



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:09 pm BST

PDB ID : 5J88
Title : Structure of the E coli 70S ribosome with the U1060A mutation in 16S rRNA
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.32 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

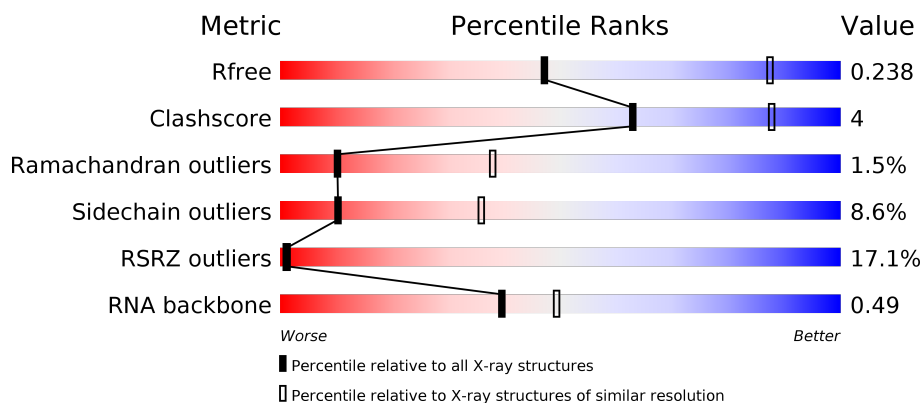
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)
RNA backbone	3102	1125 (3.74-2.90)

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	1534	<div> <div>7%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	BA	1534	<div> <div>17%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
2	AB	224	<div> <div>25%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	BB	224	<div> <div>20%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	129	
11	BK	129	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	


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Mol	Chain	Length	Quality of chain
42	CO	127	
42	DO	127	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	100	
48	DU	100	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	76	
51	DX	76	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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
1	2MG	BA	966	-	-	-	X
1	5MC	BA	967	-	-	-	X
56	MG	AA	1603	-	-	-	X
56	MG	AA	1604	-	-	-	X
56	MG	AA	1605	-	-	-	X
56	MG	AA	1615	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	AA	1621	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1623	-	-	-	X
56	MG	AA	1625	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1627	-	-	-	X
56	MG	AA	1660	-	-	-	X
56	MG	AA	1665	-	-	-	X
56	MG	BA	1623	-	-	-	X
56	MG	BA	1624	-	-	-	X
56	MG	BA	1625	-	-	-	X
56	MG	BA	1626	-	-	-	X
56	MG	BA	1637	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3075	-	-	-	X
56	MG	CA	3077	-	-	-	X
56	MG	CA	3104	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3116	-	-	-	X
56	MG	CA	3123	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	CA	3145	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3154	-	-	-	X
56	MG	DA	3130	-	-	-	X
56	MG	DA	3156	-	-	-	X
56	MG	DA	3163	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3182	-	-	-	X
58	MPD	DE	301	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	AA	1675	-	-	-	X
59	PUT	DA	3195	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DP	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	DA	3002	-	-	-	X
62	EDO	DA	3198	-	-	-	X
66	ACY	DA	3202	-	-	X	-
68	TRS	DA	3220	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295119 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32932	14695	6044	10659	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32910	14685	6039	10653	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1060	A	U	conflict	GB 675819282
BA	1060	A	U	conflict	GB 675819282

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- 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	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- 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
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- 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	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
33	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
35	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
36	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
38	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
39	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
40	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
41	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
42	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
43	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
44	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CR	117	Total	C	N	O		0	0	0
			947	604	192	151				
45	DR	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
46	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
50	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
51	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
52	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
53	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 54 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 55 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

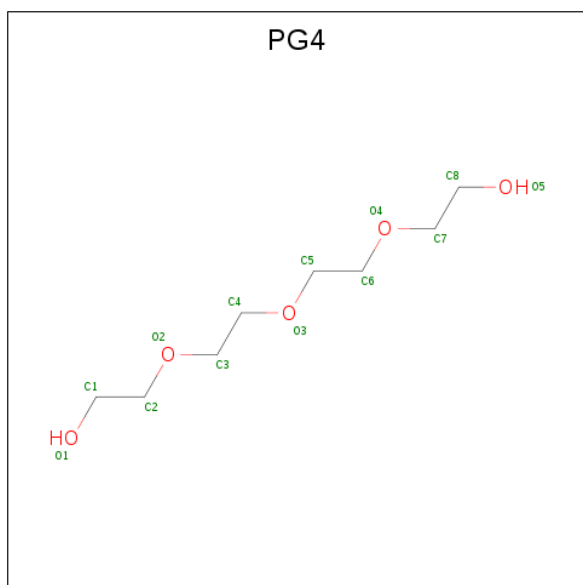
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	41	Total	Mg	0	0
			41	41		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		
56	AA	70	Total	Mg	0	0
			70	70		
56	DA	184	Total	Mg	0	0
			184	184		

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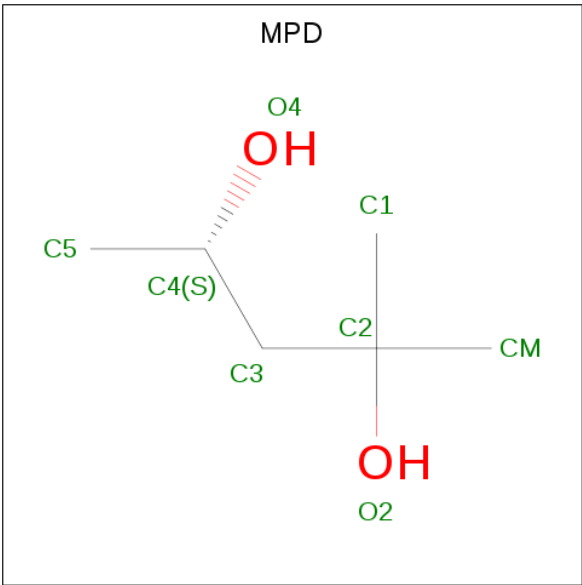
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	1	Total	Mg	0	0
			1	1		

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



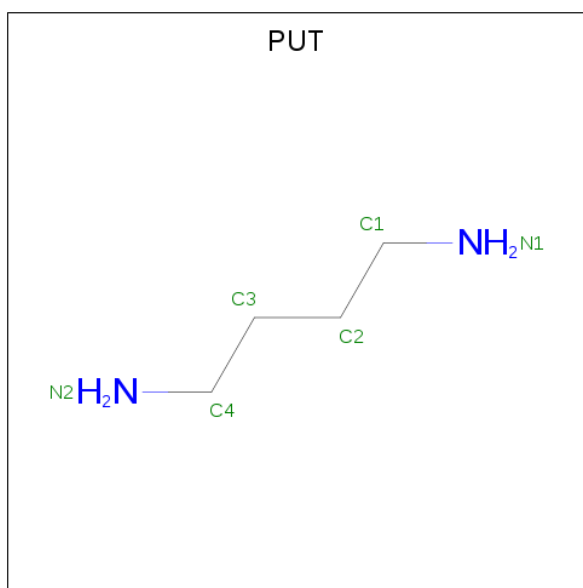
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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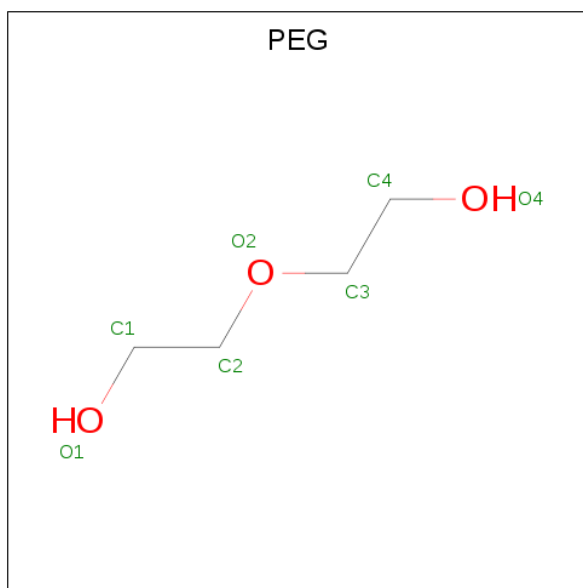
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C5	1	Total	Zn	0	0
			1	1		
60	AB	1	Total	Zn	0	0
			1	1		
60	D5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



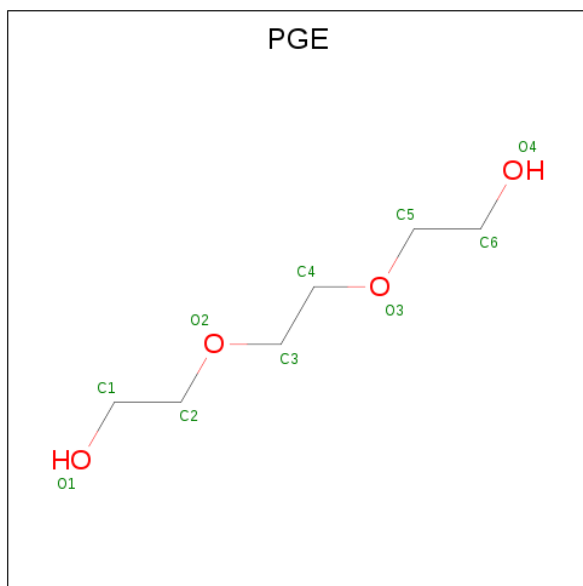
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	D0	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



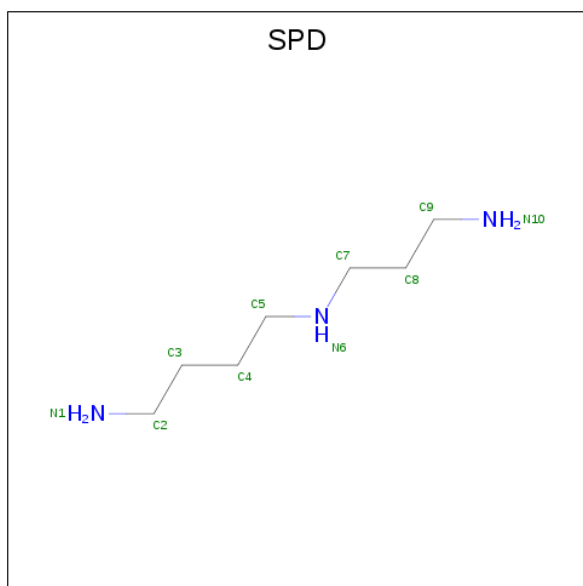
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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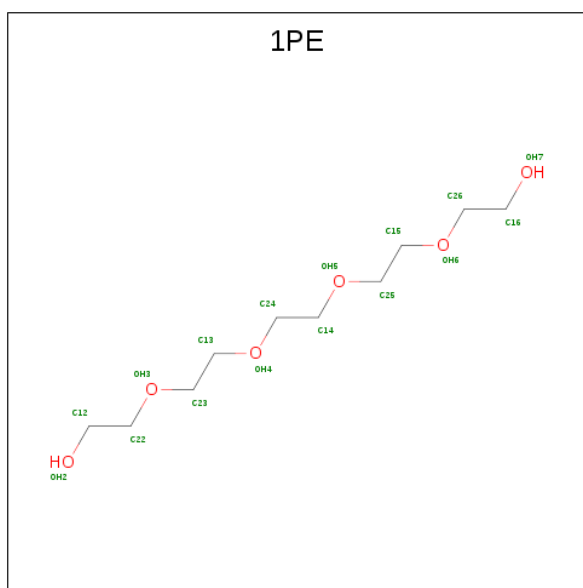
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



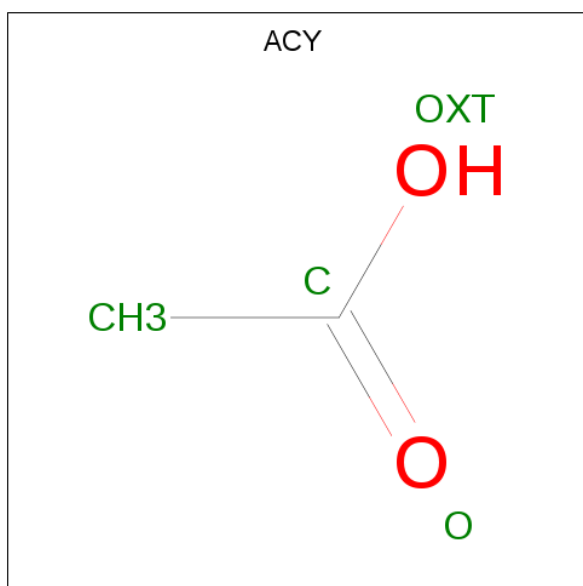
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



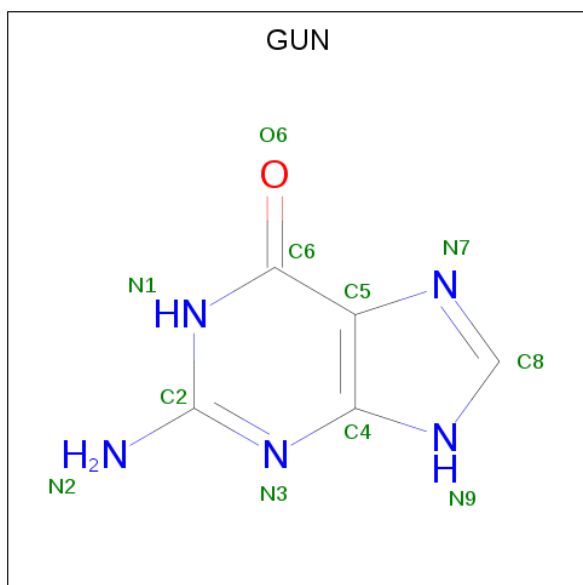
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
67	DA	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	2	Total	O	0	0
			2	2		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	3	Total	O	0	0
			3	3		
69	AK	5	Total	O	0	0
			5	5		
69	AL	7	Total	O	0	0
			7	7		
69	AM	4	Total	O	0	0
			4	4		
69	AN	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	1	Total 1	O 1	0	0
69	AP	1	Total 1	O 1	0	0
69	AQ	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	4	Total 4	O 4	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	3	Total 3	O 3	0	0
69	BL	3	Total 3	O 3	0	0
69	BN	1	Total 1	O 1	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	4	Total 4	O 4	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	5	Total 5	O 5	0	0
69	D1	37	Total 37	O 37	0	0
69	D2	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	30	Total 30	O 30	0	0
69	D4	40	Total 40	O 40	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	11	Total 11	O 11	0	0
69	CD	4	Total 4	O 4	0	0
69	CA	696	Total 696	O 696	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	97	Total 97	O 97	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	54	Total 54	O 54	0	0
69	DF	13	Total 13	O 13	0	0
69	DG	9	Total 9	O 9	0	0

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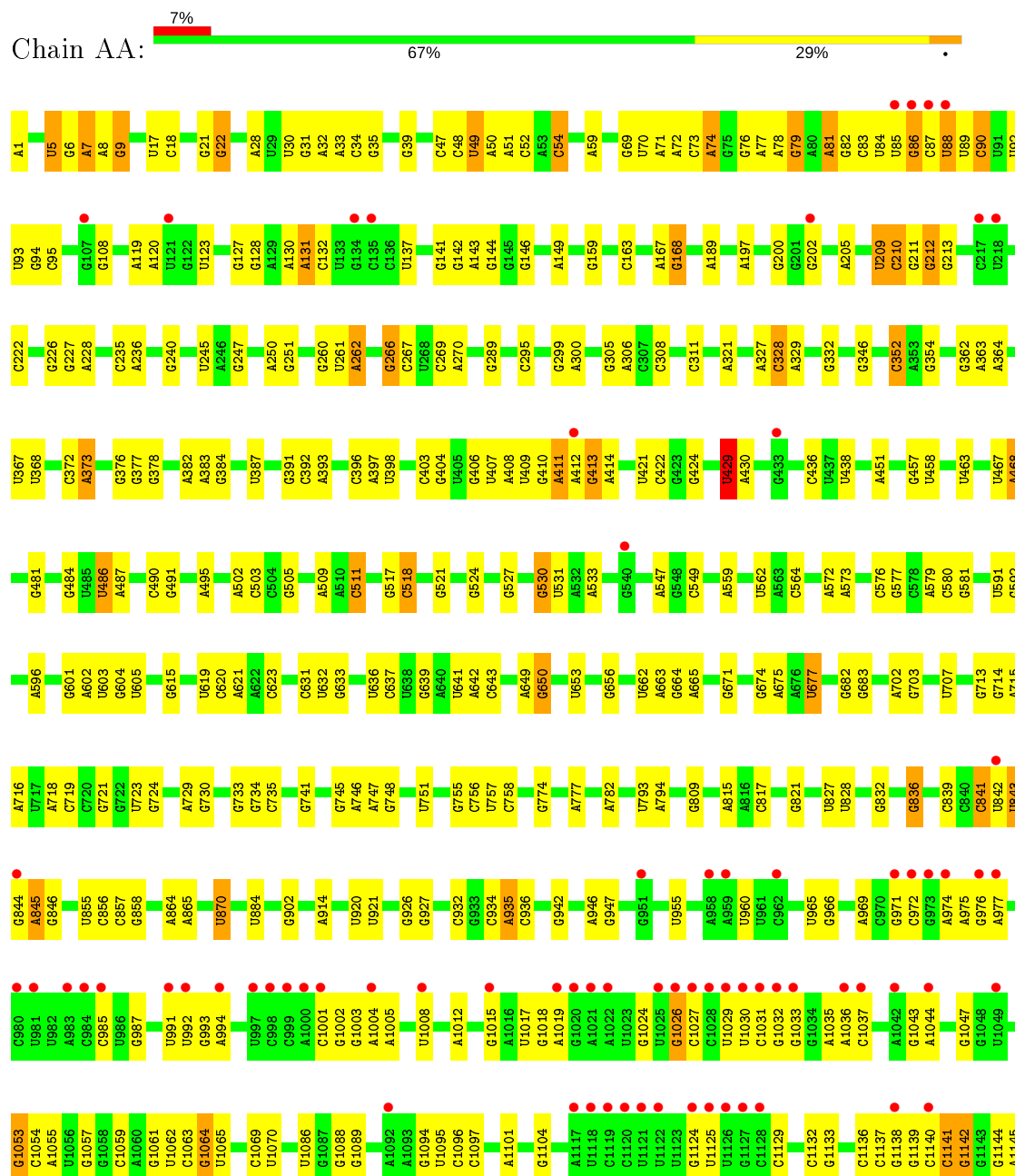
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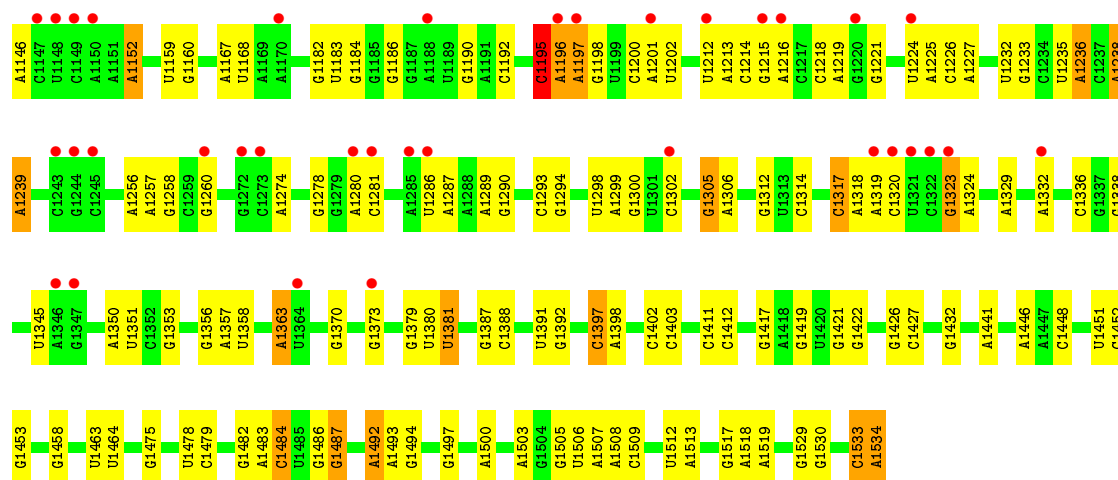
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DH	2	Total 2	O 2	0	0
69	DK	61	Total 61	O 61	0	0
69	DL	50	Total 50	O 50	0	0
69	DM	60	Total 60	O 60	0	0
69	DN	81	Total 81	O 81	0	0
69	DO	42	Total 42	O 42	0	0
69	DP	42	Total 42	O 42	0	0
69	DQ	32	Total 32	O 32	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	52	Total 52	O 52	0	0
69	DT	65	Total 65	O 65	0	0
69	DU	24	Total 24	O 24	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	33	Total 33	O 33	0	0
69	DX	33	Total 33	O 33	0	0
69	DY	11	Total 11	O 11	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	203	Total 203	O 203	0	0
69	DA	4824	Total 4824	O 4824	0	0

3 Residue-property plots [i](#)

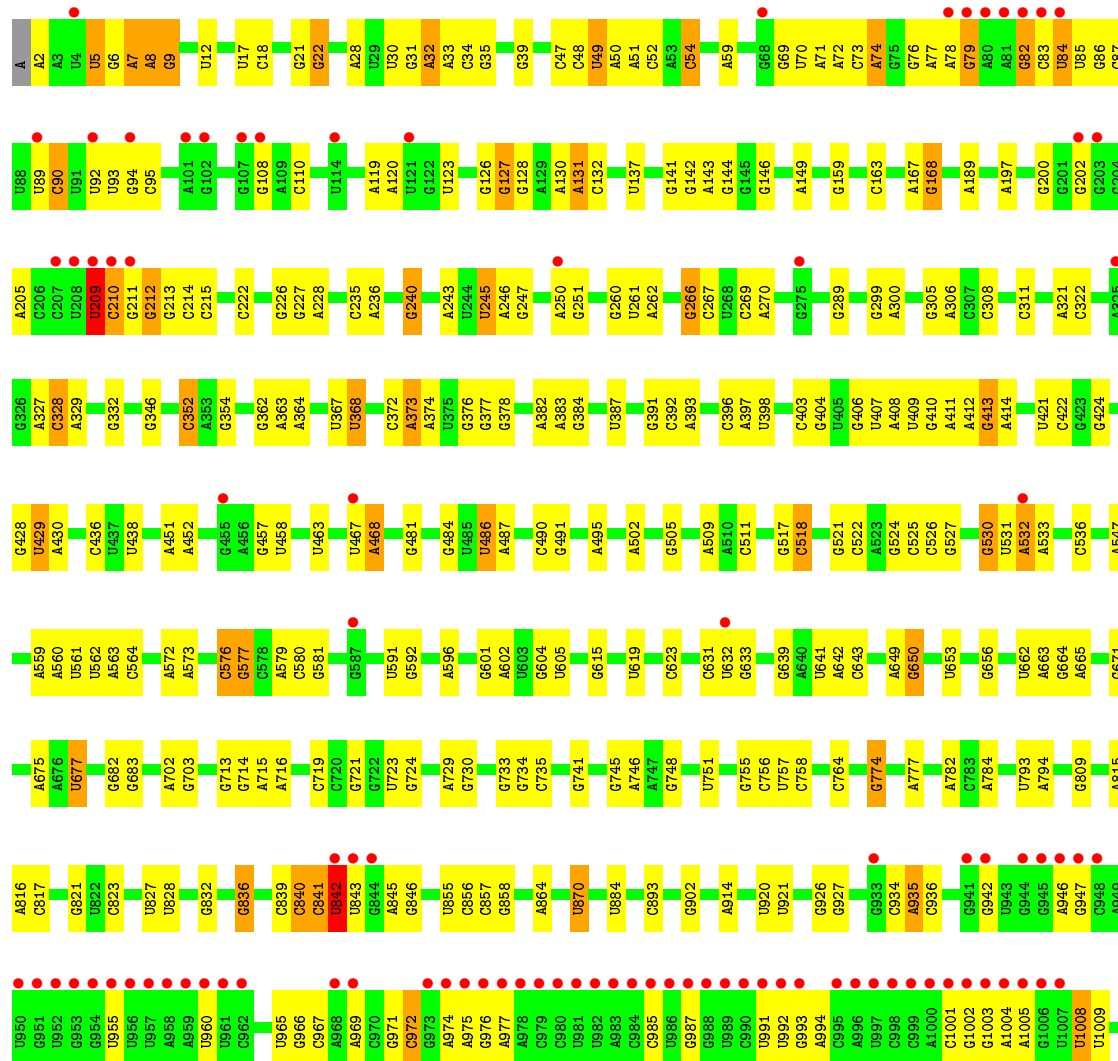
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

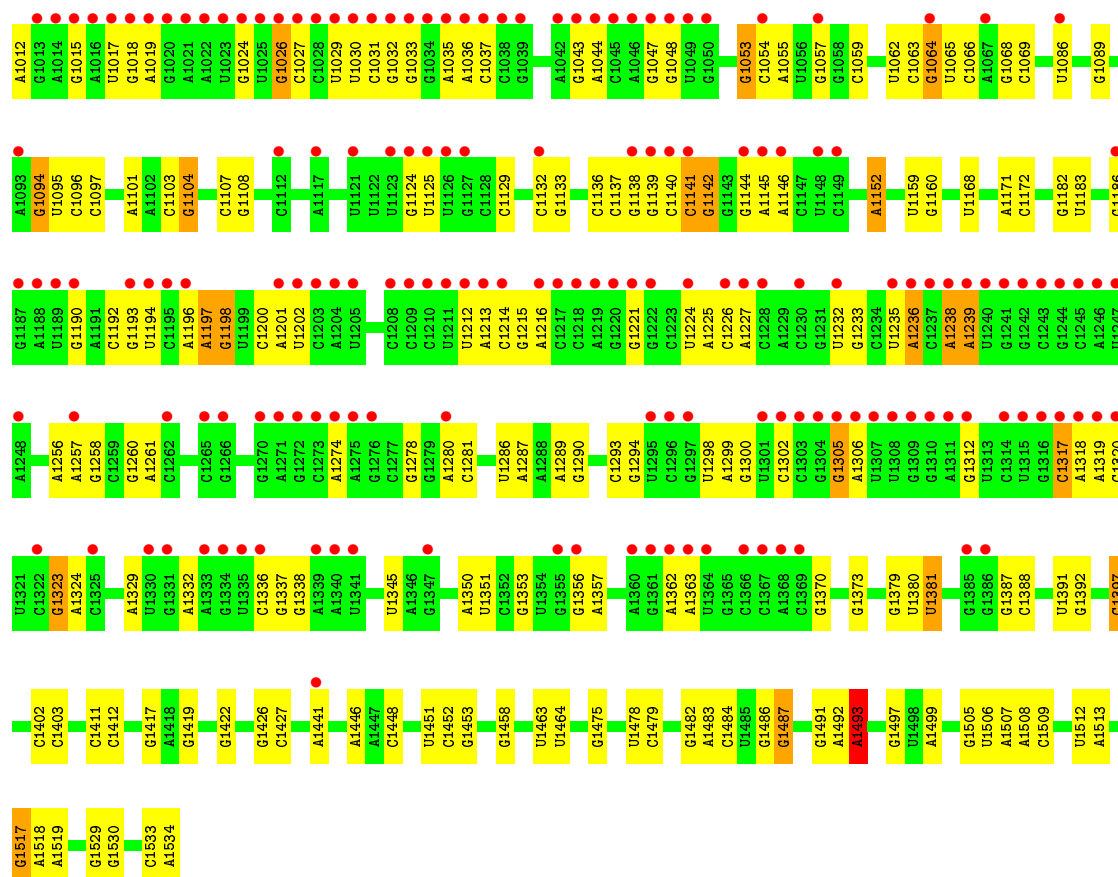
• Molecule 1: 16S rRNA



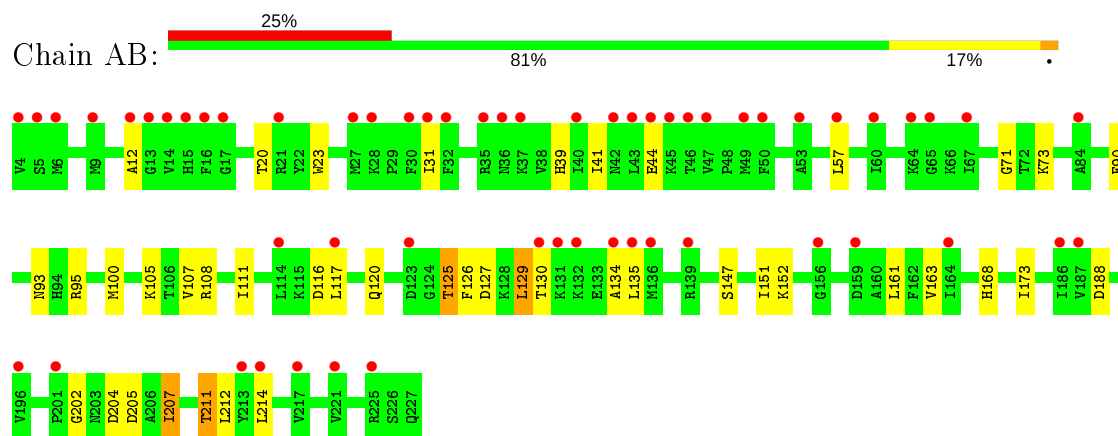


• Molecule 1: 16S rRNA

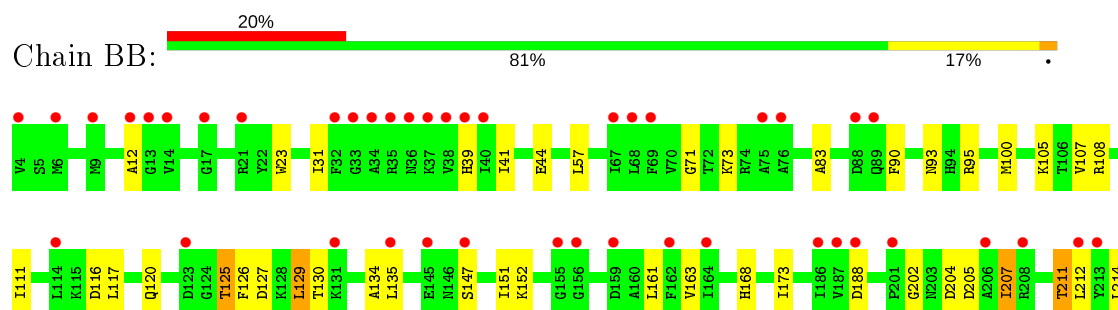




• Molecule 2: 30S ribosomal protein S2

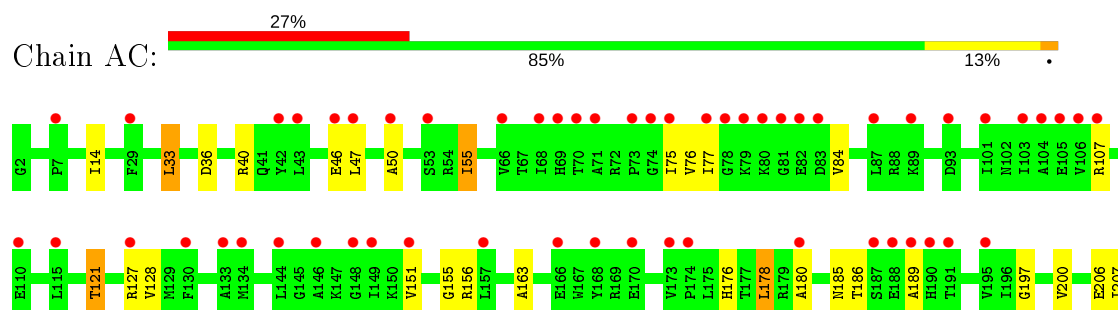


• Molecule 2: 30S ribosomal protein S2

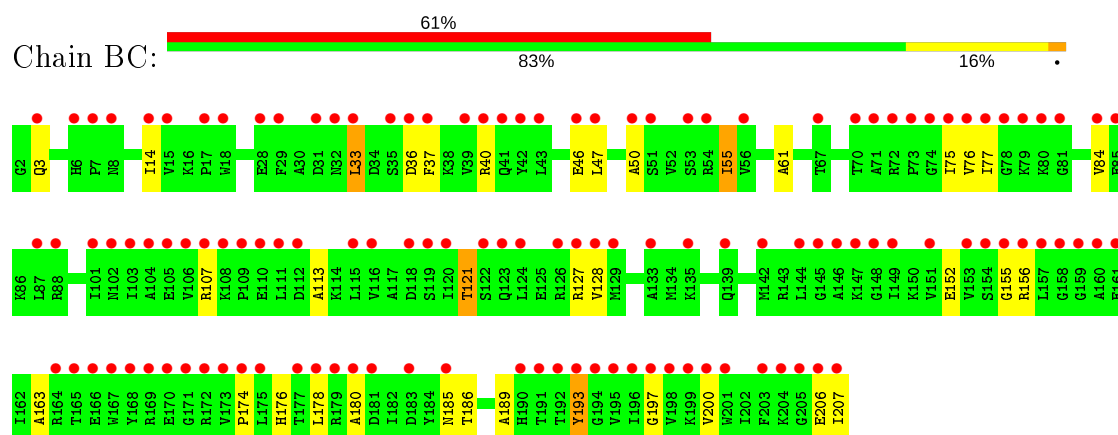




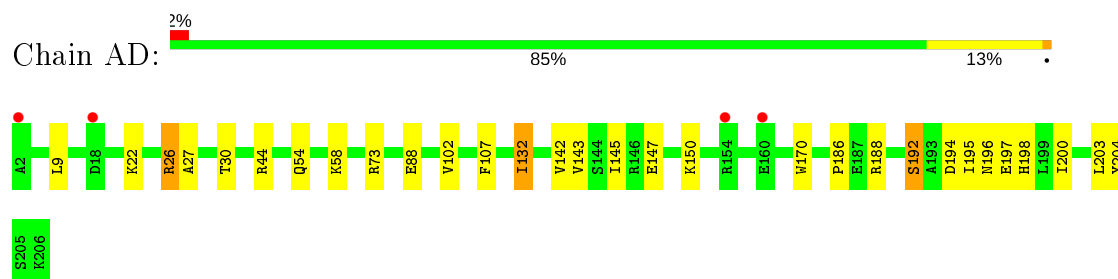
- Molecule 3: 30S ribosomal protein S3



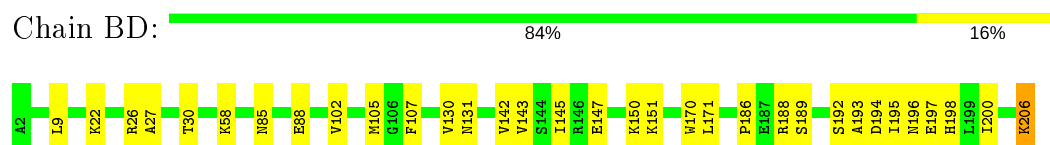
- Molecule 3: 30S ribosomal protein S3



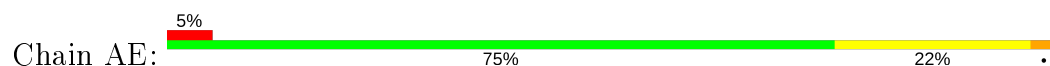
- Molecule 4: 30S ribosomal protein S4

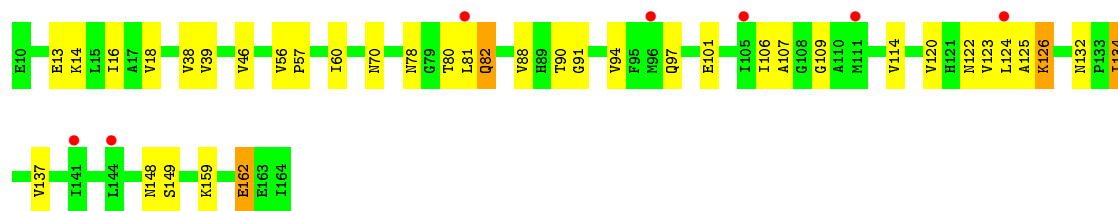


- Molecule 4: 30S ribosomal protein S4

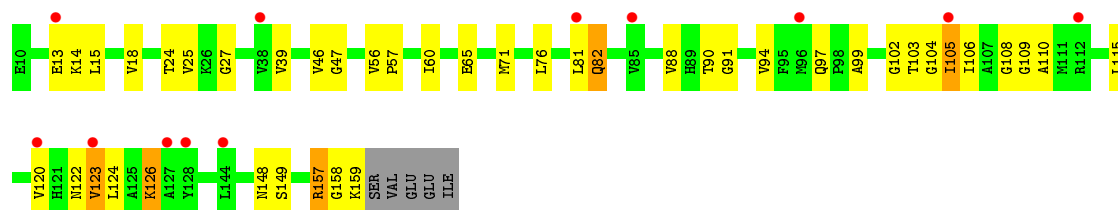


- Molecule 5: 30S ribosomal protein S5

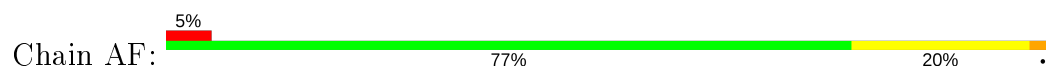




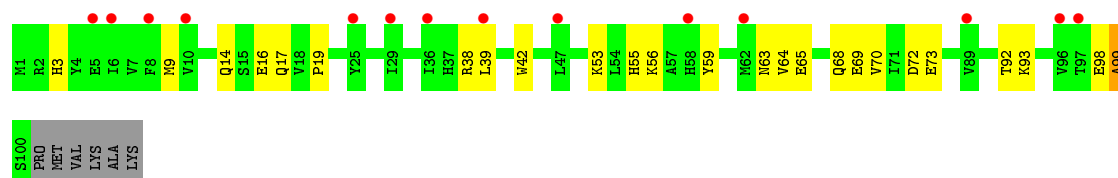
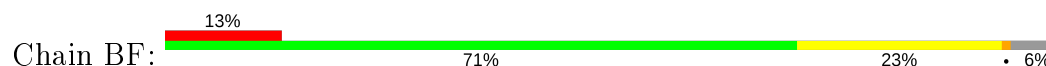
• Molecule 5: 30S ribosomal protein S5



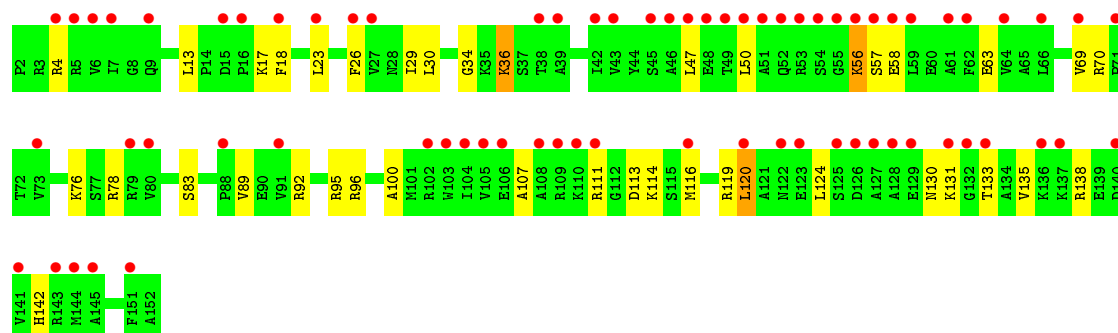
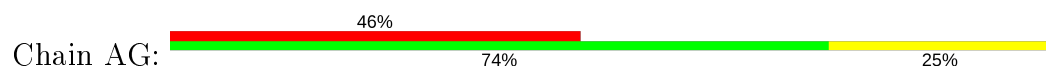
• Molecule 6: 30S ribosomal protein S6



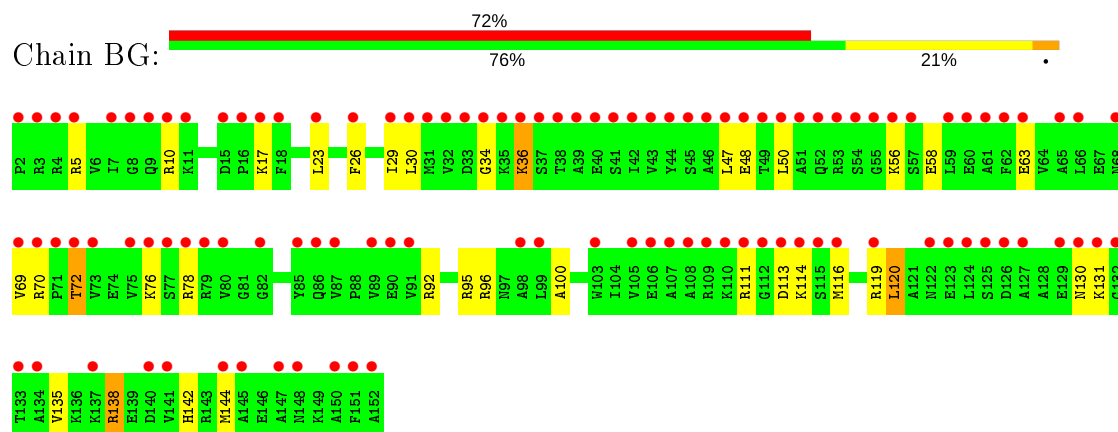
• Molecule 6: 30S ribosomal protein S6



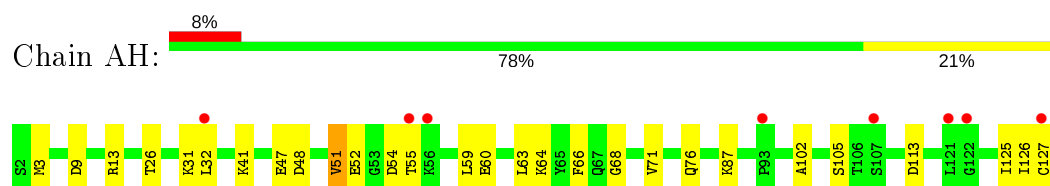
• Molecule 7: 30S ribosomal protein S7



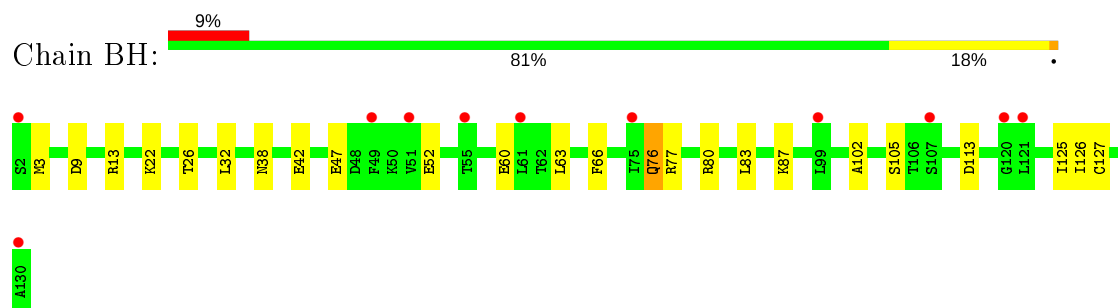
- Molecule 7: 30S ribosomal protein S7



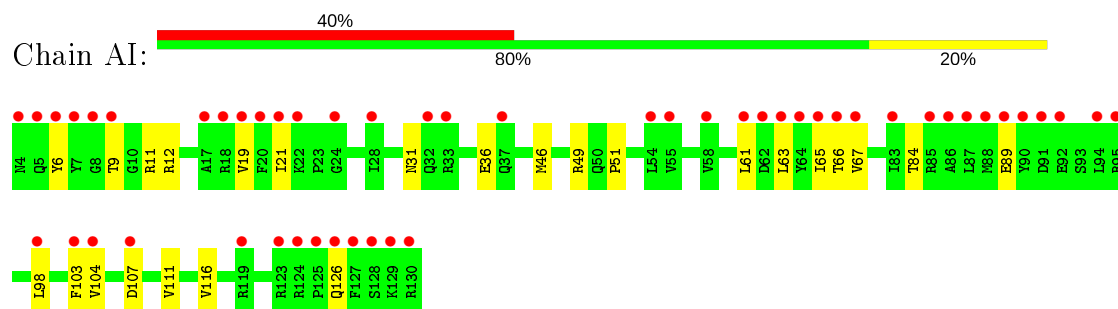
- Molecule 8: 30S ribosomal protein S8



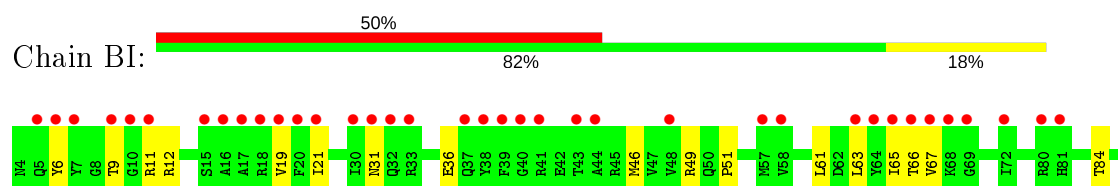
- Molecule 8: 30S ribosomal protein S8

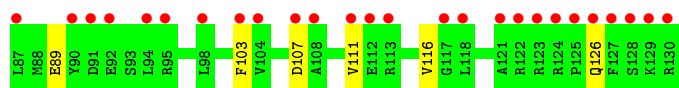


- Molecule 9: 30S ribosomal protein S9

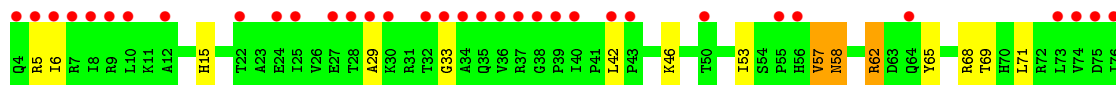
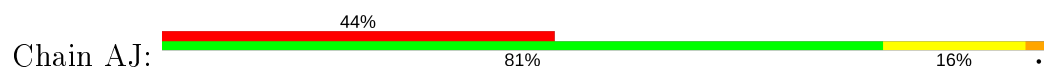


- Molecule 9: 30S ribosomal protein S9

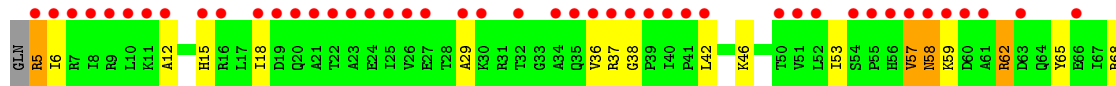
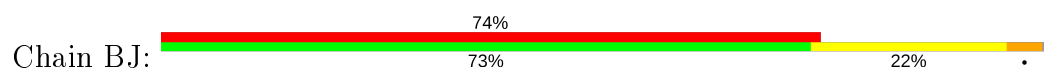




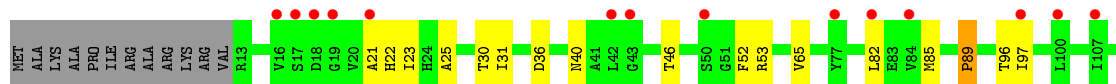
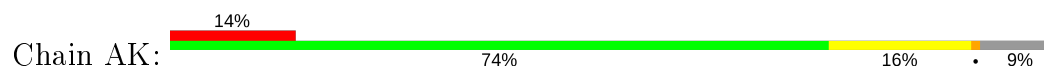
- Molecule 10: 30S ribosomal protein S10



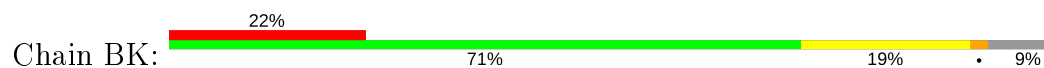
- Molecule 10: 30S ribosomal protein S10



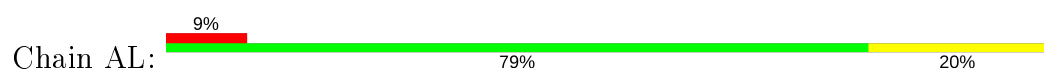
- Molecule 11: 30S ribosomal protein S11

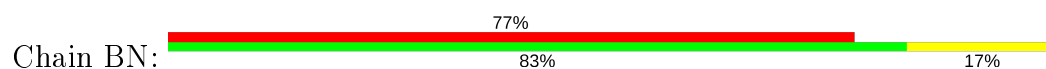


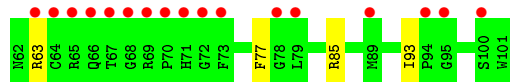
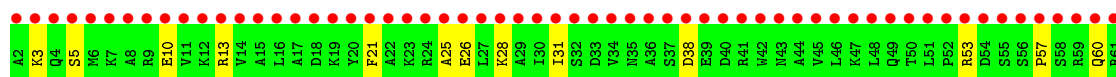
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



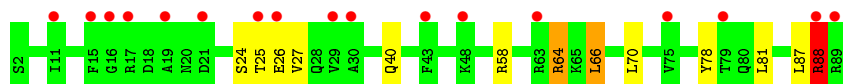
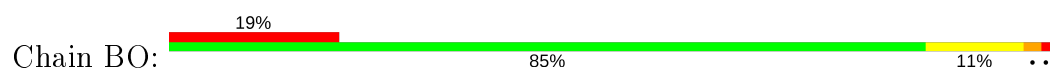




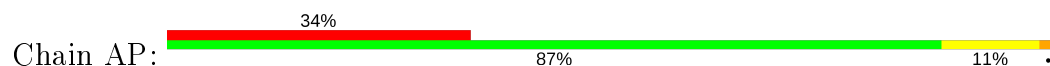
- Molecule 15: 30S ribosomal protein S15



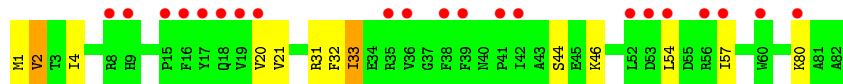
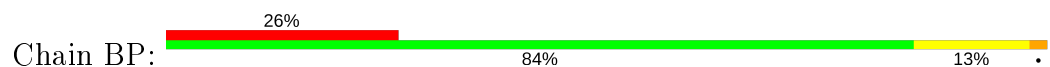
- Molecule 15: 30S ribosomal protein S15



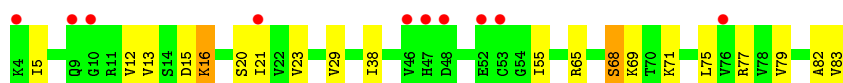
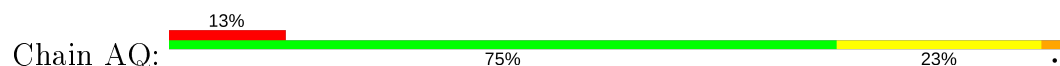
- Molecule 16: 30S ribosomal protein S16



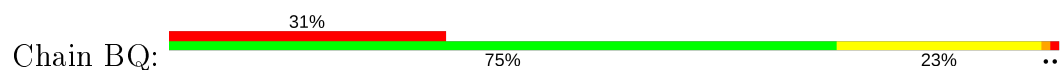
- Molecule 16: 30S ribosomal protein S16

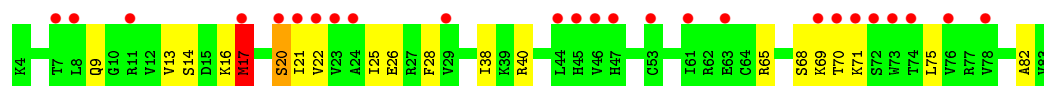


- Molecule 17: 30S ribosomal protein S17

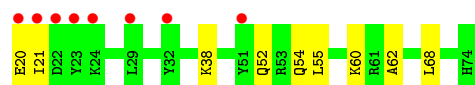
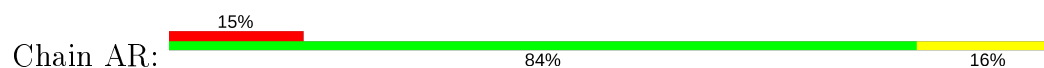


- Molecule 17: 30S ribosomal protein S17

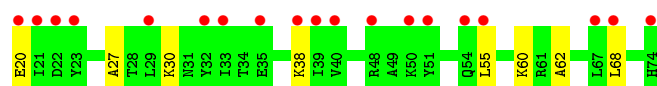
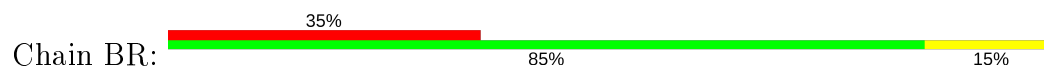




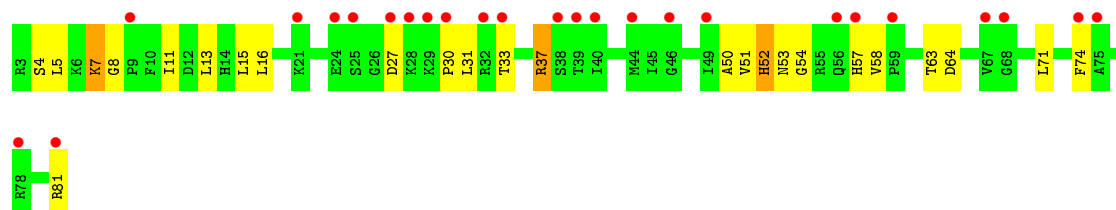
- Molecule 18: 30S ribosomal protein S18



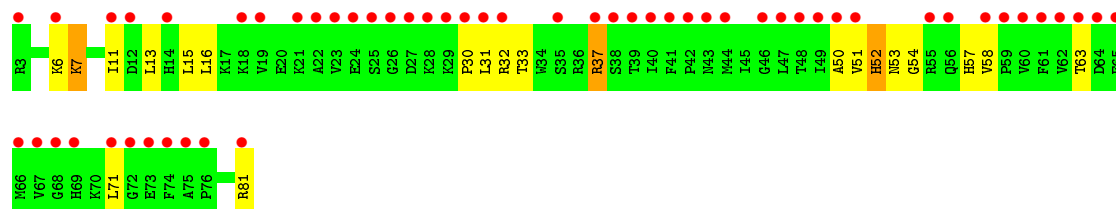
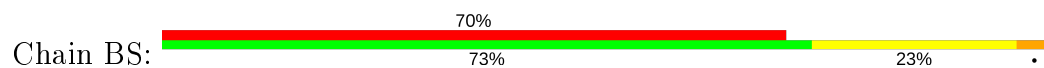
- Molecule 18: 30S ribosomal protein S18



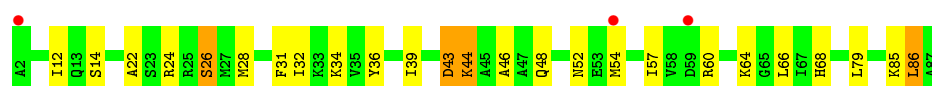
- Molecule 19: 30S ribosomal protein S19



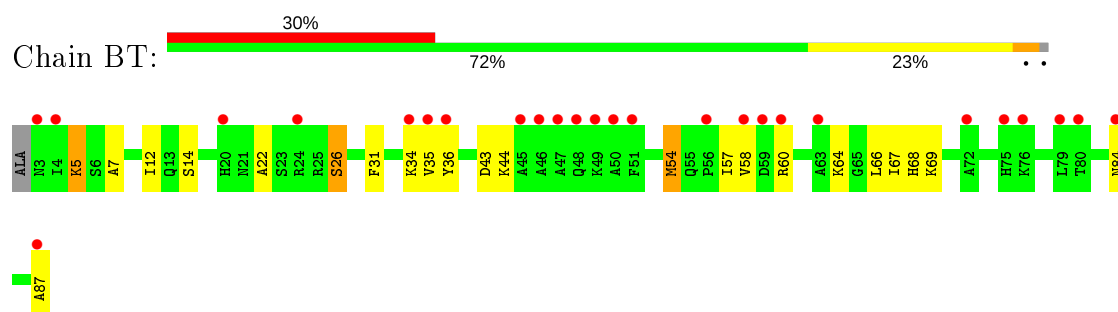
- Molecule 19: 30S ribosomal protein S19



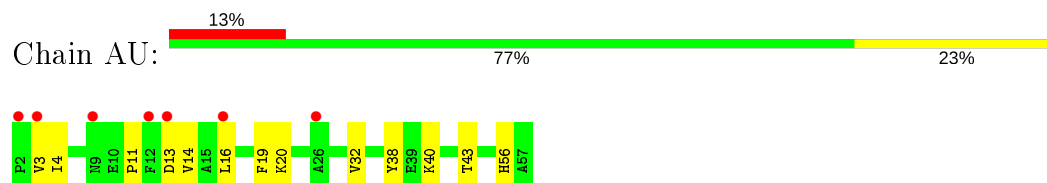
- Molecule 20: 30S ribosomal protein S20



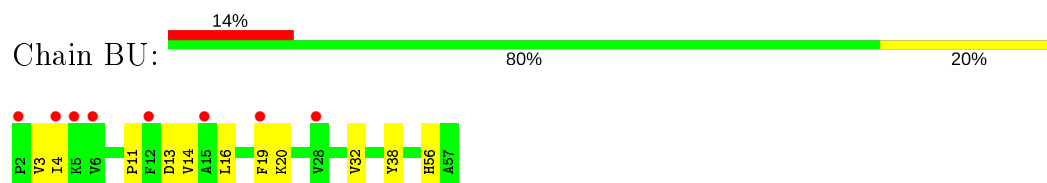
- Molecule 20: 30S ribosomal protein S20



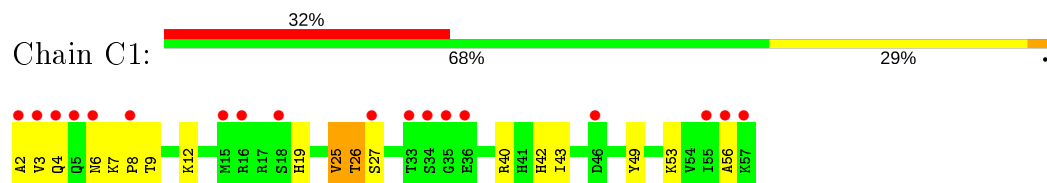
- Molecule 21: 30S ribosomal protein S21



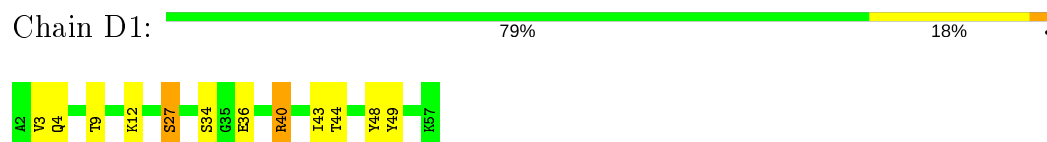
- Molecule 21: 30S ribosomal protein S21



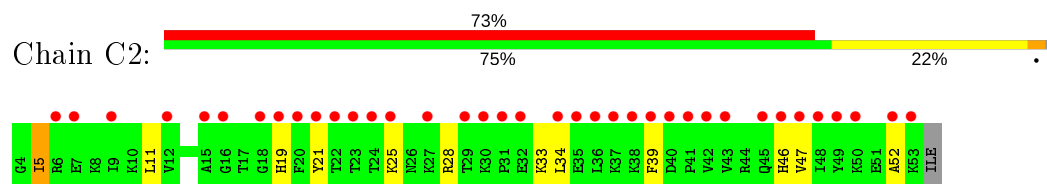
- Molecule 22: 50S ribosomal protein L32



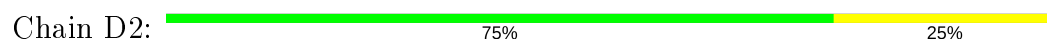
- Molecule 22: 50S ribosomal protein L32



- Molecule 23: 50S ribosomal protein L33

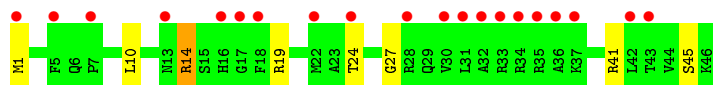
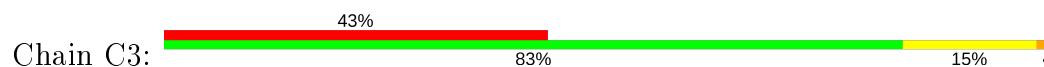


- Molecule 23: 50S ribosomal protein L33

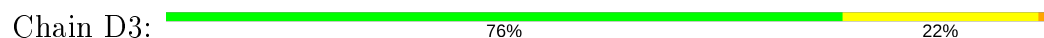




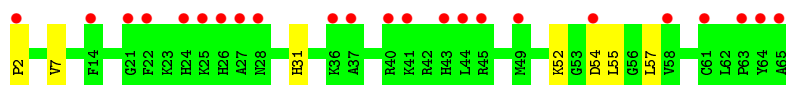
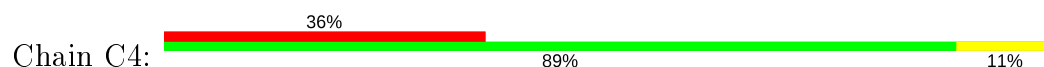
- Molecule 24: 50S ribosomal protein L34



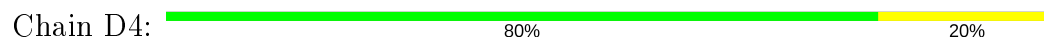
- Molecule 24: 50S ribosomal protein L34



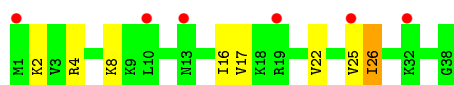
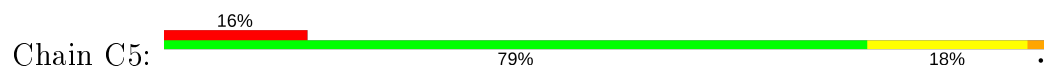
- Molecule 25: 50S ribosomal protein L35



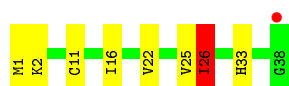
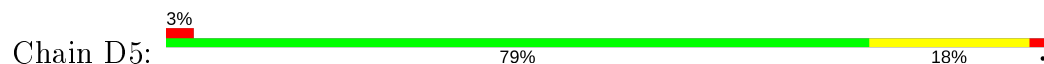
- Molecule 25: 50S ribosomal protein L35



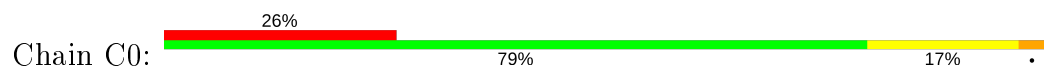
- Molecule 26: 50S ribosomal protein L36



- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L30

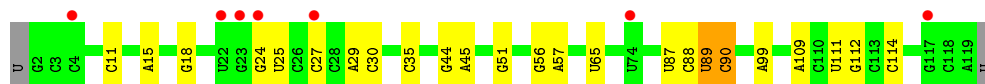
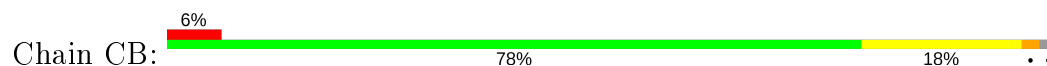




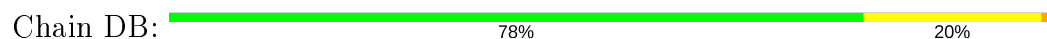
- Molecule 27: 50S ribosomal protein L30



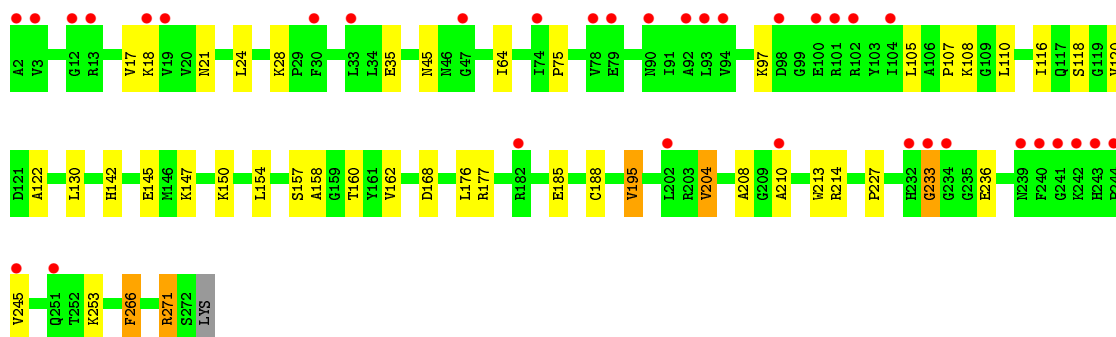
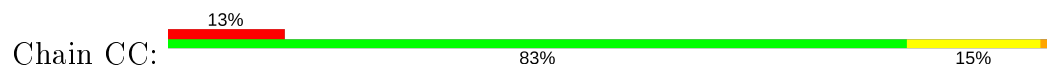
- Molecule 28: 5S rRNA



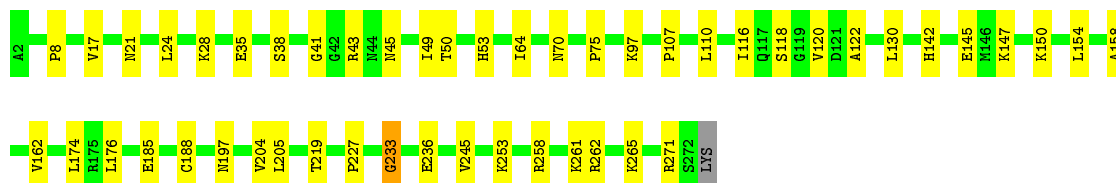
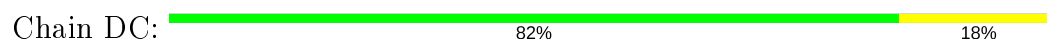
- Molecule 28: 5S rRNA



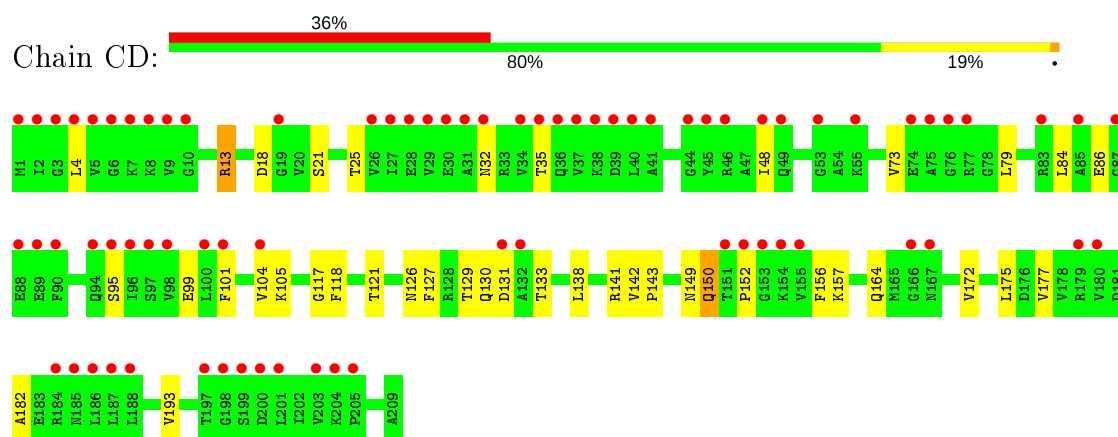
- Molecule 29: 50S ribosomal protein L2



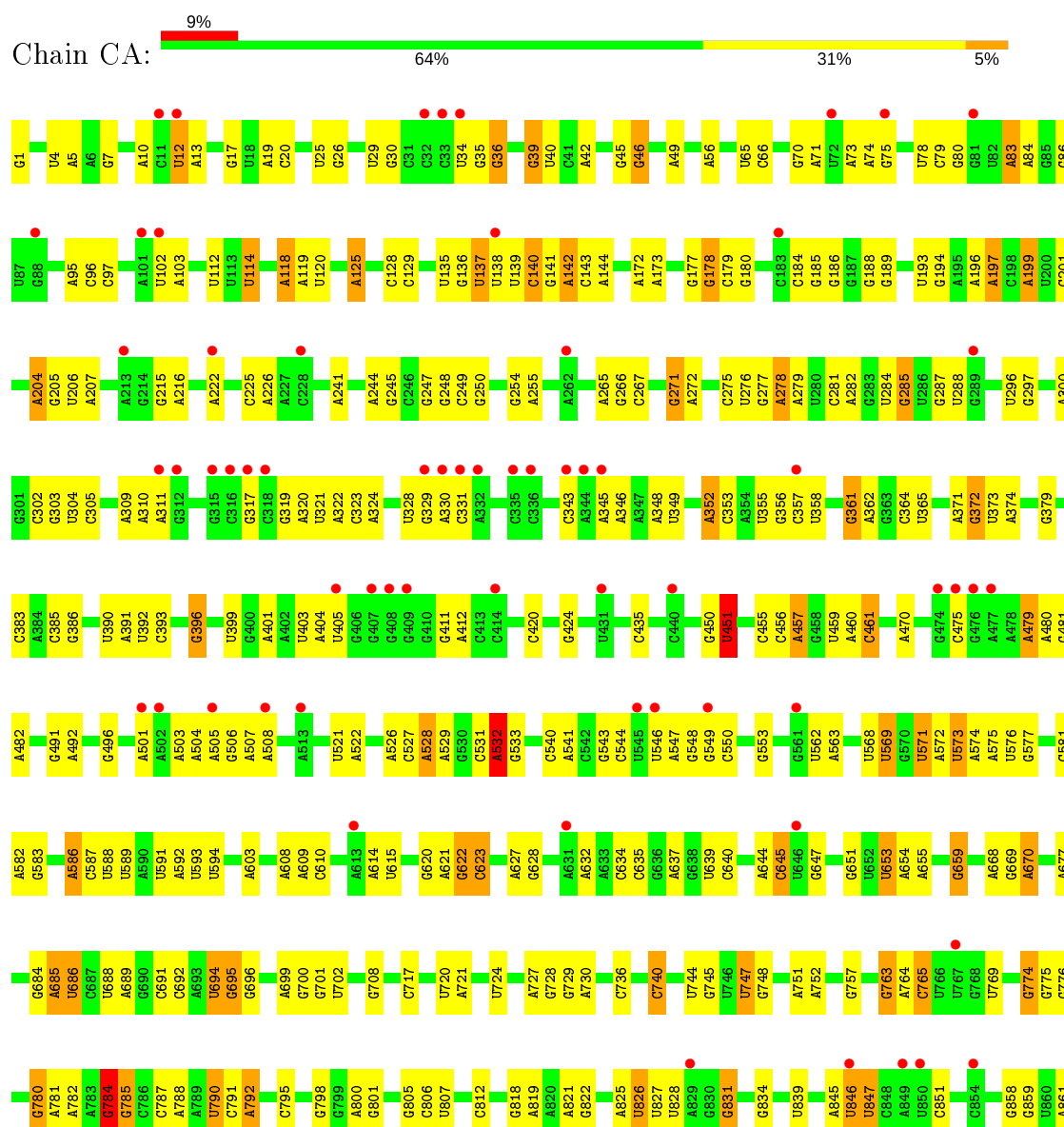
- Molecule 29: 50S ribosomal protein L2

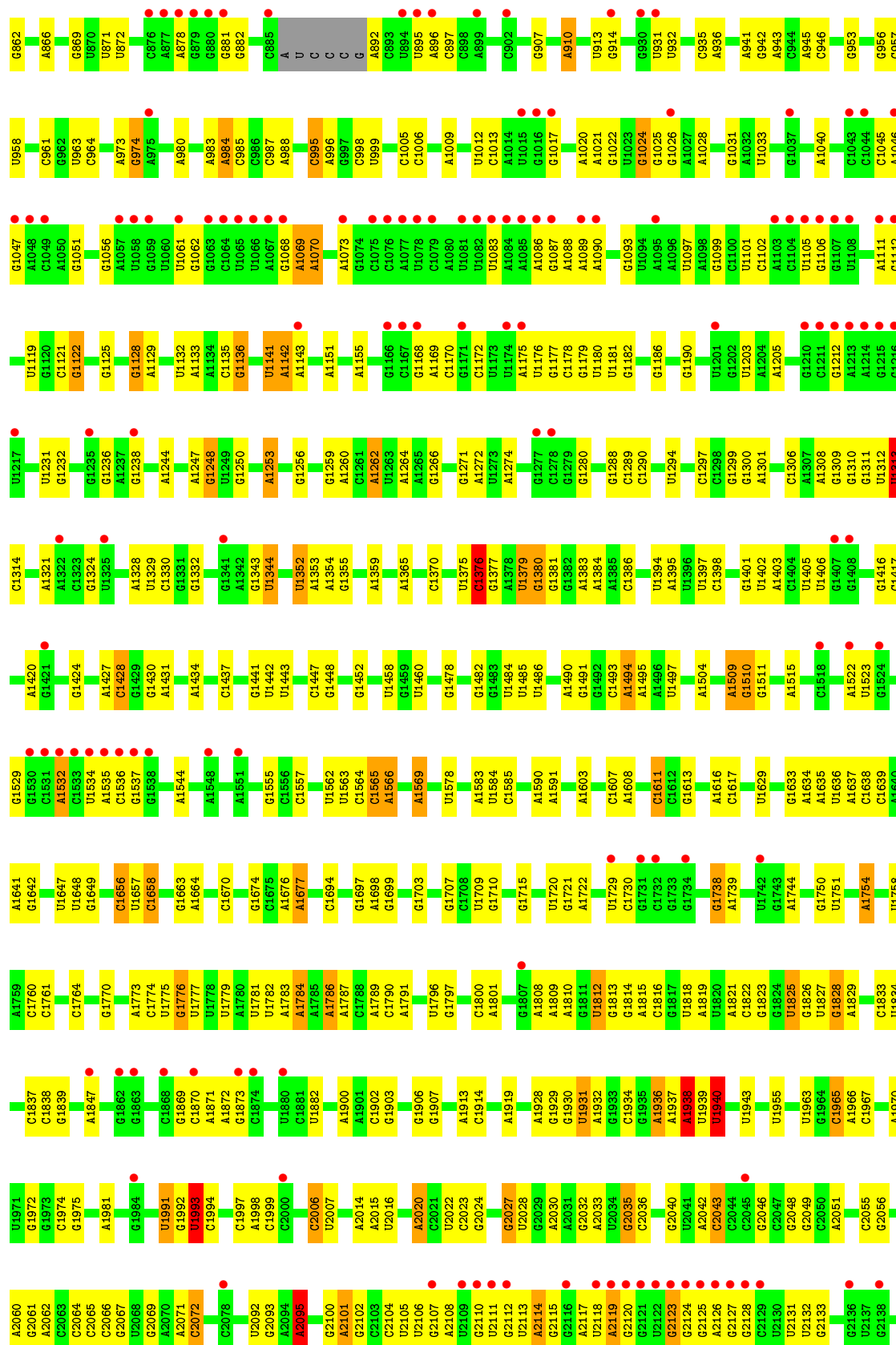


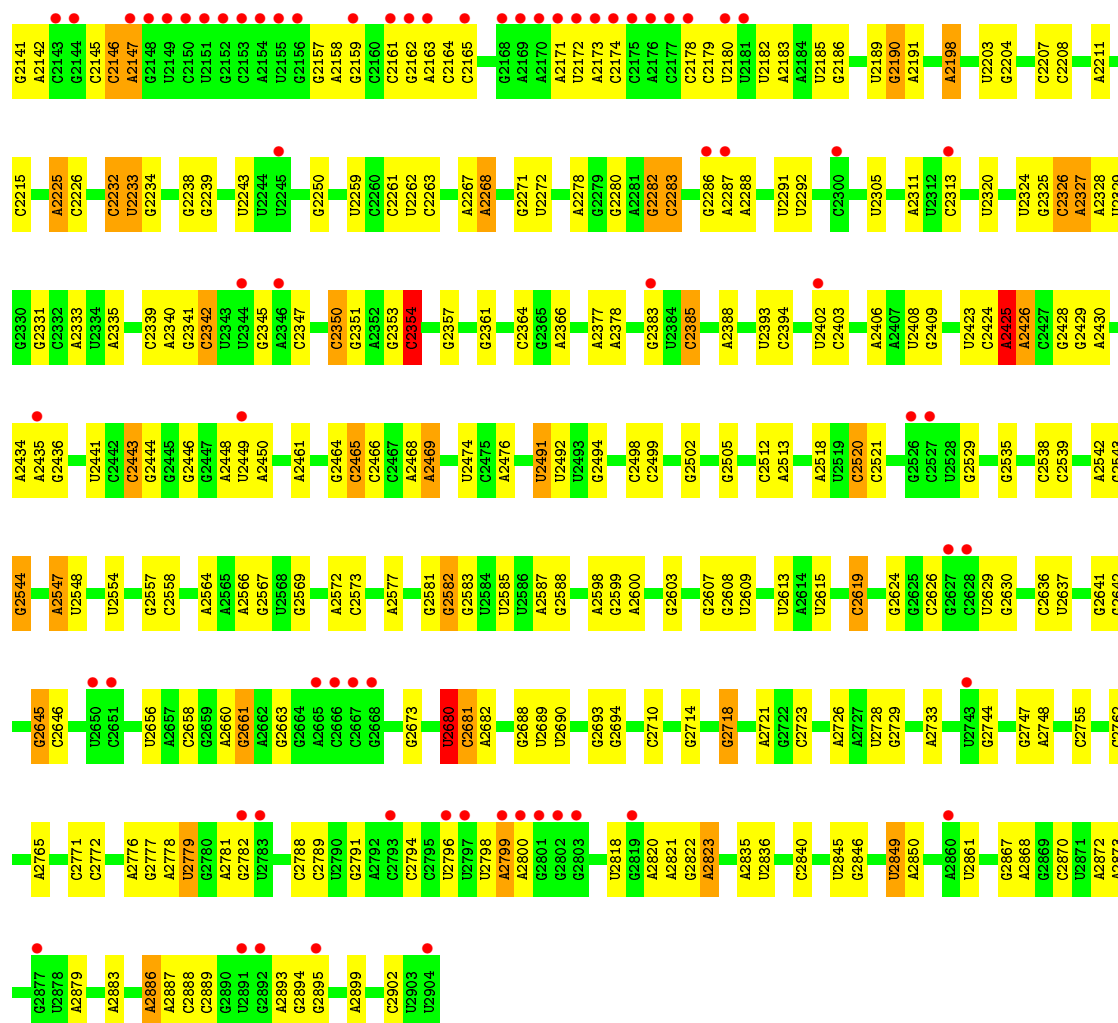
- Molecule 30: 50S ribosomal protein L3



• Molecule 31: 23S rRNA







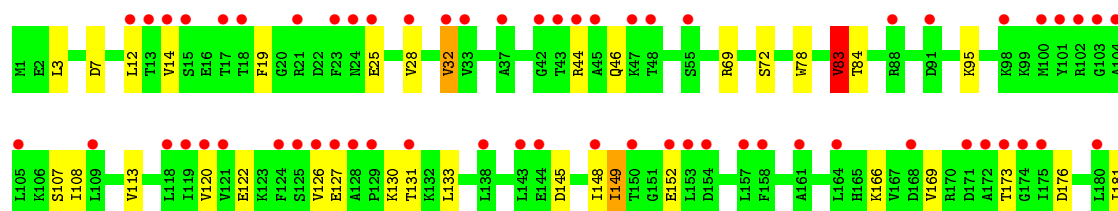
• Molecule 32: 50S ribosomal protein L3

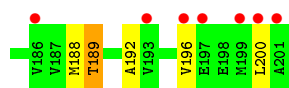
Chain DD: 79% 20%



• Molecule 33: 50S ribosomal protein L4

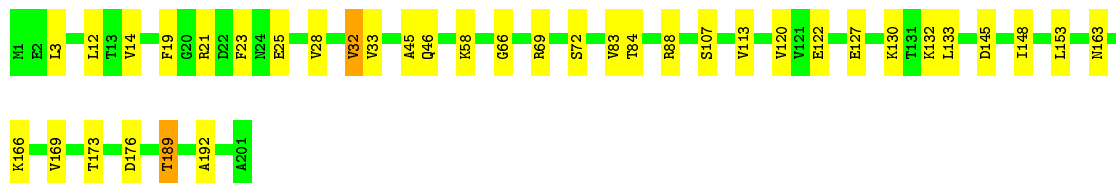
Chain CE: 34% 80% 18%





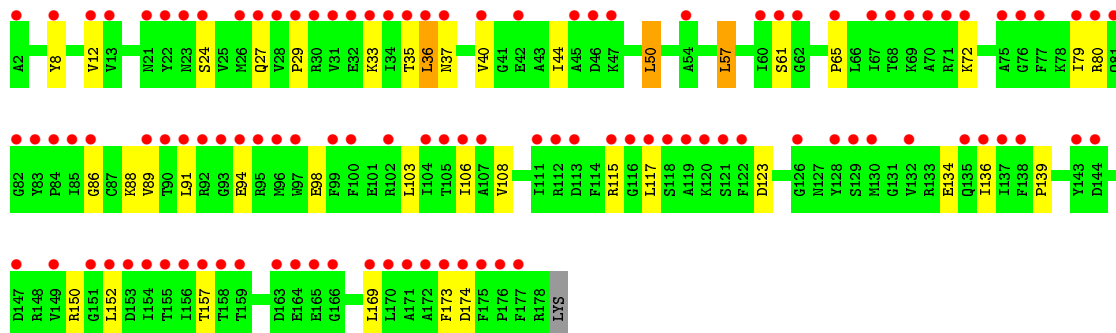
- Molecule 33: 50S ribosomal protein L4

Chain DE: 82% 17%



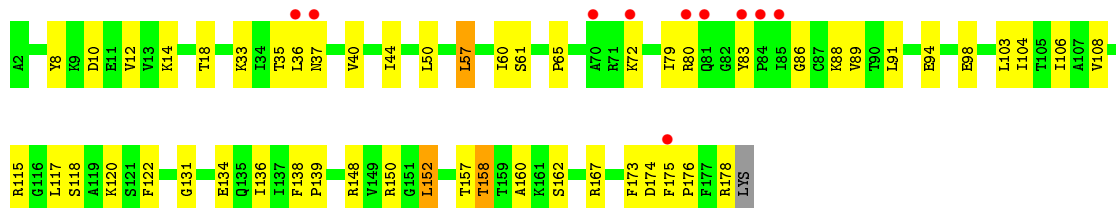
- Molecule 34: 50S ribosomal protein L5

Chain CF: 61% 78% 20%



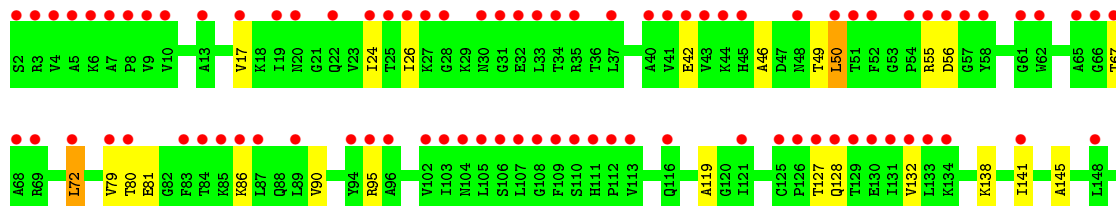
- Molecule 34: 50S ribosomal protein L5

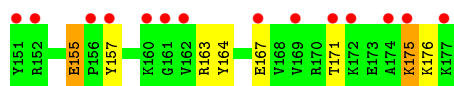
Chain DF: 6% 70% 28%



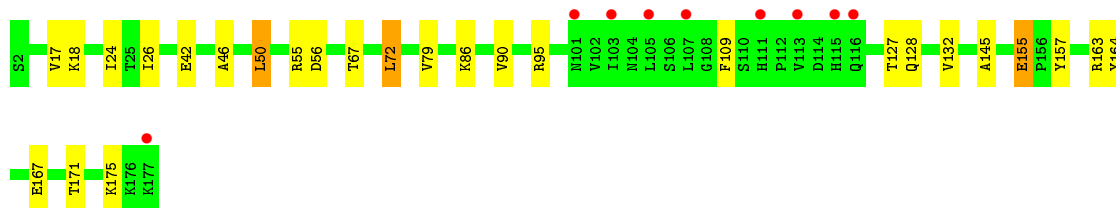
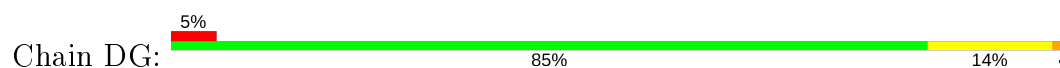
- Molecule 35: 50S ribosomal protein L6

Chain CG: 57% 82% 16%

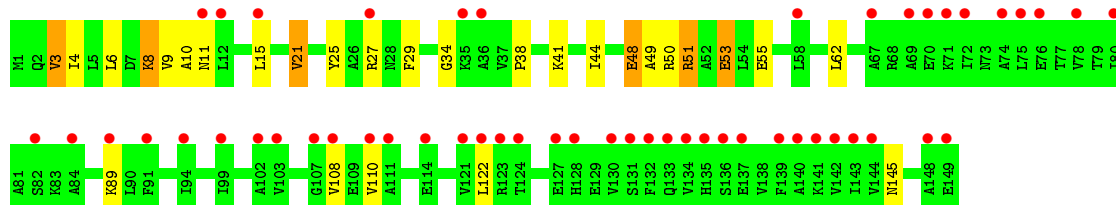
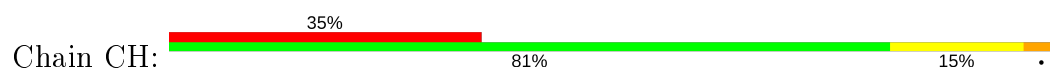




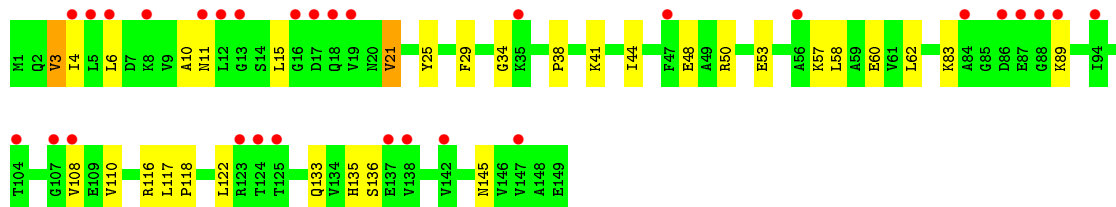
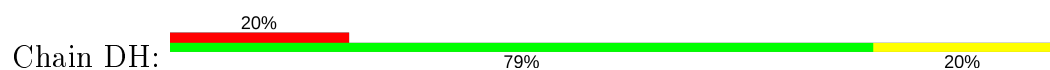
- Molecule 35: 50S ribosomal protein L6



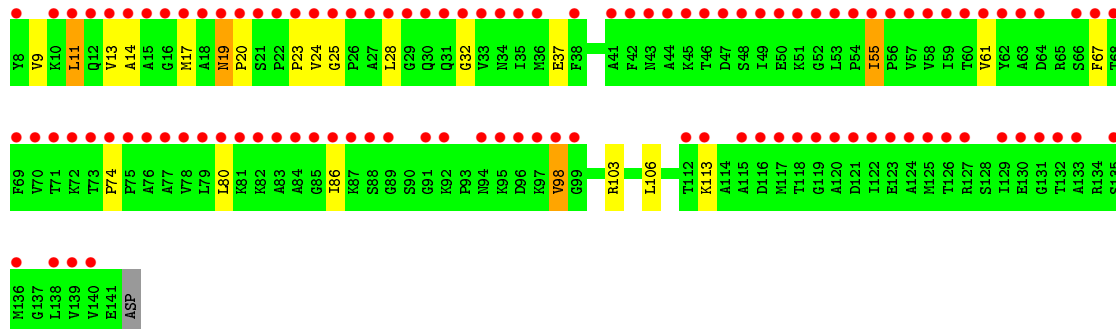
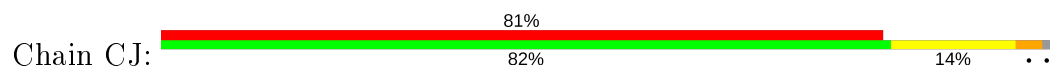
- Molecule 36: 50S ribosomal protein L9



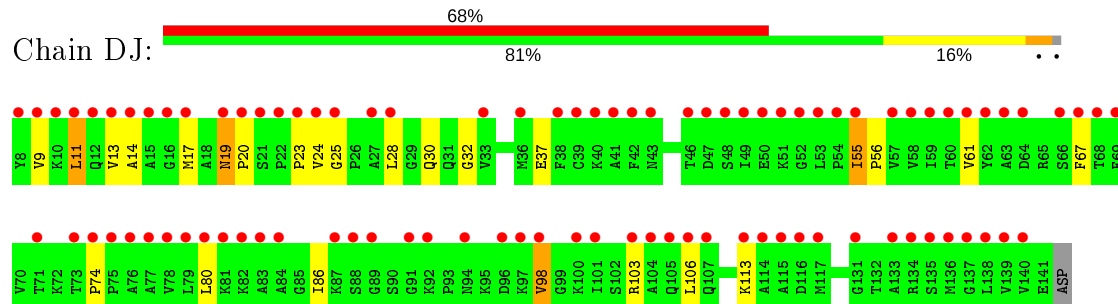
- Molecule 36: 50S ribosomal protein L9



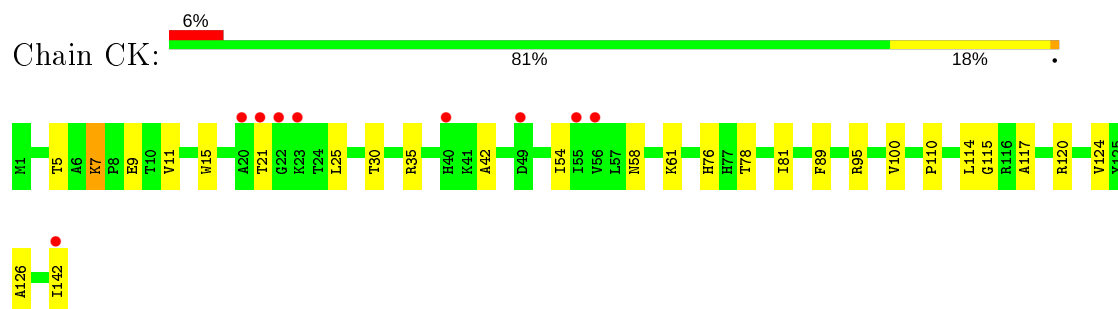
- Molecule 37: 50S ribosomal protein L11



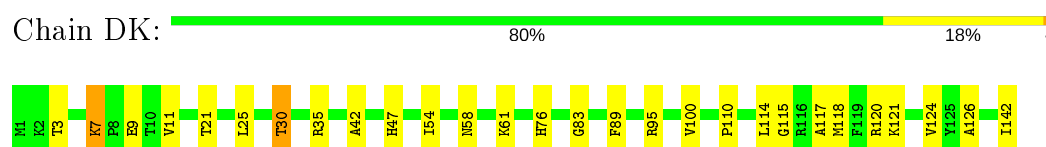
- Molecule 37: 50S ribosomal protein L11



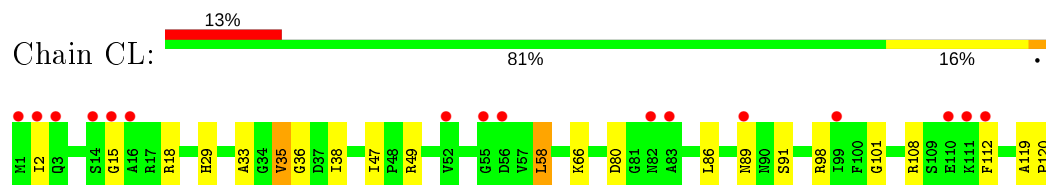
- Molecule 38: 50S ribosomal protein L13



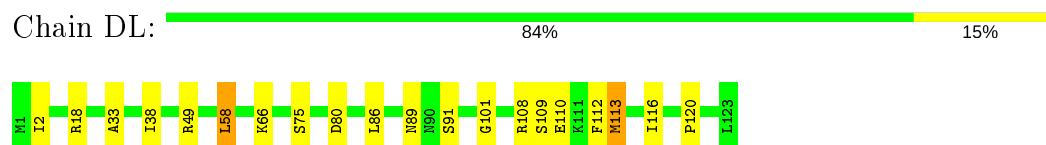
- Molecule 38: 50S ribosomal protein L13



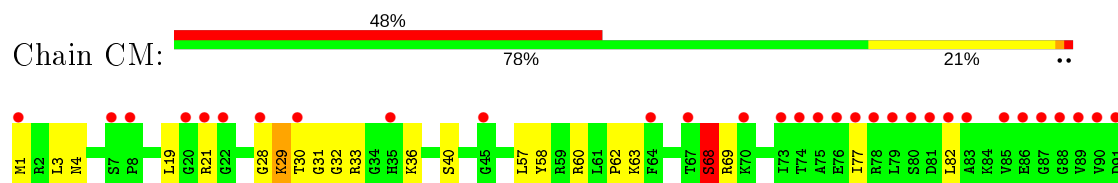
- Molecule 39: 50S ribosomal protein L14



- Molecule 39: 50S ribosomal protein L14

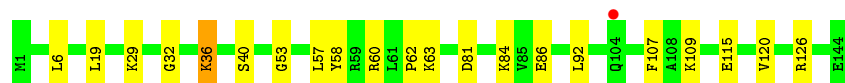
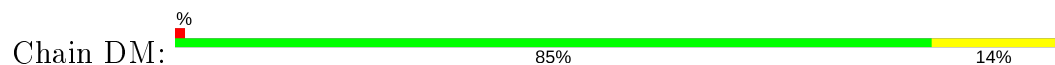


- Molecule 40: 50S ribosomal protein L15

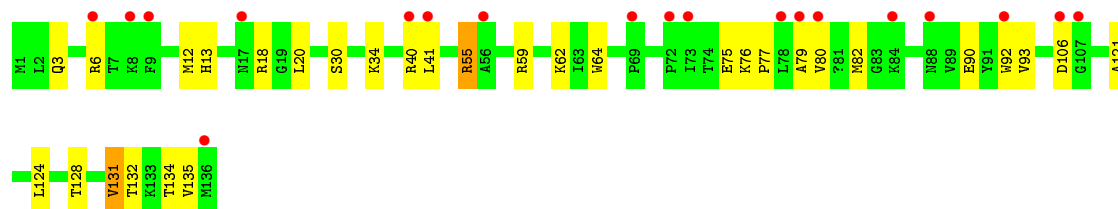
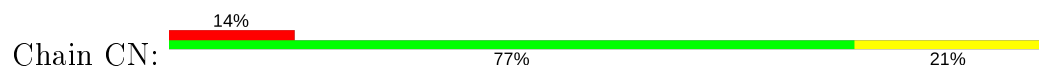




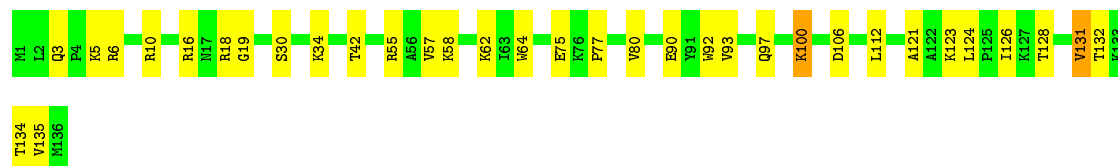
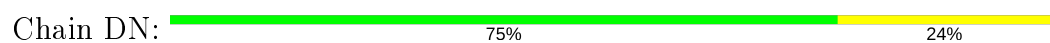
- Molecule 40: 50S ribosomal protein L15



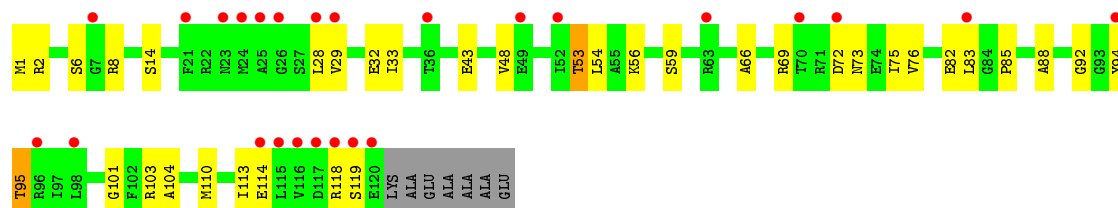
- Molecule 41: 50S ribosomal protein L16



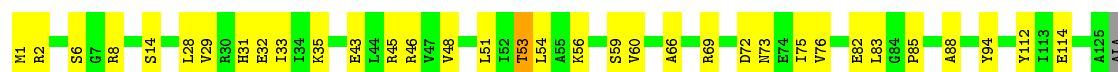
- Molecule 41: 50S ribosomal protein L16



- Molecule 42: 50S ribosomal protein L17

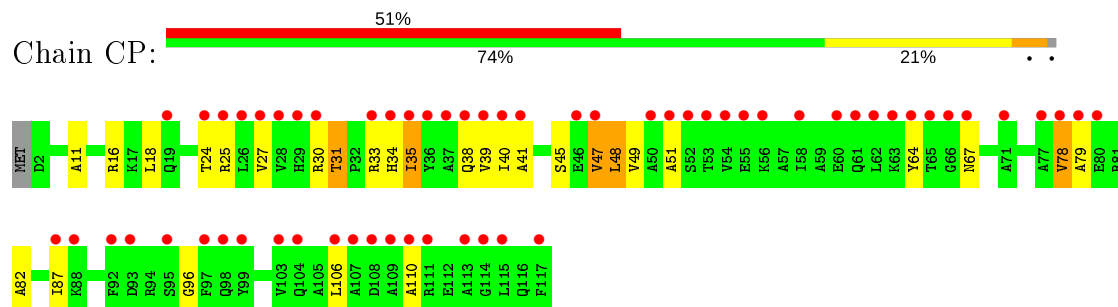


- Molecule 42: 50S ribosomal protein L17

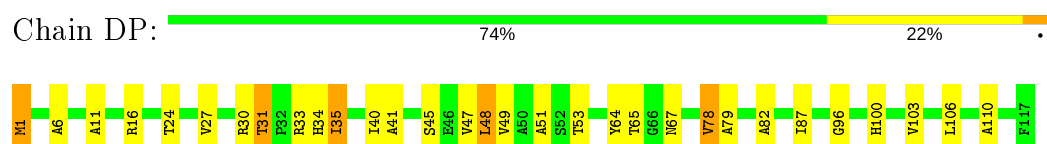


GLU

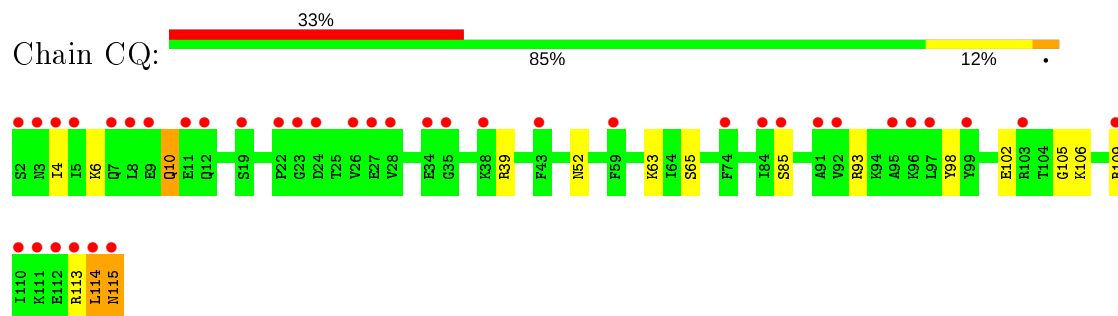
- Molecule 43: 50S ribosomal protein L18



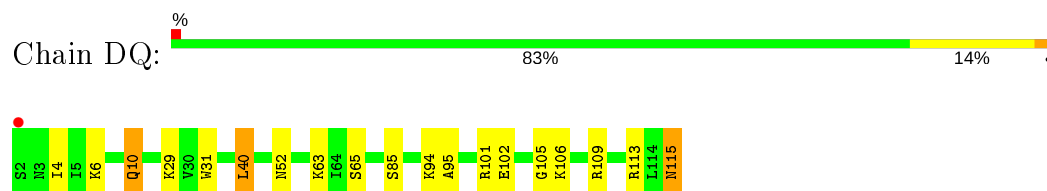
- Molecule 43: 50S ribosomal protein L18



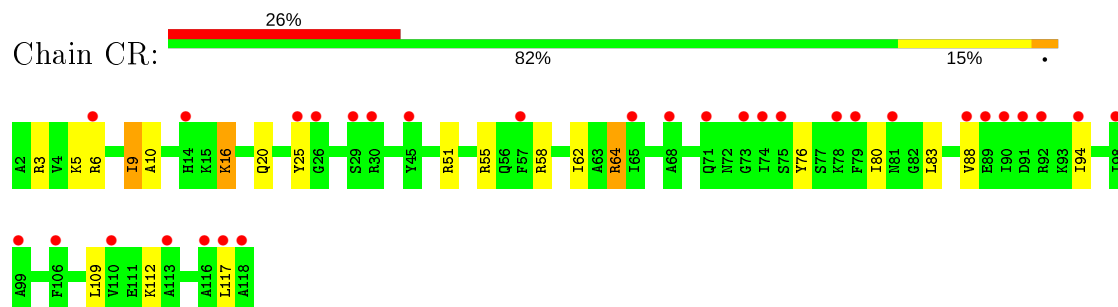
- Molecule 44: 50S ribosomal protein L19




- Molecule 44: 50S ribosomal protein L19



- Molecule 45: 50S ribosomal protein L20




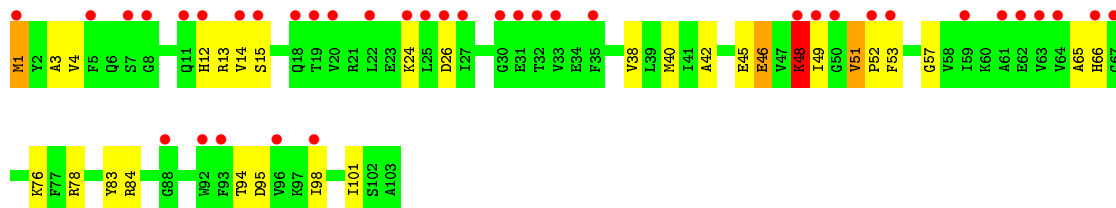
- Molecule 45: 50S ribosomal protein L20

Chain DR:  79% 19%



- Molecule 46: 50S ribosomal protein L21

Chain CS:  37% 71% 25%



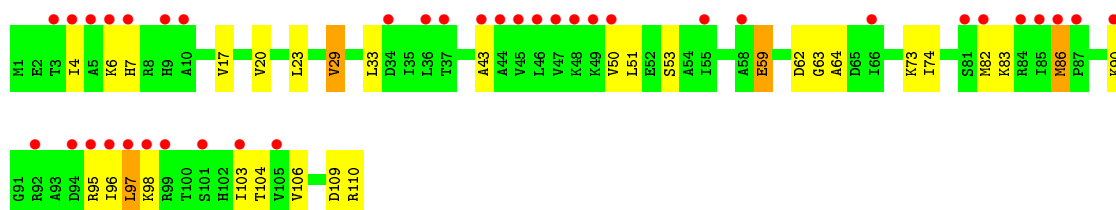
- Molecule 46: 50S ribosomal protein L21

Chain DS:  71% 26%




- Molecule 47: 50S ribosomal protein L22

Chain CT:  35% 72% 25%




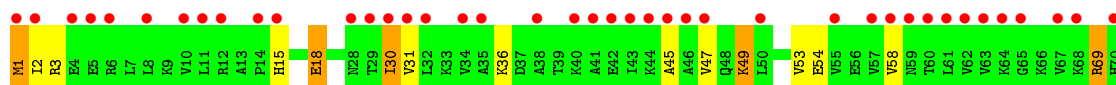
- Molecule 47: 50S ribosomal protein L22

Chain DT:  78% 22%



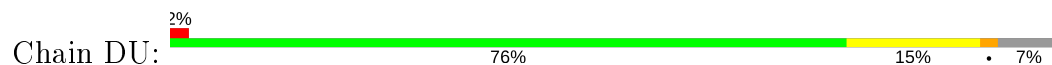
- Molecule 48: 50S ribosomal protein L23

Chain CU:  54% 70% 18% 5% 7%

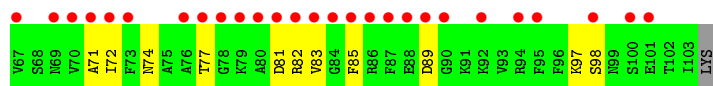
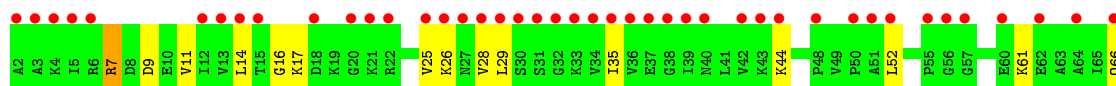
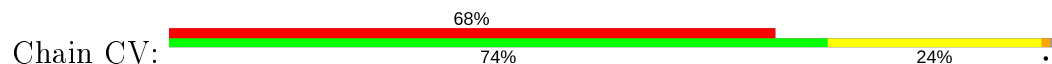




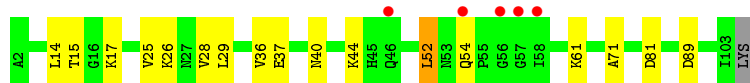
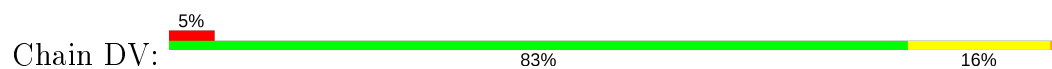
- Molecule 48: 50S ribosomal protein L23



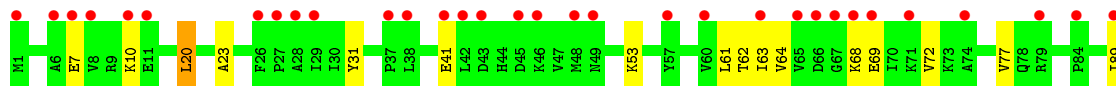
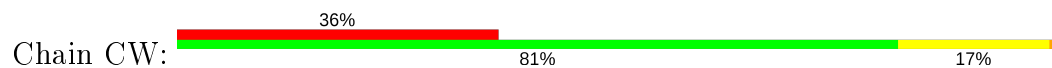
- Molecule 49: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24



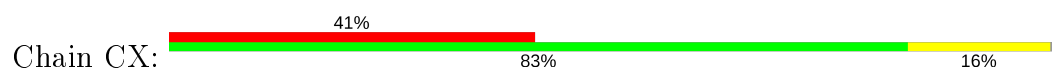
- Molecule 50: 50S ribosomal protein L25

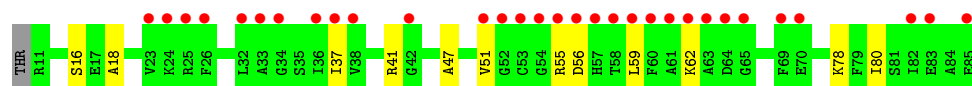


- Molecule 50: 50S ribosomal protein L25



- Molecule 51: 50S ribosomal protein L27





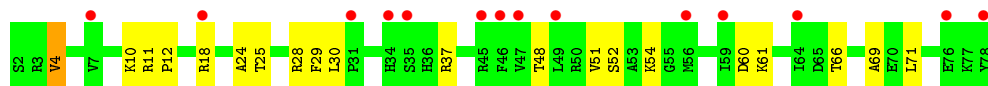
- Molecule 51: 50S ribosomal protein L27

Chain DX: 79% 20% .



- Molecule 52: 50S ribosomal protein L28

Chain CY: 18% 74% 25% .



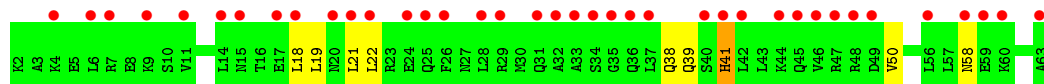
- Molecule 52: 50S ribosomal protein L28

Chain DY: % 81% 18% .



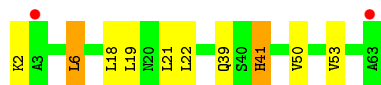
- Molecule 53: 50S ribosomal protein L29

Chain CZ: 61% 85% 13% .



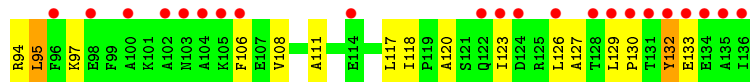
- Molecule 53: 50S ribosomal protein L29

Chain DZ: 3% 84% 13% .



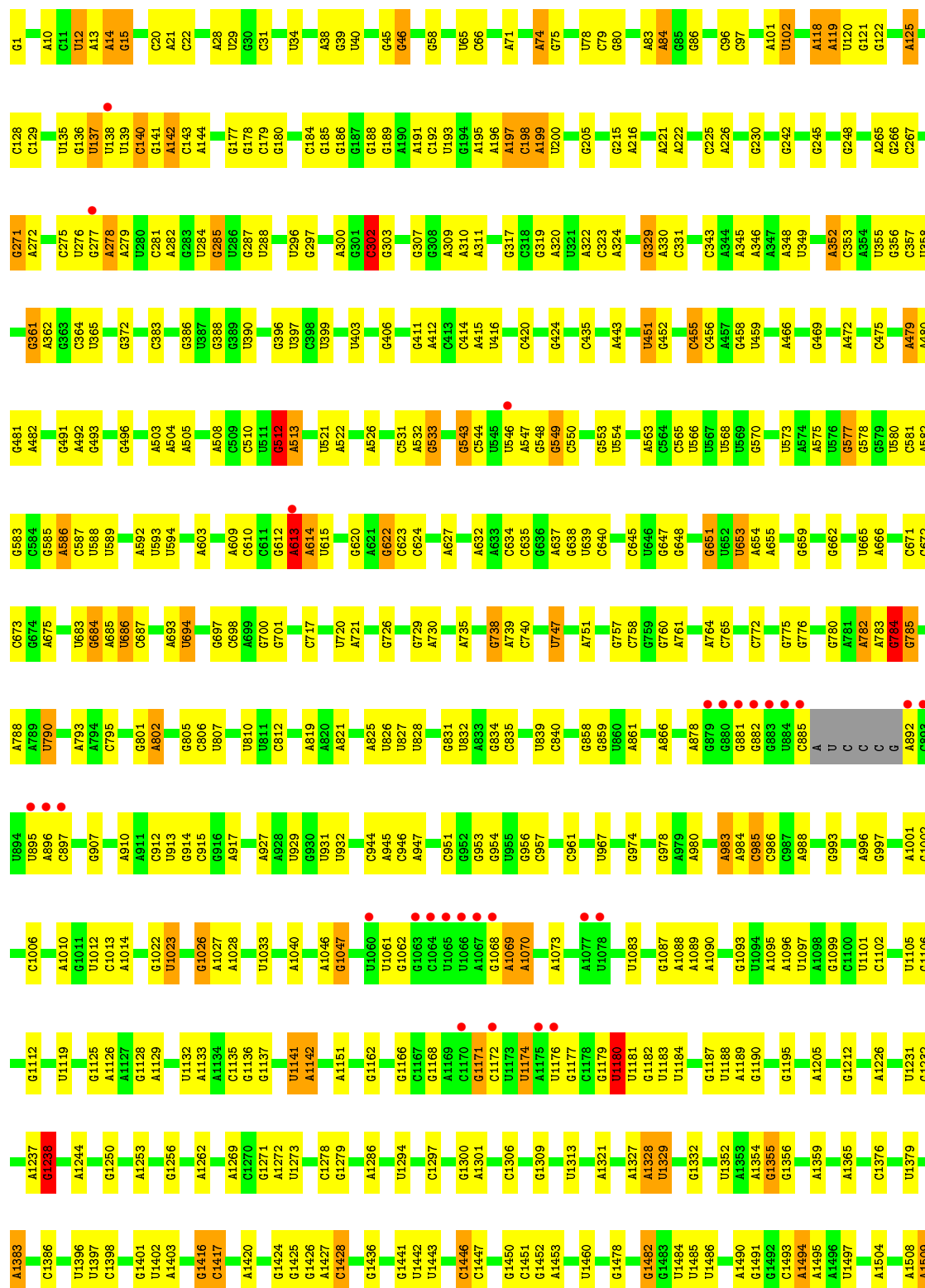
- Molecule 54: 50S ribosomal protein L10

Chain DI: 29% 66% 28% 6% .



• Molecule 55: 23S rRNA

Chain DA: 3% 67% 28% 5%



A2887	U2783	G2673	A2439	A2340	A2225	U2131	C2050	C1961	U1796	G1649	G1510
C2888	U2784	C2681	G2440	C2341	U2233	U2132	A2051	U1797	G1797	G1659	G1511
G2895	C2788	C2682	U2441	C2342	G2234	G2133	A2052	U1798	U1798	A1515	A1515
C2901	U2789	U2689	G2442	U2343	G2235	G2134	G2055	C1965	G1799	G1663	U1523
C2902	U2790	U2690	G2443	U2344	G2236	A2135	G2056	C1966	C1800	A1664	G1529
U	G2791	U2695	U2444	C2345	G2237	G2140	G2057	C1967	A1801	A1665	G1530
	U2796		A2445	C2350	U2243	G2141	A2060	A1970	A1808	G1674	
	U2797	C2703	A2450	C2351	G2255	A2142	G2061	U1971	A1812	A1676	A1532
	U2798	C2704	A2461	G2354	G2256	C2146	A2062	G1972	A1813	A1677	U1533
	A2799	A2705	G2464	C2355	U2258	C2147	C2063	G1973	G1813		U1534
A2800	G2706		C2465	G2356	U2259	A2147	C2064	G1974		G1682	A1535
			A2469	G2357	U2260	U2149	C2065	G1975	C1816		G1536
	G2714		A2577	C2364	U2261	G2150	G2066	U1976	G1826	C1694	G1537
	C2715		G2578	A2365	U2262	C2151	G2067	U1979	G1826	G1695	
	G2719		U2473	A2366	U2263	G2152	G2068	U1980	A1829		A1544
	U2720		U2474	A2367		C2153	G2069	A1981	G1699		C1547
	U2721		U2475	A2377	A2268			C1985	C1832	U1714	U1544
	G2722		A2476	A2378	A2273	G2157	A2077	C1985	C1833	G1715	
	C2723		U2477	A2381	A2274	A2158	G2082	U1991	A1847	U1720	C1557
	A2821		A2478	A2382	A2275	G2159	G2083	G1992	G1721	C1558	
	G2822		U2479	G2382	A2276	C2161	G2087	U1993	A1853	A1722	
	A2823		C2480	U2383	G2279	G2162	G2093	C1997	G1869	U1729	U1562
	C2824		G2484	C2384	A2280	A2163	A2094	C1997	C1870	C1730	U1563
	G2825		U2491	U2385	A2281	C2164	A2095	A2005	A1871	A1566	A1566
			U2492	U2386	C2283	C2165	C2096	G2010	A1872		
	C2830		U2493	A2388	G2286	U2166	A2097	G2010	G1873	G1738	A1569
	A2835		G2607	U2393	A2287	U2167	G2100	A2014	A1885	U1744	U1578
	U2836		G2608	C2394	A2288	G2168	G2101	A2015	U1886	A1745	A1583
	G2844		G2502	U2402	U2292	A2169	G2102	A2019	A1900	U1746	U1584
	U2845		U2505	C2403	U2305	U2172	U2105	A2019	A1900	U1747	
	G2846		U2506	A2406	U2306	A2173	U2106	A2020	G1906	G1750	A1586
	U2847		U2512	U2407	G2308	C2174	G2107	C2023	G1907		G1587
	U2849		A2516	U2408	U2309	C2175	A2108	U2026	G1753	G1753	U1588
	A2851		G2517	G2409	A2311	A2176	U2109	U2026	A1913	A1754	U1589
	G2852		A2518	G2410	U2312	C2177	G2110	G2027	C1914	A1755	A1590
			U2519	A2418	U2313	C2178	U2111	G2027	A1927	U1758	A1591
	U2861		C2520	U2419	U2320	U2179	U2112	A2030	A1928	U1758	C1604
			U2522	U2420	U2321	U2180	U2113	A2031	A1928	A1759	
	U2866		U2523	U2421	U2322	U2181	A2114	G2032	G1929	C1764	C1607
	G2867		A2524	U2422	U2323	U2182	G2115	A2033	G1930	A1608	A1608
	A2868		C2424	U2423	G2325	A2183	G2116	U2034	U1931	A1773	C1612
	G2869		A2425	U2424	A2326	A2184	U2117	G2035	A1932	C1774	G1613
	C2870		A2426	U2425	A2327	U2185	U2118	G2036		U1775	A1614
	U2871		A2427	A2426	U2328	G2186	A2119	G2037	G1935		
	A2872		G2427	A2427	U2329	A2186	G2120	G2038	A1938	U1778	G1622
	A2873		G2428	G2428	U2330	A2188	G2121	G2038	U1939	G1622	
			U2429	A2429	U2331	A2189	U2122	A2042	U1940	U1781	A1641
	A2879		A2434	A2434	U2332	G2204	G2123	C2043	C1941	U1782	G1642
			A2435	A2435	U2333	A2211	G2124	C2047	A1962	A1783	
	A2883		G2436	G2436	U2334	U2220	G2125	G2048	U1965	A1784	U1647
	U2884		G2437	G2437	A2335		G2126	G2049		A1785	U1648
			U2438	U2438	C2339		G2128				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.55Å 433.65Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.32 48.13 – 3.32	Depositor EDS
% Data completeness (in resolution range)	83.3 (48.13-3.32) 83.3 (48.13-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	40.28 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.176 , 0.219 0.191 , 0.238	Depositor DCC
R_{free} test set	2784 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 128.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295119	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, D2T, UR3, 7MG, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, H2U, SPD, EDO, MEQ, OMU, PUT, 4OC, PSU

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	1.02	13/36596 (0.0%)	0.86	4/57086 (0.0%)
1	BA	1.01	12/36571 (0.0%)	0.86	3/57047 (0.0%)
2	AB	0.45	0/1784	0.65	0/2403
2	BB	0.43	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.66	0/2225
3	BC	0.48	0/1652	0.66	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.46	0/1665	0.69	0/2227
5	AE	0.47	0/1157	0.78	0/1557
5	BE	0.45	0/1118	0.81	0/1504
6	AF	0.44	0/881	0.71	0/1189
6	BF	0.45	0/835	0.76	0/1128
7	AG	0.49	0/1196	0.65	0/1602
7	BG	0.48	0/1196	0.64	0/1602
8	AH	0.42	0/989	0.68	0/1326
8	BH	0.41	0/989	0.67	0/1326
9	AI	0.44	0/1034	0.67	0/1375
9	BI	0.45	0/1034	0.66	0/1375
10	AJ	0.46	0/806	0.67	0/1089
10	BJ	0.52	0/797	0.71	0/1077
11	AK	0.47	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.45	0/960	0.74	0/1286
12	BL	0.43	0/960	0.72	0/1286
13	AM	0.51	0/893	0.74	1/1193 (0.1%)
13	BM	0.53	0/893	0.73	0/1193
14	AN	0.48	0/817	0.65	0/1088
14	BN	0.47	0/817	0.65	0/1088
15	AO	0.47	0/722	0.65	0/964
15	BO	0.43	0/722	0.64	0/964
16	AP	0.48	0/659	0.73	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.47	0/659	0.75	0/884
17	AQ	0.47	0/658	0.73	0/881
17	BQ	0.47	0/658	0.75	0/881
18	AR	0.50	0/463	0.70	0/621
18	BR	0.49	0/463	0.69	0/621
19	AS	0.51	0/653	0.63	0/877
19	BS	0.51	0/653	0.64	0/877
20	AT	0.47	0/676	0.68	0/895
20	BT	0.50	0/671	0.70	0/888
21	AU	0.42	0/472	0.62	0/627
21	BU	0.40	0/472	0.63	0/627
22	C1	0.49	0/450	0.69	0/599
22	D1	0.61	0/450	0.75	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.49	0/421	0.70	0/561
24	C3	0.44	0/380	0.71	0/498
24	D3	0.54	0/380	0.74	0/498
25	C4	0.44	0/513	0.64	0/676
25	D4	0.52	0/513	0.68	0/676
26	C5	0.44	0/303	0.74	0/397
26	D5	0.60	1/303 (0.3%)	0.75	0/397
27	C0	0.53	0/453	0.75	0/605
27	D0	0.61	0/467	0.79	0/623
28	CB	1.01	1/2828 (0.0%)	0.90	1/4410 (0.0%)
28	DB	1.10	3/2872 (0.1%)	0.91	0/4478
29	CC	0.45	0/2121	0.74	0/2852
29	DC	0.49	0/2121	0.75	0/2852
30	CD	0.44	0/1586	0.68	0/2134
31	CA	1.05	65/69165 (0.1%)	0.88	16/107896 (0.0%)
32	DD	0.53	0/1576	0.70	0/2119
33	CE	0.43	0/1571	0.72	0/2113
33	DE	0.48	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.69	0/1926
34	DF	0.47	0/1434	0.73	0/1926
35	CG	0.41	0/1343	0.68	1/1816 (0.1%)
35	DG	0.45	0/1343	0.67	0/1816
36	CH	0.46	0/1121	0.72	1/1515 (0.1%)
36	DH	0.47	0/1121	0.70	0/1515
37	CJ	0.54	0/993	0.68	0/1341
37	DJ	0.54	0/993	0.68	0/1341
38	CK	0.43	0/1152	0.71	0/1551
38	DK	0.58	0/1152	0.75	0/1551
39	CL	0.47	0/947	0.75	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DL	0.53	0/955	0.77	0/1279
40	CM	0.45	0/1062	0.73	1/1413 (0.1%)
40	DM	0.51	0/1062	0.71	0/1413
41	CN	0.45	0/1081	0.72	0/1443
41	DN	0.55	0/1092	0.78	0/1457
42	CO	0.45	0/973	0.72	0/1301
42	DO	0.59	0/1006	0.78	0/1345
43	CP	0.44	0/902	0.70	0/1209
43	DP	0.51	0/910	0.70	0/1219
44	CQ	0.42	0/929	0.75	0/1242
44	DQ	0.50	0/929	0.74	0/1242
45	CR	0.47	0/960	0.70	0/1278
45	DR	0.61	0/960	0.75	0/1278
46	CS	0.45	0/829	0.77	0/1107
46	DS	0.59	0/829	0.82	0/1107
47	CT	0.42	0/864	0.78	0/1156
47	DT	0.57	0/864	0.80	0/1156
48	CU	0.46	0/744	0.72	0/994
48	DU	0.52	0/744	0.72	0/994
49	CV	0.47	0/787	0.79	0/1051
49	DV	0.49	0/787	0.82	0/1051
50	CW	0.42	0/766	0.69	0/1025
50	DW	0.52	0/766	0.71	0/1025
51	CX	0.39	0/576	0.66	0/762
51	DX	0.51	0/598	0.69	0/790
52	CY	0.40	0/635	0.70	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.44	0/502	0.69	0/667
53	DZ	0.50	0/502	0.69	0/667
54	DI	0.52	0/1037	0.78	1/1402 (0.1%)
55	DA	1.19	83/69364 (0.1%)	0.93	24/108207 (0.0%)
All	All	0.95	178/309271 (0.1%)	0.85	53/462220 (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
10	BJ	0	1
28	DB	0	1
31	CA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DA	0	26
All	All	0	29

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-10.08	1.26	1.42
31	CA	2225	A	C3'-O3'	9.82	1.55	1.42
31	CA	1936	A	N9-C4	-9.23	1.32	1.37
55	DA	2097	A	O5'-C5'	-8.54	1.29	1.42
55	DA	2585	U	C1'-N1	8.38	1.61	1.48

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	9.57	115.86	108.20
31	CA	2425	A	P-O3'-C3'	8.79	130.24	119.70
31	CA	271	G	P-O3'-C3'	7.72	128.96	119.70
1	BA	2	A	OP1-P-OP2	-7.50	108.34	119.60
1	AA	1	A	OP1-P-OP2	-7.15	108.88	119.60

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	BJ	37	ARG	Mainchain
31	CA	780	G	Sidechain
55	DA	329	G	Sidechain
55	DA	452	G	Sidechain
28	DB	13	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32932	0	16593	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	32910	0	16582	182	0
2	AB	1753	0	1780	14	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	18	0
4	BD	1643	0	1707	19	0
5	AE	1144	0	1185	17	0
5	BE	1105	0	1148	26	0
6	AF	862	0	864	12	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	17	0
7	BG	1182	0	1238	16	0
8	AH	979	0	1031	9	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	11	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	8	0
10	BJ	787	0	828	11	0
11	AK	877	0	887	11	0
11	BK	877	0	887	13	0
12	AL	957	0	1017	14	0
12	BL	957	0	1017	16	0
13	AM	884	0	941	11	0
13	BM	884	0	941	14	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	3	0
15	BO	714	0	734	7	0
16	AP	649	0	666	5	0
16	BP	649	0	666	8	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	5	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	11	0
20	BT	665	0	714	8	0
21	AU	465	0	491	6	0
21	BU	465	0	491	5	0
22	C1	444	0	458	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	10	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	7	0
25	C4	504	0	572	3	0
25	D4	504	0	572	7	0
26	C5	302	0	340	5	0
26	D5	302	0	340	4	0
27	C0	449	0	488	4	0
27	D0	463	0	504	7	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	10	0
29	CC	2082	0	2154	24	0
29	DC	2082	0	2154	22	0
30	CD	1565	0	1616	22	0
31	CA	62229	0	31319	399	0
32	DD	1576	0	1627	29	0
33	CE	1552	0	1619	20	0
33	DE	1552	0	1619	20	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	26	0
35	CG	1323	0	1371	16	0
35	DG	1323	0	1371	14	0
36	CH	1110	0	1148	9	0
36	DH	1110	0	1148	10	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	10	0
38	CK	1129	0	1162	13	0
38	DK	1129	0	1162	14	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	7	0
40	CM	1053	0	1129	21	0
40	DM	1053	0	1129	16	0
41	CN	1075	0	1154	15	0
41	DN	1092	0	1177	17	0
42	CO	960	0	1000	16	0
42	DO	993	0	1034	16	0
43	CP	892	0	923	14	0
43	DP	900	0	935	17	0
44	CQ	917	0	962	8	0
44	DQ	917	0	962	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CR	947	0	1019	13	0
45	DR	947	0	1019	20	0
46	CS	816	0	839	16	0
46	DS	816	0	839	20	0
47	CT	857	0	922	16	0
47	DT	857	0	922	14	0
48	CU	738	0	807	9	0
48	DU	738	0	807	6	0
49	CV	779	0	831	12	0
49	DV	779	0	831	8	0
50	CW	753	0	780	6	0
50	DW	753	0	780	7	0
51	CX	569	0	581	8	0
51	DX	591	0	606	14	0
52	CY	625	0	652	11	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	5	0
53	DZ	501	0	531	6	0
54	DI	1023	0	1052	26	0
55	DA	62423	0	31411	382	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	0	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	1	0
57	DS	13	0	18	0	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	4	0
58	DT	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	1	0
61	DA	42	0	60	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	1	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	4	0
62	DB	8	0	12	0	0
63	D1	10	0	14	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	2	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	3	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	5	0	0	0	0
69	AL	7	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	1	0
69	AO	1	0	0	0	0
69	AP	1	0	0	0	0
69	AQ	1	0	0	0	0
69	AS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AT	2	0	0	0	0
69	AU	4	0	0	0	0
69	BA	287	0	0	2	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0
69	BL	3	0	0	0	0
69	BN	1	0	0	0	0
69	BO	1	0	0	0	0
69	BP	4	0	0	0	0
69	BR	1	0	0	0	0
69	BT	5	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	CA	696	0	0	3	0
69	CB	13	0	0	0	0
69	CC	11	0	0	0	0
69	CD	4	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	2	0
69	D1	37	0	0	0	0
69	D2	5	0	0	0	0
69	D3	30	0	0	0	0
69	D4	40	0	0	1	0
69	D5	13	0	0	1	0
69	DA	4824	0	0	39	0
69	DB	203	0	0	3	0
69	DC	100	0	0	1	0
69	DD	97	0	0	5	0
69	DE	54	0	0	2	0
69	DF	13	0	0	1	0
69	DG	9	0	0	0	0
69	DH	2	0	0	0	0
69	DK	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DL	50	0	0	0	0
69	DM	60	0	0	0	0
69	DN	81	0	0	1	0
69	DO	42	0	0	1	0
69	DP	42	0	0	2	0
69	DQ	32	0	0	1	0
69	DR	68	0	0	3	0
69	DS	52	0	0	5	0
69	DT	65	0	0	1	0
69	DU	24	0	0	0	0
69	DV	19	0	0	1	0
69	DW	33	0	0	1	0
69	DX	33	0	0	2	0
69	DY	11	0	0	1	0
69	DZ	7	0	0	0	0
All	All	295119	0	194415	2066	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 2066 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)
26:D5:26:ILE:CD1	26:D5:26:ILE:CG1	1.85	1.50
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.16
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.62	0.99
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.44	0.95
31:CA:1311:G:H21	31:CA:1603:A:H62	1.16	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	6	30
2	BB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	6	30
3	AC	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	15	47
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	10	38
4	AD	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	12	40
5	BE	148/155 (96%)	126 (85%)	17 (12%)	5 (3%)	3	23
6	AF	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	47
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	4	24
7	AG	149/151 (99%)	137 (92%)	10 (7%)	2 (1%)	12	40
7	BG	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	12	40
8	AH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	37
8	BH	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	51
9	AI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
9	BI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
10	AJ	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	4	24
10	BJ	96/99 (97%)	78 (81%)	14 (15%)	4 (4%)	3	18
11	AK	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	17	49
11	BK	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	17	49
12	AL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	9	36
12	BL	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	9	36
13	AM	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	3	22
13	BM	112/114 (98%)	96 (86%)	10 (9%)	6 (5%)	2	13
14	AN	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	47
14	BN	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	47
15	AO	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	BO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	43
16	AP	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	5	28
16	BP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	3	20
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	3	20
17	BQ	78/80 (98%)	69 (88%)	5 (6%)	4 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	6 (8%)	3 (4%)	3	20
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	5	28
20	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	BT	83/86 (96%)	78 (94%)	4 (5%)	1 (1%)	13	43
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	45 (83%)	6 (11%)	3 (6%)	2	12
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	4 (8%)	1 (2%)	7	32
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6	30
24	D3	44/46 (96%)	44 (100%)	0	0	100	100
25	C4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	37
25	D4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	37
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	3	22
27	D0	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
29	CC	269/272 (99%)	243 (90%)	21 (8%)	5 (2%)	8	34
29	DC	269/272 (99%)	245 (91%)	19 (7%)	5 (2%)	8	34
30	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	11	39
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
33	CE	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	29	61
33	DE	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
34	CF	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
34	DF	175/178 (98%)	163 (93%)	12 (7%)	0	100	100
35	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	6	30
35	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	25	57
36	CH	147/149 (99%)	129 (88%)	12 (8%)	6 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DH	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	5	27
37	CJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	25
37	DJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	25
38	CK	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	7	32
38	DK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	7	32
39	CL	120/123 (98%)	111 (92%)	7 (6%)	2 (2%)	9	36
39	DL	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	19	51
40	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	3	18
40	DM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	32
41	CN	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	DN	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	CO	118/127 (93%)	98 (83%)	16 (14%)	4 (3%)	3	23
42	DO	123/127 (97%)	106 (86%)	16 (13%)	1 (1%)	19	51
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	CQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	49
44	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	49
45	CR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
45	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
46	CS	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	7	33
46	DS	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	15	47
47	CT	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
47	DT	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	49
48	CU	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	14	45
48	DU	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	14	45
49	CV	100/103 (97%)	85 (85%)	12 (12%)	3 (3%)	4	25
49	DV	100/103 (97%)	87 (87%)	11 (11%)	2 (2%)	7	33
50	CW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	45
50	DW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	45
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	CY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
52	DY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
53	CZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	36
53	DZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	36
54	DI	133/135 (98%)	112 (84%)	17 (13%)	4 (3%)	4	25
All	All	11407/11679 (98%)	10425 (91%)	815 (7%)	167 (2%)	10	38

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	ARG
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA

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	186/186 (100%)	168 (90%)	18 (10%)	8	30
2	BB	186/186 (100%)	168 (90%)	18 (10%)	8	30
3	AC	170/170 (100%)	158 (93%)	12 (7%)	14	44
3	BC	170/170 (100%)	155 (91%)	15 (9%)	10	34
4	AD	172/172 (100%)	163 (95%)	9 (5%)	23	55
4	BD	172/172 (100%)	162 (94%)	10 (6%)	20	51
5	AE	118/118 (100%)	102 (86%)	16 (14%)	3	16
5	BE	113/118 (96%)	97 (86%)	16 (14%)	3	15
6	AF	92/92 (100%)	83 (90%)	9 (10%)	8	29
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	22
7	AG	124/124 (100%)	108 (87%)	16 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BG	124/124 (100%)	107 (86%)	17 (14%)	3	16
8	AH	104/104 (100%)	92 (88%)	12 (12%)	5	22
8	BH	104/104 (100%)	93 (89%)	11 (11%)	6	25
9	AI	105/105 (100%)	97 (92%)	8 (8%)	13	40
9	BI	105/105 (100%)	97 (92%)	8 (8%)	13	40
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	15	45
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	7	26
11	AK	90/99 (91%)	86 (96%)	4 (4%)	28	60
11	BK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	AL	102/102 (100%)	96 (94%)	6 (6%)	19	50
12	BL	102/102 (100%)	95 (93%)	7 (7%)	15	45
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	21
13	BM	92/92 (100%)	81 (88%)	11 (12%)	5	21
14	AN	83/83 (100%)	81 (98%)	2 (2%)	49	74
14	BN	83/83 (100%)	81 (98%)	2 (2%)	49	74
15	AO	76/76 (100%)	71 (93%)	5 (7%)	16	47
15	BO	76/76 (100%)	68 (90%)	8 (10%)	7	26
16	AP	65/65 (100%)	60 (92%)	5 (8%)	13	40
16	BP	65/65 (100%)	61 (94%)	4 (6%)	18	49
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	20
17	BQ	74/74 (100%)	64 (86%)	10 (14%)	4	17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	76
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	28
19	BS	70/70 (100%)	64 (91%)	6 (9%)	10	36
20	AT	65/65 (100%)	54 (83%)	11 (17%)	2	9
20	BT	65/65 (100%)	54 (83%)	11 (17%)	2	9
21	AU	48/48 (100%)	44 (92%)	4 (8%)	11	37
21	BU	48/48 (100%)	44 (92%)	4 (8%)	11	37
22	C1	47/47 (100%)	46 (98%)	1 (2%)	53	76
22	D1	47/47 (100%)	45 (96%)	2 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	C2	45/46 (98%)	42 (93%)	3 (7%)	16	46
23	D2	45/46 (98%)	41 (91%)	4 (9%)	9	33
24	C3	38/38 (100%)	35 (92%)	3 (8%)	12	39
24	D3	38/38 (100%)	35 (92%)	3 (8%)	12	39
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19	50
25	D4	51/51 (100%)	47 (92%)	4 (8%)	12	39
26	C5	34/34 (100%)	31 (91%)	3 (9%)	10	34
26	D5	34/34 (100%)	31 (91%)	3 (9%)	10	34
27	C0	48/48 (100%)	42 (88%)	6 (12%)	4	19
27	D0	49/48 (102%)	44 (90%)	5 (10%)	7	27
29	CC	216/217 (100%)	202 (94%)	14 (6%)	17	47
29	DC	216/217 (100%)	204 (94%)	12 (6%)	21	53
30	CD	164/164 (100%)	154 (94%)	10 (6%)	18	49
32	DD	163/163 (100%)	153 (94%)	10 (6%)	18	49
33	CE	165/165 (100%)	147 (89%)	18 (11%)	6	25
33	DE	165/165 (100%)	153 (93%)	12 (7%)	14	42
34	CF	148/149 (99%)	131 (88%)	17 (12%)	5	22
34	DF	148/149 (99%)	132 (89%)	16 (11%)	6	25
35	CG	137/137 (100%)	129 (94%)	8 (6%)	20	51
35	DG	137/137 (100%)	129 (94%)	8 (6%)	20	51
36	CH	114/114 (100%)	100 (88%)	14 (12%)	4	20
36	DH	114/114 (100%)	101 (89%)	13 (11%)	5	22
37	CJ	104/105 (99%)	95 (91%)	9 (9%)	10	35
37	DJ	104/105 (99%)	95 (91%)	9 (9%)	10	35
38	CK	116/116 (100%)	110 (95%)	6 (5%)	23	55
38	DK	116/116 (100%)	111 (96%)	5 (4%)	29	61
39	CL	103/104 (99%)	95 (92%)	8 (8%)	12	39
39	DL	104/104 (100%)	93 (89%)	11 (11%)	6	25
40	CM	103/103 (100%)	94 (91%)	9 (9%)	10	35
40	DM	103/103 (100%)	97 (94%)	6 (6%)	20	51
41	CN	108/108 (100%)	98 (91%)	10 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DN	109/108 (101%)	98 (90%)	11 (10%)	7	28
42	CO	100/103 (97%)	92 (92%)	8 (8%)	12	38
42	DO	102/103 (99%)	94 (92%)	8 (8%)	12	39
43	CP	86/87 (99%)	77 (90%)	9 (10%)	7	26
43	DP	87/87 (100%)	78 (90%)	9 (10%)	7	27
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	11	37
44	DQ	99/99 (100%)	92 (93%)	7 (7%)	14	44
45	CR	89/89 (100%)	81 (91%)	8 (9%)	9	33
45	DR	89/89 (100%)	83 (93%)	6 (7%)	16	46
46	CS	84/84 (100%)	74 (88%)	10 (12%)	5	21
46	DS	84/84 (100%)	75 (89%)	9 (11%)	6	25
47	CT	93/93 (100%)	83 (89%)	10 (11%)	6	25
47	DT	93/93 (100%)	85 (91%)	8 (9%)	10	36
48	CU	80/84 (95%)	67 (84%)	13 (16%)	2	10
48	DU	80/84 (95%)	72 (90%)	8 (10%)	7	28
49	CV	83/84 (99%)	75 (90%)	8 (10%)	8	30
49	DV	83/84 (99%)	77 (93%)	6 (7%)	14	43
50	CW	78/78 (100%)	70 (90%)	8 (10%)	7	27
50	DW	78/78 (100%)	72 (92%)	6 (8%)	13	40
51	CX	56/58 (97%)	54 (96%)	2 (4%)	35	65
51	DX	58/58 (100%)	54 (93%)	4 (7%)	15	45
52	CY	67/67 (100%)	63 (94%)	4 (6%)	19	50
52	DY	67/67 (100%)	62 (92%)	5 (8%)	13	41
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	41
53	DZ	54/54 (100%)	51 (94%)	3 (6%)	21	53
54	DI	103/103 (100%)	91 (88%)	12 (12%)	5	21
All	All	9461/9514 (99%)	8645 (91%)	816 (9%)	10	36

5 of 816 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	BT	66	LEU
33	CE	149	ILE

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Mol	Chain	Res	Type
45	DR	117	LEU
23	D2	12	VAL
30	CD	32	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
5	BE	89	HIS
16	BP	63	GLN
42	DO	13	ASN
5	BE	97	GLN
7	BG	142	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	296 (19%)	48 (3%)
1	BA	1529/1534 (99%)	300 (19%)	52 (3%)
28	CB	117/120 (97%)	13 (11%)	2 (1%)
28	DB	119/120 (99%)	13 (10%)	1 (0%)
31	CA	2892/2904 (99%)	572 (19%)	110 (3%)
55	DA	2880/2904 (99%)	490 (17%)	73 (2%)
All	All	9067/9116 (99%)	1684 (18%)	286 (3%)

5 of 1684 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 286 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	603	A
31	CA	1300	G
55	DA	1939	5MU
31	CA	684	G

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Mol	Chain	Res	Type
31	CA	973	A

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

75 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
55	2MA	DA	2503	55,56	17,25,26	0.95	0	19,37,40	1.93	4 (21%)
55	PSU	DA	2457	55	17,21,22	1.39	3 (17%)	20,30,33	5.27	4 (20%)
31	OMC	CA	2498	31,56	15,22,23	0.94	1 (6%)	17,31,34	1.11	1 (5%)
1	2MG	BA	966	1	19,26,27	1.31	2 (10%)	21,38,41	2.43	4 (19%)
55	PSU	DA	2504	55	17,21,22	1.24	3 (17%)	20,30,33	5.30	4 (20%)
55	7MG	DA	2069	55	22,26,27	1.71	3 (13%)	28,39,42	2.37	6 (21%)
1	2MG	BA	1207	1	19,26,27	1.22	2 (10%)	21,38,41	2.40	4 (19%)
31	PSU	CA	955	31	17,21,22	1.17	2 (11%)	20,30,33	5.31	5 (25%)
1	2MG	AA	1516	1	19,26,27	1.15	2 (10%)	21,38,41	2.40	4 (19%)
1	MA6	AA	1518	1	19,26,27	0.86	0	18,38,41	1.25	1 (5%)
31	PSU	CA	2504	31	17,21,22	1.22	3 (17%)	20,30,33	5.32	4 (20%)
41	4D4	DN	81[B]	-	9,11,12	1.73	2 (22%)	8,13,15	2.07	2 (25%)
41	4D4	DN	81[A]	-	9,11,12	1.60	1 (11%)	8,13,15	2.99	2 (25%)
31	2MG	CA	1835	31	19,26,27	1.14	2 (10%)	21,38,41	2.38	4 (19%)
1	4OC	BA	1402	1	16,23,24	0.79	1 (6%)	17,32,35	0.84	1 (5%)
55	6MZ	DA	2030	55	18,25,26	0.78	0	16,36,39	0.98	1 (6%)
1	UR3	BA	1498	1	14,22,23	1.01	1 (7%)	15,32,35	0.56	0
31	2MA	CA	2503	31	17,25,26	0.98	0	19,37,40	2.01	4 (21%)
1	MA6	BA	1519	1	19,26,27	0.90	0	18,38,41	0.87	0
1	2MG	AA	966	1	19,26,27	1.38	2 (10%)	21,38,41	2.34	3 (14%)
55	PSU	DA	2604	55	17,21,22	1.51	4 (23%)	20,30,33	5.31	4 (20%)
55	PSU	DA	2580	55	17,21,22	1.31	2 (11%)	20,30,33	5.35	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	CA	2580	31	17,21,22	1.39	3 (17%)	20,30,33	5.32	5 (25%)
1	PSU	BA	516	1	17,21,22	1.39	3 (17%)	20,30,33	5.29	4 (20%)
32	MEQ	DD	150[B]	32	8,9,10	1.65	1 (12%)	5,10,12	1.46	1 (20%)
55	PSU	DA	1911	55	17,21,22	1.28	2 (11%)	20,30,33	5.26	4 (20%)
55	OMC	DA	2498	55,56	15,22,23	1.25	2 (13%)	17,31,34	1.10	1 (5%)
12	D2T	BL	89	12	4,9,10	0.66	0	3,11,13	0.88	0
1	2MG	BA	1516	1	19,26,27	1.20	2 (10%)	21,38,41	2.42	4 (19%)
1	5MC	AA	1407	1	15,22,23	0.80	1 (6%)	19,32,35	1.21	2 (10%)
31	PSU	CA	1911	31	17,21,22	1.26	2 (11%)	20,30,33	5.30	4 (20%)
32	MEQ	DD	150[A]	32	8,9,10	0.39	0	5,10,12	0.54	0
55	OMG	DA	2251	55	18,26,27	1.01	1 (5%)	20,38,41	2.50	5 (25%)
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	1.36	1 (5%)
55	PSU	DA	2605	55	17,21,22	1.26	2 (11%)	20,30,33	5.27	4 (20%)
55	5MU	DA	747	55	15,22,23	1.22	2 (13%)	16,32,35	3.70	1 (6%)
1	5MC	AA	967	1	15,22,23	0.87	1 (6%)	19,32,35	1.16	2 (10%)
1	7MG	BA	527	1	22,26,27	1.73	3 (13%)	28,39,42	2.47	8 (28%)
55	2MG	DA	1835	55	19,26,27	1.25	2 (10%)	21,38,41	2.43	4 (19%)
1	7MG	AA	527	1	22,26,27	1.61	3 (13%)	28,39,42	2.50	7 (25%)
31	PSU	CA	746	31,56	17,21,22	1.44	3 (17%)	20,30,33	5.32	4 (20%)
31	PSU	CA	2457	31	17,21,22	1.59	4 (23%)	20,30,33	5.30	4 (20%)
55	5MC	DA	1962	55	15,22,23	1.10	2 (13%)	19,32,35	1.19	2 (10%)
55	PSU	DA	955	55	17,21,22	1.43	3 (17%)	20,30,33	5.32	5 (25%)
31	3TD	CA	1915	31	17,22,23	1.29	4 (23%)	19,32,35	1.51	2 (10%)
31	5MU	CA	1939	31	15,22,23	1.20	2 (13%)	16,32,35	3.65	1 (6%)
31	PSU	CA	1917	31	17,21,22	1.28	2 (11%)	20,30,33	5.32	4 (20%)
31	5MC	CA	1962	31	15,22,23	0.74	0	19,32,35	1.20	2 (10%)
1	5MC	BA	1407	1	15,22,23	0.90	0	19,32,35	1.17	2 (10%)
55	PSU	DA	746	55,56	17,21,22	1.75	4 (23%)	20,30,33	5.31	5 (25%)
12	D2T	AL	89	12	4,9,10	0.59	0	3,11,13	0.94	0
55	PSU	DA	1917	55	17,21,22	1.44	3 (17%)	20,30,33	5.29	4 (20%)
31	PSU	CA	2605	31	17,21,22	1.21	2 (11%)	20,30,33	5.34	4 (20%)
31	6MZ	CA	1618	31	18,25,26	0.90	1 (5%)	16,36,39	1.04	1 (6%)
1	2MG	AA	1207	1	19,26,27	1.18	2 (10%)	21,38,41	2.39	4 (19%)
41	4D4	CN	81	41	9,11,12	2.26	2 (22%)	8,13,15	2.20	2 (25%)
31	6MZ	CA	2030	31	18,25,26	0.71	0	16,36,39	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	2MG	DA	2445	55	19,26,27	1.14	1 (5%)	21,38,41	2.40	4 (19%)
1	PSU	AA	516	1,56	17,21,22	1.40	3 (17%)	20,30,33	5.32	4 (20%)
55	6MZ	DA	1618	55	18,25,26	1.09	0	16,36,39	2.01	2 (12%)
55	1MG	DA	745	55	18,26,27	1.15	2 (11%)	19,39,42	1.20	2 (10%)
1	MA6	AA	1519	1	19,26,27	0.93	1 (5%)	18,38,41	0.90	1 (5%)
31	7MG	CA	2069	31	22,26,27	1.70	4 (18%)	28,39,42	2.37	7 (25%)
31	OMG	CA	2251	31	18,26,27	1.27	2 (11%)	20,38,41	2.51	4 (20%)
31	1MG	CA	745	31	18,26,27	1.20	2 (11%)	19,39,42	1.29	2 (10%)
1	UR3	AA	1498	1	14,22,23	1.05	1 (7%)	15,32,35	0.53	0
1	4OC	AA	1402	1	16,23,24	0.79	1 (6%)	17,32,35	0.79	1 (5%)
55	3TD	DA	1915	55	17,22,23	1.28	2 (11%)	19,32,35	1.50	2 (10%)
31	OMU	CA	2552	31	14,22,23	1.27	2 (14%)	14,31,34	1.16	1 (7%)
31	5MU	CA	747	31	15,22,23	1.13	1 (6%)	16,32,35	3.68	2 (12%)
55	5MU	DA	1939	55	15,22,23	1.58	2 (13%)	16,32,35	3.68	2 (12%)
55	OMU	DA	2552	55	14,22,23	1.28	2 (14%)	14,31,34	1.10	1 (7%)
1	5MC	BA	967	1	15,22,23	0.87	0	19,32,35	1.16	2 (10%)
31	2MG	CA	2445	31	19,26,27	1.22	1 (5%)	21,38,41	2.31	3 (14%)
55	H2U	DA	2449	55	18,21,22	0.84	0	21,30,33	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	2MA	DA	2503	55,56	-	2/3/25/26	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	2/7/27/28	0/2/2/2
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
55	PSU	DA	2504	55	-	2/7/25/26	0/2/2/2
55	7MG	DA	2069	55	-	2/7/37/38	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	PSU	CA	2504	31	-	2/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	4/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	4D4	DN	81[A]	-	-	1/11/12/14	-
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/5/25/26	0/2/2/2
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
55	PSU	DA	2604	55	-	1/7/25/26	0/2/2/2
55	PSU	DA	2580	55	-	2/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	3/8/9/11	-
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/7/27/28	0/2/2/2
12	D2T	BL	89	12	-	3/3/12/14	-
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
55	OMG	DA	2251	55	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/5/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	2MG	DA	1835	55	-	0/5/27/28	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
31	PSU	CA	746	31,56	-	1/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/5/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	2/5/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/5/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/5/25/26	0/2/2/2
55	PSU	DA	746	55,56	-	3/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/3/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
55	2MG	DA	2445	55	-	2/5/27/28	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
31	7MG	CA	2069	31	-	1/7/37/38	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/7/27/28	0/2/2/2
31	5MU	CA	747	31	-	0/5/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/5/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/7/27/28	0/2/2/2
1	5MC	BA	967	1	-	0/5/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	CN	81	4D4	CZ-NE	6.18	1.45	1.33
55	DA	2069	7MG	C8-N9	-5.42	1.33	1.45
1	BA	527	7MG	C8-N9	-5.38	1.33	1.45
31	CA	2069	7MG	C8-N9	-5.23	1.33	1.45
1	AA	527	7MG	C8-N9	-5.21	1.33	1.45

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	955	PSU	N1-C2-N3	-17.20	114.76	128.43
31	CA	2605	PSU	N1-C2-N3	-17.19	114.76	128.43
31	CA	1917	PSU	N1-C2-N3	-17.17	114.78	128.43
1	AA	516	PSU	N1-C2-N3	-17.17	114.78	128.43
31	CA	746	PSU	N1-C2-N3	-17.15	114.79	128.43

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	CA	2498	OMC	C2'-C1'-N1-C6
41	DN	81[B]	4D4	CA-CB-CG-CD
41	DN	81[A]	4D4	O-C-CA-CB
32	DD	150[B]	MEQ	N-CA-CB-CG
12	BL	89	D2T	O-C-CA-CB

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	BA	1402	4OC	1	0
55	DA	2030	6MZ	2	0
1	BA	1519	MA6	1	0
32	DD	150[B]	MEQ	1	0
55	DA	2498	OMC	1	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
55	DA	747	5MU	1	0
31	CA	1939	5MU	1	0
31	CA	2030	6MZ	5	0
1	AA	1519	MA6	1	0
31	CA	745	1MG	1	0
1	AA	1402	4OC	1	0
31	CA	747	5MU	1	0
1	BA	967	5MC	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	GUN	DA	3211	-	9,12,12	1.55	2 (22%)	8,17,17	3.91	4 (50%)
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.07	0
59	PUT	AA	1672	-	5,5,5	0.08	0	4,4,4	0.14	0
62	EDO	DA	3003	-	3,3,3	0.68	0	2,2,2	0.32	0
59	PUT	DA	3213	-	5,5,5	0.24	0	4,4,4	0.18	0
59	PUT	AA	1675	-	5,5,5	0.18	0	4,4,4	0.08	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.16	0
59	PUT	DM	201	-	5,5,5	0.22	0	4,4,4	0.27	0
59	PUT	AA	1674	-	5,5,5	0.15	0	4,4,4	0.12	0
58	MPD	DA	3204	-	7,7,7	0.71	0	9,10,10	0.51	0
59	PUT	DA	3222	-	5,5,5	0.27	0	4,4,4	0.50	0
57	PG4	DA	3216	-	12,12,12	0.14	0	11,11,11	0.15	0
62	EDO	DA	3197	-	3,3,3	0.67	0	2,2,2	0.16	0
57	PG4	AA	1670	-	12,12,12	0.18	0	11,11,11	0.20	0
62	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.22	0
64	SPD	DA	3187	-	9,9,9	0.12	0	8,8,8	0.21	0
63	PGE	D1	102	-	9,9,9	0.11	0	8,8,8	0.13	0
62	EDO	DA	3002	-	3,3,3	0.63	0	2,2,2	0.15	0
57	PG4	DA	3193	-	12,12,12	0.28	0	11,11,11	0.26	0
66	ACY	DA	3191	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
57	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.19	0
62	EDO	DA	3215	-	3,3,3	0.72	0	2,2,2	0.23	0
63	PGE	DA	3214	-	9,9,9	0.24	0	8,8,8	0.34	0
61	PEG	DP	201	-	6,6,6	0.16	0	5,5,5	0.13	0
64	SPD	DA	3224	-	9,9,9	0.13	0	8,8,8	0.23	0
66	ACY	DA	3202	-	1,3,3	0.01	0	0,3,3	0.00	-
57	PG4	DS	202	-	12,12,12	0.19	0	11,11,11	0.23	0
61	PEG	DA	3218	-	6,6,6	0.15	0	5,5,5	0.08	0
57	PG4	DQ	202	-	12,12,12	0.13	0	11,11,11	0.15	0
68	TRS	DA	3220	-	7,7,7	0.23	0	9,9,9	0.22	0
61	PEG	DA	3200	-	6,6,6	0.23	0	5,5,5	0.09	0
59	PUT	DA	3189	-	5,5,5	0.09	0	4,4,4	0.22	0
61	PEG	DA	3201	-	6,6,6	0.14	0	5,5,5	0.15	0
58	MPD	DA	3207	-	7,7,7	0.37	0	9,10,10	0.52	0
61	PEG	DQ	201	-	6,6,6	0.22	0	5,5,5	0.12	0
65	1PE	DA	3203	-	15,15,15	0.21	0	14,14,14	0.25	0
58	MPD	DA	3210	-	7,7,7	0.82	0	9,10,10	0.34	0
62	EDO	DA	3209	-	3,3,3	0.53	0	2,2,2	0.33	0
59	PUT	DA	3188	-	5,5,5	0.12	0	4,4,4	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DN	201	-	7,7,7	1.17	1 (14%)	9,10,10	0.51	0
63	PGE	DA	3225	-	9,9,9	0.26	0	8,8,8	0.31	0
63	PGE	DA	3217	-	9,9,9	0.22	0	8,8,8	0.19	0
59	PUT	DA	3223	-	5,5,5	0.20	0	4,4,4	0.17	0
58	MPD	DT	202	-	7,7,7	0.78	0	9,10,10	0.50	0
59	PUT	DA	3221	-	5,5,5	0.25	0	4,4,4	0.13	0
63	PGE	DS	201	-	9,9,9	0.22	0	8,8,8	0.18	0
59	PUT	DA	3184	-	5,5,5	0.17	0	4,4,4	0.21	0
61	PEG	DA	3199	-	6,6,6	0.18	0	5,5,5	0.12	0
66	ACY	DA	3196	-	1,3,3	4.11	1 (100%)	0,3,3	0.00	-
61	PEG	DA	3226	-	6,6,6	0.20	0	5,5,5	0.06	0
63	PGE	DD	301	-	9,9,9	0.21	0	8,8,8	0.16	0
58	MPD	DE	301	-	7,7,7	0.67	0	9,10,10	0.43	0
63	PGE	D3	101	-	9,9,9	0.22	0	8,8,8	0.11	0
58	MPD	DA	3190	-	7,7,7	0.53	0	9,10,10	0.45	0
59	PUT	DA	3205	-	5,5,5	0.18	0	4,4,4	0.16	0
62	EDO	DA	3194	-	3,3,3	0.74	0	2,2,2	0.13	0
59	PUT	DA	3212	-	5,5,5	0.25	0	4,4,4	0.13	0
59	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.16	0
62	EDO	DA	3198	-	3,3,3	0.76	0	2,2,2	0.25	0
61	PEG	AL	201	-	6,6,6	0.19	0	5,5,5	0.15	0
62	EDO	DB	210	-	3,3,3	0.69	0	2,2,2	0.15	0
57	PG4	DR	201	-	12,12,12	0.22	0	11,11,11	0.25	0
62	EDO	DB	211	-	3,3,3	0.59	0	2,2,2	0.31	0
62	EDO	D0	101	-	3,3,3	0.63	0	2,2,2	0.55	0
58	MPD	DK	201	-	7,7,7	1.02	1 (14%)	9,10,10	0.37	0
61	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.20	0
59	PUT	DA	3195	-	5,5,5	0.28	0	4,4,4	0.25	0
58	MPD	DT	201	-	7,7,7	0.76	0	9,10,10	0.30	0
58	MPD	DA	3192	-	7,7,7	0.84	0	9,10,10	0.65	0
58	MPD	DE	302	-	7,7,7	0.96	1 (14%)	9,10,10	0.72	0
62	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.31	0
64	SPD	DA	3183	-	9,9,9	0.22	0	8,8,8	0.34	0
58	MPD	AA	1676	-	7,7,7	0.74	0	9,10,10	0.54	0
63	PGE	DU	201	-	9,9,9	0.32	0	8,8,8	0.29	0
59	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.09	0
63	PGE	DA	3186	-	9,9,9	0.33	0	8,8,8	0.35	0
58	MPD	DS	203	-	7,7,7	0.36	0	9,10,10	0.38	0
64	SPD	DA	3206	-	9,9,9	0.23	0	8,8,8	0.21	0
58	MPD	AA	1671	-	7,7,7	0.43	0	9,10,10	0.49	0
61	PEG	DA	3227	-	6,6,6	0.24	0	5,5,5	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GUN	DA	3211	-	-	-	0/2/2/2
61	PEG	DL	201	-	-	3/4/4/4	-
59	PUT	AA	1672	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-
59	PUT	DA	3213	-	-	1/3/3/3	-
59	PUT	AA	1675	-	-	1/3/3/3	-
65	1PE	DA	3185	-	-	4/13/13/13	-
59	PUT	DM	201	-	-	0/3/3/3	-
59	PUT	AA	1674	-	-	0/3/3/3	-
58	MPD	DA	3204	-	-	2/5/5/5	-
59	PUT	DA	3222	-	-	0/3/3/3	-
57	PG4	DA	3216	-	-	5/10/10/10	-
62	EDO	DA	3197	-	-	0/1/1/1	-
57	PG4	AA	1670	-	-	6/10/10/10	-
62	EDO	D1	101	-	-	0/1/1/1	-
64	SPD	DA	3187	-	-	2/7/7/7	-
63	PGE	D1	102	-	-	5/7/7/7	-
62	EDO	DA	3002	-	-	0/1/1/1	-
57	PG4	DA	3193	-	-	4/10/10/10	-
57	PG4	BA	1642	-	-	5/10/10/10	-
62	EDO	DA	3215	-	-	0/1/1/1	-
63	PGE	DA	3214	-	-	4/7/7/7	-
61	PEG	DP	201	-	-	1/4/4/4	-
64	SPD	DA	3224	-	-	3/7/7/7	-
57	PG4	DS	202	-	-	4/10/10/10	-
61	PEG	DA	3218	-	-	1/4/4/4	-
57	PG4	DQ	202	-	-	1/10/10/10	-
68	TRS	DA	3220	-	-	0/9/9/9	-
61	PEG	DA	3200	-	-	1/4/4/4	-
59	PUT	DA	3189	-	-	0/3/3/3	-
61	PEG	DA	3201	-	-	1/4/4/4	-
58	MPD	DA	3207	-	-	2/5/5/5	-
61	PEG	DQ	201	-	-	2/4/4/4	-
65	1PE	DA	3203	-	-	5/13/13/13	-
58	MPD	DA	3210	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	EDO	DA	3209	-	-	0/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
58	MPD	DN	201	-	-	0/5/5/5	-
63	PGE	DA	3225	-	-	4/7/7/7	-
63	PGE	DA	3217	-	-	3/7/7/7	-
59	PUT	DA	3223	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	1/5/5/5	-
59	PUT	DA	3221	-	-	0/3/3/3	-
63	PGE	DS	201	-	-	4/7/7/7	-
59	PUT	DA	3184	-	-	1/3/3/3	-
61	PEG	DA	3199	-	-	2/4/4/4	-
61	PEG	DA	3226	-	-	0/4/4/4	-
63	PGE	DD	301	-	-	5/7/7/7	-
58	MPD	DE	301	-	-	2/5/5/5	-
63	PGE	D3	101	-	-	4/7/7/7	-
58	MPD	DA	3190	-	-	1/5/5/5	-
59	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3194	-	-	0/1/1/1	-
59	PUT	DA	3212	-	-	0/3/3/3	-
59	PUT	DA	3219	-	-	0/3/3/3	-
62	EDO	DA	3198	-	-	1/1/1/1	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	EDO	DB	210	-	-	1/1/1/1	-
57	PG4	DR	201	-	-	4/10/10/10	-
62	EDO	DB	211	-	-	0/1/1/1	-
62	EDO	D0	101	-	-	0/1/1/1	-
58	MPD	DK	201	-	-	5/5/5/5	-
61	PEG	D3	102	-	-	1/4/4/4	-
59	PUT	DA	3195	-	-	0/3/3/3	-
58	MPD	DT	201	-	-	1/5/5/5	-
58	MPD	DA	3192	-	-	2/5/5/5	-
58	MPD	DE	302	-	-	3/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
64	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	AA	1676	-	-	1/5/5/5	-
63	PGE	DU	201	-	-	4/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
63	PGE	DA	3186	-	-	2/7/7/7	-
58	MPD	DS	203	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	SPD	DA	3206	-	-	2/7/7/7	-
58	MPD	AA	1671	-	-	0/5/5/5	-
61	PEG	DA	3227	-	-	0/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	CH3-C	4.11	1.54	1.48
67	DA	3211	GUN	C6-N1	3.70	1.39	1.33
58	DN	201	MPD	C3-C2	2.72	1.61	1.53
58	DK	201	MPD	C3-C2	2.38	1.60	1.53
58	DE	302	MPD	C3-C2	2.25	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3211	GUN	C5-C6-N1	-8.01	112.48	123.43
67	DA	3211	GUN	C6-N1-C2	5.91	125.32	115.93
67	DA	3211	GUN	N3-C2-N1	-3.30	122.82	127.22
67	DA	3211	GUN	C6-C5-C4	-2.97	117.96	120.80

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DE	302	MPD	C1-C2-C3-C4
58	DE	302	MPD	O2-C2-C3-C4
57	BA	1642	PG4	O4-C7-C8-O5
63	DA	3225	PGE	O2-C3-C4-O3
63	DS	201	PGE	O2-C3-C4-O3

There are no ring outliers.

19 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3213	PUT	1	0
65	DA	3185	1PE	1	0
62	DA	3002	EDO	1	0
57	BA	1642	PG4	1	0
63	DA	3214	PGE	1	0
66	DA	3202	ACY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	DA	3220	TRS	1	0
61	DA	3201	PEG	1	0
61	DQ	201	PEG	1	0
63	DA	3225	PGE	4	0
59	DA	3223	PUT	1	0
62	DA	3194	EDO	3	0
59	DA	3212	PUT	1	0
59	DA	3219	PUT	1	0
57	DR	201	PG4	1	0
61	D3	102	PEG	1	0
58	DA	3192	MPD	2	0
63	DU	201	PGE	1	0
58	DS	203	MPD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1523/1534 (99%)	0.32	109 (7%) 15 16	65, 138, 270, 291	0
1	BA	1522/1534 (99%)	0.84	261 (17%) 1 1	86, 162, 293, 294	0
2	AB	224/224 (100%)	1.18	57 (25%) 0 0	108, 156, 231, 272	0
2	BB	224/224 (100%)	1.03	44 (19%) 1 0	138, 181, 229, 262	0
3	AC	206/206 (100%)	1.32	56 (27%) 0 0	138, 174, 208, 228	0
3	BC	206/206 (100%)	3.38	125 (60%) 0 0	223, 253, 269, 279	0
4	AD	205/205 (100%)	0.24	4 (1%) 65 64	100, 145, 174, 190	0
4	BD	205/205 (100%)	-0.21	0 100 100	71, 100, 137, 174	0
5	AE	155/155 (100%)	0.39	7 (4%) 33 33	83, 119, 150, 176	0
5	BE	150/155 (96%)	0.43	12 (8%) 12 12	92, 125, 168, 236	0
6	AF	106/106 (100%)	0.01	5 (4%) 31 31	89, 126, 149, 187	0
6	BF	100/106 (94%)	0.73	14 (14%) 2 2	135, 162, 188, 196	0
7	AG	151/151 (100%)	1.99	70 (46%) 0 0	159, 186, 216, 229	0
7	BG	151/151 (100%)	4.00	108 (71%) 0 0	198, 247, 263, 268	0
8	AH	129/129 (100%)	0.48	10 (7%) 13 13	89, 122, 148, 158	0
8	BH	129/129 (100%)	0.33	11 (8%) 10 11	119, 151, 179, 192	0
9	AI	127/127 (100%)	2.23	51 (40%) 0 0	168, 196, 251, 270	0
9	BI	127/127 (100%)	2.80	63 (49%) 0 0	198, 234, 277, 283	0
10	AJ	99/99 (100%)	2.36	44 (44%) 0 0	169, 190, 228, 238	0
10	BJ	98/99 (98%)	4.87	73 (74%) 0 0	209, 248, 280, 287	0
11	AK	117/129 (90%)	0.76	18 (15%) 2 1	77, 139, 174, 190	0
11	BK	117/129 (90%)	1.20	28 (23%) 0 0	111, 166, 186, 202	0
12	AL	122/123 (99%)	0.47	11 (9%) 9 10	78, 112, 137, 178	0
12	BL	122/123 (99%)	0.62	12 (9%) 7 7	96, 121, 148, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	2.14	53 (46%) 0 0	167, 198, 220, 233	0
13	BM	114/114 (100%)	4.71	103 (90%) 0 0	254, 271, 288, 292	0
14	AN	100/100 (100%)	2.49	51 (51%) 0 0	166, 188, 252, 260	0
14	BN	100/100 (100%)	4.56	77 (77%) 0 0	226, 252, 282, 288	0
15	AO	88/88 (100%)	0.30	7 (7%) 12 12	75, 109, 142, 169	0
15	BO	88/88 (100%)	0.94	17 (19%) 1 0	127, 160, 180, 197	0
16	AP	82/82 (100%)	1.41	28 (34%) 0 0	88, 128, 168, 195	0
16	BP	82/82 (100%)	1.12	21 (25%) 0 0	106, 136, 168, 184	0
17	AQ	80/80 (100%)	0.57	10 (12%) 3 3	86, 115, 149, 157	0
17	BQ	80/80 (100%)	1.41	25 (31%) 0 0	120, 159, 182, 197	0
18	AR	55/55 (100%)	0.71	8 (14%) 2 2	86, 116, 172, 194	0
18	BR	55/55 (100%)	1.75	19 (34%) 0 0	126, 143, 173, 216	0
19	AS	79/79 (100%)	1.36	25 (31%) 0 0	180, 201, 215, 222	0
19	BS	79/79 (100%)	4.58	55 (69%) 0 0	229, 265, 274, 278	0
20	AT	86/86 (100%)	0.24	3 (3%) 44 42	91, 122, 151, 161	0
20	BT	85/86 (98%)	1.67	26 (30%) 0 0	136, 157, 183, 193	0
21	AU	56/56 (100%)	1.15	7 (12%) 3 3	114, 146, 208, 223	0
21	BU	56/56 (100%)	0.65	8 (14%) 2 2	112, 151, 191, 204	0
22	C1	56/56 (100%)	1.67	18 (32%) 0 0	131, 187, 206, 219	0
22	D1	56/56 (100%)	-0.35	0 100 100	31, 57, 81, 120	0
23	C2	50/51 (98%)	3.48	37 (74%) 0 0	179, 197, 215, 237	0
23	D2	51/51 (100%)	0.18	0 100 100	81, 98, 130, 145	0
24	C3	46/46 (100%)	1.91	20 (43%) 0 0	129, 153, 170, 177	0
24	D3	46/46 (100%)	-0.11	0 100 100	42, 51, 71, 143	0
25	C4	64/64 (100%)	1.43	23 (35%) 0 0	145, 165, 182, 187	0
25	D4	64/64 (100%)	-0.18	0 100 100	51, 64, 78, 105	0
26	C5	38/38 (100%)	1.26	6 (15%) 2 1	126, 153, 166, 174	0
26	D5	38/38 (100%)	0.07	1 (2%) 56 53	52, 68, 95, 120	0
27	C0	58/58 (100%)	1.24	15 (25%) 0 0	123, 142, 171, 180	0
27	D0	58/58 (100%)	-0.34	0 100 100	36, 49, 85, 112	0
28	CB	118/120 (98%)	0.58	7 (5%) 22 23	134, 208, 253, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.18	0 100 100	45, 87, 138, 167	0
29	CC	271/272 (99%)	0.70	35 (12%) 3 3	102, 130, 160, 176	0
29	DC	271/272 (99%)	-0.18	0 100 100	42, 75, 106, 142	0
30	CD	209/209 (100%)	1.64	75 (35%) 0 0	100, 154, 179, 193	0
31	CA	2876/2904 (99%)	0.63	271 (9%) 8 9	92, 184, 267, 286	0
32	DD	208/209 (99%)	-0.24	0 100 100	27, 55, 93, 121	0
33	CE	201/201 (100%)	1.60	68 (33%) 0 0	133, 193, 233, 243	0
33	DE	201/201 (100%)	-0.06	0 100 100	30, 82, 132, 150	0
34	CF	177/178 (99%)	2.60	109 (61%) 0 0	212, 233, 249, 254	0
34	DF	177/178 (99%)	0.33	10 (5%) 24 24	79, 120, 170, 188	0
35	CG	176/176 (100%)	2.55	100 (56%) 0 0	168, 196, 232, 244	0
35	DG	176/176 (100%)	0.08	9 (5%) 28 27	57, 93, 122, 156	0
36	CH	149/149 (100%)	1.57	52 (34%) 0 0	131, 172, 197, 208	0
36	DH	149/149 (100%)	1.18	30 (20%) 1 0	83, 173, 211, 231	0
37	CJ	134/135 (99%)	5.46	110 (82%) 0 0	259, 279, 289, 291	0
37	DJ	134/135 (99%)	3.81	92 (68%) 0 0	228, 249, 266, 272	0
38	CK	142/142 (100%)	0.65	9 (6%) 20 21	115, 144, 168, 182	0
38	DK	142/142 (100%)	-0.32	0 100 100	28, 49, 82, 106	0
39	CL	122/123 (99%)	0.68	16 (13%) 3 3	105, 133, 168, 181	0
39	DL	123/123 (100%)	-0.23	0 100 100	43, 62, 95, 135	0
40	CM	144/144 (100%)	2.54	69 (47%) 0 0	131, 195, 243, 260	0
40	DM	144/144 (100%)	-0.18	1 (0%) 87 89	26, 78, 114, 152	0
41	CN	135/136 (99%)	0.88	19 (14%) 2 2	107, 145, 176, 205	0
41	DN	135/136 (99%)	-0.38	0 100 100	36, 59, 90, 112	0
42	CO	120/127 (94%)	1.25	25 (20%) 1 0	127, 158, 186, 233	0
42	DO	125/127 (98%)	-0.26	0 100 100	33, 52, 96, 155	0
43	CP	116/117 (99%)	2.36	60 (51%) 0 0	165, 195, 217, 223	0
43	DP	117/117 (100%)	-0.09	0 100 100	56, 84, 121, 136	0
44	CQ	114/114 (100%)	1.49	38 (33%) 0 0	124, 150, 174, 186	0
44	DQ	114/114 (100%)	-0.22	1 (0%) 84 85	47, 72, 105, 135	0
45	CR	117/117 (100%)	1.35	31 (26%) 0 0	117, 144, 166, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.17	0 100 100	24, 41, 63, 114	0
46	CS	103/103 (100%)	1.93	38 (36%) 0 0	117, 159, 195, 202	0
46	DS	103/103 (100%)	-0.24	0 100 100	30, 55, 92, 126	0
47	CT	110/110 (100%)	1.58	38 (34%) 0 0	140, 171, 196, 207	0
47	DT	110/110 (100%)	-0.28	0 100 100	26, 45, 79, 128	0
48	CU	93/100 (93%)	2.62	54 (58%) 0 0	159, 194, 219, 229	0
48	DU	93/100 (93%)	0.26	2 (2%) 62 60	51, 73, 136, 154	0
49	CV	102/103 (99%)	3.12	70 (68%) 0 0	157, 198, 231, 242	0
49	DV	102/103 (99%)	0.08	5 (4%) 29 29	57, 82, 126, 156	0
50	CW	94/94 (100%)	1.56	34 (36%) 0 0	133, 172, 186, 192	0
50	DW	94/94 (100%)	-0.30	0 100 100	43, 73, 110, 119	0
51	CX	75/76 (98%)	1.94	31 (41%) 0 0	129, 161, 175, 206	0
51	DX	76/76 (100%)	-0.35	0 100 100	36, 62, 92, 157	0
52	CY	77/77 (100%)	0.86	14 (18%) 1 1	120, 145, 173, 185	0
52	DY	77/77 (100%)	-0.10	1 (1%) 77 77	56, 76, 111, 130	0
53	CZ	62/62 (100%)	2.61	38 (61%) 0 0	177, 199, 210, 217	0
53	DZ	62/62 (100%)	0.33	2 (3%) 47 46	65, 97, 136, 174	0
54	DI	135/135 (100%)	1.29	39 (28%) 0 0	104, 179, 244, 266	1 (0%)
55	DA	2873/2904 (98%)	0.06	78 (2%) 54 53	29, 65, 231, 294	0
All	All	20634/20795 (99%)	0.86	3537 (17%) 1 1	24, 144, 266, 294	1 (0%)

The worst 5 of 3537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	CJ	13	VAL	34.4
9	BI	126	GLN	26.3
9	BI	128	SER	23.0
37	DJ	54	PRO	20.5
1	BA	1302	C	20.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	966	24/25	0.43	0.57	258,264,268,268	0
1	5MC	BA	967	21/22	0.55	0.61	258,263,266,266	0
1	2MG	BA	1207	24/25	0.70	0.39	256,257,258,259	0
1	5MC	AA	967	21/22	0.75	0.28	214,216,219,220	0
1	2MG	AA	966	24/25	0.78	0.24	211,213,215,216	0
1	2MG	AA	1207	24/25	0.80	0.19	234,239,241,243	0
31	3TD	CA	1915	21/22	0.87	0.19	162,165,170,171	0
31	OMU	CA	2552	21/22	0.87	0.44	106,111,115,116	0
31	PSU	CA	746	20/21	0.90	0.19	135,137,142,142	0
1	PSU	BA	516	20/21	0.90	0.14	111,121,128,129	0
31	PSU	CA	1917	20/21	0.91	0.17	132,140,149,149	0
31	PSU	CA	955	20/21	0.91	0.17	126,130,135,136	0
31	PSU	CA	1911	20/21	0.92	0.14	152,158,159,161	0
31	OMC	CA	2498	21/22	0.92	0.29	116,124,130,132	0
31	5MU	CA	747	21/22	0.92	0.17	131,134,136,137	0
31	OMG	CA	2251	24/25	0.92	0.26	111,114,115,116	0
41	4D4	CN	81	12/13	0.92	0.42	118,121,132,133	0
31	PSU	CA	2504	20/21	0.93	0.21	106,114,117,120	0
1	MA6	BA	1518	24/25	0.93	0.24	91,97,102,103	0
1	2MG	BA	1516	24/25	0.93	0.19	105,110,116,117	0
31	2MA	CA	2503	23/24	0.94	0.23	117,126,137,138	0
31	6MZ	CA	1618	23/24	0.94	0.29	160,164,168,172	0
1	MA6	BA	1519	24/25	0.94	0.24	100,102,107,110	0
31	6MZ	CA	2030	23/24	0.94	0.19	117,125,134,134	0
31	7MG	CA	2069	24/25	0.94	0.20	104,111,124,124	0
31	2MG	CA	1835	24/25	0.94	0.21	100,103,106,110	0
1	4OC	BA	1402	22/23	0.94	0.19	111,116,127,128	0
12	D2T	BL	89	10/11	0.94	0.39	106,110,113,114	0
1	PSU	AA	516	20/21	0.94	0.15	135,138,139,141	0
31	1MG	CA	745	24/25	0.94	0.17	123,126,132,134	0
31	2MG	CA	2445	24/25	0.94	0.28	103,109,112,114	0
1	UR3	BA	1498	21/22	0.95	0.14	118,122,126,127	0
1	5MC	BA	1407	21/22	0.95	0.14	111,121,124,125	0
12	D2T	AL	89	10/11	0.95	0.29	109,114,125,128	0
55	PSU	DA	1911	20/21	0.95	0.14	107,118,120,121	0
1	7MG	BA	527	24/25	0.95	0.18	100,108,118,120	0
31	PSU	CA	2580	20/21	0.95	0.18	118,125,130,131	0
31	5MU	CA	1939	21/22	0.95	0.17	95,99,105,107	0
31	PSU	CA	2457	20/21	0.96	0.19	118,122,126,127	0
1	4OC	AA	1402	22/23	0.96	0.17	94,99,103,104	0
55	3TD	DA	1915	21/22	0.96	0.12	133,140,146,147	0
1	5MC	AA	1407	21/22	0.96	0.16	80,88,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	PSU	CA	2605	20/21	0.96	0.17	97,101,106,106	0
1	2MG	AA	1516	24/25	0.96	0.17	74,82,84,86	0
55	2MG	DA	1835	24/25	0.96	0.21	59,65,71,72	0
1	7MG	AA	527	24/25	0.96	0.16	102,109,115,118	0
31	5MC	CA	1962	21/22	0.96	0.20	103,106,110,112	0
1	MA6	AA	1518	24/25	0.97	0.16	67,77,81,85	0
1	MA6	AA	1519	24/25	0.97	0.20	72,76,80,81	0
55	PSU	DA	1917	20/21	0.97	0.13	109,113,119,119	0
1	UR3	AA	1498	21/22	0.97	0.18	86,92,97,100	0
41	4D4	DN	81[B]	12/13	0.98	0.23	37,45,50,50	9
55	5MC	DA	1962	21/22	0.98	0.19	46,61,65,66	0
41	4D4	DN	81[A]	12/13	0.98	0.23	49,59,65,66	9
55	PSU	DA	2605	20/21	0.98	0.17	51,59,64,65	0
55	PSU	DA	2504	20/21	0.98	0.19	50,51,54,56	0
55	2MG	DA	2445	24/25	0.99	0.20	39,45,50,62	0
55	OMC	DA	2498	21/22	0.99	0.21	37,39,46,47	0
55	6MZ	DA	1618	23/24	0.99	0.20	34,42,47,49	0
55	1MG	DA	745	24/25	0.99	0.19	31,37,42,44	0
32	MEQ	DD	150[B]	10/11	0.99	0.28	35,38,44,45	10
55	5MU	DA	747	21/22	0.99	0.19	41,43,52,58	0
55	PSU	DA	2457	20/21	0.99	0.18	44,46,52,53	0
55	6MZ	DA	2030	23/24	0.99	0.20	27,33,38,40	0
55	5MU	DA	1939	21/22	0.99	0.20	53,58,65,69	0
55	PSU	DA	2604	20/21	0.99	0.17	58,63,70,72	0
55	PSU	DA	2580	20/21	0.99	0.20	30,35,41,43	0
55	7MG	DA	2069	24/25	0.99	0.18	41,48,53,53	0
55	OMU	DA	2552	21/22	0.99	0.21	45,48,52,57	0
32	MEQ	DD	150[A]	10/11	0.99	0.28	31,32,37,37	10
55	OMG	DA	2251	24/25	0.99	0.18	29,48,54,62	0
55	PSU	DA	955	20/21	0.99	0.19	32,35,39,41	0
55	2MA	DA	2503	23/24	0.99	0.21	44,51,58,62	0
55	H2U	DA	2449	20/21	0.99	0.23	33,39,46,46	0
55	PSU	DA	746	20/21	1.00	0.18	38,44,46,47	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
56	MG	CA	3132	1/1	0.17	0.62	157,157,157,157	0
56	MG	CA	3139	1/1	0.17	0.83	140,140,140,140	0
56	MG	BA	1624	1/1	0.17	2.21	293,293,293,293	0
56	MG	AA	1628	1/1	0.23	0.26	137,137,137,137	0
56	MG	AA	1622	1/1	0.24	0.84	106,106,106,106	0
56	MG	AA	1627	1/1	0.27	1.21	115,115,115,115	0
56	MG	DA	3130	1/1	0.27	0.89	109,109,109,109	0
56	MG	BA	1637	1/1	0.28	0.54	121,121,121,121	0
59	PUT	AA	1675	6/6	0.36	0.61	172,174,174,175	0
56	MG	CA	3154	1/1	0.38	0.71	110,110,110,110	0
56	MG	CA	3124	1/1	0.40	0.28	159,159,159,159	0
56	MG	CA	3061	1/1	0.42	0.20	270,270,270,270	0
56	MG	CA	3104	1/1	0.46	0.46	249,249,249,249	0
56	MG	CA	3007	1/1	0.47	0.66	257,257,257,257	0
61	PEG	DQ	201	7/7	0.51	0.82	162,166,170,170	0
56	MG	DA	3168	1/1	0.51	0.54	119,119,119,119	0
56	MG	AA	1603	1/1	0.52	0.67	111,111,111,111	0
56	MG	AA	1616	1/1	0.52	0.69	105,105,105,105	0
59	PUT	AA	1672	6/6	0.53	0.30	149,150,150,150	0
56	MG	CA	3075	1/1	0.54	1.12	231,231,231,231	0
56	MG	AA	1618	1/1	0.54	0.11	172,172,172,172	0
56	MG	DA	3156	1/1	0.55	0.69	83,83,83,83	0
56	MG	DA	3152	1/1	0.56	0.27	115,115,115,115	0
56	MG	CA	3126	1/1	0.57	0.35	115,115,115,115	0
56	MG	DA	3137	1/1	0.59	0.34	61,61,61,61	0
56	MG	CA	3145	1/1	0.60	0.98	78,78,78,78	0
56	MG	DA	3163	1/1	0.60	0.52	87,87,87,87	0
56	MG	CA	3105	1/1	0.61	0.18	252,252,252,252	0
56	MG	CA	3135	1/1	0.61	0.48	78,78,78,78	0
57	PG4	DR	201	13/13	0.61	0.34	156,168,173,173	0
56	MG	AA	1660	1/1	0.62	0.53	283,283,283,283	0
56	MG	BA	1623	1/1	0.62	0.86	277,277,277,277	0
56	MG	AA	1623	1/1	0.63	0.77	87,87,87,87	0
56	MG	AA	1621	1/1	0.64	0.50	97,97,97,97	0
61	PEG	AL	201	7/7	0.64	0.30	132,133,135,136	0
61	PEG	D3	102	7/7	0.66	1.33	136,138,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1615	1/1	0.68	0.67	129,129,129,129	0
58	MPD	DE	301	8/8	0.69	1.05	172,174,179,179	0
56	MG	CA	3056	1/1	0.69	0.48	77,77,77,77	0
61	PEG	DP	201	7/7	0.69	0.69	149,153,164,165	0
68	TRS	DA	3220	8/8	0.69	0.80	184,187,190,191	0
56	MG	DA	3147	1/1	0.69	0.29	108,108,108,108	0
56	MG	CA	3140	1/1	0.69	0.54	108,108,108,108	0
59	PUT	DA	3195	6/6	0.69	0.44	100,104,108,108	0
56	MG	AA	1626	1/1	0.70	0.95	120,120,120,120	0
64	SPD	DA	3206	10/10	0.71	0.23	142,143,144,144	0
62	EDO	DA	3002	4/4	0.71	0.61	176,176,176,177	0
56	MG	DA	3182	1/1	0.71	0.43	55,55,55,55	0
56	MG	BA	1626	1/1	0.72	0.91	255,255,255,255	0
61	PEG	DA	3200	7/7	0.72	0.35	124,124,125,125	0
56	MG	CA	3026	1/1	0.73	1.05	245,245,245,245	0
62	EDO	DA	3198	4/4	0.73	0.43	109,110,112,112	0
58	MPD	DT	202	8/8	0.75	0.37	138,139,144,145	0
56	MG	CA	3116	1/1	0.75	0.41	92,92,92,92	0
56	MG	CA	3113	1/1	0.76	0.44	76,76,76,76	0
56	MG	DA	3162	1/1	0.76	0.30	79,79,79,79	0
56	MG	AA	1665	1/1	0.76	0.71	274,274,274,274	0
56	MG	CA	3092	1/1	0.76	0.08	163,163,163,163	0
62	EDO	DB	210	4/4	0.76	0.39	125,126,126,127	0
56	MG	AA	1604	1/1	0.77	0.66	79,79,79,79	0
61	PEG	DA	3218	7/7	0.77	0.28	179,180,181,181	0
56	MG	BA	1625	1/1	0.77	0.77	288,288,288,288	0
56	MG	AA	1625	1/1	0.77	0.58	83,83,83,83	0
59	PUT	AA	1673	6/6	0.77	0.67	142,145,148,150	0
56	MG	CA	3022	1/1	0.78	0.71	259,259,259,259	0
56	MG	CA	3077	1/1	0.78	0.44	244,244,244,244	0
56	MG	CA	3055	1/1	0.78	0.11	193,193,193,193	0
59	PUT	AA	1674	6/6	0.79	0.77	109,113,116,117	0
56	MG	AA	1659	1/1	0.79	0.33	273,273,273,273	0
56	MG	AA	1605	1/1	0.79	0.52	87,87,87,87	0
56	MG	CA	3123	1/1	0.80	0.69	142,142,142,142	0
56	MG	CA	3122	1/1	0.80	0.53	89,89,89,89	0
56	MG	DA	3170	1/1	0.80	0.18	59,59,59,59	0
56	MG	DA	3123	1/1	0.80	0.36	84,84,84,84	0
62	EDO	DA	3003	4/4	0.80	0.28	135,137,140,141	0
56	MG	CA	3130	1/1	0.80	0.13	84,84,84,84	0
56	MG	BA	1635	1/1	0.80	0.16	209,209,209,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1602	1/1	0.80	0.44	78,78,78,78	0
56	MG	CA	3009	1/1	0.80	0.15	259,259,259,259	0
56	MG	DA	3134	1/1	0.81	0.60	98,98,98,98	0
56	MG	BA	1638	1/1	0.81	0.44	65,65,65,65	0
56	MG	CA	3006	1/1	0.81	0.10	221,221,221,221	0
57	PG4	AA	1670	13/13	0.81	0.26	111,116,118,119	0
63	PGE	DA	3225	10/10	0.81	0.39	100,120,131,131	0
61	PEG	DA	3201	7/7	0.81	0.47	146,150,151,152	0
56	MG	CA	3080	1/1	0.81	0.11	108,108,108,108	0
56	MG	DA	3155	1/1	0.81	0.41	86,86,86,86	0
59	PUT	DA	3221	6/6	0.82	0.46	112,120,122,122	0
63	PGE	D3	101	10/10	0.82	0.54	121,123,125,126	0
56	MG	AA	1663	1/1	0.82	0.24	230,230,230,230	0
56	MG	DA	3148	1/1	0.82	0.22	67,67,67,67	0
59	PUT	DA	3213	6/6	0.82	0.27	156,156,157,157	0
56	MG	AA	1610	1/1	0.82	0.28	99,99,99,99	0
56	MG	CA	3093	1/1	0.82	0.16	143,143,143,143	0
56	MG	CA	3034	1/1	0.82	0.14	228,228,228,228	0
56	MG	CA	3151	1/1	0.82	0.54	102,102,102,102	0
56	MG	AA	1620	1/1	0.82	0.80	116,116,116,116	0
56	MG	BA	1606	1/1	0.83	0.17	270,270,270,270	0
56	MG	AA	1624	1/1	0.83	0.30	82,82,82,82	0
63	PGE	D1	102	10/10	0.83	0.36	142,145,152,153	0
62	EDO	DA	3194	4/4	0.83	0.31	89,90,90,90	0
58	MPD	DK	201	8/8	0.83	0.27	125,126,127,127	0
56	MG	DA	3178	1/1	0.83	0.33	93,93,93,93	0
56	MG	DA	3176	1/1	0.84	0.31	81,81,81,81	0
56	MG	CA	3071	1/1	0.84	0.35	228,228,228,228	0
61	PEG	DA	3199	7/7	0.84	0.46	99,106,112,113	0
56	MG	AA	1642	1/1	0.84	0.77	275,275,275,275	0
56	MG	DA	3154	1/1	0.84	0.35	60,60,60,60	0
56	MG	CA	3125	1/1	0.84	0.28	136,136,136,136	0
57	PG4	DQ	202	13/13	0.84	0.26	84,89,100,101	0
61	PEG	DA	3227	7/7	0.84	0.34	109,114,120,120	0
56	MG	DA	3157	1/1	0.84	0.26	74,74,74,74	0
56	MG	AA	1601	1/1	0.84	0.75	62,62,62,62	0
56	MG	CA	3119	1/1	0.84	0.37	100,100,100,100	0
59	PUT	DA	3212	6/6	0.85	0.22	114,115,117,117	0
58	MPD	DA	3204	8/8	0.85	0.61	116,119,125,127	0
56	MG	BA	1630	1/1	0.85	0.07	197,197,197,197	0
56	MG	CA	3110	1/1	0.85	0.35	129,129,129,129	0
56	MG	BA	1604	1/1	0.85	0.49	257,257,257,257	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1641	1/1	0.85	0.37	140,140,140,140	0
56	MG	CA	3094	1/1	0.86	0.11	132,132,132,132	0
63	PGE	DU	201	10/10	0.86	0.45	135,141,147,147	0
56	MG	CA	3146	1/1	0.86	0.10	174,174,174,174	0
63	PGE	DA	3214	10/10	0.86	0.60	67,87,91,92	0
56	MG	DA	3158	1/1	0.86	0.49	107,107,107,107	0
59	PUT	DA	3219	6/6	0.86	0.29	100,102,103,103	0
56	MG	AA	1609	1/1	0.86	0.55	107,107,107,107	0
56	MG	BA	1634	1/1	0.86	0.10	216,216,216,216	0
56	MG	CA	3019	1/1	0.86	0.21	87,87,87,87	0
56	MG	CA	3067	1/1	0.86	0.21	274,274,274,274	0
58	MPD	AA	1676	8/8	0.86	0.63	145,146,148,148	0
56	MG	CA	3142	1/1	0.86	0.17	102,102,102,102	0
56	MG	DA	3160	1/1	0.86	0.36	64,64,64,64	0
56	MG	CA	3128	1/1	0.86	0.35	116,116,116,116	0
56	MG	DA	3171	1/1	0.86	0.82	111,111,111,111	0
56	MG	CA	3131	1/1	0.87	0.34	123,123,123,123	0
61	PEG	DA	3226	7/7	0.87	0.32	125,126,131,131	0
56	MG	CA	3156	1/1	0.87	0.16	263,263,263,263	0
58	MPD	DT	201	8/8	0.87	0.31	110,115,125,126	0
63	PGE	DS	201	10/10	0.87	0.34	96,99,101,101	0
56	MG	CB	201	1/1	0.87	0.06	235,235,235,235	0
56	MG	CA	3060	1/1	0.87	0.42	238,238,238,238	0
56	MG	AA	1677	1/1	0.87	0.08	101,101,101,101	0
56	MG	CA	3133	1/1	0.87	0.32	110,110,110,110	0
56	MG	CA	3118	1/1	0.87	0.52	87,87,87,87	0
56	MG	CA	3001	1/1	0.87	0.30	291,291,291,291	0
62	EDO	DA	3215	4/4	0.88	0.32	64,67,70,73	0
56	MG	CA	3021	1/1	0.88	1.30	253,253,253,253	0
61	PEG	DL	201	7/7	0.88	0.31	102,103,109,110	0
56	MG	CA	3072	1/1	0.88	1.07	258,258,258,258	0
56	MG	CA	3111	1/1	0.88	0.29	103,103,103,103	0
57	PG4	DA	3193	13/13	0.88	0.96	109,113,119,120	0
56	MG	BA	1636	1/1	0.88	0.47	77,77,77,77	0
56	MG	DA	3128	1/1	0.88	1.11	57,57,57,57	0
58	MPD	DA	3190	8/8	0.89	0.31	100,102,103,106	0
58	MPD	DA	3207	8/8	0.89	0.44	121,125,128,129	0
57	PG4	BA	1642	13/13	0.89	0.45	113,117,132,132	0
57	PG4	DA	3216	13/13	0.89	0.28	111,122,132,134	0
56	MG	CA	3141	1/1	0.89	0.22	78,78,78,78	0
56	MG	AA	1606	1/1	0.89	0.14	124,124,124,124	0
56	MG	CA	3054	1/1	0.89	0.12	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3014	1/1	0.89	0.19	273,273,273,273	0
56	MG	BA	1612	1/1	0.89	0.22	262,262,262,262	0
56	MG	AA	1656	1/1	0.89	0.11	274,274,274,274	0
56	MG	CA	3030	1/1	0.89	0.09	82,82,82,82	0
56	MG	CA	3048	1/1	0.89	0.16	147,147,147,147	0
56	MG	DA	3129	1/1	0.89	0.22	51,51,51,51	0
56	MG	DA	3133	1/1	0.89	0.26	52,52,52,52	0
56	MG	DA	3180	1/1	0.89	0.80	77,77,77,77	0
63	PGE	DD	301	10/10	0.89	0.31	120,122,129,130	0
56	MG	AA	1654	1/1	0.89	0.14	178,178,178,178	0
56	MG	CA	3107	1/1	0.90	0.34	81,81,81,81	0
56	MG	AA	1661	1/1	0.90	0.68	223,223,223,223	0
56	MG	BA	1619	1/1	0.90	0.48	228,228,228,228	0
63	PGE	DA	3217	10/10	0.90	0.34	87,89,93,94	0
56	MG	DA	3172	1/1	0.90	0.38	85,85,85,85	0
56	MG	DA	3124	1/1	0.90	0.52	90,90,90,90	0
57	PG4	DS	202	13/13	0.90	0.31	72,73,85,86	0
56	MG	CA	3147	1/1	0.90	0.25	36,36,36,36	1
56	MG	DA	3098	1/1	0.90	0.21	246,246,246,246	0
56	MG	CA	3148	1/1	0.90	0.42	43,43,43,43	1
56	MG	DA	3161	1/1	0.90	0.22	73,73,73,73	0
56	MG	DA	3165	1/1	0.90	0.27	63,63,63,63	0
56	MG	CA	3008	1/1	0.90	0.09	202,202,202,202	0
58	MPD	DN	201	8/8	0.91	0.35	109,117,119,121	0
62	EDO	D1	101	4/4	0.91	0.23	70,71,73,75	0
56	MG	DA	3153	1/1	0.91	0.28	102,102,102,102	0
56	MG	BA	1603	1/1	0.91	0.21	278,278,278,278	0
56	MG	BA	1629	1/1	0.91	1.35	217,217,217,217	0
56	MG	CA	3047	1/1	0.91	0.26	100,100,100,100	0
56	MG	CA	3052	1/1	0.91	0.07	124,124,124,124	0
56	MG	CA	3137	1/1	0.91	0.31	164,164,164,164	0
56	MG	AA	1613	1/1	0.91	0.62	80,80,80,80	0
56	MG	AA	1647	1/1	0.91	0.30	145,145,145,145	0
56	MG	DA	3125	1/1	0.91	0.22	51,51,51,51	0
56	MG	CA	3138	1/1	0.91	0.12	98,98,98,98	0
62	EDO	DA	3209	4/4	0.91	0.62	94,96,98,99	0
56	MG	CA	3057	1/1	0.91	0.14	111,111,111,111	0
58	MPD	AA	1671	8/8	0.91	0.70	143,144,147,148	0
56	MG	DA	3001	1/1	0.91	0.45	47,47,47,47	0
67	GUN	DA	3211	11/11	0.91	0.26	116,122,123,124	0
56	MG	AA	1658	1/1	0.91	0.34	212,212,212,212	0
64	SPD	DA	3224	10/10	0.91	0.30	58,71,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3070	1/1	0.91	0.31	234,234,234,234	0
56	MG	AA	1614	1/1	0.92	0.13	83,83,83,83	0
56	MG	CA	3053	1/1	0.92	0.11	86,86,86,86	0
56	MG	CA	3121	1/1	0.92	0.23	83,83,83,83	0
59	PUT	DA	3222	6/6	0.92	0.31	77,81,83,83	0
56	MG	CA	3064	1/1	0.92	0.29	271,271,271,271	0
59	PUT	DA	3184	6/6	0.92	0.43	65,70,74,74	0
56	MG	CA	3028	1/1	0.92	0.80	284,284,284,284	0
59	PUT	DA	3205	6/6	0.92	0.30	106,108,108,109	0
56	MG	CA	3038	1/1	0.92	0.17	252,252,252,252	0
56	MG	CA	3039	1/1	0.92	0.58	190,190,190,190	0
56	MG	DA	3131	1/1	0.92	0.24	83,83,83,83	0
56	MG	CA	3083	1/1	0.92	0.35	254,254,254,254	0
56	MG	CA	3117	1/1	0.92	0.13	59,59,59,59	0
56	MG	AA	1612	1/1	0.92	0.36	77,77,77,77	0
56	MG	DA	3138	1/1	0.92	0.34	29,29,29,29	1
56	MG	CA	3149	1/1	0.92	0.44	76,76,76,76	0
56	MG	CA	3090	1/1	0.92	0.16	187,187,187,187	0
56	MG	CA	3120	1/1	0.92	0.13	130,130,130,130	0
56	MG	DB	206	1/1	0.92	0.31	73,73,73,73	0
56	MG	CA	3032	1/1	0.92	0.35	197,197,197,197	0
65	1PE	DA	3203	16/16	0.92	0.30	98,105,109,109	0
56	MG	CB	203	1/1	0.92	0.15	237,237,237,237	0
56	MG	CA	3002	1/1	0.92	0.15	224,224,224,224	0
62	EDO	D0	101	4/4	0.92	0.26	79,80,85,89	0
58	MPD	DA	3210	8/8	0.92	0.30	110,118,123,125	0
56	MG	CA	3096	1/1	0.92	0.08	89,89,89,89	0
56	MG	BA	1639	1/1	0.92	0.27	117,117,117,117	0
56	MG	CA	3152	1/1	0.92	0.16	160,160,160,160	0
56	MG	CA	3059	1/1	0.92	0.10	118,118,118,118	0
56	MG	CA	3099	1/1	0.93	0.12	174,174,174,174	0
56	MG	CA	3018	1/1	0.93	0.10	147,147,147,147	0
56	MG	DA	3126	1/1	0.93	0.31	77,77,77,77	0
56	MG	CA	3010	1/1	0.93	0.10	259,259,259,259	0
56	MG	DA	3143	1/1	0.93	0.31	63,63,63,63	0
56	MG	CA	3068	1/1	0.93	0.26	174,174,174,174	0
56	MG	AA	1638	1/1	0.93	0.14	142,142,142,142	0
56	MG	CA	3155	1/1	0.93	0.26	181,181,181,181	0
56	MG	CA	3036	1/1	0.93	0.15	227,227,227,227	0
56	MG	BA	1627	1/1	0.93	0.68	203,203,203,203	0
58	MPD	DE	302	8/8	0.93	0.41	101,102,103,104	0
56	MG	DA	3062	1/1	0.93	0.28	269,269,269,269	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3087	1/1	0.93	0.17	232,232,232,232	0
56	MG	CA	3134	1/1	0.93	0.12	167,167,167,167	0
56	MG	DA	3144	1/1	0.93	0.63	79,79,79,79	0
62	EDO	DA	3197	4/4	0.93	0.29	75,76,77,77	0
64	SPD	DA	3183	10/10	0.93	0.45	80,95,97,98	0
59	PUT	DA	3188	6/6	0.93	0.20	89,93,93,94	0
56	MG	CA	3109	1/1	0.93	0.34	67,67,67,67	0
56	MG	CA	3129	1/1	0.93	0.13	135,135,135,135	0
56	MG	DA	3146	1/1	0.93	0.28	76,76,76,76	0
60	ZN	C5	101	1/1	0.93	0.07	175,175,175,175	0
56	MG	DA	3121	1/1	0.94	0.53	111,111,111,111	0
56	MG	CA	3136	1/1	0.94	0.24	107,107,107,107	0
56	MG	AA	1617	1/1	0.94	0.21	88,88,88,88	0
56	MG	CA	3040	1/1	0.94	0.13	122,122,122,122	0
56	MG	BA	1610	1/1	0.94	0.07	107,107,107,107	0
56	MG	CA	3106	1/1	0.94	0.13	74,74,74,74	0
56	MG	AA	1662	1/1	0.94	0.20	164,164,164,164	0
56	MG	DA	3179	1/1	0.94	1.13	85,85,85,85	0
56	MG	AA	1641	1/1	0.94	0.06	122,122,122,122	0
56	MG	CA	3062	1/1	0.94	0.11	168,168,168,168	0
56	MG	DA	3132	1/1	0.94	0.21	56,56,56,56	0
56	MG	CA	3066	1/1	0.94	0.11	91,91,91,91	0
56	MG	CA	3003	1/1	0.94	1.80	272,272,272,272	0
56	MG	AA	1611	1/1	0.94	0.15	133,133,133,133	0
56	MG	CA	3084	1/1	0.94	0.21	172,172,172,172	0
56	MG	CA	3031	1/1	0.94	0.19	128,128,128,128	0
56	MG	CA	3085	1/1	0.94	0.08	116,116,116,116	0
56	MG	AA	1608	1/1	0.94	0.36	128,128,128,128	0
64	SPD	DA	3187	10/10	0.94	0.26	78,82,85,85	0
65	1PE	DA	3185	16/16	0.94	0.21	74,89,123,123	0
56	MG	BA	1633	1/1	0.94	0.55	237,237,237,237	0
56	MG	DB	207	1/1	0.94	0.77	92,92,92,92	0
56	MG	BA	1620	1/1	0.94	0.12	172,172,172,172	0
56	MG	DB	204	1/1	0.94	0.16	85,85,85,85	0
56	MG	DA	3145	1/1	0.95	0.20	45,45,45,45	0
56	MG	AA	1634	1/1	0.95	0.33	179,179,179,179	0
56	MG	DA	3079	1/1	0.95	0.32	179,179,179,179	0
56	MG	CA	3004	1/1	0.95	0.11	192,192,192,192	0
56	MG	BA	1616	1/1	0.95	0.12	151,151,151,151	0
63	PGE	DA	3186	10/10	0.95	0.20	58,65,71,71	0
59	PUT	DA	3189	6/6	0.95	0.25	49,55,59,62	0
59	PUT	DM	201	6/6	0.95	0.21	63,66,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1653	1/1	0.95	0.06	108,108,108,108	0
56	MG	DA	3118	1/1	0.95	0.10	31,31,31,31	0
66	ACY	DA	3191	4/4	0.95	0.25	79,80,81,81	0
56	MG	CA	3114	1/1	0.95	0.31	67,67,67,67	0
56	MG	DA	3141	1/1	0.95	0.41	80,80,80,80	0
60	ZN	AB	301	1/1	0.95	0.04	165,165,165,165	0
56	MG	CA	3029	1/1	0.95	0.17	143,143,143,143	0
56	MG	CA	3046	1/1	0.95	0.13	99,99,99,99	0
56	MG	DA	3080	1/1	0.95	0.10	195,195,195,195	0
56	MG	DA	3164	1/1	0.95	0.26	78,78,78,78	0
58	MPD	DA	3192	8/8	0.95	0.57	84,90,92,94	0
56	MG	CA	3101	1/1	0.95	0.12	239,239,239,239	0
56	MG	AA	1619	1/1	0.95	0.54	122,122,122,122	0
56	MG	DB	205	1/1	0.95	0.66	148,148,148,148	0
56	MG	CA	3058	1/1	0.95	0.14	124,124,124,124	0
56	MG	AA	1637	1/1	0.95	0.15	106,106,106,106	0
56	MG	DA	3033	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3023	1/1	0.95	0.39	255,255,255,255	0
56	MG	AA	1607	1/1	0.95	0.47	90,90,90,90	0
56	MG	AA	1657	1/1	0.95	0.46	134,134,134,134	0
56	MG	CA	3108	1/1	0.96	0.23	89,89,89,89	0
56	MG	CA	3020	1/1	0.96	0.15	116,116,116,116	0
56	MG	CA	3153	1/1	0.96	0.20	77,77,77,77	0
56	MG	DA	3007	1/1	0.96	0.09	127,127,127,127	0
56	MG	CA	3150	1/1	0.96	0.77	79,79,79,79	0
56	MG	AA	1664	1/1	0.96	0.71	265,265,265,265	0
56	MG	AA	1630	1/1	0.96	0.20	205,205,205,205	0
56	MG	AA	1648	1/1	0.96	0.05	84,84,84,84	0
56	MG	DA	3177	1/1	0.96	0.36	52,52,52,52	0
56	MG	AA	1668	1/1	0.96	0.13	110,110,110,110	0
56	MG	DA	3142	1/1	0.96	0.26	80,80,80,80	0
56	MG	AA	1635	1/1	0.96	0.14	220,220,220,220	0
56	MG	CA	3112	1/1	0.96	0.36	103,103,103,103	0
56	MG	DA	3008	1/1	0.96	0.12	280,280,280,280	0
56	MG	DB	209	1/1	0.96	0.15	83,83,83,83	0
56	MG	CA	3097	1/1	0.96	0.14	112,112,112,112	0
56	MG	DA	3174	1/1	0.96	0.23	87,87,87,87	0
56	MG	CA	3065	1/1	0.96	0.15	115,115,115,115	0
56	MG	DA	3095	1/1	0.96	0.14	65,65,65,65	0
56	MG	AA	1640	1/1	0.96	0.10	131,131,131,131	0
56	MG	DB	201	1/1	0.96	0.11	121,121,121,121	0
62	EDO	DB	211	4/4	0.96	0.22	131,131,132,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3143	1/1	0.96	0.14	72,72,72,72	0
56	MG	DA	3175	1/1	0.96	0.60	115,115,115,115	0
56	MG	CA	3082	1/1	0.96	0.26	168,168,168,168	0
56	MG	BA	1607	1/1	0.96	0.24	280,280,280,280	0
56	MG	CA	3050	1/1	0.96	0.18	166,166,166,166	0
56	MG	BA	1617	1/1	0.96	0.12	165,165,165,165	0
66	ACY	DA	3196	4/4	0.96	0.24	61,69,69,72	0
56	MG	CA	3051	1/1	0.96	0.39	248,248,248,248	0
56	MG	BA	1622	1/1	0.96	0.10	240,240,240,240	0
56	MG	DA	3120	1/1	0.96	0.55	66,66,66,66	0
56	MG	CA	3103	1/1	0.96	0.15	176,176,176,176	0
56	MG	BA	1609	1/1	0.96	0.14	156,156,156,156	0
56	MG	DA	3044	1/1	0.97	0.08	124,124,124,124	0
56	MG	DA	3149	1/1	0.97	0.24	96,96,96,96	0
56	MG	CA	3073	1/1	0.97	0.23	139,139,139,139	0
56	MG	CA	3005	1/1	0.97	0.37	233,233,233,233	0
56	MG	CA	3127	1/1	0.97	0.14	73,73,73,73	0
56	MG	BA	1631	1/1	0.97	0.11	132,132,132,132	0
56	MG	DA	3097	1/1	0.97	0.11	75,75,75,75	0
56	MG	DA	3012	1/1	0.97	0.14	141,141,141,141	0
56	MG	CA	3033	1/1	0.97	0.09	150,150,150,150	0
56	MG	BA	1618	1/1	0.97	0.22	172,172,172,172	0
56	MG	DA	3166	1/1	0.97	0.34	74,74,74,74	0
56	MG	CA	3016	1/1	0.97	0.90	218,218,218,218	0
56	MG	AA	1655	1/1	0.97	0.08	152,152,152,152	0
56	MG	DD	302	1/1	0.97	0.22	62,62,62,62	0
56	MG	BA	1628	1/1	0.97	0.15	120,120,120,120	0
56	MG	CA	3095	1/1	0.97	0.12	174,174,174,174	0
56	MG	AA	1649	1/1	0.97	0.06	111,111,111,111	0
59	PUT	DA	3223	6/6	0.97	0.19	75,81,84,84	0
56	MG	BA	1602	1/1	0.97	0.11	102,102,102,102	0
56	MG	DA	3122	1/1	0.97	0.28	48,48,48,48	0
56	MG	DR	202	1/1	0.97	0.30	269,269,269,269	0
66	ACY	DA	3202	4/4	0.97	0.19	93,96,96,97	0
56	MG	BA	1601	1/1	0.97	0.22	135,135,135,135	0
56	MG	CA	3012	1/1	0.97	0.14	115,115,115,115	0
56	MG	DA	3139	1/1	0.97	0.13	42,42,42,42	0
56	MG	CA	3115	1/1	0.97	0.30	111,111,111,111	0
56	MG	CA	3027	1/1	0.97	0.21	88,88,88,88	0
56	MG	CA	3063	1/1	0.97	0.13	155,155,155,155	0
56	MG	CA	3017	1/1	0.97	0.12	192,192,192,192	0
56	MG	CA	3081	1/1	0.97	0.16	254,254,254,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1650	1/1	0.97	0.13	115,115,115,115	0
56	MG	DA	3167	1/1	0.97	0.43	97,97,97,97	0
56	MG	CA	3079	1/1	0.97	0.28	131,131,131,131	0
62	EDO	DA	3208	4/4	0.97	0.21	111,113,113,113	0
56	MG	DA	3135	1/1	0.97	0.17	146,146,146,146	0
56	MG	AA	1645	1/1	0.97	0.13	70,70,70,70	0
56	MG	DA	3173	1/1	0.97	0.87	100,100,100,100	0
56	MG	DA	3117	1/1	0.97	0.12	70,70,70,70	0
56	MG	CA	3091	1/1	0.97	0.09	81,81,81,81	0
56	MG	AA	1632	1/1	0.97	0.10	162,162,162,162	0
56	MG	DA	3099	1/1	0.97	0.19	45,45,45,45	0
56	MG	DA	3181	1/1	0.97	0.29	66,66,66,66	0
56	MG	CA	3078	1/1	0.98	0.30	198,198,198,198	0
56	MG	CA	3025	1/1	0.98	0.13	133,133,133,133	0
56	MG	CA	3074	1/1	0.98	0.10	145,145,145,145	0
56	MG	CA	3037	1/1	0.98	0.27	234,234,234,234	0
56	MG	CA	3069	1/1	0.98	0.14	107,107,107,107	0
56	MG	DA	3054	1/1	0.98	0.17	167,167,167,167	0
56	MG	CA	3049	1/1	0.98	0.12	53,53,53,53	0
56	MG	DA	3048	1/1	0.98	0.12	59,59,59,59	0
56	MG	AA	1652	1/1	0.98	0.26	42,42,42,42	0
56	MG	DA	3108	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3030	1/1	0.98	0.20	88,88,88,88	0
56	MG	DA	3004	1/1	0.98	0.14	149,149,149,149	0
56	MG	CA	3044	1/1	0.98	0.17	113,113,113,113	0
56	MG	DA	3085	1/1	0.98	0.14	100,100,100,100	0
56	MG	BA	1605	1/1	0.98	0.08	136,136,136,136	0
56	MG	DA	3127	1/1	0.98	0.45	69,69,69,69	0
56	MG	CA	3024	1/1	0.98	0.06	85,85,85,85	0
56	MG	BA	1611	1/1	0.98	0.13	84,84,84,84	0
56	MG	CA	3015	1/1	0.98	0.22	84,84,84,84	0
56	MG	AA	1667	1/1	0.98	0.14	76,76,76,76	0
56	MG	DA	3231	1/1	0.98	0.26	70,70,70,70	0
56	MG	DA	3094	1/1	0.98	0.19	29,29,29,29	0
56	MG	DA	3031	1/1	0.98	0.16	51,51,51,51	0
56	MG	CA	3042	1/1	0.98	0.06	96,96,96,96	0
56	MG	DA	3067	1/1	0.98	0.11	75,75,75,75	0
56	MG	DA	3071	1/1	0.98	0.08	56,56,56,56	0
56	MG	BA	1608	1/1	0.98	0.19	144,144,144,144	0
56	MG	DA	3111	1/1	0.98	0.47	283,283,283,283	0
56	MG	BA	1614	1/1	0.98	0.14	217,217,217,217	0
56	MG	CA	3100	1/1	0.98	0.25	243,243,243,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3011	1/1	0.98	0.17	95,95,95,95	0
56	MG	DA	3115	1/1	0.98	0.20	52,52,52,52	0
56	MG	CA	3144	1/1	0.98	0.06	66,66,66,66	0
56	MG	DA	3151	1/1	0.98	0.26	48,48,48,48	0
56	MG	AA	1643	1/1	0.98	0.14	70,70,70,70	0
56	MG	DA	3053	1/1	0.98	0.10	54,54,54,54	0
56	MG	AA	1639	1/1	0.98	0.50	225,225,225,225	0
56	MG	DA	3043	1/1	0.98	0.14	40,40,40,40	0
56	MG	AA	1631	1/1	0.98	0.09	75,75,75,75	0
56	MG	AA	1636	1/1	0.98	0.39	209,209,209,209	0
56	MG	DA	3150	1/1	0.98	0.08	72,72,72,72	0
56	MG	CA	3045	1/1	0.98	0.08	167,167,167,167	0
56	MG	DA	3088	1/1	0.98	0.09	75,75,75,75	0
58	MPD	DS	203	8/8	0.98	0.22	62,64,65,67	0
56	MG	BA	1615	1/1	0.98	0.16	103,103,103,103	0
56	MG	DA	3159	1/1	0.98	0.14	131,131,131,131	0
56	MG	DA	3169	1/1	0.98	0.11	41,41,41,41	0
56	MG	CA	3086	1/1	0.98	0.21	106,106,106,106	0
56	MG	CA	3043	1/1	0.99	0.06	90,90,90,90	0
56	MG	DA	3026	1/1	0.99	0.18	228,228,228,228	0
56	MG	DA	3103	1/1	0.99	0.15	59,59,59,59	0
56	MG	DA	3089	1/1	0.99	0.15	24,24,24,24	0
56	MG	DA	3228	1/1	0.99	0.14	18,18,18,18	0
56	MG	DA	3102	1/1	0.99	0.13	32,32,32,32	0
56	MG	DA	3060	1/1	0.99	0.14	23,23,23,23	0
56	MG	DA	3074	1/1	0.99	0.12	54,54,54,54	0
56	MG	DA	3038	1/1	0.99	0.11	35,35,35,35	0
56	MG	DA	3051	1/1	0.99	0.13	37,37,37,37	0
56	MG	DA	3029	1/1	0.99	0.21	44,44,44,44	0
56	MG	DB	208	1/1	0.99	0.17	57,57,57,57	0
56	MG	DA	3010	1/1	0.99	0.11	48,48,48,48	0
56	MG	DA	3025	1/1	0.99	0.11	57,57,57,57	0
56	MG	DA	3016	1/1	0.99	0.16	74,74,74,74	0
56	MG	DA	3136	1/1	0.99	0.18	72,72,72,72	0
56	MG	DA	3086	1/1	0.99	0.09	82,82,82,82	0
56	MG	DA	3059	1/1	0.99	0.07	25,25,25,25	0
56	MG	AA	1644	1/1	0.99	0.14	180,180,180,180	0
56	MG	DA	3023	1/1	0.99	0.23	57,57,57,57	0
56	MG	CA	3098	1/1	0.99	0.07	98,98,98,98	0
56	MG	DA	3006	1/1	0.99	0.11	266,266,266,266	0
56	MG	DA	3112	1/1	0.99	0.18	46,46,46,46	0
56	MG	DA	3070	1/1	0.99	0.12	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1632	1/1	0.99	0.12	74,74,74,74	0
56	MG	DA	3077	1/1	0.99	0.12	71,71,71,71	0
56	MG	BA	1640	1/1	0.99	0.08	103,103,103,103	0
56	MG	AA	1669	1/1	0.99	0.25	239,239,239,239	0
56	MG	DA	3015	1/1	0.99	0.16	78,78,78,78	0
56	MG	DA	3107	1/1	0.99	0.15	50,50,50,50	0
56	MG	CB	202	1/1	0.99	0.08	116,116,116,116	0
56	MG	CA	3041	1/1	0.99	0.08	50,50,50,50	0
56	MG	DA	3066	1/1	0.99	0.12	43,43,43,43	0
56	MG	AA	1651	1/1	0.99	0.12	75,75,75,75	0
56	MG	DA	3082	1/1	0.99	0.11	109,109,109,109	0
56	MG	AA	1646	1/1	0.99	0.12	80,80,80,80	0
56	MG	DA	3014	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3028	1/1	0.99	0.10	116,116,116,116	0
56	MG	DA	3040	1/1	0.99	0.09	55,55,55,55	0
56	MG	DA	3114	1/1	0.99	0.08	52,52,52,52	0
56	MG	DA	3140	1/1	0.99	0.18	51,51,51,51	0
56	MG	DM	202	1/1	0.99	0.04	90,90,90,90	0
56	MG	DA	3020	1/1	0.99	0.06	69,69,69,69	0
56	MG	CA	3089	1/1	0.99	0.21	64,64,64,64	0
56	MG	DA	3035	1/1	0.99	0.14	24,24,24,24	0
56	MG	CA	3102	1/1	0.99	0.11	99,99,99,99	0
56	MG	DA	3078	1/1	0.99	0.06	47,47,47,47	0
56	MG	DB	202	1/1	0.99	0.10	56,56,56,56	0
56	MG	DA	3068	1/1	0.99	0.20	43,43,43,43	0
56	MG	DA	3017	1/1	0.99	0.12	34,34,34,34	0
56	MG	DA	3081	1/1	0.99	0.07	46,46,46,46	0
56	MG	AA	1633	1/1	0.99	0.12	116,116,116,116	0
56	MG	DA	3047	1/1	0.99	0.13	42,42,42,42	0
56	MG	DA	3083	1/1	0.99	0.07	57,57,57,57	0
56	MG	DA	3105	1/1	0.99	0.17	33,33,33,33	0
56	MG	DA	3092	1/1	0.99	0.12	50,50,50,50	0
56	MG	DA	3106	1/1	0.99	0.16	45,45,45,45	0
56	MG	CA	3088	1/1	0.99	0.13	86,86,86,86	0
56	MG	DA	3009	1/1	0.99	0.12	39,39,39,39	0
56	MG	DA	3027	1/1	0.99	0.20	49,49,49,49	0
56	MG	CA	3035	1/1	0.99	0.20	100,100,100,100	0
56	MG	BA	1621	1/1	0.99	0.17	45,45,45,45	0
56	MG	DA	3229	1/1	0.99	0.08	107,107,107,107	0
56	MG	CA	3013	1/1	0.99	0.11	71,71,71,71	0
56	MG	DA	3096	1/1	0.99	0.13	28,28,28,28	0
56	MG	DA	3022	1/1	0.99	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3113	1/1	0.99	0.16	113,113,113,113	0
56	MG	DB	203	1/1	0.99	0.10	88,88,88,88	0
56	MG	AA	1629	1/1	0.99	0.10	110,110,110,110	0
56	MG	DA	3063	1/1	0.99	0.15	111,111,111,111	0
56	MG	DA	3018	1/1	0.99	0.10	95,95,95,95	0
56	MG	DA	3055	1/1	0.99	0.26	52,52,52,52	0
56	MG	DA	3050	1/1	0.99	0.13	41,41,41,41	0
56	MG	DA	3052	1/1	0.99	0.29	251,251,251,251	0
56	MG	DA	3076	1/1	0.99	0.19	46,46,46,46	0
56	MG	DA	3090	1/1	0.99	0.17	26,26,26,26	0
56	MG	DA	3045	1/1	0.99	0.10	73,73,73,73	0
56	MG	DA	3042	1/1	0.99	0.11	87,87,87,87	0
56	MG	DA	3093	1/1	0.99	0.17	23,23,23,23	0
56	MG	DA	3061	1/1	0.99	0.14	44,44,44,44	0
56	MG	DA	3032	1/1	0.99	0.19	33,33,33,33	0
56	MG	DA	3109	1/1	0.99	0.16	38,38,38,38	0
56	MG	DA	3056	1/1	0.99	0.22	55,55,55,55	0
56	MG	DA	3013	1/1	0.99	0.20	13,13,13,13	0
56	MG	DA	3005	1/1	0.99	0.13	67,67,67,67	0
56	MG	DA	3116	1/1	0.99	0.10	72,72,72,72	0
56	MG	DA	3101	1/1	0.99	0.15	90,90,90,90	0
56	MG	CA	3076	1/1	0.99	0.31	218,218,218,218	0
56	MG	BA	1613	1/1	0.99	0.26	149,149,149,149	0
56	MG	AA	1666	1/1	0.99	0.07	100,100,100,100	0
56	MG	DA	3034	1/1	1.00	0.16	44,44,44,44	0
56	MG	DA	3041	1/1	1.00	0.23	22,22,22,22	0
56	MG	DA	3065	1/1	1.00	0.13	41,41,41,41	0
60	ZN	D5	101	1/1	1.00	0.10	84,84,84,84	0
56	MG	DA	3039	1/1	1.00	0.11	34,34,34,34	0
56	MG	DA	3037	1/1	1.00	0.16	13,13,13,13	0
56	MG	DA	3046	1/1	1.00	0.18	27,27,27,27	0
56	MG	DA	3049	1/1	1.00	0.13	52,52,52,52	0
56	MG	DA	3084	1/1	1.00	0.18	55,55,55,55	0
56	MG	DA	3104	1/1	1.00	0.22	43,43,43,43	0
56	MG	DA	3036	1/1	1.00	0.18	32,32,32,32	0
56	MG	DA	3019	1/1	1.00	0.26	16,16,16,16	0
56	MG	DA	3024	1/1	1.00	0.17	44,44,44,44	0
56	MG	DA	3058	1/1	1.00	0.09	66,66,66,66	0
56	MG	DA	3087	1/1	1.00	0.19	32,32,32,32	0
56	MG	DA	3073	1/1	1.00	0.16	40,40,40,40	0
56	MG	DA	3110	1/1	1.00	0.16	31,31,31,31	0
56	MG	DA	3057	1/1	1.00	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3091	1/1	1.00	0.13	29,29,29,29	0
56	MG	DA	3011	1/1	1.00	0.10	23,23,23,23	0
56	MG	DA	3021	1/1	1.00	0.14	31,31,31,31	0
56	MG	DA	3069	1/1	1.00	0.10	64,64,64,64	0
56	MG	DA	3072	1/1	1.00	0.20	86,86,86,86	0
56	MG	DA	3100	1/1	1.00	0.20	34,34,34,34	0
56	MG	DA	3075	1/1	1.00	0.18	25,25,25,25	0
56	MG	DA	3064	1/1	1.00	0.14	75,75,75,75	0
56	MG	DA	3230	1/1	1.00	0.13	76,76,76,76	0
56	MG	DA	3119	1/1	1.00	0.30	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.