wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 06:57 PM EDT

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

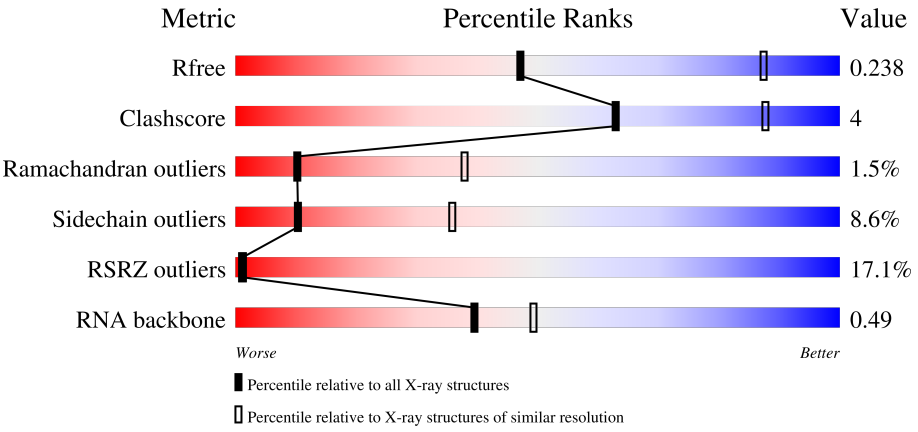
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 67% 29% .
1	BA	1534	17% 66% 29% .
2	AB	224	25% 81% 17% .
2	BB	224	20% 81% 17% .

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Mol	Chain	Length	Quality of chain
3	AC	206	27% 85% 13%
3	BC	206	61% 83% 16%
4	AD	205	2% 85% 13%
4	BD	205	84% 16%
5	AE	155	5% 75% 22%
5	BE	155	8% 69% 25%
6	AF	106	5% 77% 20%
6	BF	106	13% 71% 23% 6%
7	AG	151	46% 74% 25%
7	BG	151	72% 76% 21%
8	AH	129	8% 78% 21%
8	BH	129	9% 81% 18%
9	AI	127	40% 80% 20%
9	BI	127	50% 82% 18%
10	AJ	99	44% 81% 16%
10	BJ	99	74% 73% 22%
11	AK	129	14% 74% 16% 9%
11	BK	129	22% 71% 19% 9%
12	AL	123	9% 78% 20%
12	BL	123	10% 76% 22%
13	AM	114	46% 75% 24%
13	BM	114	90% 70% 25% 5%
14	AN	100	51% 83% 17%
14	BN	100	77% 83% 17%
15	AO	88	8% 92% 7%

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Mol	Chain	Length	Quality of chain
15	BO	88	19% 85% 11%
16	AP	82	34% 87% 11%
16	BP	82	26% 84% 13%
17	AQ	80	12% 75% 22%
17	BQ	80	31% 75% 22%
18	AR	55	15% 84% 16%
18	BR	55	35% 85% 15%
19	AS	79	32% 68% 28%
19	BS	79	70% 73% 23%
20	AT	86	3% 71% 24% 5%
20	BT	86	30% 72% 23%
21	AU	56	12% 77% 23%
21	BU	56	14% 80% 20%
22	C1	56	32% 68% 29%
22	D1	56	79% 18%
23	C2	51	73% 75% 22%
23	D2	51	75% 25%
24	C3	46	43% 83% 15%
24	D3	46	76% 22%
25	C4	64	36% 89% 11%
25	D4	64	80% 20%
26	C5	38	16% 79% 18%
26	D5	38	3% 79% 18%
27	C0	58	26% 79% 17%
27	D0	58	74% 24%

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Mol	Chain	Length	Quality of chain
28	CB	120	6% 78% 18%
28	DB	120	78% 20%
29	CC	272	13% 83% 15%
29	DC	272	82% 18%
30	CD	209	36% 80% 19%
31	CA	2904	9% 64% 31% 5%
32	DD	209	79% 20%
33	CE	201	34% 80% 18%
33	DE	201	82% 17%
34	CF	178	61% 78% 20%
34	DF	178	6% 70% 28%
35	CG	176	57% 82% 16%
35	DG	176	5% 85% 14%
36	CH	149	35% 81% 15%
36	DH	149	20% 79% 20%
37	CJ	135	81% 82% 14%
37	DJ	135	68% 81% 16%
38	CK	142	6% 81% 18%
38	DK	142	80% 18%
39	CL	123	13% 81% 16%
39	DL	123	84% 15%
40	CM	144	48% 78% 21%
40	DM	144	% 85% 14%
41	CN	136	14% 76% 22%
41	DN	136	74% 24%

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Mol	Chain	Length	Quality of chain
42	CO	127	20% 66% 27% 6%
42	DO	127	72% 26%
43	CP	117	51% 74% 21%
43	DP	117	74% 22%
44	CQ	114	33% 85% 12%
44	DQ	114	% 83% 14%
45	CR	117	26% 82% 15%
45	DR	117	79% 19%
46	CS	103	37% 71% 25%
46	DS	103	71% 26%
47	CT	110	35% 72% 25%
47	DT	110	78% 22%
48	CU	100	54% 70% 18% 5% 7%
48	DU	100	2% 76% 15% 7%
49	CV	103	68% 74% 24%
49	DV	103	5% 83% 16%
50	CW	94	36% 81% 17%
50	DW	94	82% 16%
51	CX	76	41% 83% 16%
51	DX	76	79% 20%
52	CY	77	18% 74% 25%
52	DY	77	% 81% 18%
53	CZ	62	61% 85% 13%
53	DZ	62	3% 84% 13%
54	DI	135	29% 66% 28% 6%

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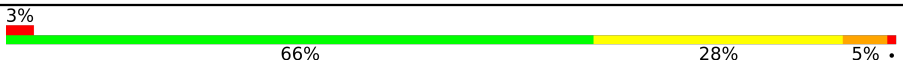
Mol	Chain	Length	Quality of chain
55	DA	2904	

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	3196	-	X	-	-
66	ACY	DA	3202	-	-	X	-
68	TRS	DA	3220	-	-	-	X

2 Entry composition (i)

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 857	C 532	N 166	O 156	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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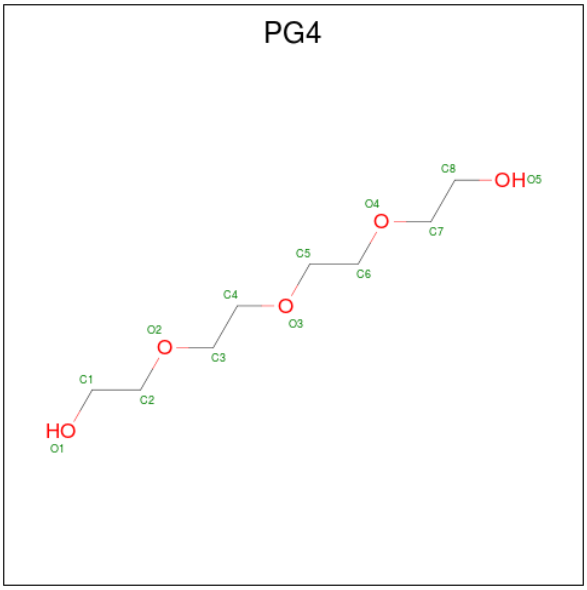
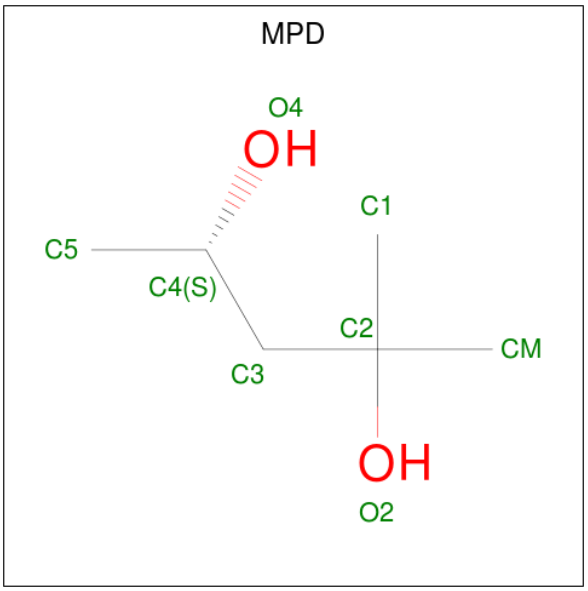
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DB	9	Total Mg 9 9	0	0
56	DA	184	Total Mg 184 184	0	0

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



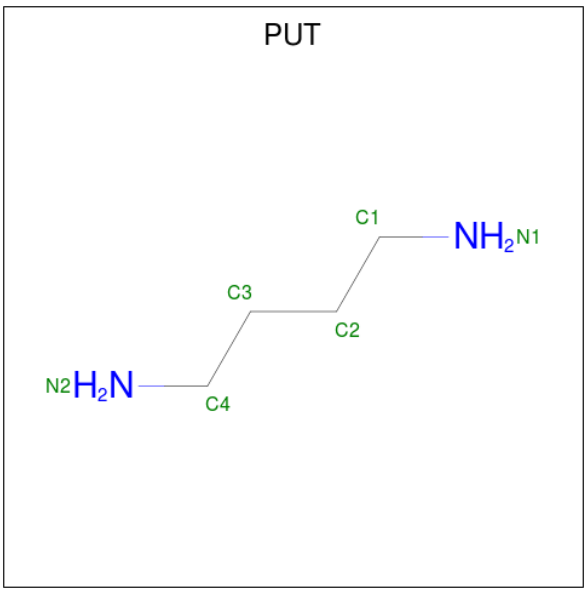
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0

- 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 8 6 2	0	0
58	AA	1	Total C O 8 6 2	0	0
58	DE	1	Total C O 8 6 2	0	0
58	DE	1	Total C O 8 6 2	0	0
58	DK	1	Total C O 8 6 2	0	0
58	DN	1	Total C O 8 6 2	0	0
58	DS	1	Total C O 8 6 2	0	0
58	DT	1	Total C O 8 6 2	0	0
58	DT	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0

- Molecule 59 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



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

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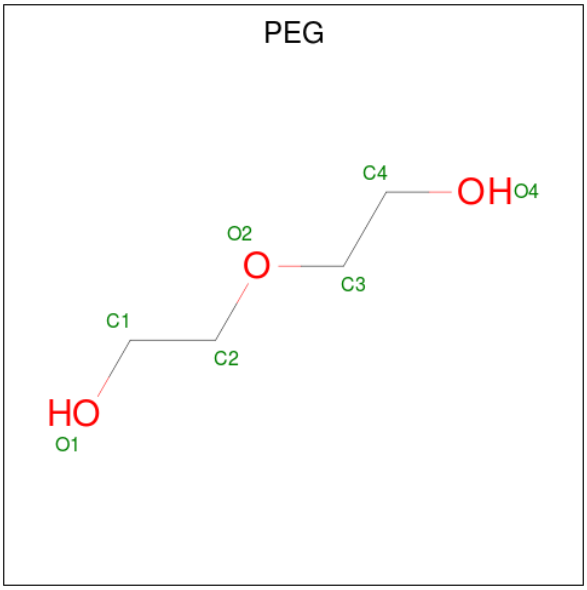
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

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

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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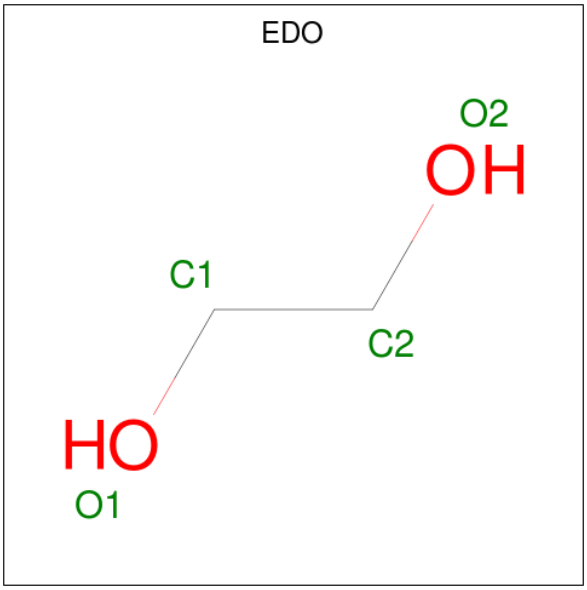
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DP	1	Total C O 7 4 3	0	0
61	DQ	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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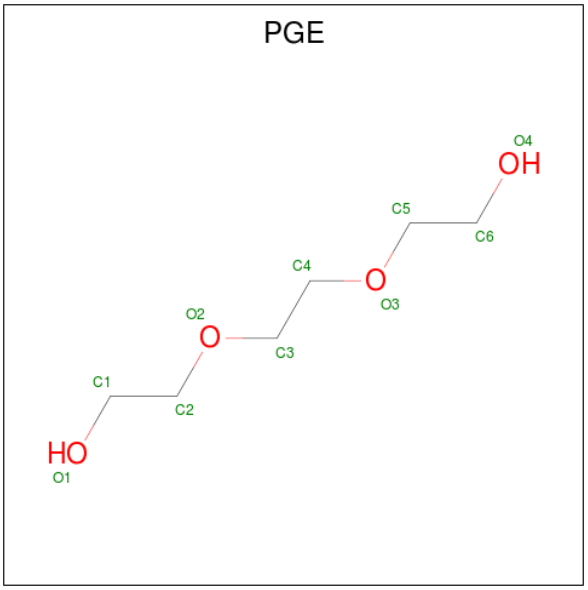
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DB	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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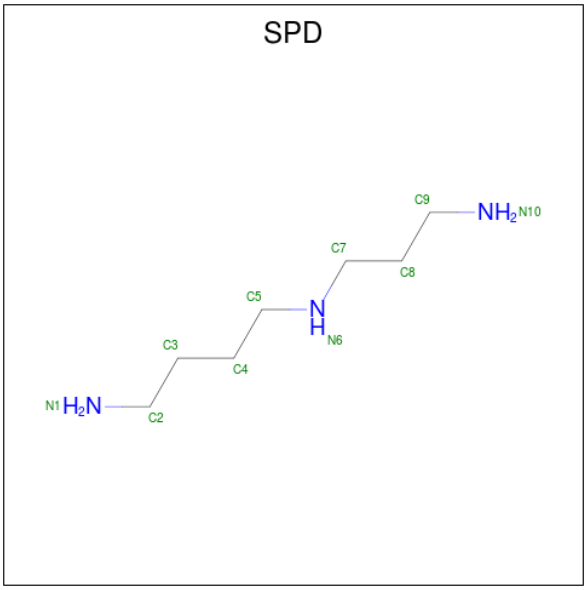
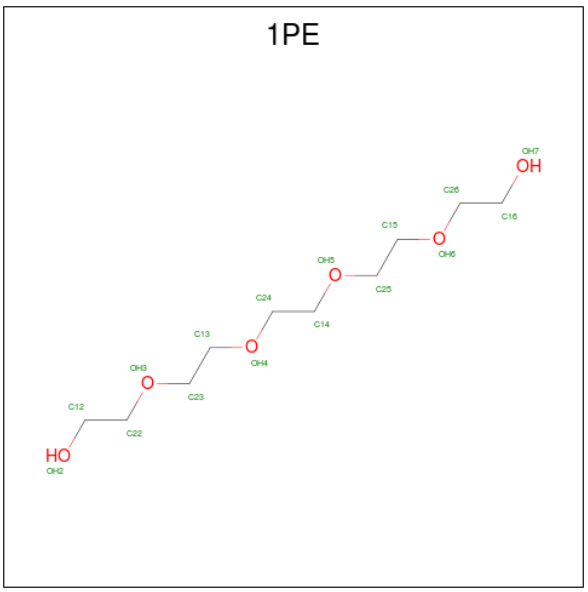
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	DD	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0

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



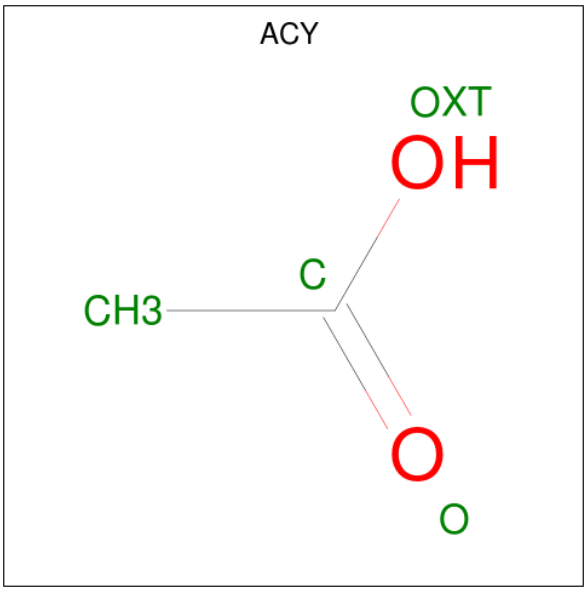
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

- 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 16 10 6	0	0
65	DA	1	Total C O 16 10 6	0	0

- 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 4 2 2	0	0

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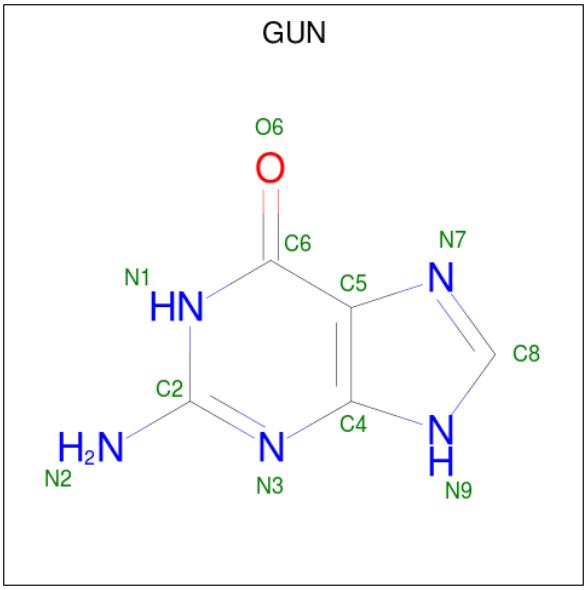
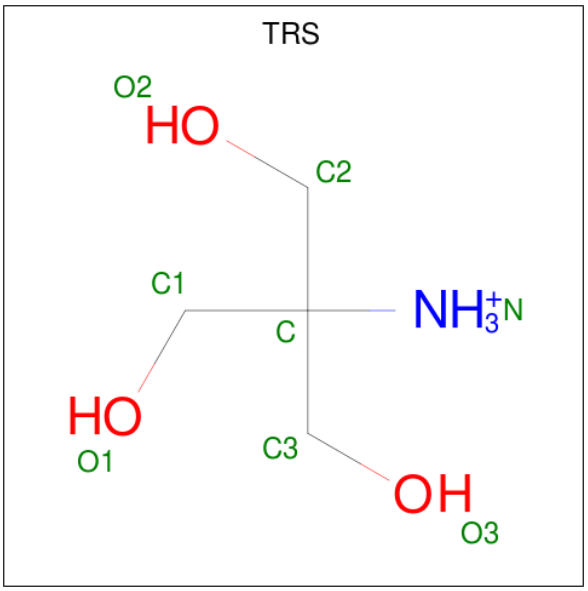
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0

- 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 11 5 5 1	0	0

- 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 8 4 1 3	0	0

- Molecule 69 is water.

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

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

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

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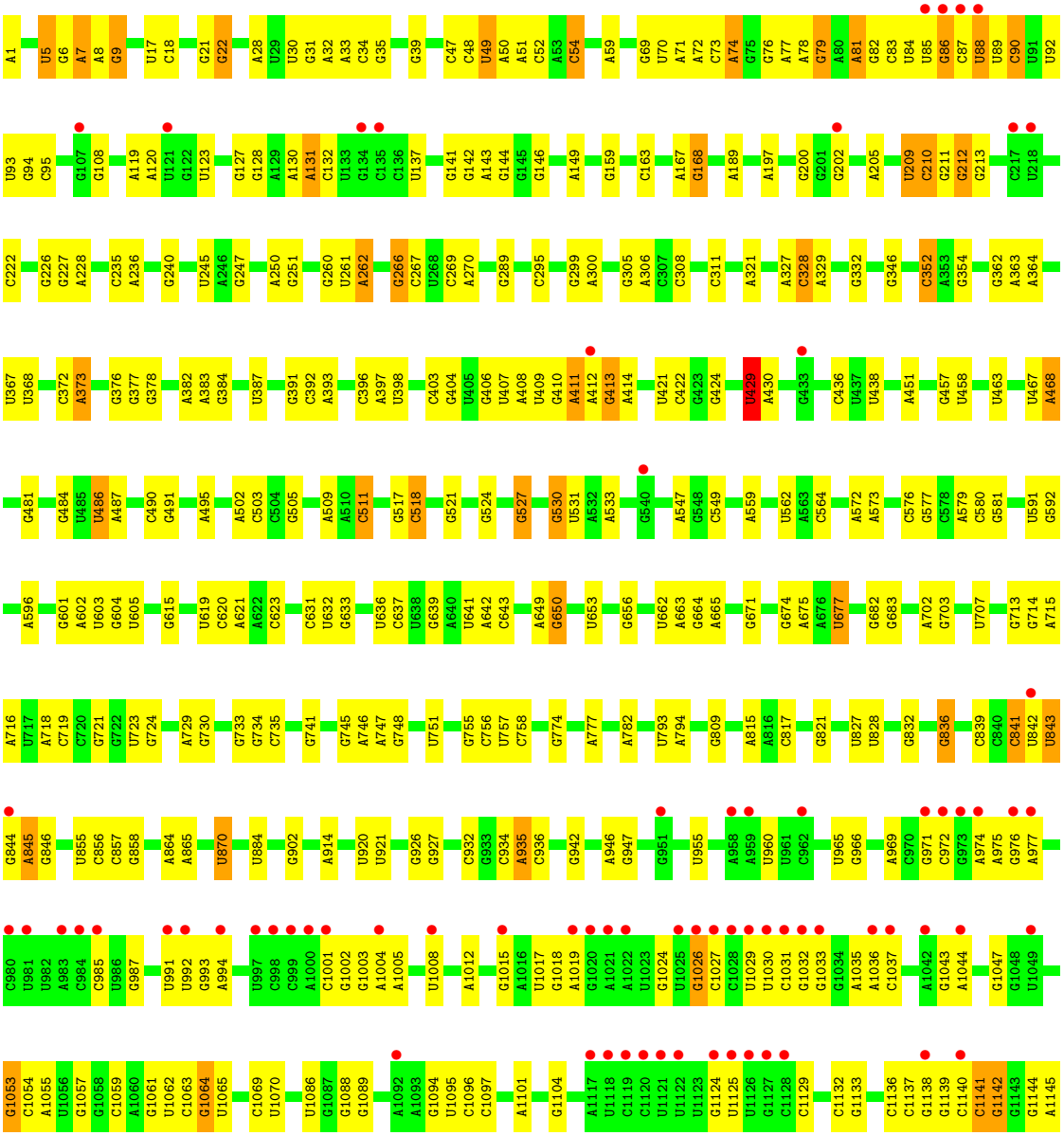
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DH	2	Total O 2 2	0	0
69	DK	61	Total O 61 61	0	0
69	DL	50	Total O 50 50	0	0
69	DM	60	Total O 60 60	0	0
69	DN	81	Total O 81 81	0	0
69	DO	42	Total O 42 42	0	0
69	DP	42	Total O 42 42	0	0
69	DQ	32	Total O 32 32	0	0
69	DR	68	Total O 68 68	0	0
69	DS	52	Total O 52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

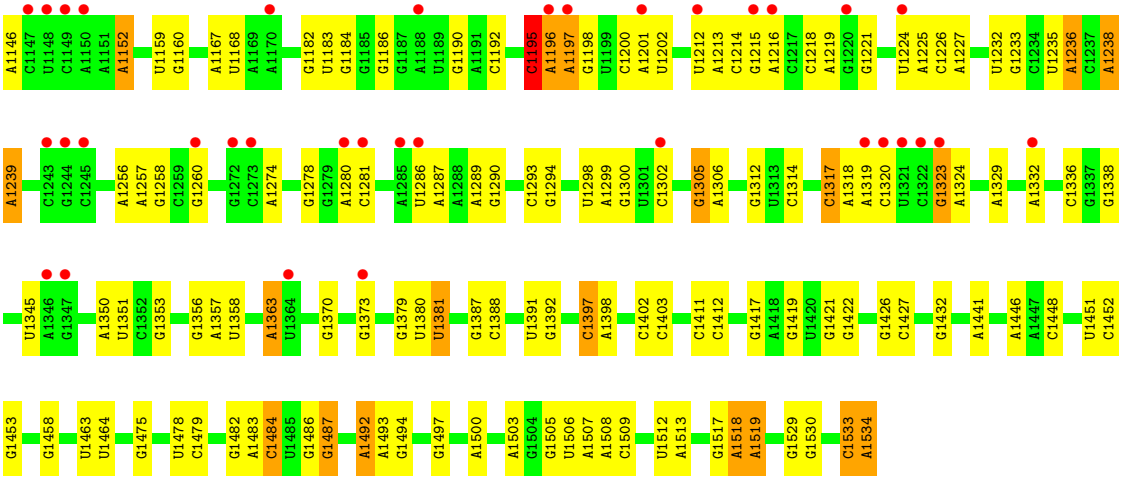
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

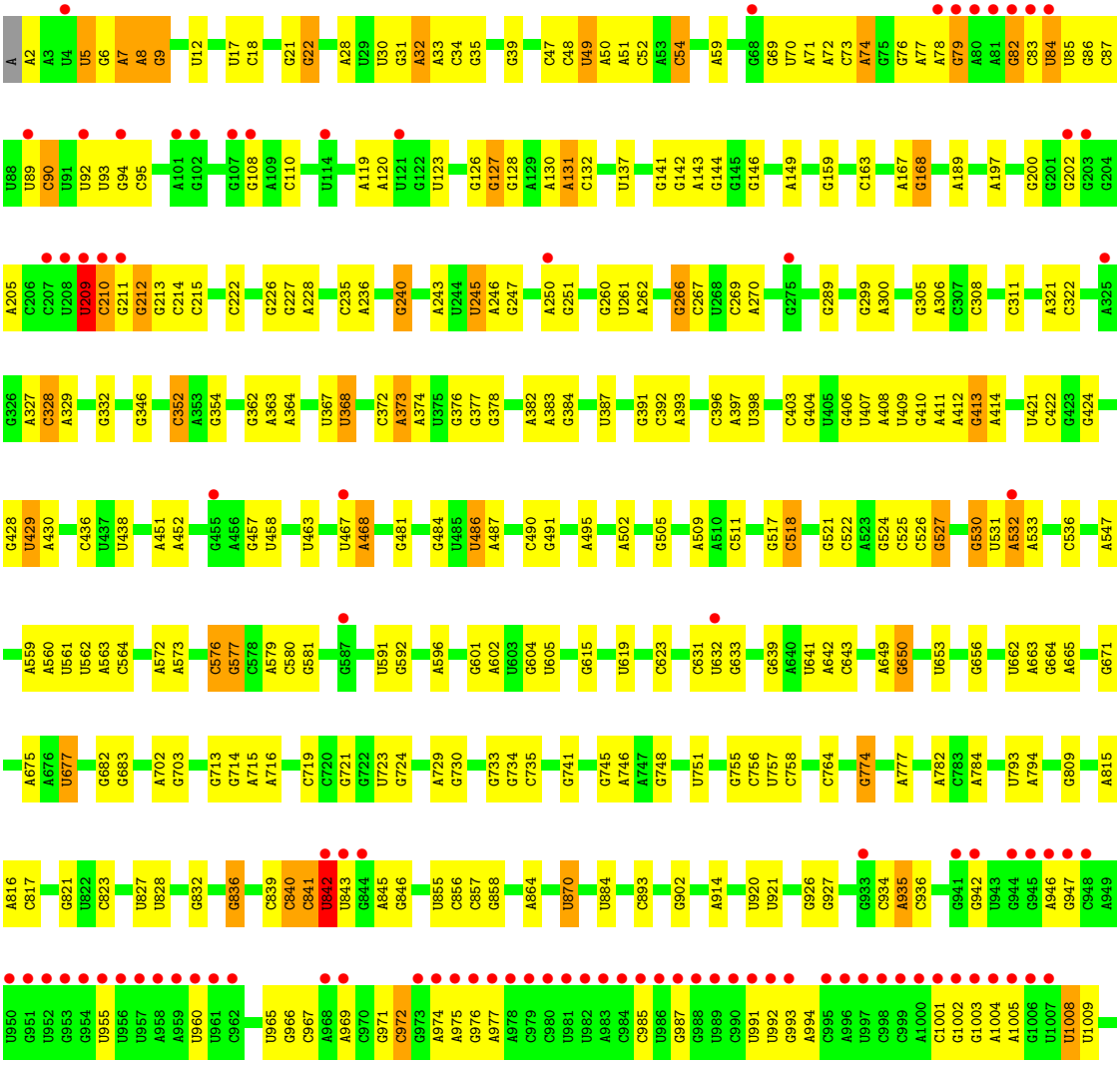
Chain AA:

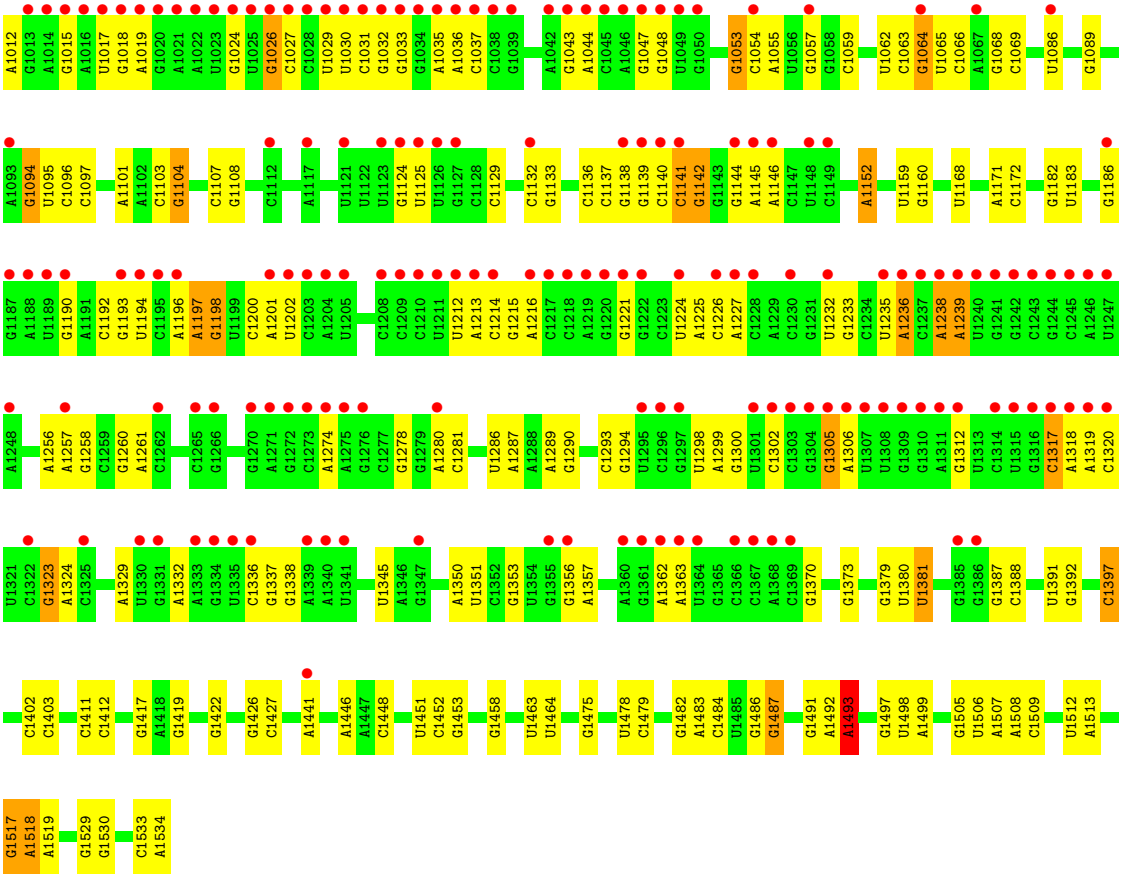




• Molecule 1: 16S rRNA

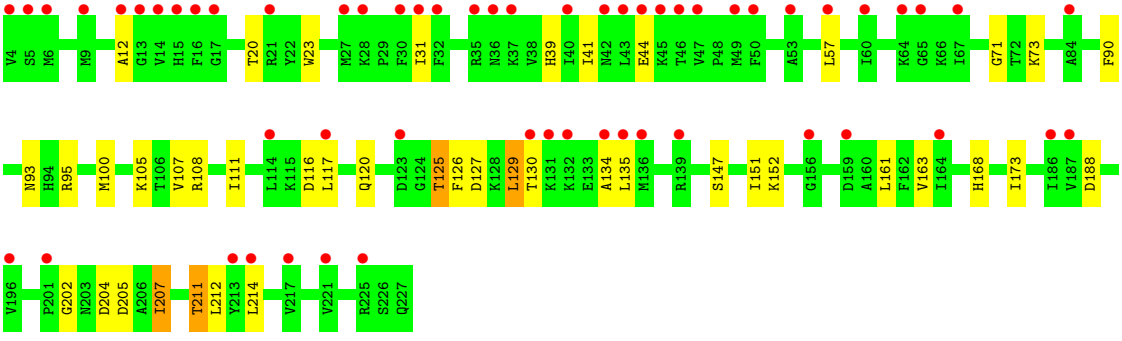
Chain BA:





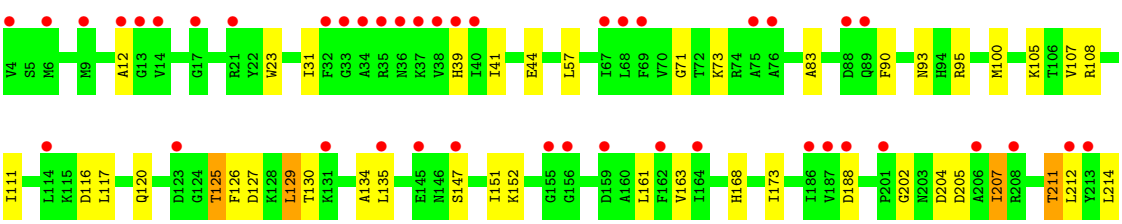
• Molecule 2: 30S ribosomal protein S2

Chain AB:



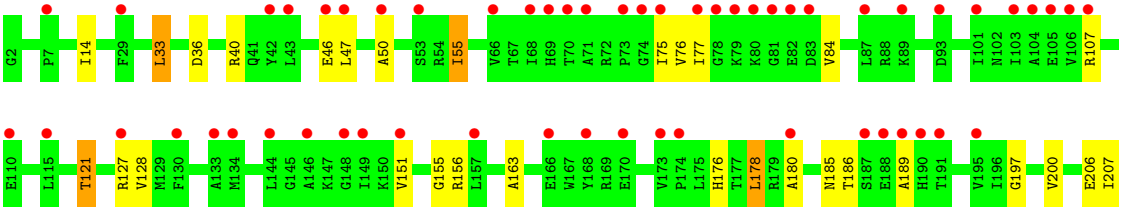
• Molecule 2: 30S ribosomal protein S2

Chain BB:



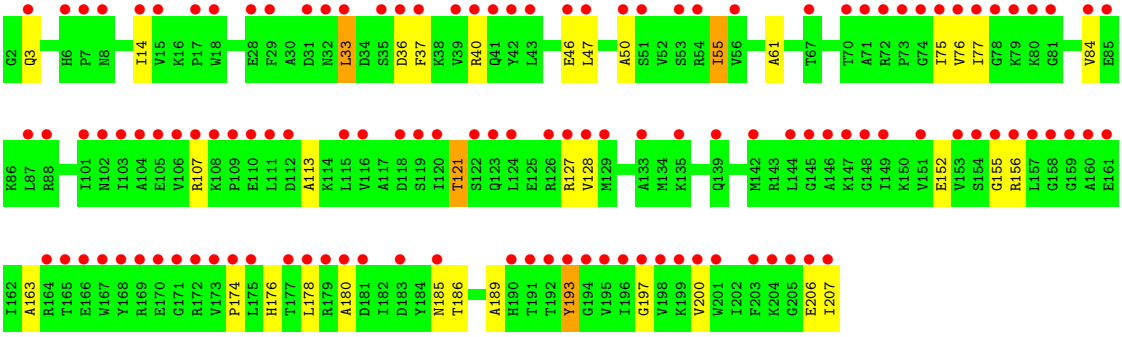
• Molecule 3: 30S ribosomal protein S3

Chain AC:



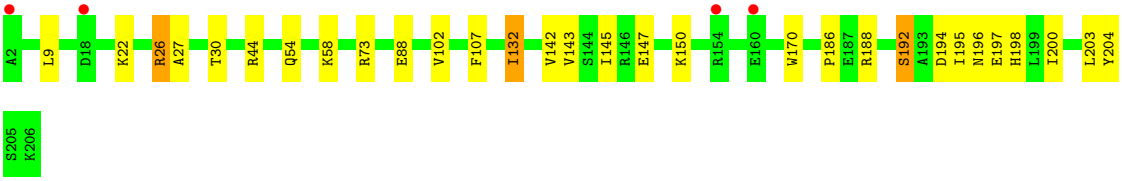
• Molecule 3: 30S ribosomal protein S3

Chain BC:



• Molecule 4: 30S ribosomal protein S4

Chain AD:

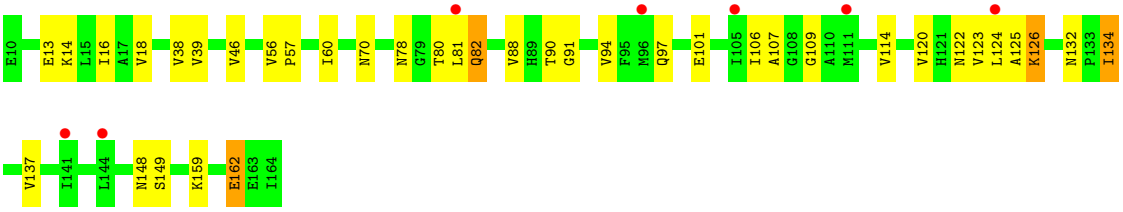


• Molecule 4: 30S ribosomal protein S4

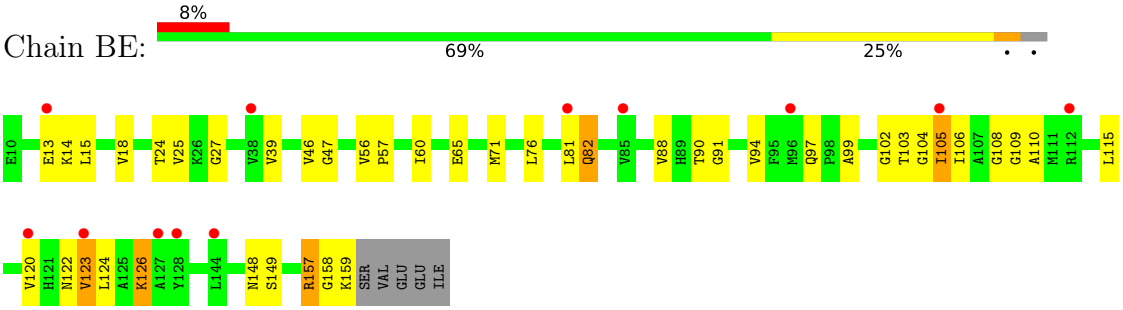
Chain BD:

• Molecule 5: 30S ribosomal protein S5

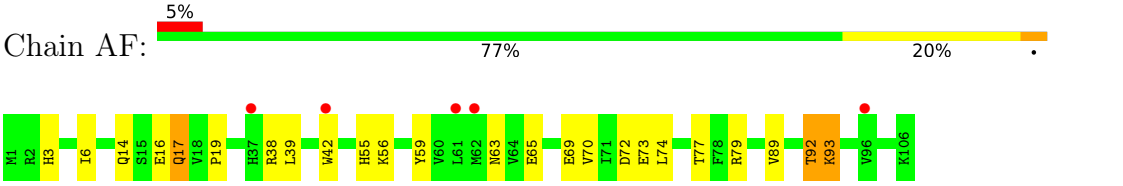
Chain AE:



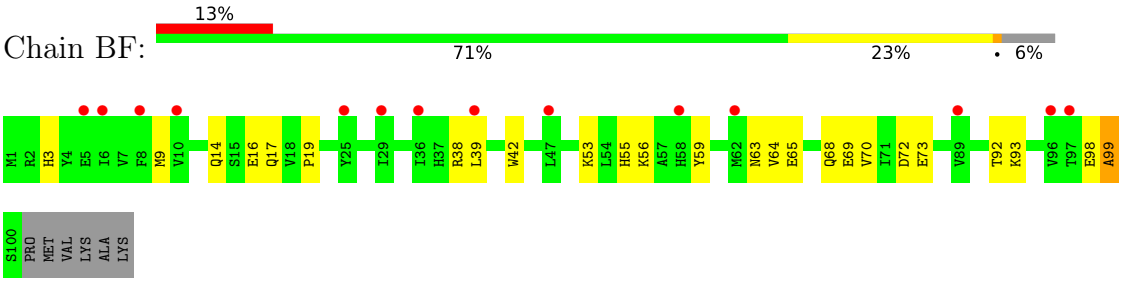
• Molecule 5: 30S ribosomal protein S5



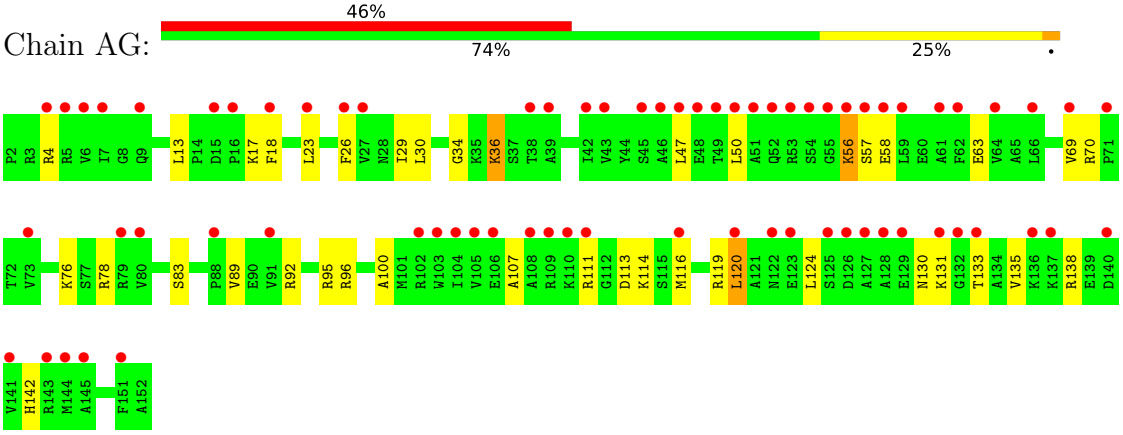
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

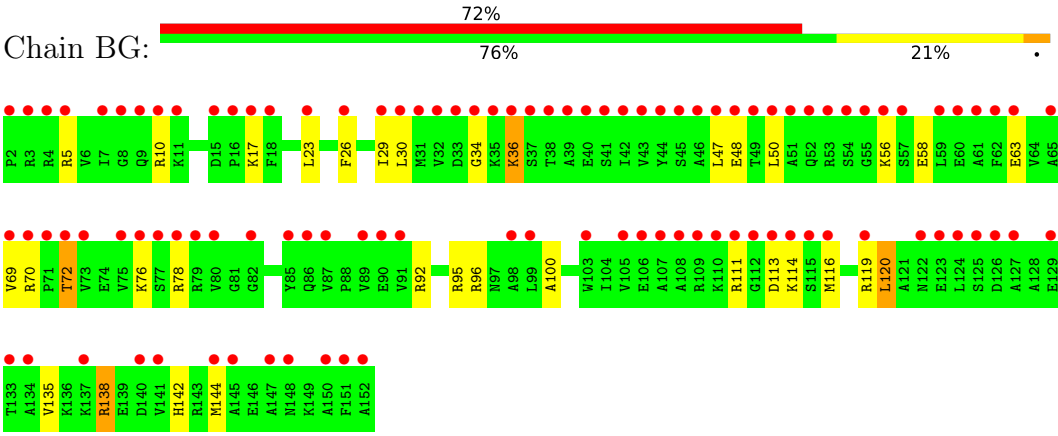


• Molecule 7: 30S ribosomal protein S7



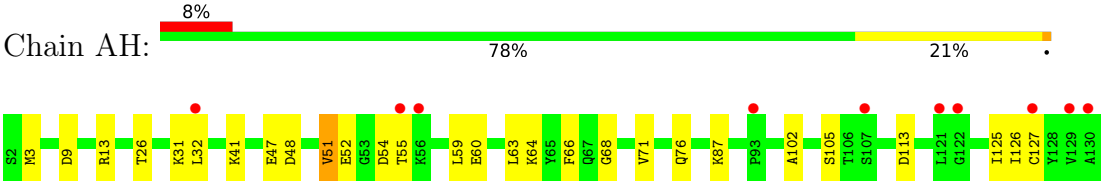
• Molecule 7: 30S ribosomal protein S7

Chain BG:



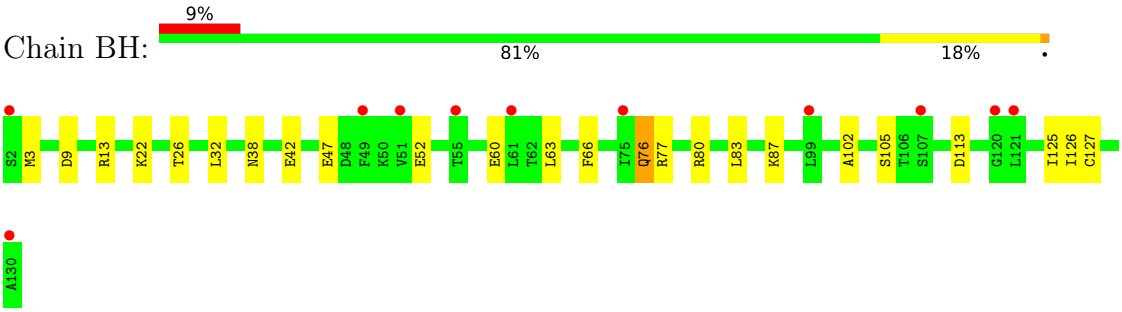
• Molecule 8: 30S ribosomal protein S8

Chain AH:



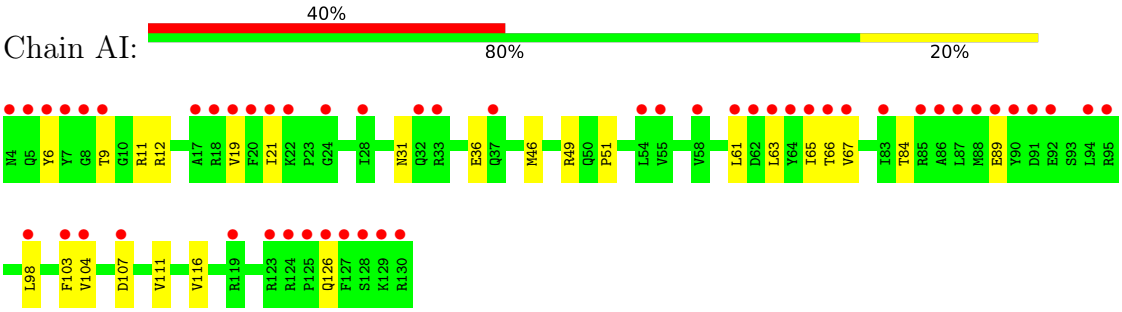
• Molecule 8: 30S ribosomal protein S8

Chain BH:



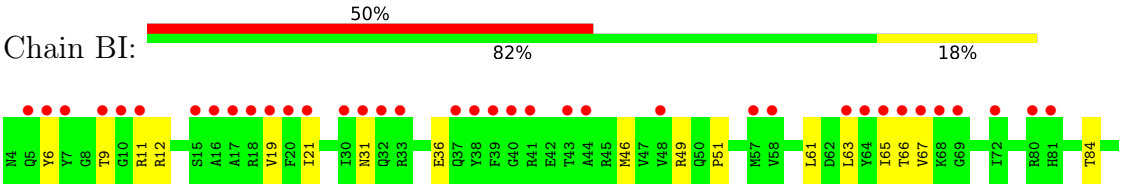
• Molecule 9: 30S ribosomal protein S9

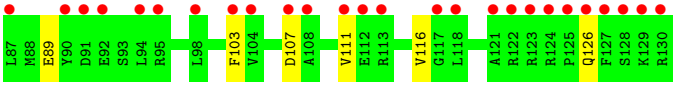
Chain AI:



• Molecule 9: 30S ribosomal protein S9

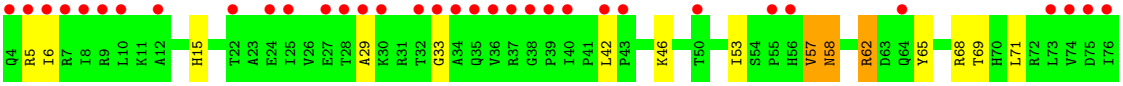
Chain BI:

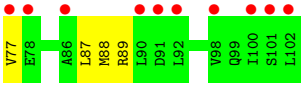




• Molecule 10: 30S ribosomal protein S10

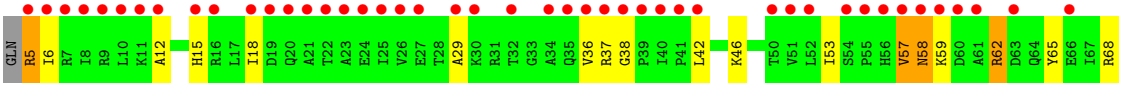
Chain AJ:

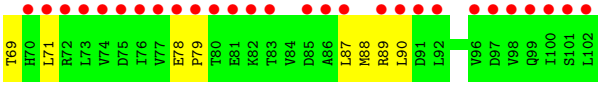




• Molecule 10: 30S ribosomal protein S10

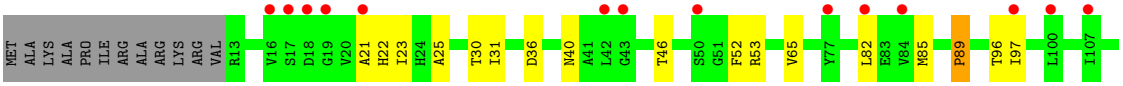
Chain BJ:





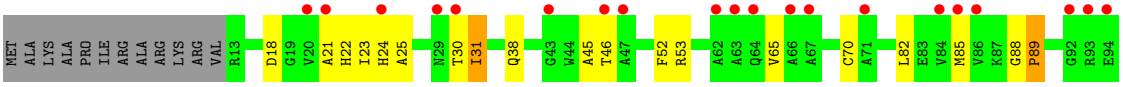
• Molecule 11: 30S ribosomal protein S11

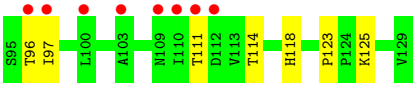
Chain AK:



• Molecule 11: 30S ribosomal protein S11

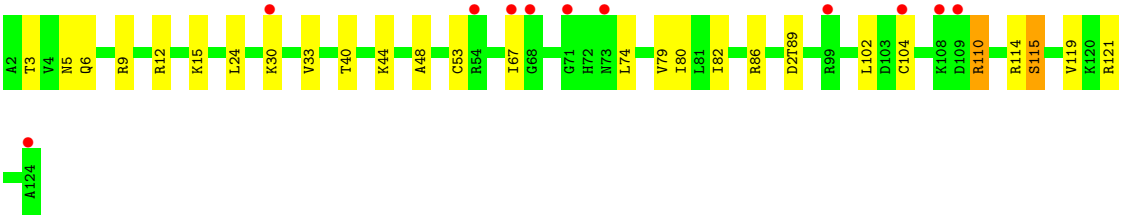
Chain BK:





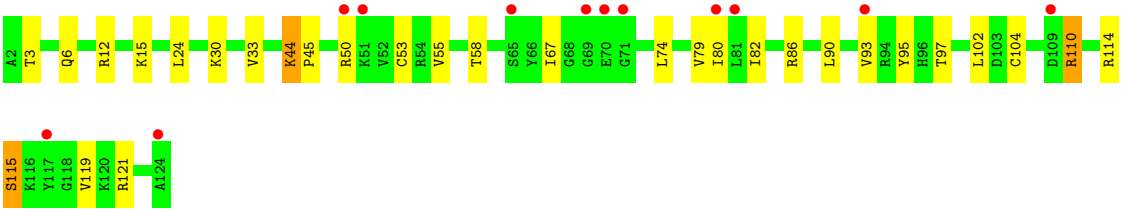
• Molecule 12: 30S ribosomal protein S12

Chain AL:



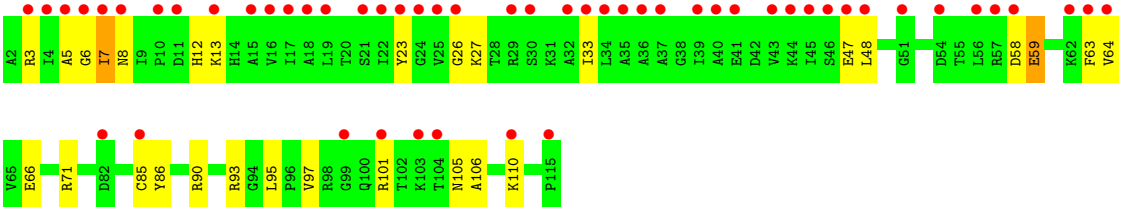
• Molecule 12: 30S ribosomal protein S12

Chain BL:



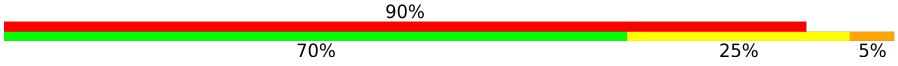
• Molecule 13: 30S ribosomal protein S13

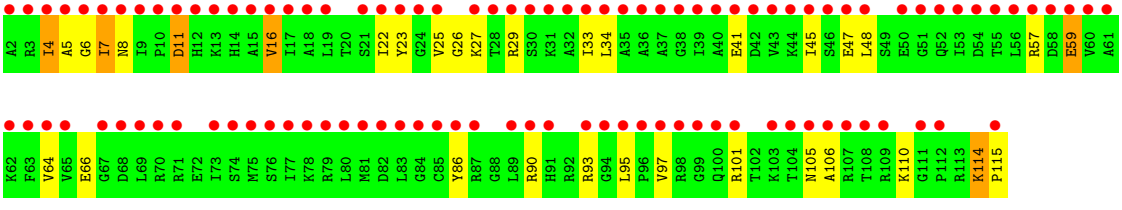
Chain AM:



• Molecule 13: 30S ribosomal protein S13

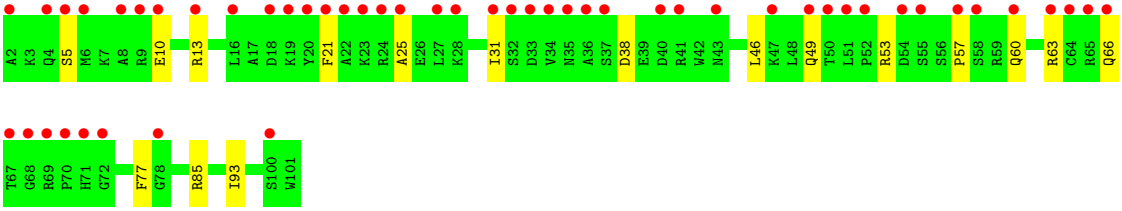
Chain BM:





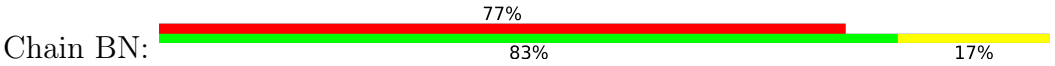
• Molecule 14: 30S ribosomal protein S14

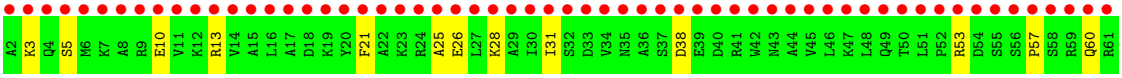
Chain AN:

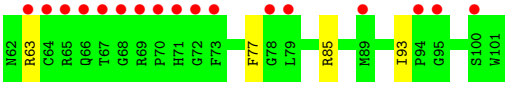


• Molecule 14: 30S ribosomal protein S14

Chain BN:

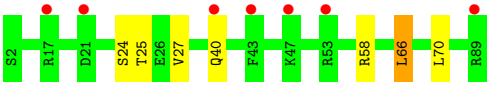






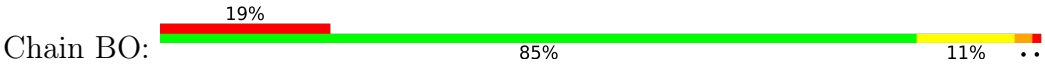
• Molecule 15: 30S ribosomal protein S15

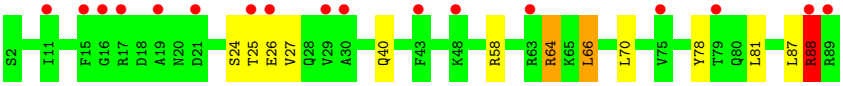
Chain AO:



• Molecule 15: 30S ribosomal protein S15

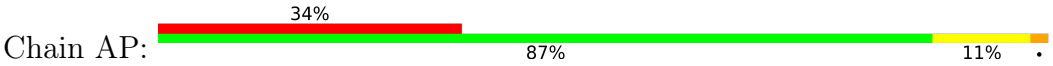
Chain BO:

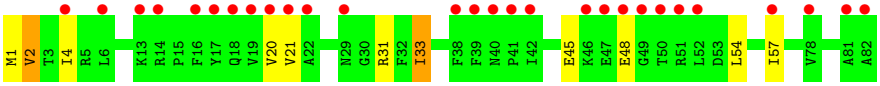




• Molecule 16: 30S ribosomal protein S16

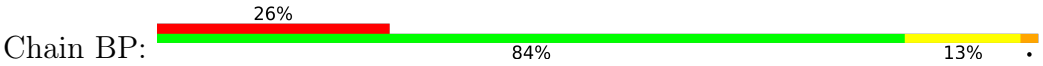
Chain AP:

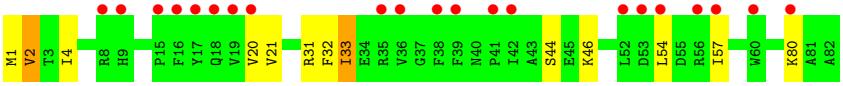




• Molecule 16: 30S ribosomal protein S16

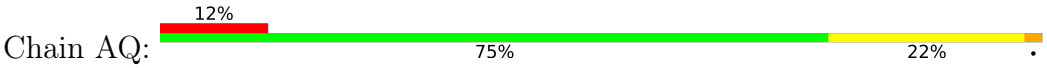
Chain BP:

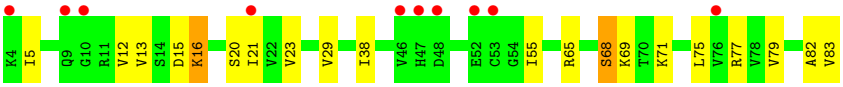




• Molecule 17: 30S ribosomal protein S17

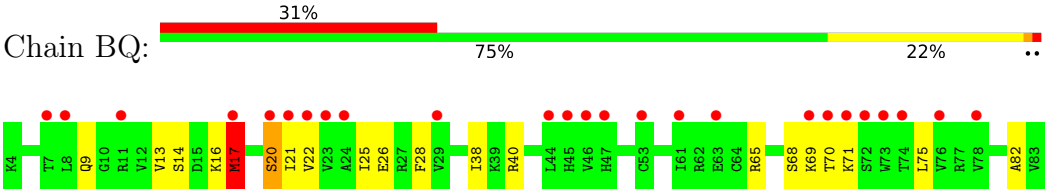
Chain AQ:





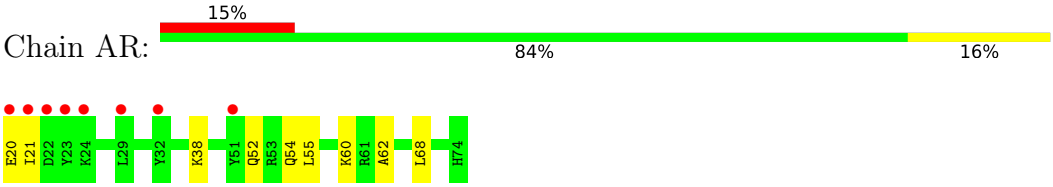
• Molecule 17: 30S ribosomal protein S17

Chain BQ:



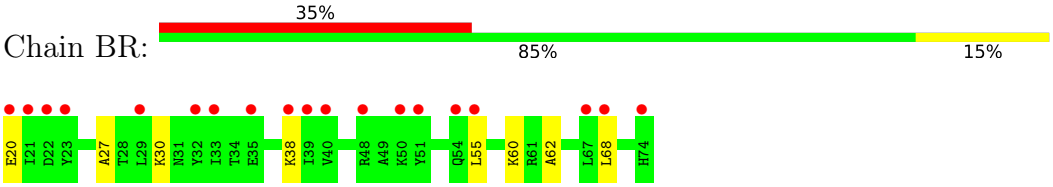
• Molecule 18: 30S ribosomal protein S18

Chain AR:



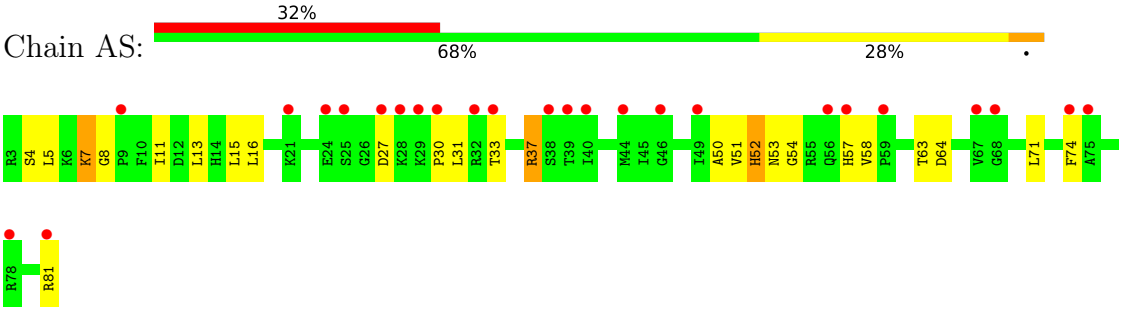
• Molecule 18: 30S ribosomal protein S18

Chain BR:



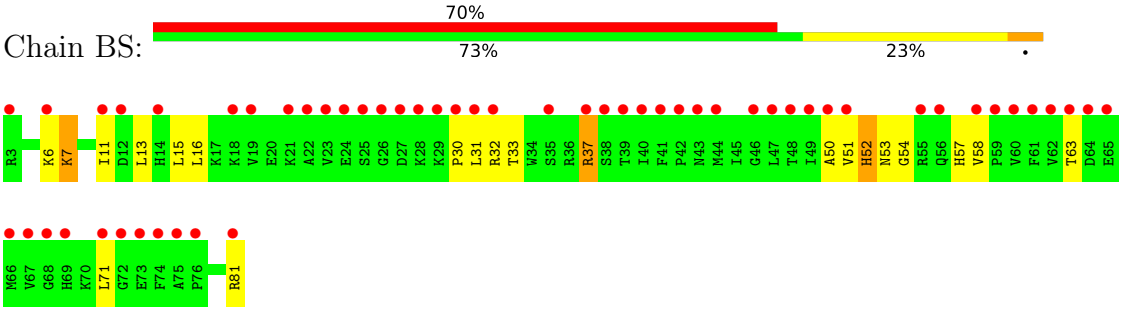
• Molecule 19: 30S ribosomal protein S19

Chain AS:



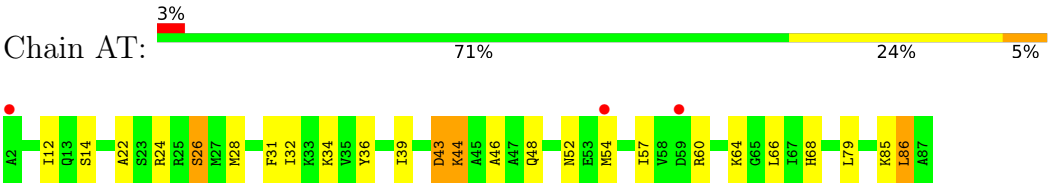
• Molecule 19: 30S ribosomal protein S19

Chain BS:



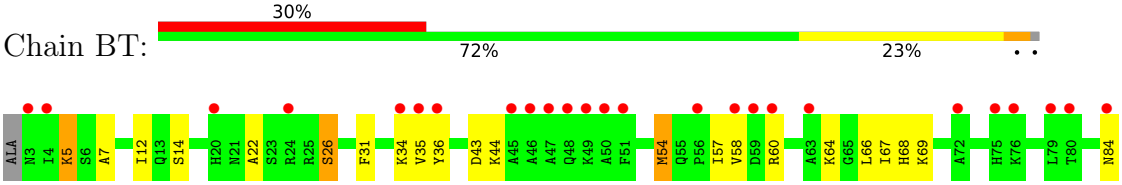
• Molecule 20: 30S ribosomal protein S20

Chain AT:



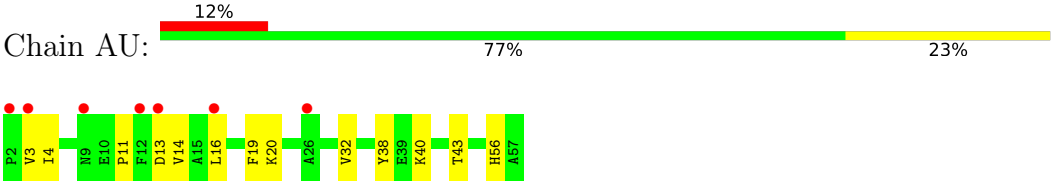
• Molecule 20: 30S ribosomal protein S20

Chain BT:



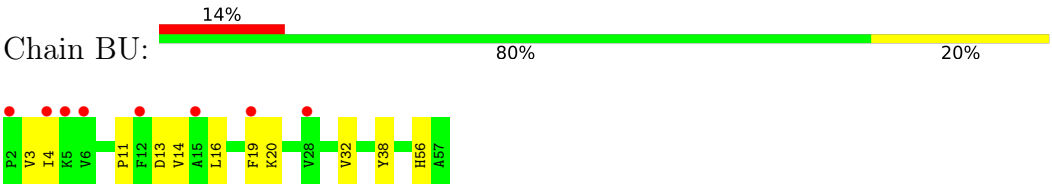
• Molecule 21: 30S ribosomal protein S21

Chain AU:



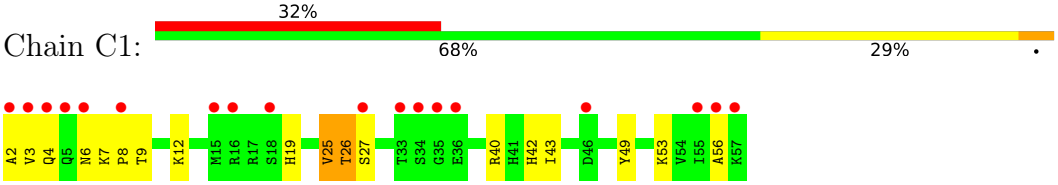
• Molecule 21: 30S ribosomal protein S21

Chain BU:



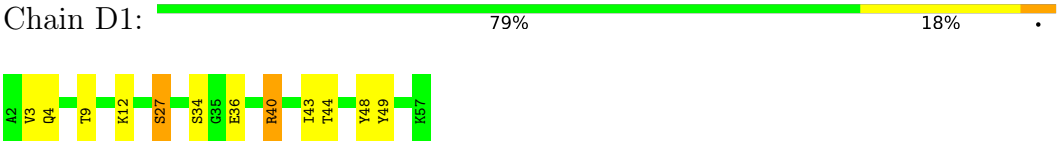
• Molecule 22: 50S ribosomal protein L32

Chain C1:



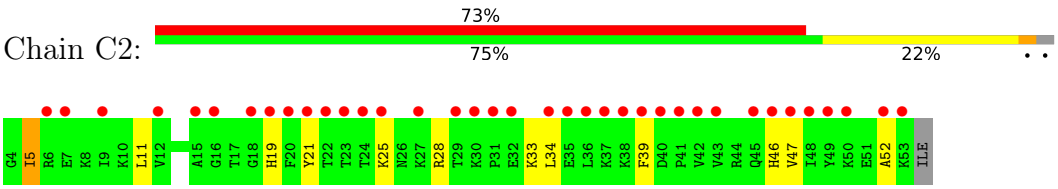
• Molecule 22: 50S ribosomal protein L32

Chain D1:



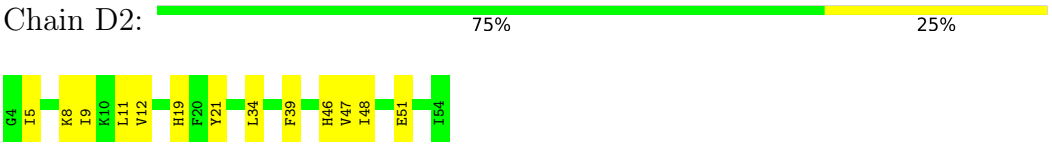
• Molecule 23: 50S ribosomal protein L33

Chain C2:



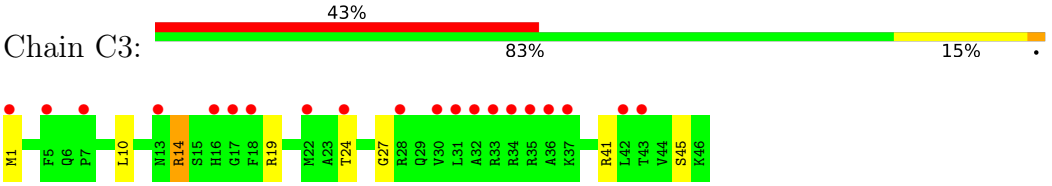
• Molecule 23: 50S ribosomal protein L33

Chain D2:



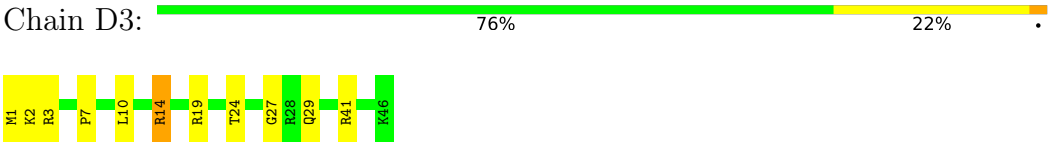
• Molecule 24: 50S ribosomal protein L34

Chain C3:



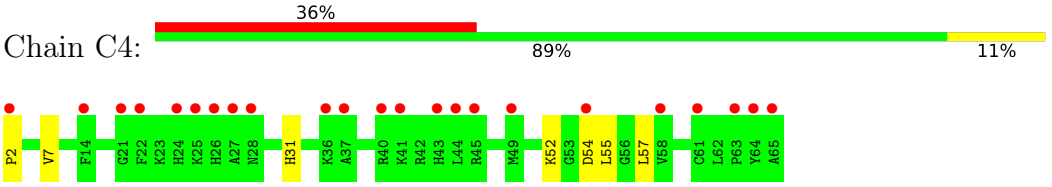
• Molecule 24: 50S ribosomal protein L34

Chain D3:



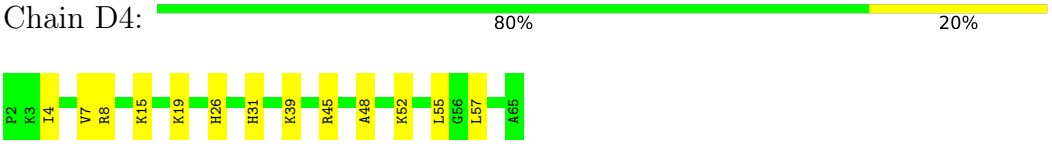
• Molecule 25: 50S ribosomal protein L35

Chain C4:



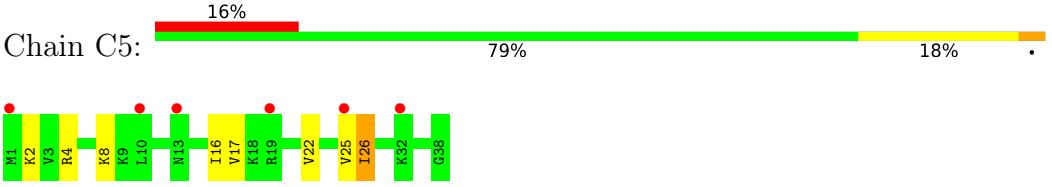
• Molecule 25: 50S ribosomal protein L35

Chain D4:



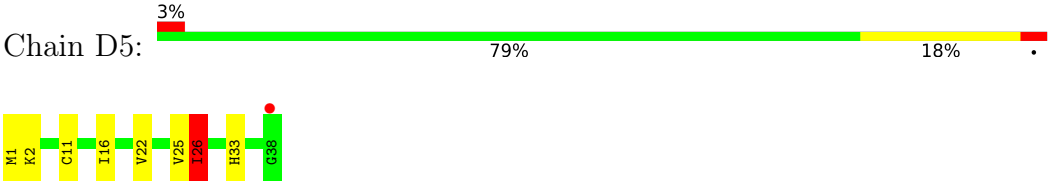
• Molecule 26: 50S ribosomal protein L36

Chain C5:



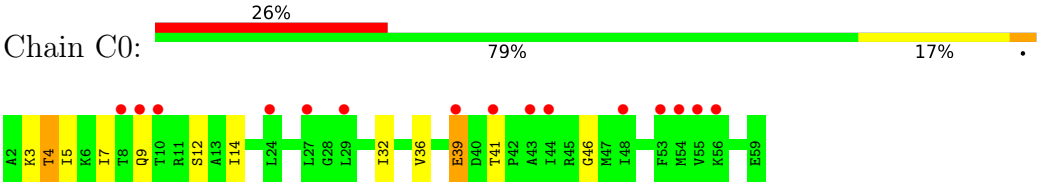
• Molecule 26: 50S ribosomal protein L36

Chain D5:



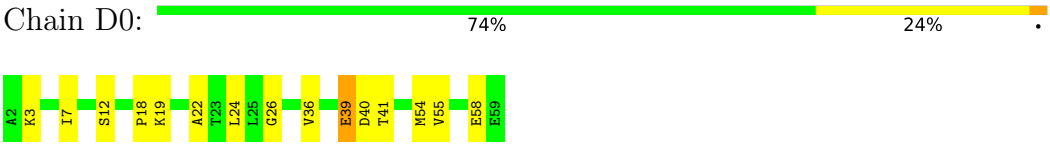
• Molecule 27: 50S ribosomal protein L30

Chain C0:



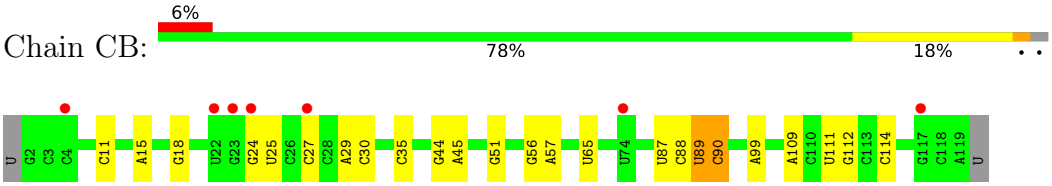
• Molecule 27: 50S ribosomal protein L30

Chain D0:



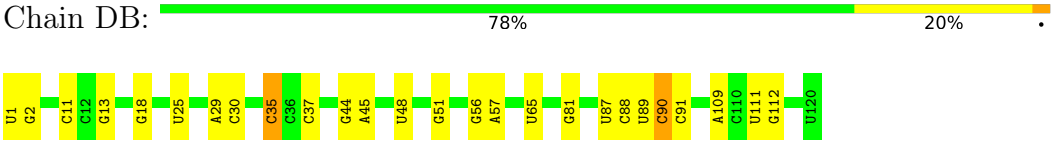
• Molecule 28: 5S rRNA

Chain CB:



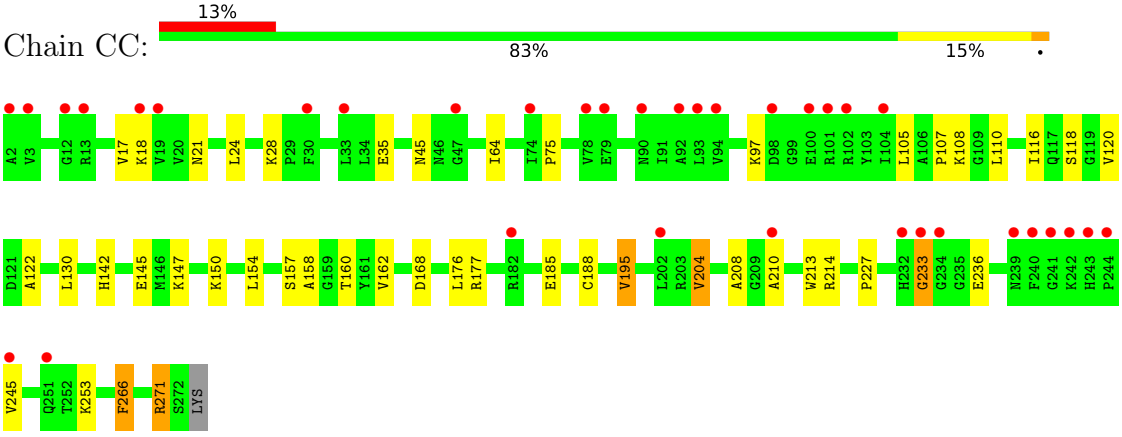
• Molecule 28: 5S rRNA

Chain DB:



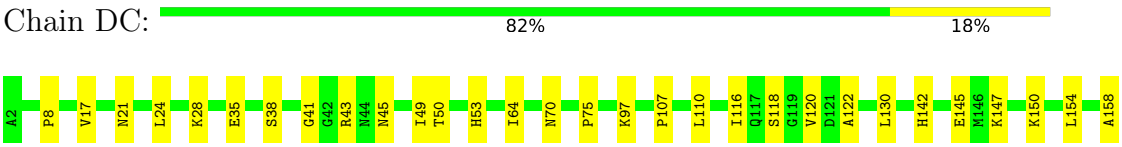
• Molecule 29: 50S ribosomal protein L2

Chain CC:

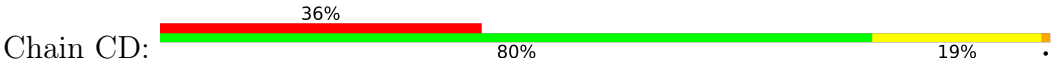


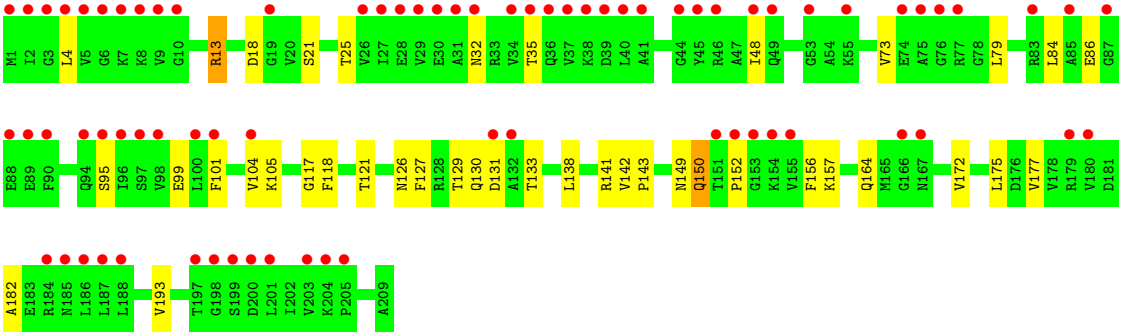
• Molecule 29: 50S ribosomal protein L2

Chain DC:

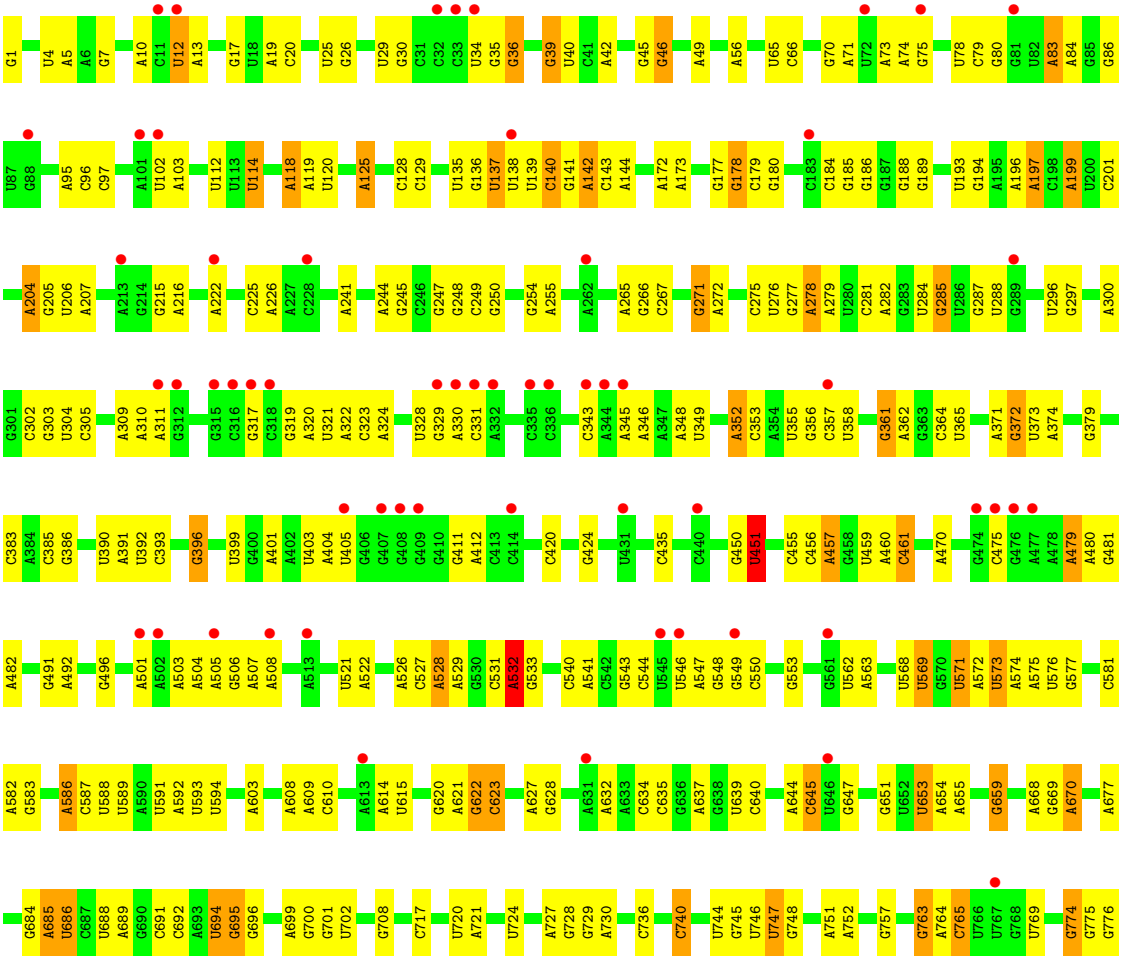


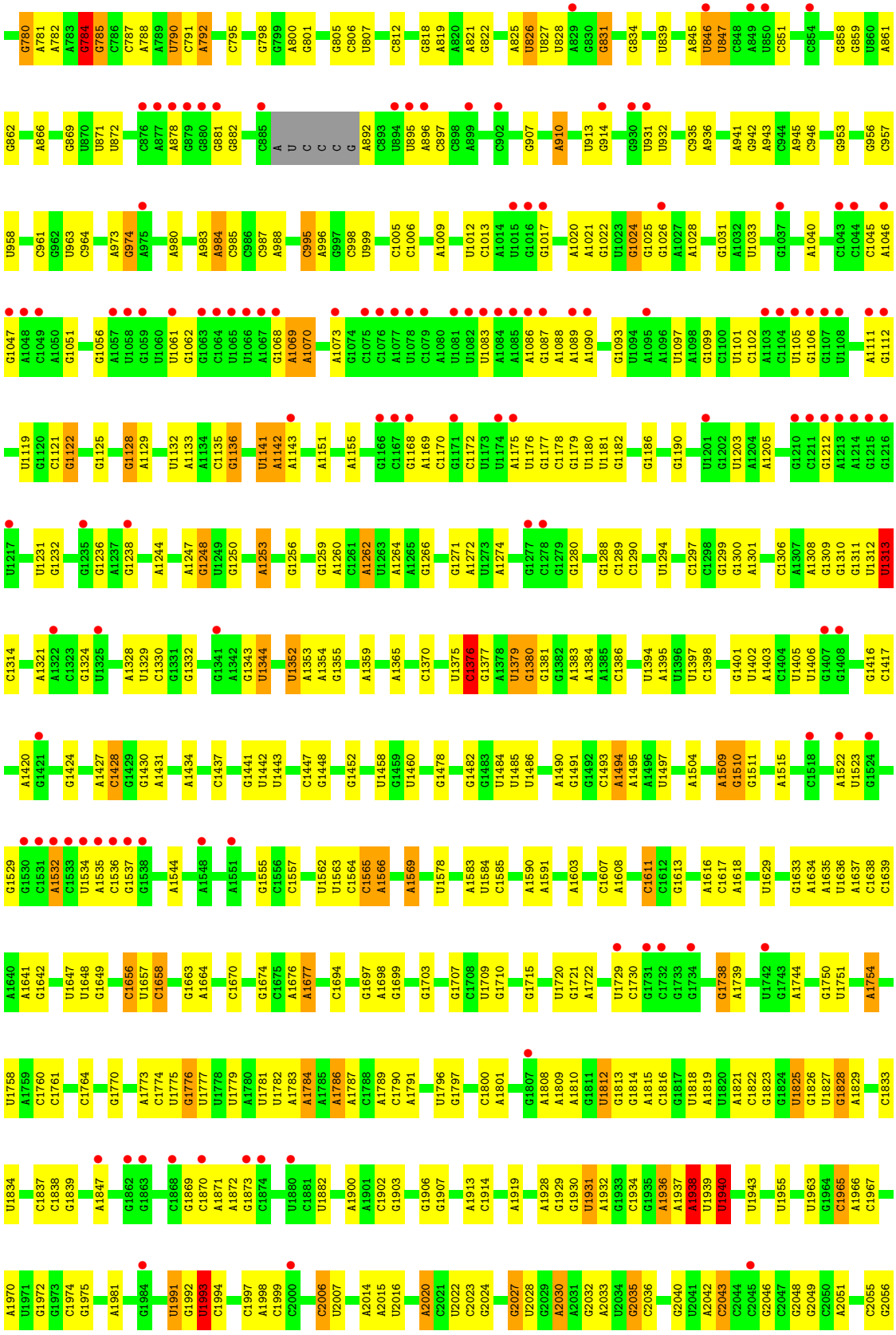
• Molecule 30: 50S ribosomal protein L3





• Molecule 31: 23S rRNA

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G862 A866 G869 U870 U871 U872 C876 A877 A878 G879 G880 G881 G882 C885 A U C C C G A892 C893 U894 U895 A896 C897 C898 A899 C902 G907 A910 U913 G914 G930 U931 U932 C935 A936 A941 G942 A943 C944 A945 C946 G953 G956 C957
U958 C961 G962 U963 C964 A973 G974 A975 A980 A983 A984 C985 C986 C987 A988 C995 A996 G997 C998 U999 C1005 C1006 A1009 U1012 C1013 A1014 U1015 G1016 G1017 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 A1028 G1031 A1032 U1033 G1037 A1040 C1043 C1044 C1045 A1046
G1047 A1048 C1049 A1050 G1051 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 A1111 G1112
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U1217 U1231 G1232 G1235 G1236 A1237 G1238 A1244 A1247 G1248 U1249 G1250 A1253 G1256 G1259 A1260 C1261 A1262 U1263 A1264 A1265 G1266 G1271 A1272 U1273 A1274 G1277 C1278 G1279 G1280 G1288 C1289 C1290 U1294 C1297 C1298 G1299 G1300 A1301 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313
C1314 A1321 A1322 C1323 G1324 U1325 A1328 U1329 C1330 G1331 G1332 G1341 A1342 G1343 U1344 U1352 A1353 A1354 G1355 A1359 A1365 C1370 U1375 C1376 G1377 A1378 U1379 G1380 G1381 G1382 A1383 A1384 A1385 C1386 U1394 A1395 U1396 U1397 C1398 G1401 U1402 A1403 C1404 U1405 U1406 G1407 G1408 G1416 C1417
A1420 G1421 G1424 A1427 C1428 G1429 G1430 A1431 A1434 C1437 G1441 U1442 U1443 C1447 G1448 G1452 U1458 G1459 U1460 G1478 G1482 G1483 U1484 U1485 U1486 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1504 A1509 G1510 G1511 A1515 C1518 A1522 U1523 G1524
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A1640 A1641 G1642 U1647 U1648 G1649 C1656 U1657 C1658 G1663 A1664 C1670 G1674 C1675 A1676 A1677 C1694 G1697 A1698 G1699 G1703 G1707 C1708 U1709 G1710 G1715 U1720 G1721 A1722 U1729 C1730 G1731 C1732 G1733 G1734 G1738 A1739 U1742 G1743 A1744 G1750 U1751 A1754
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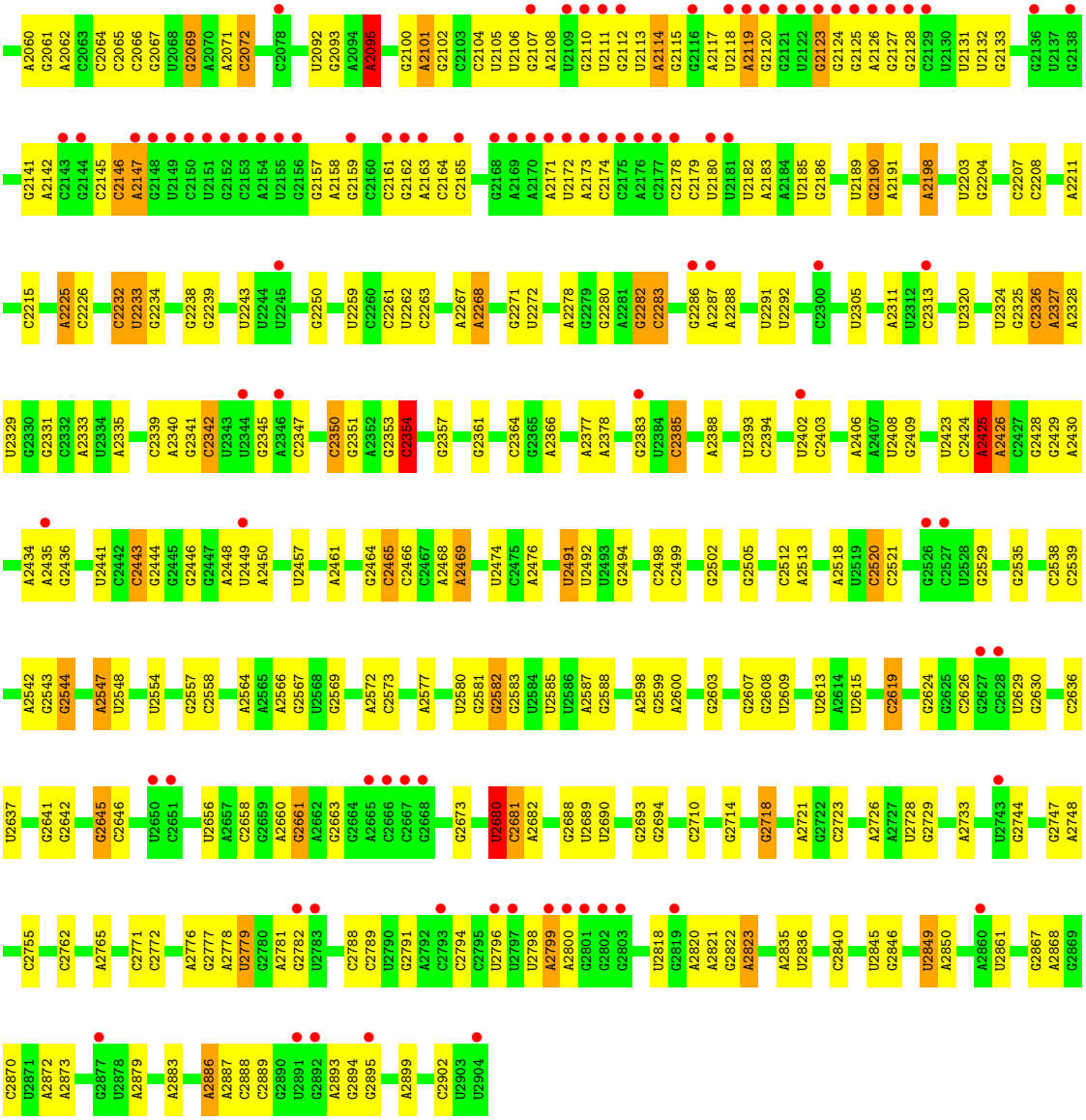
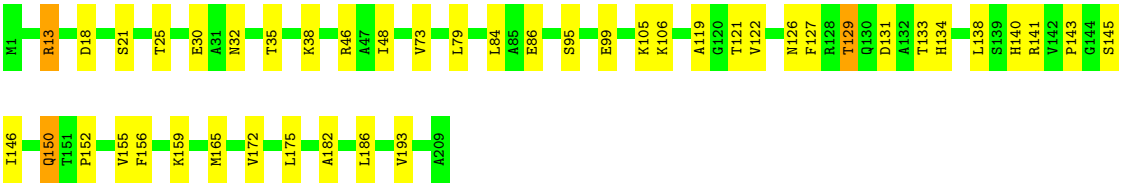


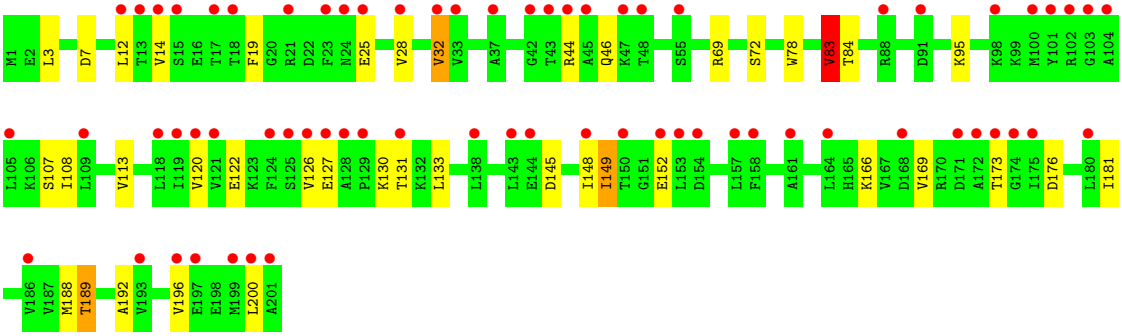
• Molecule 32: 50S ribosomal protein L3

Chain DD:



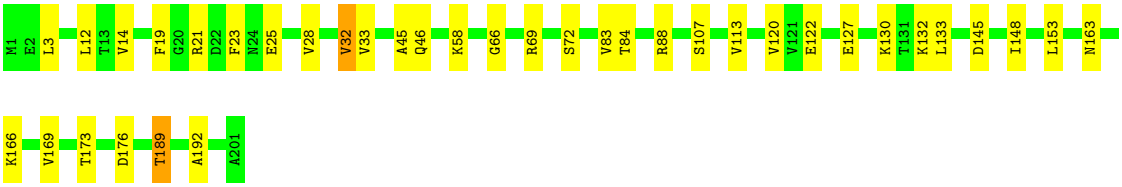
• Molecule 33: 50S ribosomal protein L4

Chain CE:



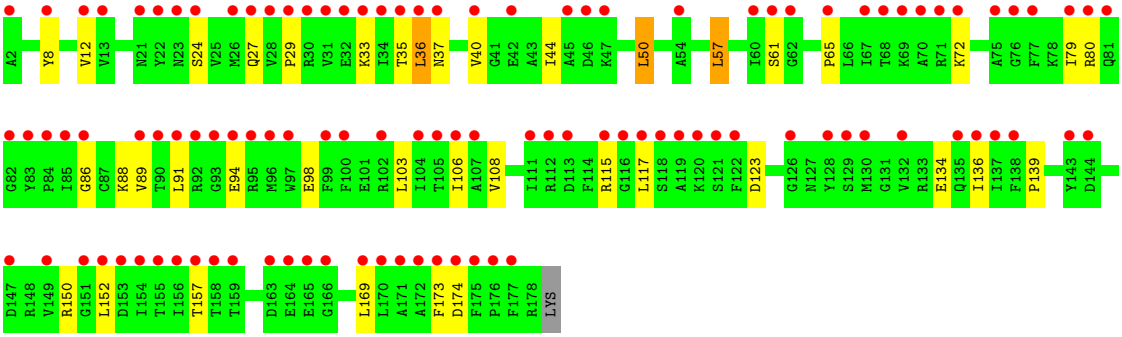
• Molecule 33: 50S ribosomal protein L4

Chain DE:



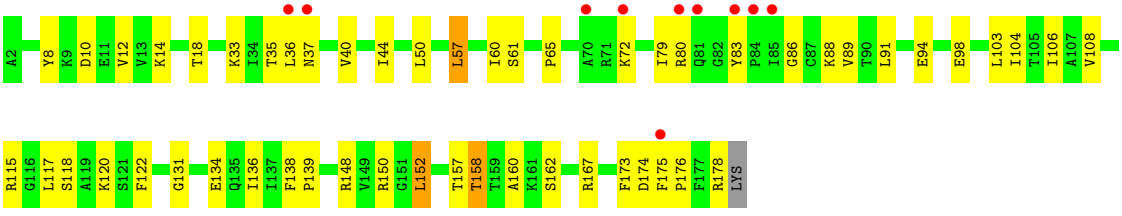
• Molecule 34: 50S ribosomal protein L5

Chain CF:



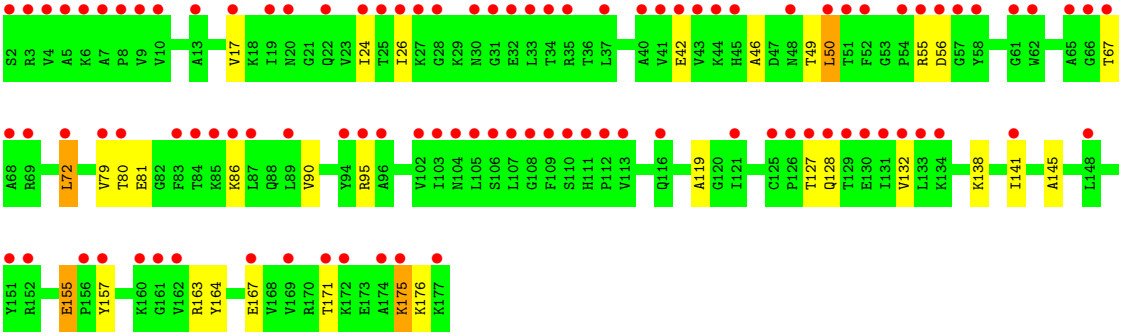
• Molecule 34: 50S ribosomal protein L5

Chain DF:

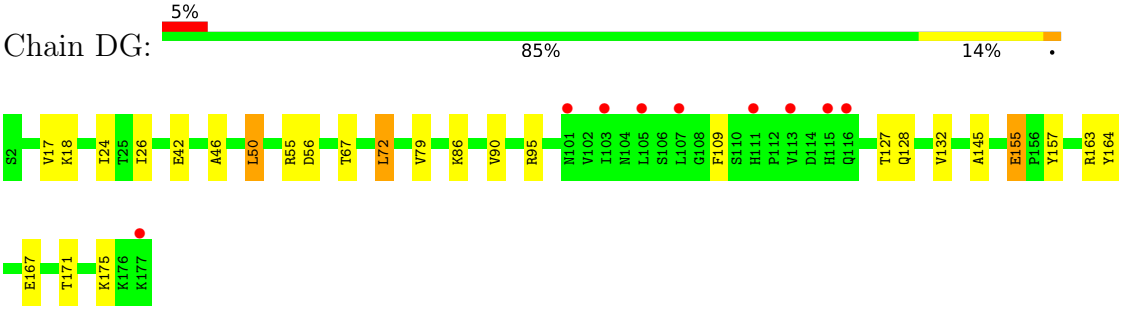


• Molecule 35: 50S ribosomal protein L6

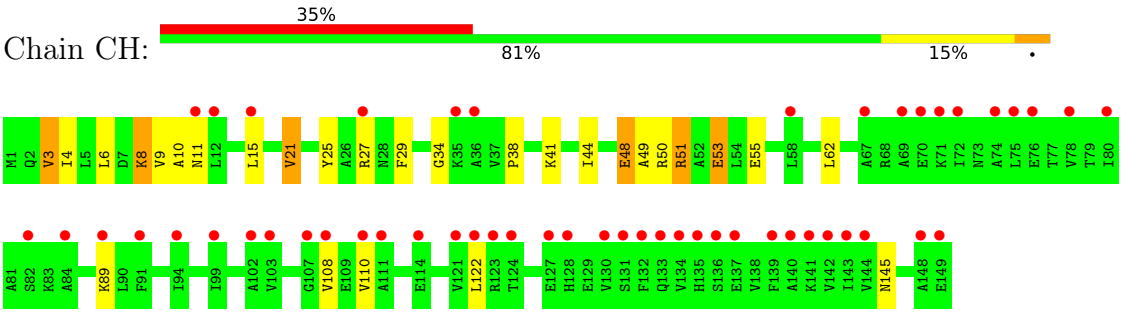
Chain CG:



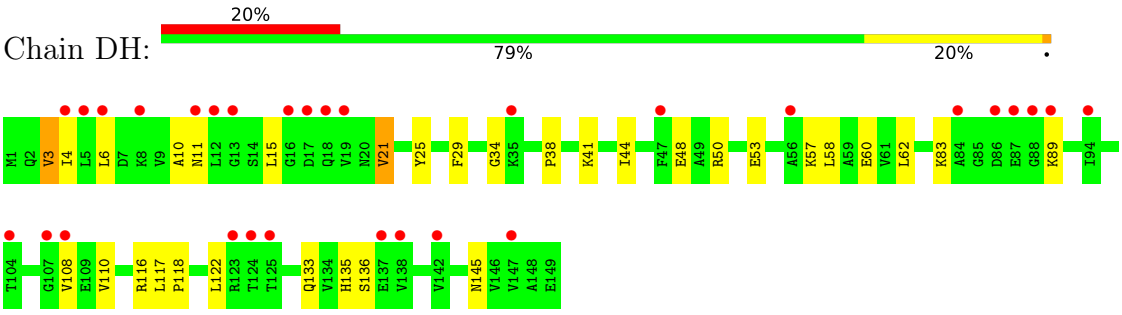
• Molecule 35: 50S ribosomal protein L6



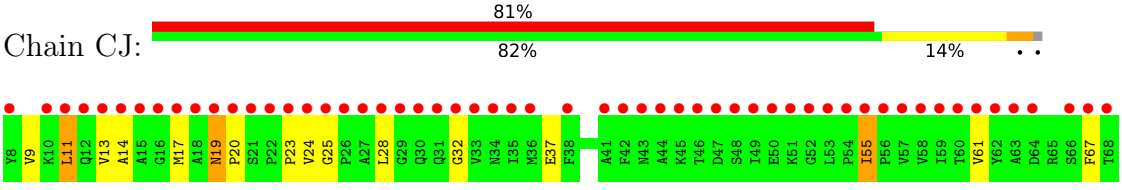
• Molecule 36: 50S ribosomal protein L9

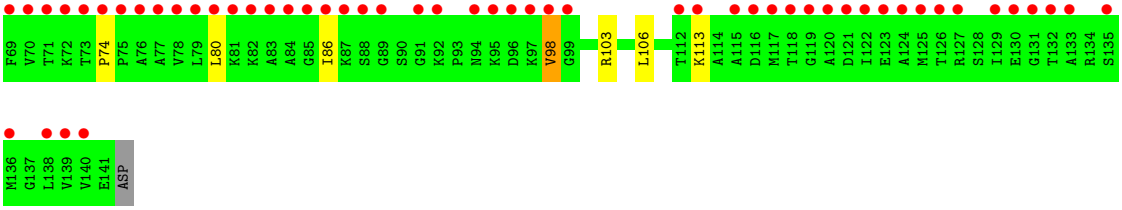


• Molecule 36: 50S ribosomal protein L9



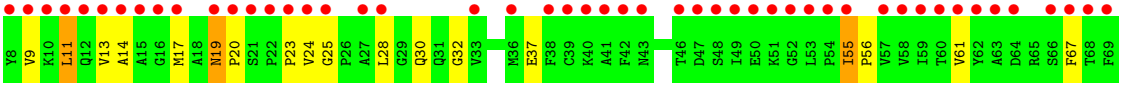
• Molecule 37: 50S ribosomal protein L11

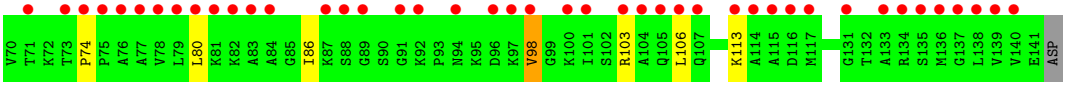




• Molecule 37: 50S ribosomal protein L11

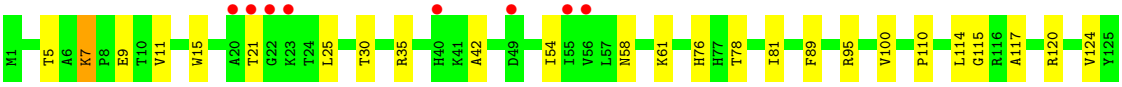
Chain DJ:





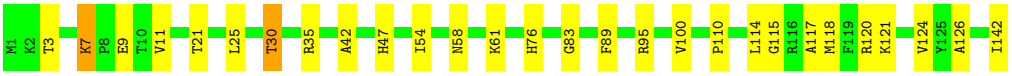
• Molecule 38: 50S ribosomal protein L13

Chain CK:



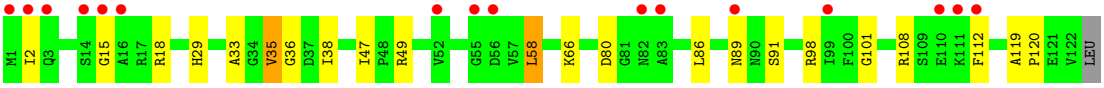
• Molecule 38: 50S ribosomal protein L13

Chain DK:



• Molecule 39: 50S ribosomal protein L14

Chain CL:

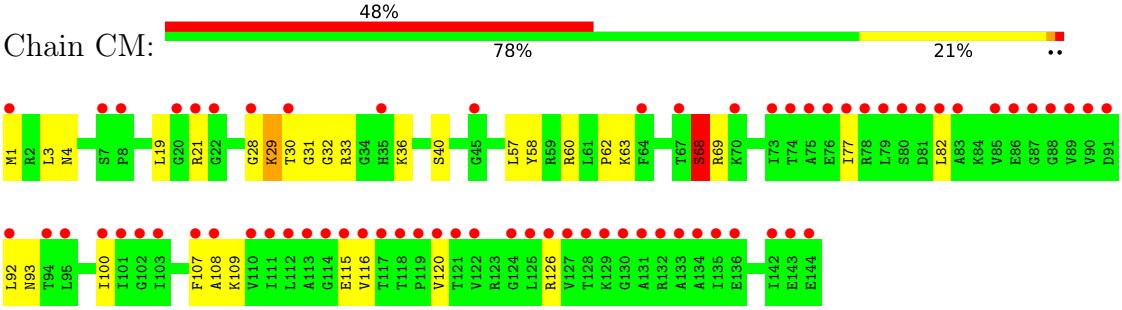


• Molecule 39: 50S ribosomal protein L14

Chain DL:

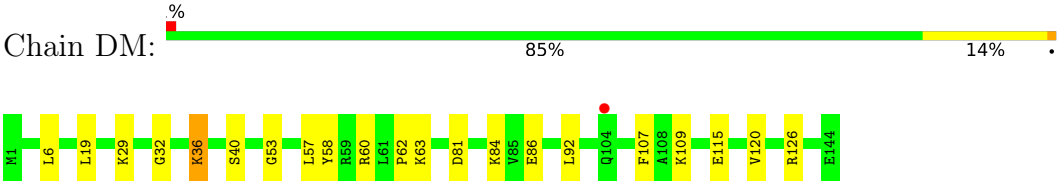
• Molecule 40: 50S ribosomal protein L15

Chain CM:



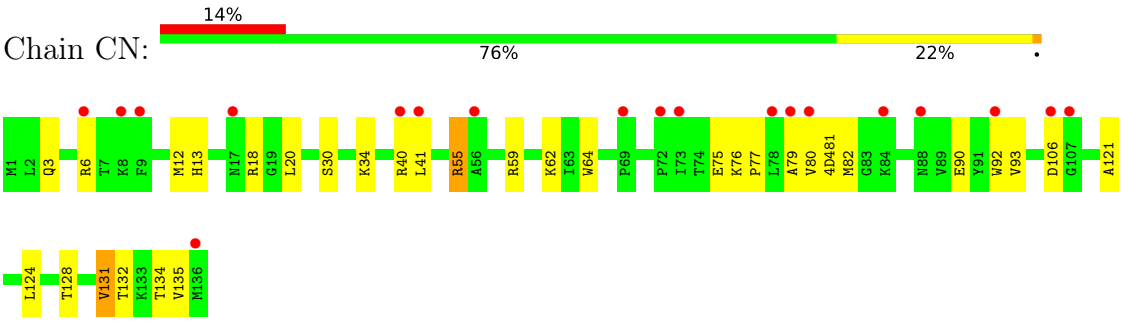
• Molecule 40: 50S ribosomal protein L15

Chain DM:



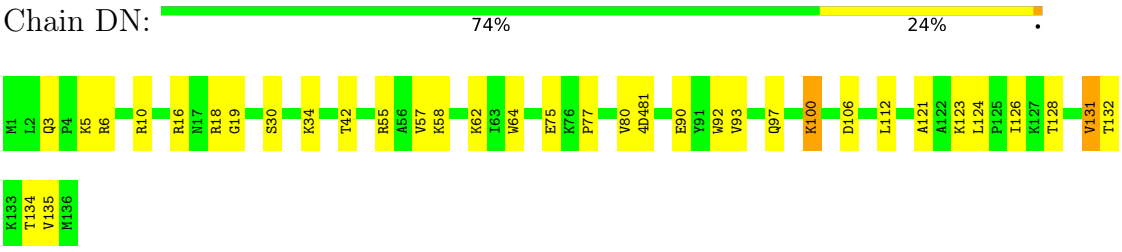
• Molecule 41: 50S ribosomal protein L16

Chain CN:



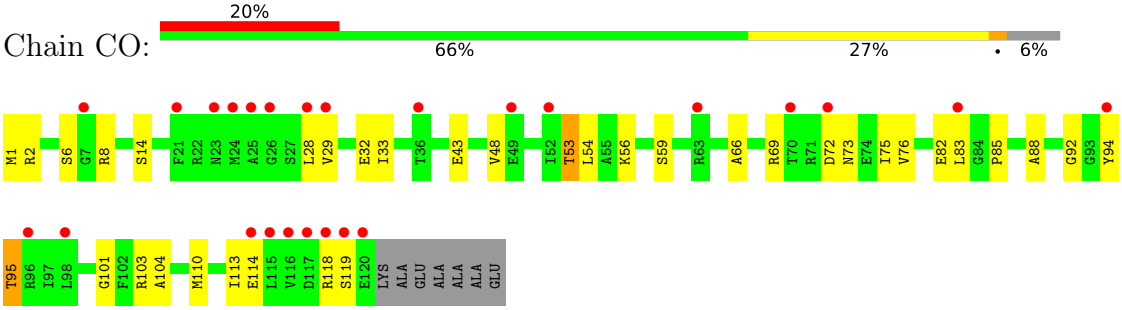
• Molecule 41: 50S ribosomal protein L16

Chain DN:



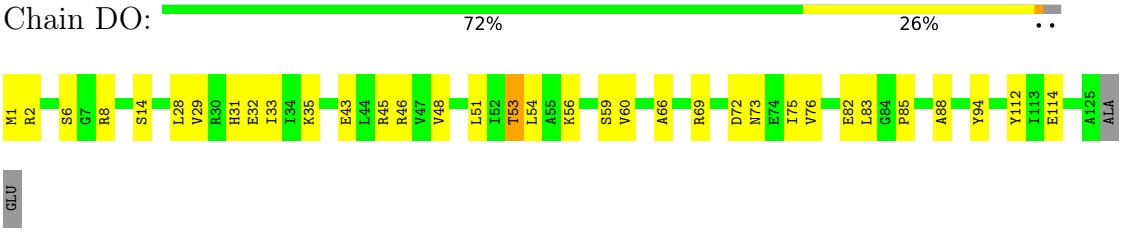
• Molecule 42: 50S ribosomal protein L17

Chain CO:



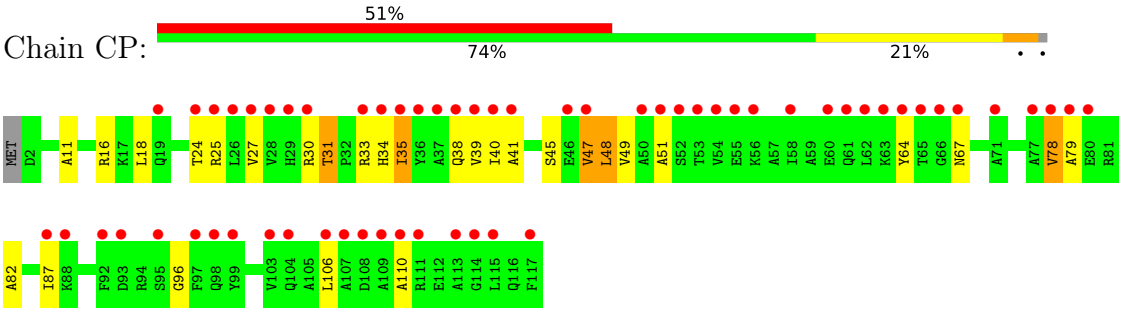
• Molecule 42: 50S ribosomal protein L17

Chain DO:



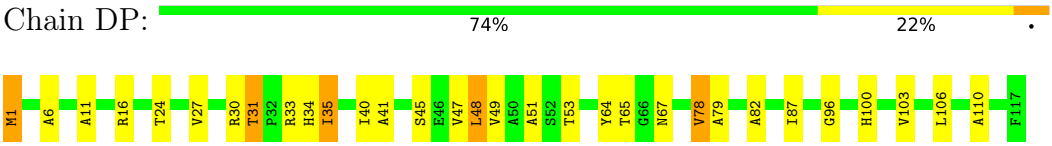
• Molecule 43: 50S ribosomal protein L18

Chain CP:



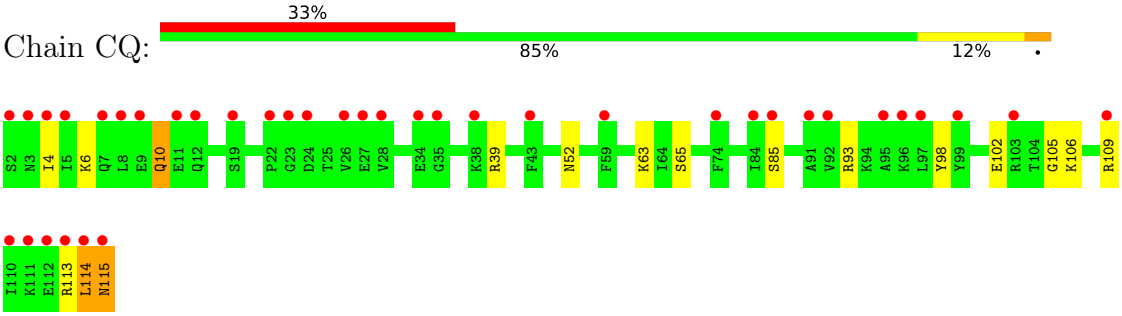
• Molecule 43: 50S ribosomal protein L18

Chain DP:



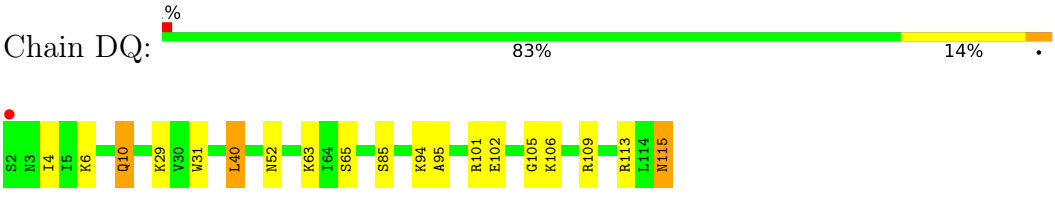
• Molecule 44: 50S ribosomal protein L19

Chain CQ:



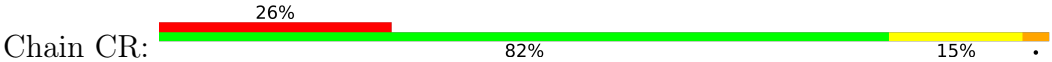
• Molecule 44: 50S ribosomal protein L19

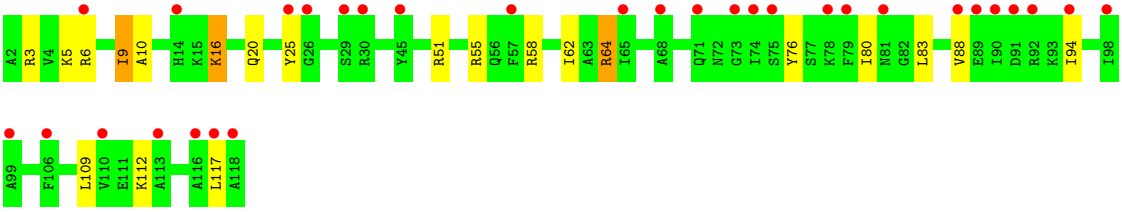
Chain DQ:



• Molecule 45: 50S ribosomal protein L20

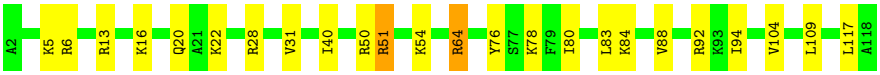
Chain CR:





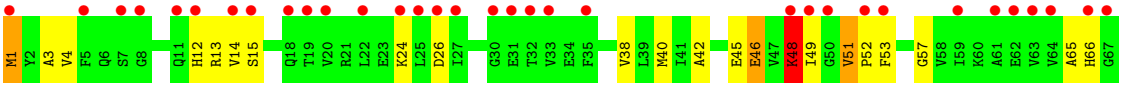
• Molecule 45: 50S ribosomal protein L20

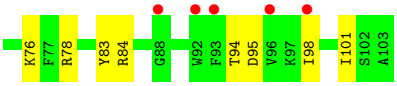
Chain DR:



• Molecule 46: 50S ribosomal protein L21

Chain CS:



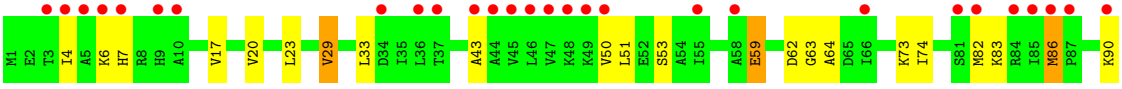


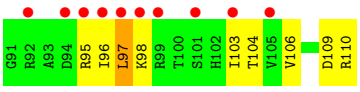
• Molecule 46: 50S ribosomal protein L21

Chain DS:

• Molecule 47: 50S ribosomal protein L22

Chain CT:



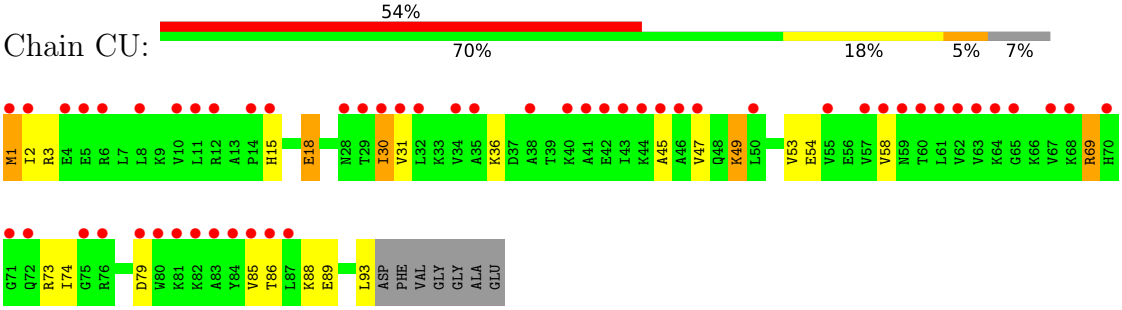


• Molecule 47: 50S ribosomal protein L22

Chain DT:

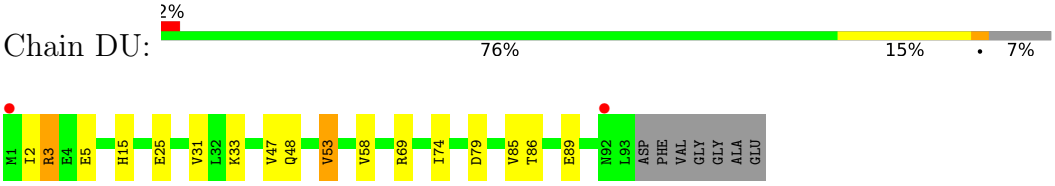
• Molecule 48: 50S ribosomal protein L23

Chain CU:



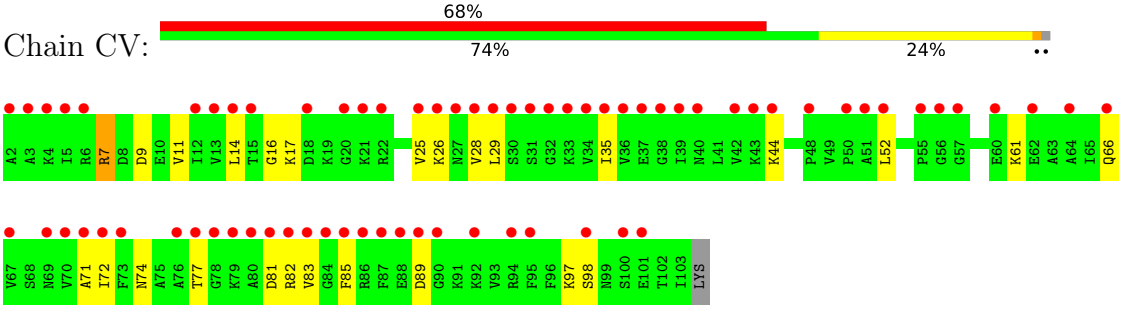
• Molecule 48: 50S ribosomal protein L23

Chain DU:



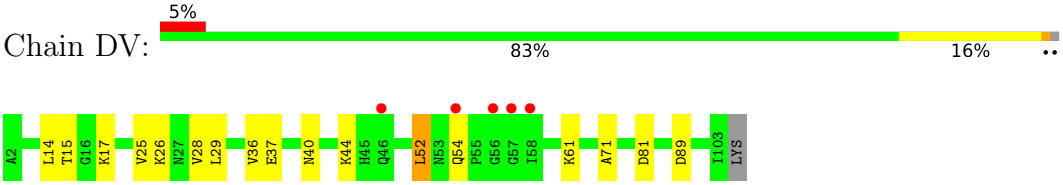
• Molecule 49: 50S ribosomal protein L24

Chain CV:



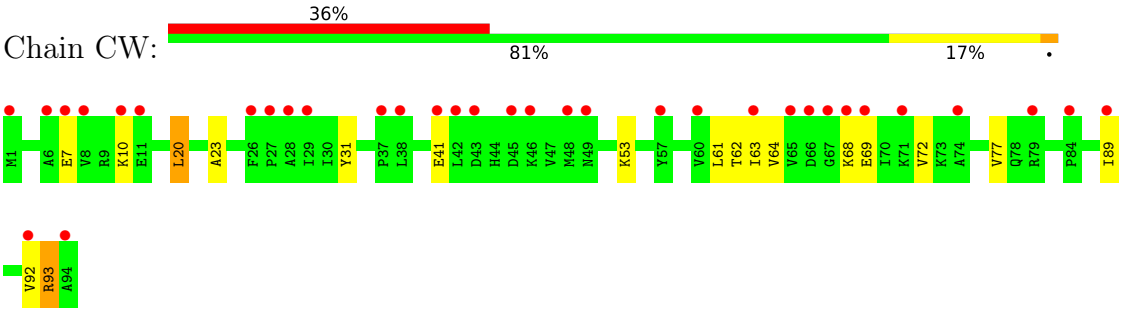
• Molecule 49: 50S ribosomal protein L24

Chain DV:



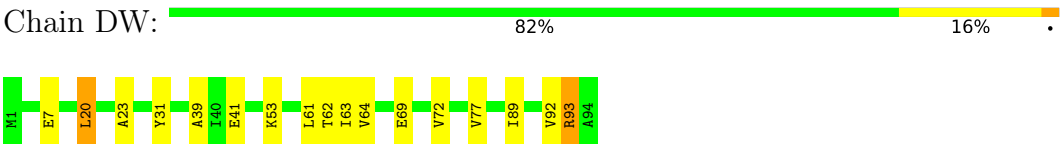
• Molecule 50: 50S ribosomal protein L25

Chain CW:



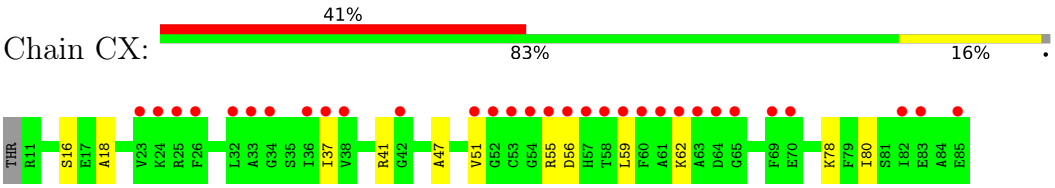
• Molecule 50: 50S ribosomal protein L25

Chain DW:



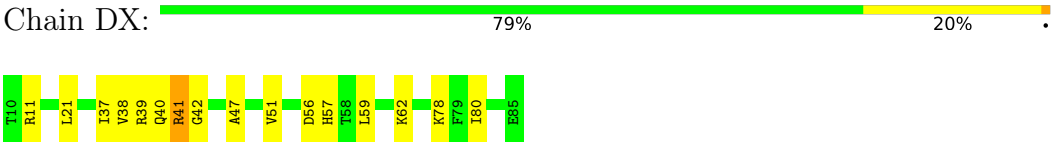
• Molecule 51: 50S ribosomal protein L27

Chain CX:



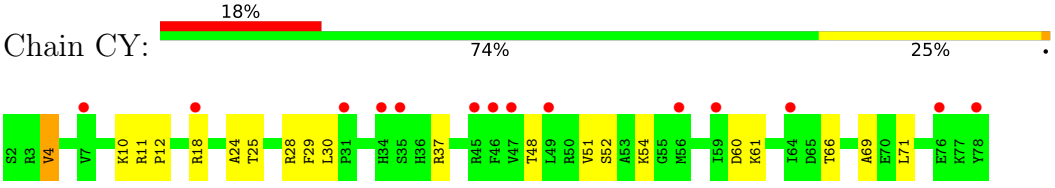
• Molecule 51: 50S ribosomal protein L27

Chain DX:



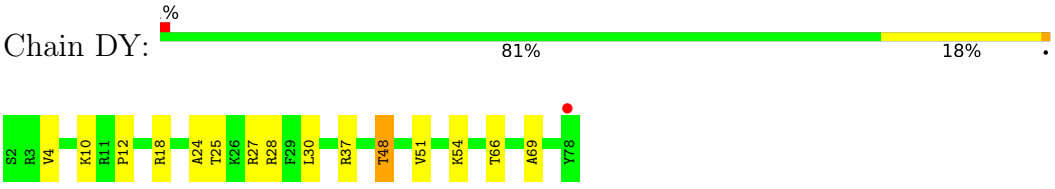
• Molecule 52: 50S ribosomal protein L28

Chain CY:



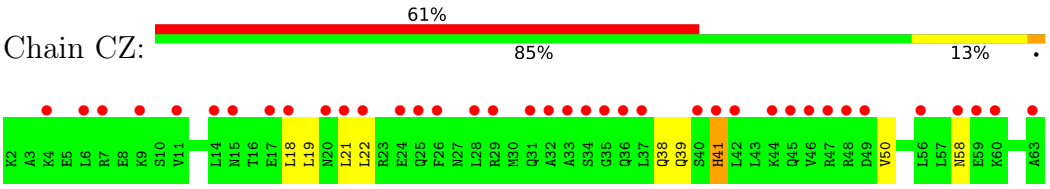
• Molecule 52: 50S ribosomal protein L28

Chain DY:



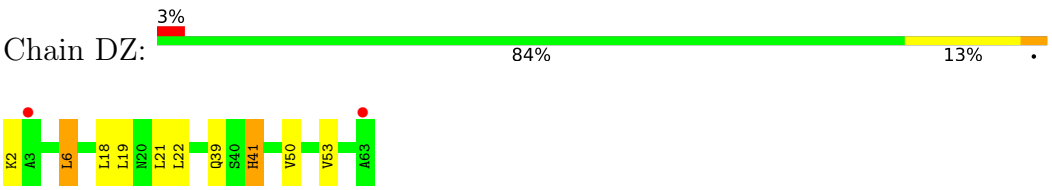
• Molecule 53: 50S ribosomal protein L29

Chain CZ:



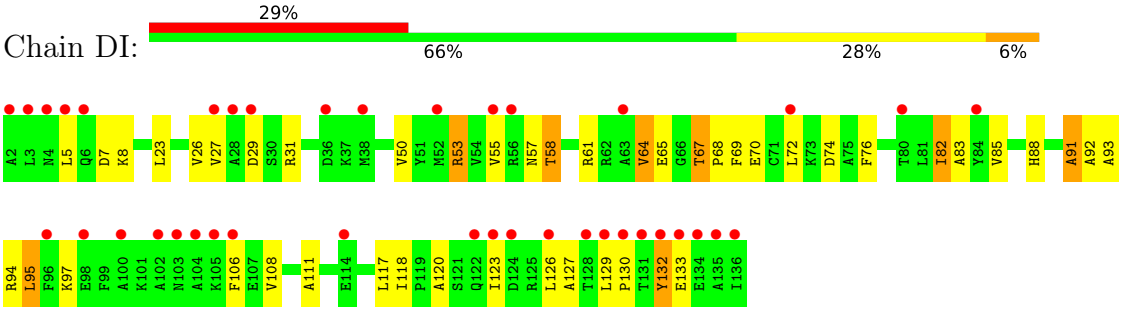
• Molecule 53: 50S ribosomal protein L29

Chain DZ:



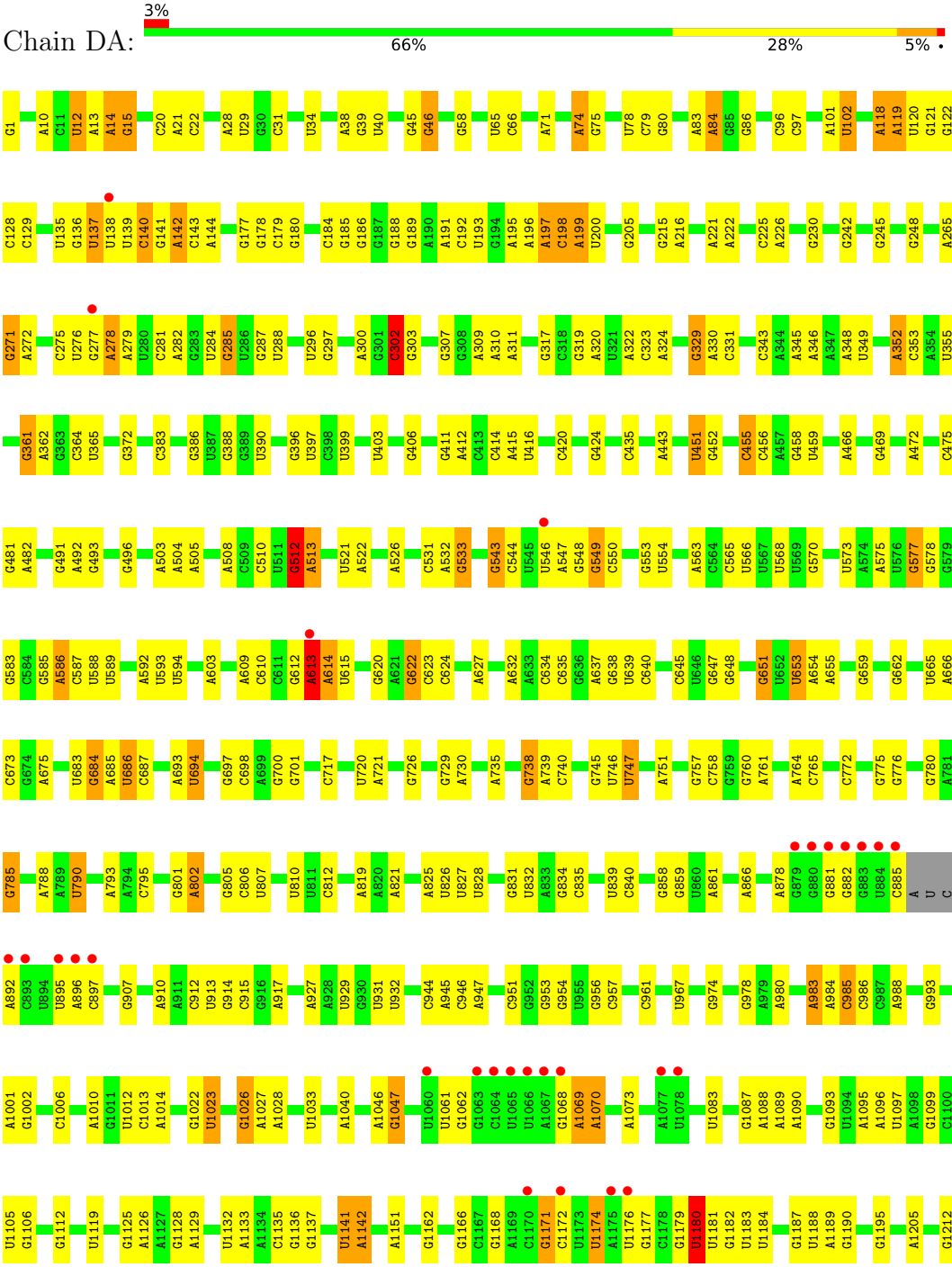
• Molecule 54: 50S ribosomal protein L10

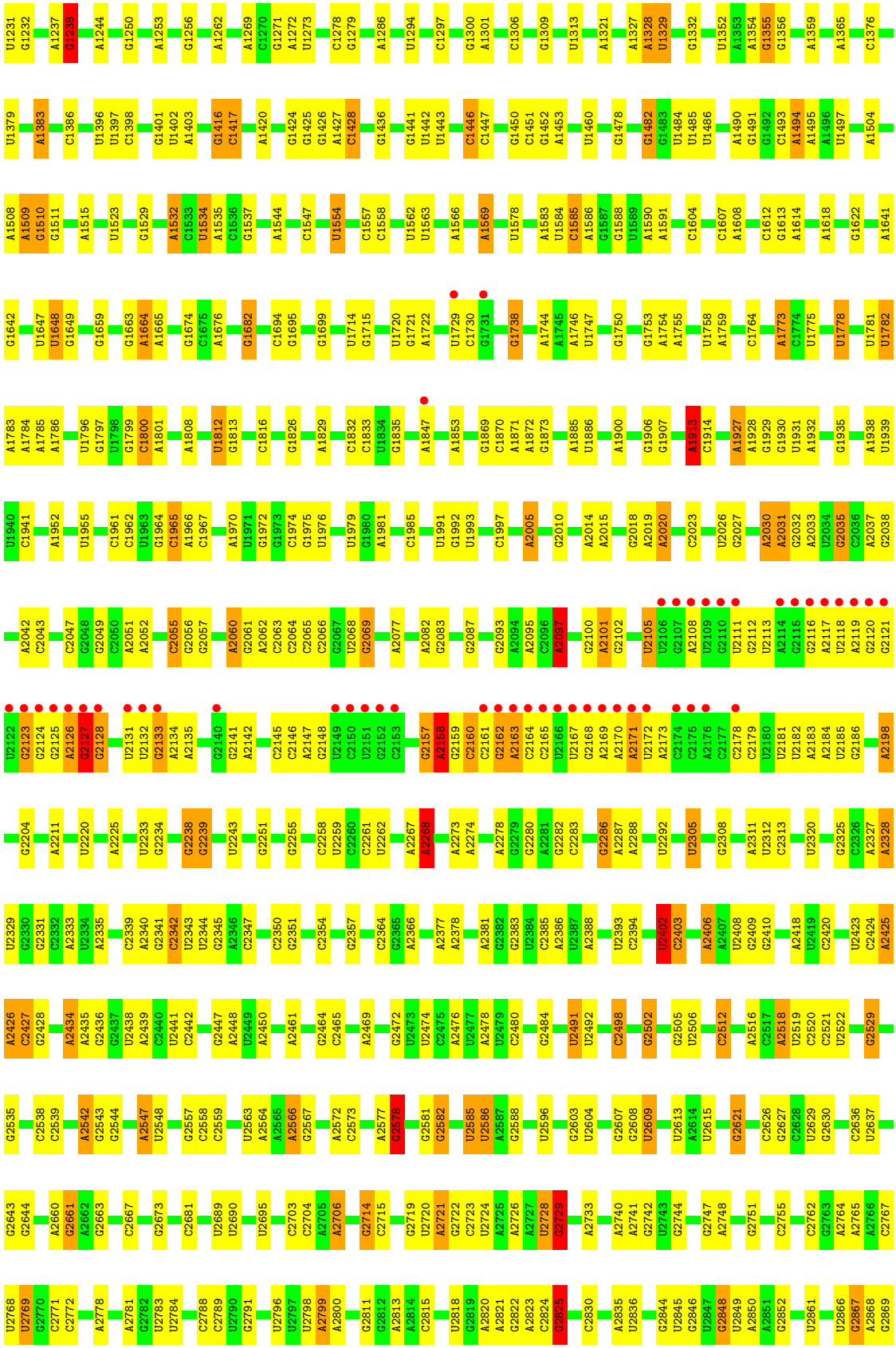
Chain DI:

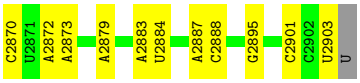


• Molecule 55: 23S rRNA

Chain DA:






C2870
U2871
A2872
A2873
A2879
A2883
U2884
A2887
C2888
G2895
C2901
C2902
U2903
U

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PSU, MEQ, PG4, D2T, OMG, MG, 5MC, PUT, ACY, 4OC, MA6, 6MZ, EDO, 4D4, 1MG, PEG, OMC, OMU, PGE, TRS, 5MU, GUN, 3TD, 1PE, 2MG, H2U, MPD, SPD, UR3, 2MA, ZN, 7MG

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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	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 (i)

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
34	CF	37	ASN
45	CR	109	LEU

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Mol	Chain	Res	Type
52	DY	48	THR
34	CF	152	LEU
34	CF	36	LEU

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

Mol	Chain	Res	Type
52	CY	16	ASN
37	DJ	30	GLN
44	DQ	115	ASN
22	C1	42	HIS
22	C1	6	ASN

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
55	DA	603	A
55	DA	984	A
55	DA	1800	C
1	BA	1380	U

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Mol	Chain	Res	Type
1	BA	1345	U

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

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	$\#\|Z\| > 2$
1	5MC	AA	967	1	18,22,23	0.35	0	26,32,35	0.40	0
31	1MG	CA	745	31	18,26,27	0.86	0	19,39,42	0.57	0
55	7MG	DA	2069	55	22,26,27	5.02	1 (4%)	29,39,42	2.10	6 (20%)
55	PSU	DA	1911	55	18,21,22	0.42	0	22,30,33	0.43	0
55	OMC	DA	2498	55,56	19,22,23	0.78	1 (5%)	26,31,34	0.44	0
1	PSU	BA	516	1	18,21,22	0.50	0	22,30,33	0.47	0
41	4D4	DN	81[B]	-	9,11,12	1.73	2 (22%)	8,13,15	2.07	2 (25%)
55	PSU	DA	2580	55	18,21,22	0.66	0	22,30,33	0.61	0
55	1MG	DA	745	55	18,26,27	1.05	1 (5%)	19,39,42	0.47	0
55	PSU	DA	2457	55	18,21,22	0.59	0	22,30,33	0.51	0
1	MA6	AA	1519	1	19,26,27	0.93	1 (5%)	18,38,41	0.90	1 (5%)
1	MA6	BA	1519	1	19,26,27	0.90	0	18,38,41	0.87	0
55	5MU	DA	1939	55	19,22,23	0.71	0	28,32,35	0.39	0
55	PSU	DA	2605	55	18,21,22	0.48	0	22,30,33	0.52	0
1	4OC	AA	1402	1	20,23,24	0.35	0	26,32,35	0.46	0
1	2MG	AA	1207	1	18,26,27	0.77	0	16,38,41	0.55	0
31	OMG	CA	2251	31	18,26,27	0.92	0	19,38,41	0.63	0
55	PSU	DA	2504	55	18,21,22	0.47	0	22,30,33	0.39	0
1	2MG	BA	966	1	18,26,27	0.83	0	16,38,41	0.64	0
1	2MG	BA	1207	1	18,26,27	0.78	0	16,38,41	0.53	0
55	PSU	DA	955	55	18,21,22	0.71	0	22,30,33	0.53	0
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	1.36	1 (5%)
31	2MG	CA	1835	31	18,26,27	0.87	0	16,38,41	0.55	0
31	2MA	CA	2503	31	17,25,26	0.82	0	17,37,40	0.51	0
31	PSU	CA	2580	31	18,21,22	0.64	0	22,30,33	0.76	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PSU	CA	746	31,56	18,21,22	0.75	1 (5%)	22,30,33	0.42	0
32	MEQ	DD	150[B]	32	8,9,10	1.65	1 (12%)	5,10,12	1.46	1 (20%)
1	2MG	AA	966	1	18,26,27	0.81	0	16,38,41	0.65	0
55	OMG	DA	2251	55	18,26,27	1.08	1 (5%)	19,38,41	0.56	0
31	PSU	CA	955	31	18,21,22	0.39	0	22,30,33	0.59	0
31	PSU	CA	2504	31	18,21,22	0.38	0	22,30,33	0.44	0
55	2MA	DA	2503	55,56	17,25,26	0.94	0	17,37,40	0.49	0
31	5MU	CA	747	31	19,22,23	0.27	0	28,32,35	0.27	0
31	PSU	CA	1911	31	18,21,22	0.40	0	22,30,33	0.43	0
55	PSU	DA	2604	55	18,21,22	0.83	1 (5%)	22,30,33	0.52	0
41	4D4	DN	81[A]	-	9,11,12	1.60	1 (11%)	8,13,15	2.99	2 (25%)
1	5MC	BA	1407	1	18,22,23	0.37	0	26,32,35	0.45	0
31	PSU	CA	1917	31	18,21,22	0.44	0	22,30,33	0.39	0
55	PSU	DA	1917	55	18,21,22	0.56	0	22,30,33	0.41	0
1	7MG	BA	527	1	22,26,27	5.00	2 (9%)	29,39,42	2.32	6 (20%)
1	4OC	BA	1402	1	20,23,24	0.42	0	26,32,35	0.47	0
55	H2U	DA	2449	55	18,21,22	0.84	0	21,30,33	0.45	0
31	6MZ	CA	2030	31	18,25,26	0.71	0	16,36,39	0.85	1 (6%)
41	4D4	CN	81	41	9,11,12	2.26	2 (22%)	8,13,15	2.20	2 (25%)
31	6MZ	CA	1618	31	18,25,26	0.90	1 (5%)	16,36,39	1.04	1 (6%)
31	5MU	CA	1939	31	19,22,23	0.55	0	28,32,35	0.36	0
55	5MU	DA	747	55	19,22,23	0.50	0	28,32,35	0.35	0
12	D2T	AL	89	12	7,9,10	0.94	1 (14%)	6,11,13	0.74	0
1	5MC	AA	1407	1	18,22,23	0.30	0	26,32,35	0.45	0
1	UR3	AA	1498	1	19,22,23	0.63	0	26,32,35	0.54	0
55	PSU	DA	746	55,56	18,21,22	1.15	2 (11%)	22,30,33	0.38	0
31	OMU	CA	2552	31	19,22,23	0.31	0	26,31,34	0.38	0
55	OMU	DA	2552	55	19,22,23	0.59	0	26,31,34	0.32	0
1	MA6	AA	1518	1	19,26,27	0.86	0	18,38,41	1.25	1 (5%)
32	MEQ	DD	150[A]	32	8,9,10	0.39	0	5,10,12	0.54	0
55	6MZ	DA	2030	55	18,25,26	0.78	0	16,36,39	0.98	1 (6%)
55	6MZ	DA	1618	55	18,25,26	1.09	0	16,36,39	2.01	2 (12%)
31	PSU	CA	2457	31	18,21,22	0.94	1 (5%)	22,30,33	0.40	0
55	5MC	DA	1962	55	18,22,23	0.78	1 (5%)	26,32,35	0.45	0
12	D2T	BL	89	12	7,9,10	0.85	0	6,11,13	0.66	0
1	2MG	AA	1516	1	18,26,27	0.70	0	16,38,41	0.62	0
1	UR3	BA	1498	1	19,22,23	0.58	0	26,32,35	0.65	1 (3%)
1	2MG	BA	1516	1	18,26,27	0.76	0	16,38,41	0.61	0
31	5MC	CA	1962	31	18,22,23	0.27	0	26,32,35	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	2MG	DA	2445	55	18,26,27	1.00	0	16,38,41	0.65	0
1	PSU	AA	516	56,1	18,21,22	0.45	0	22,30,33	0.48	0
31	7MG	CA	2069	31	22,26,27	4.97	3 (13%)	29,39,42	2.13	6 (20%)
31	PSU	CA	2605	31	18,21,22	0.35	0	22,30,33	0.52	0
1	5MC	BA	967	1	18,22,23	0.35	0	26,32,35	0.39	0
55	3TD	DA	1915	55	18,22,23	0.43	0	22,32,35	0.58	0
55	2MG	DA	1835	55	18,26,27	0.90	1 (5%)	16,38,41	0.70	1 (6%)
31	3TD	CA	1915	31	18,22,23	0.47	0	22,32,35	0.56	0
31	OMC	CA	2498	31,56	19,22,23	0.42	0	26,31,34	0.36	0
1	7MG	AA	527	1	22,26,27	4.88	2 (9%)	29,39,42	2.33	6 (20%)
31	2MG	CA	2445	31	18,26,27	0.97	0	16,38,41	0.53	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
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
55	7MG	DA	2069	55	-	2/7/37/38	0/3/3/3
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/9/27/28	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	4/11/12/14	-
55	PSU	DA	2580	55	-	1/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
55	PSU	DA	2504	55	-	2/7/25/26	0/2/2/2
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	746	31,56	-	3/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	3/8/9/11	-
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
55	OMG	DA	2251	55	-	0/5/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	2/7/25/26	0/2/2/2
55	2MA	DA	2503	55,56	-	2/3/25/26	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2604	55	-	1/7/25/26	0/2/2/2
41	4D4	DN	81[A]	-	-	1/11/12/14	-
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
31	5MU	CA	1939	31	-	2/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	746	55,56	-	1/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
55	OMU	DA	2552	55	-	0/9/27/28	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	6/7/12/14	-
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
55	2MG	DA	2445	55	-	2/5/27/28	0/3/3/3
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
31	7MG	CA	2069	31	-	1/7/37/38	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	2MG	DA	1835	55	-	0/5/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	2/9/27/28	0/2/2/2
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2069	7MG	C8-N9	-23.31	1.33	1.46
1	BA	527	7MG	C8-N9	-23.13	1.33	1.46
31	CA	2069	7MG	C8-N9	-22.50	1.33	1.46
1	AA	527	7MG	C8-N9	-22.43	1.33	1.46
41	CN	81	4D4	CZ-NE	6.18	1.45	1.33

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DA	1618	6MZ	C9-N6-C6	-7.16	116.70	122.87
1	AA	527	7MG	C6-C5-N7	-6.55	121.61	131.91
41	DN	81[A]	4D4	NE-CZ-NH2	6.55	132.21	120.70
1	BA	527	7MG	C6-C5-N7	-6.50	121.70	131.91
1	BA	527	7MG	C6-C5-C4	-5.91	110.43	122.62

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	O-C-CA-CB
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	O-C-CA-CB
12	BL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1

There are no ring outliers.

16 monomers are involved in 22 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
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	DD	301	-	9,9,9	0.21	0	8,8,8	0.16	0
59	PUT	DA	3205	-	5,5,5	0.18	0	4,4,4	0.16	0
62	EDO	DA	3209	-	3,3,3	0.53	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
64	SPD	DA	3206	-	9,9,9	0.23	0	8,8,8	0.21	0
59	PUT	DA	3188	-	5,5,5	0.12	0	4,4,4	0.17	0
59	PUT	AA	1675	-	5,5,5	0.18	0	4,4,4	0.08	0
58	MPD	DA	3192	-	7,7,7	0.84	0	9,10,10	0.65	0
59	PUT	DA	3213	-	5,5,5	0.24	0	4,4,4	0.18	0
62	EDO	D0	101	-	3,3,3	0.63	0	2,2,2	0.55	0
62	EDO	DB	211	-	3,3,3	0.59	0	2,2,2	0.31	0
61	PEG	DA	3200	-	6,6,6	0.23	0	5,5,5	0.09	0
61	PEG	DQ	201	-	6,6,6	0.22	0	5,5,5	0.12	0
63	PGE	DU	201	-	9,9,9	0.32	0	8,8,8	0.29	0
58	MPD	DA	3190	-	7,7,7	0.53	0	9,10,10	0.45	0
58	MPD	DA	3210	-	7,7,7	0.82	0	9,10,10	0.34	0
58	MPD	DE	301	-	7,7,7	0.67	0	9,10,10	0.43	0
64	SPD	DA	3183	-	9,9,9	0.22	0	8,8,8	0.34	0
62	EDO	DB	210	-	3,3,3	0.69	0	2,2,2	0.15	0
61	PEG	DA	3218	-	6,6,6	0.15	0	5,5,5	0.08	0
64	SPD	DA	3224	-	9,9,9	0.13	0	8,8,8	0.23	0
63	PGE	DA	3186	-	9,9,9	0.33	0	8,8,8	0.35	0
62	EDO	DA	3198	-	3,3,3	0.76	0	2,2,2	0.25	0
62	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.31	0
57	PG4	DA	3216	-	12,12,12	0.14	0	11,11,11	0.15	0
63	PGE	DA	3225	-	9,9,9	0.26	0	8,8,8	0.31	0
63	PGE	DS	201	-	9,9,9	0.22	0	8,8,8	0.18	0
59	PUT	DA	3212	-	5,5,5	0.25	0	4,4,4	0.13	0
61	PEG	AL	201	-	6,6,6	0.19	0	5,5,5	0.15	0
64	SPD	DA	3187	-	9,9,9	0.12	0	8,8,8	0.21	0
59	PUT	DA	3184	-	5,5,5	0.17	0	4,4,4	0.21	0
61	PEG	DA	3201	-	6,6,6	0.14	0	5,5,5	0.15	0
58	MPD	AA	1676	-	7,7,7	0.74	0	9,10,10	0.54	0
57	PG4	DQ	202	-	12,12,12	0.13	0	11,11,11	0.15	0
62	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.22	0
58	MPD	DA	3207	-	7,7,7	0.37	0	9,10,10	0.52	0
66	ACY	DA	3191	-	3,3,3	0.63	0	3,3,3	1.38	0
61	PEG	DA	3199	-	6,6,6	0.18	0	5,5,5	0.12	0
57	PG4	DR	201	-	12,12,12	0.22	0	11,11,11	0.25	0
61	PEG	DA	3226	-	6,6,6	0.20	0	5,5,5	0.06	0
58	MPD	DS	203	-	7,7,7	0.36	0	9,10,10	0.38	0
59	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.09	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	3195	-	5,5,5	0.28	0	4,4,4	0.25	0
58	MPD	DN	201	-	7,7,7	1.17	1 (14%)	9,10,10	0.51	0
59	PUT	AA	1672	-	5,5,5	0.08	0	4,4,4	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	EDO	DA	3215	-	3,3,3	0.72	0	2,2,2	0.23	0
63	PGE	D1	102	-	9,9,9	0.11	0	8,8,8	0.13	0
61	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.20	0
58	MPD	DE	302	-	7,7,7	0.96	1 (14%)	9,10,10	0.72	0
66	ACY	DA	3202	-	3,3,3	0.65	0	3,3,3	0.93	0
57	PG4	DS	202	-	12,12,12	0.19	0	11,11,11	0.23	0
59	PUT	DA	3222	-	5,5,5	0.27	0	4,4,4	0.50	0
61	PEG	DP	201	-	6,6,6	0.16	0	5,5,5	0.13	0
61	PEG	DA	3227	-	6,6,6	0.24	0	5,5,5	0.16	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.16	0
63	PGE	DA	3214	-	9,9,9	0.24	0	8,8,8	0.34	0
58	MPD	DT	201	-	7,7,7	0.76	0	9,10,10	0.30	0
59	PUT	DA	3189	-	5,5,5	0.09	0	4,4,4	0.22	0
66	ACY	DA	3196	-	3,3,3	2.69	1 (33%)	3,3,3	1.91	2 (66%)
68	TRS	DA	3220	-	7,7,7	0.23	0	9,9,9	0.22	0
62	EDO	DA	3003	-	3,3,3	0.68	0	2,2,2	0.32	0
63	PGE	D3	101	-	9,9,9	0.22	0	8,8,8	0.11	0
63	PGE	DA	3217	-	9,9,9	0.22	0	8,8,8	0.19	0
57	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.19	0
62	EDO	DA	3194	-	3,3,3	0.74	0	2,2,2	0.13	0
58	MPD	AA	1671	-	7,7,7	0.43	0	9,10,10	0.49	0
59	PUT	DA	3223	-	5,5,5	0.20	0	4,4,4	0.17	0
59	PUT	DM	201	-	5,5,5	0.22	0	4,4,4	0.27	0
62	EDO	DA	3197	-	3,3,3	0.67	0	2,2,2	0.16	0
65	1PE	DA	3203	-	15,15,15	0.21	0	14,14,14	0.25	0
67	GUN	DA	3211	-	7,12,12	0.66	0	8,17,17	0.56	0
59	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.16	0
58	MPD	DK	201	-	7,7,7	1.02	1 (14%)	9,10,10	0.37	0
57	PG4	AA	1670	-	12,12,12	0.18	0	11,11,11	0.20	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
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.07	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
58	MPD	DT	202	-	-	1/5/5/5	-
59	PUT	DA	3221	-	-	0/3/3/3	-
63	PGE	DD	301	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3209	-	-	0/1/1/1	-
64	SPD	DA	3206	-	-	2/7/7/7	-
59	PUT	DA	3188	-	-	0/3/3/3	-
59	PUT	AA	1675	-	-	1/3/3/3	-
58	MPD	DA	3192	-	-	2/5/5/5	-
59	PUT	DA	3213	-	-	1/3/3/3	-
62	EDO	D0	101	-	-	0/1/1/1	-
62	EDO	DB	211	-	-	0/1/1/1	-
61	PEG	DA	3200	-	-	1/4/4/4	-
61	PEG	DQ	201	-	-	2/4/4/4	-
63	PGE	DU	201	-	-	4/7/7/7	-
58	MPD	DA	3190	-	-	1/5/5/5	-
58	MPD	DA	3210	-	-	2/5/5/5	-
58	MPD	DE	301	-	-	2/5/5/5	-
64	SPD	DA	3183	-	-	3/7/7/7	-
62	EDO	DB	210	-	-	1/1/1/1	-
61	PEG	DA	3218	-	-	1/4/4/4	-
64	SPD	DA	3224	-	-	3/7/7/7	-
63	PGE	DA	3186	-	-	2/7/7/7	-
62	EDO	DA	3198	-	-	1/1/1/1	-
62	EDO	DA	3208	-	-	0/1/1/1	-
57	PG4	DA	3216	-	-	5/10/10/10	-
63	PGE	DA	3225	-	-	4/7/7/7	-
63	PGE	DS	201	-	-	4/7/7/7	-
59	PUT	DA	3212	-	-	0/3/3/3	-
61	PEG	AL	201	-	-	2/4/4/4	-
64	SPD	DA	3187	-	-	2/7/7/7	-
59	PUT	DA	3184	-	-	1/3/3/3	-
61	PEG	DA	3201	-	-	1/4/4/4	-
58	MPD	AA	1676	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
62	EDO	D1	101	-	-	0/1/1/1	-
58	MPD	DA	3207	-	-	2/5/5/5	-
61	PEG	DA	3199	-	-	2/4/4/4	-
57	PG4	DR	201	-	-	4/10/10/10	-
61	PEG	DA	3226	-	-	0/4/4/4	-
58	MPD	DS	203	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	AA	1673	-	-	0/3/3/3	-
59	PUT	AA	1674	-	-	0/3/3/3	-
58	MPD	DA	3204	-	-	2/5/5/5	-
59	PUT	DA	3195	-	-	0/3/3/3	-
58	MPD	DN	201	-	-	0/5/5/5	-
59	PUT	AA	1672	-	-	0/3/3/3	-
62	EDO	DA	3215	-	-	0/1/1/1	-
63	PGE	D1	102	-	-	5/7/7/7	-
61	PEG	D3	102	-	-	1/4/4/4	-
58	MPD	DE	302	-	-	3/5/5/5	-
57	PG4	DS	202	-	-	4/10/10/10	-
59	PUT	DA	3222	-	-	0/3/3/3	-
61	PEG	DP	201	-	-	1/4/4/4	-
61	PEG	DA	3227	-	-	0/4/4/4	-
65	1PE	DA	3185	-	-	4/13/13/13	-
63	PGE	DA	3214	-	-	4/7/7/7	-
58	MPD	DT	201	-	-	1/5/5/5	-
59	PUT	DA	3189	-	-	0/3/3/3	-
68	TRS	DA	3220	-	-	0/9/9/9	-
62	EDO	DA	3003	-	-	1/1/1/1	-
63	PGE	D3	101	-	-	4/7/7/7	-
63	PGE	DA	3217	-	-	3/7/7/7	-
57	PG4	BA	1642	-	-	5/10/10/10	-
62	EDO	DA	3194	-	-	0/1/1/1	-
58	MPD	AA	1671	-	-	0/5/5/5	-
59	PUT	DA	3223	-	-	1/3/3/3	-
59	PUT	DM	201	-	-	0/3/3/3	-
62	EDO	DA	3197	-	-	0/1/1/1	-
65	1PE	DA	3203	-	-	5/13/13/13	-
67	GUN	DA	3211	-	-	-	0/2/2/2
59	PUT	DA	3219	-	-	0/3/3/3	-
58	MPD	DK	201	-	-	5/5/5/5	-
57	PG4	AA	1670	-	-	6/10/10/10	-
62	EDO	DA	3002	-	-	0/1/1/1	-
57	PG4	DA	3193	-	-	4/10/10/10	-
61	PEG	DL	201	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.47	1.42	1.22
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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	DA	3196	ACY	OXT-C-CH3	2.45	125.31	115.18
66	DA	3196	ACY	O-C-CH3	-2.21	113.72	122.33

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
58	DA	3192	MPD	2	0
59	DA	3213	PUT	1	0
61	DQ	201	PEG	1	0
63	DU	201	PGE	1	0
63	DA	3225	PGE	4	0
59	DA	3212	PUT	1	0
61	DA	3201	PEG	1	0
57	DR	201	PG4	1	0
58	DS	203	MPD	4	0
61	D3	102	PEG	1	0
66	DA	3202	ACY	2	0
65	DA	3185	1PE	1	0
63	DA	3214	PGE	1	0
68	DA	3220	TRS	1	0
57	BA	1642	PG4	1	0
62	DA	3194	EDO	3	0
59	DA	3223	PUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3219	PUT	1	0
62	DA	3002	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	78, 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	82, 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	132, 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	64, 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
1	PSU	BA	516	20/21	0.90	0.14	111,121,128,129	0
31	PSU	CA	746	20/21	0.90	0.19	135,137,142,142	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	OMG	CA	2251	24/25	0.92	0.26	111,114,115,116	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
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	2MG	BA	1516	24/25	0.93	0.19	105,110,116,117	0
1	MA6	BA	1518	24/25	0.93	0.24	91,97,102,103	0
31	1MG	CA	745	24/25	0.94	0.17	123,126,132,134	0
1	PSU	AA	516	20/21	0.94	0.15	135,138,139,141	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
1	4OC	BA	1402	22/23	0.94	0.19	111,116,127,128	0
31	2MG	CA	2445	24/25	0.94	0.28	103,109,112,114	0
1	MA6	BA	1519	24/25	0.94	0.24	100,102,107,110	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
31	2MG	CA	1835	24/25	0.94	0.21	100,103,106,110	0
12	D2T	BL	89	10/11	0.94	0.39	106,110,113,114	0
31	5MU	CA	1939	21/22	0.95	0.17	95,99,105,107	0
1	7MG	BA	527	24/25	0.95	0.18	100,108,118,120	0
1	5MC	BA	1407	21/22	0.95	0.14	111,121,124,125	0
1	UR3	BA	1498	21/22	0.95	0.14	118,122,126,127	0
31	PSU	CA	2580	20/21	0.95	0.18	118,125,130,131	0
55	PSU	DA	1911	20/21	0.95	0.14	107,118,120,121	0
12	D2T	AL	89	10/11	0.95	0.29	109,114,125,128	0
1	2MG	AA	1516	24/25	0.96	0.17	74,82,84,86	0
1	7MG	AA	527	24/25	0.96	0.16	102,109,115,118	0
1	4OC	AA	1402	22/23	0.96	0.17	94,99,103,104	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(Å^2)	Q<0.9
31	PSU	CA	2605	20/21	0.96	0.17	97,101,106,106	0
55	2MG	DA	1835	24/25	0.96	0.21	59,65,71,72	0
31	PSU	CA	2457	20/21	0.96	0.19	118,122,126,127	0
55	3TD	DA	1915	21/22	0.96	0.12	133,140,146,147	0
31	5MC	CA	1962	21/22	0.96	0.20	103,106,110,112	0
1	UR3	AA	1498	21/22	0.97	0.18	86,92,97,100	0
1	MA6	AA	1518	24/25	0.97	0.16	67,77,81,85	0
55	PSU	DA	1917	20/21	0.97	0.13	109,113,119,119	0
1	MA6	AA	1519	24/25	0.97	0.20	72,76,80,81	0
55	PSU	DA	2504	20/21	0.98	0.19	50,51,54,56	0
55	PSU	DA	2605	20/21	0.98	0.17	51,59,64,65	0
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
41	4D4	DN	81[B]	12/13	0.98	0.23	37,45,50,50	9
55	5MU	DA	1939	21/22	0.99	0.20	53,58,65,69	0
55	PSU	DA	955	20/21	0.99	0.19	32,35,39,41	0
55	6MZ	DA	2030	23/24	0.99	0.20	27,33,38,40	0
55	7MG	DA	2069	24/25	0.99	0.18	41,48,53,53	0
55	OMG	DA	2251	24/25	0.99	0.18	29,48,54,62	0
55	2MG	DA	2445	24/25	0.99	0.20	39,45,50,62	0
55	H2U	DA	2449	20/21	0.99	0.23	33,39,46,46	0
55	PSU	DA	2457	20/21	0.99	0.18	44,46,52,53	0
55	OMC	DA	2498	21/22	0.99	0.21	37,39,46,47	0
55	2MA	DA	2503	23/24	0.99	0.21	44,51,58,62	0
55	6MZ	DA	1618	23/24	0.99	0.20	34,42,47,49	0
55	OMU	DA	2552	21/22	0.99	0.21	45,48,52,57	0
55	PSU	DA	2580	20/21	0.99	0.20	30,35,41,43	0
55	PSU	DA	2604	20/21	0.99	0.17	58,63,70,72	0
32	MEQ	DD	150[A]	10/11	0.99	0.28	31,32,37,37	10
32	MEQ	DD	150[B]	10/11	0.99	0.28	35,38,44,45	10
55	1MG	DA	745	24/25	0.99	0.19	31,37,42,44	0
55	5MU	DA	747	21/22	0.99	0.19	41,43,52,58	0
55	PSU	DA	746	20/21	1.00	0.18	38,44,46,47	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	BA	1624	1/1	0.17	2.21	293,293,293,293	0
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	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
56	MG	DA	3168	1/1	0.51	0.54	119,119,119,119	0
61	PEG	DQ	201	7/7	0.51	0.82	162,166,170,170	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	AA	1618	1/1	0.54	0.11	172,172,172,172	0
56	MG	CA	3075	1/1	0.54	1.12	231,231,231,231	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	3135	1/1	0.61	0.48	78,78,78,78	0
56	MG	CA	3105	1/1	0.61	0.18	252,252,252,252	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
61	PEG	AL	201	7/7	0.64	0.30	132,133,135,136	0
56	MG	AA	1621	1/1	0.64	0.50	97,97,97,97	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(Å^2)	Q<0.9
56	MG	AA	1615	1/1	0.68	0.67	129,129,129,129	0
56	MG	CA	3056	1/1	0.69	0.48	77,77,77,77	0
59	PUT	DA	3195	6/6	0.69	0.44	100,104,108,108	0
56	MG	CA	3140	1/1	0.69	0.54	108,108,108,108	0
58	MPD	DE	301	8/8	0.69	1.05	172,174,179,179	0
61	PEG	DP	201	7/7	0.69	0.69	149,153,164,165	0
56	MG	DA	3147	1/1	0.69	0.29	108,108,108,108	0
68	TRS	DA	3220	8/8	0.69	0.80	184,187,190,191	0
56	MG	AA	1626	1/1	0.70	0.95	120,120,120,120	0
62	EDO	DA	3002	4/4	0.71	0.61	176,176,176,177	0
64	SPD	DA	3206	10/10	0.71	0.23	142,143,144,144	0
56	MG	DA	3182	1/1	0.71	0.43	55,55,55,55	0
61	PEG	DA	3200	7/7	0.72	0.35	124,124,125,125	0
56	MG	BA	1626	1/1	0.72	0.91	255,255,255,255	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
56	MG	CA	3116	1/1	0.75	0.41	92,92,92,92	0
58	MPD	DT	202	8/8	0.75	0.37	138,139,144,145	0
62	EDO	DB	210	4/4	0.76	0.39	125,126,126,127	0
56	MG	CA	3092	1/1	0.76	0.08	163,163,163,163	0
56	MG	DA	3162	1/1	0.76	0.30	79,79,79,79	0
56	MG	CA	3113	1/1	0.76	0.44	76,76,76,76	0
56	MG	AA	1665	1/1	0.76	0.71	274,274,274,274	0
59	PUT	AA	1673	6/6	0.77	0.67	142,145,148,150	0
56	MG	AA	1625	1/1	0.77	0.58	83,83,83,83	0
56	MG	AA	1604	1/1	0.77	0.66	79,79,79,79	0
56	MG	BA	1625	1/1	0.77	0.77	288,288,288,288	0
61	PEG	DA	3218	7/7	0.77	0.28	179,180,181,181	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
56	MG	AA	1659	1/1	0.79	0.33	273,273,273,273	0
59	PUT	AA	1674	6/6	0.79	0.77	109,113,116,117	0
56	MG	AA	1605	1/1	0.79	0.52	87,87,87,87	0
56	MG	CA	3130	1/1	0.80	0.13	84,84,84,84	0
56	MG	DA	3123	1/1	0.80	0.36	84,84,84,84	0
56	MG	CA	3009	1/1	0.80	0.15	259,259,259,259	0
56	MG	DA	3170	1/1	0.80	0.18	59,59,59,59	0
56	MG	CA	3122	1/1	0.80	0.53	89,89,89,89	0
62	EDO	DA	3003	4/4	0.80	0.28	135,137,140,141	0
56	MG	CA	3123	1/1	0.80	0.69	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1602	1/1	0.80	0.44	78,78,78,78	0
56	MG	BA	1635	1/1	0.80	0.16	209,209,209,209	0
56	MG	BA	1638	1/1	0.81	0.44	65,65,65,65	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
56	MG	DA	3134	1/1	0.81	0.60	98,98,98,98	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
56	MG	CA	3006	1/1	0.81	0.10	221,221,221,221	0
61	PEG	DA	3201	7/7	0.81	0.47	146,150,151,152	0
56	MG	CA	3034	1/1	0.82	0.14	228,228,228,228	0
56	MG	AA	1610	1/1	0.82	0.28	99,99,99,99	0
59	PUT	DA	3213	6/6	0.82	0.27	156,156,157,157	0
59	PUT	DA	3221	6/6	0.82	0.46	112,120,122,122	0
56	MG	AA	1663	1/1	0.82	0.24	230,230,230,230	0
56	MG	AA	1620	1/1	0.82	0.80	116,116,116,116	0
63	PGE	D3	101	10/10	0.82	0.54	121,123,125,126	0
56	MG	CA	3151	1/1	0.82	0.54	102,102,102,102	0
56	MG	DA	3148	1/1	0.82	0.22	67,67,67,67	0
56	MG	CA	3093	1/1	0.82	0.16	143,143,143,143	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
58	MPD	DK	201	8/8	0.83	0.27	125,126,127,127	0
56	MG	BA	1606	1/1	0.83	0.17	270,270,270,270	0
56	MG	DA	3178	1/1	0.83	0.33	93,93,93,93	0
62	EDO	DA	3194	4/4	0.83	0.31	89,90,90,90	0
61	PEG	DA	3227	7/7	0.84	0.34	109,114,120,120	0
56	MG	CA	3071	1/1	0.84	0.35	228,228,228,228	0
56	MG	CA	3125	1/1	0.84	0.28	136,136,136,136	0
56	MG	CA	3119	1/1	0.84	0.37	100,100,100,100	0
56	MG	DA	3154	1/1	0.84	0.35	60,60,60,60	0
56	MG	DA	3176	1/1	0.84	0.31	81,81,81,81	0
56	MG	AA	1642	1/1	0.84	0.77	275,275,275,275	0
61	PEG	DA	3199	7/7	0.84	0.46	99,106,112,113	0
56	MG	AA	1601	1/1	0.84	0.75	62,62,62,62	0
56	MG	DA	3157	1/1	0.84	0.26	74,74,74,74	0
57	PG4	DQ	202	13/13	0.84	0.26	84,89,100,101	0
56	MG	CA	3110	1/1	0.85	0.35	129,129,129,129	0
58	MPD	DA	3204	8/8	0.85	0.61	116,119,125,127	0
59	PUT	DA	3212	6/6	0.85	0.22	114,115,117,117	0
56	MG	BA	1641	1/1	0.85	0.37	140,140,140,140	0
56	MG	BA	1630	1/1	0.85	0.07	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	1604	1/1	0.85	0.49	257,257,257,257	0
56	MG	AA	1609	1/1	0.86	0.55	107,107,107,107	0
56	MG	CA	3094	1/1	0.86	0.11	132,132,132,132	0
56	MG	CA	3019	1/1	0.86	0.21	87,87,87,87	0
56	MG	DA	3158	1/1	0.86	0.49	107,107,107,107	0
56	MG	DA	3160	1/1	0.86	0.36	64,64,64,64	0
59	PUT	DA	3219	6/6	0.86	0.29	100,102,103,103	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	CA	3128	1/1	0.86	0.35	116,116,116,116	0
56	MG	CA	3146	1/1	0.86	0.10	174,174,174,174	0
63	PGE	DU	201	10/10	0.86	0.45	135,141,147,147	0
63	PGE	DA	3214	10/10	0.86	0.60	67,87,91,92	0
56	MG	CA	3067	1/1	0.86	0.21	274,274,274,274	0
56	MG	DA	3171	1/1	0.86	0.82	111,111,111,111	0
56	MG	BA	1634	1/1	0.86	0.10	216,216,216,216	0
56	MG	CA	3156	1/1	0.87	0.16	263,263,263,263	0
56	MG	CA	3001	1/1	0.87	0.30	291,291,291,291	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
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	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	CB	201	1/1	0.87	0.06	235,235,235,235	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
61	PEG	DL	201	7/7	0.88	0.31	102,103,109,110	0
57	PG4	DA	3193	13/13	0.88	0.96	109,113,119,120	0
56	MG	CA	3111	1/1	0.88	0.29	103,103,103,103	0
56	MG	DA	3128	1/1	0.88	1.11	57,57,57,57	0
56	MG	CA	3021	1/1	0.88	1.30	253,253,253,253	0
56	MG	BA	1636	1/1	0.88	0.47	77,77,77,77	0
56	MG	CA	3072	1/1	0.88	1.07	258,258,258,258	0
62	EDO	DA	3215	4/4	0.88	0.32	64,67,70,73	0
56	MG	DA	3129	1/1	0.89	0.22	51,51,51,51	0
57	PG4	BA	1642	13/13	0.89	0.45	113,117,132,132	0
56	MG	CA	3141	1/1	0.89	0.22	78,78,78,78	0
56	MG	DA	3133	1/1	0.89	0.26	52,52,52,52	0
56	MG	AA	1606	1/1	0.89	0.14	124,124,124,124	0
57	PG4	DA	3216	13/13	0.89	0.28	111,122,132,134	0
56	MG	BA	1612	1/1	0.89	0.22	262,262,262,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3030	1/1	0.89	0.09	82,82,82,82	0
56	MG	CA	3014	1/1	0.89	0.19	273,273,273,273	0
56	MG	CA	3048	1/1	0.89	0.16	147,147,147,147	0
63	PGE	DD	301	10/10	0.89	0.31	120,122,129,130	0
56	MG	CA	3054	1/1	0.89	0.12	122,122,122,122	0
58	MPD	DA	3190	8/8	0.89	0.31	100,102,103,106	0
56	MG	AA	1654	1/1	0.89	0.14	178,178,178,178	0
58	MPD	DA	3207	8/8	0.89	0.44	121,125,128,129	0
56	MG	DA	3180	1/1	0.89	0.80	77,77,77,77	0
56	MG	AA	1656	1/1	0.89	0.11	274,274,274,274	0
56	MG	DA	3165	1/1	0.90	0.27	63,63,63,63	0
56	MG	CA	3148	1/1	0.90	0.42	43,43,43,43	1
57	PG4	DS	202	13/13	0.90	0.31	72,73,85,86	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	DA	3172	1/1	0.90	0.38	85,85,85,85	0
56	MG	CA	3008	1/1	0.90	0.09	202,202,202,202	0
56	MG	DA	3098	1/1	0.90	0.21	246,246,246,246	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	3161	1/1	0.90	0.22	73,73,73,73	0
56	MG	DA	3124	1/1	0.90	0.52	90,90,90,90	0
56	MG	CA	3147	1/1	0.90	0.25	36,36,36,36	1
62	EDO	D1	101	4/4	0.91	0.23	70,71,73,75	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
58	MPD	AA	1671	8/8	0.91	0.70	143,144,147,148	0
56	MG	CA	3138	1/1	0.91	0.12	98,98,98,98	0
56	MG	DA	3001	1/1	0.91	0.45	47,47,47,47	0
62	EDO	DA	3209	4/4	0.91	0.62	94,96,98,99	0
56	MG	DA	3153	1/1	0.91	0.28	102,102,102,102	0
58	MPD	DN	201	8/8	0.91	0.35	109,117,119,121	0
56	MG	AA	1647	1/1	0.91	0.30	145,145,145,145	0
56	MG	AA	1658	1/1	0.91	0.34	212,212,212,212	0
56	MG	BA	1603	1/1	0.91	0.21	278,278,278,278	0
56	MG	DA	3125	1/1	0.91	0.22	51,51,51,51	0
56	MG	CA	3057	1/1	0.91	0.14	111,111,111,111	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	AA	1613	1/1	0.91	0.62	80,80,80,80	0
64	SPD	DA	3224	10/10	0.91	0.30	58,71,88,88	0
67	GUN	DA	3211	11/11	0.91	0.26	116,122,123,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3070	1/1	0.91	0.31	234,234,234,234	0
56	MG	CA	3152	1/1	0.92	0.16	160,160,160,160	0
56	MG	CA	3038	1/1	0.92	0.17	252,252,252,252	0
56	MG	CA	3096	1/1	0.92	0.08	89,89,89,89	0
56	MG	DB	206	1/1	0.92	0.31	73,73,73,73	0
56	MG	CA	3039	1/1	0.92	0.58	190,190,190,190	0
56	MG	CA	3064	1/1	0.92	0.29	271,271,271,271	0
56	MG	AA	1612	1/1	0.92	0.36	77,77,77,77	0
56	MG	CB	203	1/1	0.92	0.15	237,237,237,237	0
62	EDO	D0	101	4/4	0.92	0.26	79,80,85,89	0
56	MG	BA	1639	1/1	0.92	0.27	117,117,117,117	0
56	MG	CA	3053	1/1	0.92	0.11	86,86,86,86	0
58	MPD	DA	3210	8/8	0.92	0.30	110,118,123,125	0
56	MG	CA	3028	1/1	0.92	0.80	284,284,284,284	0
56	MG	CA	3117	1/1	0.92	0.13	59,59,59,59	0
56	MG	DA	3131	1/1	0.92	0.24	83,83,83,83	0
56	MG	CA	3002	1/1	0.92	0.15	224,224,224,224	0
59	PUT	DA	3184	6/6	0.92	0.43	65,70,74,74	0
56	MG	CA	3032	1/1	0.92	0.35	197,197,197,197	0
59	PUT	DA	3205	6/6	0.92	0.30	106,108,108,109	0
56	MG	CA	3120	1/1	0.92	0.13	130,130,130,130	0
56	MG	DA	3138	1/1	0.92	0.34	29,29,29,29	1
56	MG	CA	3121	1/1	0.92	0.23	83,83,83,83	0
56	MG	CA	3083	1/1	0.92	0.35	254,254,254,254	0
59	PUT	DA	3222	6/6	0.92	0.31	77,81,83,83	0
56	MG	CA	3090	1/1	0.92	0.16	187,187,187,187	0
56	MG	AA	1614	1/1	0.92	0.13	83,83,83,83	0
65	1PE	DA	3203	16/16	0.92	0.30	98,105,109,109	0
56	MG	CA	3149	1/1	0.92	0.44	76,76,76,76	0
56	MG	CA	3059	1/1	0.92	0.10	118,118,118,118	0
56	MG	CA	3129	1/1	0.93	0.13	135,135,135,135	0
56	MG	CA	3087	1/1	0.93	0.17	232,232,232,232	0
56	MG	DA	3143	1/1	0.93	0.31	63,63,63,63	0
58	MPD	DE	302	8/8	0.93	0.41	101,102,103,104	0
62	EDO	DA	3197	4/4	0.93	0.29	75,76,77,77	0
56	MG	DA	3144	1/1	0.93	0.63	79,79,79,79	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	3062	1/1	0.93	0.28	269,269,269,269	0
56	MG	CA	3010	1/1	0.93	0.10	259,259,259,259	0
56	MG	CA	3109	1/1	0.93	0.34	67,67,67,67	0
56	MG	BA	1627	1/1	0.93	0.68	203,203,203,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3134	1/1	0.93	0.12	167,167,167,167	0
56	MG	DA	3126	1/1	0.93	0.31	77,77,77,77	0
56	MG	CA	3018	1/1	0.93	0.10	147,147,147,147	0
56	MG	CA	3036	1/1	0.93	0.15	227,227,227,227	0
64	SPD	DA	3183	10/10	0.93	0.45	80,95,97,98	0
56	MG	CA	3068	1/1	0.93	0.26	174,174,174,174	0
56	MG	CA	3099	1/1	0.93	0.12	174,174,174,174	0
56	MG	CA	3155	1/1	0.93	0.26	181,181,181,181	0
59	PUT	DA	3188	6/6	0.93	0.20	89,93,93,94	0
56	MG	AA	1638	1/1	0.93	0.14	142,142,142,142	0
56	MG	AA	1611	1/1	0.94	0.15	133,133,133,133	0
56	MG	DA	3121	1/1	0.94	0.53	111,111,111,111	0
56	MG	AA	1608	1/1	0.94	0.36	128,128,128,128	0
56	MG	BA	1620	1/1	0.94	0.12	172,172,172,172	0
56	MG	CA	3031	1/1	0.94	0.19	128,128,128,128	0
56	MG	BA	1633	1/1	0.94	0.55	237,237,237,237	0
56	MG	CA	3106	1/1	0.94	0.13	74,74,74,74	0
56	MG	AA	1641	1/1	0.94	0.06	122,122,122,122	0
56	MG	AA	1662	1/1	0.94	0.20	164,164,164,164	0
56	MG	AA	1617	1/1	0.94	0.21	88,88,88,88	0
56	MG	DA	3132	1/1	0.94	0.21	56,56,56,56	0
56	MG	CA	3003	1/1	0.94	1.80	272,272,272,272	0
56	MG	CA	3084	1/1	0.94	0.21	172,172,172,172	0
56	MG	CA	3085	1/1	0.94	0.08	116,116,116,116	0
56	MG	CA	3040	1/1	0.94	0.13	122,122,122,122	0
56	MG	CA	3062	1/1	0.94	0.11	168,168,168,168	0
56	MG	DB	204	1/1	0.94	0.16	85,85,85,85	0
64	SPD	DA	3187	10/10	0.94	0.26	78,82,85,85	0
56	MG	DA	3179	1/1	0.94	1.13	85,85,85,85	0
56	MG	CA	3136	1/1	0.94	0.24	107,107,107,107	0
65	1PE	DA	3185	16/16	0.94	0.21	74,89,123,123	0
56	MG	DB	207	1/1	0.94	0.77	92,92,92,92	0
56	MG	BA	1610	1/1	0.94	0.07	107,107,107,107	0
56	MG	CA	3066	1/1	0.94	0.11	91,91,91,91	0
56	MG	DA	3118	1/1	0.95	0.10	31,31,31,31	0
56	MG	CA	3004	1/1	0.95	0.11	192,192,192,192	0
59	PUT	DM	201	6/6	0.95	0.21	63,66,74,75	0
56	MG	AA	1653	1/1	0.95	0.06	108,108,108,108	0
56	MG	AA	1619	1/1	0.95	0.54	122,122,122,122	0
59	PUT	DA	3189	6/6	0.95	0.25	49,55,59,62	0
56	MG	CA	3058	1/1	0.95	0.14	124,124,124,124	0
56	MG	CA	3101	1/1	0.95	0.12	239,239,239,239	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	CA	3046	1/1	0.95	0.13	99,99,99,99	0
56	MG	AA	1657	1/1	0.95	0.46	134,134,134,134	0
56	MG	DB	205	1/1	0.95	0.66	148,148,148,148	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
63	PGE	DA	3186	10/10	0.95	0.20	58,65,71,71	0
56	MG	DA	3164	1/1	0.95	0.26	78,78,78,78	0
56	MG	AA	1634	1/1	0.95	0.33	179,179,179,179	0
56	MG	BA	1616	1/1	0.95	0.12	151,151,151,151	0
56	MG	DA	3033	1/1	0.95	0.13	46,46,46,46	0
56	MG	DA	3141	1/1	0.95	0.41	80,80,80,80	0
58	MPD	DA	3192	8/8	0.95	0.57	84,90,92,94	0
56	MG	AA	1637	1/1	0.95	0.15	106,106,106,106	0
56	MG	DA	3079	1/1	0.95	0.32	179,179,179,179	0
56	MG	DA	3145	1/1	0.95	0.20	45,45,45,45	0
66	ACY	DA	3191	4/4	0.95	0.25	79,80,81,81	0
56	MG	DA	3080	1/1	0.95	0.10	195,195,195,195	0
56	MG	CA	3114	1/1	0.95	0.31	67,67,67,67	0
56	MG	CA	3103	1/1	0.96	0.15	176,176,176,176	0
56	MG	DA	3120	1/1	0.96	0.55	66,66,66,66	0
56	MG	BA	1622	1/1	0.96	0.10	240,240,240,240	0
56	MG	AA	1664	1/1	0.96	0.71	265,265,265,265	0
56	MG	BA	1607	1/1	0.96	0.24	280,280,280,280	0
56	MG	CA	3082	1/1	0.96	0.26	168,168,168,168	0
56	MG	CA	3150	1/1	0.96	0.77	79,79,79,79	0
62	EDO	DB	211	4/4	0.96	0.22	131,131,132,133	0
56	MG	CA	3108	1/1	0.96	0.23	89,89,89,89	0
56	MG	BA	1609	1/1	0.96	0.14	156,156,156,156	0
56	MG	CA	3153	1/1	0.96	0.20	77,77,77,77	0
56	MG	AA	1640	1/1	0.96	0.10	131,131,131,131	0
56	MG	AA	1668	1/1	0.96	0.13	110,110,110,110	0
56	MG	DA	3174	1/1	0.96	0.23	87,87,87,87	0
56	MG	DA	3175	1/1	0.96	0.60	115,115,115,115	0
56	MG	CA	3112	1/1	0.96	0.36	103,103,103,103	0
56	MG	DA	3177	1/1	0.96	0.36	52,52,52,52	0
56	MG	DB	201	1/1	0.96	0.11	121,121,121,121	0
56	MG	CA	3050	1/1	0.96	0.18	166,166,166,166	0
56	MG	CA	3065	1/1	0.96	0.15	115,115,115,115	0
56	MG	CA	3051	1/1	0.96	0.39	248,248,248,248	0
56	MG	DA	3142	1/1	0.96	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1648	1/1	0.96	0.05	84,84,84,84	0
56	MG	DB	209	1/1	0.96	0.15	83,83,83,83	0
56	MG	BA	1617	1/1	0.96	0.12	165,165,165,165	0
56	MG	DA	3007	1/1	0.96	0.09	127,127,127,127	0
56	MG	DA	3008	1/1	0.96	0.12	280,280,280,280	0
56	MG	AA	1630	1/1	0.96	0.20	205,205,205,205	0
56	MG	CA	3097	1/1	0.96	0.14	112,112,112,112	0
56	MG	AA	1635	1/1	0.96	0.14	220,220,220,220	0
56	MG	CA	3020	1/1	0.96	0.15	116,116,116,116	0
66	ACY	DA	3196	4/4	0.96	0.24	61,69,69,72	0
56	MG	DA	3095	1/1	0.96	0.14	65,65,65,65	0
56	MG	CA	3143	1/1	0.96	0.14	72,72,72,72	0
56	MG	AA	1650	1/1	0.97	0.13	115,115,115,115	0
56	MG	DA	3139	1/1	0.97	0.13	42,42,42,42	0
56	MG	BA	1601	1/1	0.97	0.22	135,135,135,135	0
56	MG	BA	1602	1/1	0.97	0.11	102,102,102,102	0
56	MG	CA	3115	1/1	0.97	0.30	111,111,111,111	0
56	MG	CA	3063	1/1	0.97	0.13	155,155,155,155	0
56	MG	DA	3012	1/1	0.97	0.14	141,141,141,141	0
56	MG	CA	3091	1/1	0.97	0.09	81,81,81,81	0
56	MG	DA	3044	1/1	0.97	0.08	124,124,124,124	0
56	MG	AA	1632	1/1	0.97	0.10	162,162,162,162	0
56	MG	DA	3149	1/1	0.97	0.24	96,96,96,96	0
56	MG	CA	3005	1/1	0.97	0.37	233,233,233,233	0
56	MG	AA	1645	1/1	0.97	0.13	70,70,70,70	0
56	MG	CA	3095	1/1	0.97	0.12	174,174,174,174	0
56	MG	DA	3097	1/1	0.97	0.11	75,75,75,75	0
56	MG	BA	1618	1/1	0.97	0.22	172,172,172,172	0
56	MG	DA	3099	1/1	0.97	0.19	45,45,45,45	0
56	MG	DA	3117	1/1	0.97	0.12	70,70,70,70	0
56	MG	CA	3027	1/1	0.97	0.21	88,88,88,88	0
62	EDO	DA	3208	4/4	0.97	0.21	111,113,113,113	0
56	MG	BA	1628	1/1	0.97	0.15	120,120,120,120	0
56	MG	AA	1655	1/1	0.97	0.08	152,152,152,152	0
56	MG	DA	3122	1/1	0.97	0.28	48,48,48,48	0
56	MG	AA	1649	1/1	0.97	0.06	111,111,111,111	0
56	MG	CA	3127	1/1	0.97	0.14	73,73,73,73	0
56	MG	DA	3166	1/1	0.97	0.34	74,74,74,74	0
56	MG	DA	3167	1/1	0.97	0.43	97,97,97,97	0
56	MG	CA	3073	1/1	0.97	0.23	139,139,139,139	0
56	MG	CA	3012	1/1	0.97	0.14	115,115,115,115	0
56	MG	BA	1631	1/1	0.97	0.11	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3079	1/1	0.97	0.28	131,131,131,131	0
56	MG	DA	3173	1/1	0.97	0.87	100,100,100,100	0
56	MG	DD	302	1/1	0.97	0.22	62,62,62,62	0
56	MG	DR	202	1/1	0.97	0.30	269,269,269,269	0
56	MG	CA	3033	1/1	0.97	0.09	150,150,150,150	0
56	MG	CA	3081	1/1	0.97	0.16	254,254,254,254	0
56	MG	CA	3016	1/1	0.97	0.90	218,218,218,218	0
59	PUT	DA	3223	6/6	0.97	0.19	75,81,84,84	0
56	MG	DA	3135	1/1	0.97	0.17	146,146,146,146	0
66	ACY	DA	3202	4/4	0.97	0.19	93,96,96,97	0
56	MG	CA	3017	1/1	0.97	0.12	192,192,192,192	0
56	MG	DA	3181	1/1	0.97	0.29	66,66,66,66	0
56	MG	CA	3015	1/1	0.98	0.22	84,84,84,84	0
56	MG	BA	1608	1/1	0.98	0.19	144,144,144,144	0
56	MG	CA	3078	1/1	0.98	0.30	198,198,198,198	0
56	MG	AA	1636	1/1	0.98	0.39	209,209,209,209	0
56	MG	AA	1639	1/1	0.98	0.50	225,225,225,225	0
56	MG	DA	3127	1/1	0.98	0.45	69,69,69,69	0
56	MG	BA	1611	1/1	0.98	0.13	84,84,84,84	0
56	MG	AA	1643	1/1	0.98	0.14	70,70,70,70	0
56	MG	CA	3037	1/1	0.98	0.27	234,234,234,234	0
56	MG	BA	1614	1/1	0.98	0.14	217,217,217,217	0
56	MG	BA	1615	1/1	0.98	0.16	103,103,103,103	0
56	MG	DA	3004	1/1	0.98	0.14	149,149,149,149	0
56	MG	CA	3086	1/1	0.98	0.21	106,106,106,106	0
56	MG	DA	3231	1/1	0.98	0.26	70,70,70,70	0
56	MG	AA	1667	1/1	0.98	0.14	76,76,76,76	0
56	MG	CA	3042	1/1	0.98	0.06	96,96,96,96	0
56	MG	DA	3030	1/1	0.98	0.20	88,88,88,88	0
56	MG	DA	3031	1/1	0.98	0.16	51,51,51,51	0
56	MG	CA	3044	1/1	0.98	0.17	113,113,113,113	0
56	MG	DA	3043	1/1	0.98	0.14	40,40,40,40	0
56	MG	CA	3144	1/1	0.98	0.06	66,66,66,66	0
56	MG	DA	3048	1/1	0.98	0.12	59,59,59,59	0
56	MG	DA	3053	1/1	0.98	0.10	54,54,54,54	0
56	MG	DA	3054	1/1	0.98	0.17	167,167,167,167	0
56	MG	CA	3045	1/1	0.98	0.08	167,167,167,167	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
58	MPD	DS	203	8/8	0.98	0.22	62,64,65,67	0
56	MG	DA	3150	1/1	0.98	0.08	72,72,72,72	0
56	MG	DA	3151	1/1	0.98	0.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3024	1/1	0.98	0.06	85,85,85,85	0
56	MG	CA	3025	1/1	0.98	0.13	133,133,133,133	0
56	MG	DA	3085	1/1	0.98	0.14	100,100,100,100	0
56	MG	DA	3088	1/1	0.98	0.09	75,75,75,75	0
56	MG	DA	3094	1/1	0.98	0.19	29,29,29,29	0
56	MG	BA	1605	1/1	0.98	0.08	136,136,136,136	0
56	MG	CA	3069	1/1	0.98	0.14	107,107,107,107	0
56	MG	DA	3159	1/1	0.98	0.14	131,131,131,131	0
56	MG	CA	3049	1/1	0.98	0.12	53,53,53,53	0
56	MG	CA	3011	1/1	0.98	0.17	95,95,95,95	0
56	MG	DA	3108	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3111	1/1	0.98	0.47	283,283,283,283	0
56	MG	DA	3115	1/1	0.98	0.20	52,52,52,52	0
56	MG	CA	3100	1/1	0.98	0.25	243,243,243,243	0
56	MG	AA	1631	1/1	0.98	0.09	75,75,75,75	0
56	MG	AA	1652	1/1	0.98	0.26	42,42,42,42	0
56	MG	CA	3074	1/1	0.98	0.10	145,145,145,145	0
56	MG	DA	3169	1/1	0.98	0.11	41,41,41,41	0
56	MG	DA	3083	1/1	0.99	0.07	57,57,57,57	0
56	MG	DB	203	1/1	0.99	0.10	88,88,88,88	0
56	MG	DA	3086	1/1	0.99	0.09	82,82,82,82	0
56	MG	AA	1629	1/1	0.99	0.10	110,110,110,110	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	3229	1/1	0.99	0.08	107,107,107,107	0
56	MG	DA	3090	1/1	0.99	0.17	26,26,26,26	0
56	MG	DA	3092	1/1	0.99	0.12	50,50,50,50	0
56	MG	DA	3093	1/1	0.99	0.17	23,23,23,23	0
56	MG	CA	3098	1/1	0.99	0.07	98,98,98,98	0
56	MG	AA	1646	1/1	0.99	0.12	80,80,80,80	0
56	MG	DA	3096	1/1	0.99	0.13	28,28,28,28	0
56	MG	AA	1666	1/1	0.99	0.07	100,100,100,100	0
56	MG	DB	208	1/1	0.99	0.17	57,57,57,57	0
56	MG	AA	1651	1/1	0.99	0.12	75,75,75,75	0
56	MG	DA	3101	1/1	0.99	0.15	90,90,90,90	0
56	MG	DA	3102	1/1	0.99	0.13	32,32,32,32	0
56	MG	DA	3103	1/1	0.99	0.15	59,59,59,59	0
56	MG	DA	3105	1/1	0.99	0.17	33,33,33,33	0
56	MG	DA	3106	1/1	0.99	0.16	45,45,45,45	0
56	MG	DA	3107	1/1	0.99	0.15	50,50,50,50	0
56	MG	CA	3102	1/1	0.99	0.11	99,99,99,99	0
56	MG	DA	3109	1/1	0.99	0.16	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1633	1/1	0.99	0.12	116,116,116,116	0
56	MG	DA	3112	1/1	0.99	0.18	46,46,46,46	0
56	MG	DA	3113	1/1	0.99	0.16	113,113,113,113	0
56	MG	DA	3114	1/1	0.99	0.08	52,52,52,52	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	3006	1/1	0.99	0.11	266,266,266,266	0
56	MG	BA	1640	1/1	0.99	0.08	103,103,103,103	0
56	MG	CA	3035	1/1	0.99	0.20	100,100,100,100	0
56	MG	DA	3009	1/1	0.99	0.12	39,39,39,39	0
56	MG	DA	3010	1/1	0.99	0.11	48,48,48,48	0
56	MG	BA	1621	1/1	0.99	0.17	45,45,45,45	0
56	MG	DA	3013	1/1	0.99	0.20	13,13,13,13	0
56	MG	DA	3014	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3015	1/1	0.99	0.16	78,78,78,78	0
56	MG	DA	3016	1/1	0.99	0.16	74,74,74,74	0
56	MG	DA	3017	1/1	0.99	0.12	34,34,34,34	0
56	MG	DA	3018	1/1	0.99	0.10	95,95,95,95	0
56	MG	DA	3020	1/1	0.99	0.06	69,69,69,69	0
56	MG	DA	3022	1/1	0.99	0.13	40,40,40,40	0
56	MG	DA	3023	1/1	0.99	0.23	57,57,57,57	0
56	MG	DA	3025	1/1	0.99	0.11	57,57,57,57	0
56	MG	DA	3026	1/1	0.99	0.18	228,228,228,228	0
56	MG	DA	3027	1/1	0.99	0.20	49,49,49,49	0
56	MG	DA	3136	1/1	0.99	0.18	72,72,72,72	0
56	MG	DA	3028	1/1	0.99	0.10	116,116,116,116	0
56	MG	DA	3029	1/1	0.99	0.21	44,44,44,44	0
56	MG	BA	1613	1/1	0.99	0.26	149,149,149,149	0
56	MG	DA	3140	1/1	0.99	0.18	51,51,51,51	0
56	MG	CB	202	1/1	0.99	0.08	116,116,116,116	0
56	MG	DA	3032	1/1	0.99	0.19	33,33,33,33	0
56	MG	CA	3088	1/1	0.99	0.13	86,86,86,86	0
56	MG	DA	3035	1/1	0.99	0.14	24,24,24,24	0
56	MG	DA	3038	1/1	0.99	0.11	35,35,35,35	0
56	MG	DA	3040	1/1	0.99	0.09	55,55,55,55	0
56	MG	DA	3042	1/1	0.99	0.11	87,87,87,87	0
56	MG	CA	3089	1/1	0.99	0.21	64,64,64,64	0
56	MG	BA	1632	1/1	0.99	0.12	74,74,74,74	0
56	MG	DA	3045	1/1	0.99	0.10	73,73,73,73	0
56	MG	DA	3047	1/1	0.99	0.13	42,42,42,42	0
56	MG	CA	3013	1/1	0.99	0.11	71,71,71,71	0
56	MG	DA	3050	1/1	0.99	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3051	1/1	0.99	0.13	37,37,37,37	0
56	MG	DA	3052	1/1	0.99	0.29	251,251,251,251	0
56	MG	CA	3041	1/1	0.99	0.08	50,50,50,50	0
56	MG	AA	1669	1/1	0.99	0.25	239,239,239,239	0
56	MG	DA	3055	1/1	0.99	0.26	52,52,52,52	0
56	MG	DA	3056	1/1	0.99	0.22	55,55,55,55	0
56	MG	DA	3059	1/1	0.99	0.07	25,25,25,25	0
56	MG	DA	3060	1/1	0.99	0.14	23,23,23,23	0
56	MG	DA	3061	1/1	0.99	0.14	44,44,44,44	0
56	MG	CA	3043	1/1	0.99	0.06	90,90,90,90	0
56	MG	DA	3063	1/1	0.99	0.15	111,111,111,111	0
56	MG	DA	3066	1/1	0.99	0.12	43,43,43,43	0
56	MG	DM	202	1/1	0.99	0.04	90,90,90,90	0
56	MG	DA	3068	1/1	0.99	0.20	43,43,43,43	0
56	MG	DA	3070	1/1	0.99	0.12	151,151,151,151	0
56	MG	CA	3076	1/1	0.99	0.31	218,218,218,218	0
56	MG	DA	3074	1/1	0.99	0.12	54,54,54,54	0
56	MG	DA	3076	1/1	0.99	0.19	46,46,46,46	0
56	MG	DA	3077	1/1	0.99	0.12	71,71,71,71	0
56	MG	DA	3078	1/1	0.99	0.06	47,47,47,47	0
56	MG	AA	1644	1/1	0.99	0.14	180,180,180,180	0
56	MG	DB	202	1/1	0.99	0.10	56,56,56,56	0
56	MG	DA	3081	1/1	0.99	0.07	46,46,46,46	0
56	MG	DA	3082	1/1	0.99	0.11	109,109,109,109	0
56	MG	DA	3084	1/1	1.00	0.18	55,55,55,55	0
56	MG	DA	3065	1/1	1.00	0.13	41,41,41,41	0
56	MG	DA	3110	1/1	1.00	0.16	31,31,31,31	0
56	MG	DA	3024	1/1	1.00	0.17	44,44,44,44	0
56	MG	DA	3087	1/1	1.00	0.19	32,32,32,32	0
56	MG	DA	3041	1/1	1.00	0.23	22,22,22,22	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	3091	1/1	1.00	0.13	29,29,29,29	0
56	MG	DA	3034	1/1	1.00	0.16	44,44,44,44	0
56	MG	DA	3019	1/1	1.00	0.26	16,16,16,16	0
56	MG	DA	3119	1/1	1.00	0.30	41,41,41,41	0
60	ZN	D5	101	1/1	1.00	0.10	84,84,84,84	0
56	MG	DA	3072	1/1	1.00	0.20	86,86,86,86	0
56	MG	DA	3073	1/1	1.00	0.16	40,40,40,40	0
56	MG	DA	3036	1/1	1.00	0.18	32,32,32,32	0
56	MG	DA	3075	1/1	1.00	0.18	25,25,25,25	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(Å^2)	Q<0.9
56	MG	DA	3058	1/1	1.00	0.09	66,66,66,66	0
56	MG	DA	3100	1/1	1.00	0.20	34,34,34,34	0
56	MG	DA	3046	1/1	1.00	0.18	27,27,27,27	0
56	MG	DA	3037	1/1	1.00	0.16	13,13,13,13	0
56	MG	DA	3011	1/1	1.00	0.10	23,23,23,23	0
56	MG	DA	3104	1/1	1.00	0.22	43,43,43,43	0
56	MG	DA	3049	1/1	1.00	0.13	52,52,52,52	0
56	MG	DA	3039	1/1	1.00	0.11	34,34,34,34	0
56	MG	DA	3230	1/1	1.00	0.13	76,76,76,76	0
56	MG	DA	3064	1/1	1.00	0.14	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.