	0.68	0.24	74,74,74,74	1
57	MG	DA	3170	1/1	0.68	0.62	60,60,60,60	0
57	MG	CA	1716	1/1	0.68	0.76	68,68,68,68	1
57	MG	CA	1676	1/1	0.68	0.45	71,71,71,71	0
57	MG	CA	1691	1/1	0.68	0.24	110,110,110,110	0
57	MG	AA	1635	1/1	0.68	0.26	92,92,92,92	0
57	MG	BA	3230	1/1	0.68	0.48	97,97,97,97	0
57	MG	BA	3247	1/1	0.69	0.34	49,49,49,49	0
57	MG	DA	3012	1/1	0.69	0.28	45,45,45,45	0
57	MG	DN	201	1/1	0.69	2.50	129,129,129,129	0
57	MG	DA	3267	1/1	0.69	0.17	71,71,71,71	0
57	MG	DB	202	1/1	0.69	0.30	113,113,113,113	0
57	MG	BA	3162	1/1	0.69	0.12	79,79,79,79	0
57	MG	DA	3166	1/1	0.69	0.41	75,75,75,75	0
57	MG	BA	3267	1/1	0.70	0.41	56,56,56,56	0
57	MG	CA	1763	1/1	0.70	0.24	98,98,98,98	0
57	MG	DA	3290	1/1	0.70	1.14	73,73,73,73	0
57	MG	DA	3210	1/1	0.70	0.54	96,96,96,96	0
57	MG	AA	1689	1/1	0.70	0.48	118,118,118,118	0
57	MG	AA	1666	1/1	0.70	0.42	93,93,93,93	0
57	MG	DA	3400	1/1	0.70	0.34	77,77,77,77	0
57	MG	AA	1740	1/1	0.70	0.31	87,87,87,87	0
57	MG	BA	3163	1/1	0.70	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1640	1/1	0.70	0.34	76,76,76,76	0
57	MG	CA	1764	1/1	0.71	0.23	68,68,68,68	1
57	MG	DA	3379	1/1	0.71	0.55	105,105,105,105	0
57	MG	AA	1625	1/1	0.71	0.46	65,65,65,65	0
57	MG	BA	3324	1/1	0.71	0.44	39,39,39,39	1
57	MG	CA	1752	1/1	0.71	0.19	112,112,112,112	1
57	MG	AA	1781	1/1	0.71	0.25	63,63,63,63	0
57	MG	AA	1607	1/1	0.71	0.31	64,64,64,64	0
57	MG	BA	3216	1/1	0.71	0.33	80,80,80,80	0
57	MG	CA	1786	1/1	0.71	0.12	71,71,71,71	1
57	MG	DA	3139	1/1	0.71	1.40	112,112,112,112	0
57	MG	AX	102	1/1	0.71	0.35	83,83,83,83	0
57	MG	BA	3376	1/1	0.71	0.46	81,81,81,81	0
57	MG	AA	1683	1/1	0.71	0.24	101,101,101,101	0
57	MG	DA	3004	1/1	0.71	0.69	86,86,86,86	0
57	MG	DA	3358	1/1	0.71	0.78	94,94,94,94	0
57	MG	DA	3248	1/1	0.71	0.24	90,90,90,90	0
57	MG	CA	1678	1/1	0.71	0.41	94,94,94,94	0
57	MG	CA	1698	1/1	0.72	0.12	86,86,86,86	0
57	MG	BA	3223	1/1	0.72	0.50	64,64,64,64	0
57	MG	CA	1612	1/1	0.72	0.16	91,91,91,91	0
57	MG	CA	1756	1/1	0.72	0.36	53,53,53,53	0
57	MG	CA	1617	1/1	0.72	0.55	81,81,81,81	0
57	MG	AW	106	1/1	0.72	0.27	102,102,102,102	1
57	MG	AW	105	1/1	0.72	0.41	154,154,154,154	1
57	MG	DA	3160	1/1	0.72	0.44	67,67,67,67	0
57	MG	DC	301	1/1	0.72	0.23	91,91,91,91	1
57	MG	AA	1631	1/1	0.72	0.38	54,54,54,54	0
57	MG	AA	1734	1/1	0.72	0.80	102,102,102,102	0
57	MG	DA	3222	1/1	0.72	0.53	95,95,95,95	0
57	MG	AV	103	1/1	0.72	0.44	81,81,81,81	0
57	MG	AA	1601	1/1	0.72	0.26	90,90,90,90	0
57	MG	BB	201	1/1	0.73	0.38	87,87,87,87	0
57	MG	DA	3328	1/1	0.73	0.55	50,50,50,50	0
57	MG	CA	1709	1/1	0.73	0.35	73,73,73,73	0
57	MG	AA	1706	1/1	0.73	0.43	108,108,108,108	0
57	MG	CA	1609	1/1	0.73	0.66	61,61,61,61	0
57	MG	CA	1666	1/1	0.73	0.67	87,87,87,87	0
57	MG	CA	1643	1/1	0.73	0.19	157,157,157,157	0
57	MG	CA	1682	1/1	0.73	0.73	90,90,90,90	0
57	MG	AA	1777	1/1	0.73	0.29	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3273	1/1	0.73	0.19	59,59,59,59	0
57	MG	DA	3161	1/1	0.73	0.35	65,65,65,65	0
57	MG	BA	3283	1/1	0.73	0.25	33,33,33,33	0
57	MG	CA	1798	1/1	0.73	0.23	55,55,55,55	0
57	MG	CA	1711	1/1	0.73	0.16	74,74,74,74	0
57	MG	CA	1731	1/1	0.74	0.31	85,85,85,85	0
57	MG	DA	3229	1/1	0.74	0.62	92,92,92,92	0
57	MG	BA	3345	1/1	0.74	0.41	69,69,69,69	1
57	MG	CA	1657	1/1	0.74	0.35	86,86,86,86	0
57	MG	BU	201	1/1	0.74	0.40	166,166,166,166	1
57	MG	DA	3304	1/1	0.74	0.42	49,49,49,49	0
57	MG	BA	3297	1/1	0.74	0.76	77,77,77,77	0
57	MG	AA	1721	1/1	0.74	0.49	90,90,90,90	0
57	MG	DA	3291	1/1	0.74	0.25	58,58,58,58	0
57	MG	DA	3188	1/1	0.74	1.99	111,111,111,111	0
57	MG	CA	1685	1/1	0.74	0.20	62,62,62,62	0
57	MG	BA	3291	1/1	0.74	0.37	42,42,42,42	0
57	MG	CA	1660	1/1	0.75	0.35	59,59,59,59	0
57	MG	CA	1690	1/1	0.75	0.85	110,110,110,110	0
57	MG	CA	1780	1/1	0.75	0.55	32,32,32,32	1
57	MG	AA	1707	1/1	0.75	0.31	116,116,116,116	0
57	MG	BA	3264	1/1	0.75	0.27	58,58,58,58	0
57	MG	AA	1754	1/1	0.75	0.34	64,64,64,64	0
57	MG	DA	3393	1/1	0.75	0.52	109,109,109,109	1
57	MG	CA	1645	1/1	0.75	0.73	66,66,66,66	0
57	MG	BA	3195	1/1	0.75	1.13	79,79,79,79	0
57	MG	DA	3049	1/1	0.75	0.77	71,71,71,71	0
57	MG	D2	602	1/1	0.75	0.32	99,99,99,99	0
57	MG	DA	3087	1/1	0.75	0.40	84,84,84,84	0
57	MG	DA	3270	1/1	0.75	0.28	87,87,87,87	0
57	MG	AA	1773	1/1	0.75	0.37	72,72,72,72	0
57	MG	DA	3059	1/1	0.76	0.37	46,46,46,46	0
57	MG	BA	3340	1/1	0.76	0.61	90,90,90,90	1
57	MG	AW	104	1/1	0.76	0.11	60,60,60,60	1
57	MG	BA	3151	1/1	0.76	0.45	45,45,45,45	1
57	MG	DA	3389	1/1	0.76	0.94	113,113,113,113	0
57	MG	CA	1622	1/1	0.76	0.46	117,117,117,117	0
57	MG	AA	1679	1/1	0.76	0.48	56,56,56,56	0
57	MG	CA	1665	1/1	0.76	0.35	68,68,68,68	0
57	MG	AA	1715	1/1	0.76	0.67	39,39,39,39	1
57	MG	DA	3090	1/1	0.76	0.88	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3282	1/1	0.76	0.21	50,50,50,50	0
57	MG	DA	3119	1/1	0.76	0.36	86,86,86,86	0
57	MG	AA	1726	1/1	0.76	0.26	71,71,71,71	0
57	MG	AA	1793	1/1	0.76	0.34	91,91,91,91	0
57	MG	BA	3127	1/1	0.76	0.33	44,44,44,44	1
57	MG	DA	3319	1/1	0.76	0.54	102,102,102,102	1
57	MG	DA	3373	1/1	0.76	0.18	98,98,98,98	0
57	MG	BA	3224	1/1	0.76	0.34	91,91,91,91	0
57	MG	BA	3295	1/1	0.76	0.44	64,64,64,64	0
57	MG	BA	3047	1/1	0.76	0.82	72,72,72,72	0
57	MG	AA	1646	1/1	0.76	0.65	82,82,82,82	0
57	MG	DA	3416	1/1	0.76	0.12	81,81,81,81	0
57	MG	AA	1602	1/1	0.76	0.28	97,97,97,97	0
57	MG	DA	3239	1/1	0.77	0.98	79,79,79,79	0
57	MG	AA	1751	1/1	0.77	0.42	72,72,72,72	1
57	MG	DA	3354	1/1	0.77	0.13	84,84,84,84	0
57	MG	BA	3152	1/1	0.77	0.46	93,93,93,93	0
57	MG	AA	1702	1/1	0.77	1.05	126,126,126,126	0
57	MG	BA	3253	1/1	0.77	0.37	87,87,87,87	0
57	MG	BA	3289	1/1	0.77	0.23	79,79,79,79	0
57	MG	BA	3360	1/1	0.77	0.39	140,140,140,140	0
57	MG	DA	3338	1/1	0.77	0.30	74,74,74,74	0
57	MG	CA	1759	1/1	0.77	0.67	67,67,67,67	1
57	MG	CA	1729	1/1	0.77	0.20	70,70,70,70	1
57	MG	CA	1606	1/1	0.77	0.32	78,78,78,78	0
57	MG	CA	1735	1/1	0.77	0.50	90,90,90,90	0
57	MG	AA	1732	1/1	0.77	0.52	61,61,61,61	0
57	MG	CA	1652	1/1	0.77	0.72	52,52,52,52	0
57	MG	AA	1772	1/1	0.77	0.33	85,85,85,85	0
57	MG	DA	3227	1/1	0.77	1.36	136,136,136,136	0
57	MG	AA	1690	1/1	0.78	0.37	81,81,81,81	0
57	MG	AA	1753	1/1	0.78	0.16	103,103,103,103	0
57	MG	DB	213	1/1	0.78	0.51	93,93,93,93	0
57	MG	DA	3307	1/1	0.78	0.44	51,51,51,51	0
57	MG	D7	102	1/1	0.78	0.84	62,62,62,62	1
57	MG	DA	3198	1/1	0.78	0.38	58,58,58,58	1
57	MG	DA	3122	1/1	0.78	0.68	77,77,77,77	0
57	MG	DA	3299	1/1	0.78	0.52	93,93,93,93	0
57	MG	BA	3200	1/1	0.78	0.25	52,52,52,52	0
57	MG	DA	3259	1/1	0.78	0.35	56,56,56,56	0
57	MG	CA	1765	1/1	0.78	0.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3260	1/1	0.78	0.99	81,81,81,81	0
57	MG	BA	3418	1/1	0.78	0.08	59,59,59,59	0
57	MG	BA	3176	1/1	0.78	0.40	97,97,97,97	0
57	MG	DA	3135	1/1	0.78	0.28	39,39,39,39	0
57	MG	DA	3006	1/1	0.78	0.42	23,23,23,23	0
57	MG	BA	3143	1/1	0.78	0.31	49,49,49,49	1
57	MG	BA	3067	1/1	0.78	0.76	53,53,53,53	0
57	MG	DA	3033	1/1	0.78	0.40	70,70,70,70	0
57	MG	BA	3225	1/1	0.78	0.67	128,128,128,128	0
57	MG	BN	201	1/1	0.78	0.62	64,64,64,64	0
57	MG	BA	3353	1/1	0.78	0.47	79,79,79,79	0
57	MG	DA	3217	1/1	0.78	0.26	62,62,62,62	0
57	MG	CA	1725	1/1	0.78	0.34	116,116,116,116	1
57	MG	CA	1632	1/1	0.79	0.34	54,54,54,54	1
57	MG	AA	1621	1/1	0.79	0.26	50,50,50,50	0
57	MG	AA	1681	1/1	0.79	1.02	86,86,86,86	0
57	MG	CA	1647	1/1	0.79	0.52	68,68,68,68	0
57	MG	CA	1654	1/1	0.79	0.59	69,69,69,69	0
57	MG	DA	3243	1/1	0.79	0.73	76,76,76,76	0
57	MG	AA	1643	1/1	0.79	0.30	84,84,84,84	0
57	MG	DA	3111	1/1	0.79	1.59	111,111,111,111	0
57	MG	AA	1795	1/1	0.79	0.51	128,128,128,128	0
57	MG	BA	3399	1/1	0.79	0.58	64,64,64,64	0
57	MG	BA	3006	1/1	0.79	0.91	66,66,66,66	0
57	MG	CA	1613	1/1	0.79	0.54	51,51,51,51	0
57	MG	CA	1684	1/1	0.79	0.10	94,94,94,94	0
57	MG	AA	1700	1/1	0.79	0.64	79,79,79,79	0
57	MG	BA	3241	1/1	0.79	0.51	70,70,70,70	0
57	MG	AA	1775	1/1	0.80	0.57	92,92,92,92	0
57	MG	DA	3315	1/1	0.80	0.32	85,85,85,85	1
57	MG	CA	1740	1/1	0.80	0.44	61,61,61,61	1
57	MG	CA	1720	1/1	0.80	0.23	89,89,89,89	0
57	MG	DA	3342	1/1	0.80	0.27	90,90,90,90	0
57	MG	DB	209	1/1	0.80	0.56	7,7,7,7	1
57	MG	BA	3226	1/1	0.80	0.17	58,58,58,58	0
57	MG	AA	1748	1/1	0.80	0.35	144,144,144,144	1
57	MG	AA	1673	1/1	0.80	1.32	76,76,76,76	1
57	MG	BA	3107	1/1	0.80	0.45	44,44,44,44	0
57	MG	AA	1727	1/1	0.80	0.44	54,54,54,54	1
57	MG	AA	1648	1/1	0.80	0.32	87,87,87,87	0
57	MG	BA	3281	1/1	0.80	0.38	53,53,53,53	0
57	MG	DA	3262	1/1	0.80	0.56	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3159	1/1	0.80	0.32	37,37,37,37	0
57	MG	AA	1616	1/1	0.80	0.84	70,70,70,70	0
57	MG	CA	1775	1/1	0.80	0.22	79,79,79,79	0
57	MG	DA	3317	1/1	0.80	0.33	55,55,55,55	1
57	MG	CW	106	1/1	0.81	0.17	86,86,86,86	1
57	MG	BA	3415	1/1	0.81	0.37	77,77,77,77	0
57	MG	AA	1770	1/1	0.81	0.39	163,163,163,163	0
57	MG	CA	1733	1/1	0.81	0.52	81,81,81,81	1
57	MG	CA	1646	1/1	0.81	0.20	81,81,81,81	0
57	MG	DA	3114	1/1	0.81	0.28	29,29,29,29	0
57	MG	AA	1724	1/1	0.81	0.29	68,68,68,68	1
57	MG	CA	1681	1/1	0.81	0.54	49,49,49,49	0
57	MG	DB	208	1/1	0.81	1.57	76,76,76,76	1
57	MG	BA	3248	1/1	0.81	0.28	50,50,50,50	1
57	MG	DA	3070	1/1	0.81	0.72	94,94,94,94	0
57	MG	DA	3253	1/1	0.81	0.52	86,86,86,86	1
57	MG	BA	3150	1/1	0.81	0.43	64,64,64,64	0
57	MG	DA	3101	1/1	0.81	0.36	67,67,67,67	0
57	MG	CA	1648	1/1	0.81	0.55	83,83,83,83	0
57	MG	DA	3412	1/1	0.81	0.36	74,74,74,74	0
57	MG	DA	3190	1/1	0.81	0.26	67,67,67,67	0
57	MG	CA	1671	1/1	0.81	0.30	58,58,58,58	0
57	MG	DA	3285	1/1	0.81	0.21	71,71,71,71	0
57	MG	CA	1779	1/1	0.81	0.26	115,115,115,115	0
57	MG	DA	3376	1/1	0.81	0.46	110,110,110,110	0
57	MG	DA	3118	1/1	0.81	0.62	62,62,62,62	0
57	MG	BA	3393	1/1	0.81	0.38	74,74,74,74	0
57	MG	DA	3098	1/1	0.81	0.59	38,38,38,38	0
57	MG	BA	3367	1/1	0.81	0.36	1,1,1,1	1
57	MG	AA	1708	1/1	0.81	0.41	72,72,72,72	0
57	MG	AA	1742	1/1	0.81	0.42	100,100,100,100	0
57	MG	DA	3205	1/1	0.81	0.25	37,37,37,37	0
57	MG	CA	1615	1/1	0.82	1.52	70,70,70,70	0
57	MG	DA	3238	1/1	0.82	0.33	56,56,56,56	0
57	MG	BA	3368	1/1	0.82	0.22	61,61,61,61	0
57	MG	DA	3349	1/1	0.82	0.32	41,41,41,41	1
57	MG	BA	3285	1/1	0.82	0.54	89,89,89,89	0
57	MG	AA	1617	1/1	0.82	0.71	51,51,51,51	0
57	MG	CA	1742	1/1	0.82	0.21	70,70,70,70	0
57	MG	DA	3147	1/1	0.82	0.32	59,59,59,59	0
57	MG	DA	3406	1/1	0.82	0.18	51,51,51,51	0
57	MG	CA	1788	1/1	0.82	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1705	1/1	0.82	0.51	63,63,63,63	0
57	MG	DA	3138	1/1	0.82	0.28	68,68,68,68	0
57	MG	BA	3041	1/1	0.82	0.29	96,96,96,96	0
57	MG	BA	3366	1/1	0.82	0.46	112,112,112,112	0
57	MG	CW	102	1/1	0.82	0.10	112,112,112,112	0
57	MG	CA	1694	1/1	0.82	0.37	116,116,116,116	0
57	MG	DA	3327	1/1	0.82	0.98	64,64,64,64	1
57	MG	BA	3406	1/1	0.82	0.27	38,38,38,38	1
57	MG	DA	3297	1/1	0.82	0.45	71,71,71,71	0
57	MG	AV	105	1/1	0.82	0.77	89,89,89,89	0
57	MG	BA	3110	1/1	0.82	0.21	44,44,44,44	0
57	MG	DA	3172	1/1	0.82	0.27	58,58,58,58	0
57	MG	DA	3240	1/1	0.82	0.47	56,56,56,56	0
57	MG	BA	3100	1/1	0.82	0.48	49,49,49,49	0
57	MG	DA	3051	1/1	0.82	0.26	75,75,75,75	0
57	MG	AA	1759	1/1	0.82	0.36	96,96,96,96	0
57	MG	AA	1655	1/1	0.82	0.36	74,74,74,74	0
57	MG	AA	1762	1/1	0.82	0.40	80,80,80,80	1
57	MG	DA	3226	1/1	0.82	0.33	88,88,88,88	0
57	MG	DA	3294	1/1	0.82	0.26	54,54,54,54	0
57	MG	AA	1731	1/1	0.82	0.54	73,73,73,73	1
57	MG	B0	101	1/1	0.82	0.31	50,50,50,50	0
57	MG	DA	3398	1/1	0.83	0.61	86,86,86,86	0
57	MG	CA	1736	1/1	0.83	0.53	73,73,73,73	0
57	MG	BA	3188	1/1	0.83	0.24	64,64,64,64	0
57	MG	CA	1669	1/1	0.83	0.33	81,81,81,81	0
57	MG	DA	3341	1/1	0.83	0.27	54,54,54,54	0
57	MG	DA	3195	1/1	0.83	0.16	89,89,89,89	0
57	MG	BA	3014	1/1	0.83	0.23	61,61,61,61	0
57	MG	DA	3144	1/1	0.83	0.38	63,63,63,63	1
57	MG	AA	1710	1/1	0.83	0.27	71,71,71,71	0
57	MG	DA	3225	1/1	0.83	0.57	71,71,71,71	0
57	MG	AA	1623	1/1	0.83	0.54	70,70,70,70	0
57	MG	CA	1664	1/1	0.83	0.54	53,53,53,53	0
57	MG	BA	3080	1/1	0.83	0.29	26,26,26,26	0
57	MG	DA	3154	1/1	0.83	0.32	60,60,60,60	0
57	MG	BA	3305	1/1	0.83	1.33	101,101,101,101	0
57	MG	AA	1682	1/1	0.83	0.40	131,131,131,131	0
57	MG	DA	3019	1/1	0.83	0.50	29,29,29,29	0
57	MG	AA	1758	1/1	0.83	0.30	97,97,97,97	0
57	MG	BA	3250	1/1	0.83	0.23	76,76,76,76	0
57	MG	BA	3211	1/1	0.83	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3214	1/1	0.83	0.26	129,129,129,129	0
57	MG	DA	3365	1/1	0.83	0.26	19,19,19,19	0
57	MG	DA	3123	1/1	0.84	0.40	89,89,89,89	0
57	MG	CA	1630	1/1	0.84	0.29	84,84,84,84	0
57	MG	AA	1684	1/1	0.84	0.19	74,74,74,74	0
57	MG	BA	3282	1/1	0.84	0.51	23,23,23,23	0
57	MG	BA	3290	1/1	0.84	0.62	78,78,78,78	1
57	MG	DA	3212	1/1	0.84	0.94	91,91,91,91	0
57	MG	DA	3177	1/1	0.84	0.48	77,77,77,77	0
57	MG	CV	105	1/1	0.84	0.14	65,65,65,65	0
57	MG	BA	3394	1/1	0.84	0.41	81,81,81,81	1
57	MG	B5	102	1/1	0.84	0.49	58,58,58,58	1
57	MG	BA	3212	1/1	0.84	0.36	88,88,88,88	0
57	MG	DA	3223	1/1	0.84	0.64	46,46,46,46	1
57	MG	BA	3317	1/1	0.84	0.16	167,167,167,167	0
57	MG	DA	3127	1/1	0.84	0.46	67,67,67,67	0
57	MG	DA	3002	1/1	0.84	0.23	69,69,69,69	0
57	MG	CA	1757	1/1	0.84	0.49	128,128,128,128	0
57	MG	DA	3213	1/1	0.84	0.37	89,89,89,89	0
57	MG	DA	3256	1/1	0.84	0.26	79,79,79,79	0
57	MG	BB	207	1/1	0.84	0.43	29,29,29,29	1
57	MG	BA	3322	1/1	0.84	0.67	42,42,42,42	1
57	MG	AA	1668	1/1	0.84	0.29	51,51,51,51	0
57	MG	CA	1767	1/1	0.84	0.23	97,97,97,97	0
57	MG	BA	3275	1/1	0.84	0.58	98,98,98,98	0
57	MG	CA	1778	1/1	0.84	0.37	66,66,66,66	0
57	MG	CA	1782	1/1	0.84	0.33	77,77,77,77	0
57	MG	DA	3312	1/1	0.84	0.20	56,56,56,56	1
57	MG	DA	3015	1/1	0.84	0.45	79,79,79,79	0
57	MG	D2	601	1/1	0.84	0.30	35,35,35,35	1
57	MG	BA	3228	1/1	0.84	0.41	51,51,51,51	0
57	MG	DA	3221	1/1	0.85	0.52	50,50,50,50	0
57	MG	BA	3338	1/1	0.85	0.35	52,52,52,52	0
57	MG	CV	103	1/1	0.85	0.59	74,74,74,74	0
57	MG	CA	1714	1/1	0.85	0.12	62,62,62,62	0
57	MG	BA	3326	1/1	0.85	0.28	46,46,46,46	1
57	MG	BA	3313	1/1	0.85	0.31	162,162,162,162	0
57	MG	CA	1700	1/1	0.85	0.09	101,101,101,101	0
57	MG	AA	1654	1/1	0.85	0.29	52,52,52,52	1
57	MG	DA	3388	1/1	0.85	0.25	68,68,68,68	0
57	MG	CA	1753	1/1	0.85	0.35	130,130,130,130	1
57	MG	CA	1785	1/1	0.85	0.30	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3048	1/1	0.85	0.67	33,33,33,33	0
57	MG	BA	3220	1/1	0.85	0.49	95,95,95,95	0
57	MG	BA	3351	1/1	0.85	0.25	135,135,135,135	0
57	MG	AA	1790	1/1	0.85	0.13	63,63,63,63	0
57	MG	AA	1735	1/1	0.85	0.29	108,108,108,108	0
57	MG	BB	213	1/1	0.85	0.32	87,87,87,87	0
57	MG	DA	3162	1/1	0.85	0.27	77,77,77,77	0
57	MG	DA	3164	1/1	0.85	0.21	84,84,84,84	0
57	MG	DA	3325	1/1	0.85	0.30	83,83,83,83	1
57	MG	DA	3408	1/1	0.85	0.38	44,44,44,44	0
57	MG	BA	3187	1/1	0.85	0.41	108,108,108,108	0
57	MG	AA	1670	1/1	0.85	0.38	49,49,49,49	0
57	MG	DA	3329	1/1	0.85	0.42	140,140,140,140	0
57	MG	BA	3356	1/1	0.85	0.19	41,41,41,41	0
57	MG	AA	1656	1/1	0.86	0.76	97,97,97,97	0
57	MG	BA	3389	1/1	0.86	0.35	62,62,62,62	0
57	MG	BA	3244	1/1	0.86	0.36	88,88,88,88	0
57	MG	BA	3001	1/1	0.86	0.22	33,33,33,33	0
57	MG	AA	1712	1/1	0.86	0.30	61,61,61,61	0
57	MG	DA	3178	1/1	0.86	0.21	88,88,88,88	0
57	MG	AN	101	1/1	0.86	0.24	50,50,50,50	0
57	MG	DA	3339	1/1	0.86	0.29	57,57,57,57	1
57	MG	BA	3170	1/1	0.86	0.34	61,61,61,61	0
57	MG	DA	3301	1/1	0.86	0.77	84,84,84,84	0
57	MG	DA	3020	1/1	0.86	0.33	59,59,59,59	0
57	MG	BA	3167	1/1	0.86	0.37	32,32,32,32	1
57	MG	CA	1799	1/1	0.86	0.32	75,75,75,75	0
57	MG	CA	1614	1/1	0.86	1.00	89,89,89,89	0
57	MG	AA	1664	1/1	0.86	0.33	47,47,47,47	0
57	MG	BA	3194	1/1	0.86	0.27	42,42,42,42	0
57	MG	CA	1777	1/1	0.86	1.28	135,135,135,135	0
57	MG	BA	3252	1/1	0.86	0.27	79,79,79,79	0
57	MG	CA	1719	1/1	0.86	0.62	93,93,93,93	0
57	MG	CA	1773	1/1	0.86	0.76	55,55,55,55	0
57	MG	CA	1737	1/1	0.86	0.26	87,87,87,87	0
57	MG	BB	202	1/1	0.86	0.38	92,92,92,92	0
57	MG	CA	1686	1/1	0.86	0.33	43,43,43,43	0
57	MG	DA	3249	1/1	0.86	0.37	60,60,60,60	0
57	MG	DA	3001	1/1	0.86	0.18	42,42,42,42	0
57	MG	DA	3383	1/1	0.86	0.39	67,67,67,67	0
57	MG	DA	3255	1/1	0.86	0.27	61,61,61,61	0
57	MG	BA	3384	1/1	0.86	0.35	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1771	1/1	0.86	0.53	40,40,40,40	0
57	MG	BA	3010	1/1	0.86	0.40	41,41,41,41	0
57	MG	DA	3146	1/1	0.86	0.31	55,55,55,55	0
57	MG	DA	3182	1/1	0.86	0.59	60,60,60,60	0
57	MG	CA	1677	1/1	0.87	0.14	48,48,48,48	0
57	MG	DB	211	1/1	0.87	0.25	119,119,119,119	0
57	MG	DA	3007	1/1	0.87	0.71	59,59,59,59	0
57	MG	CA	1783	1/1	0.87	0.37	105,105,105,105	0
57	MG	DA	3252	1/1	0.87	0.12	95,95,95,95	0
57	MG	DA	3179	1/1	0.87	0.18	80,80,80,80	0
57	MG	DA	3218	1/1	0.87	0.40	94,94,94,94	0
57	MG	DA	3086	1/1	0.87	0.29	56,56,56,56	0
57	MG	DA	3132	1/1	0.87	0.34	41,41,41,41	0
57	MG	DA	3175	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	3121	1/1	0.87	0.41	83,83,83,83	0
57	MG	DV	201	1/1	0.87	0.28	70,70,70,70	0
57	MG	AA	1722	1/1	0.87	0.15	75,75,75,75	0
57	MG	BA	3257	1/1	0.87	0.58	61,61,61,61	0
57	MG	BA	3318	1/1	0.87	0.36	70,70,70,70	1
57	MG	DO	201	1/1	0.87	0.37	85,85,85,85	0
57	MG	D5	101	1/1	0.87	0.24	51,51,51,51	0
57	MG	DA	3216	1/1	0.87	0.50	74,74,74,74	0
57	MG	AW	101	1/1	0.87	0.26	157,157,157,157	0
57	MG	DA	3116	1/1	0.87	0.75	50,50,50,50	0
57	MG	AA	1713	1/1	0.87	0.15	53,53,53,53	0
57	MG	DA	3269	1/1	0.87	0.36	47,47,47,47	0
57	MG	DA	3201	1/1	0.87	1.32	88,88,88,88	0
57	MG	BA	3121	1/1	0.87	0.34	40,40,40,40	0
57	MG	CA	1661	1/1	0.87	0.59	56,56,56,56	0
57	MG	CA	1708	1/1	0.87	0.11	89,89,89,89	0
57	MG	DA	3413	1/1	0.87	0.21	84,84,84,84	0
57	MG	DA	3092	1/1	0.87	0.37	46,46,46,46	0
57	MG	DA	3266	1/1	0.87	0.24	84,84,84,84	0
57	MG	AA	1750	1/1	0.87	0.29	62,62,62,62	1
57	MG	DA	3272	1/1	0.87	0.53	108,108,108,108	0
57	MG	CA	1707	1/1	0.87	0.34	119,119,119,119	0
57	MG	CA	1687	1/1	0.88	0.44	84,84,84,84	0
57	MG	BA	3277	1/1	0.88	0.78	35,35,35,35	1
57	MG	DA	3351	1/1	0.88	0.49	94,94,94,94	0
57	MG	AA	1729	1/1	0.88	0.46	69,69,69,69	0
57	MG	AA	1755	1/1	0.88	0.35	84,84,84,84	0
57	MG	AA	1797	1/1	0.88	0.53	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3137	1/1	0.88	0.18	33,33,33,33	0
57	MG	BA	3131	1/1	0.88	0.26	31,31,31,31	0
57	MG	DA	3057	1/1	0.88	0.26	31,31,31,31	0
57	MG	BA	3003	1/1	0.88	0.89	85,85,85,85	0
57	MG	CA	1768	1/1	0.88	0.35	72,72,72,72	0
57	MG	CA	1755	1/1	0.88	0.16	107,107,107,107	0
57	MG	BA	3120	1/1	0.88	0.32	90,90,90,90	0
57	MG	DB	205	1/1	0.88	0.12	55,55,55,55	0
57	MG	CA	1766	1/1	0.88	0.15	96,96,96,96	0
57	MG	BA	3135	1/1	0.88	0.67	36,36,36,36	0
57	MG	BA	3403	1/1	0.88	0.23	65,65,65,65	0
57	MG	AA	1644	1/1	0.88	0.32	110,110,110,110	0
57	MG	BA	3118	1/1	0.88	0.24	68,68,68,68	0
57	MG	DA	3141	1/1	0.88	0.43	67,67,67,67	0
57	MG	AA	1611	1/1	0.88	0.20	63,63,63,63	0
57	MG	DA	3277	1/1	0.88	0.67	63,63,63,63	0
57	MG	BA	3334	1/1	0.88	0.35	79,79,79,79	0
57	MG	DA	3047	1/1	0.88	0.34	28,28,28,28	0
57	MG	AA	1720	1/1	0.88	0.28	137,137,137,137	0
57	MG	DA	3346	1/1	0.88	0.23	54,54,54,54	0
57	MG	DB	207	1/1	0.88	0.31	49,49,49,49	1
57	MG	CA	1702	1/1	0.88	0.40	66,66,66,66	0
57	MG	AA	1659	1/1	0.88	0.36	42,42,42,42	0
57	MG	DA	3169	1/1	0.88	0.52	43,43,43,43	1
57	MG	DA	3073	1/1	0.88	0.19	36,36,36,36	0
57	MG	BA	3246	1/1	0.88	0.21	74,74,74,74	0
57	MG	DA	3352	1/1	0.88	0.49	20,20,20,20	1
57	MG	DA	3035	1/1	0.88	0.12	55,55,55,55	0
57	MG	CA	1738	1/1	0.88	0.24	62,62,62,62	0
57	MG	AA	1634	1/1	0.88	0.79	73,73,73,73	0
57	MG	CA	1776	1/1	0.88	0.18	46,46,46,46	0
57	MG	CA	1667	1/1	0.88	0.48	55,55,55,55	0
57	MG	CA	1616	1/1	0.88	0.41	43,43,43,43	0
57	MG	AA	1695	1/1	0.88	0.16	52,52,52,52	0
57	MG	BA	3320	1/1	0.89	0.25	141,141,141,141	0
57	MG	DA	3375	1/1	0.89	0.16	83,83,83,83	0
57	MG	DA	3265	1/1	0.89	0.27	71,71,71,71	0
57	MG	DF	301	1/1	0.89	0.12	56,56,56,56	0
57	MG	CA	1611	1/1	0.89	0.36	110,110,110,110	0
57	MG	BA	3382	1/1	0.89	0.23	31,31,31,31	0
57	MG	DA	3063	1/1	0.89	0.50	32,32,32,32	0
57	MG	BO	201	1/1	0.89	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1739	1/1	0.89	0.29	115,115,115,115	0
57	MG	BA	3153	1/1	0.89	0.40	20,20,20,20	1
57	MG	BA	3071	1/1	0.89	0.30	52,52,52,52	0
57	MG	BA	3242	1/1	0.89	0.49	60,60,60,60	0
57	MG	AA	1645	1/1	0.89	0.53	41,41,41,41	0
57	MG	DA	3263	1/1	0.89	0.86	69,69,69,69	0
57	MG	DA	3183	1/1	0.89	0.29	96,96,96,96	0
57	MG	DA	3387	1/1	0.89	0.52	66,66,66,66	0
57	MG	BA	3266	1/1	0.89	0.32	50,50,50,50	0
57	MG	BA	3323	1/1	0.89	0.34	86,86,86,86	1
57	MG	BA	3314	1/1	0.89	0.43	92,92,92,92	1
57	MG	AA	1792	1/1	0.89	0.51	58,58,58,58	0
57	MG	CA	1789	1/1	0.89	0.56	64,64,64,64	1
57	MG	AA	1693	1/1	0.89	0.15	54,54,54,54	0
57	MG	DA	3150	1/1	0.89	0.30	65,65,65,65	1
57	MG	AA	1752	1/1	0.89	0.32	120,120,120,120	1
57	MG	BA	3296	1/1	0.89	0.21	66,66,66,66	0
57	MG	CA	1603	1/1	0.89	0.20	68,68,68,68	0
57	MG	DA	3021	1/1	0.89	0.17	35,35,35,35	0
57	MG	DA	3283	1/1	0.89	0.26	77,77,77,77	0
57	MG	CW	101	1/1	0.89	0.41	144,144,144,144	0
57	MG	AA	1703	1/1	0.89	0.14	38,38,38,38	0
57	MG	CA	1634	1/1	0.89	0.59	53,53,53,53	0
57	MG	DA	3165	1/1	0.89	0.20	78,78,78,78	0
57	MG	BA	3288	1/1	0.90	0.74	59,59,59,59	0
57	MG	DA	3401	1/1	0.90	0.15	57,57,57,57	0
57	MG	BA	3375	1/1	0.90	0.22	21,21,21,21	1
57	MG	DX	101	1/1	0.90	0.34	45,45,45,45	0
57	MG	CX	103	1/1	0.90	0.23	108,108,108,108	0
57	MG	D1	101	1/1	0.90	0.21	29,29,29,29	1
57	MG	BA	3164	1/1	0.90	0.18	56,56,56,56	0
57	MG	DA	3292	1/1	0.90	0.89	51,51,51,51	1
57	MG	DA	3306	1/1	0.90	0.17	51,51,51,51	0
57	MG	BA	3380	1/1	0.90	0.69	54,54,54,54	0
57	MG	AA	1620	1/1	0.90	0.15	54,54,54,54	0
57	MG	DA	3335	1/1	0.90	0.26	80,80,80,80	0
57	MG	DA	3054	1/1	0.90	0.46	90,90,90,90	0
57	MG	AA	1728	1/1	0.90	0.30	67,67,67,67	0
57	MG	BA	3201	1/1	0.90	0.11	35,35,35,35	0
57	MG	BA	3180	1/1	0.90	0.38	50,50,50,50	0
57	MG	BA	3215	1/1	0.90	0.31	33,33,33,33	0
57	MG	AA	1671	1/1	0.90	0.30	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3004	1/1	0.90	0.33	42,42,42,42	0
57	MG	CA	1750	1/1	0.90	0.37	77,77,77,77	1
57	MG	DA	3224	1/1	0.90	0.17	85,85,85,85	0
57	MG	BA	3387	1/1	0.90	0.65	119,119,119,119	0
57	MG	BA	3301	1/1	0.90	0.37	57,57,57,57	0
57	MG	CA	1604	1/1	0.90	0.18	63,63,63,63	0
57	MG	BA	3243	1/1	0.90	0.16	65,65,65,65	0
57	MG	BA	3236	1/1	0.90	0.19	44,44,44,44	0
57	MG	CA	1692	1/1	0.90	0.19	59,59,59,59	0
57	MG	DA	3381	1/1	0.90	0.14	45,45,45,45	0
57	MG	BA	3214	1/1	0.90	0.50	83,83,83,83	0
57	MG	DA	3211	1/1	0.90	0.30	45,45,45,45	0
57	MG	BA	3255	1/1	0.90	0.32	37,37,37,37	0
57	MG	CX	101	1/1	0.90	0.59	123,123,123,123	0
57	MG	CA	1638	1/1	0.90	0.27	42,42,42,42	0
57	MG	BA	3161	1/1	0.90	0.23	86,86,86,86	0
57	MG	BA	3086	1/1	0.90	0.40	32,32,32,32	0
57	MG	DA	3230	1/1	0.90	0.68	71,71,71,71	0
57	MG	BA	3175	1/1	0.90	0.34	46,46,46,46	0
57	MG	BA	3141	1/1	0.90	0.27	56,56,56,56	0
57	MG	DA	3034	1/1	0.90	0.51	52,52,52,52	0
58	PAR	CA	1800	42/42	0.90	0.25	86,91,109,113	0
57	MG	DA	3068	1/1	0.90	0.36	98,98,98,98	0
57	MG	DA	3194	1/1	0.90	0.12	59,59,59,59	0
57	MG	CA	1635	1/1	0.91	0.19	74,74,74,74	0
57	MG	DA	3031	1/1	0.91	0.34	41,41,41,41	0
57	MG	AL	201	1/1	0.91	0.38	81,81,81,81	0
57	MG	AA	1766	1/1	0.91	0.27	67,67,67,67	0
57	MG	BA	3172	1/1	0.91	0.21	52,52,52,52	0
57	MG	BA	3365	1/1	0.91	0.19	1,1,1,1	0
57	MG	DA	3187	1/1	0.91	0.17	55,55,55,55	0
57	MG	DA	3287	1/1	0.91	0.28	148,148,148,148	0
57	MG	CA	1762	1/1	0.91	0.41	84,84,84,84	0
57	MG	AA	1730	1/1	0.91	0.27	107,107,107,107	0
57	MG	DA	3112	1/1	0.91	0.36	39,39,39,39	0
57	MG	BA	3379	1/1	0.91	0.23	36,36,36,36	0
57	MG	AA	1786	1/1	0.91	0.27	108,108,108,108	0
57	MG	BA	3113	1/1	0.91	0.24	3,3,3,3	0
57	MG	DB	206	1/1	0.91	0.11	75,75,75,75	0
57	MG	CA	1675	1/1	0.91	0.19	92,92,92,92	0
57	MG	BA	3341	1/1	0.91	0.20	40,40,40,40	0
57	MG	DA	3199	1/1	0.91	0.99	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3318	1/1	0.91	0.19	138,138,138,138	0
57	MG	CA	1770	1/1	0.91	0.42	94,94,94,94	0
57	MG	BE	301	1/1	0.91	0.22	30,30,30,30	0
57	MG	BA	3134	1/1	0.91	0.20	10,10,10,10	0
57	MG	DA	3278	1/1	0.91	0.29	54,54,54,54	0
57	MG	BA	3249	1/1	0.91	0.41	114,114,114,114	0
57	MG	BA	3390	1/1	0.91	0.27	37,37,37,37	0
57	MG	BA	3402	1/1	0.91	0.11	63,63,63,63	0
57	MG	AA	1685	1/1	0.91	0.23	42,42,42,42	0
57	MG	DA	3200	1/1	0.91	0.20	59,59,59,59	0
57	MG	DA	3368	1/1	0.91	0.39	45,45,45,45	1
57	MG	DA	3041	1/1	0.91	0.21	46,46,46,46	0
57	MG	BA	3062	1/1	0.91	0.57	31,31,31,31	0
57	MG	BA	3319	1/1	0.91	0.24	3,3,3,3	1
57	MG	CA	1734	1/1	0.91	0.69	67,67,67,67	0
57	MG	DA	3148	1/1	0.91	0.54	46,46,46,46	0
57	MG	AA	1774	1/1	0.91	0.33	88,88,88,88	0
57	MG	AA	1699	1/1	0.91	0.15	78,78,78,78	0
57	MG	DA	3109	1/1	0.91	0.21	29,29,29,29	0
57	MG	BA	3156	1/1	0.91	0.12	20,20,20,20	0
57	MG	CA	1610	1/1	0.91	0.10	88,88,88,88	0
57	MG	AA	1647	1/1	0.91	0.21	74,74,74,74	0
57	MG	D5	102	1/1	0.91	0.31	39,39,39,39	1
57	MG	CE	201	1/1	0.91	0.15	90,90,90,90	0
57	MG	CA	1749	1/1	0.91	0.16	98,98,98,98	0
57	MG	DA	3402	1/1	0.91	0.41	125,125,125,125	0
57	MG	AA	1628	1/1	0.91	0.10	37,37,37,37	0
57	MG	DA	3142	1/1	0.91	0.47	65,65,65,65	0
57	MG	BA	3171	1/1	0.91	0.11	31,31,31,31	0
57	MG	DA	3396	1/1	0.91	0.21	145,145,145,145	0
57	MG	AA	1723	1/1	0.91	0.74	79,79,79,79	1
57	MG	BA	3409	1/1	0.91	0.36	20,20,20,20	0
57	MG	BA	3217	1/1	0.91	0.25	78,78,78,78	0
57	MG	BF	301	1/1	0.91	0.20	41,41,41,41	0
57	MG	BA	3268	1/1	0.91	0.30	34,34,34,34	0
57	MG	AA	1662	1/1	0.91	0.08	95,95,95,95	0
57	MG	BA	3298	1/1	0.91	0.47	69,69,69,69	0
57	MG	BA	3057	1/1	0.91	0.48	85,85,85,85	0
57	MG	DA	3050	1/1	0.91	0.17	69,69,69,69	1
57	MG	CN	101	1/1	0.91	0.15	57,57,57,57	0
57	MG	CA	1704	1/1	0.91	0.34	114,114,114,114	0
57	MG	DA	3334	1/1	0.92	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1697	1/1	0.92	0.16	72,72,72,72	0
57	MG	BA	3033	1/1	0.92	0.37	33,33,33,33	0
57	MG	BA	3352	1/1	0.92	0.73	23,23,23,23	1
57	MG	CA	1747	1/1	0.92	0.49	62,62,62,62	0
57	MG	CA	1662	1/1	0.92	0.69	80,80,80,80	0
57	MG	BA	3265	1/1	0.92	0.18	30,30,30,30	0
57	MG	AA	1665	1/1	0.92	0.43	53,53,53,53	0
57	MG	BA	3105	1/1	0.92	0.46	50,50,50,50	0
57	MG	BA	3174	1/1	0.92	0.25	55,55,55,55	0
57	MG	DA	3103	1/1	0.92	0.43	34,34,34,34	0
57	MG	CA	1792	1/1	0.92	0.12	95,95,95,95	0
57	MG	AA	1627	1/1	0.92	0.26	54,54,54,54	0
57	MG	DA	3025	1/1	0.92	0.48	13,13,13,13	0
57	MG	BA	3269	1/1	0.92	0.28	38,38,38,38	0
57	MG	BA	3273	1/1	0.92	0.12	75,75,75,75	0
57	MG	BB	212	1/1	0.92	0.23	31,31,31,31	1
57	MG	DA	3140	1/1	0.92	0.26	90,90,90,90	0
57	MG	BA	3005	1/1	0.92	0.42	7,7,7,7	0
57	MG	DA	3345	1/1	0.92	0.43	43,43,43,43	1
57	MG	DA	3155	1/1	0.92	0.41	21,21,21,21	1
57	MG	DA	3310	1/1	0.92	0.41	54,54,54,54	1
57	MG	AA	1612	1/1	0.92	0.31	67,67,67,67	0
57	MG	DA	3257	1/1	0.92	0.14	52,52,52,52	0
57	MG	BB	204	1/1	0.92	0.25	106,106,106,106	0
57	MG	BA	3231	1/1	0.92	0.67	38,38,38,38	0
57	MG	B2	601	1/1	0.92	0.22	55,55,55,55	1
57	MG	DA	3411	1/1	0.92	0.08	46,46,46,46	0
57	MG	DA	3233	1/1	0.92	0.45	36,36,36,36	0
57	MG	DA	3069	1/1	0.92	0.27	75,75,75,75	0
57	MG	BA	3056	1/1	0.92	0.34	17,17,17,17	0
57	MG	DA	3125	1/1	0.92	0.18	53,53,53,53	0
57	MG	BA	3408	1/1	0.92	0.20	43,43,43,43	0
57	MG	AA	1610	1/1	0.92	0.60	49,49,49,49	0
57	MG	BA	3052	1/1	0.92	0.33	13,13,13,13	0
57	MG	BA	3125	1/1	0.92	0.26	62,62,62,62	0
57	MG	CA	1787	1/1	0.92	0.13	66,66,66,66	0
57	MG	CA	1760	1/1	0.92	0.32	145,145,145,145	0
57	MG	DA	3244	1/1	0.92	0.35	62,62,62,62	0
57	MG	DB	212	1/1	0.92	0.50	99,99,99,99	1
57	MG	BA	3330	1/1	0.92	0.24	85,85,85,85	1
57	MG	CA	1794	1/1	0.92	0.61	81,81,81,81	0
57	MG	BA	3404	1/1	0.92	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3422	1/1	0.92	0.30	120,120,120,120	0
57	MG	DA	3288	1/1	0.92	0.66	37,37,37,37	0
57	MG	DA	3314	1/1	0.92	0.20	141,141,141,141	0
57	MG	AA	1698	1/1	0.92	0.14	42,42,42,42	0
57	MG	AA	1680	1/1	0.92	0.58	53,53,53,53	0
57	MG	DA	3380	1/1	0.92	0.41	52,52,52,52	0
57	MG	AA	1660	1/1	0.92	0.38	43,43,43,43	0
57	MG	AA	1658	1/1	0.92	0.19	25,25,25,25	0
57	MG	CA	1658	1/1	0.92	0.23	78,78,78,78	0
57	MG	BA	3210	1/1	0.92	1.03	84,84,84,84	0
57	MG	DA	3028	1/1	0.92	0.44	47,47,47,47	0
57	MG	CA	1627	1/1	0.92	0.34	78,78,78,78	0
57	MG	AA	1745	1/1	0.92	0.47	62,62,62,62	0
57	MG	BA	3361	1/1	0.92	0.13	28,28,28,28	0
57	MG	BA	3193	1/1	0.92	0.18	40,40,40,40	0
57	MG	BB	208	1/1	0.92	1.03	61,61,61,61	1
57	MG	CA	1717	1/1	0.92	0.12	82,82,82,82	0
57	MG	BA	3219	1/1	0.92	0.58	30,30,30,30	0
57	MG	BA	3166	1/1	0.92	0.07	31,31,31,31	0
57	MG	BA	3262	1/1	0.92	0.15	100,100,100,100	0
57	MG	CA	1601	1/1	0.92	0.29	140,140,140,140	0
57	MG	AA	1716	1/1	0.93	0.18	86,86,86,86	0
57	MG	BA	3309	1/1	0.93	0.12	112,112,112,112	1
57	MG	BA	3263	1/1	0.93	0.63	77,77,77,77	0
57	MG	BA	3332	1/1	0.93	0.49	29,29,29,29	0
57	MG	DA	3189	1/1	0.93	0.31	69,69,69,69	0
57	MG	AA	1718	1/1	0.93	0.18	72,72,72,72	0
57	MG	BA	3274	1/1	0.93	0.72	85,85,85,85	0
57	MG	DA	3298	1/1	0.93	0.17	56,56,56,56	0
57	MG	AA	1618	1/1	0.93	0.32	38,38,38,38	0
57	MG	DA	3219	1/1	0.93	0.35	99,99,99,99	0
57	MG	DA	3407	1/1	0.93	0.20	45,45,45,45	0
57	MG	DA	3386	1/1	0.93	0.74	115,115,115,115	0
57	MG	DB	210	1/1	0.93	0.27	74,74,74,74	0
57	MG	DA	3275	1/1	0.93	0.10	98,98,98,98	0
57	MG	BA	3346	1/1	0.93	0.38	67,67,67,67	0
57	MG	BA	3190	1/1	0.93	0.29	51,51,51,51	0
57	MG	BA	3146	1/1	0.93	0.22	57,57,57,57	0
57	MG	BA	3122	1/1	0.93	0.51	94,94,94,94	0
57	MG	AI	201	1/1	0.93	0.24	109,109,109,109	0
57	MG	BA	3271	1/1	0.93	0.49	43,43,43,43	0
57	MG	AA	1756	1/1	0.93	0.27	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1765	1/1	0.93	0.21	94,94,94,94	0
57	MG	CA	1693	1/1	0.93	0.12	87,87,87,87	0
57	MG	CA	1718	1/1	0.93	0.15	67,67,67,67	0
57	MG	BA	3302	1/1	0.93	0.24	26,26,26,26	0
57	MG	AE	201	1/1	0.93	0.11	101,101,101,101	0
57	MG	BA	3400	1/1	0.93	0.15	47,47,47,47	0
57	MG	BA	3032	1/1	0.93	0.23	45,45,45,45	0
57	MG	CA	1722	1/1	0.93	0.47	121,121,121,121	0
57	MG	BA	3401	1/1	0.93	0.29	81,81,81,81	0
57	MG	DA	3149	1/1	0.93	0.29	57,57,57,57	0
57	MG	AA	1663	1/1	0.93	0.57	47,47,47,47	0
57	MG	BA	3017	1/1	0.93	0.19	9,9,9,9	0
57	MG	DA	3029	1/1	0.93	0.41	40,40,40,40	0
57	MG	CA	1672	1/1	0.93	0.23	59,59,59,59	0
57	MG	AA	1760	1/1	0.93	0.43	90,90,90,90	0
57	MG	DA	3395	1/1	0.93	0.41	49,49,49,49	0
57	MG	AA	1669	1/1	0.93	0.27	57,57,57,57	0
57	MG	BA	3126	1/1	0.93	0.27	39,39,39,39	0
57	MG	DA	3080	1/1	0.93	0.14	63,63,63,63	0
57	MG	DA	3336	1/1	0.93	0.17	77,77,77,77	1
57	MG	DA	3027	1/1	0.93	0.42	37,37,37,37	0
57	MG	DA	3232	1/1	0.93	0.27	93,93,93,93	0
57	MG	DA	3384	1/1	0.93	0.23	115,115,115,115	0
57	MG	DA	3053	1/1	0.93	0.17	26,26,26,26	0
57	MG	CA	1699	1/1	0.93	0.14	50,50,50,50	0
57	MG	DA	3308	1/1	0.93	0.17	53,53,53,53	0
57	MG	BA	3192	1/1	0.93	0.17	21,21,21,21	0
57	MG	DA	3071	1/1	0.93	0.56	23,23,23,23	0
57	MG	DA	3085	1/1	0.93	0.14	32,32,32,32	0
57	MG	BA	3124	1/1	0.93	0.25	46,46,46,46	0
57	MG	BA	3053	1/1	0.93	0.47	64,64,64,64	0
57	MG	BA	3133	1/1	0.93	0.22	19,19,19,19	0
57	MG	B7	101	1/1	0.93	0.30	45,45,45,45	1
57	MG	DA	3113	1/1	0.93	0.40	27,27,27,27	0
57	MG	CA	1608	1/1	0.93	0.19	39,39,39,39	0
57	MG	CA	1769	1/1	0.93	0.29	27,27,27,27	0
57	MG	CA	1744	1/1	0.93	0.67	63,63,63,63	0
57	MG	DA	3008	1/1	0.93	0.26	36,36,36,36	0
57	MG	BA	3374	1/1	0.93	0.07	92,92,92,92	0
57	MG	DA	3105	1/1	0.93	0.28	54,54,54,54	0
57	MG	BA	3207	1/1	0.93	0.17	45,45,45,45	0
57	MG	BA	3128	1/1	0.93	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3143	1/1	0.94	0.41	18,18,18,18	0
57	MG	BA	3280	1/1	0.94	0.12	28,28,28,28	0
57	MG	DA	3320	1/1	0.94	0.30	34,34,34,34	1
57	MG	CA	1618	1/1	0.94	0.28	53,53,53,53	0
57	MG	CA	1696	1/1	0.94	0.55	108,108,108,108	0
57	MG	AA	1632	1/1	0.94	0.42	34,34,34,34	1
57	MG	AA	1719	1/1	0.94	0.50	52,52,52,52	0
57	MG	DA	3191	1/1	0.94	0.23	41,41,41,41	0
57	MG	DA	3115	1/1	0.94	0.26	22,22,22,22	0
57	MG	DA	3158	1/1	0.94	0.53	48,48,48,48	0
57	MG	BA	3208	1/1	0.94	0.44	61,61,61,61	0
57	MG	CA	1637	1/1	0.94	0.12	83,83,83,83	0
57	MG	DA	3100	1/1	0.94	0.20	63,63,63,63	0
57	MG	DA	3350	1/1	0.94	0.12	89,89,89,89	1
57	MG	BA	3168	1/1	0.94	0.49	87,87,87,87	0
57	MG	BA	3221	1/1	0.94	0.59	80,80,80,80	1
57	MG	BA	3284	1/1	0.94	0.65	53,53,53,53	0
57	MG	AA	1768	1/1	0.94	0.43	71,71,71,71	0
57	MG	BA	3091	1/1	0.94	0.47	41,41,41,41	0
57	MG	DA	3099	1/1	0.94	0.29	40,40,40,40	0
57	MG	DD	302	1/1	0.94	0.32	46,46,46,46	0
57	MG	B1	101	1/1	0.94	0.11	41,41,41,41	1
57	MG	CW	105	1/1	0.94	0.32	70,70,70,70	1
57	MG	CA	1659	1/1	0.94	0.18	42,42,42,42	0
57	MG	DA	3048	1/1	0.94	0.67	61,61,61,61	0
57	MG	DA	3040	1/1	0.94	0.20	25,25,25,25	0
57	MG	CA	1772	1/1	0.94	0.24	77,77,77,77	0
57	MG	CA	1741	1/1	0.94	0.20	53,53,53,53	0
57	MG	DA	3362	1/1	0.94	0.35	112,112,112,112	0
57	MG	DA	3397	1/1	0.94	0.74	101,101,101,101	0
57	MG	DA	3046	1/1	0.94	0.54	30,30,30,30	0
57	MG	DA	3134	1/1	0.94	0.20	57,57,57,57	0
57	MG	BA	3144	1/1	0.94	0.22	58,58,58,58	0
57	MG	B2	602	1/1	0.94	0.51	55,55,55,55	0
57	MG	BA	3413	1/1	0.94	0.55	33,33,33,33	0
57	MG	BA	3258	1/1	0.94	0.35	32,32,32,32	0
57	MG	AW	103	1/1	0.94	0.10	106,106,106,106	0
57	MG	BA	3378	1/1	0.94	0.41	8,8,8,8	0
57	MG	DD	301	1/1	0.94	0.26	38,38,38,38	0
57	MG	DA	3176	1/1	0.94	0.35	69,69,69,69	0
57	MG	DA	3421	1/1	0.94	0.20	168,168,168,168	0
57	MG	BA	3085	1/1	0.94	0.24	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3005	1/1	0.94	0.27	52,52,52,52	0
57	MG	BA	3204	1/1	0.94	0.24	33,33,33,33	0
57	MG	DA	3003	1/1	0.94	0.22	91,91,91,91	0
57	MG	AA	1794	1/1	0.94	0.16	126,126,126,126	0
57	MG	DA	3180	1/1	0.94	0.17	35,35,35,35	0
57	MG	DA	3081	1/1	0.94	0.32	38,38,38,38	0
58	PAR	AA	1799	42/42	0.94	0.23	60,65,83,87	0
57	MG	BA	3016	1/1	0.94	0.46	28,28,28,28	0
57	MG	DA	3184	1/1	0.94	0.29	36,36,36,36	0
57	MG	DA	3207	1/1	0.94	0.26	67,67,67,67	0
57	MG	DA	3251	1/1	0.94	0.17	96,96,96,96	0
57	MG	BA	3407	1/1	0.94	0.20	52,52,52,52	0
57	MG	DA	3356	1/1	0.94	0.15	57,57,57,57	0
57	MG	BA	3083	1/1	0.94	0.38	30,30,30,30	0
57	MG	DA	3129	1/1	0.94	0.13	22,22,22,22	0
57	MG	DA	3094	1/1	0.94	0.14	22,22,22,22	0
57	MG	BB	206	1/1	0.94	0.15	105,105,105,105	0
57	MG	DA	3096	1/1	0.94	0.23	24,24,24,24	0
57	MG	AA	1696	1/1	0.94	0.09	47,47,47,47	0
57	MG	BA	3027	1/1	0.94	0.19	30,30,30,30	0
57	MG	AA	1736	1/1	0.94	0.24	87,87,87,87	0
57	MG	AA	1650	1/1	0.94	0.22	99,99,99,99	0
57	MG	BA	3157	1/1	0.94	0.38	74,74,74,74	0
57	MG	DA	3337	1/1	0.94	0.10	76,76,76,76	0
57	MG	DA	3102	1/1	0.94	0.46	129,129,129,129	1
57	MG	BA	3245	1/1	0.94	0.12	42,42,42,42	0
57	MG	DA	3361	1/1	0.94	0.15	64,64,64,64	0
57	MG	CA	1620	1/1	0.94	0.28	59,59,59,59	0
57	MG	DA	3332	1/1	0.94	0.43	33,33,33,33	0
57	MG	DA	3110	1/1	0.95	0.19	41,41,41,41	0
57	MG	AA	1619	1/1	0.95	0.50	65,65,65,65	0
57	MG	BA	3240	1/1	0.95	0.12	11,11,11,11	0
57	MG	DA	3126	1/1	0.95	0.14	59,59,59,59	0
57	MG	BA	3007	1/1	0.95	0.26	22,22,22,22	0
57	MG	CA	1791	1/1	0.95	0.11	85,85,85,85	1
57	MG	CA	1641	1/1	0.95	0.43	64,64,64,64	0
57	MG	DE	301	1/1	0.95	0.27	39,39,39,39	0
57	MG	DA	3286	1/1	0.95	0.82	75,75,75,75	0
57	MG	BA	3227	1/1	0.95	0.28	74,74,74,74	0
57	MG	BA	3108	1/1	0.95	0.19	4,4,4,4	0
57	MG	BA	3103	1/1	0.95	0.21	31,31,31,31	0
57	MG	CW	104	1/1	0.95	0.11	130,130,130,130	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1605	1/1	0.95	0.14	47,47,47,47	0
57	MG	AA	1784	1/1	0.95	0.04	81,81,81,81	1
57	MG	DA	3418	1/1	0.95	0.40	47,47,47,47	1
57	MG	BA	3197	1/1	0.95	0.32	46,46,46,46	0
57	MG	DA	3355	1/1	0.95	0.17	95,95,95,95	0
57	MG	CA	1663	1/1	0.95	0.07	53,53,53,53	0
57	MG	AA	1624	1/1	0.95	0.39	52,52,52,52	0
57	MG	BA	3066	1/1	0.95	0.33	26,26,26,26	0
57	MG	DA	3231	1/1	0.95	0.35	31,31,31,31	0
57	MG	DA	3061	1/1	0.95	0.28	30,30,30,30	0
57	MG	DA	3163	1/1	0.95	0.31	52,52,52,52	0
57	MG	CA	1730	1/1	0.95	0.26	43,43,43,43	0
57	MG	AA	1694	1/1	0.95	0.46	84,84,84,84	0
57	MG	AA	1791	1/1	0.95	0.23	26,26,26,26	1
57	MG	AA	1629	1/1	0.95	0.28	62,62,62,62	0
57	MG	DA	3274	1/1	0.95	0.30	60,60,60,60	0
57	MG	BA	3050	1/1	0.95	0.27	30,30,30,30	0
57	MG	BA	3023	1/1	0.95	0.34	23,23,23,23	0
57	MG	DA	3044	1/1	0.95	0.20	40,40,40,40	0
57	MG	AA	1614	1/1	0.95	0.40	14,14,14,14	0
57	MG	BB	209	1/1	0.95	0.51	1,1,1,1	1
57	MG	AA	1630	1/1	0.95	0.23	55,55,55,55	0
57	MG	BA	3292	1/1	0.95	0.18	23,23,23,23	0
57	MG	BX	102	1/1	0.95	0.32	104,104,104,104	0
57	MG	CA	1695	1/1	0.95	0.36	54,54,54,54	0
57	MG	BA	3276	1/1	0.95	0.30	49,49,49,49	0
57	MG	AA	1709	1/1	0.95	0.06	49,49,49,49	0
57	MG	DA	3093	1/1	0.95	0.23	36,36,36,36	0
57	MG	BA	3370	1/1	0.95	0.40	113,113,113,113	0
57	MG	BA	3369	1/1	0.95	0.33	53,53,53,53	1
57	MG	DA	3206	1/1	0.95	0.20	33,33,33,33	0
57	MG	BA	3104	1/1	0.95	0.29	20,20,20,20	0
57	MG	CA	1774	1/1	0.95	0.19	121,121,121,121	0
57	MG	BA	3082	1/1	0.95	0.30	37,37,37,37	0
57	MG	BA	3037	1/1	0.95	0.25	23,23,23,23	0
57	MG	DA	3258	1/1	0.95	0.39	37,37,37,37	0
57	MG	CA	1784	1/1	0.95	0.17	68,68,68,68	1
57	MG	DA	3026	1/1	0.95	0.24	19,19,19,19	0
57	MG	AA	1717	1/1	0.95	0.32	61,61,61,61	0
57	MG	BA	3015	1/1	0.95	0.35	33,33,33,33	0
57	MG	BA	3102	1/1	0.95	0.38	13,13,13,13	0
57	MG	BA	3199	1/1	0.95	0.68	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3098	1/1	0.95	0.20	6,6,6,6	0
57	MG	DA	3254	1/1	0.95	0.13	99,99,99,99	0
57	MG	CI	201	1/1	0.95	0.19	75,75,75,75	0
57	MG	DA	3215	1/1	0.95	0.08	68,68,68,68	1
57	MG	BB	203	1/1	0.95	0.48	14,14,14,14	1
57	MG	BA	3148	1/1	0.95	0.22	57,57,57,57	0
57	MG	AA	1639	1/1	0.95	0.29	99,99,99,99	0
57	MG	CA	1797	1/1	0.95	0.10	120,120,120,120	0
57	MG	BA	3181	1/1	0.95	0.32	49,49,49,49	0
57	MG	BA	3145	1/1	0.95	0.21	27,27,27,27	0
57	MG	DA	3159	1/1	0.95	0.58	70,70,70,70	0
57	MG	CA	1626	1/1	0.95	0.22	34,34,34,34	0
57	MG	BA	3031	1/1	0.95	0.45	44,44,44,44	0
57	MG	DA	3271	1/1	0.95	0.34	47,47,47,47	0
57	MG	BA	3060	1/1	0.95	0.38	1,1,1,1	0
57	MG	DA	3156	1/1	0.95	0.49	38,38,38,38	0
57	MG	DA	3074	1/1	0.95	0.28	26,26,26,26	0
57	MG	CA	1796	1/1	0.95	0.25	119,119,119,119	0
57	MG	DA	3036	1/1	0.95	0.32	32,32,32,32	0
57	MG	BA	3147	1/1	0.95	0.17	26,26,26,26	0
57	MG	DA	3145	1/1	0.95	0.44	90,90,90,90	0
57	MG	BA	3261	1/1	0.95	0.56	23,23,23,23	0
57	MG	BA	3039	1/1	0.95	0.27	14,14,14,14	0
57	MG	AA	1626	1/1	0.95	0.17	37,37,37,37	0
57	MG	DA	3018	1/1	0.96	0.31	31,31,31,31	0
57	MG	BA	3109	1/1	0.96	0.18	39,39,39,39	0
57	MG	BA	3304	1/1	0.96	0.16	81,81,81,81	0
57	MG	DA	3326	1/1	0.96	0.15	78,78,78,78	1
57	MG	CA	1651	1/1	0.96	0.17	85,85,85,85	0
57	MG	DA	3084	1/1	0.96	0.42	44,44,44,44	0
57	MG	AA	1652	1/1	0.96	0.31	82,82,82,82	0
57	MG	DA	3348	1/1	0.96	0.10	64,64,64,64	0
57	MG	DA	3235	1/1	0.96	0.29	30,30,30,30	0
57	MG	CA	1724	1/1	0.96	0.20	80,80,80,80	0
57	MG	BA	3011	1/1	0.96	0.30	32,32,32,32	0
57	MG	DB	204	1/1	0.96	0.21	90,90,90,90	0
57	MG	DA	3024	1/1	0.96	0.22	49,49,49,49	0
57	MG	AA	1697	1/1	0.96	0.30	78,78,78,78	0
57	MG	DA	3242	1/1	0.96	0.19	18,18,18,18	0
57	MG	BA	3026	1/1	0.96	0.33	8,8,8,8	0
57	MG	DA	3378	1/1	0.96	0.32	72,72,72,72	0
57	MG	BA	3344	1/1	0.96	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3130	1/1	0.96	0.33	41,41,41,41	0
57	MG	DA	3066	1/1	0.96	0.42	43,43,43,43	0
57	MG	DA	3174	1/1	0.96	0.09	53,53,53,53	0
57	MG	AA	1746	1/1	0.96	0.37	95,95,95,95	0
57	MG	BA	3063	1/1	0.96	0.15	1,1,1,1	0
57	MG	BA	3395	1/1	0.96	0.21	113,113,113,113	0
57	MG	BA	3203	1/1	0.96	0.13	30,30,30,30	0
57	MG	BA	3372	1/1	0.96	0.53	57,57,57,57	1
57	MG	AA	1788	1/1	0.96	0.23	73,73,73,73	0
57	MG	DA	3385	1/1	0.96	0.26	79,79,79,79	0
57	MG	DA	3009	1/1	0.96	0.15	45,45,45,45	0
57	MG	DA	3323	1/1	0.96	0.64	53,53,53,53	1
57	MG	BA	3106	1/1	0.96	0.28	20,20,20,20	0
57	MG	BA	3337	1/1	0.96	0.14	162,162,162,162	0
57	MG	DA	3420	1/1	0.96	0.10	137,137,137,137	1
57	MG	DA	3347	1/1	0.96	0.26	53,53,53,53	0
57	MG	BA	3205	1/1	0.96	0.30	17,17,17,17	0
57	MG	BA	3025	1/1	0.96	0.49	9,9,9,9	0
57	MG	BA	3088	1/1	0.96	0.23	21,21,21,21	0
57	MG	AA	1688	1/1	0.96	0.25	35,35,35,35	0
57	MG	DA	3394	1/1	0.96	0.13	103,103,103,103	0
57	MG	DA	3173	1/1	0.96	0.10	50,50,50,50	0
57	MG	AA	1604	1/1	0.96	0.14	55,55,55,55	0
57	MG	DA	3030	1/1	0.96	0.23	47,47,47,47	0
57	MG	CA	1732	1/1	0.96	0.09	82,82,82,82	0
57	MG	CA	1710	1/1	0.96	0.07	54,54,54,54	0
57	MG	BA	3034	1/1	0.96	0.19	40,40,40,40	0
57	MG	DA	3403	1/1	0.96	0.17	55,55,55,55	0
57	MG	DA	3167	1/1	0.96	0.13	37,37,37,37	0
57	MG	BA	3178	1/1	0.96	0.24	24,24,24,24	0
57	MG	DA	3203	1/1	0.96	0.08	56,56,56,56	0
57	MG	DA	3237	1/1	0.96	0.17	156,156,156,156	0
57	MG	BA	3154	1/1	0.96	0.33	13,13,13,13	0
57	MG	BA	3089	1/1	0.96	0.63	43,43,43,43	0
57	MG	AA	1638	1/1	0.96	0.23	36,36,36,36	0
57	MG	BA	3018	1/1	0.96	0.48	9,9,9,9	0
57	MG	BA	3398	1/1	0.96	0.36	84,84,84,84	0
57	MG	CA	1653	1/1	0.96	0.13	83,83,83,83	0
57	MG	DA	3104	1/1	0.96	0.47	37,37,37,37	0
57	MG	BA	3095	1/1	0.96	0.34	27,27,27,27	0
57	MG	DA	3060	1/1	0.96	0.30	30,30,30,30	0
57	MG	BA	3308	1/1	0.96	0.21	114,114,114,114	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3294	1/1	0.96	0.37	33,33,33,33	0
57	MG	BA	3068	1/1	0.96	0.15	38,38,38,38	0
57	MG	DA	3045	1/1	0.96	0.30	35,35,35,35	0
57	MG	AA	1686	1/1	0.96	0.57	104,104,104,104	0
57	MG	AA	1609	1/1	0.96	0.20	36,36,36,36	0
57	MG	CA	1624	1/1	0.96	0.25	55,55,55,55	0
57	MG	BA	3385	1/1	0.96	0.12	87,87,87,87	0
57	MG	BA	3272	1/1	0.96	0.27	46,46,46,46	0
57	MG	D2	603	1/1	0.96	0.29	95,95,95,95	0
57	MG	AA	1636	1/1	0.96	0.51	74,74,74,74	0
57	MG	DA	3107	1/1	0.96	0.09	32,32,32,32	0
57	MG	DA	3124	1/1	0.96	0.62	28,28,28,28	0
57	MG	DA	3013	1/1	0.96	0.36	31,31,31,31	0
57	MG	CA	1607	1/1	0.96	0.16	30,30,30,30	0
57	MG	DA	3185	1/1	0.96	0.30	33,33,33,33	0
57	MG	DA	3280	1/1	0.96	0.35	109,109,109,109	0
57	MG	BA	3092	1/1	0.96	0.27	28,28,28,28	0
57	MG	DA	3137	1/1	0.96	0.18	21,21,21,21	0
57	MG	BA	3333	1/1	0.96	0.21	40,40,40,40	0
57	MG	DA	3377	1/1	0.96	0.33	24,24,24,24	0
57	MG	BV	201	1/1	0.96	0.26	64,64,64,64	0
57	MG	AV	102	1/1	0.96	0.15	93,93,93,93	1
57	MG	AA	1675	1/1	0.96	0.59	63,63,63,63	0
57	MG	BA	3142	1/1	0.96	0.49	20,20,20,20	0
57	MG	AA	1711	1/1	0.96	0.13	73,73,73,73	0
57	MG	DA	3151	1/1	0.96	0.33	57,57,57,57	1
57	MG	BA	3306	1/1	0.96	0.11	18,18,18,18	0
57	MG	AA	1615	1/1	0.96	0.58	65,65,65,65	0
57	MG	DA	3017	1/1	0.96	0.44	31,31,31,31	0
57	MG	DA	3016	1/1	0.96	0.24	51,51,51,51	0
57	MG	AA	1605	1/1	0.96	0.12	120,120,120,120	0
57	MG	DA	3302	1/1	0.96	0.19	43,43,43,43	1
57	MG	BA	3140	1/1	0.96	0.36	66,66,66,66	0
57	MG	AA	1778	1/1	0.96	0.57	65,65,65,65	1
57	MG	BA	3038	1/1	0.96	0.15	41,41,41,41	0
59	ZN	D9	101	1/1	0.96	0.12	136,136,136,136	0
57	MG	BA	3386	1/1	0.96	0.09	76,76,76,76	0
57	MG	BA	3076	1/1	0.96	0.20	25,25,25,25	0
57	MG	DA	3204	1/1	0.96	0.39	39,39,39,39	0
57	MG	DA	3245	1/1	0.96	0.21	69,69,69,69	0
57	MG	CA	1631	1/1	0.97	0.30	65,65,65,65	0
57	MG	BA	3184	1/1	0.97	0.34	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3209	1/1	0.97	0.14	73,73,73,73	0
57	MG	DA	3303	1/1	0.97	0.30	30,30,30,30	0
57	MG	CV	102	1/1	0.97	0.19	46,46,46,46	1
57	MG	BA	3355	1/1	0.97	0.16	92,92,92,92	0
57	MG	DA	3089	1/1	0.97	0.29	26,26,26,26	0
57	MG	BA	3079	1/1	0.97	0.21	31,31,31,31	0
57	MG	BA	3405	1/1	0.97	0.34	164,164,164,164	1
57	MG	BA	3260	1/1	0.97	0.50	30,30,30,30	0
57	MG	DA	3295	1/1	0.97	0.09	78,78,78,78	0
57	MG	BA	3234	1/1	0.97	0.54	56,56,56,56	0
57	MG	AA	1676	1/1	0.97	0.13	48,48,48,48	0
57	MG	AA	1714	1/1	0.97	0.10	29,29,29,29	0
57	MG	CA	1628	1/1	0.97	0.08	81,81,81,81	0
57	MG	CA	1636	1/1	0.97	0.49	50,50,50,50	0
57	MG	CA	1642	1/1	0.97	0.27	74,74,74,74	0
57	MG	DA	3208	1/1	0.97	0.18	32,32,32,32	0
57	MG	DA	3261	1/1	0.97	0.27	95,95,95,95	0
57	MG	CA	1703	1/1	0.97	0.36	87,87,87,87	0
57	MG	BA	3117	1/1	0.97	0.56	59,59,59,59	0
57	MG	CA	1758	1/1	0.97	0.27	64,64,64,64	1
57	MG	BB	211	1/1	0.97	0.15	119,119,119,119	0
57	MG	BA	3209	1/1	0.97	0.39	14,14,14,14	0
57	MG	BA	3396	1/1	0.97	0.28	11,11,11,11	0
57	MG	B5	101	1/1	0.97	0.17	42,42,42,42	0
57	MG	BA	3069	1/1	0.97	0.53	63,63,63,63	0
57	MG	AA	1782	1/1	0.97	0.17	96,96,96,96	1
57	MG	BX	101	1/1	0.97	0.39	58,58,58,58	0
57	MG	BA	3238	1/1	0.97	0.30	51,51,51,51	0
57	MG	BA	3111	1/1	0.97	0.41	23,23,23,23	0
57	MG	DB	201	1/1	0.97	0.24	74,74,74,74	0
57	MG	DA	3082	1/1	0.97	0.28	59,59,59,59	0
57	MG	DA	3095	1/1	0.97	0.10	37,37,37,37	0
57	MG	DA	3075	1/1	0.97	0.21	37,37,37,37	0
57	MG	DA	3343	1/1	0.97	0.19	71,71,71,71	0
57	MG	BA	3354	1/1	0.97	0.14	129,129,129,129	0
57	MG	DA	3305	1/1	0.97	0.56	100,100,100,100	1
57	MG	BA	3329	1/1	0.97	0.16	126,126,126,126	0
57	MG	BA	3123	1/1	0.97	0.57	29,29,29,29	0
57	MG	CW	103	1/1	0.97	0.26	87,87,87,87	0
57	MG	DA	3322	1/1	0.97	0.22	62,62,62,62	0
57	MG	BB	210	1/1	0.97	0.32	27,27,27,27	0
57	MG	BA	3300	1/1	0.97	0.32	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3012	1/1	0.97	0.32	16,16,16,16	0
57	MG	AA	1725	1/1	0.97	0.13	104,104,104,104	0
57	MG	DA	3011	1/1	0.97	0.48	52,52,52,52	0
57	MG	BA	3206	1/1	0.97	0.25	22,22,22,22	0
57	MG	BA	3218	1/1	0.97	0.35	6,6,6,6	0
57	MG	DA	3023	1/1	0.97	0.33	20,20,20,20	0
57	MG	DA	3181	1/1	0.97	0.20	100,100,100,100	0
57	MG	CA	1751	1/1	0.97	0.16	66,66,66,66	1
57	MG	BA	3202	1/1	0.97	0.41	16,16,16,16	0
57	MG	AA	1747	1/1	0.97	0.13	135,135,135,135	0
57	MG	DA	3344	1/1	0.97	0.46	64,64,64,64	0
57	MG	BA	3072	1/1	0.97	0.10	3,3,3,3	0
57	MG	CA	1723	1/1	0.97	0.35	86,86,86,86	0
57	MG	BA	3198	1/1	0.97	0.17	51,51,51,51	0
57	MG	BA	3149	1/1	0.97	0.25	13,13,13,13	1
57	MG	BA	3173	1/1	0.97	0.22	33,33,33,33	0
57	MG	CA	1621	1/1	0.97	0.09	58,58,58,58	0
57	MG	BA	3020	1/1	0.97	0.25	28,28,28,28	0
57	MG	BA	3114	1/1	0.97	0.43	3,3,3,3	0
57	MG	DA	3097	1/1	0.97	0.08	25,25,25,25	0
57	MG	AA	1674	1/1	0.97	0.16	42,42,42,42	0
57	MG	DA	3330	1/1	0.97	0.14	51,51,51,51	1
57	MG	BA	3074	1/1	0.97	0.17	24,24,24,24	0
57	MG	DA	3417	1/1	0.97	0.08	37,37,37,37	0
57	MG	DA	3078	1/1	0.97	0.21	20,20,20,20	0
57	MG	DA	3067	1/1	0.97	0.56	46,46,46,46	0
57	MG	BA	3392	1/1	0.97	0.14	139,139,139,139	0
57	MG	DA	3043	1/1	0.97	0.19	51,51,51,51	0
57	MG	DA	3091	1/1	0.97	0.30	39,39,39,39	0
57	MG	BA	3343	1/1	0.97	0.13	37,37,37,37	0
57	MG	AA	1613	1/1	0.97	0.19	81,81,81,81	0
57	MG	BA	3316	1/1	0.97	0.22	55,55,55,55	1
57	MG	DA	3333	1/1	0.97	0.16	108,108,108,108	0
57	MG	DA	3120	1/1	0.97	0.19	39,39,39,39	0
57	MG	DA	3064	1/1	0.97	0.16	32,32,32,32	0
57	MG	CA	1639	1/1	0.97	0.17	62,62,62,62	0
57	MG	BA	3348	1/1	0.97	0.20	79,79,79,79	0
57	MG	BA	3059	1/1	0.97	0.24	9,9,9,9	0
57	MG	DA	3088	1/1	0.97	0.41	37,37,37,37	0
57	MG	BA	3381	1/1	0.97	0.39	29,29,29,29	0
57	MG	BA	3119	1/1	0.97	0.24	35,35,35,35	0
57	MG	DA	3058	1/1	0.97	0.37	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3388	1/1	0.97	0.36	12,12,12,12	0
57	MG	BA	3411	1/1	0.97	0.12	51,51,51,51	1
57	MG	BA	3043	1/1	0.97	0.20	20,20,20,20	0
57	MG	AA	1678	1/1	0.97	0.10	166,166,166,166	0
57	MG	AA	1606	1/1	0.97	0.12	34,34,34,34	0
57	MG	BA	3009	1/1	0.97	0.35	17,17,17,17	0
57	MG	BA	3097	1/1	0.98	0.28	7,7,7,7	0
57	MG	BA	3065	1/1	0.98	0.25	1,1,1,1	0
57	MG	DA	3117	1/1	0.98	0.09	16,16,16,16	0
57	MG	CA	1689	1/1	0.98	0.16	40,40,40,40	0
57	MG	BA	3303	1/1	0.98	0.18	49,49,49,49	1
57	MG	BA	3008	1/1	0.98	0.26	3,3,3,3	0
57	MG	AA	1649	1/1	0.98	0.13	56,56,56,56	1
57	MG	BA	3350	1/1	0.98	0.18	81,81,81,81	1
57	MG	DA	3079	1/1	0.98	0.14	37,37,37,37	0
57	MG	AA	1608	1/1	0.98	0.20	46,46,46,46	0
57	MG	DA	3404	1/1	0.98	0.07	97,97,97,97	1
57	MG	DA	3391	1/1	0.98	0.10	120,120,120,120	0
57	MG	DA	3077	1/1	0.98	0.13	29,29,29,29	0
57	MG	DA	3055	1/1	0.98	0.15	31,31,31,31	0
57	MG	CA	1790	1/1	0.98	0.18	48,48,48,48	0
57	MG	DA	3220	1/1	0.98	0.38	26,26,26,26	0
57	MG	BA	3191	1/1	0.98	0.19	14,14,14,14	0
57	MG	BA	3070	1/1	0.98	0.44	2,2,2,2	0
57	MG	DA	3366	1/1	0.98	0.08	29,29,29,29	1
57	MG	DA	3313	1/1	0.98	0.32	80,80,80,80	0
57	MG	BA	3412	1/1	0.98	0.10	30,30,30,30	0
57	MG	BA	3099	1/1	0.98	0.20	37,37,37,37	0
57	MG	DA	3065	1/1	0.98	0.19	17,17,17,17	0
57	MG	DA	3309	1/1	0.98	0.22	47,47,47,47	0
57	MG	DA	3037	1/1	0.98	0.22	45,45,45,45	0
57	MG	DA	3083	1/1	0.98	0.29	33,33,33,33	0
57	MG	BA	3096	1/1	0.98	0.15	1,1,1,1	0
57	MG	BA	3036	1/1	0.98	0.22	29,29,29,29	0
57	MG	BA	3064	1/1	0.98	0.34	20,20,20,20	0
57	MG	BA	3094	1/1	0.98	0.18	24,24,24,24	0
57	MG	CA	1712	1/1	0.98	0.12	81,81,81,81	0
57	MG	BA	3259	1/1	0.98	0.18	24,24,24,24	0
57	MG	BA	3410	1/1	0.98	0.45	120,120,120,120	0
57	MG	BA	3315	1/1	0.98	0.06	83,83,83,83	0
57	MG	AA	1637	1/1	0.98	0.11	58,58,58,58	0
57	MG	BD	302	1/1	0.98	0.22	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3171	1/1	0.98	0.24	43,43,43,43	0
57	MG	AA	1687	1/1	0.98	0.13	9,9,9,9	1
57	MG	BA	3045	1/1	0.98	0.41	1,1,1,1	0
57	MG	BA	3165	1/1	0.98	0.14	38,38,38,38	0
57	MG	CA	1633	1/1	0.98	0.14	42,42,42,42	0
57	MG	DA	3168	1/1	0.98	0.21	36,36,36,36	0
57	MG	CA	1715	1/1	0.98	0.12	66,66,66,66	0
57	MG	BA	3414	1/1	0.98	0.10	60,60,60,60	0
57	MG	BA	3040	1/1	0.98	0.33	20,20,20,20	0
57	MG	BA	3213	1/1	0.98	0.09	93,93,93,93	1
57	MG	DA	3022	1/1	0.98	0.33	34,34,34,34	0
57	MG	BA	3325	1/1	0.98	0.13	88,88,88,88	1
57	MG	BA	3299	1/1	0.98	0.28	46,46,46,46	1
57	MG	DA	3236	1/1	0.98	0.33	47,47,47,47	0
57	MG	BA	3061	1/1	0.98	0.31	10,10,10,10	0
57	MG	BA	3421	1/1	0.98	0.15	110,110,110,110	1
57	MG	BA	3028	1/1	0.98	0.23	12,12,12,12	0
57	MG	BA	3335	1/1	0.98	0.11	62,62,62,62	0
57	MG	CA	1781	1/1	0.98	0.08	58,58,58,58	0
57	MG	DA	3382	1/1	0.98	0.13	74,74,74,74	0
57	MG	BA	3049	1/1	0.98	0.28	84,84,84,84	1
57	MG	CA	1670	1/1	0.98	0.11	69,69,69,69	0
57	MG	DA	3374	1/1	0.98	0.12	37,37,37,37	1
57	MG	BA	3132	1/1	0.98	0.21	14,14,14,14	0
57	MG	AA	1789	1/1	0.98	0.32	81,81,81,81	1
57	MG	BA	3021	1/1	0.98	0.36	30,30,30,30	0
57	MG	AA	1785	1/1	0.98	0.18	105,105,105,105	0
57	MG	CA	1743	1/1	0.98	0.50	65,65,65,65	0
57	MG	BA	3362	1/1	0.98	0.19	85,85,85,85	0
57	MG	DA	3409	1/1	0.98	0.55	121,121,121,121	0
57	MG	BA	3019	1/1	0.98	0.28	28,28,28,28	0
57	MG	BA	3024	1/1	0.98	0.42	11,11,11,11	0
57	MG	CA	1679	1/1	0.98	0.12	86,86,86,86	0
57	MG	BA	3182	1/1	0.98	0.23	62,62,62,62	0
57	MG	BA	3183	1/1	0.98	0.32	20,20,20,20	0
57	MG	BB	205	1/1	0.98	0.20	25,25,25,25	0
57	MG	BA	3022	1/1	0.98	0.35	20,20,20,20	0
57	MG	BA	3328	1/1	0.98	0.18	168,168,168,168	0
57	MG	AA	1633	1/1	0.98	0.14	40,40,40,40	0
57	MG	AA	1691	1/1	0.98	0.11	27,27,27,27	0
57	MG	BA	3046	1/1	0.98	0.29	4,4,4,4	0
57	MG	BA	3347	1/1	0.98	0.29	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3410	1/1	0.98	0.31	87,87,87,87	1
57	MG	BA	3286	1/1	0.98	0.67	16,16,16,16	0
57	MG	DA	3062	1/1	0.98	0.32	33,33,33,33	0
57	MG	CA	1619	1/1	0.98	0.18	80,80,80,80	0
57	MG	BA	3029	1/1	0.98	0.12	40,40,40,40	0
57	MG	DA	3250	1/1	0.98	0.40	63,63,63,63	1
57	MG	BA	3185	1/1	0.98	0.22	1,1,1,1	0
57	MG	BA	3058	1/1	0.98	0.38	19,19,19,19	0
57	MG	BA	3044	1/1	0.98	0.31	1,1,1,1	0
57	MG	DA	3039	1/1	0.98	0.05	70,70,70,70	0
57	MG	BA	3321	1/1	0.98	0.14	80,80,80,80	0
57	MG	BA	3115	1/1	0.98	0.32	27,27,27,27	0
57	MG	BA	3189	1/1	0.98	0.17	8,8,8,8	0
57	MG	BA	3116	1/1	0.98	0.12	4,4,4,4	0
57	MG	DA	3131	1/1	0.98	0.21	23,23,23,23	0
57	MG	BA	3358	1/1	0.98	0.24	24,24,24,24	0
57	MG	BA	3256	1/1	0.98	0.34	11,11,11,11	0
57	MG	BA	3136	1/1	0.98	0.22	16,16,16,16	0
57	MG	DA	3076	1/1	0.98	0.33	45,45,45,45	0
57	MG	AA	1642	1/1	0.98	0.19	45,45,45,45	0
57	MG	BA	3075	1/1	0.98	0.36	31,31,31,31	0
57	MG	CA	1650	1/1	0.98	0.11	89,89,89,89	1
57	MG	DA	3014	1/1	0.98	0.19	31,31,31,31	0
57	MG	BA	3073	1/1	0.98	0.15	5,5,5,5	0
57	MG	DA	3371	1/1	0.98	0.12	61,61,61,61	1
57	MG	BA	3278	1/1	0.98	0.09	127,127,127,127	0
57	MG	DA	3056	1/1	0.98	0.34	49,49,49,49	0
57	MG	AA	1767	1/1	0.99	0.29	44,44,44,44	0
57	MG	DA	3193	1/1	0.99	0.33	48,48,48,48	0
57	MG	AX	101	1/1	0.99	0.08	118,118,118,118	0
57	MG	CA	1748	1/1	0.99	0.24	63,63,63,63	0
59	ZN	AD	302	1/1	0.99	0.24	55,55,55,55	0
57	MG	AA	1787	1/1	0.99	0.12	41,41,41,41	1
59	ZN	AN	102	1/1	0.99	0.18	109,109,109,109	0
57	MG	BA	3042	1/1	0.99	0.14	36,36,36,36	0
57	MG	BD	301	1/1	0.99	0.21	16,16,16,16	0
59	ZN	CD	301	1/1	0.99	0.23	55,55,55,55	0
57	MG	DA	3316	1/1	0.99	0.09	88,88,88,88	0
57	MG	DA	3133	1/1	0.99	0.22	35,35,35,35	0
57	MG	CV	101	1/1	0.99	0.21	20,20,20,20	0
57	MG	DA	3010	1/1	0.99	0.35	18,18,18,18	0
57	MG	BA	3090	1/1	0.99	0.36	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3093	1/1	0.99	0.07	7,7,7,7	0
57	MG	DA	3241	1/1	0.99	0.38	32,32,32,32	0
57	MG	BA	3078	1/1	0.99	0.18	13,13,13,13	0
57	MG	BA	3055	1/1	0.99	0.32	18,18,18,18	0
57	MG	BA	3222	1/1	0.99	0.16	84,84,84,84	0
57	MG	DA	3052	1/1	0.99	0.12	30,30,30,30	0
57	MG	AA	1779	1/1	0.99	0.13	90,90,90,90	0
57	MG	AA	1692	1/1	0.99	0.13	72,72,72,72	0
57	MG	BA	3391	1/1	0.99	0.20	37,37,37,37	0
57	MG	BA	3336	1/1	0.99	0.09	105,105,105,105	1
59	ZN	B9	101	1/1	0.99	0.04	94,94,94,94	0
57	MG	AA	1780	1/1	0.99	0.35	115,115,115,115	0
57	MG	BA	3139	1/1	0.99	0.16	85,85,85,85	0
57	MG	DA	3390	1/1	0.99	0.17	48,48,48,48	0
57	MG	DA	3360	1/1	0.99	0.10	83,83,83,83	0
57	MG	BA	3087	1/1	0.99	0.21	10,10,10,10	0
57	MG	BA	3307	1/1	0.99	0.31	23,23,23,23	0
57	MG	DA	3359	1/1	0.99	0.08	62,62,62,62	1
57	MG	BA	3030	1/1	0.99	0.23	18,18,18,18	0
57	MG	BA	3081	1/1	0.99	0.20	7,7,7,7	0
57	MG	BA	3051	1/1	0.99	0.17	5,5,5,5	0
57	MG	BA	3239	1/1	0.99	0.32	20,20,20,20	0
57	MG	BA	3077	1/1	0.99	0.15	1,1,1,1	0
57	MG	CX	102	1/1	0.99	0.09	110,110,110,110	0
57	MG	DA	3234	1/1	0.99	0.15	22,22,22,22	0
57	MG	BA	3229	1/1	0.99	0.35	20,20,20,20	0
59	ZN	CN	102	1/1	0.99	0.12	120,120,120,120	0
57	MG	DA	3357	1/1	0.99	0.16	111,111,111,111	0
57	MG	BA	3287	1/1	0.99	0.51	31,31,31,31	0
57	MG	DA	3186	1/1	0.99	0.21	48,48,48,48	0
57	MG	BA	3377	1/1	0.99	0.14	126,126,126,126	0
57	MG	BA	3084	1/1	0.99	0.18	12,12,12,12	0
57	MG	BA	3359	1/1	0.99	0.16	86,86,86,86	1
57	MG	BA	3035	1/1	0.99	0.26	2,2,2,2	0
57	MG	BA	3169	1/1	0.99	0.23	18,18,18,18	0
57	MG	BA	3293	1/1	0.99	0.11	87,87,87,87	0
57	MG	DA	3363	1/1	0.99	0.14	68,68,68,68	0
57	MG	BA	3129	1/1	0.99	0.27	10,10,10,10	0
57	MG	BA	3397	1/1	0.99	0.10	73,73,73,73	0
57	MG	BA	3130	1/1	0.99	0.19	8,8,8,8	0
57	MG	BA	3054	1/1	0.99	0.15	1,1,1,1	0
57	MG	DA	3268	1/1	0.99	0.08	41,41,41,41	0

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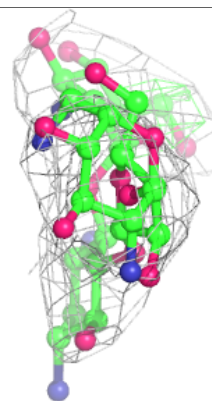
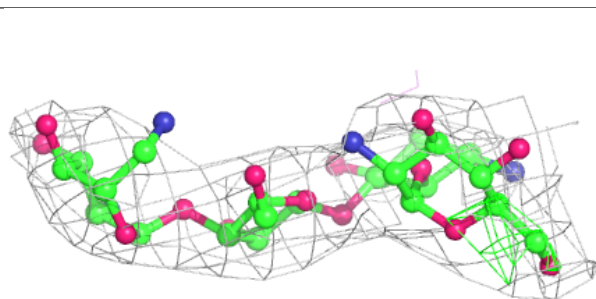
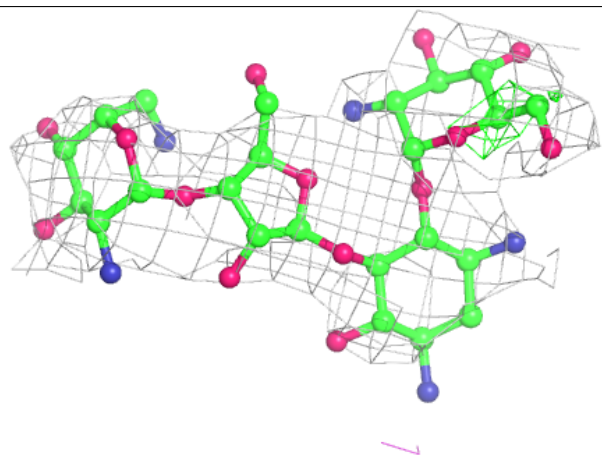
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3233	1/1	0.99	0.40	24,24,24,24	0
57	MG	BA	3363	1/1	0.99	0.15	73,73,73,73	0
57	MG	BA	3013	1/1	0.99	0.17	7,7,7,7	0
57	MG	BA	3232	1/1	0.99	0.20	27,27,27,27	0
57	MG	DA	3038	1/1	0.99	0.21	49,49,49,49	0
57	MG	BA	3112	1/1	0.99	0.40	15,15,15,15	0
57	MG	AV	101	1/1	0.99	0.14	36,36,36,36	0
57	MG	BA	3357	1/1	1.00	0.17	84,84,84,84	0
57	MG	BA	3364	1/1	1.00	0.17	35,35,35,35	0
57	MG	DA	3364	1/1	1.00	0.22	52,52,52,52	0
57	MG	BA	3002	1/1	1.00	0.16	139,139,139,139	0

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

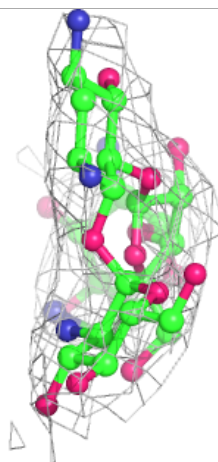
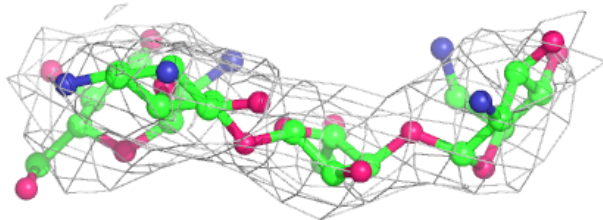
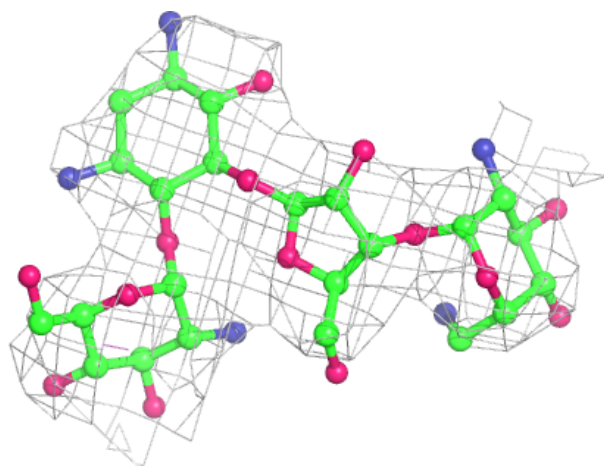
Electron density around PAR CA 1800:

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



Electron density around PAR AA 1799:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.