



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:50 am BST

PDB ID : 4V8X
Title : Structure of Thermus thermophilus ribosome
Authors : Feng, S.; Chen, Y.; Kamada, K.; Wang, H.; Tang, K.; Wang, M.; Gao, Y.G.
Deposited on : 2013-07-19
Resolution : 3.35 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
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

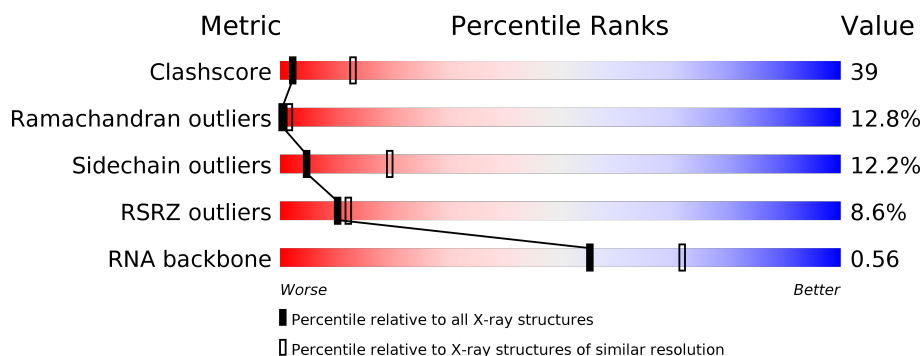
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.





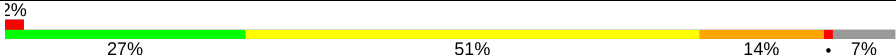
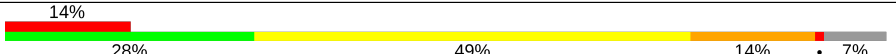
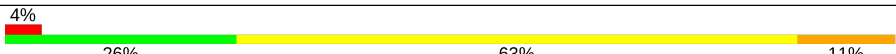
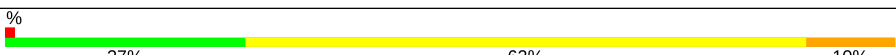
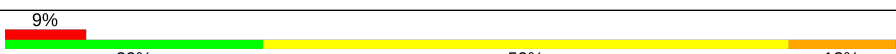
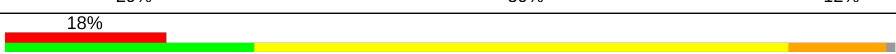
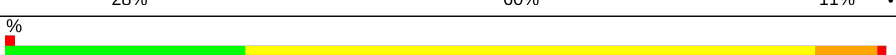
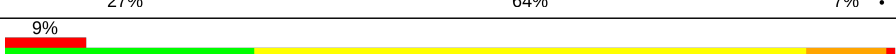
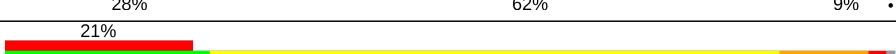
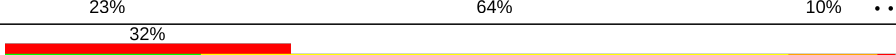
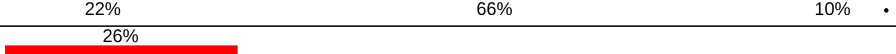
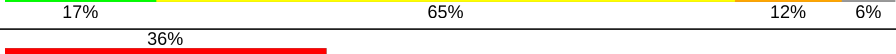
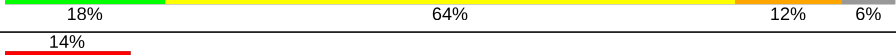
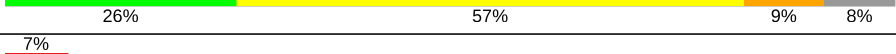



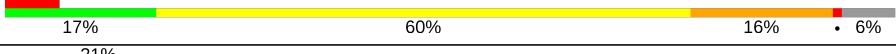
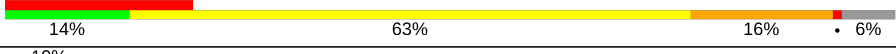
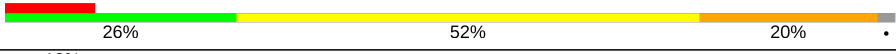
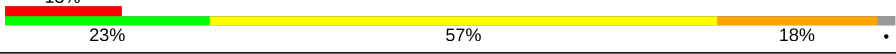


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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	1504	<div> <div>2%</div> <div>29% 60% 11%</div> </div>
1	CA	1504	<div> <div>3%</div> <div>27% 62% 10%</div> </div>
2	AB	256	<div> <div>11%</div> <div>20% 61% 11% 8%</div> </div>
2	CB	256	<div> <div>11%</div> <div>18% 63% 10% 8%</div> </div>
3	AC	239	<div> <div>6%</div> <div>21% 52% 13% 13%</div> </div>
3	CC	239	<div> <div>16%</div> <div>21% 51% 13% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
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	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	

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Mol	Chain	Length	Quality of chain
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	
23	AW	77	
23	CV	77	
23	CW	77	
24	AX	25	
25	AY	84	
25	AZ	84	
25	CY	84	
25	CZ	84	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	
28	B2	72	

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Mol	Chain	Length	Quality of chain
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2848	
36	DA	2848	
37	BB	119	
37	DB	119	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	

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Mol	Chain	Length	Quality of chain
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BI	148	
44	DI	148	
45	BJ	130	
45	DJ	130	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	

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Mol	Chain	Length	Quality of chain
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	CX	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	OMU	AX	19	-	-	X	-
24	A2M	AX	20	-	-	X	X
24	A2M	AX	21	-	-	X	-
59	OMU	CX	19	-	-	X	-
59	A2M	CX	20	-	-	X	-
59	A2M	CX	21	-	-	X	-
60	MG	AA	1601	-	-	-	X
60	MG	AA	1603	-	-	-	X
60	MG	AA	1606	-	-	-	X
60	MG	AA	1608	-	-	-	X
60	MG	AA	1612	-	-	-	X
60	MG	AA	1614	-	-	-	X
60	MG	AA	1623	-	-	-	X
60	MG	AA	1624	-	-	-	X
60	MG	AA	1625	-	-	-	X
60	MG	AA	1627	-	-	-	X
60	MG	AA	1633	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1634	-	-	-	X
60	MG	AA	1636	-	-	-	X
60	MG	AA	1641	-	-	-	X
60	MG	AA	1642	-	-	-	X
60	MG	AA	1643	-	-	-	X
60	MG	AA	1645	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1649	-	-	-	X
60	MG	AA	1650	-	-	-	X
60	MG	AA	1661	-	-	-	X
60	MG	AA	1662	-	-	-	X
60	MG	AA	1665	-	-	-	X
60	MG	AA	1667	-	-	-	X
60	MG	AA	1670	-	-	-	X
60	MG	AA	1672	-	-	-	X
60	MG	AA	1674	-	-	-	X
60	MG	AA	1675	-	-	-	X
60	MG	AA	1686	-	-	-	X
60	MG	AV	101	-	-	-	X
60	MG	B1	101	-	-	-	X
60	MG	BA	2908	-	-	-	X
60	MG	BA	2920	-	-	-	X
60	MG	BA	2949	-	-	-	X
60	MG	BA	2960	-	-	-	X
60	MG	BA	2965	-	-	-	X
60	MG	BA	2970	-	-	-	X
60	MG	BA	2973	-	-	-	X
60	MG	BA	2977	-	-	-	X
60	MG	BA	2988	-	-	-	X
60	MG	BA	2995	-	-	-	X
60	MG	BA	2996	-	-	-	X
60	MG	BA	3002	-	-	-	X
60	MG	BA	3008	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3012	-	-	-	X
60	MG	BA	3015	-	-	-	X
60	MG	BA	3017	-	-	-	X
60	MG	BA	3018	-	-	-	X
60	MG	BA	3020	-	-	-	X
60	MG	BA	3022	-	-	-	X
60	MG	BA	3030	-	-	-	X
60	MG	BA	3032	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3040	-	-	-	X
60	MG	BA	3046	-	-	-	X
60	MG	BA	3051	-	-	-	X
60	MG	BA	3053	-	-	-	X
60	MG	BA	3060	-	-	-	X
60	MG	BA	3063	-	-	-	X
60	MG	BA	3064	-	-	-	X
60	MG	BA	3066	-	-	-	X
60	MG	BA	3080	-	-	-	X
60	MG	BA	3081	-	-	-	X
60	MG	BA	3083	-	-	-	X
60	MG	BA	3084	-	-	-	X
60	MG	BA	3086	-	-	-	X
60	MG	BA	3089	-	-	-	X
60	MG	BA	3090	-	-	-	X
60	MG	BA	3093	-	-	-	X
60	MG	BA	3094	-	-	-	X
60	MG	BA	3098	-	-	-	X
60	MG	BA	3100	-	-	-	X
60	MG	BA	3101	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3106	-	-	-	X
60	MG	BA	3107	-	-	-	X
60	MG	BA	3108	-	-	-	X
60	MG	BA	3109	-	-	-	X
60	MG	BA	3114	-	-	-	X
60	MG	BA	3115	-	-	-	X
60	MG	BA	3120	-	-	-	X
60	MG	BA	3121	-	-	-	X
60	MG	BA	3123	-	-	-	X
60	MG	BA	3124	-	-	-	X
60	MG	BA	3126	-	-	-	X
60	MG	BA	3128	-	-	-	X
60	MG	BA	3129	-	-	-	X
60	MG	BB	201	-	-	-	X
60	MG	BF	301	-	-	-	X
60	MG	CA	1601	-	-	-	X
60	MG	CA	1603	-	-	-	X
60	MG	CA	1604	-	-	-	X
60	MG	CA	1606	-	-	-	X
60	MG	CA	1607	-	-	-	X
60	MG	CA	1612	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	1613	-	-	-	X
60	MG	CA	1618	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1624	-	-	-	X
60	MG	CA	1626	-	-	-	X
60	MG	CA	1627	-	-	-	X
60	MG	CA	1629	-	-	-	X
60	MG	CA	1631	-	-	-	X
60	MG	CA	1633	-	-	-	X
60	MG	CA	1636	-	-	-	X
60	MG	CA	1637	-	-	-	X
60	MG	CA	1640	-	-	-	X
60	MG	CA	1641	-	-	-	X
60	MG	CA	1644	-	-	-	X
60	MG	CA	1650	-	-	-	X
60	MG	CA	1653	-	-	-	X
60	MG	CA	1654	-	-	-	X
60	MG	CA	1662	-	-	-	X
60	MG	CA	1664	-	-	-	X
60	MG	CA	1665	-	-	-	X
60	MG	CA	1666	-	-	-	X
60	MG	CA	1667	-	-	-	X
60	MG	CA	1671	-	-	-	X
60	MG	CA	1672	-	-	-	X
60	MG	CA	1677	-	-	-	X
60	MG	CA	1678	-	-	-	X
60	MG	CA	1680	-	-	-	X
60	MG	CA	1686	-	-	-	X
60	MG	CA	1687	-	-	-	X
60	MG	CA	1688	-	-	-	X
60	MG	CA	1689	-	-	-	X
60	MG	CA	1690	-	-	-	X
60	MG	CA	1691	-	-	-	X
60	MG	CA	1692	-	-	-	X
60	MG	CA	1694	-	-	-	X
60	MG	CA	1696	-	-	-	X
60	MG	CA	1698	-	-	-	X
60	MG	CA	1700	-	-	-	X
60	MG	CA	1702	-	-	-	X
60	MG	CG	201	-	-	-	X
60	MG	CV	102	-	-	-	X
60	MG	DA	2901	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	2929	-	-	-	X
60	MG	DA	2942	-	-	-	X
60	MG	DA	2949	-	-	-	X
60	MG	DA	2962	-	-	-	X
60	MG	DA	2964	-	-	-	X
60	MG	DA	2965	-	-	-	X
60	MG	DA	2969	-	-	-	X
60	MG	DA	2972	-	-	-	X
60	MG	DA	2975	-	-	-	X
60	MG	DA	2986	-	-	-	X
60	MG	DA	2990	-	-	-	X
60	MG	DA	2991	-	-	-	X
60	MG	DA	2998	-	-	-	X
60	MG	DA	3003	-	-	-	X
60	MG	DA	3004	-	-	-	X
60	MG	DA	3009	-	-	-	X
60	MG	DA	3010	-	-	-	X
60	MG	DA	3014	-	-	-	X
60	MG	DA	3018	-	-	-	X
60	MG	DA	3019	-	-	-	X
60	MG	DA	3024	-	-	-	X
60	MG	DA	3027	-	-	-	X
60	MG	DA	3029	-	-	-	X
60	MG	DA	3031	-	-	-	X
60	MG	DA	3035	-	-	-	X
60	MG	DA	3037	-	-	-	X
60	MG	DA	3039	-	-	-	X
60	MG	DA	3041	-	-	-	X
60	MG	DA	3046	-	-	-	X
60	MG	DA	3048	-	-	-	X
60	MG	DA	3056	-	-	-	X
60	MG	DA	3057	-	-	-	X
60	MG	DA	3058	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3063	-	-	-	X
60	MG	DA	3068	-	-	-	X
60	MG	DA	3070	-	-	-	X
60	MG	DA	3071	-	-	-	X
60	MG	DA	3072	-	-	-	X
60	MG	DA	3077	-	-	-	X
60	MG	DA	3080	-	-	-	X
60	MG	DA	3081	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3082	-	-	-	X
60	MG	DA	3083	-	-	-	X
60	MG	DA	3085	-	-	-	X
60	MG	DA	3088	-	-	-	X
60	MG	DA	3089	-	-	-	X
60	MG	DA	3090	-	-	-	X
60	MG	DA	3094	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3097	-	-	-	X
60	MG	DA	3098	-	-	-	X
60	MG	DA	3099	-	-	-	X
60	MG	DA	3100	-	-	-	X
60	MG	DA	3104	-	-	-	X
60	MG	DA	3106	-	-	-	X
60	MG	DA	3114	-	-	-	X
60	MG	DA	3115	-	-	-	X
60	MG	DA	3117	-	-	-	X
60	MG	DA	3122	-	-	-	X
60	MG	DA	3124	-	-	-	X
60	MG	DA	3125	-	-	-	X
60	MG	DA	3132	-	-	-	X
60	MG	DA	3135	-	-	-	X
60	MG	DA	3137	-	-	-	X
60	MG	DA	3141	-	-	-	X
60	MG	DB	201	-	-	-	X
60	MG	DR	201	-	-	-	X
60	MG	DX	101	-	-	-	X
61	ZN	AD	301	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298206 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
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	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	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			
13	CM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

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

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 transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 23 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP *AP*AP*UP*G U2M A2M A2MP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			239	111	49	69	10			

- Molecule 25 is a protein called TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	AZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
25	CY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	CZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
33	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
36	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
38	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
43	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				
45	DJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			
49	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
52	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is a RNA chain called BACTERIAL TOXIN YOEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	10	Total 217	C 101	N 44	O 63	P 9	0	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	236	Total 236	Mg 236	0	0
60	CA	103	Total 103	Mg 103	0	0
60	DF	1	Total 1	Mg 1	0	0
60	CV	2	Total 2	Mg 2	0	0
60	B1	2	Total 2	Mg 2	0	0
60	BP	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	DR	1	Total 1	Mg 1	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BB	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	AA	103	Total 103	Mg 103	0	0
60	CG	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DX	1	Total 1	Mg 1	0	0
60	DA	242	Total 242	Mg 242	0	0
60	AL	1	Total 1	Mg 1	0	0
60	D1	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	B0	1	Total 1	Mg 1	0	0
60	CL	1	Total 1	Mg 1	0	0
60	DB	1	Total 1	Mg 1	0	0

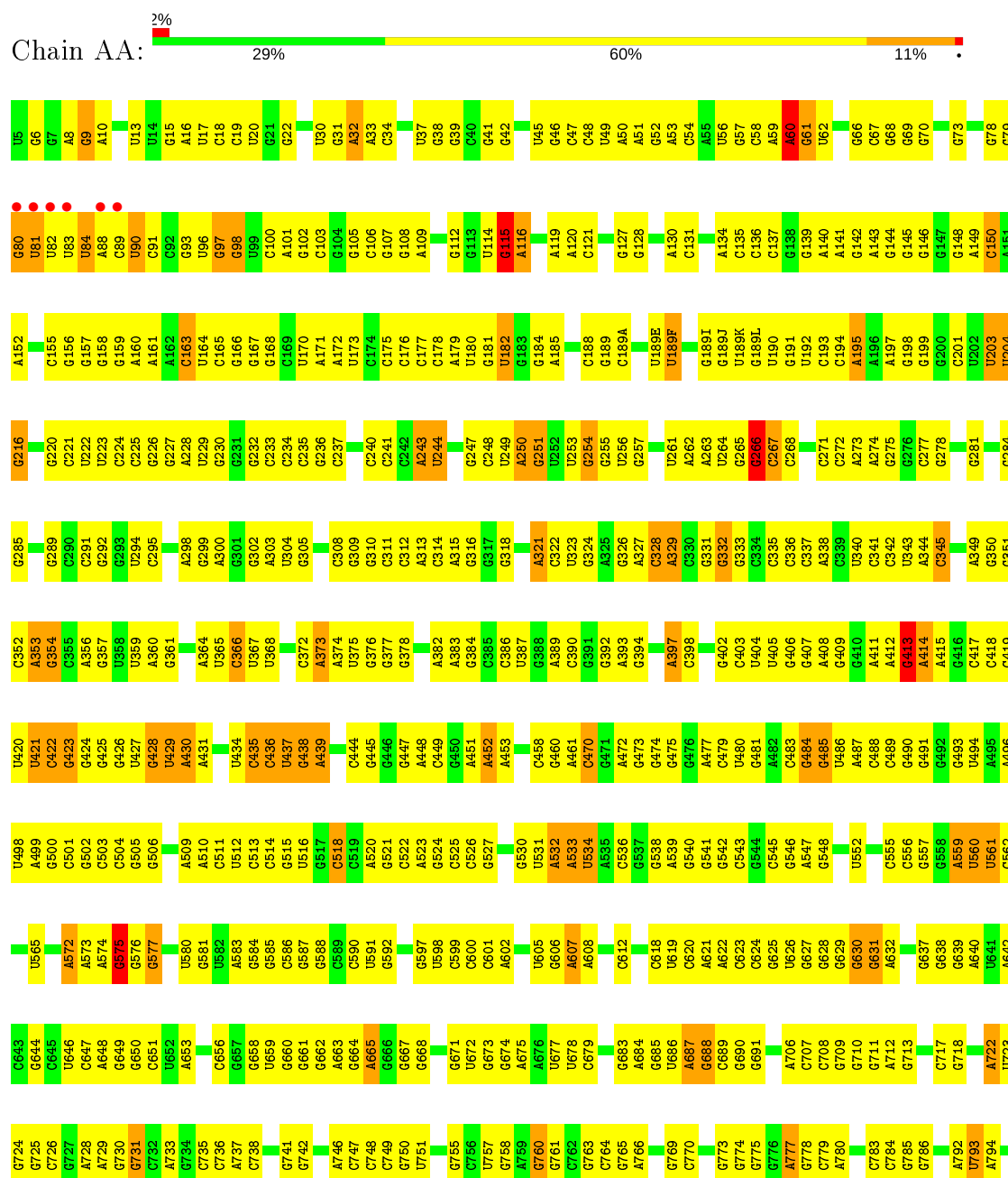
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

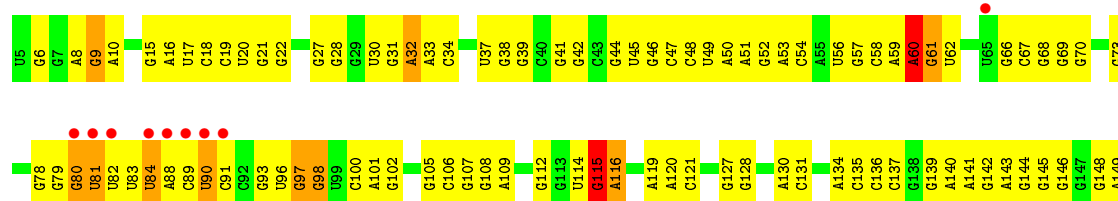
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CN	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0

3 Residue-property plots

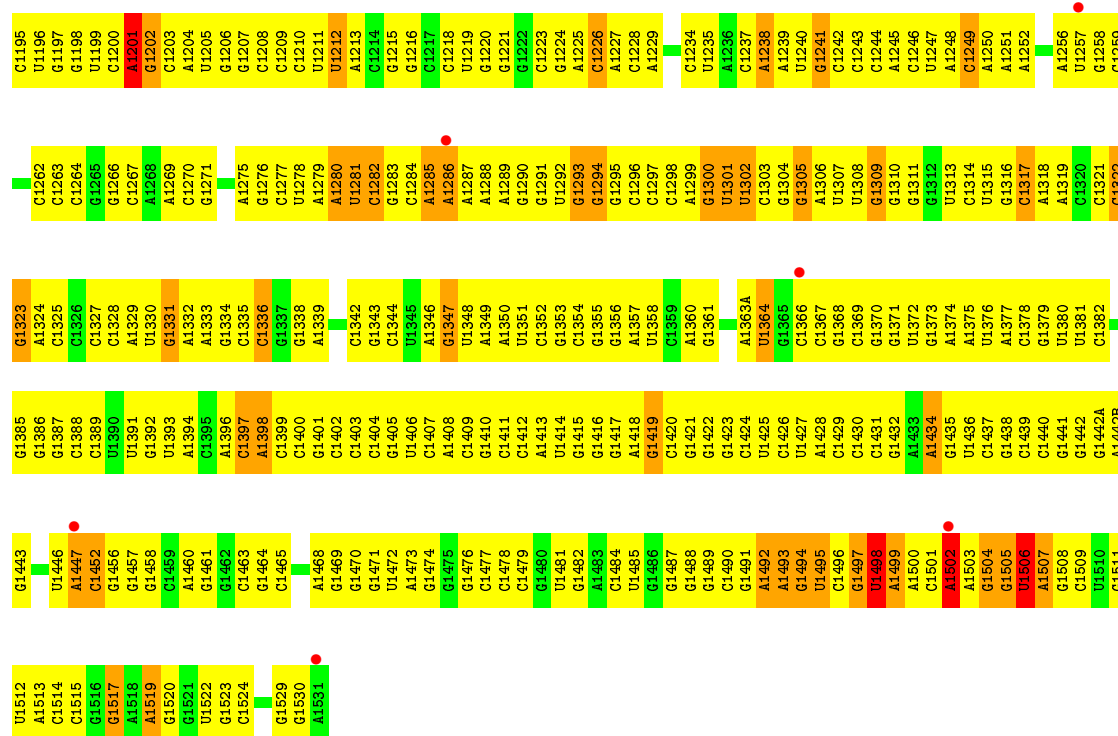
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S ribosomal RNA

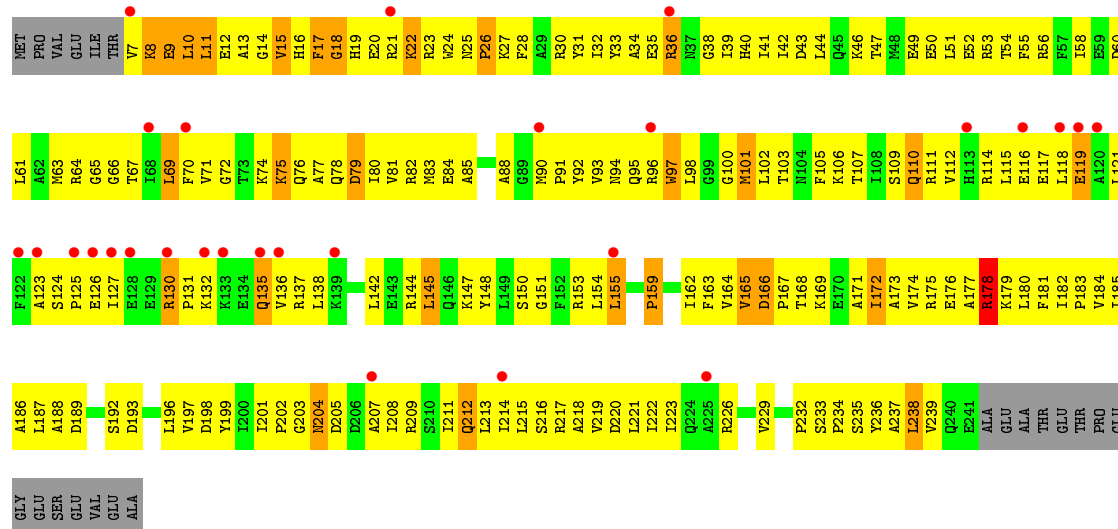




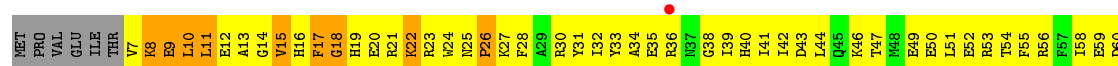


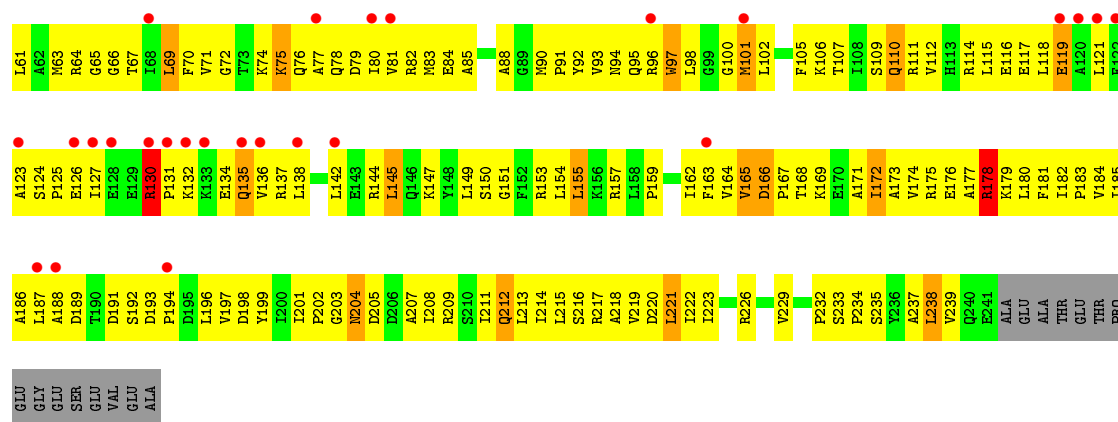


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

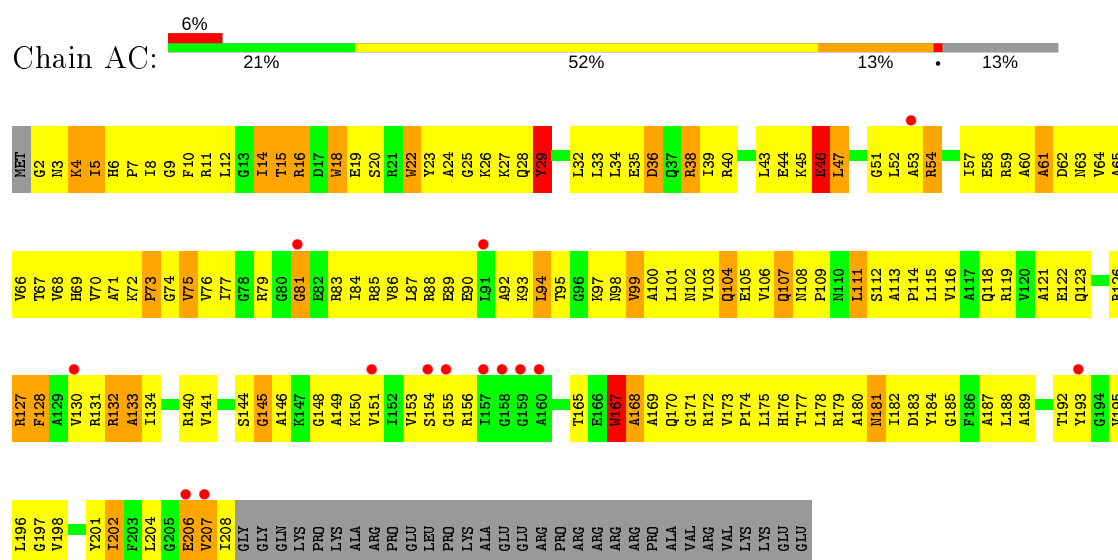


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

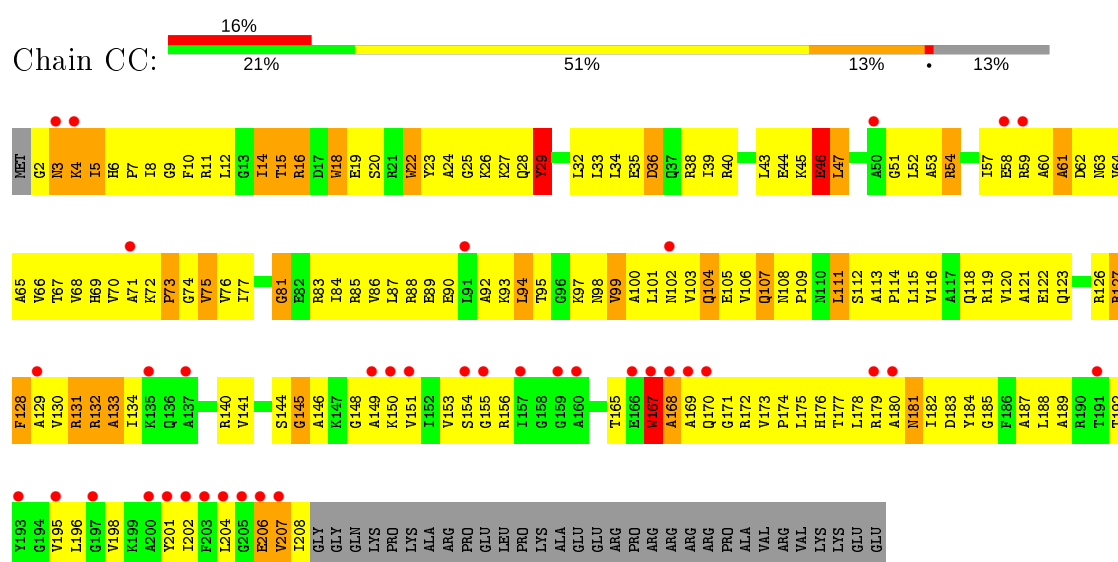




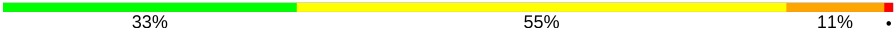
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

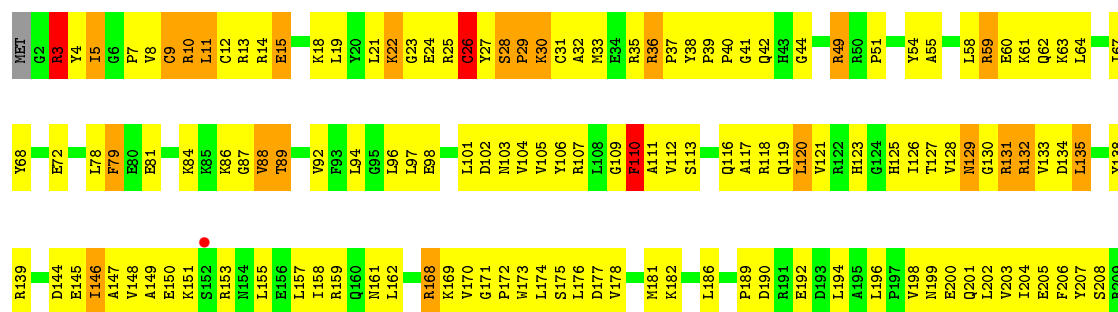


• Molecule 4: 30S RIBOSOMAL PROTEIN S4



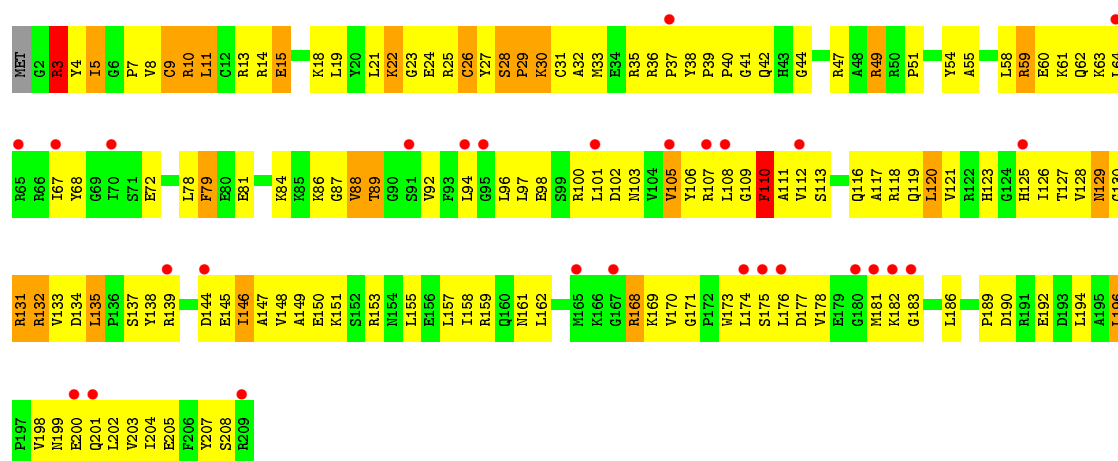
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 



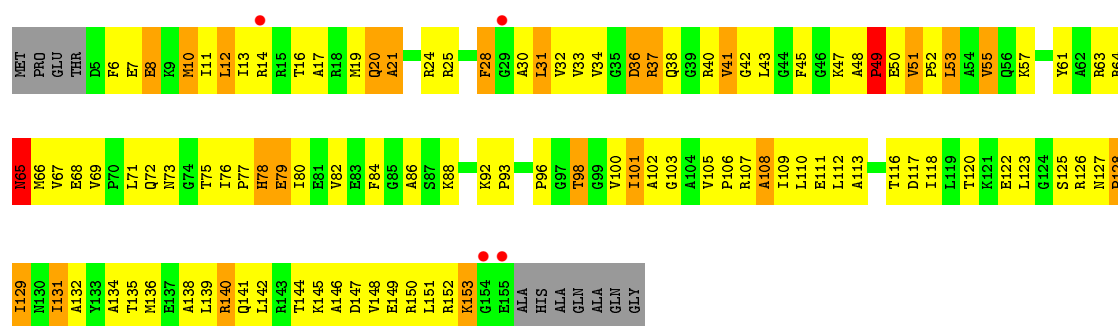
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD: 



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

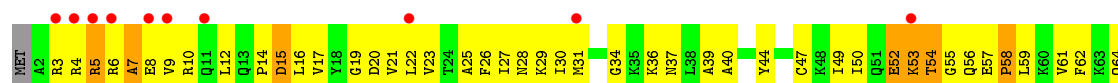
Chain AE: 

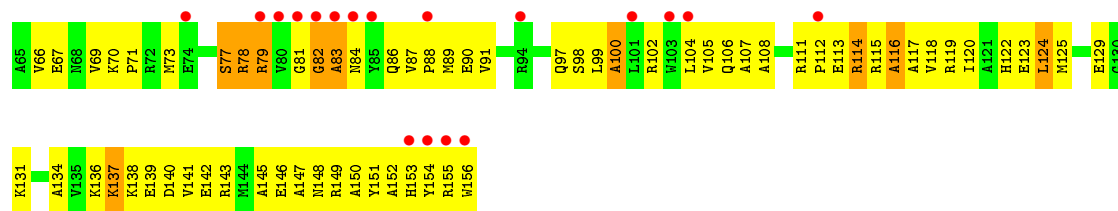


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

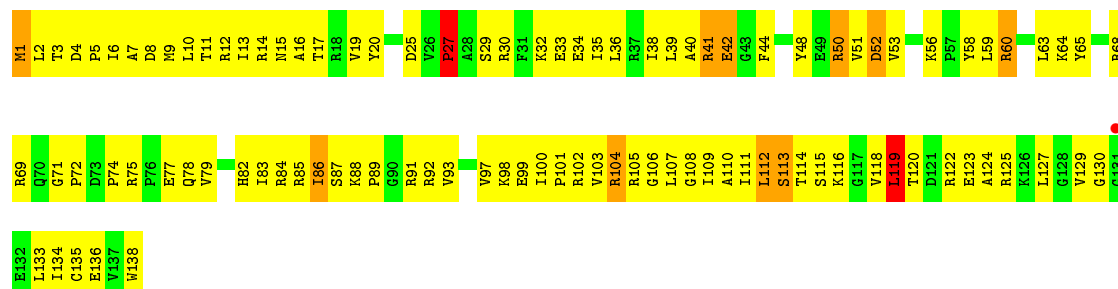
Chain CE: 



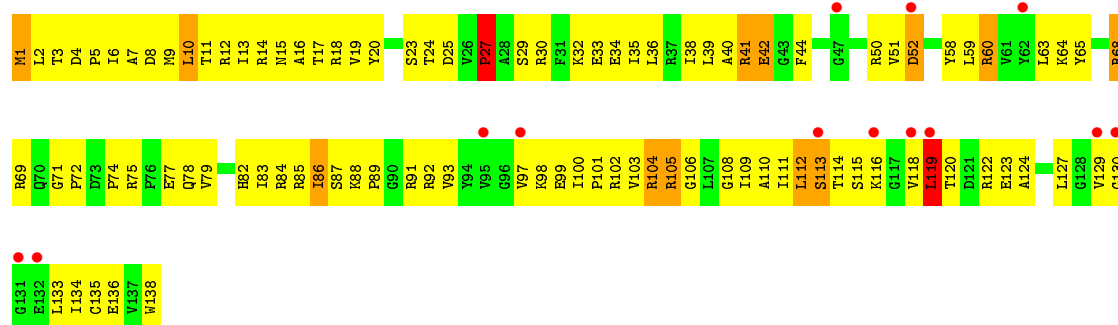




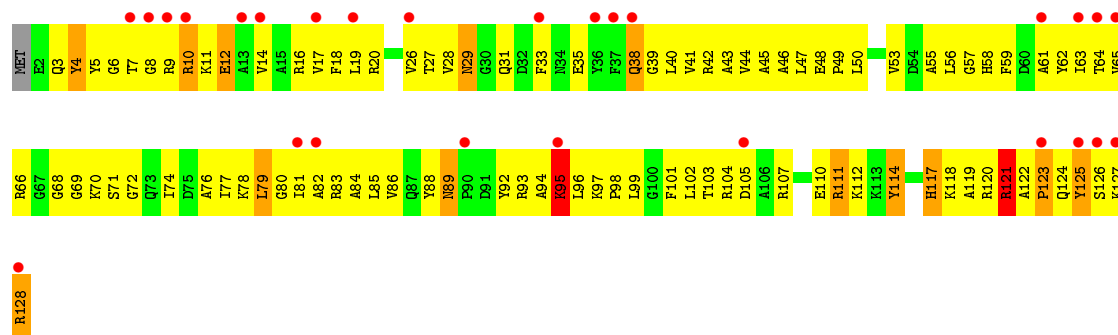
● Molecule 8: 30S RIBOSOMAL PROTEIN S8



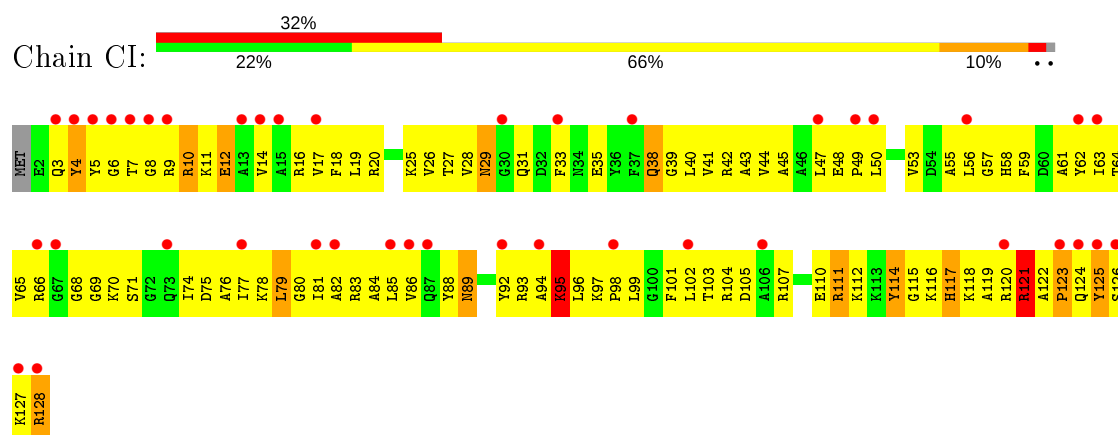
● Molecule 8: 30S RIBOSOMAL PROTEIN S8



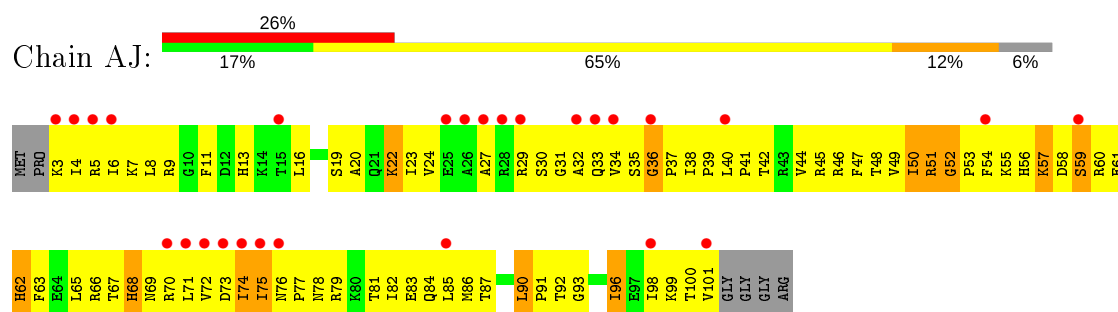
● Molecule 9: 30S RIBOSOMAL PROTEIN S9



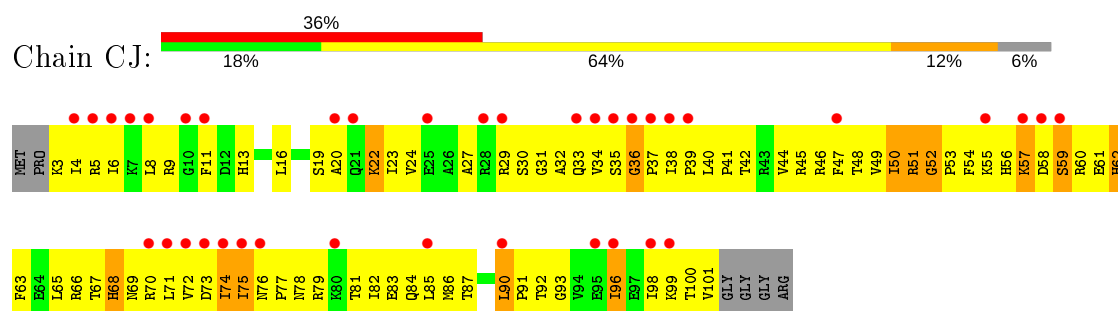
● Molecule 9: 30S RIBOSOMAL PROTEIN S9



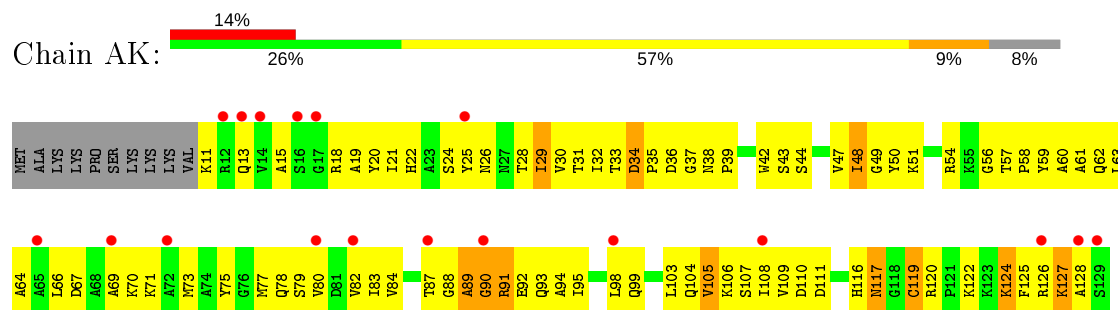
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

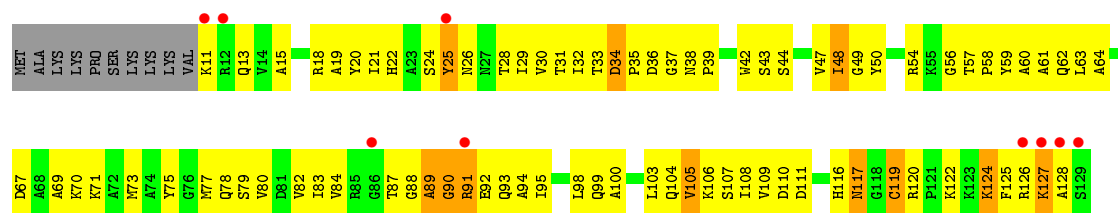


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

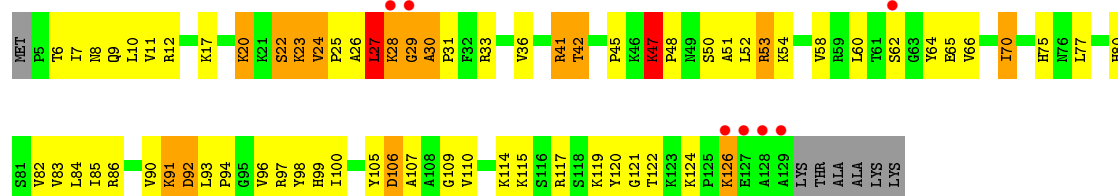


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

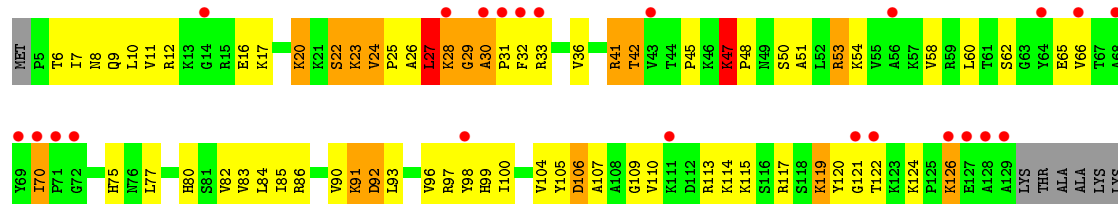




• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

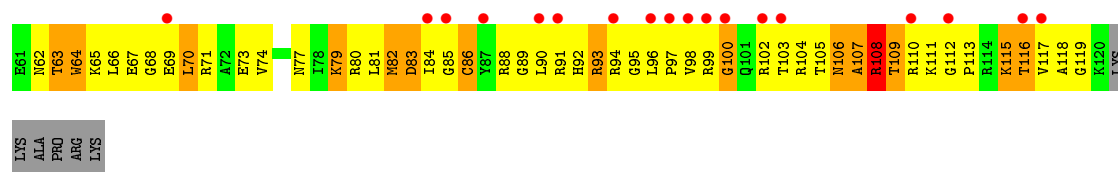


• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13





• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

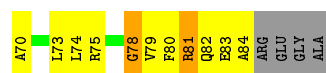


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

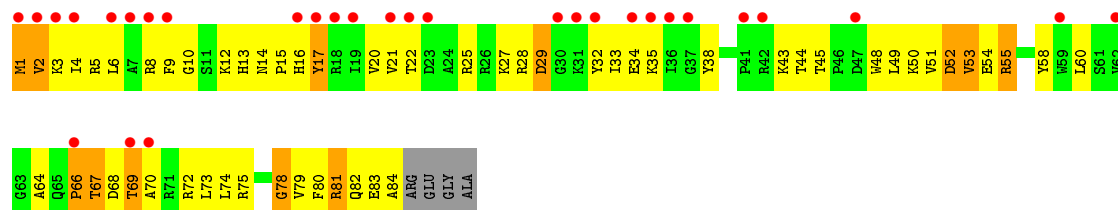


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

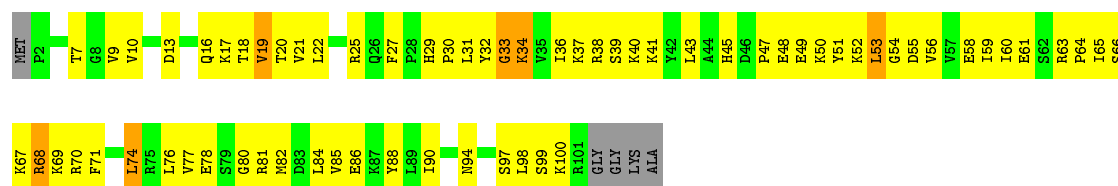




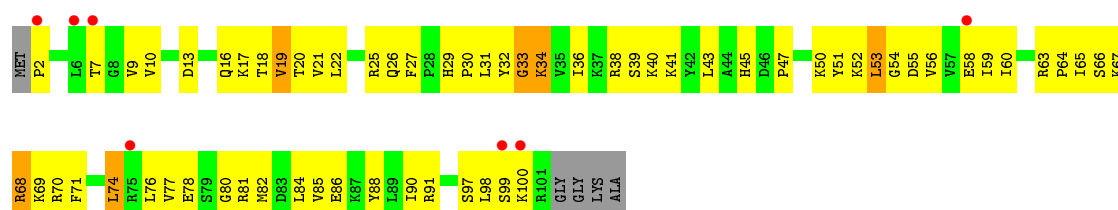
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



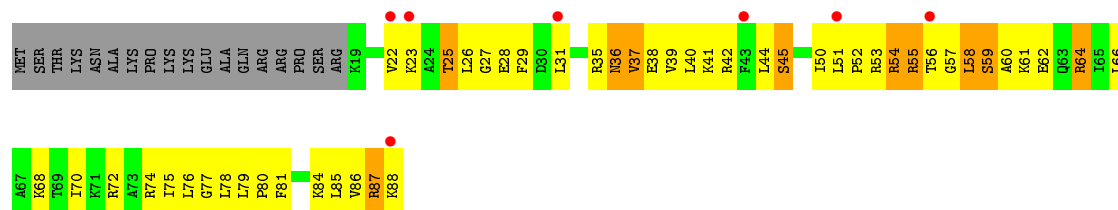
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



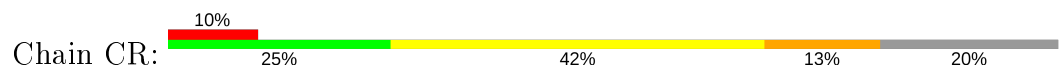
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

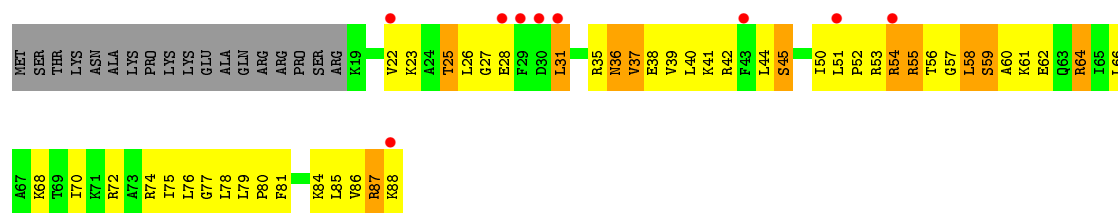


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

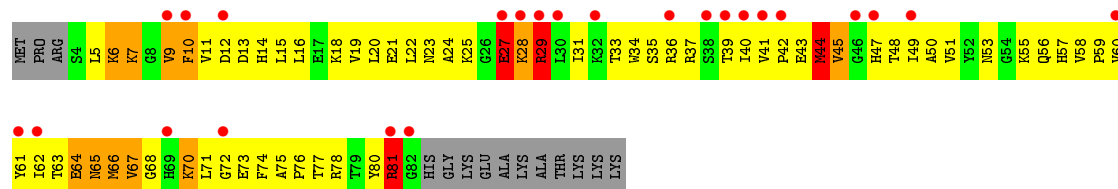
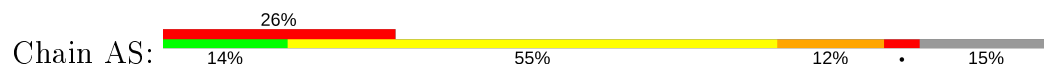


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

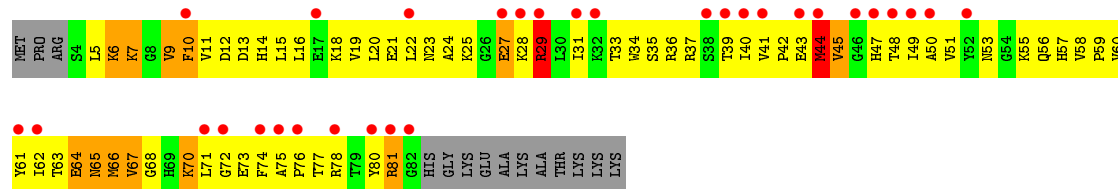
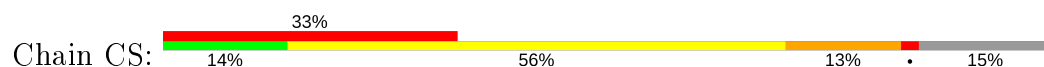




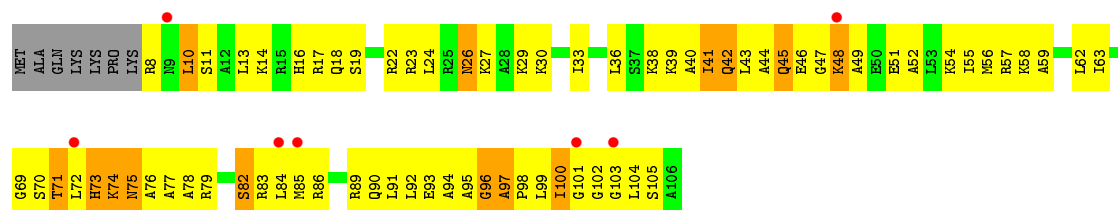
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



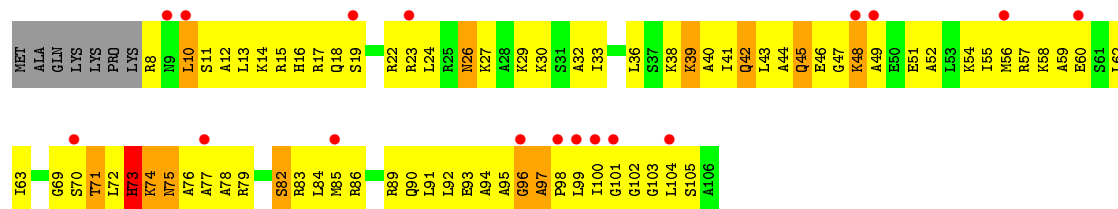
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



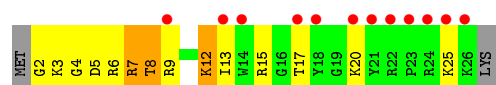
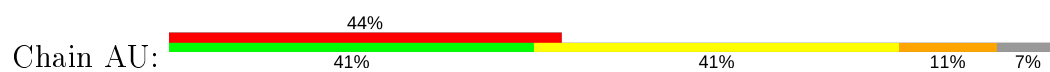
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



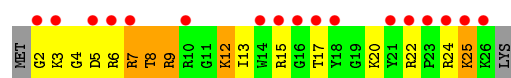
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



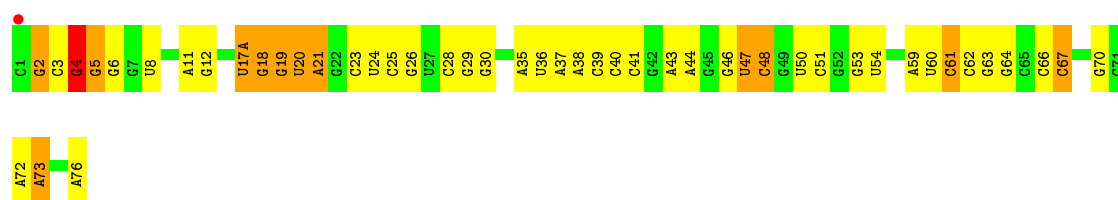
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



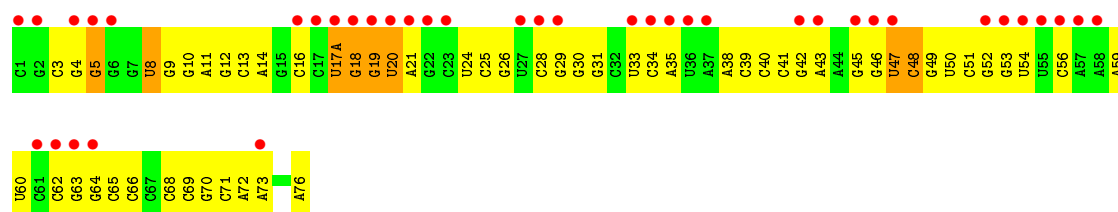
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



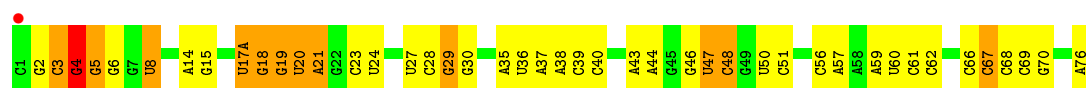
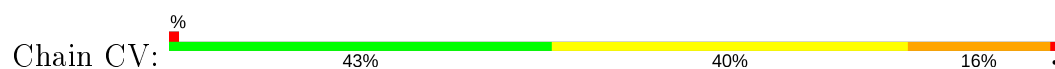
- Molecule 22: transfer RNA



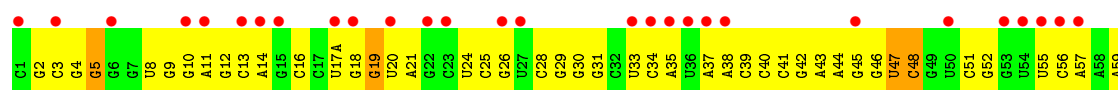
- Molecule 23: transfer RNA

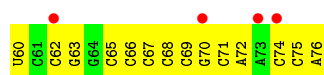


- Molecule 23: transfer RNA

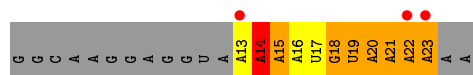


- Molecule 23: transfer RNA

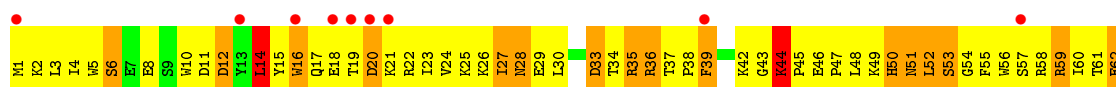
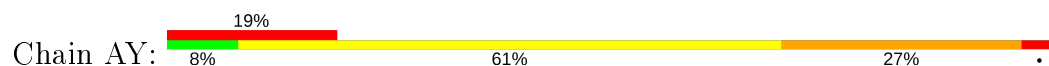




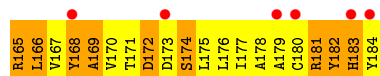
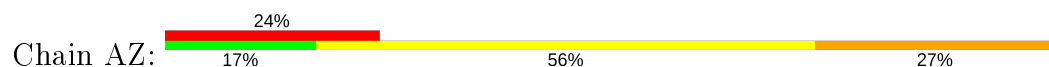
- Molecule 24: 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP*AP*AP*UP*GU2M A2M A2MP*AP*AP*AP*A)-3'



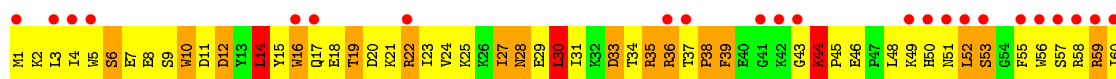
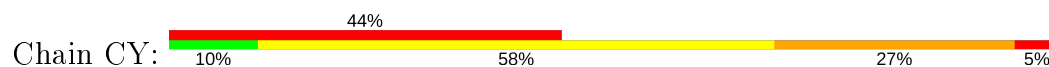
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM



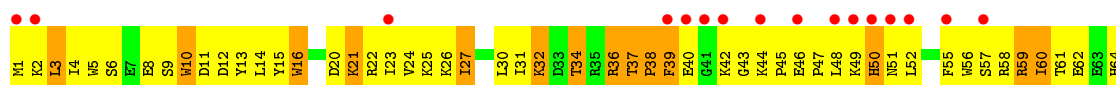
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

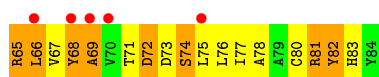


- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM



- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

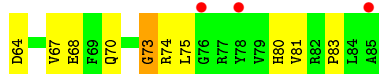




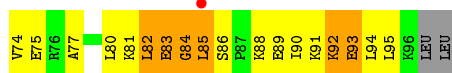
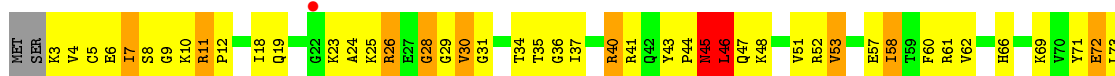
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



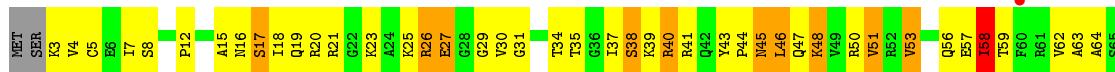
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



• Molecule 27: 50S RIBOSOMAL PROTEIN L28

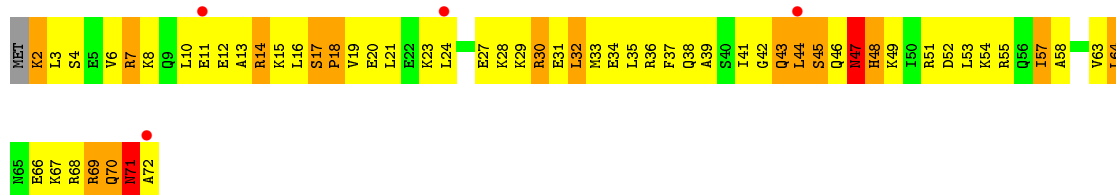


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

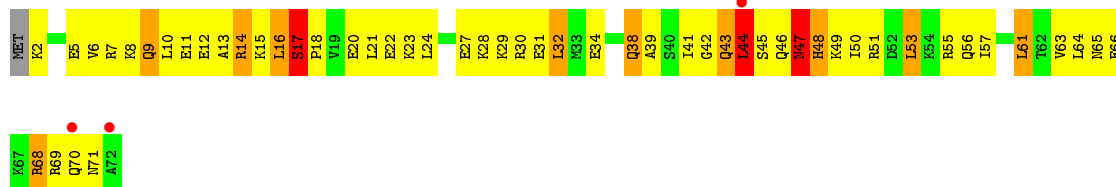


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

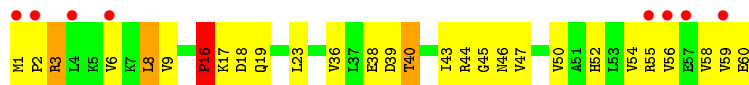




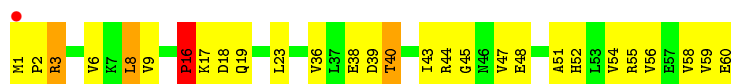
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



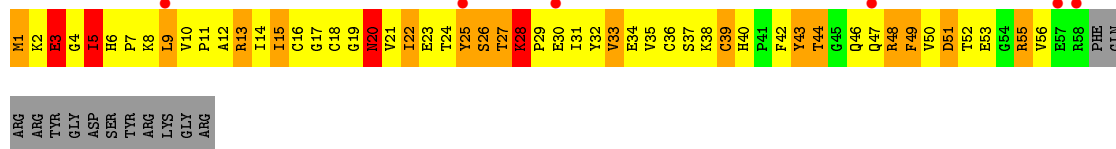
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



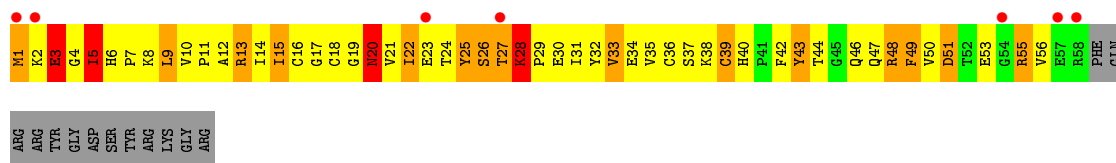
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



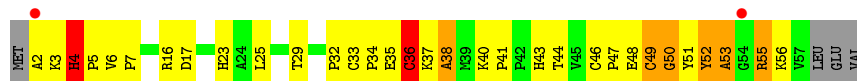
- Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5: 



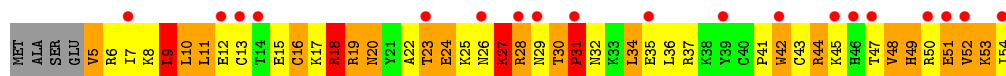
- Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7: 

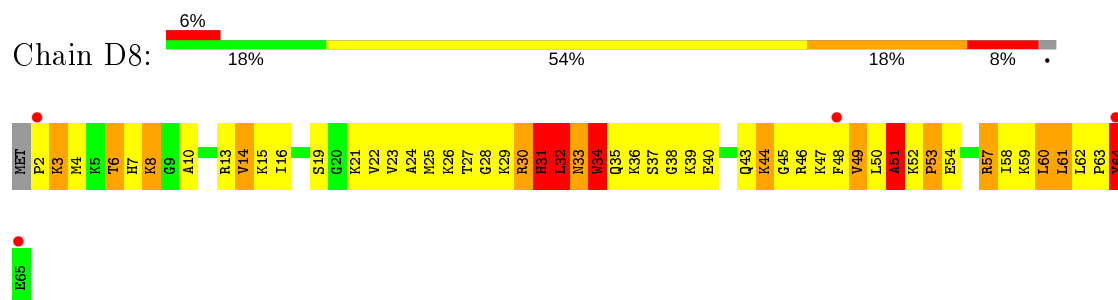


- Molecule 34: 50S RIBOSOMAL PROTEIN L35

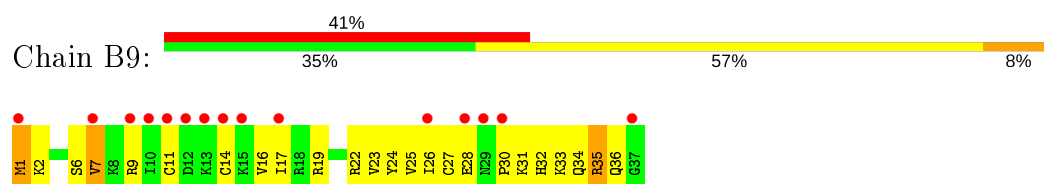
Chain B8: 



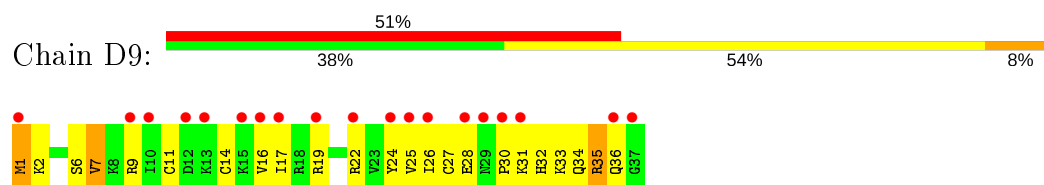
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



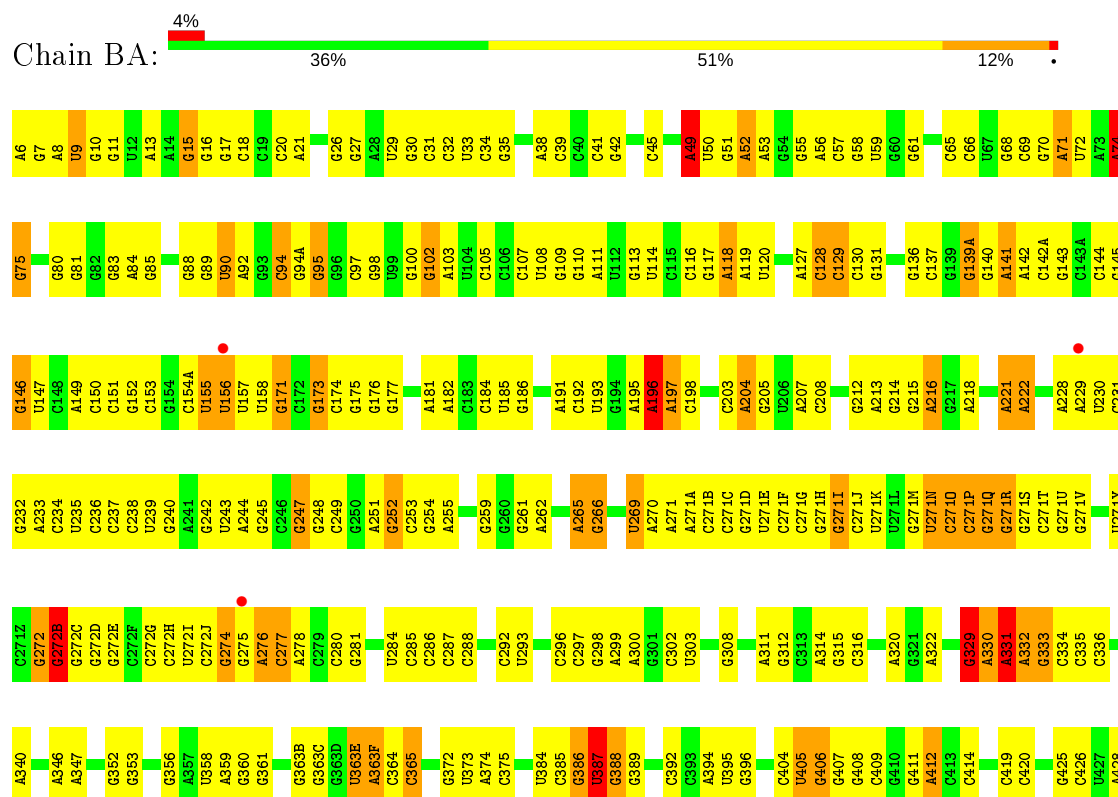
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

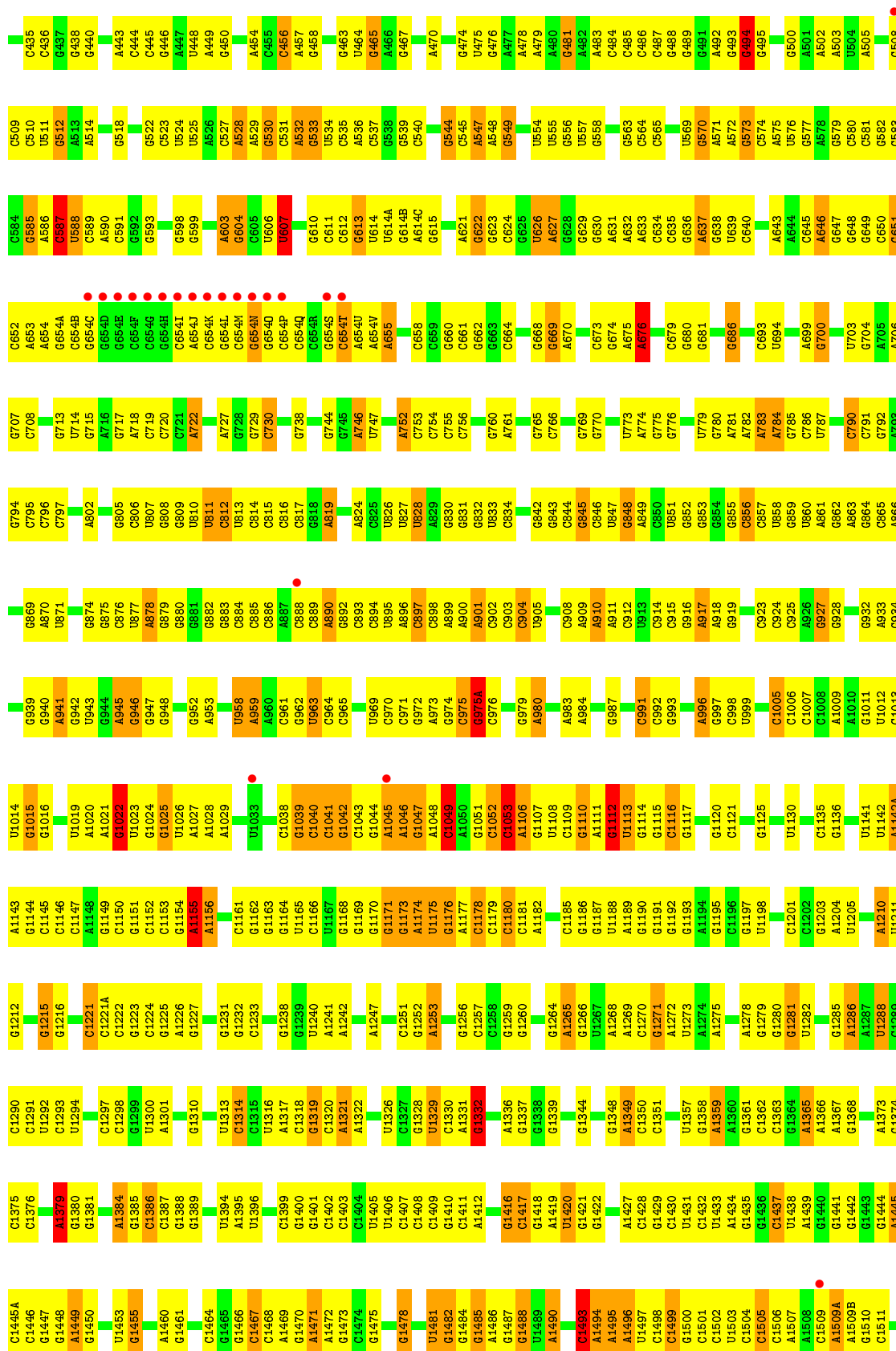


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

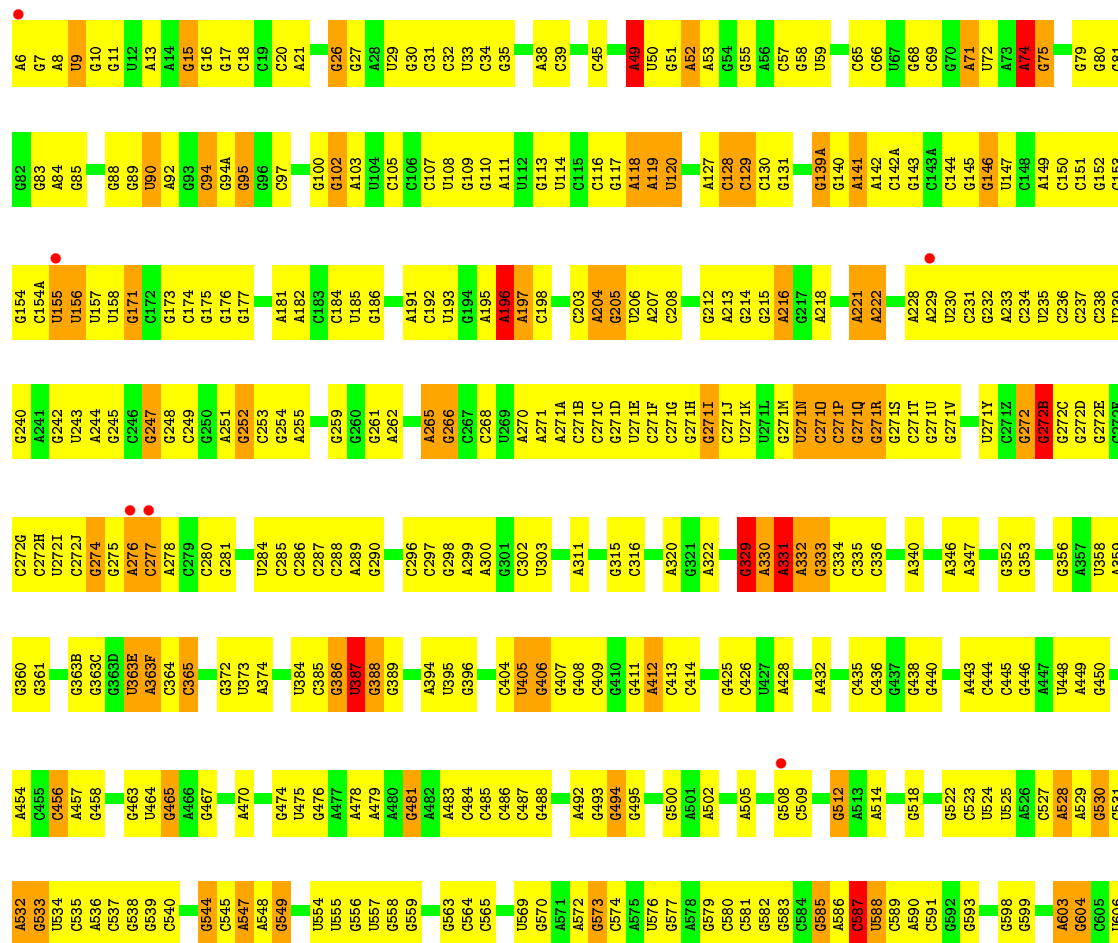


- Molecule 36: 23S ribosomal RNA



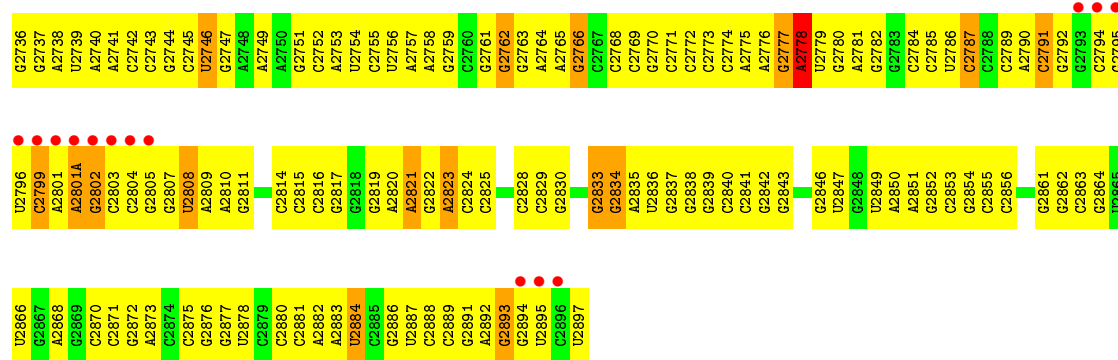


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G2405	U2406	G2407	U2408	G2409	G2410	A2411	G2415	U2419	G2420	G2421	A2422	U2423	G2424	G2425	A2426	G2427	G2428	G2429	A2430	U2438	A2439	G2440	C2441	C2442	G2443	G2444	A2448	U2449	A2450	G2451	G2452	A2453	G2454	U2457	G2461	U2462	C2463	C2464	C2465	G2466	G2467	G2468	A2469	U2470	G2471	U2472	G2473	G2474	C2475	A2476	U2477	A2478																																																																										
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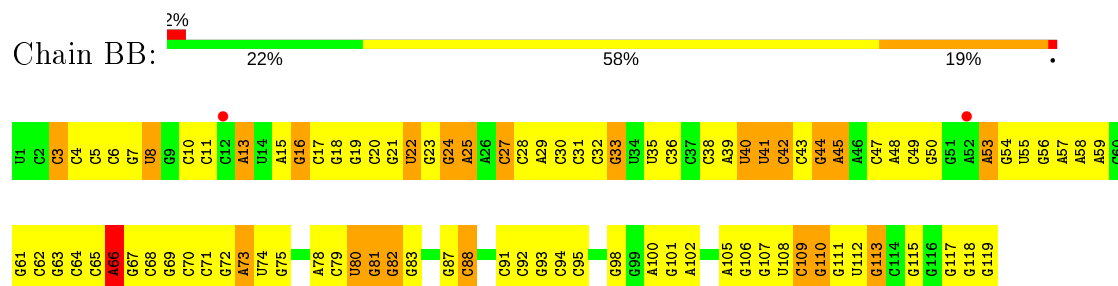


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A1609	G1541	G1473	A1253	G1166	G1042	C961	C989	C817	G745	C654T	C611
A1610	G1542	G1474	G1256	U1167	C1043	G962	A990	G818	G746	A654U	C612
A1614	U1543	G1475	G1257	G1168	G1044	U963	G992	A819	U747	A654V	G613
A1615	A1544		G1258	G1169	A1045	C964	C993	G823	U748	A655	U614
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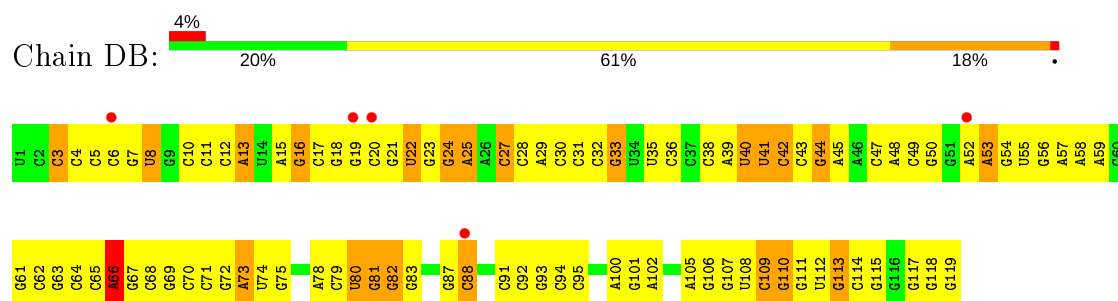




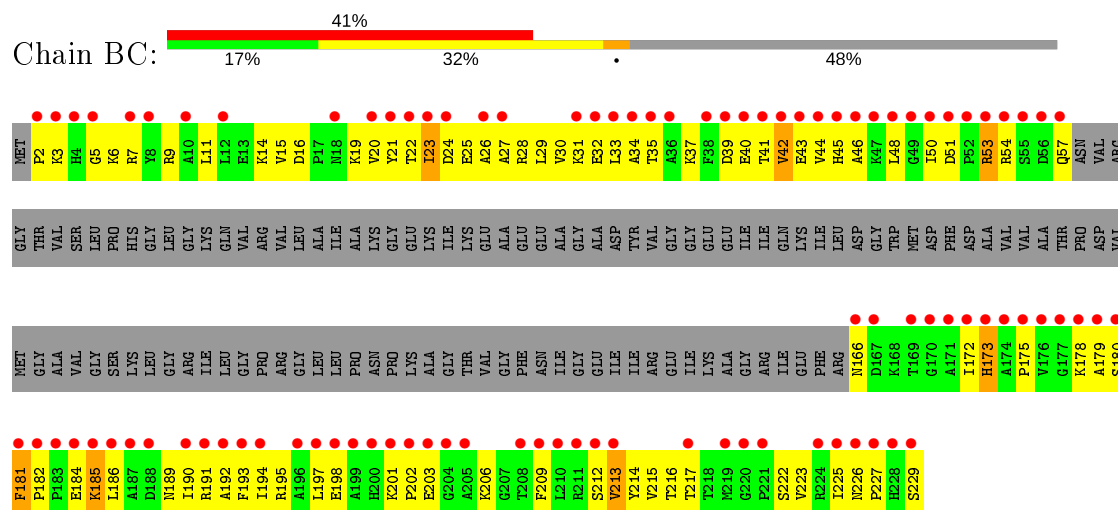
• Molecule 37: 5S ribosomal RNA



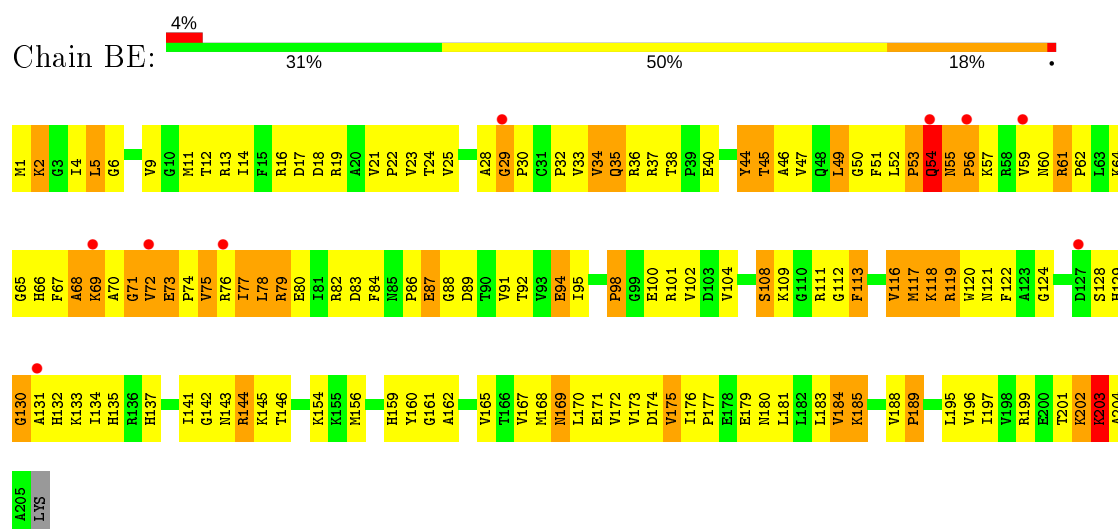
• Molecule 37: 5S ribosomal RNA



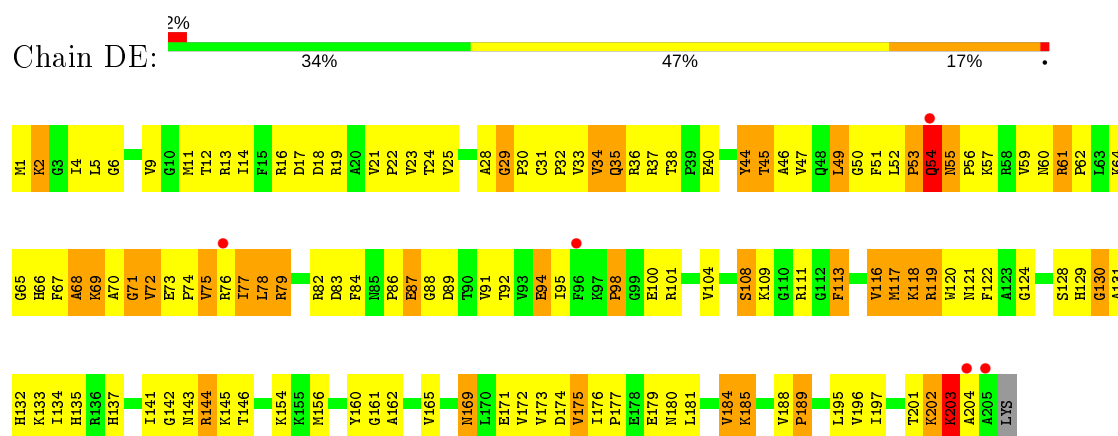
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



• Molecule 38: 50S RIBOSOMAL PROTEIN L1



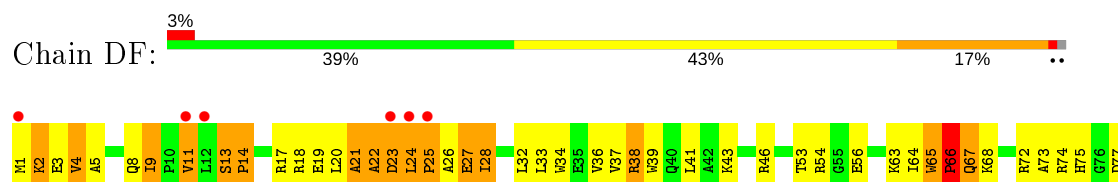
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

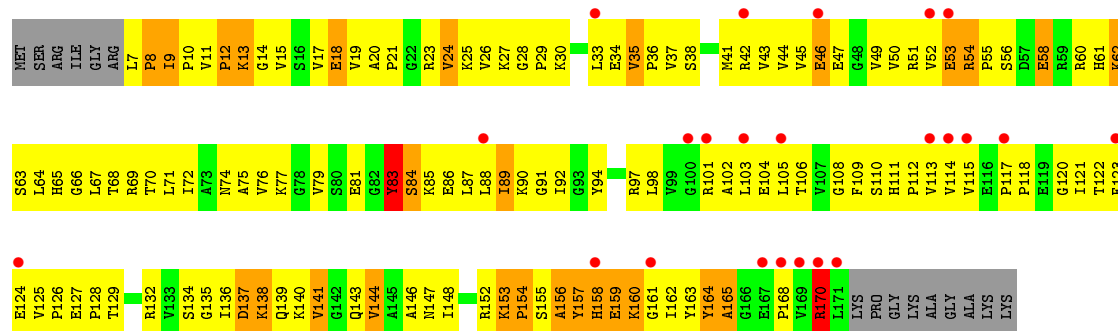


• Molecule 41: 50S RIBOSOMAL PROTEIN L4




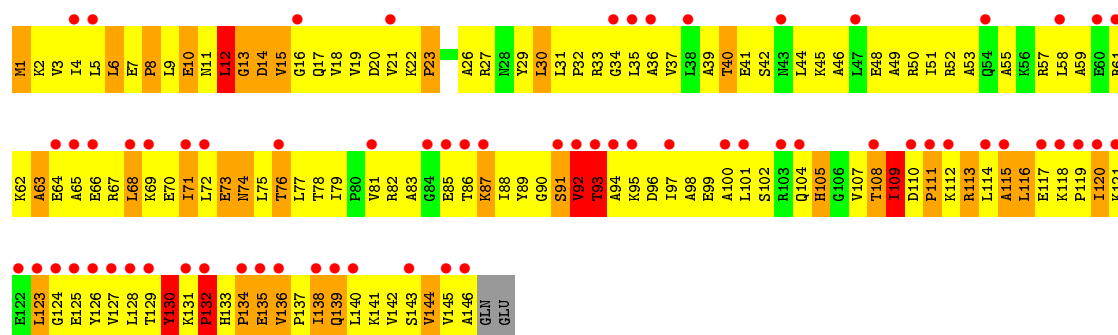


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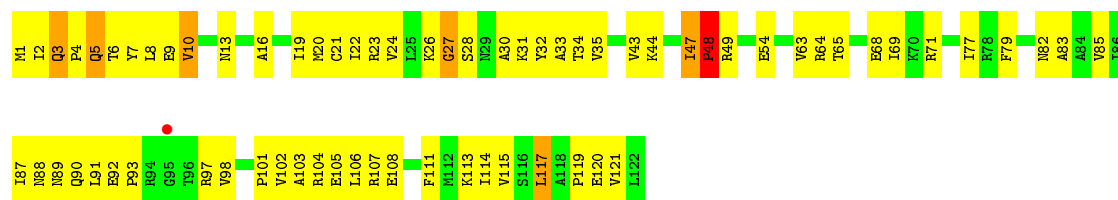


• Molecule 44: 50S RIBOSOMAL PROTEIN L9

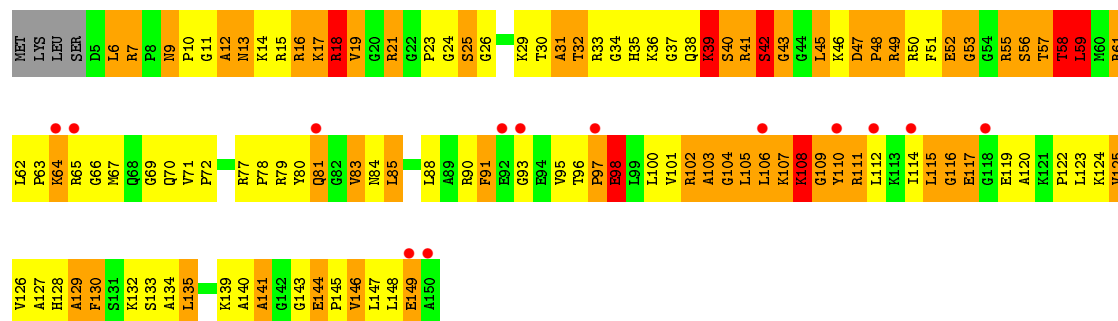
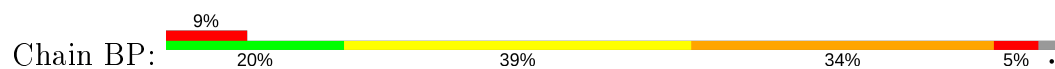
Chain BI: 



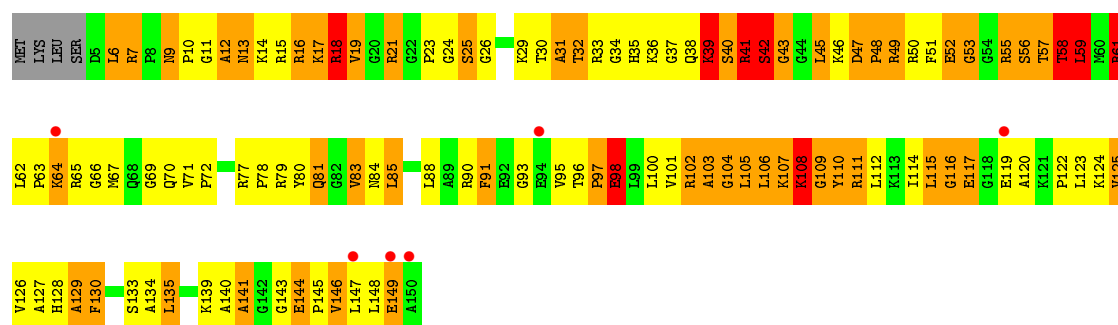
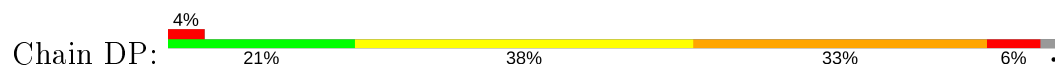




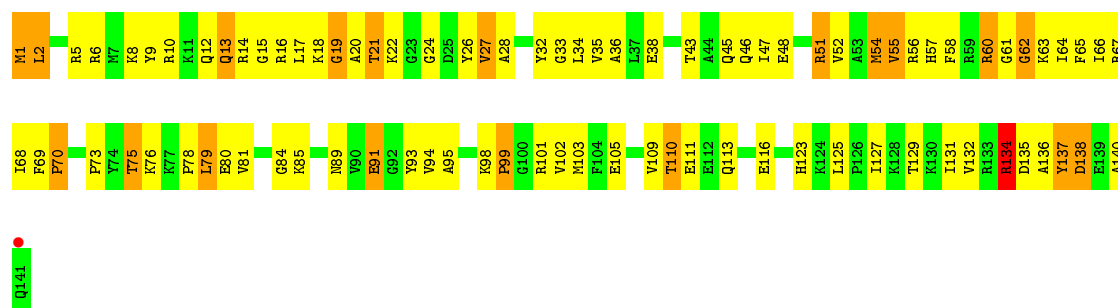
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



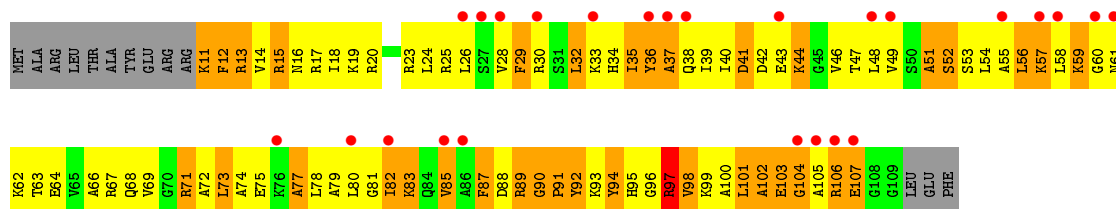
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



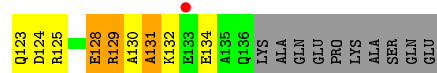
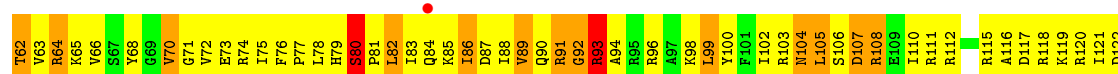
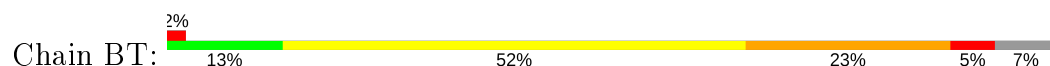
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



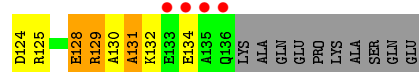
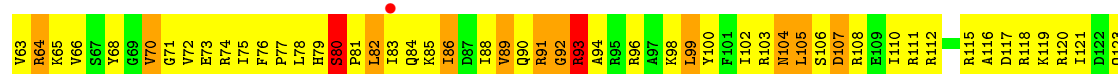
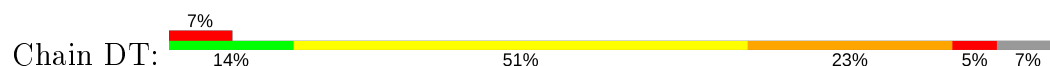
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



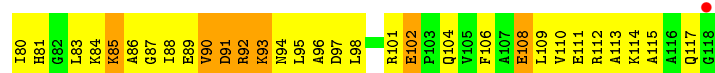
● Molecule 52: 50S RIBOSOMAL PROTEIN L19



● Molecule 52: 50S RIBOSOMAL PROTEIN L19

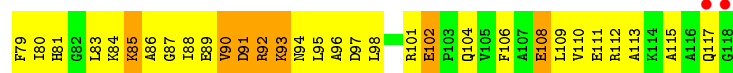


● Molecule 53: 50S RIBOSOMAL PROTEIN L20

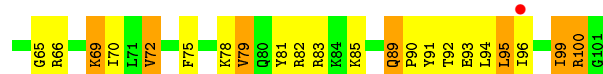
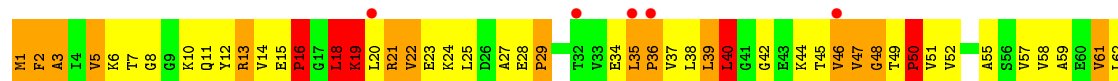


● Molecule 53: 50S RIBOSOMAL PROTEIN L20

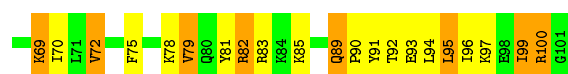
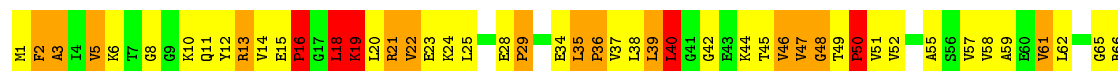




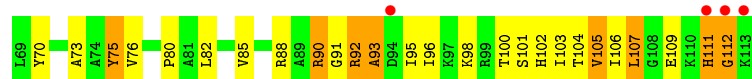
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



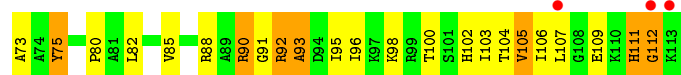
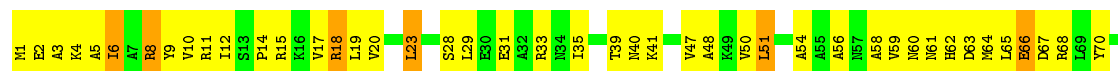
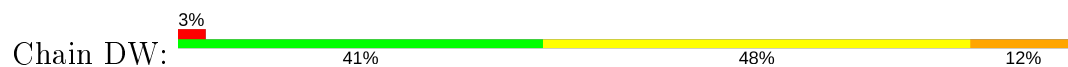
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



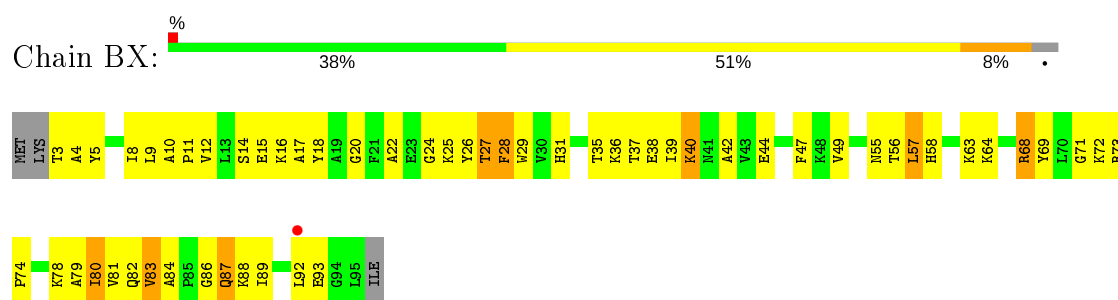
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



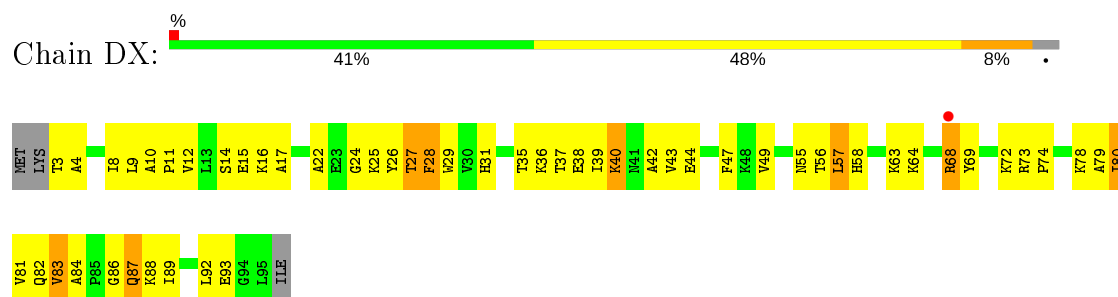
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



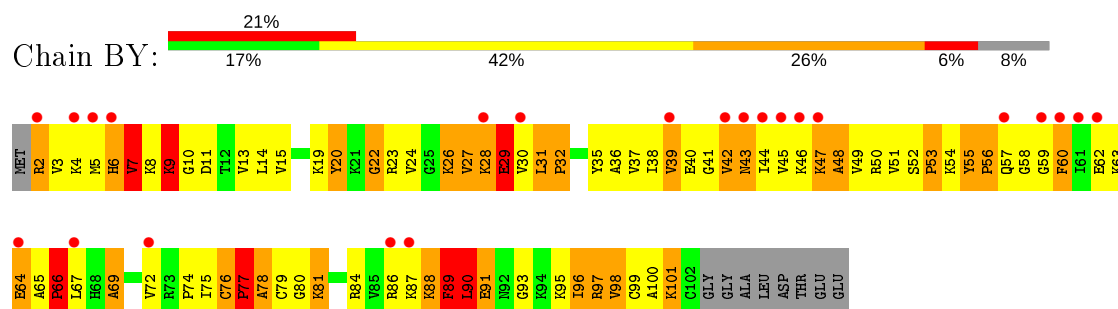
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



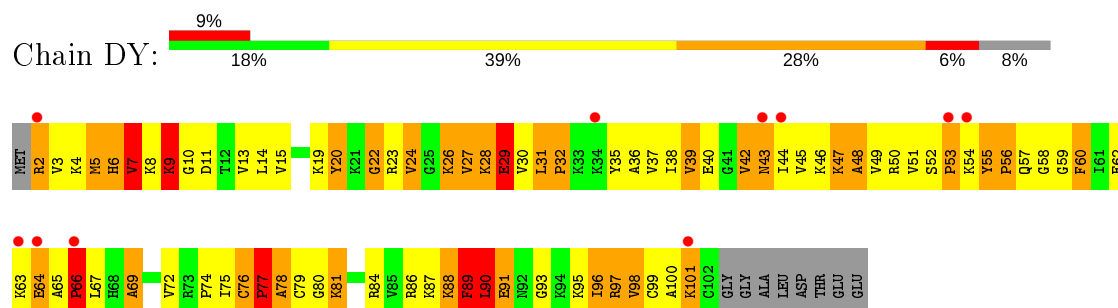
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



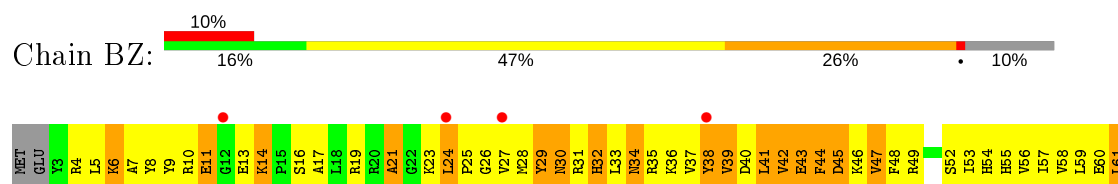
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

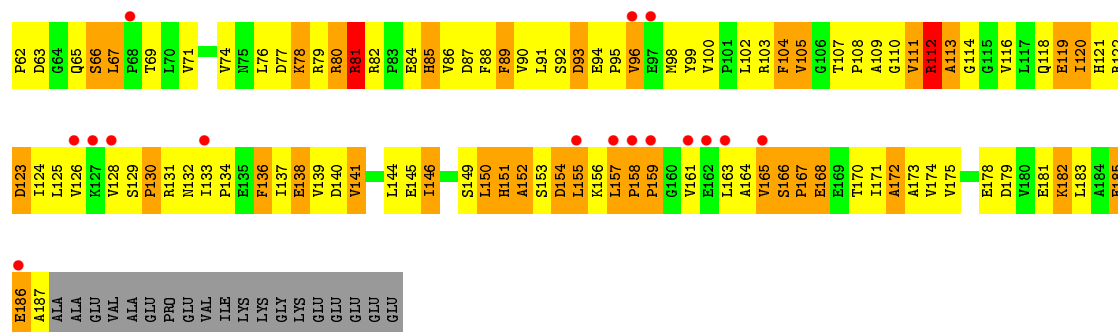


• Molecule 57: 50S RIBOSOMAL PROTEIN L24

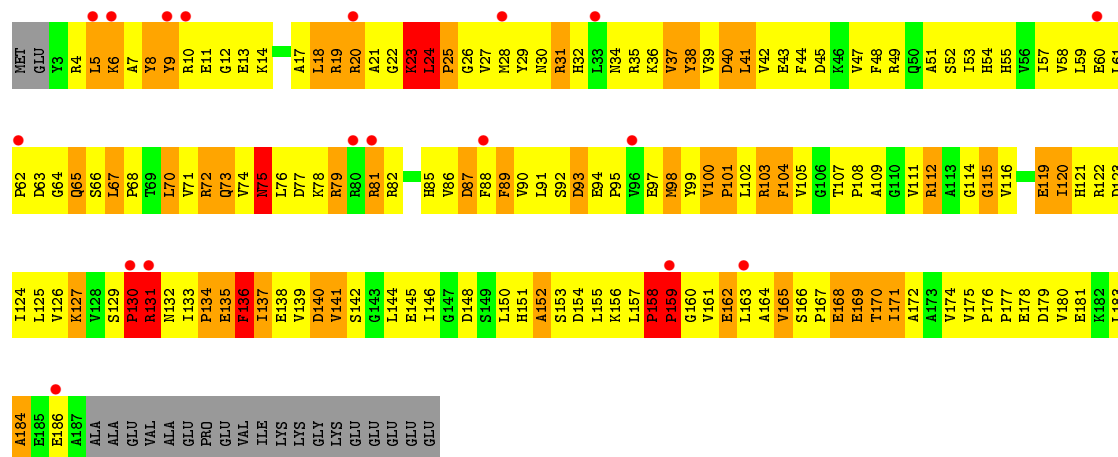
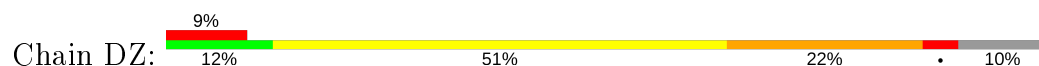


• Molecule 58: 50S RIBOSOMAL PROTEIN L25





• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 59: BACTERIAL TOXIN YOEB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.59Å 455.43Å 616.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.35 49.79 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.79-3.35) 99.7 (49.79-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.261 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	298206	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 5MU, ZN, MG, OMU, A2M

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	0.43	1/36190 (0.0%)	0.69	13/56486 (0.0%)
1	CA	0.41	1/36190 (0.0%)	0.70	15/56486 (0.0%)
2	AB	0.33	0/1936	0.62	0/2611
2	CB	0.33	0/1936	0.61	0/2611
3	AC	0.33	0/1637	0.59	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.38	0/1733	0.67	1/2318 (0.0%)
4	CD	0.35	0/1733	0.64	0/2318
5	AE	0.38	0/1163	0.67	0/1566
5	CE	0.37	0/1163	0.65	0/1566
6	AF	0.34	0/856	0.64	0/1154
6	CF	0.35	0/856	0.64	0/1154
7	AG	0.32	0/1276	0.55	0/1709
7	CG	0.30	0/1276	0.55	0/1709
8	AH	0.35	0/1136	0.69	0/1527
8	CH	0.33	0/1136	0.68	0/1527
9	AI	0.33	0/1027	0.60	0/1373
9	CI	0.32	0/1027	0.61	0/1373
10	AJ	0.35	0/808	0.62	0/1087
10	CJ	0.33	0/808	0.61	0/1087
11	AK	0.33	0/900	0.61	0/1213
11	CK	0.35	0/900	0.61	0/1213
12	AL	0.42	0/987	0.75	0/1322
12	CL	0.43	0/987	0.74	1/1322 (0.1%)
13	AM	0.33	0/943	0.84	3/1256 (0.2%)
13	CM	0.33	0/943	0.85	3/1256 (0.2%)
14	AN	0.36	0/501	0.94	3/664 (0.5%)
14	CN	0.37	0/501	0.92	3/664 (0.5%)
15	AO	0.36	0/745	0.61	0/992
15	CO	0.38	0/745	0.61	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.36	0/717	0.61	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/837	0.66	0/1119
17	CQ	0.37	0/837	0.65	0/1119
18	AR	0.37	0/579	1.06	3/768 (0.4%)
18	CR	0.36	0/579	0.97	3/768 (0.4%)
19	AS	0.43	0/643	0.92	3/867 (0.3%)
19	CS	0.51	0/643	0.98	3/867 (0.3%)
20	AT	0.35	0/765	0.61	0/1007
20	CT	0.32	0/765	0.60	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.49	0/1810	0.70	0/2821
23	AW	0.39	0/1832	0.69	0/2855
23	CV	0.44	0/1832	0.72	1/2855 (0.0%)
23	CW	0.37	0/1832	0.69	0/2855
24	AX	0.41	0/194	0.65	0/301
25	AY	0.41	0/742	0.63	1/1002 (0.1%)
25	AZ	0.40	0/743	0.63	0/1002
25	CY	0.48	0/742	0.69	2/1002 (0.2%)
25	CZ	0.47	0/743	0.64	0/1002
26	B0	0.39	0/671	0.68	0/892
26	D0	0.39	0/671	0.69	0/892
27	B1	0.43	0/739	0.81	1/983 (0.1%)
27	D1	0.47	0/739	0.78	0/983
28	B2	0.38	0/600	0.68	0/793
28	D2	0.47	0/600	0.76	1/793 (0.1%)
29	B3	0.38	0/473	0.65	0/636
29	D3	0.40	0/473	0.66	0/636
30	B4	0.39	0/461	0.70	0/623
30	D4	0.40	0/461	0.69	0/623
31	B5	0.51	0/442	0.86	0/598
31	D5	0.54	0/442	0.85	0/598
32	B6	0.46	0/440	0.83	0/586
32	D6	0.51	0/440	0.85	0/586
33	B7	0.48	0/418	0.68	0/552
33	D7	0.54	0/418	0.69	0/552
34	B8	0.57	0/516	0.97	4/681 (0.6%)
34	D8	0.56	0/516	0.97	5/681 (0.7%)
35	B9	0.36	0/310	0.61	0/407
35	D9	0.36	0/310	0.62	0/407
36	BA	0.53	5/68704 (0.0%)	0.74	50/107260 (0.0%)
36	DA	0.56	3/68704 (0.0%)	0.75	57/107260 (0.1%)
37	BB	0.39	0/2853	0.69	0/4451
37	DB	0.41	0/2853	0.70	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BC	0.31	0/956	0.55	0/1288
38	DC	0.31	0/956	0.55	0/1288
39	BD	0.47	0/2155	0.82	2/2907 (0.1%)
39	DD	0.51	0/2155	0.83	3/2907 (0.1%)
40	BE	0.46	0/1597	0.78	1/2155 (0.0%)
40	DE	0.47	0/1597	0.78	1/2155 (0.0%)
41	BF	0.46	0/1659	0.76	1/2246 (0.0%)
41	DF	0.48	0/1659	0.76	1/2246 (0.0%)
42	BG	0.36	0/1498	0.66	0/2013
42	DG	0.42	0/1498	0.79	1/2013 (0.0%)
43	BH	0.38	0/1285	0.71	0/1741
43	DH	0.40	0/1285	0.72	0/1741
44	BI	0.37	0/1147	0.87	3/1553 (0.2%)
44	DI	0.39	0/1147	0.88	3/1553 (0.2%)
46	BN	0.42	0/1132	0.74	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.45	0/943	0.69	0/1269
47	DO	0.41	0/943	0.67	0/1269
48	BP	0.53	0/1131	1.06	6/1504 (0.4%)
48	DP	0.55	0/1131	1.08	7/1504 (0.5%)
49	BQ	0.44	0/1134	0.68	0/1517
49	DQ	0.42	0/1134	0.68	0/1517
50	BR	0.42	0/974	0.77	2/1302 (0.2%)
50	DR	0.44	0/974	0.79	2/1302 (0.2%)
51	BS	0.40	0/779	0.69	0/1038
51	DS	0.41	0/779	0.69	0/1038
52	BT	0.48	0/1138	0.83	3/1521 (0.2%)
52	DT	0.45	0/1138	0.81	3/1521 (0.2%)
53	BU	0.44	0/975	0.75	0/1297
53	DU	0.47	0/975	0.75	0/1297
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.75	0/1057
55	BW	0.44	0/907	0.72	0/1216
55	DW	0.46	0/907	0.74	0/1216
56	BX	0.44	0/740	0.69	0/995
56	DX	0.47	0/740	0.71	0/995
57	BY	0.51	0/789	0.79	1/1053 (0.1%)
57	DY	0.55	0/789	0.80	1/1053 (0.1%)
58	BZ	0.38	0/1500	0.71	0/2037
58	DZ	0.40	0/1500	0.74	1/2037 (0.0%)
59	CX	0.44	0/169	0.70	0/262
All	All	0.48	10/321535 (0.0%)	0.73	220/480333 (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	1	15
1	CA	0	13
22	AV	0	1
23	CV	0	2
24	AX	0	1
36	BA	7	51
36	DA	7	58
37	BB	0	2
37	DB	0	2
59	CX	0	1
All	All	15	146

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	975(A)	G	O3'-P	-12.04	1.46	1.61
1	AA	413	G	O3'-P	-8.20	1.51	1.61
1	CA	413	G	O3'-P	-7.59	1.52	1.61
36	BA	783	A	C5-C6	-5.78	1.35	1.41
36	BA	2506	U	N1-C2	5.66	1.43	1.38

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AR	64	ARG	NE-CZ-NH2	-15.72	112.44	120.30
19	CS	81	ARG	NE-CZ-NH1	15.12	127.86	120.30
18	AR	64	ARG	NE-CZ-NH1	14.85	127.73	120.30
13	CM	29	ARG	NE-CZ-NH2	-13.53	113.53	120.30
13	CM	29	ARG	NE-CZ-NH1	13.37	126.99	120.30

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	115	G	C3'
36	BA	49	A	C3'
36	BA	331	A	C3'
36	BA	752	A	C3'
36	BA	1799	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	U	Sidechain
1	AA	254	G	Sidechain
1	AA	318	G	Sidechain
1	AA	436	C	Sidechain
1	AA	575	G	Sidechain

5.2 Too-close contacts [i](#)

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	16317	1251	0
1	CA	32329	0	16317	1322	1
2	AB	1901	0	1951	294	0
2	CB	1901	0	1951	300	0
3	AC	1613	0	1677	234	0
3	CC	1613	0	1677	234	0
4	AD	1703	0	1766	193	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	133	0
6	AF	843	0	857	109	0
6	CF	843	0	857	111	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	136	0
8	AH	1116	0	1177	129	0
8	CH	1116	0	1177	125	0
9	AI	1010	0	1035	149	0
9	CI	1010	0	1035	152	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	162	0
11	AK	885	0	904	107	0
11	CK	885	0	904	106	0
12	AL	971	0	1057	109	0
12	CL	971	0	1057	112	0
13	AM	938	0	991	143	0
13	CM	938	0	991	152	0
14	AN	492	0	530	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	531	70	0
15	AO	734	0	771	75	0
15	CO	734	0	771	70	0
16	AP	701	0	720	69	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	75	0
17	CQ	824	0	891	73	0
18	AR	574	0	644	84	0
18	CR	574	0	644	82	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	85	0
20	CT	763	0	861	95	0
21	AU	209	0	221	23	0
21	CU	209	0	221	25	0
22	AV	1641	0	839	55	0
23	AW	1640	0	837	57	0
23	CV	1640	0	837	55	0
23	CW	1640	0	837	64	0
24	AX	239	0	127	94	0
25	AY	722	0	713	147	0
25	AZ	723	0	710	110	0
25	CY	722	0	713	149	0
25	CZ	723	0	713	103	0
26	B0	662	0	688	79	0
26	D0	662	0	688	75	0
27	B1	732	0	808	87	0
27	D1	732	0	808	91	0
28	B2	598	0	653	88	0
28	D2	598	0	653	67	0
29	B3	468	0	523	27	0
29	D3	468	0	523	27	0
30	B4	451	0	449	126	0
30	D4	451	0	449	109	0
31	B5	428	0	445	65	0
31	D5	428	0	445	65	0
32	B6	433	0	461	109	0
32	D6	433	0	461	110	0
33	B7	410	0	454	29	0
33	D7	410	0	454	27	0
34	B8	508	0	576	119	0
34	D8	508	0	576	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B9	307	0	338	34	0
35	D9	307	0	338	31	0
36	BA	61341	0	30927	1969	0
36	DA	61341	0	30928	1948	0
37	BB	2551	0	1295	125	0
37	DB	2551	0	1295	119	0
38	BC	937	0	957	96	0
38	DC	937	0	957	101	0
39	BD	2105	0	2182	253	0
39	DD	2105	0	2182	266	0
40	BE	1564	0	1629	215	0
40	DE	1564	0	1629	213	0
41	BF	1624	0	1677	185	0
41	DF	1624	0	1677	168	0
42	BG	1474	0	1534	329	0
42	DG	1474	0	1534	389	0
43	BH	1260	0	1326	180	0
43	DH	1260	0	1326	175	0
44	BI	1132	0	1218	282	1
44	DI	1132	0	1218	279	0
45	BJ	651	0	177	28	0
45	DJ	651	0	174	64	0
46	BN	1105	0	1180	154	0
46	DN	1105	0	1180	160	0
47	BO	933	0	996	86	0
47	DO	933	0	996	97	0
48	BP	1114	0	1187	297	0
48	DP	1114	0	1187	294	0
49	BQ	1113	0	1171	105	0
49	DQ	1113	0	1171	112	0
50	BR	960	0	1021	139	0
50	DR	960	0	1021	130	0
51	BS	771	0	832	166	0
51	DS	771	0	832	173	0
52	BT	1124	0	1181	226	0
52	DT	1124	0	1181	211	0
53	BU	958	0	1014	125	0
53	DU	958	0	1015	123	0
54	BV	779	0	852	135	0
54	DV	779	0	852	139	0
55	BW	896	0	953	90	0
55	DW	896	0	953	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	74	0
56	DX	726	0	778	71	0
57	BY	776	0	870	182	0
57	DY	776	0	870	176	0
58	BZ	1468	0	1492	253	0
58	DZ	1468	0	1492	348	0
59	CX	217	0	116	77	0
60	AA	103	0	0	0	0
60	AL	1	0	0	0	0
60	AV	1	0	0	0	0
60	AX	1	0	0	0	0
60	B0	1	0	0	0	0
60	B1	2	0	0	0	0
60	B5	2	0	0	0	0
60	BA	236	0	0	0	0
60	BB	2	0	0	0	0
60	BF	1	0	0	0	0
60	BP	1	0	0	0	0
60	BX	1	0	0	0	0
60	CA	103	0	0	0	0
60	CG	1	0	0	0	0
60	CL	1	0	0	0	0
60	CV	2	0	0	0	0
60	D1	1	0	0	0	0
60	D5	1	0	0	0	0
60	DA	242	0	0	0	0
60	DB	1	0	0	0	0
60	DF	1	0	0	0	0
60	DR	1	0	0	0	0
60	DX	1	0	0	0	0
61	AD	1	0	0	2	0
61	AN	1	0	0	0	0
61	CD	1	0	0	1	0
61	CN	1	0	0	1	0
All	All	298206	0	202858	19516	1

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 19516 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)
24:AX:19:OMU:CM2	25:AY:51:ASN:HD21	1.10	1.58
4:CD:26:CYS:SG	61:CD:301:ZN:ZN	1.01	1.49
1:AA:1493:A:C8	24:AX:20:A2M:HM'3	1.49	1.48
1:AA:1493:A:C8	24:AX:20:A2M:CM'	1.98	1.46
1:AA:1493:A:N7	24:AX:20:A2M:CM'	1.89	1.34

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BI:121:LYS:NZ	1:CA:358:U:OP1[4_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	128 (55%)	77 (33%)	28 (12%)	0	2
2	CB	233/256 (91%)	129 (55%)	75 (32%)	29 (12%)	0	2
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	1
3	CC	205/239 (86%)	125 (61%)	53 (26%)	27 (13%)	0	1
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	6
4	CD	206/209 (99%)	139 (68%)	51 (25%)	16 (8%)	1	6
5	AE	149/162 (92%)	106 (71%)	31 (21%)	12 (8%)	1	6
5	CE	149/162 (92%)	107 (72%)	29 (20%)	13 (9%)	1	5
6	AF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	8
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	8
7	AG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	2
7	CG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	2
8	AH	136/138 (99%)	99 (73%)	25 (18%)	12 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	0	4
9	AI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	4
9	CI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	4
10	AJ	97/105 (92%)	69 (71%)	21 (22%)	7 (7%)	1	8
10	CJ	97/105 (92%)	72 (74%)	18 (19%)	7 (7%)	1	8
11	AK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	0	4
11	CK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	0	4
12	AL	123/132 (93%)	87 (71%)	26 (21%)	10 (8%)	1	6
12	CL	123/132 (93%)	88 (72%)	25 (20%)	10 (8%)	1	6
13	AM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
13	CM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
14	CN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
15	AO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	8
15	CO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	8
16	AP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	7
16	CP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	7
17	AQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	15
17	CQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	15
18	AR	68/88 (77%)	41 (60%)	17 (25%)	10 (15%)	0	1
18	CR	68/88 (77%)	42 (62%)	16 (24%)	10 (15%)	0	1
19	AS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
19	CS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
20	AT	97/106 (92%)	59 (61%)	26 (27%)	12 (12%)	0	2
20	CT	97/106 (92%)	58 (60%)	26 (27%)	13 (13%)	0	1
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	1
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
25	AY	82/84 (98%)	53 (65%)	13 (16%)	16 (20%)	0	0
25	AZ	82/84 (98%)	54 (66%)	20 (24%)	8 (10%)	0	4
25	CY	82/84 (98%)	50 (61%)	16 (20%)	16 (20%)	0	0
25	CZ	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	15
26	D0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	1	11
27	B1	92/98 (94%)	67 (73%)	12 (13%)	13 (14%)	0	1
27	D1	92/98 (94%)	66 (72%)	14 (15%)	12 (13%)	0	1
28	B2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	1
28	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	0	2
29	B3	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3	23
29	D3	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	23
30	B4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
30	D4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
31	B5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	1
31	D5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	1
32	B6	48/54 (89%)	25 (52%)	7 (15%)	16 (33%)	0	0
32	D6	48/54 (89%)	26 (54%)	7 (15%)	15 (31%)	0	0
33	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	32
33	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
34	B8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
34	D8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
35	B9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	5
35	D9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	5
38	BC	116/229 (51%)	84 (72%)	26 (22%)	6 (5%)	2	14
38	DC	116/229 (51%)	85 (73%)	25 (22%)	6 (5%)	2	14
39	BD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	0	3
39	DD	270/276 (98%)	202 (75%)	41 (15%)	27 (10%)	0	3
40	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
40	DE	203/206 (98%)	145 (71%)	35 (17%)	23 (11%)	0	2
41	BF	206/210 (98%)	155 (75%)	29 (14%)	22 (11%)	0	3
41	DF	206/210 (98%)	157 (76%)	26 (13%)	23 (11%)	0	2
42	BG	177/182 (97%)	105 (59%)	33 (19%)	39 (22%)	0	0
42	DG	177/182 (97%)	80 (45%)	47 (27%)	50 (28%)	0	0
43	BH	163/180 (91%)	98 (60%)	39 (24%)	26 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DH	163/180 (91%)	98 (60%)	38 (23%)	27 (17%)	0	1
44	BI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	0
44	DI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	0
46	BN	137/140 (98%)	96 (70%)	23 (17%)	18 (13%)	0	1
46	DN	137/140 (98%)	95 (69%)	25 (18%)	17 (12%)	0	2
47	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	29
47	DO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	5	29
48	BP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
49	BQ	139/141 (99%)	109 (78%)	17 (12%)	13 (9%)	0	4
49	DQ	139/141 (99%)	107 (77%)	20 (14%)	12 (9%)	1	5
50	BR	115/118 (98%)	89 (77%)	14 (12%)	12 (10%)	0	3
50	DR	115/118 (98%)	89 (77%)	13 (11%)	13 (11%)	0	2
51	BS	97/112 (87%)	51 (53%)	23 (24%)	23 (24%)	0	0
51	DS	97/112 (87%)	50 (52%)	23 (24%)	24 (25%)	0	0
52	BT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	0
52	DT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	0
53	BU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	14
53	DU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	14
54	BV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	1
54	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	1
55	BW	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	2	13
55	DW	111/113 (98%)	96 (86%)	9 (8%)	6 (5%)	2	13
56	BX	91/96 (95%)	71 (78%)	17 (19%)	3 (3%)	4	24
56	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	4	24
57	BY	99/110 (90%)	42 (42%)	25 (25%)	32 (32%)	0	0
57	DY	99/110 (90%)	41 (41%)	26 (26%)	32 (32%)	0	0
58	BZ	183/206 (89%)	102 (56%)	40 (22%)	41 (22%)	0	0
58	DZ	183/206 (89%)	85 (46%)	58 (32%)	40 (22%)	0	0
All	All	11928/12922 (92%)	7972 (67%)	2431 (20%)	1525 (13%)	0	2

5 of 1525 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	75	LYS
2	AB	123	ALA
2	AB	155	LEU

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%)	189 (94%)	13 (6%)	17	48
2	CB	202/220 (92%)	191 (95%)	11 (5%)	22	54
3	AC	160/188 (85%)	146 (91%)	14 (9%)	10	34
3	CC	160/188 (85%)	147 (92%)	13 (8%)	11	38
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	29
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	29
5	AE	115/123 (94%)	98 (85%)	17 (15%)	3	13
5	CE	115/123 (94%)	98 (85%)	17 (15%)	3	13
6	AF	90/90 (100%)	84 (93%)	6 (7%)	16	47
6	CF	90/90 (100%)	84 (93%)	6 (7%)	16	47
7	AG	126/127 (99%)	120 (95%)	6 (5%)	25	57
7	CG	126/127 (99%)	121 (96%)	5 (4%)	31	62
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	37
8	CH	119/119 (100%)	108 (91%)	11 (9%)	9	32
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	32
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	32
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	12	39
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	12	39
11	AK	90/99 (91%)	87 (97%)	3 (3%)	38	67
11	CK	90/99 (91%)	87 (97%)	3 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	95 (91%)	9 (9%)	10	35
12	CL	104/109 (95%)	95 (91%)	9 (9%)	10	35
13	AM	94/101 (93%)	83 (88%)	11 (12%)	5	21
13	CM	94/101 (93%)	83 (88%)	11 (12%)	5	21
14	AN	49/50 (98%)	46 (94%)	3 (6%)	18	50
14	CN	49/50 (98%)	46 (94%)	3 (6%)	18	50
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	CO	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	30
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
18	AR	61/77 (79%)	61 (100%)	0	100	100
18	CR	61/77 (79%)	60 (98%)	1 (2%)	62	81
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	17
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	21
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	26
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	32
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	26
25	AY	78/78 (100%)	65 (83%)	13 (17%)	2	9
25	AZ	78/78 (100%)	57 (73%)	21 (27%)	0	1
25	CY	78/78 (100%)	64 (82%)	14 (18%)	2	7
25	CZ	78/78 (100%)	56 (72%)	22 (28%)	0	1
26	B0	66/67 (98%)	56 (85%)	10 (15%)	3	12
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	12
27	B1	78/83 (94%)	69 (88%)	9 (12%)	5	22
27	D1	78/83 (94%)	66 (85%)	12 (15%)	2	12
28	B2	66/67 (98%)	56 (85%)	10 (15%)	3	12
28	D2	66/67 (98%)	56 (85%)	10 (15%)	3	12
29	B3	51/52 (98%)	46 (90%)	5 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D3	51/52 (98%)	46 (90%)	5 (10%)	8	30
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	2
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	2
31	B5	47/52 (90%)	42 (89%)	5 (11%)	6	26
31	D5	47/52 (90%)	42 (89%)	5 (11%)	6	26
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	3
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	1
33	B7	40/42 (95%)	36 (90%)	4 (10%)	7	29
33	D7	40/42 (95%)	36 (90%)	4 (10%)	7	29
34	B8	53/55 (96%)	42 (79%)	11 (21%)	1	4
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	34/34 (100%)	32 (94%)	2 (6%)	19	51
35	D9	34/34 (100%)	32 (94%)	2 (6%)	19	51
38	BC	99/181 (55%)	96 (97%)	3 (3%)	41	69
38	DC	99/181 (55%)	96 (97%)	3 (3%)	41	69
39	BD	213/218 (98%)	188 (88%)	25 (12%)	5	21
39	DD	213/218 (98%)	187 (88%)	26 (12%)	5	19
40	BE	165/166 (99%)	143 (87%)	22 (13%)	4	16
40	DE	165/166 (99%)	144 (87%)	21 (13%)	4	18
41	BF	165/166 (99%)	145 (88%)	20 (12%)	5	20
41	DF	165/166 (99%)	145 (88%)	20 (12%)	5	20
42	BG	155/156 (99%)	137 (88%)	18 (12%)	5	21
42	DG	155/156 (99%)	121 (78%)	34 (22%)	1	3
43	BH	137/148 (93%)	127 (93%)	10 (7%)	14	43
43	DH	137/148 (93%)	127 (93%)	10 (7%)	14	43
44	BI	122/124 (98%)	105 (86%)	17 (14%)	3	15
44	DI	122/124 (98%)	105 (86%)	17 (14%)	3	15
46	BN	117/119 (98%)	98 (84%)	19 (16%)	2	10
46	DN	117/119 (98%)	98 (84%)	19 (16%)	2	10
47	BO	100/100 (100%)	94 (94%)	6 (6%)	19	50
47	DO	100/100 (100%)	94 (94%)	6 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BP	112/116 (97%)	84 (75%)	28 (25%)	0	2
48	DP	112/116 (97%)	84 (75%)	28 (25%)	0	2
49	BQ	110/111 (99%)	95 (86%)	15 (14%)	3	16
49	DQ	110/111 (99%)	95 (86%)	15 (14%)	3	16
50	BR	100/101 (99%)	83 (83%)	17 (17%)	2	9
50	DR	100/101 (99%)	83 (83%)	17 (17%)	2	9
51	BS	77/88 (88%)	60 (78%)	17 (22%)	1	3
51	DS	77/88 (88%)	60 (78%)	17 (22%)	1	3
52	BT	118/127 (93%)	98 (83%)	20 (17%)	2	9
52	DT	118/127 (93%)	99 (84%)	19 (16%)	2	10
53	BU	92/94 (98%)	83 (90%)	9 (10%)	8	30
53	DU	92/94 (98%)	83 (90%)	9 (10%)	8	30
54	BV	82/82 (100%)	61 (74%)	21 (26%)	0	2
54	DV	82/82 (100%)	62 (76%)	20 (24%)	0	2
55	BW	91/92 (99%)	78 (86%)	13 (14%)	3	14
55	DW	91/92 (99%)	77 (85%)	14 (15%)	2	12
56	BX	74/78 (95%)	68 (92%)	6 (8%)	11	38
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	38
57	BY	84/91 (92%)	67 (80%)	17 (20%)	1	4
57	DY	84/91 (92%)	67 (80%)	17 (20%)	1	4
58	BZ	162/179 (90%)	137 (85%)	25 (15%)	2	12
58	DZ	162/179 (90%)	131 (81%)	31 (19%)	1	5
All	All	10102/10740 (94%)	8871 (88%)	1231 (12%)	5	19

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	BX	27	THR
9	CI	95	LYS
53	DU	74	LEU
57	BY	60	PHE
3	CC	131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	14	HIS
4	CD	123	HIS
50	DR	61	HIS
54	BV	11	GLN
2	CB	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	214 (14%)	30 (1%)
1	CA	1503/1504 (99%)	209 (13%)	31 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	10 (13%)	1 (1%)
23	CV	76/77 (98%)	12 (15%)	0
23	CW	76/77 (98%)	10 (13%)	1 (1%)
24	AX	10/25 (40%)	8 (80%)	1 (10%)
36	BA	2847/2848 (99%)	500 (17%)	49 (1%)
36	DA	2847/2848 (99%)	498 (17%)	47 (1%)
37	BB	118/119 (99%)	25 (21%)	2 (1%)
37	DB	118/119 (99%)	25 (21%)	2 (1%)
59	CX	9/10 (90%)	6 (66%)	2 (22%)
All	All	9259/9285 (99%)	1532 (16%)	166 (1%)

5 of 1532 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2439	A
1	CA	366	C
36	DA	2191	G
36	BA	2481	G
1	CA	60	A

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

7 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
24	A2M	AX	20	60,24	18,25,26	0.61	0	18,36,39	1.35	1 (5%)
59	A2M	CX	21	59	18,25,26	0.62	0	18,36,39	0.79	0
24	A2M	AX	21	24	18,25,26	0.62	0	18,36,39	1.74	2 (11%)
22	5MU	AV	54	22	15,22,23	1.18	2 (13%)	16,32,35	3.74	1 (6%)
59	OMU	CX	19	59	14,22,23	1.29	2 (14%)	14,31,34	1.42	2 (14%)
24	OMU	AX	19	24	14,22,23	1.32	3 (21%)	14,31,34	1.60	2 (14%)
59	A2M	CX	20	59	18,25,26	0.62	0	18,36,39	1.25	2 (11%)

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
24	A2M	AX	20	60,24	-	2/5/27/28	0/3/3/3
59	A2M	CX	21	59	-	3/5/27/28	0/3/3/3
24	A2M	AX	21	24	-	2/5/27/28	0/3/3/3
22	5MU	AV	54	22	-	0/5/25/26	0/2/2/2
59	OMU	CX	19	59	-	1/7/27/28	0/2/2/2
24	OMU	AX	19	24	-	2/7/27/28	0/2/2/2
59	A2M	CX	20	59	-	2/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	19	OMU	C4-N3	3.31	1.38	1.33
59	CX	19	OMU	C4-N3	3.28	1.38	1.33
22	AV	54	5MU	C4-N3	3.22	1.38	1.33
24	AX	19	OMU	O2'-CM2	-2.18	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CX	19	OMU	C6-N1	2.12	1.38	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	54	5MU	C4-N3-C2	14.57	127.44	115.14
24	AX	21	A2M	CM'-O2'-C2'	-6.75	96.81	114.52
24	AX	20	A2M	CM'-O2'-C2'	-4.87	101.75	114.52
59	CX	20	A2M	CM'-O2'-C2'	-4.43	102.89	114.52
24	AX	19	OMU	CM2-O2'-C2'	-4.34	103.14	114.52

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AX	20	A2M	O4'-C4'-C5'-O5'
59	CX	21	A2M	C4'-C5'-O5'-P
59	CX	21	A2M	C3'-C4'-C5'-O5'
24	AX	21	A2M	C4'-C5'-O5'-P
59	CX	19	OMU	C2'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	20	A2M	31	0
59	CX	21	A2M	20	0
24	AX	21	A2M	21	0
22	AV	54	5MU	1	0
59	CX	19	OMU	10	0
24	AX	19	OMU	14	0
59	CX	20	A2M	30	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 711 ligands modelled in this entry, 711 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.57
1	CM	69:GLU	C	70:LEU	N	4.17
1	AM	69:GLU	C	70:LEU	N	4.16
1	CM	112:GLY	C	113:PRO	N	3.94
1	AM	112:GLY	C	113:PRO	N	3.93

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	1504/1504 (100%)	0.05	31 (2%) 63 67	63, 109, 201, 216	0
1	CA	1504/1504 (100%)	0.23	44 (2%) 51 54	65, 139, 211, 216	0
2	AB	235/256 (91%)	0.53	28 (11%) 4 5	87, 146, 195, 216	0
2	CB	235/256 (91%)	0.61	27 (11%) 4 5	86, 165, 206, 216	0
3	AC	207/239 (86%)	0.42	14 (6%) 17 20	83, 143, 188, 216	0
3	CC	207/239 (86%)	0.99	38 (18%) 1 1	100, 164, 200, 216	0
4	AD	208/209 (99%)	0.09	1 (0%) 91 93	70, 104, 147, 167	0
4	CD	208/209 (99%)	0.82	28 (13%) 3 3	95, 151, 199, 216	0
5	AE	151/162 (93%)	0.35	4 (2%) 56 58	62, 102, 142, 216	0
5	CE	151/162 (93%)	0.91	22 (14%) 2 2	60, 125, 168, 210	0
6	AF	101/101 (100%)	0.16	4 (3%) 38 40	73, 128, 164, 183	0
6	CF	101/101 (100%)	-0.09	1 (0%) 82 86	63, 112, 156, 181	0
7	AG	155/156 (99%)	0.35	14 (9%) 9 11	91, 136, 181, 210	0
7	CG	155/156 (99%)	0.73	28 (18%) 1 1	91, 153, 194, 216	0
8	AH	138/138 (100%)	0.28	1 (0%) 87 91	73, 108, 147, 193	0
8	CH	138/138 (100%)	0.68	13 (9%) 8 10	89, 132, 183, 213	0
9	AI	127/128 (99%)	1.05	27 (21%) 0 1	95, 155, 190, 216	0
9	CI	127/128 (99%)	1.76	41 (32%) 0 0	113, 170, 211, 216	0
10	AJ	99/105 (94%)	1.43	27 (27%) 0 0	88, 159, 208, 216	0
10	CJ	99/105 (94%)	2.07	38 (38%) 0 0	122, 174, 215, 216	0
11	AK	119/129 (92%)	0.93	18 (15%) 2 2	70, 120, 170, 212	0
11	CK	119/129 (92%)	0.39	9 (7%) 13 16	70, 120, 167, 195	0
12	AL	125/132 (94%)	0.48	7 (5%) 24 26	60, 89, 139, 216	0
12	CL	125/132 (94%)	0.88	23 (18%) 1 1	77, 113, 157, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	119/126 (94%)	0.47	8 (6%) 17 20	80, 143, 183, 216	0
13	CM	119/126 (94%)	1.12	26 (21%) 0 1	97, 167, 210, 216	0
14	AN	60/61 (98%)	0.70	6 (10%) 7 8	84, 136, 187, 204	0
14	CN	60/61 (98%)	0.74	8 (13%) 3 4	92, 154, 192, 206	0
15	AO	88/89 (98%)	0.32	2 (2%) 60 63	66, 108, 148, 177	0
15	CO	88/89 (98%)	0.13	2 (2%) 60 63	70, 114, 149, 174	0
16	AP	84/88 (95%)	0.50	2 (2%) 59 61	70, 94, 143, 199	0
16	CP	84/88 (95%)	1.76	30 (35%) 0 0	99, 138, 175, 208	0
17	AQ	100/105 (95%)	0.15	0 100 100	70, 99, 129, 161	0
17	CQ	100/105 (95%)	0.55	7 (7%) 16 18	90, 125, 158, 179	0
18	AR	70/88 (79%)	0.85	7 (10%) 7 8	87, 128, 170, 181	0
18	CR	70/88 (79%)	0.87	9 (12%) 3 4	77, 118, 168, 186	0
19	AS	79/93 (84%)	1.43	24 (30%) 0 0	111, 163, 209, 216	0
19	CS	79/93 (84%)	2.10	31 (39%) 0 0	122, 169, 213, 216	0
20	AT	99/106 (93%)	0.46	7 (7%) 16 18	71, 107, 163, 187	0
20	CT	99/106 (93%)	1.06	17 (17%) 1 1	93, 143, 181, 216	0
21	AU	25/27 (92%)	2.34	12 (48%) 0 0	99, 143, 176, 193	0
21	CU	25/27 (92%)	3.20	17 (68%) 0 0	102, 155, 182, 191	0
22	AV	76/77 (98%)	-0.22	1 (1%) 77 80	71, 108, 162, 206	0
23	AW	77/77 (100%)	2.31	39 (50%) 0 0	151, 218, 220, 221	0
23	CV	77/77 (100%)	-0.12	1 (1%) 77 80	76, 126, 184, 211	0
23	CW	77/77 (100%)	1.85	32 (41%) 0 0	151, 218, 220, 221	0
24	AX	8/25 (32%)	1.89	3 (37%) 0 0	52, 100, 165, 180	0
25	AY	84/84 (100%)	1.08	16 (19%) 1 1	105, 142, 171, 199	0
25	AZ	84/84 (100%)	0.99	20 (23%) 0 0	121, 166, 197, 200	0
25	CY	84/84 (100%)	1.97	37 (44%) 0 0	103, 160, 194, 200	0
25	CZ	84/84 (100%)	1.30	21 (25%) 0 0	132, 182, 200, 200	0
26	B0	84/85 (98%)	0.62	10 (11%) 4 5	69, 103, 160, 207	0
26	D0	84/85 (98%)	1.02	10 (11%) 4 5	76, 107, 163, 198	0
27	B1	94/98 (95%)	0.30	2 (2%) 63 67	55, 87, 144, 208	0
27	D1	94/98 (95%)	0.30	2 (2%) 63 67	53, 83, 132, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B2	71/72 (98%)	0.26	4 (5%) 24 26	81, 122, 156, 205	0
28	D2	71/72 (98%)	-0.12	3 (4%) 36 38	51, 84, 123, 188	0
29	B3	60/60 (100%)	0.97	8 (13%) 3 4	66, 97, 144, 212	0
29	D3	60/60 (100%)	0.29	1 (1%) 70 73	61, 93, 159, 199	0
30	B4	58/71 (81%)	0.29	6 (10%) 6 7	104, 171, 212, 216	0
30	D4	58/71 (81%)	0.83	7 (12%) 4 4	145, 180, 214, 216	0
31	B5	56/60 (93%)	0.19	4 (7%) 16 18	49, 92, 147, 216	0
31	D5	56/60 (93%)	0.01	2 (3%) 42 45	49, 83, 151, 216	0
32	B6	50/54 (92%)	1.81	19 (38%) 0 0	89, 132, 180, 183	0
32	D6	50/54 (92%)	1.37	13 (26%) 0 0	97, 140, 188, 210	0
33	B7	48/49 (97%)	0.09	1 (2%) 63 67	50, 73, 123, 163	0
33	D7	48/49 (97%)	0.11	2 (4%) 36 38	42, 57, 101, 161	0
34	B8	64/65 (98%)	0.47	4 (6%) 20 22	57, 85, 144, 170	0
34	D8	64/65 (98%)	0.45	4 (6%) 20 22	48, 85, 142, 210	0
35	B9	37/37 (100%)	2.06	15 (40%) 0 0	94, 118, 163, 186	0
35	D9	37/37 (100%)	2.15	19 (51%) 0 0	93, 119, 162, 173	0
36	BA	2848/2848 (100%)	0.10	101 (3%) 44 46	46, 88, 203, 216	0
36	DA	2848/2848 (100%)	0.10	92 (3%) 47 50	43, 82, 203, 216	0
37	BB	119/119 (100%)	-0.12	2 (1%) 70 73	88, 144, 195, 212	0
37	DB	119/119 (100%)	0.30	5 (4%) 36 38	90, 173, 210, 216	0
38	BC	120/229 (52%)	4.07	95 (79%) 0 0	139, 202, 216, 216	0
38	DC	120/229 (52%)	3.81	90 (75%) 0 0	145, 202, 216, 216	0
39	BD	272/276 (98%)	0.08	2 (0%) 87 91	45, 83, 120, 188	0
39	DD	272/276 (98%)	0.09	4 (1%) 73 76	45, 77, 113, 185	0
40	BE	205/206 (99%)	0.20	9 (4%) 34 37	50, 89, 166, 201	0
40	DE	205/206 (99%)	0.42	5 (2%) 59 61	37, 89, 146, 194	0
41	BF	208/210 (99%)	-0.05	1 (0%) 91 93	49, 88, 164, 216	0
41	DF	208/210 (99%)	0.08	7 (3%) 45 47	36, 82, 164, 211	0
42	BG	181/182 (99%)	0.49	14 (7%) 13 15	100, 143, 188, 212	0
42	DG	181/182 (99%)	1.30	50 (27%) 0 0	109, 171, 215, 216	0
43	BH	165/180 (91%)	1.68	61 (36%) 0 0	98, 166, 214, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	DH	165/180 (91%)	0.71	23 (13%) 2 3	67, 127, 186, 216	0
44	BI	146/148 (98%)	2.76	67 (45%) 0 0	84, 172, 216, 216	0
44	DI	146/148 (98%)	1.08	23 (15%) 2 2	69, 144, 211, 216	0
45	BJ	0/130	-	-	-	-
45	DJ	0/130	-	-	-	-
46	BN	139/140 (99%)	0.40	6 (4%) 35 38	63, 97, 149, 192	0
46	DN	139/140 (99%)	0.05	2 (1%) 75 78	54, 90, 144, 175	0
47	BO	122/122 (100%)	-0.01	0 100 100	48, 78, 111, 141	0
47	DO	122/122 (100%)	0.24	1 (0%) 86 89	60, 89, 121, 138	0
48	BP	146/150 (97%)	0.57	13 (8%) 9 11	51, 103, 161, 216	0
48	DP	146/150 (97%)	0.36	6 (4%) 37 39	51, 105, 162, 210	0
49	BQ	141/141 (100%)	0.05	1 (0%) 87 91	65, 96, 134, 209	0
49	DQ	141/141 (100%)	0.43	6 (4%) 35 38	67, 103, 149, 208	0
50	BR	117/118 (99%)	0.09	0 100 100	55, 89, 123, 137	0
50	DR	117/118 (99%)	0.31	4 (3%) 45 47	51, 84, 121, 145	0
51	BS	99/112 (88%)	1.04	20 (20%) 1 1	93, 141, 189, 208	0
51	DS	99/112 (88%)	1.27	25 (25%) 0 0	91, 154, 199, 216	0
52	BT	136/146 (93%)	0.19	3 (2%) 62 65	64, 97, 176, 216	0
52	DT	136/146 (93%)	0.41	10 (7%) 14 17	68, 110, 189, 215	0
53	BU	117/118 (99%)	-0.02	1 (0%) 84 87	53, 86, 139, 210	0
53	DU	117/118 (99%)	-0.07	2 (1%) 70 73	45, 75, 122, 215	0
54	BV	101/101 (100%)	0.28	6 (5%) 22 25	53, 109, 158, 206	0
54	DV	101/101 (100%)	0.08	0 100 100	38, 93, 133, 216	0
55	BW	113/113 (100%)	0.28	5 (4%) 34 37	55, 80, 132, 199	0
55	DW	113/113 (100%)	0.20	3 (2%) 54 57	40, 72, 121, 209	0
56	BX	93/96 (96%)	0.21	1 (1%) 80 84	63, 106, 136, 155	0
56	DX	93/96 (96%)	0.13	1 (1%) 80 84	55, 79, 117, 164	0
57	BY	101/110 (91%)	1.37	23 (22%) 0 0	62, 114, 180, 206	0
57	DY	101/110 (91%)	0.71	10 (9%) 7 8	56, 102, 168, 211	0
58	BZ	185/206 (89%)	0.53	20 (10%) 5 6	85, 131, 186, 216	0
58	DZ	185/206 (89%)	0.38	18 (9%) 7 9	88, 144, 202, 215	0
59	CX	7/10 (70%)	1.59	2 (28%) 0 0	110, 144, 193, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21436/22467 (95%)	0.45	1849 (8%) 10 12	36, 111, 202, 221	0

The worst 5 of 1849 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	AL	129	ALA	19.7
44	BI	119	PRO	16.5
44	BI	100	ALA	15.9
44	DI	88	ILE	15.1
5	AE	155	GLU	14.1

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
59	A2M	CX	20	23/24	0.59	0.36	168,174,200,200	0
24	A2M	AX	20	23/24	0.60	0.43	158,164,194,194	0
24	A2M	AX	21	23/24	0.83	0.35	140,147,161,184	0
24	OMU	AX	19	21/22	0.85	0.29	99,130,198,198	0
59	OMU	CX	19	21/22	0.85	0.29	117,161,200,200	0
59	A2M	CX	21	23/24	0.87	0.29	177,179,187,190	0
22	5MU	AV	54	21/22	0.93	0.23	114,133,152,153	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
60	MG	AA	1618	1/1	-0.30	0.38	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1633	1/1	-0.20	0.59	78,78,78,78	0
60	MG	CA	1640	1/1	-0.10	1.19	102,102,102,102	0
60	MG	DA	3009	1/1	-0.07	0.88	168,168,168,168	0
60	MG	CA	1607	1/1	-0.06	0.42	101,101,101,101	0
60	MG	CA	1666	1/1	-0.02	0.60	137,137,137,137	1
60	MG	CA	1647	1/1	0.02	0.32	97,97,97,97	0
60	MG	BA	3094	1/1	0.05	0.97	100,100,100,100	0
60	MG	CA	1692	1/1	0.06	0.67	117,117,117,117	0
60	MG	BA	3017	1/1	0.11	0.66	117,117,117,117	0
60	MG	CA	1627	1/1	0.13	0.68	162,162,162,162	0
60	MG	AA	1623	1/1	0.13	0.66	100,100,100,100	0
60	MG	DA	2964	1/1	0.15	1.25	109,109,109,109	0
60	MG	AA	1612	1/1	0.18	1.12	102,102,102,102	0
60	MG	AA	1642	1/1	0.18	0.67	102,102,102,102	0
60	MG	BA	3101	1/1	0.21	0.83	123,123,123,123	0
60	MG	CA	1672	1/1	0.25	0.89	109,109,109,109	0
60	MG	AA	1645	1/1	0.25	1.24	99,99,99,99	0
60	MG	CA	1637	1/1	0.26	0.57	141,141,141,141	0
60	MG	BA	3045	1/1	0.28	0.21	88,88,88,88	0
60	MG	DA	3041	1/1	0.31	2.16	154,154,154,154	0
60	MG	BA	2901	1/1	0.31	0.30	145,145,145,145	0
60	MG	AA	1662	1/1	0.31	1.06	127,127,127,127	0
60	MG	BA	3001	1/1	0.32	0.20	157,157,157,157	0
60	MG	BA	3097	1/1	0.34	0.37	88,88,88,88	0
60	MG	BA	3063	1/1	0.35	0.64	136,136,136,136	0
60	MG	DA	3082	1/1	0.35	0.77	77,77,77,77	0
60	MG	BA	3051	1/1	0.35	0.75	72,72,72,72	0
60	MG	CA	1650	1/1	0.36	1.29	127,127,127,127	0
60	MG	AA	1646	1/1	0.36	0.97	125,125,125,125	0
60	MG	BA	3086	1/1	0.36	0.61	114,114,114,114	0
60	MG	AA	1638	1/1	0.37	0.13	139,139,139,139	1
60	MG	BA	3089	1/1	0.37	0.52	155,155,155,155	0
60	MG	AA	1627	1/1	0.38	1.24	101,101,101,101	0
60	MG	CA	1626	1/1	0.39	1.39	102,102,102,102	0
60	MG	BA	2995	1/1	0.39	0.43	105,105,105,105	0
60	MG	AA	1665	1/1	0.39	2.52	121,121,121,121	0
60	MG	AA	1652	1/1	0.40	0.35	103,103,103,103	1
60	MG	AA	1603	1/1	0.40	1.36	94,94,94,94	0
60	MG	CA	1678	1/1	0.40	0.56	86,86,86,86	1
60	MG	BA	3030	1/1	0.40	0.75	96,96,96,96	0
60	MG	DA	2901	1/1	0.40	0.79	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3096	1/1	0.42	1.00	124,124,124,124	0
60	MG	CA	1698	1/1	0.43	1.21	145,145,145,145	0
60	MG	CA	1612	1/1	0.43	0.56	102,102,102,102	0
60	MG	BA	3084	1/1	0.44	0.85	126,126,126,126	0
60	MG	DA	3057	1/1	0.44	0.47	92,92,92,92	0
60	MG	BB	201	1/1	0.45	1.05	84,84,84,84	0
60	MG	CA	1667	1/1	0.45	1.45	83,83,83,83	1
60	MG	DA	3081	1/1	0.45	0.57	104,104,104,104	0
60	MG	DA	2990	1/1	0.46	0.65	88,88,88,88	0
60	MG	BA	3053	1/1	0.46	0.81	122,122,122,122	0
60	MG	BA	3046	1/1	0.46	0.49	112,112,112,112	0
60	MG	DA	3103	1/1	0.46	0.32	82,82,82,82	0
60	MG	CA	1668	1/1	0.47	0.32	93,93,93,93	0
60	MG	DA	3099	1/1	0.47	0.62	108,108,108,108	0
60	MG	DA	3122	1/1	0.47	1.24	79,79,79,79	0
60	MG	DA	2986	1/1	0.48	0.75	87,87,87,87	0
60	MG	DA	2991	1/1	0.48	0.42	126,126,126,126	0
60	MG	BA	2977	1/1	0.48	1.11	107,107,107,107	0
60	MG	DA	3048	1/1	0.49	0.62	129,129,129,129	0
60	MG	DA	3058	1/1	0.50	0.49	104,104,104,104	0
60	MG	CA	1624	1/1	0.50	1.65	119,119,119,119	0
60	MG	CA	1665	1/1	0.50	0.60	111,111,111,111	1
60	MG	AA	1643	1/1	0.51	0.65	106,106,106,106	0
60	MG	AA	1675	1/1	0.51	0.43	93,93,93,93	0
60	MG	DA	3018	1/1	0.52	0.42	114,114,114,114	0
60	MG	BA	2988	1/1	0.52	0.69	117,117,117,117	0
60	MG	DA	3114	1/1	0.52	0.76	96,96,96,96	0
60	MG	BA	3102	1/1	0.53	0.52	108,108,108,108	0
60	MG	AA	1601	1/1	0.54	0.87	100,100,100,100	0
60	MG	BA	3093	1/1	0.54	0.78	99,99,99,99	0
60	MG	CA	1634	1/1	0.54	0.34	122,122,122,122	0
60	MG	DA	3004	1/1	0.54	0.52	113,113,113,113	0
60	MG	AA	1634	1/1	0.54	1.60	120,120,120,120	0
60	MG	DA	3071	1/1	0.54	0.87	123,123,123,123	0
60	MG	DA	3117	1/1	0.55	0.92	123,123,123,123	0
60	MG	DA	3008	1/1	0.55	0.24	92,92,92,92	0
60	MG	CA	1690	1/1	0.55	0.80	100,100,100,100	0
60	MG	CA	1606	1/1	0.55	0.48	118,118,118,118	0
60	MG	BA	3088	1/1	0.56	0.39	105,105,105,105	0
60	MG	AA	1691	1/1	0.56	0.38	96,96,96,96	0
60	MG	BA	3126	1/1	0.56	1.74	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1677	1/1	0.56	0.86	88,88,88,88	0
60	MG	BA	3100	1/1	0.56	0.48	117,117,117,117	0
60	MG	BA	3098	1/1	0.57	0.68	89,89,89,89	0
60	MG	DA	3019	1/1	0.57	0.88	112,112,112,112	0
60	MG	BA	3107	1/1	0.57	0.51	87,87,87,87	0
60	MG	AA	1606	1/1	0.57	1.07	98,98,98,98	0
60	MG	CA	1691	1/1	0.57	1.46	105,105,105,105	0
60	MG	AA	1641	1/1	0.58	0.59	93,93,93,93	0
60	MG	CA	1658	1/1	0.58	0.39	93,93,93,93	0
60	MG	DA	3106	1/1	0.59	0.77	143,143,143,143	0
60	MG	DA	3141	1/1	0.59	0.67	92,92,92,92	0
60	MG	DA	3124	1/1	0.59	1.96	98,98,98,98	0
60	MG	DA	3010	1/1	0.59	0.59	92,92,92,92	0
60	MG	CA	1639	1/1	0.59	0.37	99,99,99,99	0
60	MG	CA	1686	1/1	0.59	0.54	94,94,94,94	0
60	MG	DA	3115	1/1	0.60	0.50	162,162,162,162	0
60	MG	AA	1649	1/1	0.60	0.72	124,124,124,124	0
60	MG	DA	3098	1/1	0.61	0.61	107,107,107,107	0
60	MG	DA	3135	1/1	0.61	1.42	103,103,103,103	0
60	MG	CA	1662	1/1	0.61	0.69	113,113,113,113	0
60	MG	DA	3035	1/1	0.62	0.51	105,105,105,105	0
60	MG	DA	3055	1/1	0.62	0.26	106,106,106,106	0
60	MG	CA	1702	1/1	0.62	1.22	96,96,96,96	0
60	MG	CA	1644	1/1	0.62	0.68	94,94,94,94	0
60	MG	DF	301	1/1	0.62	0.30	100,100,100,100	0
60	MG	CA	1604	1/1	0.62	0.71	115,115,115,115	0
60	MG	BA	2985	1/1	0.62	0.36	87,87,87,87	0
60	MG	CA	1700	1/1	0.62	0.52	113,113,113,113	0
60	MG	CA	1601	1/1	0.63	0.87	86,86,86,86	0
60	MG	BA	3121	1/1	0.63	0.47	112,112,112,112	0
60	MG	AA	1636	1/1	0.64	0.76	142,142,142,142	0
60	MG	DA	3088	1/1	0.64	0.80	110,110,110,110	0
60	MG	CG	201	1/1	0.65	0.53	83,83,83,83	1
60	MG	AA	1608	1/1	0.65	0.44	81,81,81,81	0
60	MG	AA	1660	1/1	0.65	0.31	105,105,105,105	0
60	MG	DA	3137	1/1	0.65	0.57	121,121,121,121	0
60	MG	DA	3090	1/1	0.65	0.69	106,106,106,106	0
60	MG	AA	1604	1/1	0.66	0.39	132,132,132,132	0
60	MG	BA	3064	1/1	0.66	0.48	86,86,86,86	0
60	MG	CA	1659	1/1	0.66	0.35	104,104,104,104	1
60	MG	BA	3124	1/1	0.67	0.84	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3068	1/1	0.67	1.07	102,102,102,102	0
60	MG	DA	3029	1/1	0.67	0.65	99,99,99,99	0
60	MG	DA	3037	1/1	0.67	0.44	74,74,74,74	0
60	MG	BA	3114	1/1	0.67	1.60	130,130,130,130	0
60	MG	CA	1653	1/1	0.67	0.61	127,127,127,127	0
60	MG	CA	1671	1/1	0.67	0.59	95,95,95,95	0
60	MG	DA	3031	1/1	0.67	0.83	92,92,92,92	0
60	MG	DA	3077	1/1	0.67	0.61	96,96,96,96	0
60	MG	DA	3063	1/1	0.67	0.92	94,94,94,94	0
60	MG	BA	3020	1/1	0.67	0.63	103,103,103,103	0
60	MG	BA	3090	1/1	0.68	1.40	123,123,123,123	0
60	MG	BA	3012	1/1	0.68	1.21	91,91,91,91	0
60	MG	AA	1672	1/1	0.68	1.41	136,136,136,136	0
60	MG	AA	1677	1/1	0.68	0.24	114,114,114,114	0
60	MG	BA	3007	1/1	0.68	0.33	125,125,125,125	0
60	MG	DR	201	1/1	0.69	1.03	117,117,117,117	0
60	MG	AA	1667	1/1	0.69	0.97	118,118,118,118	0
60	MG	DA	3080	1/1	0.69	0.74	130,130,130,130	0
60	MG	CV	102	1/1	0.69	1.68	132,132,132,132	1
60	MG	DA	3022	1/1	0.69	0.31	81,81,81,81	0
60	MG	DA	3097	1/1	0.69	0.54	112,112,112,112	0
60	MG	DA	3102	1/1	0.69	0.38	80,80,80,80	0
60	MG	DA	2972	1/1	0.69	0.60	100,100,100,100	0
60	MG	BA	3083	1/1	0.69	0.52	87,87,87,87	0
60	MG	BA	3018	1/1	0.69	1.54	109,109,109,109	0
60	MG	CA	1664	1/1	0.70	0.96	112,112,112,112	0
60	MG	DA	2965	1/1	0.70	0.57	96,96,96,96	0
60	MG	BA	3108	1/1	0.70	0.47	102,102,102,102	0
60	MG	BA	2966	1/1	0.70	0.40	92,92,92,92	0
60	MG	DA	3100	1/1	0.70	0.81	113,113,113,113	0
60	MG	BA	2970	1/1	0.70	1.24	86,86,86,86	0
60	MG	CA	1654	1/1	0.70	0.47	107,107,107,107	0
60	MG	BA	3115	1/1	0.70	0.84	85,85,85,85	0
60	MG	BA	3106	1/1	0.70	0.74	97,97,97,97	0
60	MG	AA	1686	1/1	0.70	1.39	99,99,99,99	0
60	MG	DA	2969	1/1	0.70	0.83	84,84,84,84	0
60	MG	DA	3070	1/1	0.70	0.84	79,79,79,79	0
60	MG	BA	2960	1/1	0.71	0.58	105,105,105,105	0
60	MG	AA	1624	1/1	0.71	0.66	111,111,111,111	0
60	MG	AA	1670	1/1	0.71	1.39	130,130,130,130	0
60	MG	DA	3003	1/1	0.71	0.90	69,69,69,69	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	2929	1/1	0.71	0.70	94,94,94,94	0
60	MG	CA	1696	1/1	0.71	1.18	162,162,162,162	0
60	MG	BA	2908	1/1	0.71	1.25	103,103,103,103	0
60	MG	CA	1688	1/1	0.72	0.95	103,103,103,103	0
60	MG	DA	2999	1/1	0.72	0.22	94,94,94,94	0
60	MG	DA	3094	1/1	0.72	0.45	87,87,87,87	0
60	MG	BA	3022	1/1	0.72	0.46	125,125,125,125	0
60	MG	CA	1623	1/1	0.72	0.20	82,82,82,82	0
60	MG	DA	3046	1/1	0.72	0.84	76,76,76,76	0
60	MG	CA	1633	1/1	0.72	0.66	93,93,93,93	0
60	MG	BA	3043	1/1	0.72	0.24	83,83,83,83	0
60	MG	AA	1689	1/1	0.72	0.27	98,98,98,98	0
60	MG	BA	3109	1/1	0.72	0.59	101,101,101,101	0
60	MG	DA	3014	1/1	0.72	0.78	77,77,77,77	0
60	MG	CA	1618	1/1	0.72	0.55	83,83,83,83	0
60	MG	BA	3113	1/1	0.73	0.34	126,126,126,126	0
60	MG	DA	3072	1/1	0.73	0.41	102,102,102,102	0
60	MG	DA	3017	1/1	0.73	0.12	97,97,97,97	0
60	MG	BA	3006	1/1	0.73	0.39	91,91,91,91	0
60	MG	DA	2962	1/1	0.73	0.48	89,89,89,89	0
60	MG	BA	3080	1/1	0.73	0.58	115,115,115,115	0
60	MG	CA	1641	1/1	0.73	1.46	94,94,94,94	0
60	MG	BA	3129	1/1	0.73	0.63	84,84,84,84	0
60	MG	DB	201	1/1	0.73	0.43	69,69,69,69	0
60	MG	DA	3056	1/1	0.73	0.47	126,126,126,126	0
60	MG	CA	1643	1/1	0.73	0.24	105,105,105,105	0
60	MG	DX	101	1/1	0.73	0.73	72,72,72,72	1
60	MG	CA	1616	1/1	0.73	0.17	105,105,105,105	0
60	MG	CA	1685	1/1	0.74	0.33	115,115,115,115	0
60	MG	BA	3011	1/1	0.74	0.77	106,106,106,106	0
60	MG	DA	2942	1/1	0.74	0.93	90,90,90,90	0
60	MG	DA	3024	1/1	0.74	0.72	106,106,106,106	0
60	MG	BA	2965	1/1	0.74	0.40	111,111,111,111	0
60	MG	DA	3105	1/1	0.74	0.33	93,93,93,93	0
60	MG	DA	3061	1/1	0.74	0.45	94,94,94,94	0
60	MG	BA	3008	1/1	0.74	0.67	96,96,96,96	0
60	MG	CA	1680	1/1	0.74	0.64	148,148,148,148	0
60	MG	BF	301	1/1	0.74	0.55	100,100,100,100	0
60	MG	DA	3039	1/1	0.74	0.69	85,85,85,85	0
60	MG	BA	3096	1/1	0.74	0.32	84,84,84,84	0
60	MG	CA	1699	1/1	0.74	0.38	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	2949	1/1	0.75	0.91	102,102,102,102	0
60	MG	DA	3044	1/1	0.75	0.23	79,79,79,79	0
60	MG	DA	2998	1/1	0.75	0.52	91,91,91,91	0
60	MG	BA	2975	1/1	0.75	0.32	92,92,92,92	0
60	MG	BA	3002	1/1	0.75	1.08	97,97,97,97	0
60	MG	AA	1661	1/1	0.75	0.96	94,94,94,94	0
60	MG	BA	3015	1/1	0.75	0.56	94,94,94,94	0
60	MG	CA	1670	1/1	0.75	0.09	153,153,153,153	0
60	MG	CA	1632	1/1	0.76	0.15	79,79,79,79	0
60	MG	BA	3026	1/1	0.76	0.32	85,85,85,85	0
60	MG	AA	1650	1/1	0.76	0.71	111,111,111,111	0
60	MG	CA	1636	1/1	0.76	0.51	90,90,90,90	0
60	MG	B1	101	1/1	0.76	0.56	113,113,113,113	0
60	MG	BA	3032	1/1	0.76	0.70	98,98,98,98	0
60	MG	CA	1613	1/1	0.76	0.41	89,89,89,89	0
60	MG	DA	3091	1/1	0.76	0.34	107,107,107,107	0
60	MG	AA	1674	1/1	0.76	0.97	87,87,87,87	1
60	MG	CA	1629	1/1	0.76	0.98	95,95,95,95	0
60	MG	DA	3083	1/1	0.76	1.08	112,112,112,112	0
60	MG	BA	3120	1/1	0.76	0.52	111,111,111,111	0
60	MG	CA	1622	1/1	0.76	0.51	93,93,93,93	0
60	MG	CA	1609	1/1	0.76	0.14	84,84,84,84	0
60	MG	CA	1603	1/1	0.76	0.86	113,113,113,113	0
60	MG	BA	2920	1/1	0.76	1.17	98,98,98,98	0
60	MG	DA	3002	1/1	0.77	0.36	95,95,95,95	0
60	MG	AA	1635	1/1	0.77	0.30	111,111,111,111	0
60	MG	BA	3078	1/1	0.77	0.33	104,104,104,104	0
60	MG	BA	3123	1/1	0.77	0.60	80,80,80,80	0
60	MG	AV	101	1/1	0.77	0.57	83,83,83,83	1
60	MG	BA	3035	1/1	0.77	0.18	86,86,86,86	0
60	MG	DA	2953	1/1	0.77	0.33	65,65,65,65	0
60	MG	BA	2982	1/1	0.77	0.26	100,100,100,100	0
60	MG	BA	3066	1/1	0.77	0.99	113,113,113,113	0
60	MG	AA	1622	1/1	0.77	0.28	128,128,128,128	0
60	MG	DA	3085	1/1	0.77	0.51	86,86,86,86	0
60	MG	DA	3104	1/1	0.77	0.64	118,118,118,118	0
60	MG	DA	3125	1/1	0.78	0.40	72,72,72,72	0
60	MG	DA	2975	1/1	0.78	1.21	138,138,138,138	0
60	MG	BA	2949	1/1	0.78	0.48	77,77,77,77	0
60	MG	AA	1695	1/1	0.78	0.36	105,105,105,105	0
60	MG	CA	1689	1/1	0.78	0.69	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3034	1/1	0.78	0.29	72,72,72,72	0
60	MG	AA	1614	1/1	0.78	0.58	98,98,98,98	0
60	MG	BA	3081	1/1	0.78	0.64	103,103,103,103	0
60	MG	BA	2973	1/1	0.78	0.66	92,92,92,92	0
60	MG	DA	3132	1/1	0.78	0.57	120,120,120,120	0
60	MG	CA	1694	1/1	0.79	0.94	112,112,112,112	0
60	MG	AA	1625	1/1	0.79	0.46	85,85,85,85	0
60	MG	BA	3040	1/1	0.79	1.06	99,99,99,99	0
60	MG	BA	3060	1/1	0.79	0.86	83,83,83,83	0
60	MG	CA	1687	1/1	0.79	0.41	119,119,119,119	0
60	MG	BA	3073	1/1	0.79	0.29	100,100,100,100	0
60	MG	BA	2996	1/1	0.79	1.04	106,106,106,106	0
60	MG	BA	2983	1/1	0.79	0.34	108,108,108,108	0
60	MG	DA	3043	1/1	0.79	0.30	96,96,96,96	0
60	MG	DA	3027	1/1	0.80	0.90	92,92,92,92	0
60	MG	DA	3089	1/1	0.80	1.21	92,92,92,92	0
60	MG	BA	3058	1/1	0.80	0.48	88,88,88,88	0
60	MG	CA	1669	1/1	0.80	0.28	113,113,113,113	0
60	MG	DA	2951	1/1	0.80	1.03	91,91,91,91	0
60	MG	CA	1675	1/1	0.80	0.31	122,122,122,122	0
60	MG	BA	3128	1/1	0.80	0.45	117,117,117,117	0
60	MG	AA	1651	1/1	0.80	0.32	113,113,113,113	0
60	MG	AA	1699	1/1	0.80	0.64	109,109,109,109	0
60	MG	BA	3038	1/1	0.80	0.34	90,90,90,90	0
60	MG	CA	1631	1/1	0.80	0.98	111,111,111,111	0
60	MG	DA	3128	1/1	0.80	1.26	92,92,92,92	0
60	MG	AA	1693	1/1	0.80	0.96	119,119,119,119	0
60	MG	DA	3121	1/1	0.81	0.61	104,104,104,104	0
60	MG	BA	3085	1/1	0.81	0.59	118,118,118,118	0
60	MG	AA	1609	1/1	0.81	0.86	106,106,106,106	0
60	MG	BA	3042	1/1	0.81	0.46	78,78,78,78	0
60	MG	DA	2956	1/1	0.81	0.48	63,63,63,63	0
60	MG	CA	1703	1/1	0.81	0.31	107,107,107,107	0
60	MG	CA	1652	1/1	0.81	0.77	148,148,148,148	0
60	MG	BA	2976	1/1	0.81	0.50	66,66,66,66	0
60	MG	BA	3062	1/1	0.81	0.61	89,89,89,89	0
60	MG	CA	1608	1/1	0.81	0.17	113,113,113,113	0
60	MG	CA	1660	1/1	0.81	0.84	95,95,95,95	0
60	MG	BA	2984	1/1	0.81	0.84	95,95,95,95	0
60	MG	BA	2942	1/1	0.81	0.86	107,107,107,107	0
60	MG	DA	2935	1/1	0.81	0.81	68,68,68,68	0
60	MG	CA	1663	1/1	0.81	0.37	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	2969	1/1	0.82	0.45	61,61,61,61	0
60	MG	DA	2996	1/1	0.82	0.36	63,63,63,63	0
60	MG	DA	3142	1/1	0.82	0.21	81,81,81,81	0
60	MG	B0	101	1/1	0.82	0.50	98,98,98,98	0
60	MG	BA	3118	1/1	0.82	1.47	110,110,110,110	0
60	MG	BA	2963	1/1	0.82	0.68	103,103,103,103	0
60	MG	BA	2955	1/1	0.82	1.12	109,109,109,109	0
60	MG	DA	3086	1/1	0.82	0.56	78,78,78,78	0
60	MG	DA	2961	1/1	0.82	0.61	90,90,90,90	0
60	MG	DA	2963	1/1	0.82	0.53	70,70,70,70	0
60	MG	BA	3025	1/1	0.82	0.74	95,95,95,95	0
60	MG	AA	1656	1/1	0.82	0.25	140,140,140,140	0
60	MG	AA	1671	1/1	0.82	1.00	96,96,96,96	0
60	MG	BX	101	1/1	0.83	1.30	110,110,110,110	1
60	MG	BA	3082	1/1	0.83	0.44	101,101,101,101	0
60	MG	BA	2905	1/1	0.83	0.44	58,58,58,58	0
60	MG	AA	1640	1/1	0.83	0.51	64,64,64,64	1
60	MG	DA	3013	1/1	0.83	0.98	89,89,89,89	0
60	MG	DA	3118	1/1	0.83	0.63	73,73,73,73	0
60	MG	BA	3016	1/1	0.83	0.23	102,102,102,102	0
60	MG	AA	1688	1/1	0.83	1.14	113,113,113,113	0
60	MG	BA	2992	1/1	0.83	0.54	61,61,61,61	0
60	MG	CA	1611	1/1	0.83	0.42	97,97,97,97	0
60	MG	DA	3047	1/1	0.83	0.23	112,112,112,112	0
60	MG	DA	3042	1/1	0.83	0.35	81,81,81,81	0
60	MG	DA	2980	1/1	0.83	1.16	111,111,111,111	0
60	MG	DA	3053	1/1	0.83	0.40	71,71,71,71	0
60	MG	DA	3000	1/1	0.83	0.52	77,77,77,77	0
60	MG	BA	2952	1/1	0.83	0.83	87,87,87,87	0
60	MG	BA	3049	1/1	0.84	0.44	65,65,65,65	0
60	MG	DA	3023	1/1	0.84	0.38	103,103,103,103	0
60	MG	BA	2921	1/1	0.84	0.34	98,98,98,98	0
60	MG	DA	3001	1/1	0.84	0.28	69,69,69,69	0
60	MG	AA	1620	1/1	0.84	0.24	134,134,134,134	0
60	MG	BA	2971	1/1	0.84	0.13	52,52,52,52	0
60	MG	DA	2903	1/1	0.84	1.02	85,85,85,85	0
60	MG	BA	2993	1/1	0.84	0.75	92,92,92,92	0
60	MG	BA	2930	1/1	0.84	1.33	117,117,117,117	0
60	MG	AA	1637	1/1	0.84	0.55	99,99,99,99	0
60	MG	BA	3125	1/1	0.84	0.46	91,91,91,91	0
60	MG	AA	1617	1/1	0.84	0.46	104,104,104,104	0
60	MG	BA	2997	1/1	0.84	0.13	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1697	1/1	0.84	0.86	126,126,126,126	0
60	MG	AA	1613	1/1	0.84	1.48	114,114,114,114	0
60	MG	BA	3019	1/1	0.84	0.39	74,74,74,74	0
60	MG	AA	1681	1/1	0.84	0.91	99,99,99,99	0
60	MG	BA	3037	1/1	0.84	0.82	79,79,79,79	0
60	MG	BA	3076	1/1	0.84	0.57	108,108,108,108	0
60	MG	CA	1655	1/1	0.84	0.68	111,111,111,111	0
60	MG	DA	3101	1/1	0.84	0.12	88,88,88,88	0
60	MG	BA	2950	1/1	0.84	0.93	81,81,81,81	0
60	MG	DA	3136	1/1	0.84	0.21	94,94,94,94	0
60	MG	DA	3045	1/1	0.84	0.96	104,104,104,104	0
60	MG	DA	3007	1/1	0.84	0.26	82,82,82,82	0
60	MG	B5	102	1/1	0.84	0.56	79,79,79,79	0
60	MG	DA	2981	1/1	0.85	0.83	105,105,105,105	0
60	MG	DA	3075	1/1	0.85	0.36	75,75,75,75	0
60	MG	CA	1615	1/1	0.85	0.69	127,127,127,127	0
60	MG	BA	3047	1/1	0.85	0.21	105,105,105,105	0
60	MG	D5	101	1/1	0.85	0.35	56,56,56,56	0
60	MG	BA	3024	1/1	0.85	0.45	96,96,96,96	0
60	MG	BA	3105	1/1	0.85	0.16	68,68,68,68	0
60	MG	DA	2960	1/1	0.85	0.67	59,59,59,59	0
60	MG	AA	1639	1/1	0.85	0.41	98,98,98,98	1
60	MG	DA	2940	1/1	0.85	0.73	72,72,72,72	0
60	MG	BA	3055	1/1	0.85	0.62	87,87,87,87	0
60	MG	BA	2902	1/1	0.85	0.33	155,155,155,155	0
60	MG	DA	2992	1/1	0.85	0.38	75,75,75,75	0
60	MG	BA	3029	1/1	0.85	0.33	139,139,139,139	0
60	MG	CA	1628	1/1	0.86	0.42	66,66,66,66	0
60	MG	BA	3075	1/1	0.86	0.19	100,100,100,100	0
60	MG	AA	1621	1/1	0.86	0.38	95,95,95,95	0
60	MG	CA	1610	1/1	0.86	0.20	116,116,116,116	0
60	MG	CA	1682	1/1	0.86	0.16	151,151,151,151	0
60	MG	BA	3132	1/1	0.86	0.48	116,116,116,116	0
60	MG	BA	2953	1/1	0.86	1.12	113,113,113,113	0
60	MG	AA	1663	1/1	0.86	0.77	83,83,83,83	0
60	MG	DA	2979	1/1	0.86	0.32	57,57,57,57	0
60	MG	AA	1678	1/1	0.86	0.54	121,121,121,121	0
60	MG	BA	2937	1/1	0.86	0.75	70,70,70,70	0
60	MG	DA	2984	1/1	0.86	0.60	120,120,120,120	0
60	MG	BA	3072	1/1	0.86	0.85	89,89,89,89	0
60	MG	DA	3015	1/1	0.87	0.47	76,76,76,76	0
60	MG	BA	3104	1/1	0.87	0.24	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3127	1/1	0.87	1.24	112,112,112,112	0
60	MG	BA	2919	1/1	0.87	0.50	75,75,75,75	0
60	MG	BA	3130	1/1	0.87	0.30	111,111,111,111	0
60	MG	AA	1664	1/1	0.87	0.26	90,90,90,90	0
60	MG	DA	3011	1/1	0.87	0.38	88,88,88,88	0
60	MG	AA	1648	1/1	0.87	0.72	92,92,92,92	0
60	MG	BA	2938	1/1	0.87	0.30	67,67,67,67	0
60	MG	DA	3078	1/1	0.87	0.71	122,122,122,122	0
60	MG	CA	1642	1/1	0.87	1.27	97,97,97,97	0
60	MG	BA	2932	1/1	0.87	0.36	61,61,61,61	0
60	MG	BA	3014	1/1	0.87	0.39	74,74,74,74	0
60	MG	BA	3068	1/1	0.87	1.41	103,103,103,103	0
60	MG	DA	3021	1/1	0.87	0.28	81,81,81,81	0
60	MG	BA	2994	1/1	0.87	0.27	77,77,77,77	0
60	MG	DA	3069	1/1	0.87	0.58	73,73,73,73	0
60	MG	BA	3087	1/1	0.88	0.97	112,112,112,112	0
60	MG	DA	3016	1/1	0.88	0.16	83,83,83,83	0
60	MG	AA	1657	1/1	0.88	0.34	121,121,121,121	0
60	MG	BA	2987	1/1	0.88	0.72	100,100,100,100	0
60	MG	AA	1631	1/1	0.88	0.69	87,87,87,87	0
60	MG	DA	2997	1/1	0.88	0.18	79,79,79,79	0
60	MG	DA	3025	1/1	0.88	0.56	51,51,51,51	0
60	MG	BA	3013	1/1	0.88	0.30	72,72,72,72	0
60	MG	BA	3031	1/1	0.88	0.85	108,108,108,108	0
60	MG	DA	3134	1/1	0.88	0.73	89,89,89,89	0
60	MG	BA	3023	1/1	0.88	1.15	79,79,79,79	0
60	MG	AA	1632	1/1	0.88	0.77	75,75,75,75	0
60	MG	DA	3093	1/1	0.88	0.48	86,86,86,86	0
60	MG	AA	1615	1/1	0.88	0.95	84,84,84,84	0
60	MG	BA	3122	1/1	0.88	0.74	84,84,84,84	0
60	MG	DA	3033	1/1	0.88	0.19	100,100,100,100	0
60	MG	BA	3103	1/1	0.88	1.04	107,107,107,107	0
60	MG	CA	1684	1/1	0.88	0.38	101,101,101,101	0
60	MG	BA	3079	1/1	0.88	0.88	72,72,72,72	0
60	MG	CA	1646	1/1	0.88	0.55	119,119,119,119	0
60	MG	DA	3131	1/1	0.89	0.80	102,102,102,102	0
60	MG	CA	1681	1/1	0.89	0.25	113,113,113,113	1
60	MG	DA	2978	1/1	0.89	0.53	85,85,85,85	0
60	MG	BA	3021	1/1	0.89	0.14	79,79,79,79	0
60	MG	BA	3009	1/1	0.89	0.98	117,117,117,117	0
60	MG	DA	3059	1/1	0.89	1.06	110,110,110,110	0
60	MG	DA	3112	1/1	0.89	0.81	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BB	202	1/1	0.89	0.90	117,117,117,117	0
60	MG	BA	2939	1/1	0.89	0.47	50,50,50,50	0
60	MG	AA	1629	1/1	0.89	0.52	65,65,65,65	1
60	MG	CV	101	1/1	0.89	0.40	67,67,67,67	0
60	MG	AA	1647	1/1	0.89	0.39	104,104,104,104	0
60	MG	DA	3020	1/1	0.89	0.23	50,50,50,50	0
60	MG	AA	1628	1/1	0.89	0.48	87,87,87,87	0
60	MG	DA	2985	1/1	0.89	0.26	85,85,85,85	0
60	MG	BA	2990	1/1	0.90	0.36	81,81,81,81	0
60	MG	DA	3049	1/1	0.90	0.50	85,85,85,85	0
60	MG	CA	1645	1/1	0.90	0.21	68,68,68,68	0
60	MG	AA	1703	1/1	0.90	1.31	102,102,102,102	0
60	MG	DA	2993	1/1	0.90	0.31	79,79,79,79	0
60	MG	BA	3116	1/1	0.90	0.27	91,91,91,91	0
60	MG	BA	2909	1/1	0.90	0.50	64,64,64,64	0
60	MG	BA	2945	1/1	0.90	0.93	73,73,73,73	0
60	MG	BA	2998	1/1	0.90	0.62	88,88,88,88	0
60	MG	BA	3091	1/1	0.90	0.46	79,79,79,79	0
60	MG	BA	2931	1/1	0.90	0.41	72,72,72,72	0
60	MG	BA	3092	1/1	0.90	0.57	82,82,82,82	0
60	MG	DA	3074	1/1	0.90	0.71	96,96,96,96	0
60	MG	DA	2908	1/1	0.90	0.93	83,83,83,83	0
60	MG	AA	1611	1/1	0.90	0.22	82,82,82,82	0
60	MG	AA	1701	1/1	0.90	0.65	71,71,71,71	0
60	MG	DA	2994	1/1	0.90	0.60	52,52,52,52	0
60	MG	BA	3131	1/1	0.90	0.59	79,79,79,79	0
60	MG	DA	3116	1/1	0.90	0.86	104,104,104,104	0
60	MG	DA	2995	1/1	0.91	0.74	75,75,75,75	0
60	MG	BA	3052	1/1	0.91	0.23	99,99,99,99	0
60	MG	AA	1685	1/1	0.91	0.30	66,66,66,66	0
60	MG	DA	3095	1/1	0.91	0.33	98,98,98,98	0
60	MG	DA	3130	1/1	0.91	1.38	115,115,115,115	0
60	MG	BA	2904	1/1	0.91	0.76	56,56,56,56	0
60	MG	BA	3136	1/1	0.91	0.64	106,106,106,106	0
60	MG	BA	2999	1/1	0.91	0.77	121,121,121,121	0
60	MG	AA	1673	1/1	0.91	0.09	79,79,79,79	0
60	MG	BA	2968	1/1	0.91	1.08	72,72,72,72	0
60	MG	BA	3059	1/1	0.91	0.47	95,95,95,95	0
60	MG	BA	2940	1/1	0.91	0.53	64,64,64,64	0
60	MG	BA	2916	1/1	0.91	0.30	71,71,71,71	0
60	MG	BA	2948	1/1	0.91	0.35	67,67,67,67	0
60	MG	BA	2927	1/1	0.91	0.67	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3111	1/1	0.91	0.93	103,103,103,103	0
60	MG	CA	1625	1/1	0.91	0.59	96,96,96,96	0
60	MG	DA	3138	1/1	0.91	0.42	113,113,113,113	0
60	MG	DA	2916	1/1	0.91	0.81	53,53,53,53	0
60	MG	DA	2970	1/1	0.91	0.13	47,47,47,47	0
60	MG	BA	2961	1/1	0.91	0.73	78,78,78,78	0
60	MG	BA	3028	1/1	0.91	0.46	89,89,89,89	0
60	MG	BA	3110	1/1	0.91	1.16	101,101,101,101	0
60	MG	DA	2915	1/1	0.91	0.41	64,64,64,64	0
60	MG	CA	1638	1/1	0.92	0.37	81,81,81,81	0
60	MG	DA	3054	1/1	0.92	0.79	80,80,80,80	0
60	MG	DA	2958	1/1	0.92	0.23	96,96,96,96	0
60	MG	AA	1659	1/1	0.92	1.13	113,113,113,113	0
60	MG	AA	1696	1/1	0.92	0.82	90,90,90,90	0
60	MG	AA	1668	1/1	0.92	0.61	109,109,109,109	0
60	MG	BA	2991	1/1	0.92	0.47	122,122,122,122	0
60	MG	CA	1676	1/1	0.92	0.32	119,119,119,119	0
60	MG	DA	3076	1/1	0.92	0.29	119,119,119,119	0
60	MG	DA	2913	1/1	0.92	0.49	70,70,70,70	0
60	MG	BA	3054	1/1	0.92	0.41	94,94,94,94	0
60	MG	DA	2924	1/1	0.92	0.23	87,87,87,87	0
60	MG	BA	2967	1/1	0.92	0.67	57,57,57,57	0
60	MG	AA	1619	1/1	0.92	0.17	72,72,72,72	0
60	MG	CA	1602	1/1	0.92	0.14	92,92,92,92	0
60	MG	BA	3044	1/1	0.92	0.77	108,108,108,108	0
60	MG	CA	1661	1/1	0.92	0.41	81,81,81,81	0
60	MG	DA	2922	1/1	0.92	0.41	59,59,59,59	0
61	ZN	CN	101	1/1	0.92	0.04	153,153,153,153	0
60	MG	DA	3133	1/1	0.92	0.73	87,87,87,87	0
60	MG	CA	1617	1/1	0.92	0.14	93,93,93,93	0
60	MG	AA	1607	1/1	0.92	0.16	107,107,107,107	0
60	MG	DA	2948	1/1	0.92	0.63	60,60,60,60	0
60	MG	BA	3077	1/1	0.92	0.36	84,84,84,84	0
60	MG	AA	1690	1/1	0.92	0.82	96,96,96,96	0
60	MG	CA	1648	1/1	0.92	0.14	71,71,71,71	0
60	MG	BA	2946	1/1	0.92	0.29	66,66,66,66	0
60	MG	DA	2983	1/1	0.92	0.32	93,93,93,93	0
60	MG	DA	2987	1/1	0.93	0.18	86,86,86,86	0
60	MG	AA	1683	1/1	0.93	0.43	89,89,89,89	0
60	MG	BA	3065	1/1	0.93	1.01	122,122,122,122	0
60	MG	BA	2954	1/1	0.93	0.34	66,66,66,66	0
60	MG	DA	3032	1/1	0.93	0.55	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	2933	1/1	0.93	0.66	77,77,77,77	0
60	MG	BA	3095	1/1	0.93	0.21	97,97,97,97	0
60	MG	AA	1655	1/1	0.93	0.36	94,94,94,94	1
60	MG	CA	1605	1/1	0.93	0.20	104,104,104,104	0
60	MG	BA	3074	1/1	0.93	0.20	104,104,104,104	0
60	MG	DA	2932	1/1	0.93	0.60	64,64,64,64	0
60	MG	DA	2905	1/1	0.93	0.45	59,59,59,59	0
60	MG	DA	2914	1/1	0.93	0.42	49,49,49,49	0
60	MG	DA	2947	1/1	0.93	0.18	51,51,51,51	0
60	MG	AA	1700	1/1	0.93	1.33	111,111,111,111	0
60	MG	BA	2903	1/1	0.93	0.79	97,97,97,97	0
60	MG	DA	3092	1/1	0.93	0.47	86,86,86,86	0
60	MG	BA	2989	1/1	0.93	0.68	87,87,87,87	0
60	MG	DA	2945	1/1	0.93	0.22	57,57,57,57	0
60	MG	BA	2951	1/1	0.93	0.22	63,63,63,63	0
60	MG	BA	3056	1/1	0.93	0.28	55,55,55,55	0
60	MG	DA	3030	1/1	0.93	0.31	101,101,101,101	0
60	MG	BP	201	1/1	0.93	0.21	71,71,71,71	0
60	MG	CL	201	1/1	0.93	0.51	87,87,87,87	1
60	MG	DA	2989	1/1	0.93	0.59	79,79,79,79	0
60	MG	DA	3073	1/1	0.93	0.56	87,87,87,87	0
60	MG	BA	3039	1/1	0.93	0.50	67,67,67,67	0
60	MG	BA	3061	1/1	0.93	0.62	71,71,71,71	0
60	MG	BA	2964	1/1	0.93	0.42	80,80,80,80	0
60	MG	BA	2918	1/1	0.93	0.87	64,64,64,64	0
60	MG	DA	2936	1/1	0.93	0.24	59,59,59,59	0
60	MG	DA	3119	1/1	0.93	0.90	75,75,75,75	0
60	MG	DA	3065	1/1	0.93	0.90	75,75,75,75	0
60	MG	AA	1692	1/1	0.93	1.16	101,101,101,101	0
60	MG	BA	2906	1/1	0.93	0.40	100,100,100,100	0
60	MG	BA	2957	1/1	0.93	0.38	63,63,63,63	0
60	MG	DA	2904	1/1	0.93	0.82	49,49,49,49	0
60	MG	BA	2978	1/1	0.93	0.81	134,134,134,134	0
60	MG	AA	1698	1/1	0.93	1.43	80,80,80,80	0
60	MG	AA	1687	1/1	0.93	0.20	74,74,74,74	0
60	MG	CA	1695	1/1	0.93	0.74	80,80,80,80	0
60	MG	DA	3060	1/1	0.94	0.48	107,107,107,107	0
61	ZN	AN	101	1/1	0.94	0.04	153,153,153,153	0
60	MG	DA	3062	1/1	0.94	0.38	49,49,49,49	0
60	MG	AA	1697	1/1	0.94	1.11	127,127,127,127	0
60	MG	AA	1684	1/1	0.94	0.85	103,103,103,103	0
60	MG	BA	3005	1/1	0.94	0.70	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3107	1/1	0.94	0.68	59,59,59,59	0
60	MG	BA	2962	1/1	0.94	0.76	64,64,64,64	0
60	MG	DA	3087	1/1	0.94	0.69	68,68,68,68	0
60	MG	BA	3119	1/1	0.94	0.98	99,99,99,99	0
60	MG	D1	101	1/1	0.94	0.92	92,92,92,92	0
60	MG	BA	3135	1/1	0.94	0.47	83,83,83,83	0
60	MG	BA	2956	1/1	0.94	0.61	64,64,64,64	0
60	MG	DA	3038	1/1	0.94	0.62	77,77,77,77	0
60	MG	BA	2944	1/1	0.94	0.40	58,58,58,58	0
60	MG	CA	1657	1/1	0.94	0.28	56,56,56,56	1
60	MG	AA	1666	1/1	0.94	0.27	84,84,84,84	0
60	MG	BA	2929	1/1	0.94	0.71	65,65,65,65	0
60	MG	BA	3117	1/1	0.94	0.49	72,72,72,72	0
60	MG	CA	1630	1/1	0.94	0.18	105,105,105,105	0
60	MG	CA	1673	1/1	0.94	0.48	116,116,116,116	0
60	MG	BA	3070	1/1	0.94	0.86	118,118,118,118	0
60	MG	BA	2980	1/1	0.94	0.61	82,82,82,82	0
60	MG	DA	2931	1/1	0.94	0.44	52,52,52,52	0
60	MG	DA	2950	1/1	0.94	0.36	55,55,55,55	0
60	MG	DA	3028	1/1	0.94	0.57	123,123,123,123	0
60	MG	BA	2913	1/1	0.94	0.53	59,59,59,59	0
60	MG	DA	3050	1/1	0.94	1.43	105,105,105,105	0
60	MG	BA	3069	1/1	0.94	0.18	87,87,87,87	0
60	MG	BA	3027	1/1	0.94	0.56	51,51,51,51	0
61	ZN	CD	301	1/1	0.94	0.10	106,106,106,106	0
60	MG	DA	3110	1/1	0.94	0.74	63,63,63,63	0
60	MG	AX	101	1/1	0.94	0.74	96,96,96,96	0
60	MG	DA	3126	1/1	0.94	0.79	76,76,76,76	0
60	MG	AA	1610	1/1	0.94	0.31	84,84,84,84	0
60	MG	CA	1635	1/1	0.94	0.12	98,98,98,98	0
60	MG	AA	1626	1/1	0.94	0.16	99,99,99,99	0
60	MG	CA	1620	1/1	0.94	1.10	115,115,115,115	0
60	MG	DA	2943	1/1	0.94	0.24	59,59,59,59	0
60	MG	CA	1683	1/1	0.94	0.13	93,93,93,93	0
60	MG	DA	2919	1/1	0.94	0.85	73,73,73,73	0
60	MG	CA	1651	1/1	0.94	0.10	144,144,144,144	0
60	MG	BA	2974	1/1	0.94	0.95	68,68,68,68	0
60	MG	DA	3113	1/1	0.94	0.49	96,96,96,96	0
60	MG	DA	3026	1/1	0.95	0.35	78,78,78,78	0
60	MG	DA	3036	1/1	0.95	0.50	59,59,59,59	0
60	MG	BA	2959	1/1	0.95	0.48	59,59,59,59	0
60	MG	BA	2936	1/1	0.95	0.76	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1693	1/1	0.95	0.55	65,65,65,65	0
60	MG	BA	2941	1/1	0.95	0.58	49,49,49,49	0
60	MG	BA	2943	1/1	0.95	0.80	56,56,56,56	0
60	MG	DA	2971	1/1	0.95	0.64	66,66,66,66	0
60	MG	BA	3134	1/1	0.95	0.73	75,75,75,75	0
60	MG	BA	3067	1/1	0.95	0.21	93,93,93,93	0
60	MG	DA	3120	1/1	0.95	0.49	71,71,71,71	0
60	MG	DA	2902	1/1	0.95	0.15	152,152,152,152	0
60	MG	BA	3050	1/1	0.95	0.83	116,116,116,116	0
60	MG	BA	2986	1/1	0.95	0.63	81,81,81,81	0
60	MG	DA	2938	1/1	0.95	0.34	45,45,45,45	0
60	MG	CA	1621	1/1	0.95	0.13	96,96,96,96	0
60	MG	DA	2941	1/1	0.95	0.24	45,45,45,45	0
60	MG	DA	2955	1/1	0.95	0.26	54,54,54,54	0
60	MG	BA	3041	1/1	0.95	0.52	71,71,71,71	0
60	MG	BA	2972	1/1	0.95	0.75	76,76,76,76	0
60	MG	DA	3040	1/1	0.95	0.41	64,64,64,64	0
60	MG	CA	1614	1/1	0.95	0.29	87,87,87,87	0
60	MG	BA	3036	1/1	0.95	0.30	97,97,97,97	0
60	MG	DA	3108	1/1	0.95	0.53	61,61,61,61	0
60	MG	BA	3000	1/1	0.95	0.46	52,52,52,52	1
60	MG	B5	101	1/1	0.95	0.42	76,76,76,76	0
60	MG	CA	1674	1/1	0.95	0.28	137,137,137,137	0
60	MG	BA	3057	1/1	0.95	0.52	73,73,73,73	0
60	MG	CA	1679	1/1	0.95	0.55	79,79,79,79	0
60	MG	DA	2907	1/1	0.95	0.66	51,51,51,51	0
60	MG	AA	1682	1/1	0.96	0.39	98,98,98,98	0
60	MG	AA	1653	1/1	0.96	0.40	94,94,94,94	0
60	MG	DA	2921	1/1	0.96	0.46	49,49,49,49	0
60	MG	AA	1605	1/1	0.96	0.33	66,66,66,66	0
60	MG	BA	3033	1/1	0.96	0.41	92,92,92,92	0
60	MG	DA	2909	1/1	0.96	0.68	55,55,55,55	0
60	MG	DA	2946	1/1	0.96	0.32	57,57,57,57	0
60	MG	DA	3140	1/1	0.96	0.69	77,77,77,77	0
60	MG	DA	2928	1/1	0.96	0.41	42,42,42,42	0
60	MG	DA	2974	1/1	0.96	0.70	92,92,92,92	0
60	MG	CA	1701	1/1	0.96	0.53	58,58,58,58	0
60	MG	BA	2979	1/1	0.96	0.22	103,103,103,103	0
60	MG	BA	3099	1/1	0.96	0.25	117,117,117,117	0
60	MG	BA	2925	1/1	0.96	0.32	97,97,97,97	0
60	MG	BA	2914	1/1	0.96	0.39	83,83,83,83	0
60	MG	AL	201	1/1	0.96	0.40	125,125,125,125	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3004	1/1	0.96	0.31	63,63,63,63	0
60	MG	BA	2923	1/1	0.96	0.50	78,78,78,78	0
60	MG	BA	3133	1/1	0.96	1.11	73,73,73,73	0
60	MG	AA	1676	1/1	0.96	0.25	104,104,104,104	0
60	MG	DA	2926	1/1	0.96	0.74	47,47,47,47	0
60	MG	AA	1702	1/1	0.96	0.76	74,74,74,74	0
60	MG	B1	102	1/1	0.96	0.71	83,83,83,83	0
60	MG	BA	3034	1/1	0.96	0.15	82,82,82,82	0
60	MG	DA	2918	1/1	0.96	0.66	59,59,59,59	0
60	MG	DA	2930	1/1	0.96	0.47	55,55,55,55	0
60	MG	DA	3006	1/1	0.96	0.52	65,65,65,65	0
60	MG	BA	3127	1/1	0.96	0.42	84,84,84,84	0
60	MG	BA	2907	1/1	0.96	0.56	55,55,55,55	0
60	MG	DA	2923	1/1	0.96	0.29	52,52,52,52	0
60	MG	DA	3129	1/1	0.96	0.28	113,113,113,113	0
60	MG	BA	2981	1/1	0.96	0.15	88,88,88,88	0
60	MG	DA	2954	1/1	0.96	0.25	57,57,57,57	0
60	MG	CA	1649	1/1	0.96	0.12	82,82,82,82	0
60	MG	AA	1654	1/1	0.96	0.50	139,139,139,139	0
60	MG	BA	3010	1/1	0.96	0.42	88,88,88,88	0
60	MG	AA	1694	1/1	0.96	0.54	102,102,102,102	0
60	MG	AA	1658	1/1	0.96	0.65	92,92,92,92	0
60	MG	DA	3123	1/1	0.96	0.62	82,82,82,82	0
60	MG	DA	2982	1/1	0.97	0.80	75,75,75,75	0
60	MG	DA	2925	1/1	0.97	0.42	58,58,58,58	0
60	MG	DA	2988	1/1	0.97	0.22	111,111,111,111	0
60	MG	DA	3139	1/1	0.97	0.87	69,69,69,69	0
60	MG	DA	2911	1/1	0.97	0.57	62,62,62,62	0
60	MG	DA	2906	1/1	0.97	0.33	67,67,67,67	0
60	MG	BA	2926	1/1	0.97	0.40	58,58,58,58	0
60	MG	DA	2967	1/1	0.97	0.66	51,51,51,51	0
60	MG	AA	1602	1/1	0.97	0.59	131,131,131,131	0
60	MG	DA	3064	1/1	0.97	0.24	66,66,66,66	0
60	MG	DA	2973	1/1	0.97	0.63	51,51,51,51	0
60	MG	DA	2959	1/1	0.97	0.62	61,61,61,61	0
60	MG	BA	3071	1/1	0.97	0.44	61,61,61,61	0
60	MG	AA	1679	1/1	0.97	0.61	100,100,100,100	0
60	MG	BA	2912	1/1	0.97	0.78	71,71,71,71	0
60	MG	AA	1680	1/1	0.97	0.30	75,75,75,75	0
60	MG	DA	3052	1/1	0.97	0.27	57,57,57,57	0
60	MG	AA	1616	1/1	0.97	0.40	84,84,84,84	0
60	MG	DA	2937	1/1	0.97	0.34	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3005	1/1	0.97	0.58	53,53,53,53	0
60	MG	BA	2917	1/1	0.97	0.85	58,58,58,58	0
60	MG	BA	2922	1/1	0.97	0.49	53,53,53,53	0
60	MG	AA	1669	1/1	0.97	0.28	96,96,96,96	0
60	MG	DA	2977	1/1	0.97	0.15	104,104,104,104	0
60	MG	DA	2927	1/1	0.98	0.79	52,52,52,52	0
60	MG	BA	2911	1/1	0.98	0.75	74,74,74,74	0
60	MG	DA	2933	1/1	0.98	0.50	53,53,53,53	0
60	MG	DA	3066	1/1	0.98	0.52	102,102,102,102	0
60	MG	DA	3067	1/1	0.98	0.50	52,52,52,52	0
60	MG	BA	3048	1/1	0.98	0.27	87,87,87,87	0
60	MG	CA	1619	1/1	0.98	0.10	67,67,67,67	0
60	MG	DA	2920	1/1	0.98	0.17	75,75,75,75	0
60	MG	BA	2958	1/1	0.98	0.18	76,76,76,76	0
60	MG	DA	2939	1/1	0.98	0.51	41,41,41,41	0
60	MG	DA	2917	1/1	0.98	0.86	58,58,58,58	0
60	MG	BA	2924	1/1	0.98	0.27	52,52,52,52	0
60	MG	DA	3079	1/1	0.98	0.15	131,131,131,131	0
60	MG	DA	2966	1/1	0.98	0.69	48,48,48,48	0
60	MG	DA	2912	1/1	0.98	0.52	45,45,45,45	0
60	MG	DA	3051	1/1	0.98	0.29	56,56,56,56	0
60	MG	DA	3084	1/1	0.98	0.21	103,103,103,103	0
60	MG	DA	3109	1/1	0.98	0.66	45,45,45,45	0
61	ZN	AD	301	1/1	0.98	0.17	106,106,106,106	0
60	MG	DA	2957	1/1	0.98	0.55	66,66,66,66	0
60	MG	BA	2947	1/1	0.98	0.65	88,88,88,88	0
60	MG	DA	3111	1/1	0.98	1.00	62,62,62,62	0
60	MG	DA	2952	1/1	0.98	0.47	56,56,56,56	0
60	MG	BA	3003	1/1	0.98	0.66	68,68,68,68	0
60	MG	AA	1644	1/1	0.98	0.09	141,141,141,141	0
60	MG	DA	3012	1/1	0.98	0.30	53,53,53,53	0
60	MG	BA	2915	1/1	0.98	0.35	51,51,51,51	0
60	MG	DA	2934	1/1	0.98	0.40	86,86,86,86	0
60	MG	CA	1656	1/1	0.98	0.60	90,90,90,90	0
60	MG	BA	2928	1/1	0.99	0.99	63,63,63,63	0
60	MG	BA	3112	1/1	0.99	0.64	47,47,47,47	0
60	MG	DA	2910	1/1	0.99	0.34	57,57,57,57	0
60	MG	BA	2934	1/1	0.99	0.47	55,55,55,55	0
60	MG	BA	2910	1/1	0.99	0.25	75,75,75,75	0
60	MG	DA	2944	1/1	0.99	0.41	74,74,74,74	0
60	MG	BA	2935	1/1	0.99	0.50	110,110,110,110	0
60	MG	DA	2976	1/1	0.99	0.68	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1630	1/1	0.99	0.10	109,109,109,109	1
60	MG	DA	2968	1/1	0.99	0.48	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.