



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 01:10 PM EDT

PDB ID : 5IT8 / pdb_00005it8
Title : High-resolution structure of the Escherichia coli ribosome
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-03-16
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

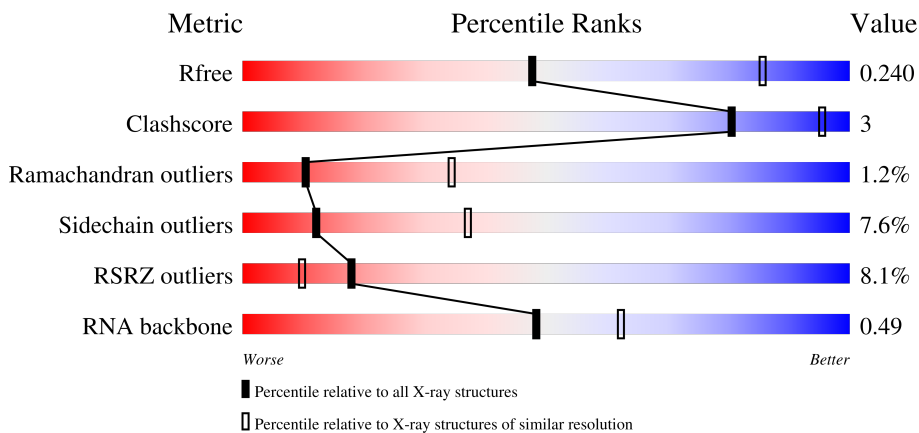
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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.














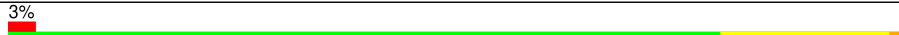

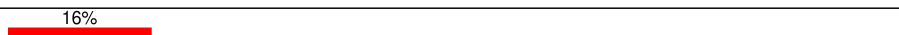
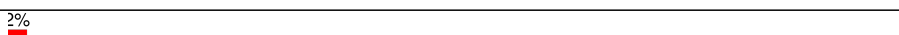
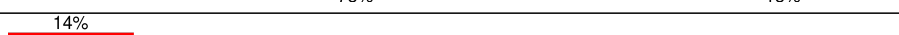

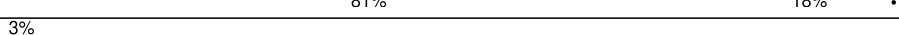







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	 5% 74% 23%
1	BA	1534	 5% 74% 23%
2	AB	224	 3% 82% 16%
2	BB	224	 4% 81% 17%




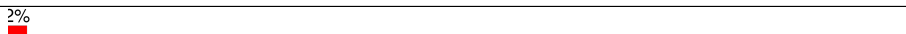
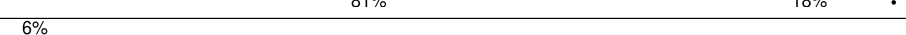
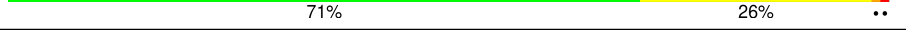



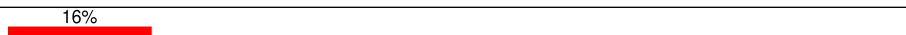
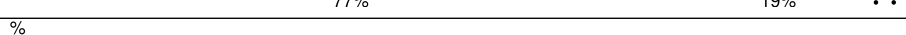




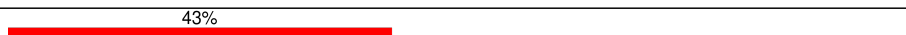






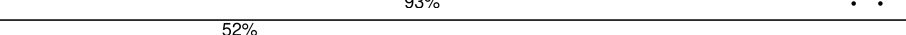
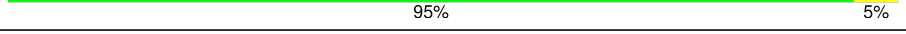

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Mol	Chain	Length	Quality of chain
3	AC	206	 85% 13% .
3	BC	206	 81% 17% .
4	AD	205	 88% 11% .
4	BD	205	 86% 14%
5	AE	155	 72% 23% 6%
5	BE	155	 67% 24% 5% . .
6	AF	106	 81% 18% .
6	BF	106	 69% 24% . . 6%
7	AG	151	 74% 23% .
7	BG	151	 15% 76% 23% .
8	AH	129	 2% 78% 20% .
8	BH	129	 3% 80% 19% .
9	AI	127	 4% 87% 12% .
9	BI	127	 16% 87% 13% .
10	AJ	99	 2% 78% 18% . .
10	BJ	99	 14% 73% 21% . . .
11	AK	117	 % 81% 18% .
11	BK	117	 3% 79% 20% .
12	AL	123	 % 82% 17% .
12	BL	123	 3% 80% 19% .
13	AM	114	 3% 78% 20% .
13	BM	114	 8% 76% 19% . .
14	AN	100	 3% 85% 14% .
14	BN	100	 16% 85% 14% .
15	AO	88	 93% 6% .


























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Mol	Chain	Length	Quality of chain
15	BO	88	 88% 13%
16	AP	82	 85% 15% 2%
16	BP	82	 78% 21% 16%
17	AQ	80	 81% 18% 2%
17	BQ	80	 71% 26% 6%
18	AR	55	 84% 15% 4%
18	BR	55	 91% 9% 4%
19	AS	79	 77% 19% 5%
19	BS	79	 77% 19% 16%
20	AT	86	 87% 10% 2%
20	BT	86	 74% 19% 19%
21	AU	56	 75% 25% 16%
21	BU	56	 75% 25% 4%
22	C1	56	 77% 20% 43%
22	D1	56	 75% 23% 4%
23	C2	51	 75% 24% 18%
23	D2	51	 80% 20% 4%
24	C3	46	 87% 11% 54%
24	D3	46	 93% 5% 2%
25	C4	64	 95% 5% 52%
25	D4	64	 92% 8% 4%
26	C5	38	 89% 11% 37%
26	D5	38	 95% 5% 4%
27	C0	58	 76% 22% 28%
27	D0	58	 84% 16% 3%


























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Mol	Chain	Length	Quality of chain
28	CB	120	 86% 12%
28	DB	120	 85% 14%
29	CC	271	 15% 83% 15%
29	DC	271	 86% 13%
30	CD	209	 28% 86% 13%
31	CA	2904	 16% 70% 27%
32	DD	209	 87% 11%
33	DA	2903	 2% 75% 22%
34	CE	201	 35% 80% 18%
34	DE	201	 86% 14%
35	CF	177	 6% 77% 19%
35	DF	177	 76% 22%
36	CG	176	 7% 89% 10%
36	DG	176	 90% 10%
37	CH	149	 3% 79% 19%
37	DH	149	 80% 19%
38	CJ	134	 19% 84% 13%
38	DJ	134	 19% 84% 13%
39	CK	142	 33% 85% 14%
39	DK	142	 91% 9%
40	CL	123	 8% 80% 17%
40	DL	123	 81% 17%
41	CM	144	 40% 74% 22%
41	DM	144	 88% 12%
42	CN	136	 15% 84% 13%

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Mol	Chain	Length	Quality of chain
42	DN	136	 87% 12%
43	CO	125	 34% 77% 17%
43	DO	125	 87% 11%
44	CP	117	 16% 83% 15%
44	DP	117	 86% 11%
45	CQ	114	 17% 88% 11%
45	DQ	114	 88% 11%
46	CR	117	 44% 86% 14%
46	DR	117	 88% 11%
47	CS	103	 31% 83% 14%
47	DS	103	 87% 12%
48	CT	110	 41% 79% 19%
48	DT	110	 79% 21%
49	CU	93	 31% 82% 14%
49	DU	93	 85% 15%
50	CV	102	 40% 79% 18%
50	DV	102	 84% 14%
51	CW	94	 6% 86% 14%
51	DW	94	 2% 87% 13%
52	CX	76	 17% 92% 7%
52	DX	76	 84% 14%
53	CY	77	 26% 78% 22%
53	DY	77	 90% 10%
54	CZ	62	 35% 85% 13%
54	DZ	62	 85% 15%

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Mol	Chain	Length	Quality of chain
55	DI	135	

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
56	MG	AA	1606	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3115	-	-	-	X
66	ACY	DA	3194	-	X	-	-

2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 295125 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
			Total	C	N	O	P			
1	AA	1534	Total 32930	C 14694	N 6041	O 10661	P 1534	0	0	0
1	BA	1533	Total 32908	C 14684	N 6036	O 10655	P 1533	0	0	0

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

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

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

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

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

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

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BJ	98	787	493	150	143	1	0	0	0

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	714	439	144	130	1	0	0	0
15	BO	88	714	439	144	130	1	0	0	0

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

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

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

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

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

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0
19	BS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AT	86	Total 670	C 414	N 138	O 115	S 3	0	0	0
20	BT	85	Total 665	C 411	N 137	O 114	S 3	0	0	0

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	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 RNA chain called 23S rRNA.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
35	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L11.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
42	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 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
49	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	CV	102	Total	C	N	O	0	0	0
			780	492	146	142			
50	DV	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

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

- Molecule 55 is a protein called 50S ribosomal protein L10.

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

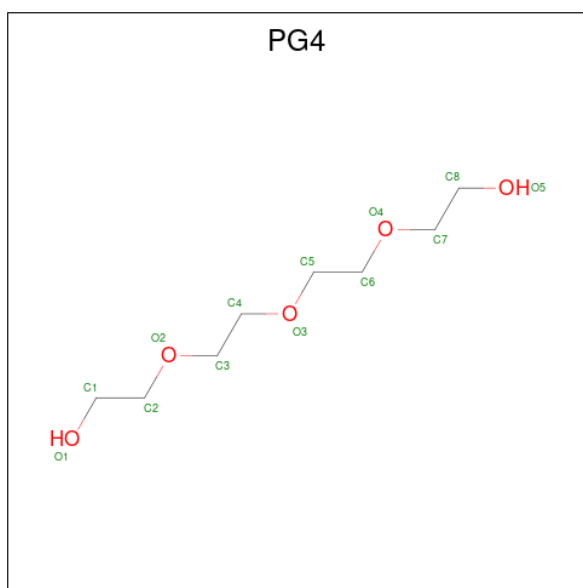
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

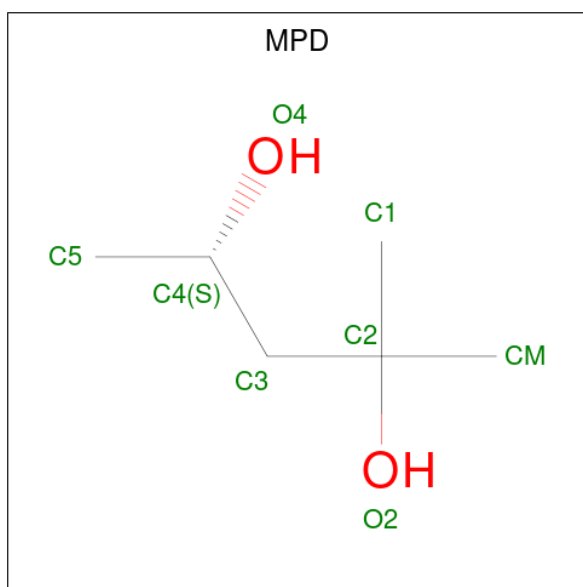
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	2	Total	Mg	0	0
			2	2		
56	DA	183	Total	Mg	0	0
			183	183		
56	DR	2	Total	Mg	0	0
			2	2		

- Molecule 57 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



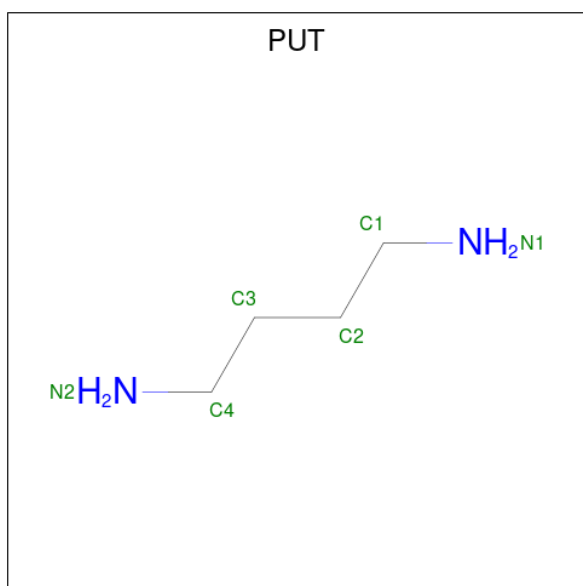
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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	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
58	DA	1	Total C O 8 6 2	0	0
58	DA	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

- Molecule 59 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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	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
59	DA	1	Total C N 6 4 2	0	0

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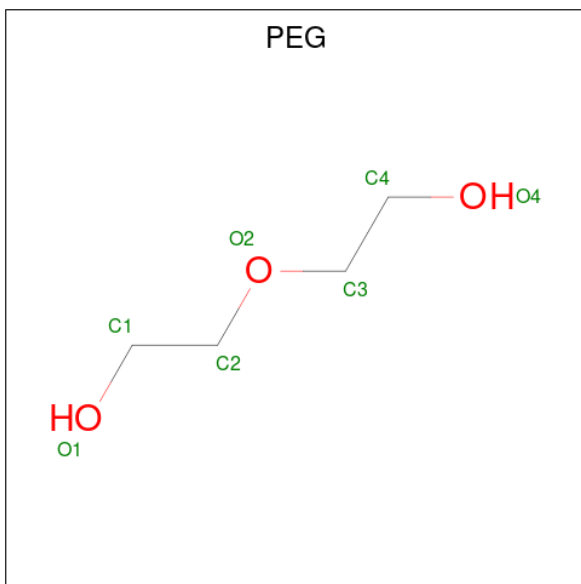
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



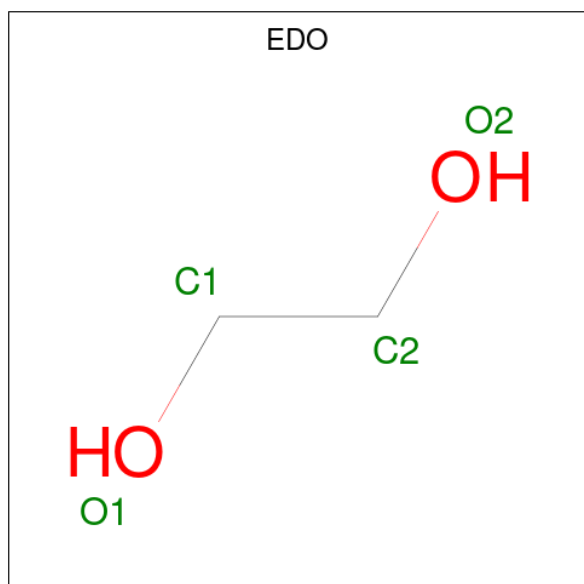
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 62 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



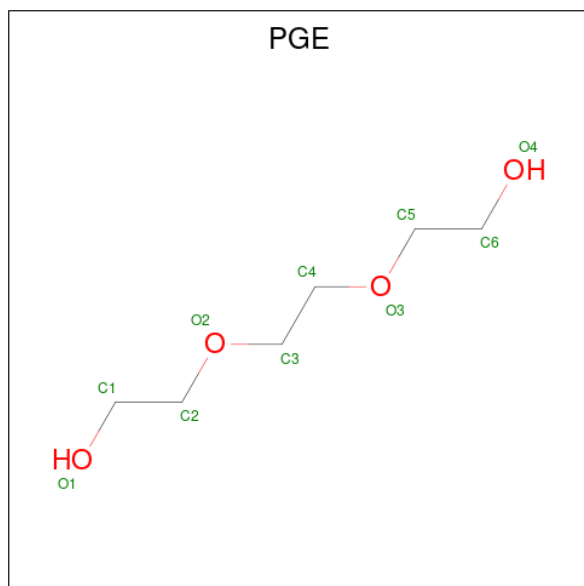
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	D1	1	Total C O 4 2 2	0	0
62	D0	1	Total C O 4 2 2	0	0
62	DB	1	Total C O 4 2 2	0	0

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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 (CCD ID: PGE) (formula: C₆H₁₄O₄).



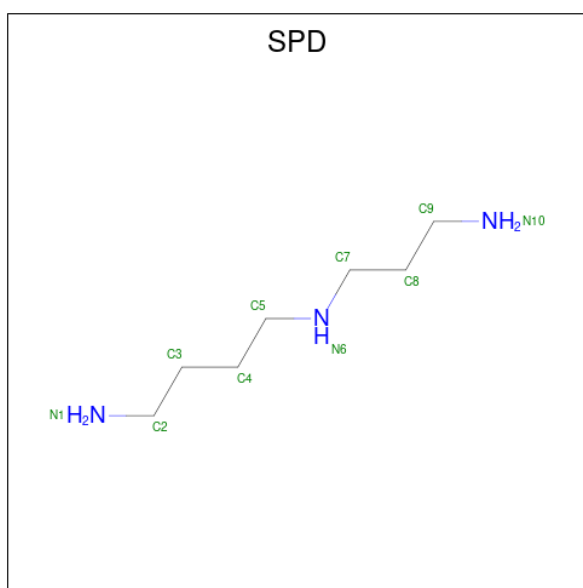
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	D3	1	Total C O 10 6 4	0	0
63	DD	1	Total C O 10 6 4	0	0

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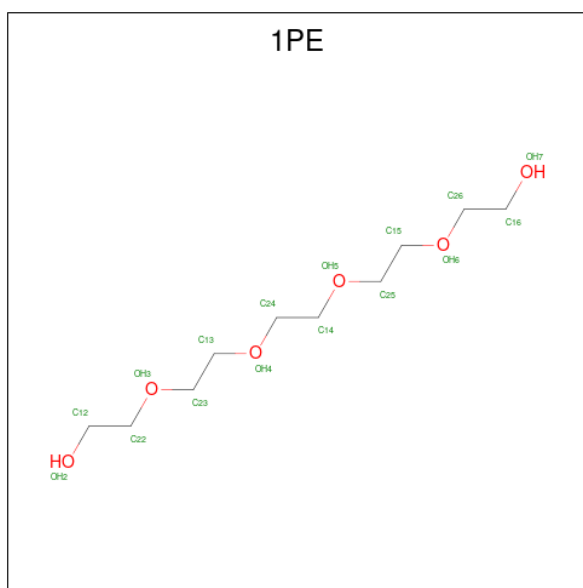
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DT	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0

- Molecule 64 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



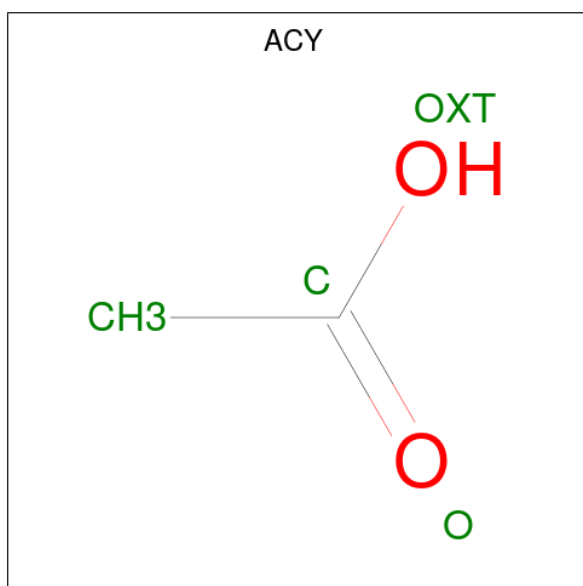
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

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



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

- Molecule 66 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



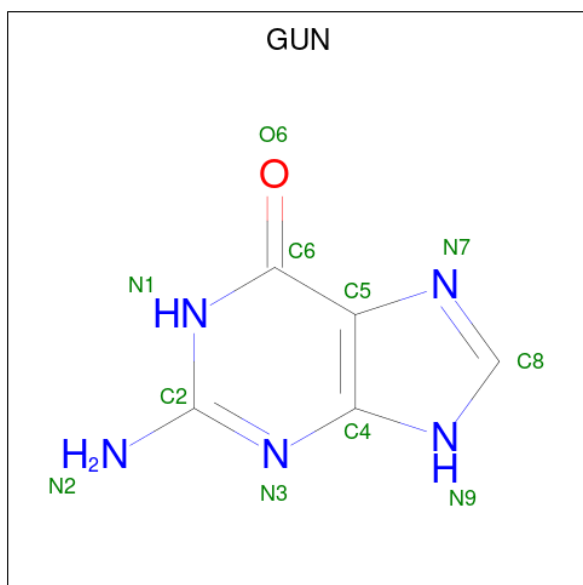
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
66	DA	1	Total	C O	0	0
			4	2 2		

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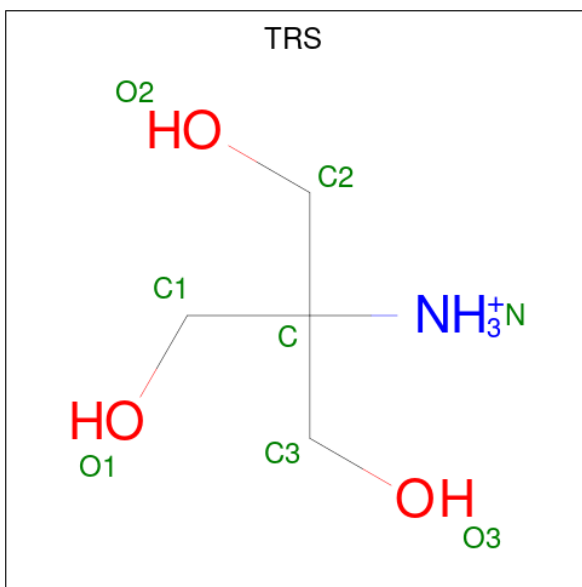
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



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

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	3	Total	O	0	0
			3	3		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	2	Total	O	0	0
			2	2		
69	AK	7	Total	O	0	0
			7	7		
69	AL	10	Total	O	0	0
			10	10		
69	AM	4	Total	O	0	0
			4	4		
69	AN	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	AO	2	Total O 2 2	0	0
69	AP	2	Total O 2 2	0	0
69	AR	1	Total O 1 1	0	0
69	AS	1	Total O 1 1	0	0
69	AT	3	Total O 3 3	0	0
69	AU	3	Total O 3 3	0	0
69	C3	3	Total O 3 3	0	0
69	C4	1	Total O 1 1	0	0
69	C5	1	Total O 1 1	0	0
69	BA	291	Total O 291 291	0	0
69	BD	11	Total O 11 11	0	0
69	BE	1	Total O 1 1	0	0
69	BF	1	Total O 1 1	0	0
69	BK	2	Total O 2 2	0	0
69	BL	2	Total O 2 2	0	0
69	BN	2	Total O 2 2	0	0
69	BO	1	Total O 1 1	0	0
69	BP	3	Total O 3 3	0	0
69	BR	1	Total O 1 1	0	0
69	BT	4	Total O 4 4	0	0
69	BU	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	28	Total 28	O 28	0	0
69	D4	39	Total 39	O 39	0	0
69	D5	9	Total 9	O 9	0	0
69	D0	21	Total 21	O 21	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	6	Total 6	O 6	0	0
69	CA	692	Total 692	O 692	0	0
69	DB	199	Total 199	O 199	0	0
69	DC	98	Total 98	O 98	0	0
69	DD	95	Total 95	O 95	0	0
69	DA	4834	Total 4834	O 4834	0	0
69	CE	7	Total 7	O 7	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0

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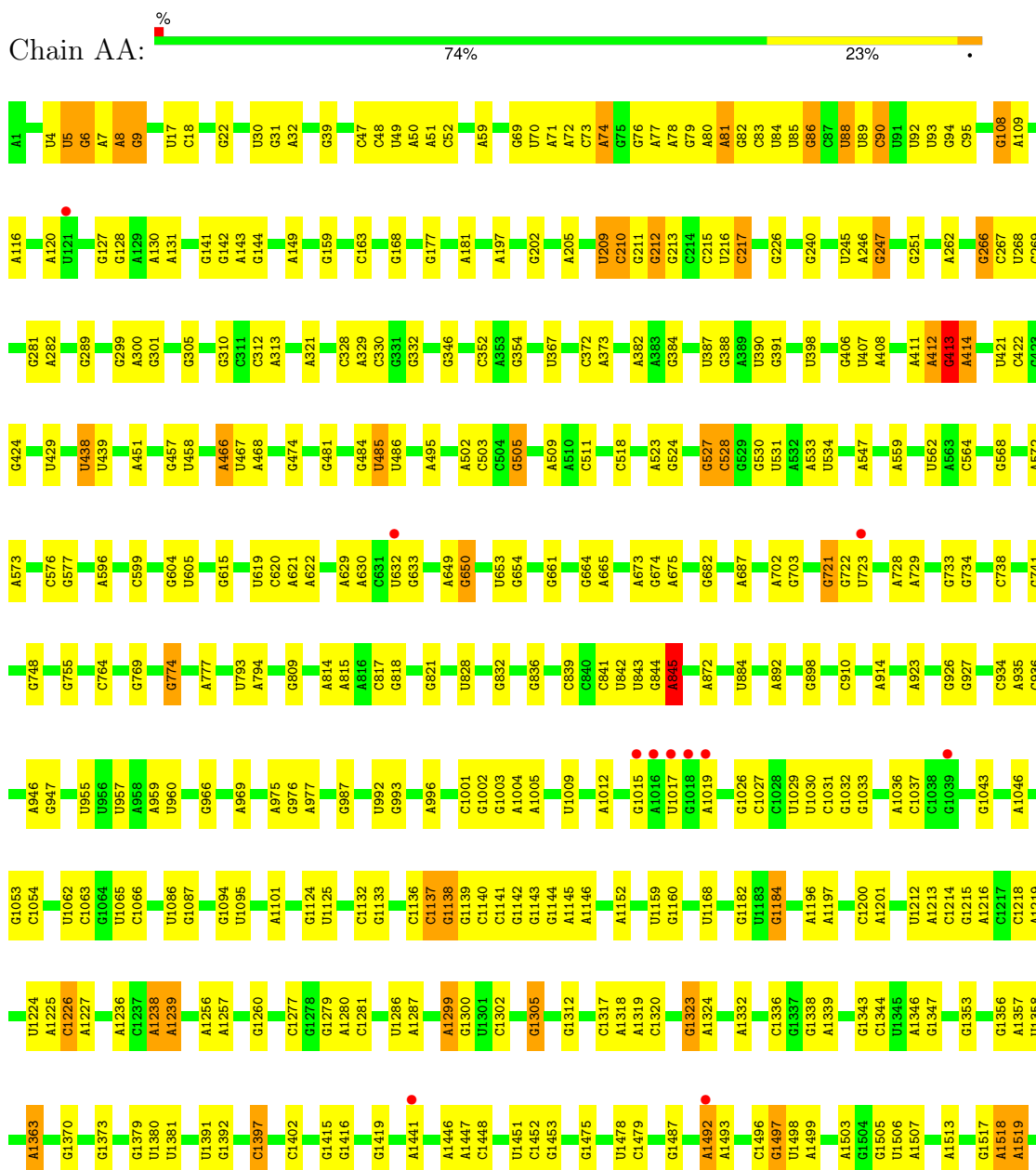
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CY	1	Total 1	O 1	0	0
69	DE	63	Total 63	O 63	0	0
69	DF	15	Total 15	O 15	0	0
69	DG	7	Total 7	O 7	0	0
69	DH	1	Total 1	O 1	0	0
69	DK	65	Total 65	O 65	0	0
69	DL	52	Total 52	O 52	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	64	Total 64	O 64	0	0
69	DO	48	Total 48	O 48	0	0
69	DP	44	Total 44	O 44	0	0
69	DQ	33	Total 33	O 33	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	48	Total 48	O 48	0	0
69	DT	62	Total 62	O 62	0	0
69	DU	22	Total 22	O 22	0	0
69	DV	18	Total 18	O 18	0	0
69	DW	34	Total 34	O 34	0	0
69	DX	31	Total 31	O 31	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	5	Total 5	O 5	0	0

3 Residue-property plots [i](#)

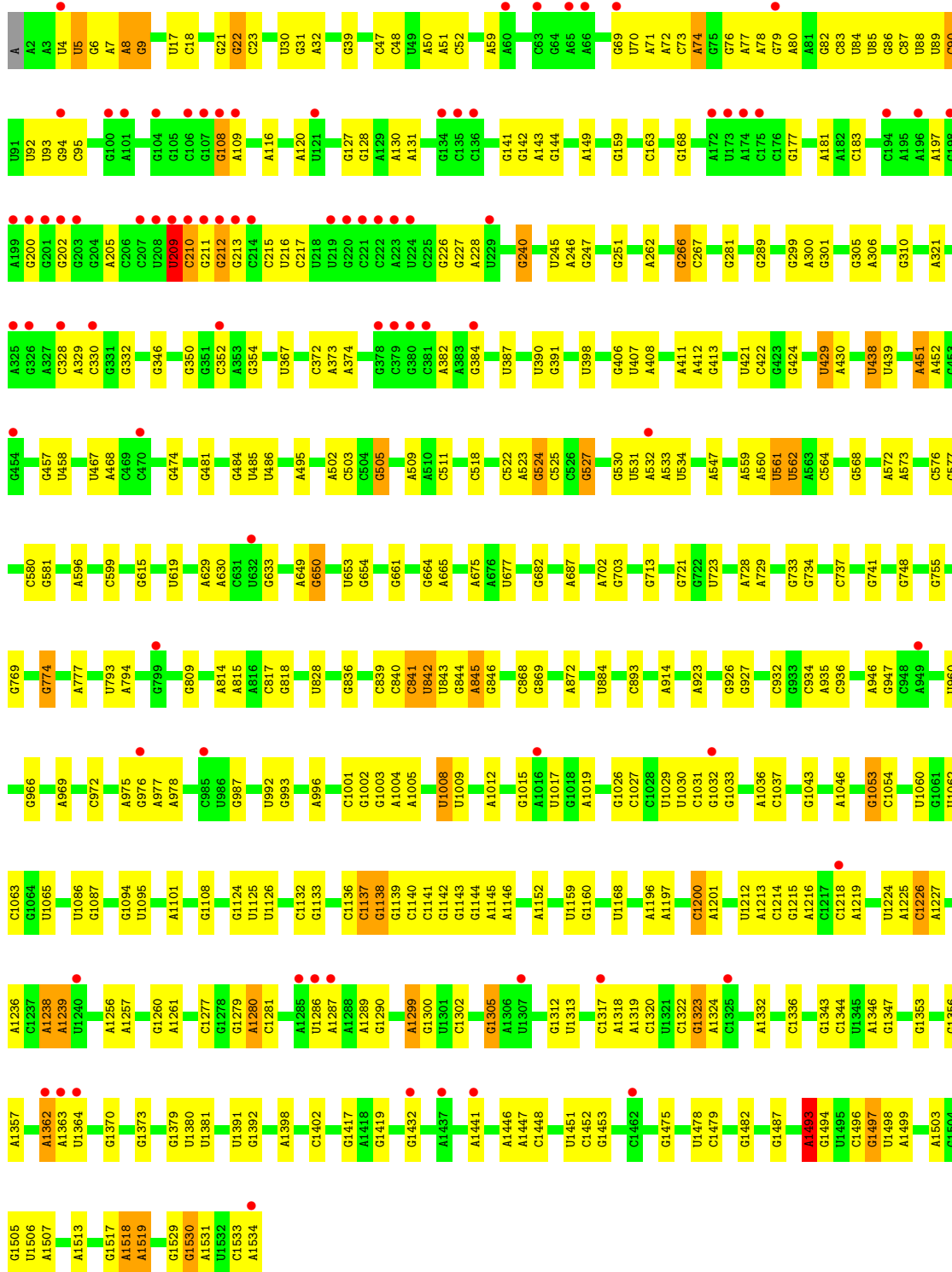
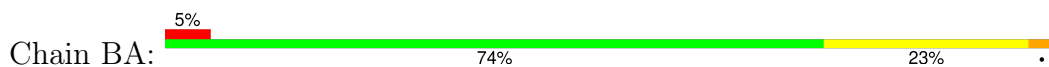
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

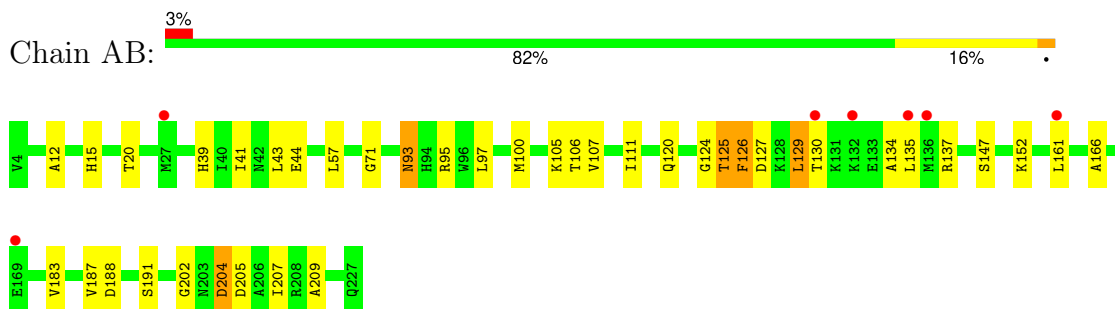


G1529
G1530
A1531
U1532
C1533
A1534

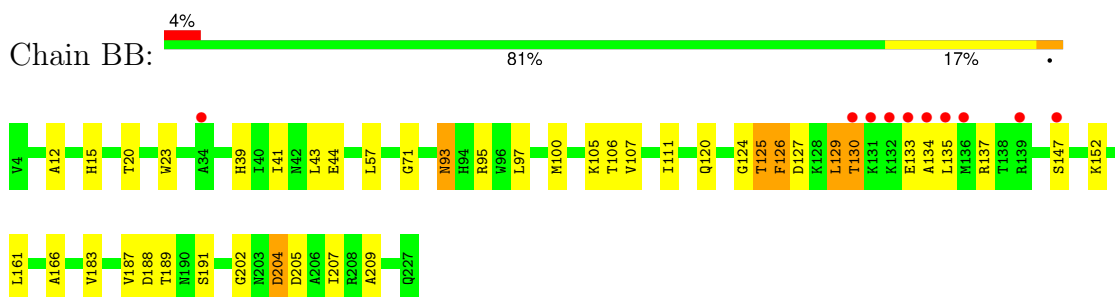
● Molecule 1: 16S rRNA



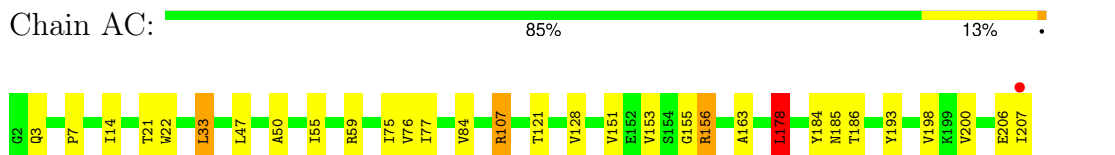
- Molecule 2: 30S ribosomal protein S2



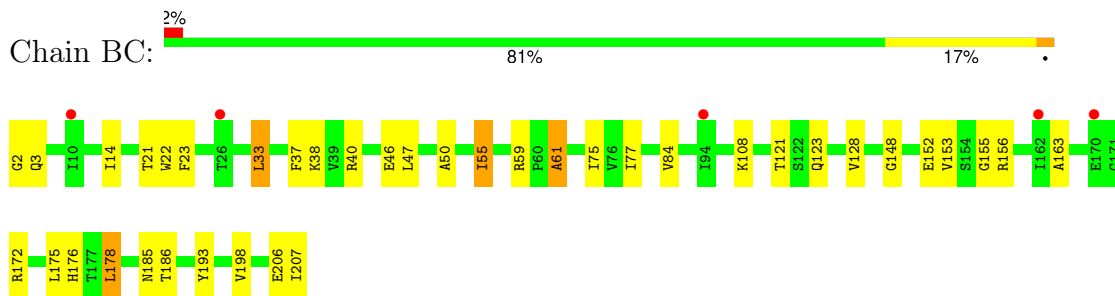
- Molecule 2: 30S ribosomal protein S2



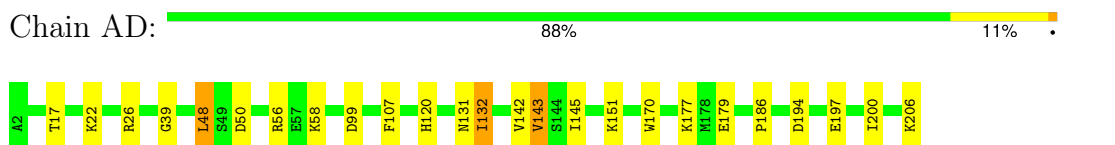
- Molecule 3: 30S ribosomal protein S3



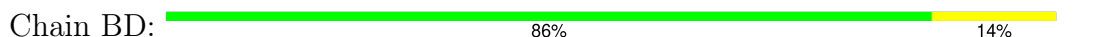
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

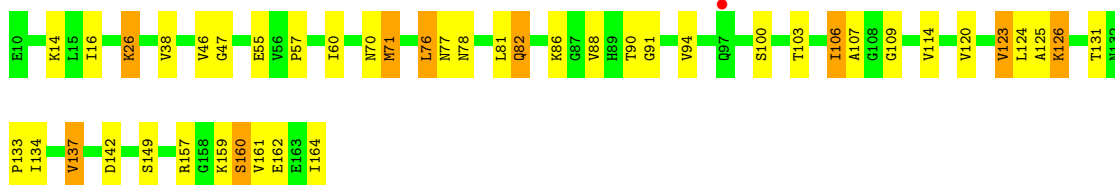


- Molecule 4: 30S ribosomal protein S4

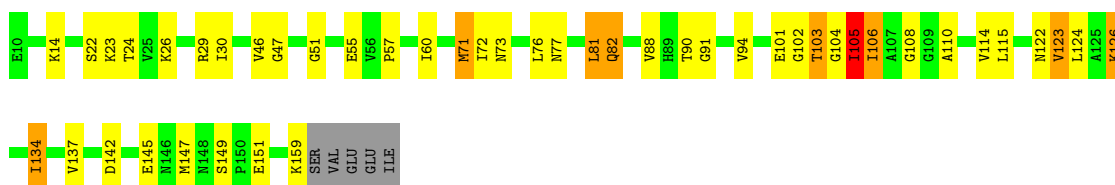




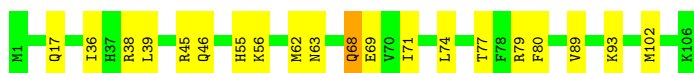
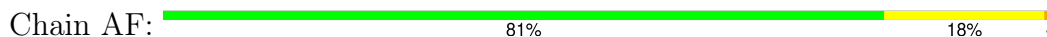
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



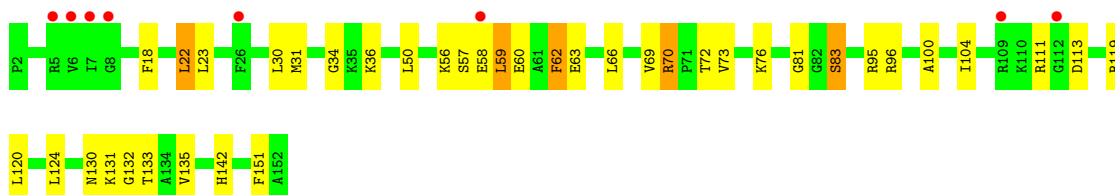
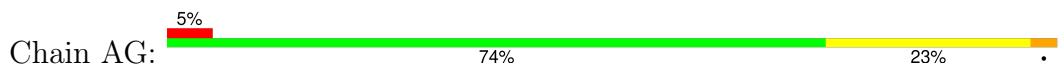
- Molecule 6: 30S ribosomal protein S6



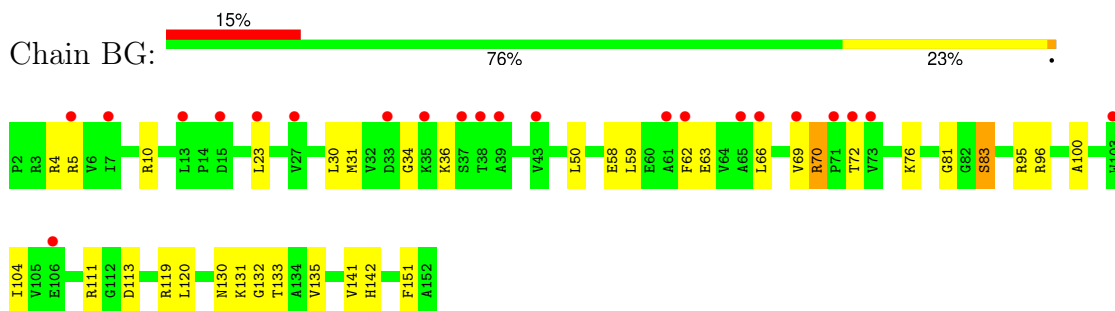
- Molecule 6: 30S ribosomal protein S6



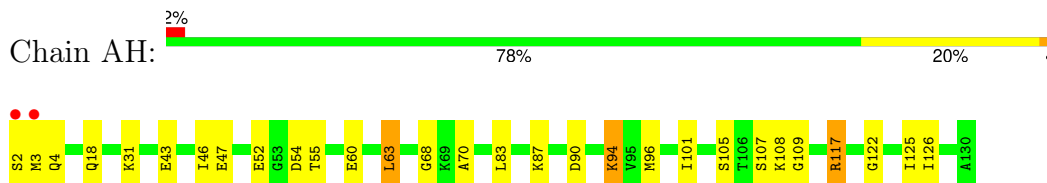
- Molecule 7: 30S ribosomal protein S7



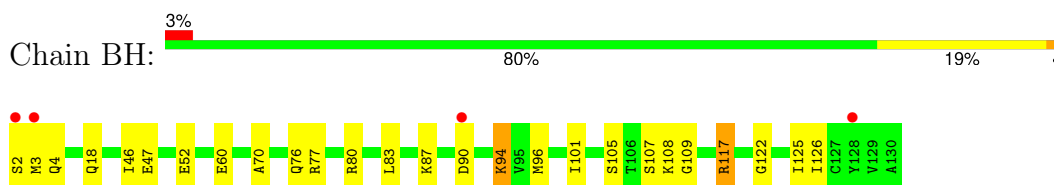
- Molecule 7: 30S ribosomal protein S7



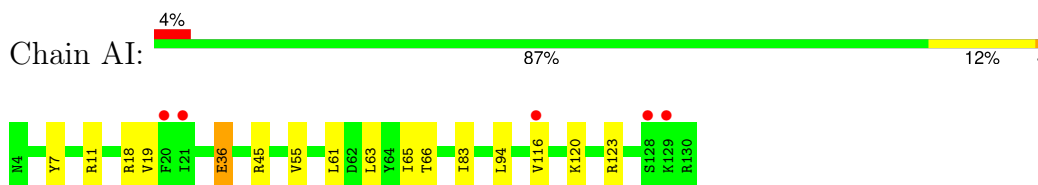
- Molecule 8: 30S ribosomal protein S8



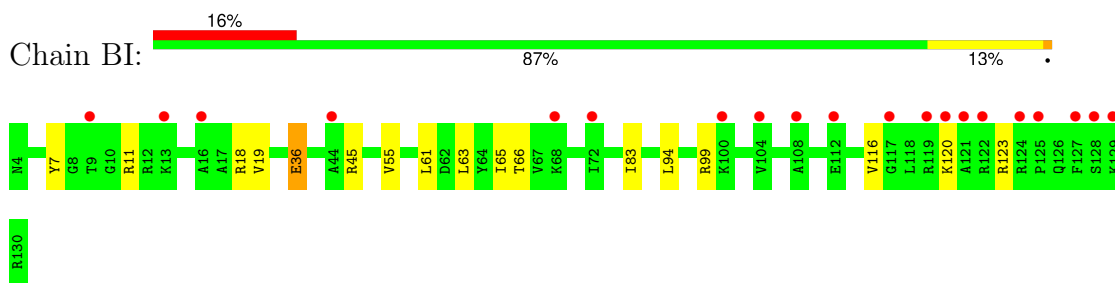
- Molecule 8: 30S ribosomal protein S8



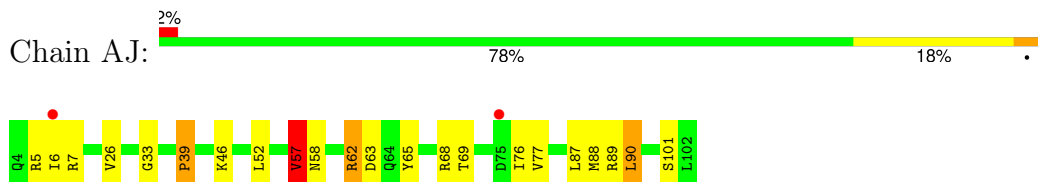
- Molecule 9: 30S ribosomal protein S9



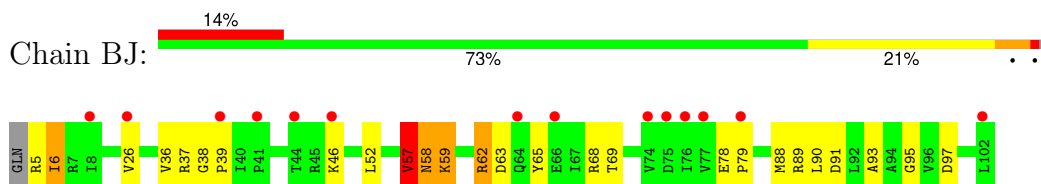
- Molecule 9: 30S ribosomal protein S9



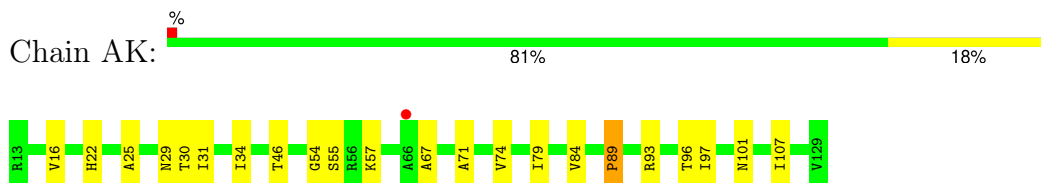
- Molecule 10: 30S ribosomal protein S10



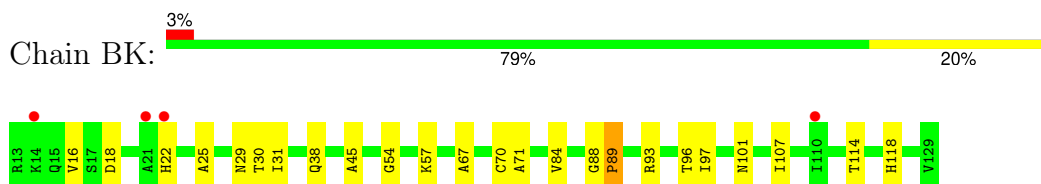
- Molecule 10: 30S ribosomal protein S10



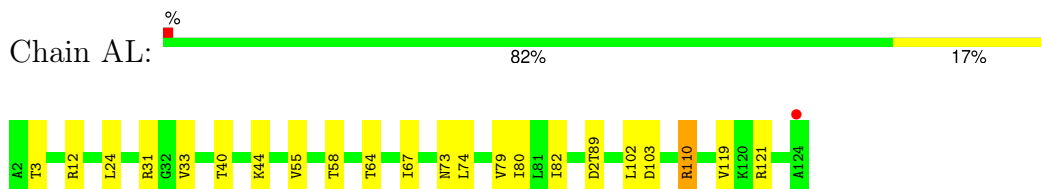
- Molecule 11: 30S ribosomal protein S11



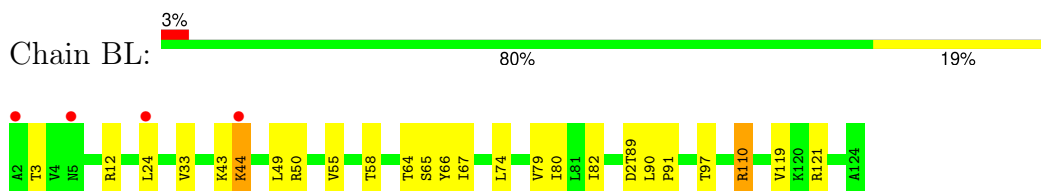
- Molecule 11: 30S ribosomal protein S11



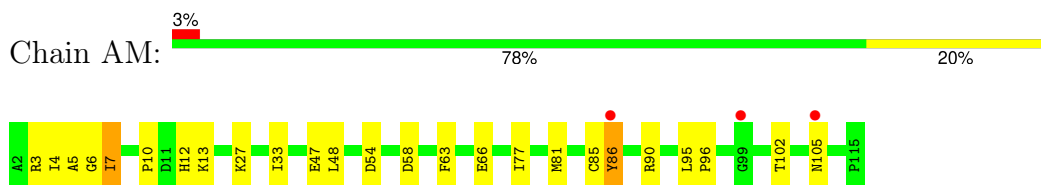
- Molecule 12: 30S ribosomal protein S12



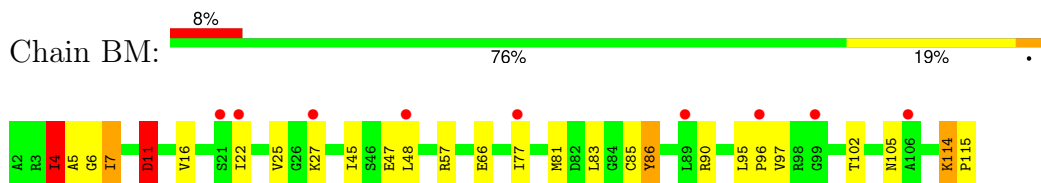
- Molecule 12: 30S ribosomal protein S12



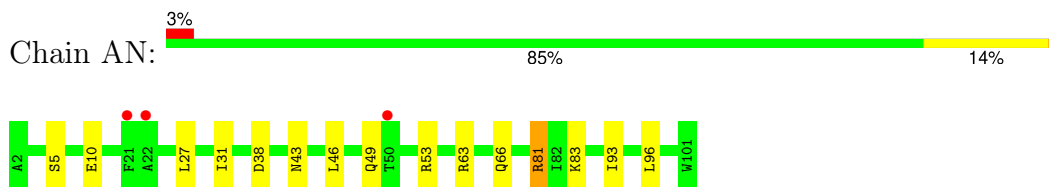
- Molecule 13: 30S ribosomal protein S13



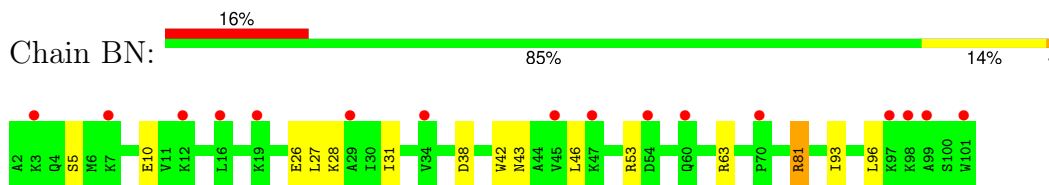
- Molecule 13: 30S ribosomal protein S13



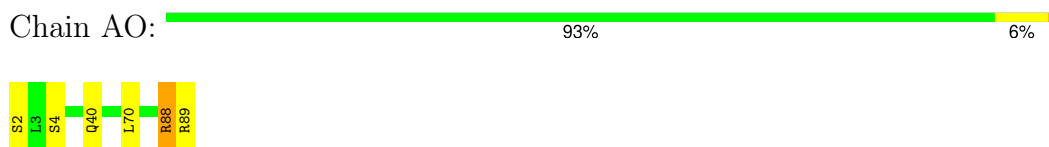
- Molecule 14: 30S ribosomal protein S14



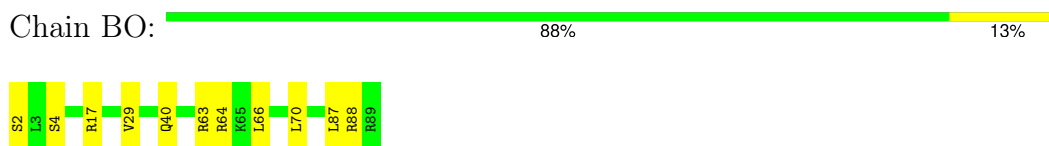
- Molecule 14: 30S ribosomal protein S14



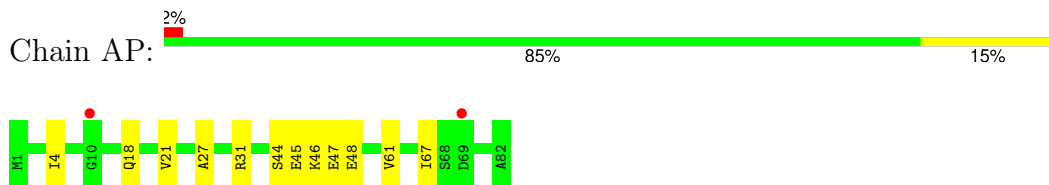
- Molecule 15: 30S ribosomal protein S15



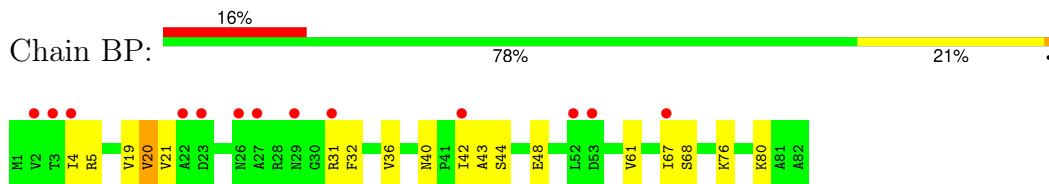
- Molecule 15: 30S ribosomal protein S15



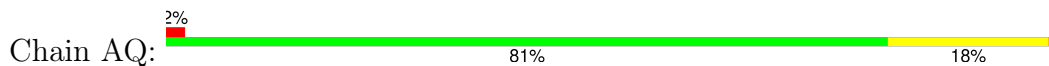
- Molecule 16: 30S ribosomal protein S16

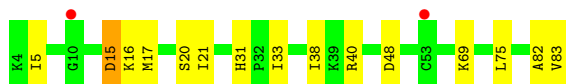


- Molecule 16: 30S ribosomal protein S16

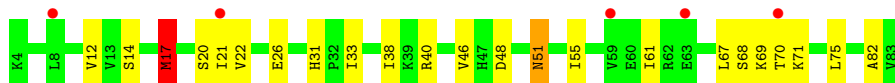
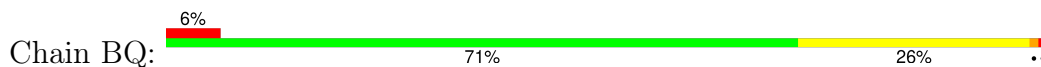


- Molecule 17: 30S ribosomal protein S17

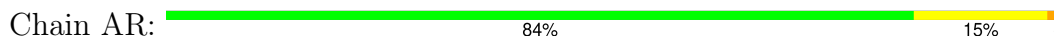




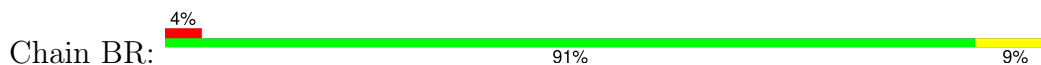
- Molecule 17: 30S ribosomal protein S17



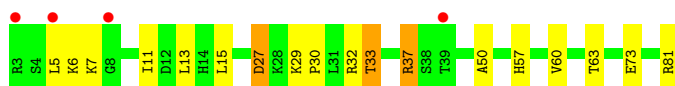
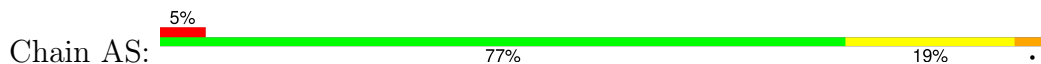
- Molecule 18: 30S ribosomal protein S18



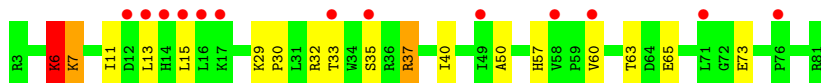
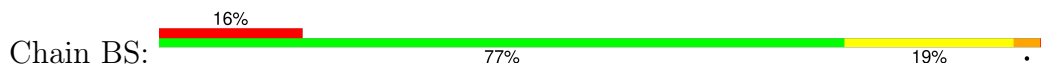
- Molecule 18: 30S ribosomal protein S18



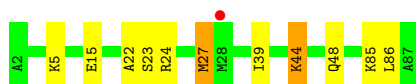
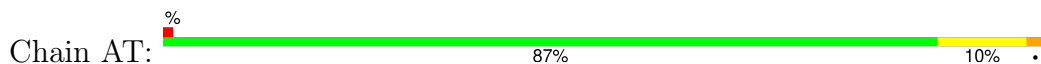
- Molecule 19: 30S ribosomal protein S19



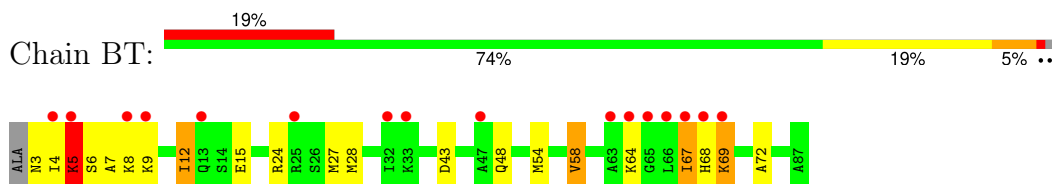
- Molecule 19: 30S ribosomal protein S19



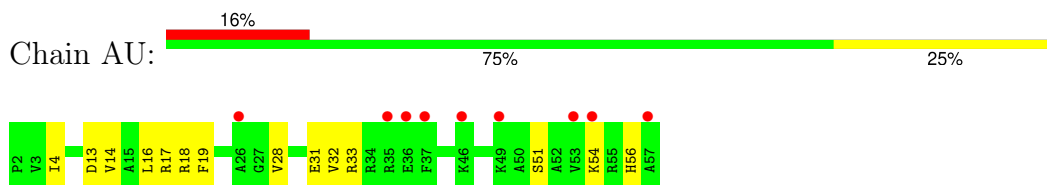
- Molecule 20: 30S ribosomal protein S20



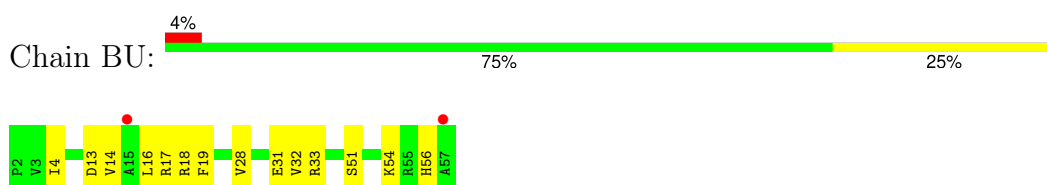
- Molecule 20: 30S ribosomal protein S20



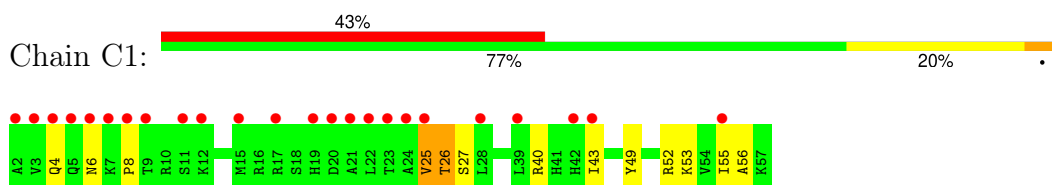
- Molecule 21: 30S ribosomal protein S21



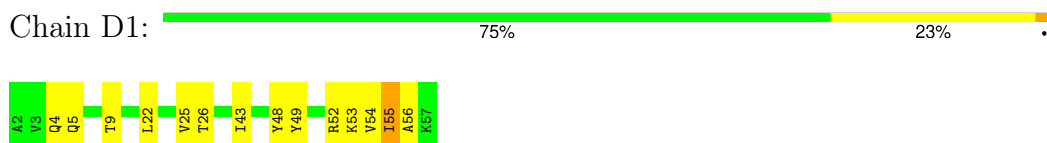
- Molecule 21: 30S ribosomal protein S21



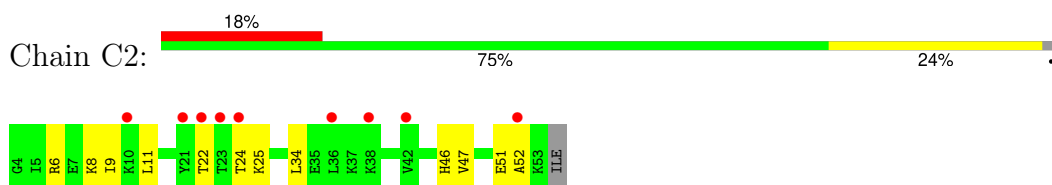
- Molecule 22: 50S ribosomal protein L32



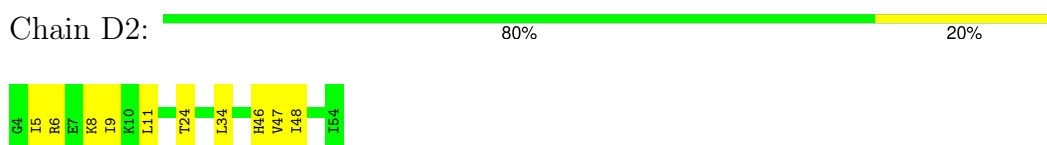
- Molecule 22: 50S ribosomal protein L32



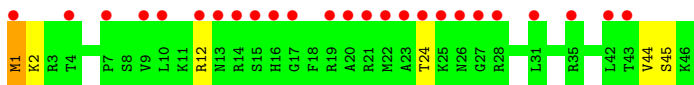
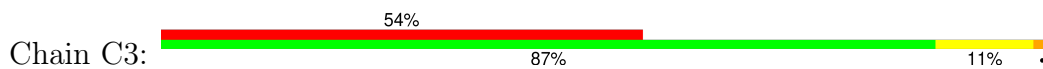
- Molecule 23: 50S ribosomal protein L33



- Molecule 23: 50S ribosomal protein L33



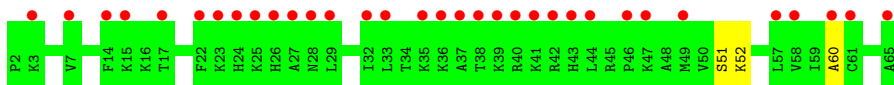
- Molecule 24: 50S ribosomal protein L34



- Molecule 24: 50S ribosomal protein L34



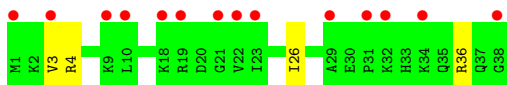
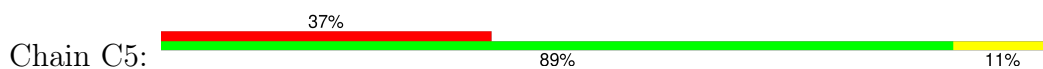
- Molecule 25: 50S ribosomal protein L35



- Molecule 25: 50S ribosomal protein L35



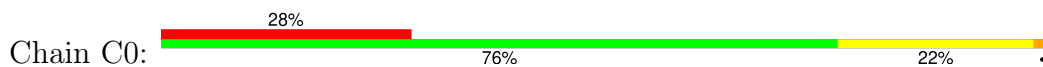
- Molecule 26: 50S ribosomal protein L36



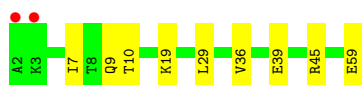
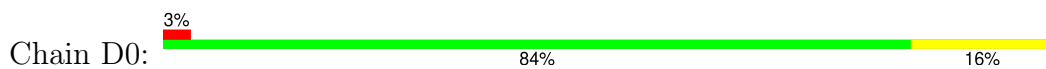
- Molecule 26: 50S ribosomal protein L36



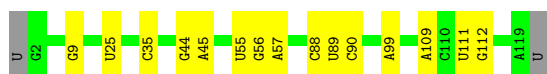
- Molecule 27: 50S ribosomal protein L30



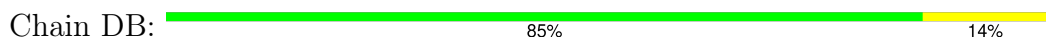
- Molecule 27: 50S ribosomal protein L30



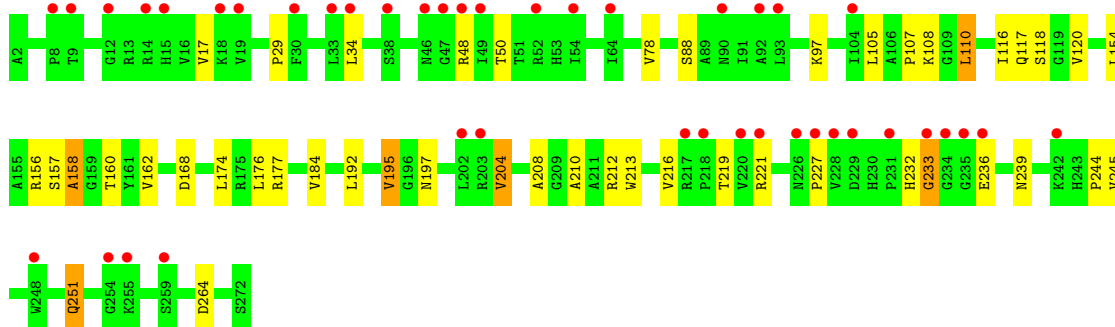
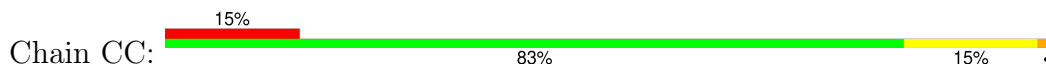
- Molecule 28: 5S rRNA



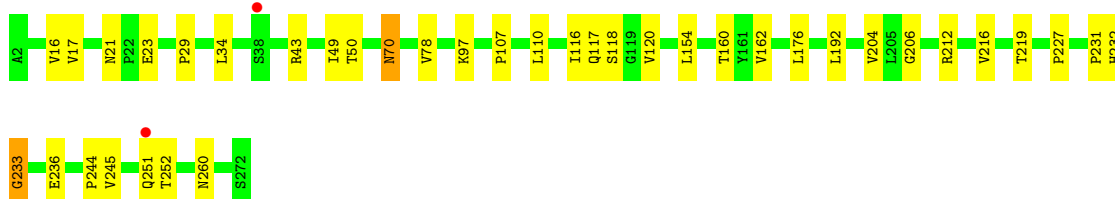
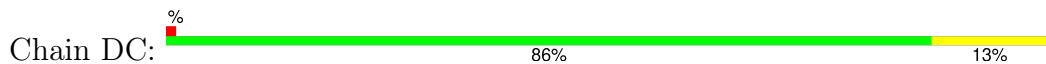
- Molecule 28: 5S rRNA



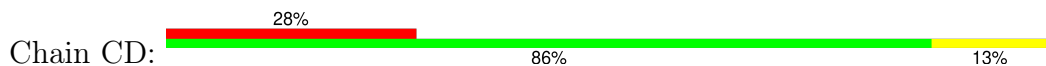
- Molecule 29: 50S ribosomal protein L2

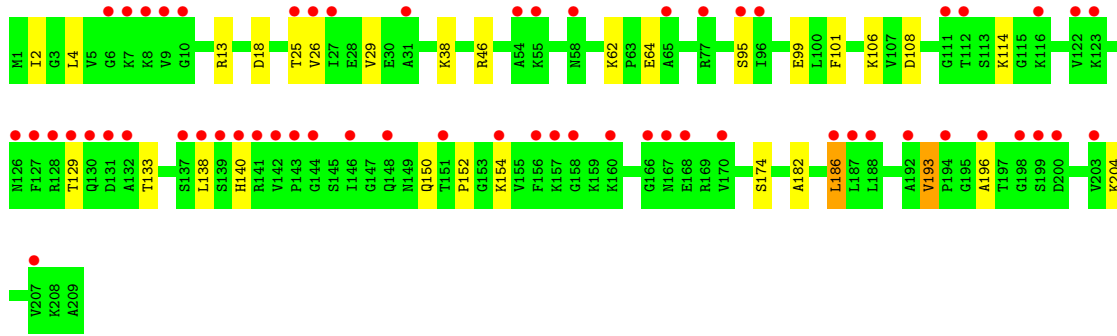


- Molecule 29: 50S ribosomal protein L2

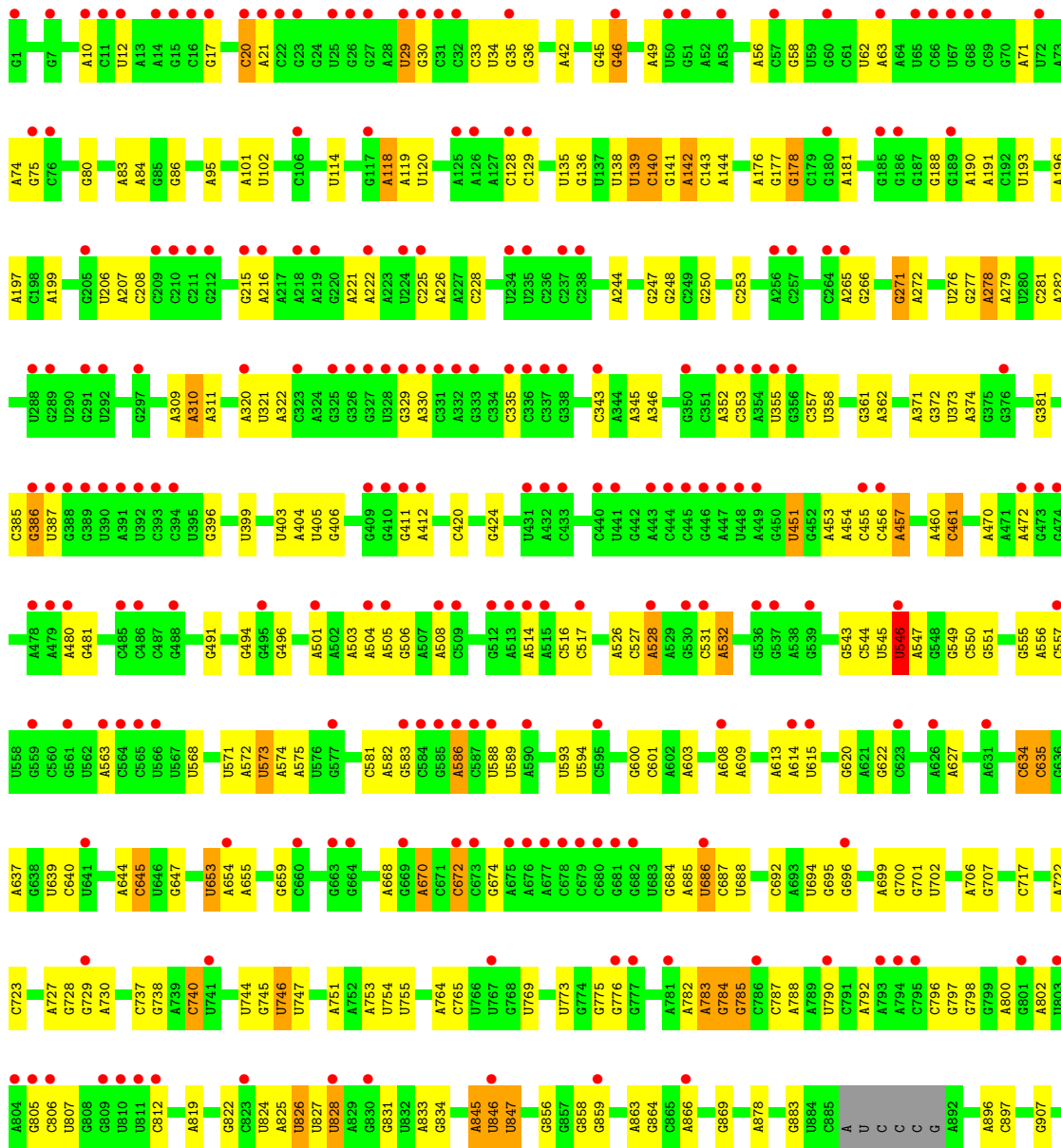


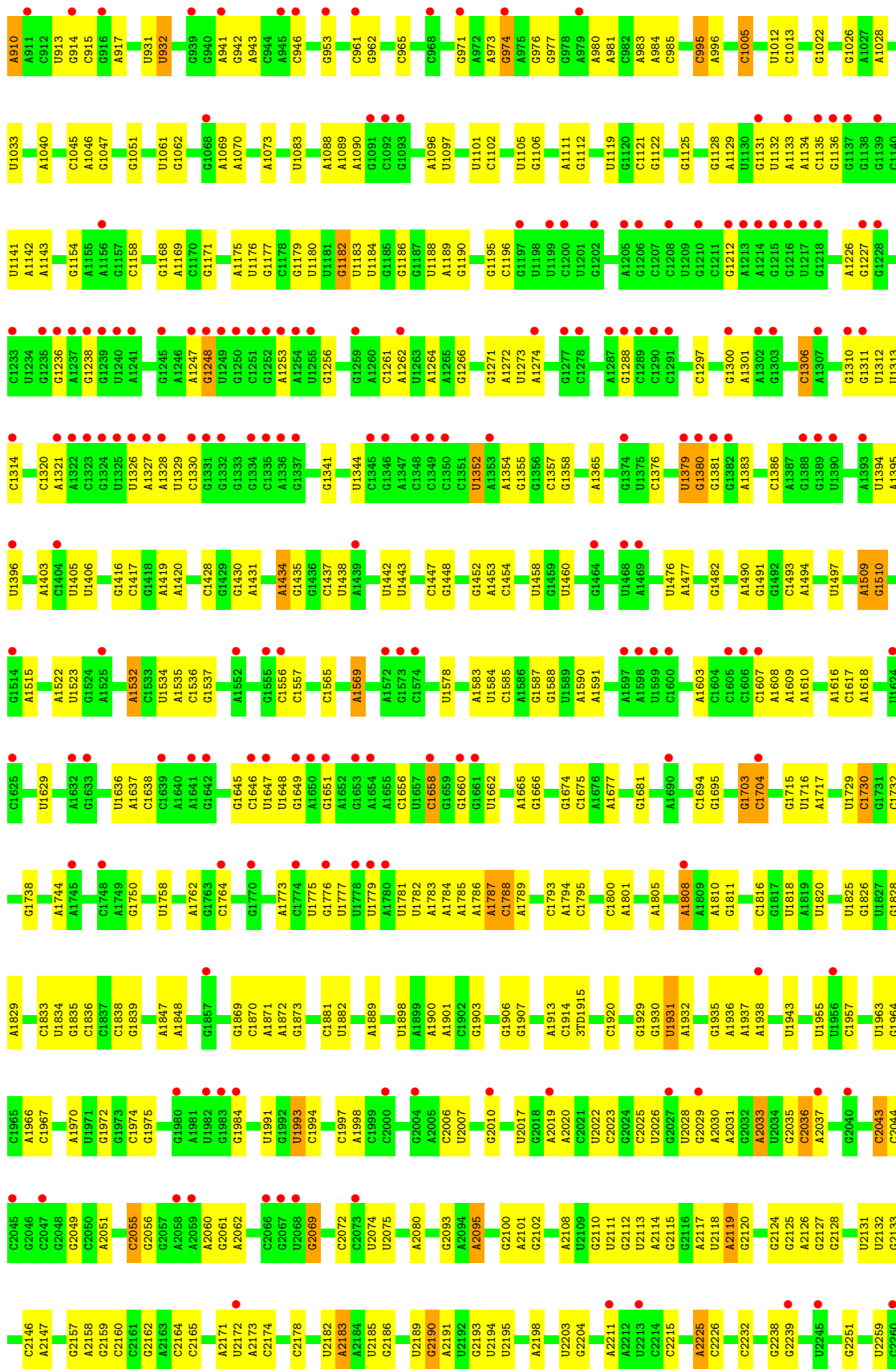
- Molecule 30: 50S ribosomal protein L3

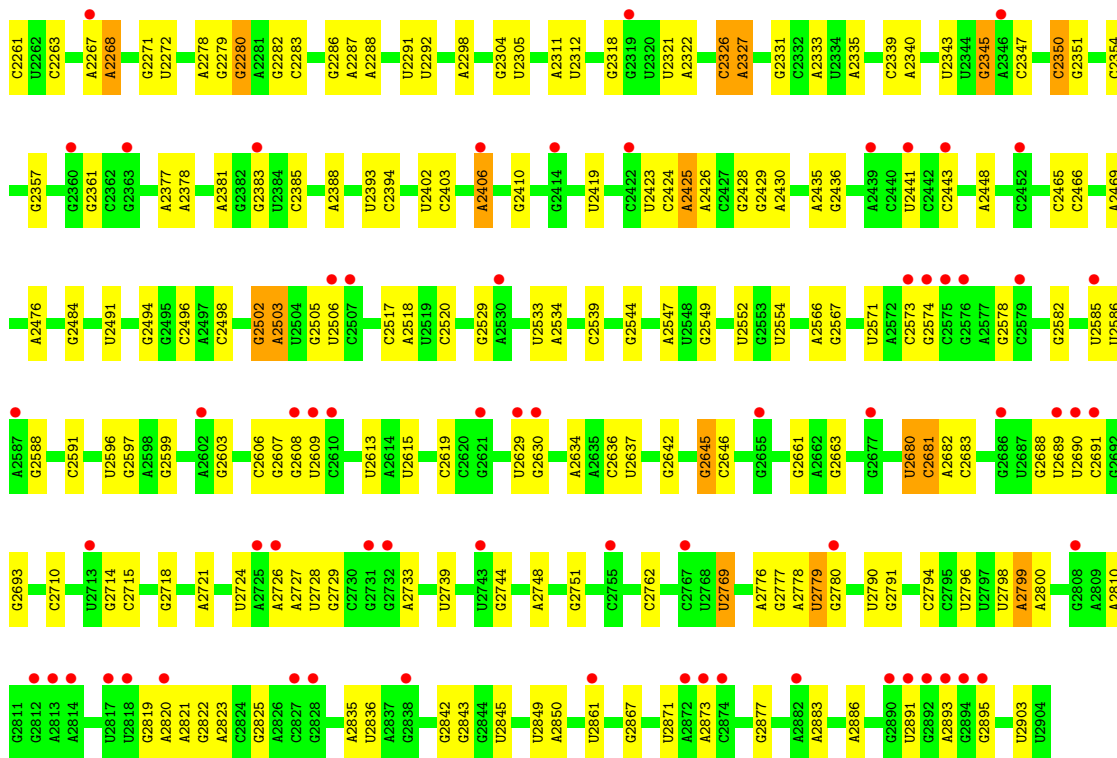




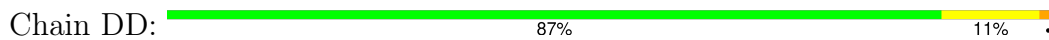
● Molecule 31: 23S rRNA



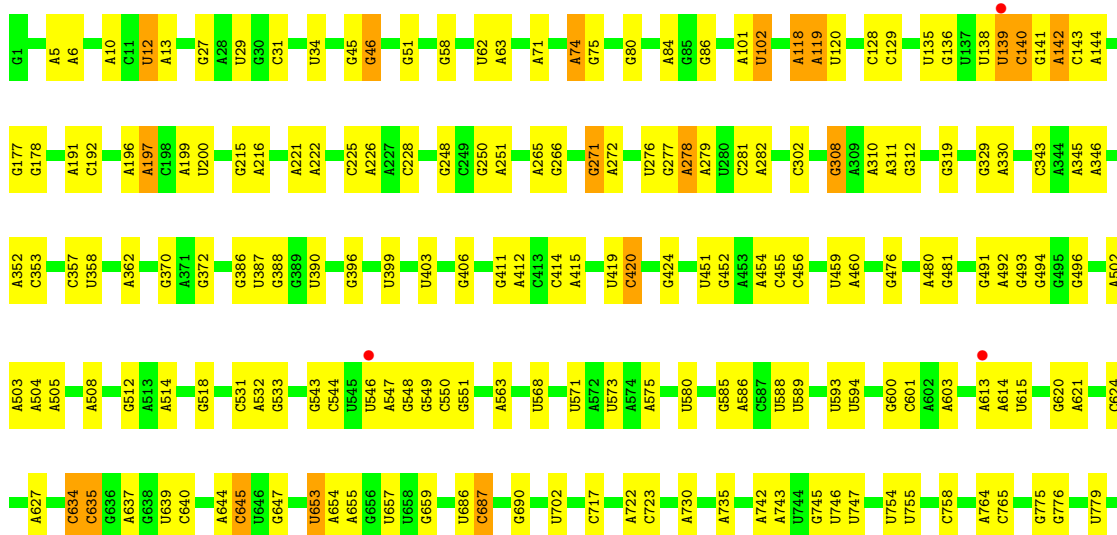
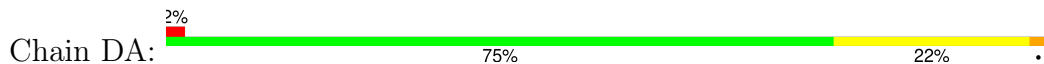


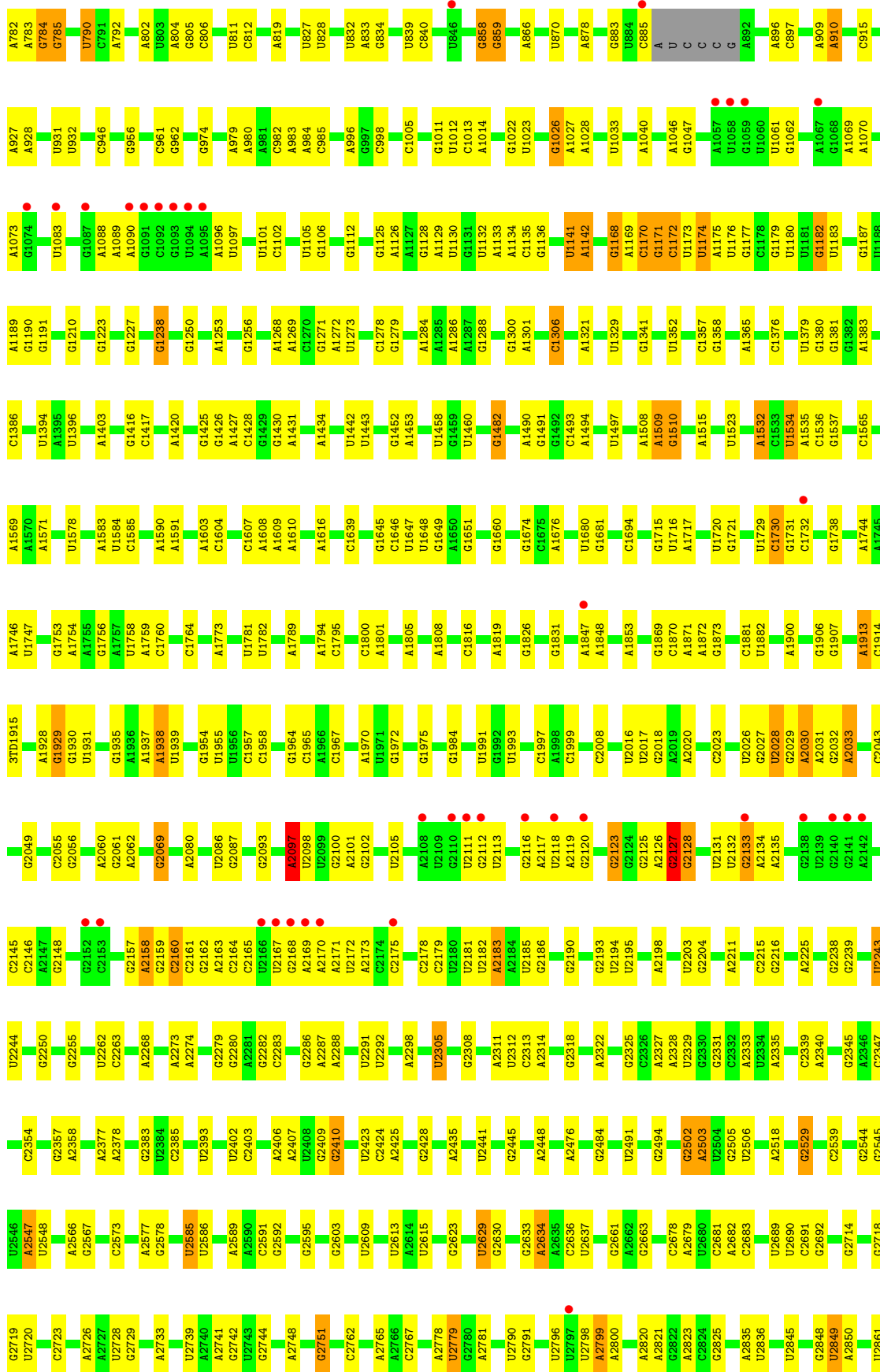


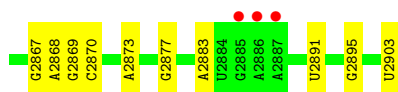
• Molecule 32: 50S ribosomal protein L3



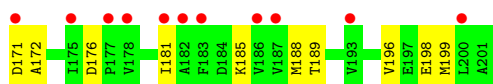
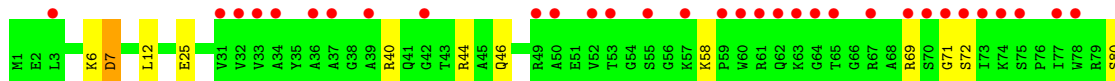
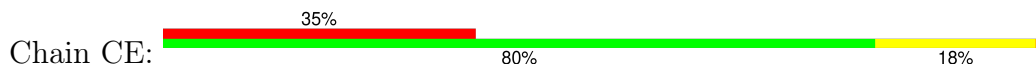
• Molecule 33: 23S rRNA



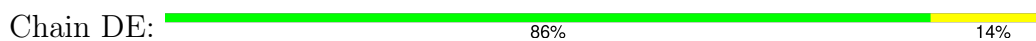




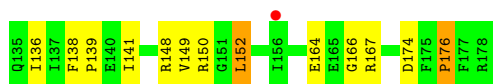
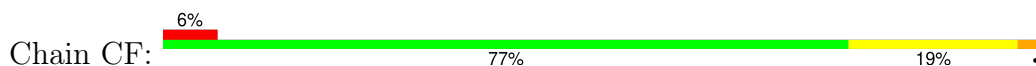
- Molecule 34: 50S ribosomal protein L4



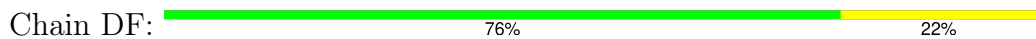
- Molecule 34: 50S ribosomal protein L4



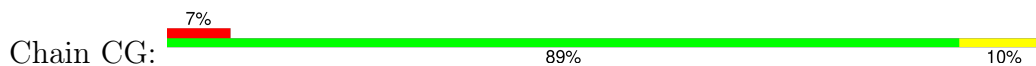
- Molecule 35: 50S ribosomal protein L5



- Molecule 35: 50S ribosomal protein L5



- Molecule 36: 50S ribosomal protein L6

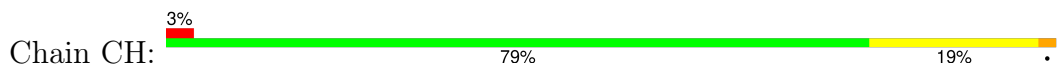




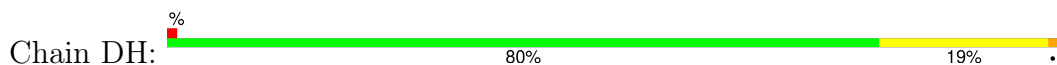
- Molecule 36: 50S ribosomal protein L6



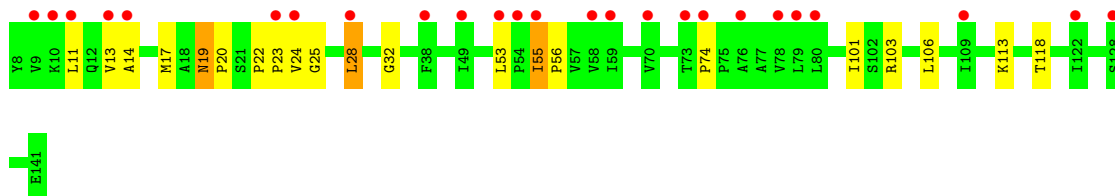
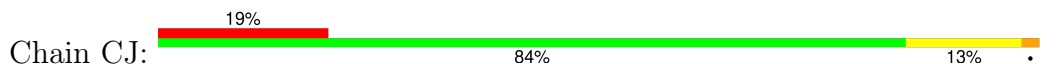
- Molecule 37: 50S ribosomal protein L9



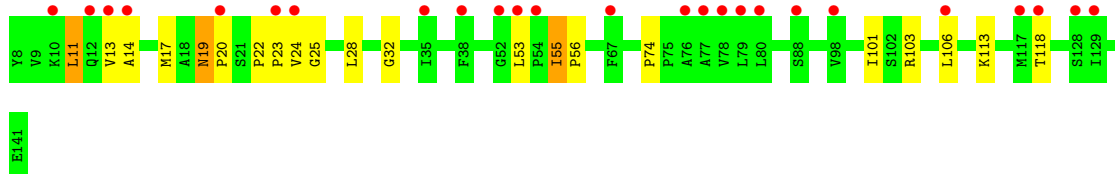
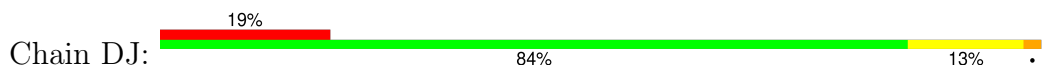
- Molecule 37: 50S ribosomal protein L9



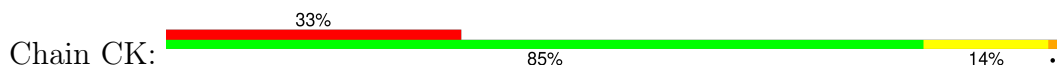
- Molecule 38: 50S ribosomal protein L11

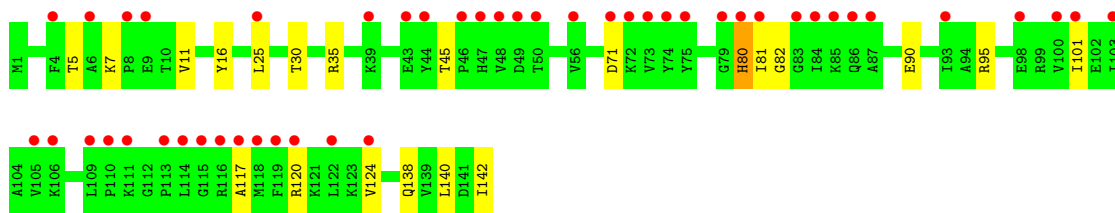


- Molecule 38: 50S ribosomal protein L11



- Molecule 39: 50S ribosomal protein L13





- Molecule 39: 50S ribosomal protein L13

Chain DK: 91% 9%



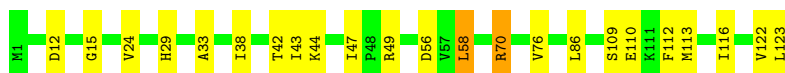
- Molecule 40: 50S ribosomal protein L14

Chain CL: 8% 80% 17% ...



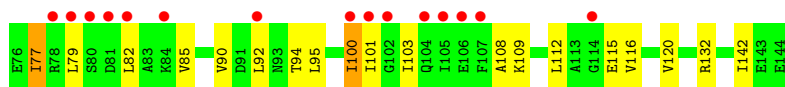
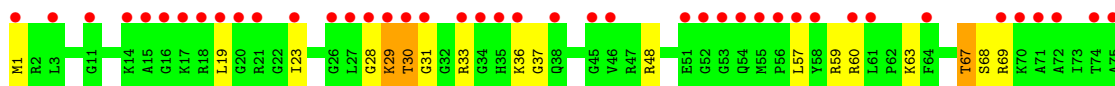
- Molecule 40: 50S ribosomal protein L14

Chain DL: 81% 17% .



- Molecule 41: 50S ribosomal protein L15

Chain CM: 40% 74% 22% .



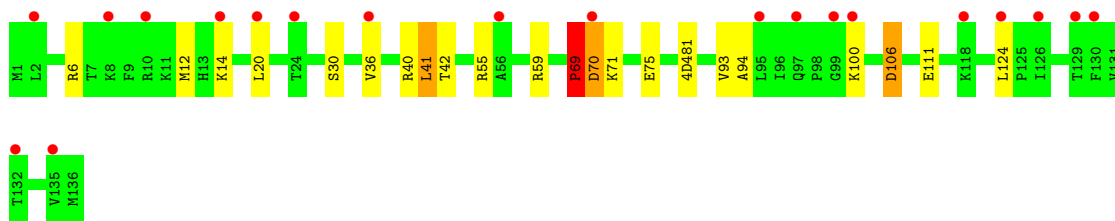
- Molecule 41: 50S ribosomal protein L15

Chain DM: 88% 12% .



- Molecule 42: 50S ribosomal protein L16

Chain CN: 15% 84% 13% ..



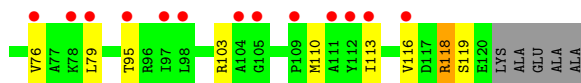
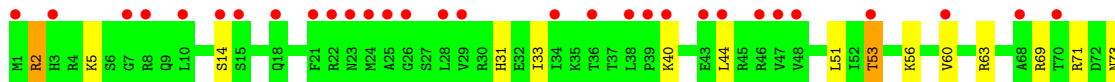
- Molecule 42: 50S ribosomal protein L16

Chain DN: 87% 12%



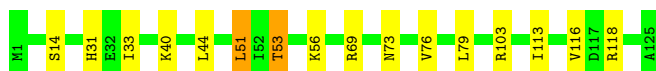
- Molecule 43: 50S ribosomal protein L17

Chain CO: 34% 77% 17%



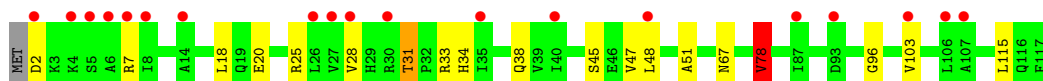
- Molecule 43: 50S ribosomal protein L17

Chain DO: 87% 11%



- Molecule 44: 50S ribosomal protein L18

Chain CP: 16% 83% 15%



- Molecule 44: 50S ribosomal protein L18

Chain DP: 86% 11%



- Molecule 45: 50S ribosomal protein L19

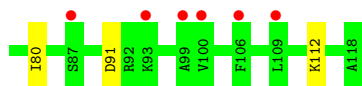
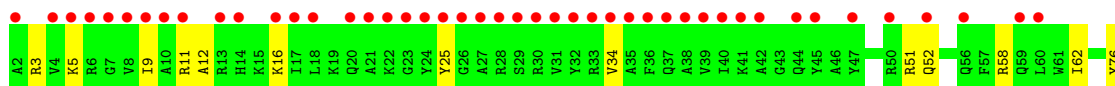
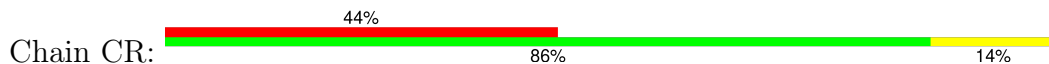
Chain CQ: 17% 88% 11%



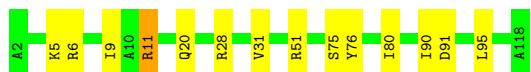
- Molecule 45: 50S ribosomal protein L19



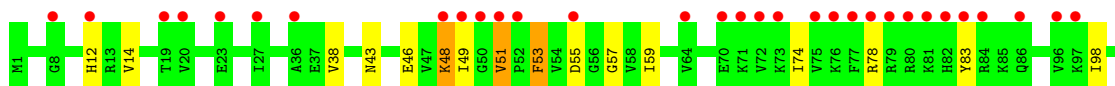
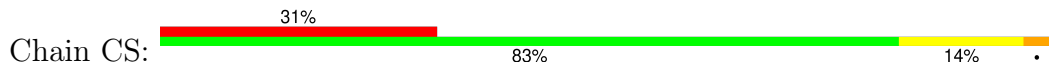
- Molecule 46: 50S ribosomal protein L20



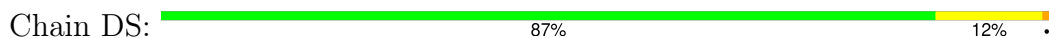
- Molecule 46: 50S ribosomal protein L20



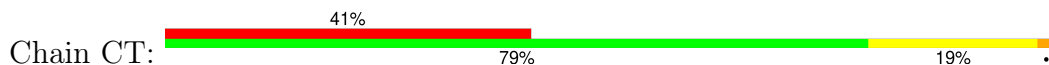
- Molecule 47: 50S ribosomal protein L21

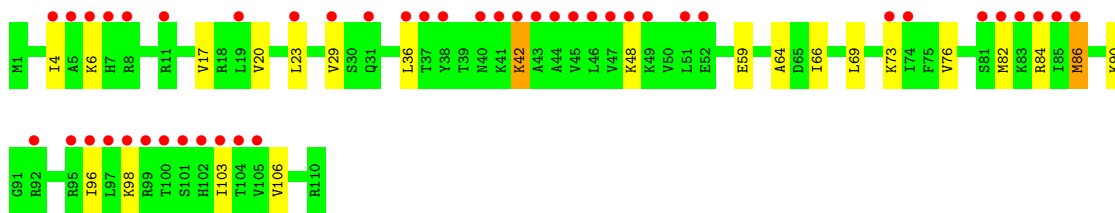


- Molecule 47: 50S ribosomal protein L21

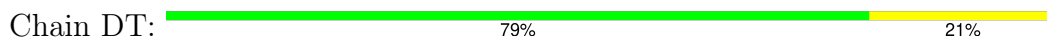


- Molecule 48: 50S ribosomal protein L22

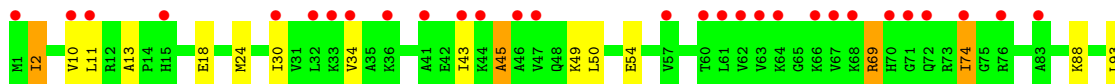
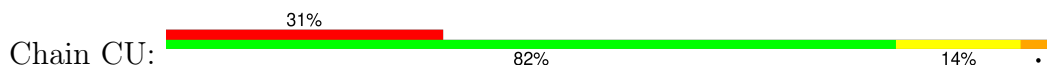




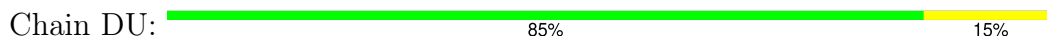
- Molecule 48: 50S ribosomal protein L22



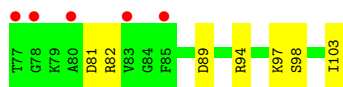
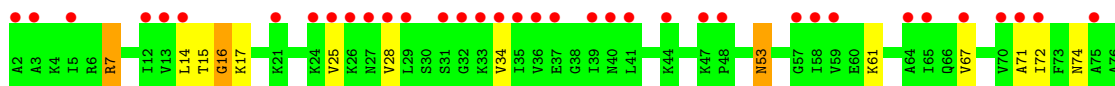
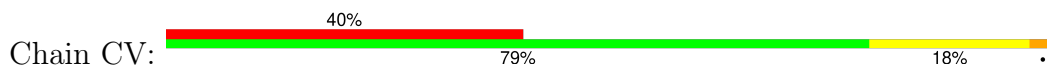
- Molecule 49: 50S ribosomal protein L23



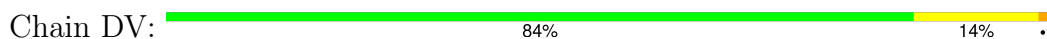
- Molecule 49: 50S ribosomal protein L23



- Molecule 50: 50S ribosomal protein L24

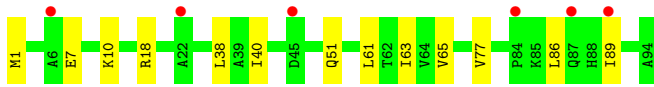


- Molecule 50: 50S ribosomal protein L24

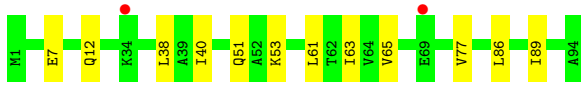
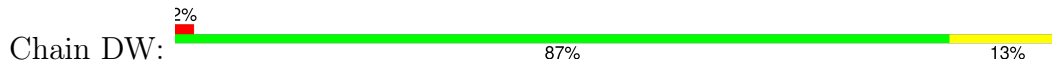


- Molecule 51: 50S ribosomal protein L25

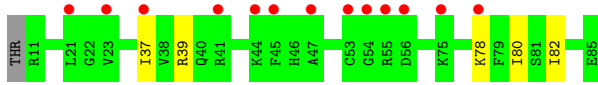




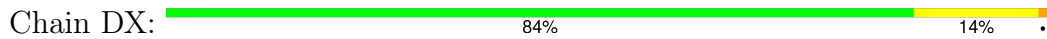
- Molecule 51: 50S ribosomal protein L25



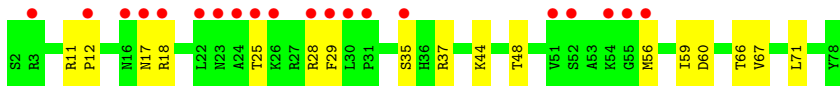
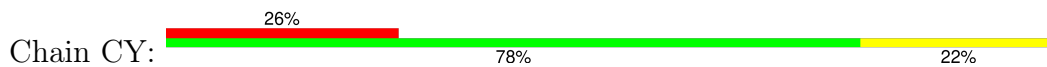
- Molecule 52: 50S ribosomal protein L27



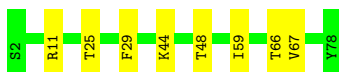
- Molecule 52: 50S ribosomal protein L27



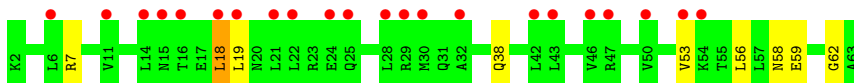
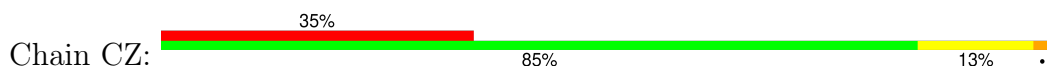
- Molecule 53: 50S ribosomal protein L28




- Molecule 53: 50S ribosomal protein L28

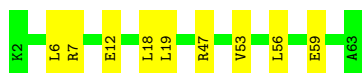


- Molecule 54: 50S ribosomal protein L29



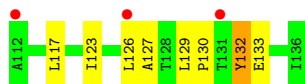
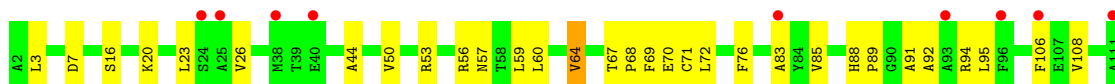
- Molecule 54: 50S ribosomal protein L29

Chain DZ:  85% 15%



● Molecule 55: 50S ribosomal protein L10

Chain DI:  9% 71% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.92Å 434.36Å 623.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 3.12 47.19 – 3.12	Depositor EDS
% Data completeness (in resolution range)	82.3 (47.19-3.12) 82.3 (47.19-3.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.94 (at 3.12Å)	Xtrriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.190 , 0.220 0.207 , 0.240	Depositor DCC
R_{free} test set	3316 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtrriage
Anisotropy	0.346	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 100.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295125	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, UR3, PSU, H2U, 4OC, OMG, EDO, 5MU, 4D4, PG4, 1MG, ZN, 6MZ, TRS, 3TD, PGE, 5MC, ACY, MEQ, OMC, D2T, SPD, PUT, PEG, GUN, MA6, 1PE, 2MG, G7M, MG, MPD, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.68	9/36593 (0.0%)	0.66	1/57081 (0.0%)
1	BA	0.68	9/36568 (0.0%)	0.66	1/57042 (0.0%)
2	AB	0.80	0/1784	1.38	5/2403 (0.2%)
2	BB	0.79	0/1784	1.38	5/2403 (0.2%)
3	AC	0.77	0/1652	1.28	4/2225 (0.2%)
3	BC	0.77	0/1652	1.29	6/2225 (0.3%)
4	AD	0.72	0/1665	1.36	5/2227 (0.2%)
4	BD	0.71	0/1665	1.36	5/2227 (0.2%)
5	AE	0.78	0/1157	1.35	10/1557 (0.6%)
5	BE	0.77	0/1118	1.36	5/1504 (0.3%)
6	AF	0.75	0/881	1.27	4/1189 (0.3%)
6	BF	0.79	0/835	1.40	10/1128 (0.9%)
7	AG	0.77	0/1196	1.38	3/1602 (0.2%)
7	BG	0.78	0/1196	1.37	3/1602 (0.2%)
8	AH	0.72	0/989	1.33	3/1326 (0.2%)
8	BH	0.73	0/989	1.32	3/1326 (0.2%)
9	AI	0.75	0/1034	1.29	0/1375
9	BI	0.74	0/1034	1.28	2/1375 (0.1%)
10	AJ	0.77	1/806 (0.1%)	1.26	2/1089 (0.2%)
10	BJ	0.86	1/797 (0.1%)	1.30	4/1077 (0.4%)
11	AK	0.75	0/893	1.24	2/1205 (0.2%)
11	BK	0.74	0/893	1.27	3/1205 (0.2%)
12	AL	0.73	0/960	1.22	2/1286 (0.2%)
12	BL	0.72	0/960	1.23	1/1286 (0.1%)
13	AM	0.84	0/893	1.50	5/1193 (0.4%)
13	BM	0.86	0/893	1.52	9/1193 (0.8%)
14	AN	0.79	0/817	1.34	0/1088
14	BN	0.76	0/817	1.33	0/1088
15	AO	0.73	0/722	1.47	1/964 (0.1%)
15	BO	0.73	0/722	1.51	0/964
16	AP	0.81	0/659	1.32	4/884 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.83	0/659	1.41	3/884 (0.3%)
17	AQ	0.77	0/658	1.22	2/881 (0.2%)
17	BQ	0.83	0/658	1.30	2/881 (0.2%)
18	AR	0.81	0/463	1.40	4/621 (0.6%)
18	BR	0.82	0/463	1.36	3/621 (0.5%)
19	AS	0.82	0/653	1.21	1/877 (0.1%)
19	BS	0.82	0/653	1.19	0/877
20	AT	0.74	0/676	1.55	4/895 (0.4%)
20	BT	0.82	0/671	1.61	2/888 (0.2%)
21	AU	0.75	0/472	1.36	2/627 (0.3%)
21	BU	0.72	0/472	1.35	2/627 (0.3%)
22	C1	0.81	0/450	1.31	2/599 (0.3%)
22	D1	0.79	0/450	1.33	0/599
23	C2	0.85	0/416	1.32	0/554
23	D2	0.82	0/421	1.28	0/561
24	C3	0.79	0/380	1.50	0/498
24	D3	0.86	0/380	1.53	0/498
25	C4	0.75	0/513	1.30	0/676
25	D4	0.82	0/513	1.33	2/676 (0.3%)
26	C5	0.77	0/303	1.13	0/397
26	D5	0.82	0/303	1.15	0/397
27	C0	0.90	0/453	1.38	0/605
27	D0	0.86	0/467	1.31	0/623
28	CB	0.68	0/2828	0.66	0/4410
28	DB	0.73	1/2872 (0.0%)	0.68	0/4478
29	CC	0.73	0/2122	1.28	6/2852 (0.2%)
29	DC	0.74	0/2122	1.25	4/2852 (0.1%)
30	CD	0.76	1/1586 (0.1%)	1.22	4/2134 (0.2%)
31	CA	0.71	53/69165 (0.1%)	0.67	5/107896 (0.0%)
32	DD	0.80	0/1576	1.22	5/2119 (0.2%)
33	DA	0.73	20/69364 (0.0%)	0.71	2/108207 (0.0%)
34	CE	0.77	0/1571	1.36	4/2113 (0.2%)
34	DE	0.78	0/1571	1.31	4/2113 (0.2%)
35	CF	0.74	0/1435	1.34	11/1926 (0.6%)
35	DF	0.75	0/1435	1.32	7/1926 (0.4%)
36	CG	0.75	0/1343	1.28	6/1816 (0.3%)
36	DG	0.73	0/1343	1.24	4/1816 (0.2%)
37	CH	0.83	0/1121	1.36	4/1515 (0.3%)
37	DH	0.83	0/1121	1.36	4/1515 (0.3%)
38	CJ	0.96	0/993	1.35	3/1341 (0.2%)
38	DJ	0.96	0/993	1.35	3/1341 (0.2%)
39	CK	0.69	0/1152	1.33	3/1551 (0.2%)
39	DK	0.78	0/1152	1.31	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	CL	0.82	0/947	1.18	1/1268 (0.1%)
40	DL	0.83	0/955	1.17	1/1279 (0.1%)
41	CM	0.78	1/1062 (0.1%)	1.37	12/1413 (0.8%)
41	DM	0.74	0/1062	1.30	5/1413 (0.4%)
42	CN	0.74	1/1081 (0.1%)	1.29	6/1443 (0.4%)
42	DN	0.78	0/1092	1.28	2/1457 (0.1%)
43	CO	0.75	0/973	1.31	0/1301
43	DO	0.81	0/1006	1.34	0/1345
44	CP	0.74	0/902	1.44	5/1209 (0.4%)
44	DP	0.75	0/910	1.42	2/1219 (0.2%)
45	CQ	0.72	0/929	1.17	0/1242
45	DQ	0.74	0/929	1.14	0/1242
46	CR	0.76	0/960	1.43	3/1278 (0.2%)
46	DR	0.85	0/960	1.40	1/1278 (0.1%)
47	CS	0.76	0/829	1.17	2/1107 (0.2%)
47	DS	0.79	0/829	1.19	0/1107
48	CT	0.76	0/864	1.37	1/1156 (0.1%)
48	DT	0.80	0/864	1.35	3/1156 (0.3%)
49	CU	0.79	0/745	1.30	3/994 (0.3%)
49	DU	0.77	0/745	1.30	5/994 (0.5%)
50	CV	0.85	0/788	1.31	4/1051 (0.4%)
50	DV	0.78	0/788	1.27	4/1051 (0.4%)
51	CW	0.73	0/766	1.23	0/1025
51	DW	0.79	0/766	1.24	0/1025
52	CX	0.70	0/576	1.16	0/762
52	DX	0.75	0/598	1.17	1/790 (0.1%)
53	CY	0.66	0/635	1.35	1/848 (0.1%)
53	DY	0.72	0/635	1.33	0/848
54	CZ	0.73	0/502	1.53	0/667
54	DZ	0.73	0/502	1.52	0/667
55	DI	0.89	0/1037	1.46	8/1402 (0.6%)
All	All	0.73	97/309273 (0.0%)	0.90	289/462210 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
33	DA	0	15
42	CN	0	1
All	All	0	17

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-8.52	1.29	1.42
33	DA	2585	U	C1'-N1	7.86	1.59	1.47
31	CA	769	U	C1'-N1	7.59	1.59	1.48
1	BA	5	U	C1'-N1	7.59	1.59	1.48
33	DA	2097	A	O5'-C5'	-7.29	1.31	1.42

The worst 5 of 289 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DI	132	TYR	CA-C-N	9.80	139.35	121.70
55	DI	132	TYR	C-N-CA	9.80	139.35	121.70
35	DF	10	ASP	CA-CB-CG	8.61	121.21	112.60
20	BT	6	SER	N-CA-C	-8.06	103.44	113.28
35	CF	134	GLU	CB-CG-CD	7.48	125.31	112.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	898	G	Sidechain
33	DA	27	G	Sidechain
33	DA	308	G	Sidechain
33	DA	452	G	Sidechain
33	DA	512	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	32930	0	16591	87	0
1	BA	32908	0	16580	89	0
2	AB	1753	0	1780	13	0
2	BB	1753	0	1780	17	0
3	AC	1625	0	1696	12	0
3	BC	1625	0	1696	15	0
4	AD	1643	0	1707	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BD	1643	0	1707	12	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	19	0
6	AF	862	0	864	7	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	14	0
7	BG	1182	0	1238	9	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	7	0
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	9	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	11	0
11	BK	877	0	887	10	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	11	0
13	AM	884	0	941	9	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	0	0
15	BO	714	0	734	1	0
16	AP	649	0	666	4	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	4	0
17	BQ	649	0	691	7	0
18	AR	456	0	478	3	0
18	BR	456	0	478	1	0
19	AS	638	0	665	6	0
19	BS	638	0	665	10	0
20	AT	670	0	719	4	0
20	BT	665	0	714	9	0
21	AU	465	0	491	5	0
21	BU	465	0	491	5	0
22	C1	444	0	458	6	0
22	D1	444	0	458	9	0
23	C2	409	0	440	4	0
23	D2	414	0	442	2	0
24	C3	377	0	418	4	0
24	D3	377	0	418	2	0
25	C4	504	0	572	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D4	504	0	572	2	0
26	C5	302	0	340	5	0
26	D5	302	0	340	1	0
27	C0	449	0	488	2	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	2	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	20	0
29	DC	2083	0	2154	17	0
30	CD	1565	0	1616	14	0
31	CA	62229	0	31318	253	0
32	DD	1576	0	1627	16	0
33	DA	62423	0	31410	188	0
34	CE	1552	0	1619	15	0
34	DE	1552	0	1619	11	0
35	CF	1411	0	1444	12	0
35	DF	1411	0	1444	13	0
36	CG	1323	0	1371	8	0
36	DG	1323	0	1371	9	0
37	CH	1110	0	1148	10	0
37	DH	1110	0	1148	7	0
38	CJ	979	0	1028	7	0
38	DJ	979	0	1028	6	0
39	CK	1129	0	1162	8	0
39	DK	1129	0	1162	3	0
40	CL	938	0	1012	10	0
40	DL	946	0	1023	10	0
41	CM	1053	0	1129	21	0
41	DM	1053	0	1129	11	0
42	CN	1075	0	1154	7	0
42	DN	1092	0	1177	7	0
43	CO	960	0	1000	10	0
43	DO	993	0	1034	8	0
44	CP	892	0	923	5	0
44	DP	900	0	935	8	0
45	CQ	917	0	962	8	0
45	DQ	917	0	962	5	0
46	CR	947	0	1019	10	0
46	DR	947	0	1019	13	0
47	CS	816	0	839	8	0
47	DS	816	0	839	8	0
48	CT	857	0	922	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	DT	857	0	922	13	0
49	CU	739	0	807	7	0
49	DU	739	0	807	3	0
50	CV	780	0	831	8	0
50	DV	780	0	831	5	0
51	CW	753	0	780	4	0
51	DW	753	0	780	5	0
52	CX	569	0	581	1	0
52	DX	591	0	606	7	0
53	CY	625	0	652	7	0
53	DY	625	0	652	2	0
54	CZ	501	0	531	3	0
54	DZ	501	0	531	3	0
55	DI	1023	0	1052	15	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	183	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	1	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	1	0
58	DA	48	0	84	1	0
58	DE	16	0	28	1	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	0	0
58	DT	8	0	14	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	2	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	D1	7	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	0	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	1	0
62	DB	8	0	12	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	2	0
63	DD	10	0	14	0	0
63	DS	10	0	14	2	0
63	DT	10	0	14	0	0
63	DU	10	0	14	0	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	1	0
69	AC	4	0	0	0	0
69	AD	3	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	2	0	0	0	0
69	AK	7	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	7	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	3	0	0	0	0
69	AU	3	0	0	0	0
69	BA	291	0	0	1	0
69	BD	11	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BL	2	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	2	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	1	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	692	0	0	5	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	7	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	21	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	28	0	0	0	0
69	D4	39	0	0	0	0
69	D5	9	0	0	0	0
69	DA	4834	0	0	14	0
69	DB	199	0	0	2	0
69	DC	98	0	0	1	0
69	DD	95	0	0	0	0
69	DE	63	0	0	1	0
69	DF	15	0	0	0	0
69	DG	7	0	0	0	0
69	DH	1	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	0	0
69	DM	62	0	0	0	0
69	DN	64	0	0	0	0
69	DO	48	0	0	0	0
69	DP	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DQ	33	0	0	0	0
69	DR	68	0	0	1	0
69	DS	48	0	0	0	0
69	DT	62	0	0	1	0
69	DU	22	0	0	0	0
69	DV	18	0	0	0	0
69	DW	34	0	0	2	0
69	DX	31	0	0	0	0
69	DY	10	0	0	0	0
69	DZ	5	0	0	1	0
All	All	295125	0	194409	1259	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 3.

The worst 5 of 1259 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)
47:CS:14:VAL:HG21	47:CS:98:ILE:HG13	1.20	1.10
33:DA:1847:A:HO2'	33:DA:1848:A:H8	1.02	0.98
2:BB:20:THR:HA	2:BB:39:HIS:CE1	1.98	0.98
47:CS:14:VAL:CG2	47:CS:98:ILE:HG13	1.96	0.96
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.04	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%)	209 (94%)	8 (4%)	5 (2%)	5	21
2	BB	222/224 (99%)	209 (94%)	8 (4%)	5 (2%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	12	39
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	8	30
4	AD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
4	BD	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
5	AE	153/155 (99%)	144 (94%)	7 (5%)	2 (1%)	9	33
5	BE	148/155 (96%)	130 (88%)	15 (10%)	3 (2%)	6	24
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	89 (91%)	7 (7%)	2 (2%)	6	24
7	AG	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	18	47
7	BG	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
8	BH	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	17
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1	6
11	AK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
11	BK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
12	AL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16	45
12	BL	120/123 (98%)	114 (95%)	4 (3%)	2 (2%)	7	28
13	AM	112/114 (98%)	101 (90%)	7 (6%)	4 (4%)	2	14
13	BM	112/114 (98%)	100 (89%)	6 (5%)	6 (5%)	1	8
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6	24
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	6	24
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	34
16	AP	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	33
16	BP	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	20
17	AQ	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	33
17	BQ	78/80 (98%)	73 (94%)	2 (3%)	3 (4%)	2	13
18	AR	53/55 (96%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	25
19	AS	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	33
19	BS	77/79 (98%)	65 (84%)	11 (14%)	1 (1%)	9	33
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	10	34
21	AU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
21	BU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
22	C1	54/56 (96%)	48 (89%)	3 (6%)	3 (6%)	1	8
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	42 (88%)	5 (10%)	1 (2%)	5	23
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	21
24	D3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
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%)	53 (95%)	1 (2%)	2 (4%)	2	14
27	D0	57/58 (98%)	55 (96%)	2 (4%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	14 (5%)	5 (2%)	6	25
29	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	30	60
30	CD	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
34	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	8	30
34	DE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	55
35	CF	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	21	50
35	DF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	21	50
36	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	5	21
36	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	21	50
37	CH	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	4	19
37	DH	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	17
38	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	17
39	CK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	23
39	DK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	9	31
40	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	16	45
40	DL	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
41	CM	142/144 (99%)	130 (92%)	8 (6%)	4 (3%)	4	19
41	DM	142/144 (99%)	136 (96%)	4 (3%)	2 (1%)	9	31
42	CN	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	16	45
42	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
43	CO	118/125 (94%)	107 (91%)	8 (7%)	3 (2%)	4	20
43	DO	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	45
44	CP	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
44	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
45	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	14	42
45	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	42
46	CR	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
46	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
47	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	17
47	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12	39
48	CT	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
48	DT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
49	CU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	DU	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
50	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	2	12
50	DV	100/102 (98%)	95 (95%)	3 (3%)	2 (2%)	6	24
51	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
51	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
52	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
52	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
53	CY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	DY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
54	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	28
54	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
55	DI	133/135 (98%)	114 (86%)	14 (10%)	5 (4%)	2	13
All	All	11407/11629 (98%)	10635 (93%)	633 (6%)	139 (1%)	10	34

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
5	AE	162	GLU
13	AM	5	ALA
22	C1	25	VAL

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%)	172 (92%)	14 (8%)	12	38
2	BB	186/186 (100%)	172 (92%)	14 (8%)	12	38
3	AC	170/170 (100%)	158 (93%)	12 (7%)	13	39
3	BC	170/170 (100%)	155 (91%)	15 (9%)	9	31
4	AD	172/172 (100%)	162 (94%)	10 (6%)	18	46
4	BD	172/172 (100%)	162 (94%)	10 (6%)	18	46
5	AE	118/118 (100%)	96 (81%)	22 (19%)	1	7
5	BE	113/118 (96%)	90 (80%)	23 (20%)	1	5
6	AF	92/92 (100%)	83 (90%)	9 (10%)	7	28
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	21
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	15
7	BG	124/124 (100%)	103 (83%)	21 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	104/104 (100%)	88 (85%)	16 (15%)	2	12
8	BH	104/104 (100%)	89 (86%)	15 (14%)	3	13
9	AI	105/105 (100%)	100 (95%)	5 (5%)	23	52
9	BI	105/105 (100%)	100 (95%)	5 (5%)	23	52
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	11	35
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	6	25
11	AK	90/90 (100%)	88 (98%)	2 (2%)	45	68
11	BK	90/90 (100%)	85 (94%)	5 (6%)	19	47
12	AL	102/102 (100%)	95 (93%)	7 (7%)	14	40
12	BL	102/102 (100%)	93 (91%)	9 (9%)	9	31
13	AM	92/92 (100%)	86 (94%)	6 (6%)	15	42
13	BM	92/92 (100%)	88 (96%)	4 (4%)	26	55
14	AN	83/83 (100%)	81 (98%)	2 (2%)	43	67
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	67
15	AO	76/76 (100%)	70 (92%)	6 (8%)	11	35
15	BO	76/76 (100%)	68 (90%)	8 (10%)	6	25
16	AP	65/65 (100%)	63 (97%)	2 (3%)	35	62
16	BP	65/65 (100%)	61 (94%)	4 (6%)	16	44
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	11	34
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6	23
18	AR	48/48 (100%)	46 (96%)	2 (4%)	26	56
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	69
19	AS	70/70 (100%)	60 (86%)	10 (14%)	3	13
19	BS	70/70 (100%)	62 (89%)	8 (11%)	5	22
20	AT	65/65 (100%)	59 (91%)	6 (9%)	8	30
20	BT	65/65 (100%)	56 (86%)	9 (14%)	3	14
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7	25
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	25
22	C1	47/47 (100%)	45 (96%)	2 (4%)	26	55
22	D1	47/47 (100%)	44 (94%)	3 (6%)	16	42
23	C2	45/46 (98%)	41 (91%)	4 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	D2	45/46 (98%)	39 (87%)	6 (13%)	4	16
24	C3	38/38 (100%)	36 (95%)	2 (5%)	20	49
24	D3	38/38 (100%)	36 (95%)	2 (5%)	20	49
25	C4	51/51 (100%)	49 (96%)	2 (4%)	28	58
25	D4	51/51 (100%)	50 (98%)	1 (2%)	48	70
26	C5	34/34 (100%)	33 (97%)	1 (3%)	37	63
26	D5	34/34 (100%)	33 (97%)	1 (3%)	37	63
27	C0	48/48 (100%)	38 (79%)	10 (21%)	1	5
27	D0	49/48 (102%)	44 (90%)	5 (10%)	7	26
29	CC	216/216 (100%)	202 (94%)	14 (6%)	15	42
29	DC	216/216 (100%)	207 (96%)	9 (4%)	26	56
30	CD	164/164 (100%)	158 (96%)	6 (4%)	30	59
32	DD	163/163 (100%)	158 (97%)	5 (3%)	35	62
34	CE	165/165 (100%)	147 (89%)	18 (11%)	6	23
34	DE	165/165 (100%)	156 (94%)	9 (6%)	19	47
35	CF	148/148 (100%)	129 (87%)	19 (13%)	4	17
35	DF	148/148 (100%)	130 (88%)	18 (12%)	5	19
36	CG	137/137 (100%)	132 (96%)	5 (4%)	31	59
36	DG	137/137 (100%)	132 (96%)	5 (4%)	31	59
37	CH	114/114 (100%)	99 (87%)	15 (13%)	4	16
37	DH	114/114 (100%)	99 (87%)	15 (13%)	4	16
38	CJ	104/104 (100%)	98 (94%)	6 (6%)	18	46
38	DJ	104/104 (100%)	97 (93%)	7 (7%)	15	41
39	CK	116/116 (100%)	110 (95%)	6 (5%)	21	49
39	DK	116/116 (100%)	112 (97%)	4 (3%)	32	60
40	CL	103/104 (99%)	95 (92%)	8 (8%)	11	36
40	DL	104/104 (100%)	97 (93%)	7 (7%)	15	41
41	CM	103/103 (100%)	95 (92%)	8 (8%)	11	36
41	DM	103/103 (100%)	96 (93%)	7 (7%)	14	40
42	CN	108/108 (100%)	100 (93%)	8 (7%)	13	38
42	DN	109/108 (101%)	105 (96%)	4 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	CO	100/102 (98%)	92 (92%)	8 (8%)	11	35
43	DO	102/102 (100%)	97 (95%)	5 (5%)	22	51
44	CP	86/87 (99%)	78 (91%)	8 (9%)	8	29
44	DP	87/87 (100%)	81 (93%)	6 (7%)	14	40
45	CQ	99/99 (100%)	93 (94%)	6 (6%)	17	44
45	DQ	99/99 (100%)	92 (93%)	7 (7%)	13	39
46	CR	89/89 (100%)	84 (94%)	5 (6%)	19	47
46	DR	89/89 (100%)	85 (96%)	4 (4%)	24	54
47	CS	84/84 (100%)	79 (94%)	5 (6%)	17	45
47	DS	84/84 (100%)	81 (96%)	3 (4%)	31	59
48	CT	93/93 (100%)	91 (98%)	2 (2%)	45	68
48	DT	93/93 (100%)	92 (99%)	1 (1%)	65	76
49	CU	80/80 (100%)	73 (91%)	7 (9%)	9	31
49	DU	80/80 (100%)	75 (94%)	5 (6%)	16	43
50	CV	83/83 (100%)	75 (90%)	8 (10%)	8	28
50	DV	83/83 (100%)	77 (93%)	6 (7%)	13	39
51	CW	78/78 (100%)	72 (92%)	6 (8%)	12	36
51	DW	78/78 (100%)	74 (95%)	4 (5%)	21	50
52	CX	56/58 (97%)	53 (95%)	3 (5%)	20	48
52	DX	58/58 (100%)	55 (95%)	3 (5%)	21	49
53	CY	67/67 (100%)	61 (91%)	6 (9%)	9	31
53	DY	67/67 (100%)	62 (92%)	5 (8%)	12	38
54	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	38
54	DZ	54/54 (100%)	50 (93%)	4 (7%)	13	38
55	DI	103/103 (100%)	96 (93%)	7 (7%)	14	40
All	All	9461/9478 (100%)	8740 (92%)	721 (8%)	12	37

5 of 721 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	CG	72	LEU
52	CX	78	LYS
37	CH	76	GLU

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Mol	Chain	Res	Type
36	CG	42	GLU
43	CO	53	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
37	DH	2	GLN
39	DK	136	GLN
53	DY	36	HIS
4	BD	41	HIS
3	BC	123	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	274 (17%)	38 (2%)
1	BA	1532/1534 (99%)	274 (17%)	44 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	12 (10%)	0
31	CA	2896/2904 (99%)	525 (18%)	94 (3%)
33	DA	2884/2903 (99%)	458 (15%)	72 (2%)
All	All	9081/9115 (99%)	1555 (17%)	248 (2%)

5 of 1555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A

5 of 248 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	973	A
33	DA	1607	C
31	CA	1647	U
33	DA	1536	C
33	DA	2282	G

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	G7M	AA	527	1	23,26,27	0.53	0	34,39,42	2.04	5 (14%)
33	2MG	DA	2445	33	23,26,27	0.49	0	33,38,41	0.36	0
42	4D4	CN	81	42	9,11,12	2.16	2 (22%)	7,13,15	2.38	2 (28%)
33	PSU	DA	2457	33	18,21,22	0.52	0	21,30,33	0.45	0
33	G7M	DA	2069	33	23,26,27	0.52	0	34,39,42	1.96	5 (14%)
31	PSU	CA	2580	31	18,21,22	0.47	0	21,30,33	0.56	0
33	PSU	DA	2605	33	18,21,22	0.40	0	21,30,33	0.59	0
1	5MC	AA	967	1	19,22,23	0.28	0	26,32,35	0.36	0
32	MEQ	DD	150[B]	32	8,9,10	1.14	1 (12%)	5,10,12	0.91	0
42	4D4	DN	81[A]	-	9,11,12	1.57	2 (22%)	7,13,15	2.66	2 (28%)
31	PSU	CA	2457	31	18,21,22	0.52	0	21,30,33	0.53	0
33	2MG	DA	1835	33	23,26,27	0.31	0	33,38,41	0.38	0
33	OMU	DA	2552	33	19,22,23	0.44	0	25,31,34	0.27	0
1	5MC	BA	967	1	19,22,23	0.30	0	26,32,35	0.36	0
31	2MA	CA	2503	31	22,25,26	0.75	0	32,37,40	1.84	6 (18%)
31	PSU	CA	2605	31	18,21,22	0.36	0	21,30,33	0.51	0
33	2MA	DA	2503	56,33	22,25,26	0.80	1 (4%)	32,37,40	1.96	6 (18%)
31	5MU	CA	747	31	19,22,23	0.21	0	27,32,35	0.32	0
1	5MC	AA	1407	1	19,22,23	0.32	0	26,32,35	0.46	0
33	5MU	DA	1939	33	19,22,23	0.62	0	27,32,35	0.43	0
1	UR3	AA	1498	1	19,22,23	0.49	0	26,32,35	0.43	0
31	2MG	CA	1835	31	23,26,27	0.34	0	33,38,41	0.38	0
31	5MU	CA	1939	31	19,22,23	0.38	0	27,32,35	0.30	0
33	OMC	DA	2498	56,33	19,22,23	0.50	0	25,31,34	0.44	0
12	D2T	BL	89	12	8,9,10	0.72	0	6,11,13	0.74	0
31	2MG	CA	2445	31	23,26,27	0.44	0	33,38,41	0.44	0
31	G7M	CA	2069	31	23,26,27	0.63	0	34,39,42	2.05	5 (14%)
33	OMG	DA	2251	33	23,26,27	0.31	0	32,38,41	0.36	0
42	4D4	DN	81[B]	-	9,11,12	1.76	1 (11%)	7,13,15	2.85	2 (28%)
31	5MC	CA	1962	31	19,22,23	0.23	0	26,32,35	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	AA	966	1	23,26,27	0.33	0	33,38,41	0.50	0
1	MA6	AA	1519	1	23,26,27	0.60	0	33,38,41	1.08	4 (12%)
1	2MG	AA	1207	1	23,26,27	0.25	0	33,38,41	0.41	0
31	6MZ	CA	2030	31	22,25,26	0.37	0	29,36,39	0.43	0
31	OMU	CA	2552	31	19,22,23	0.33	0	25,31,34	0.27	0
32	MEQ	DD	150[A]	32	8,9,10	0.43	0	5,10,12	0.66	0
1	2MG	AA	1516	1	23,26,27	0.31	0	33,38,41	0.43	0
1	5MC	BA	1407	1	19,22,23	0.38	0	26,32,35	0.45	0
33	PSU	DA	2504	33	18,21,22	0.55	0	21,30,33	0.33	0
1	4OC	BA	1402	1	20,23,24	0.35	0	25,32,35	0.54	1 (4%)
33	PSU	DA	2580	33	18,21,22	0.57	0	21,30,33	0.57	0
33	PSU	DA	1917	33	18,21,22	0.44	0	21,30,33	0.44	0
1	PSU	BA	516	1	18,21,22	0.33	0	21,30,33	0.42	0
1	MA6	BA	1518	1	23,26,27	0.44	0	33,38,41	1.18	4 (12%)
31	1MG	CA	745	31	23,26,27	1.01	1 (4%)	33,39,42	0.63	0
31	PSU	CA	2504	31	18,21,22	0.38	0	21,30,33	0.38	0
1	UR3	BA	1498	1	19,22,23	0.37	0	26,32,35	0.39	0
33	5MC	DA	1962	33	19,22,23	0.42	0	26,32,35	0.44	0
31	3TD	CA	1915	31	19,22,23	0.47	0	23,32,35	0.74	1 (4%)
33	1MG	DA	745	33	23,26,27	1.20	1 (4%)	33,39,42	0.54	0
33	3TD	DA	1915	33	19,22,23	0.43	0	23,32,35	0.77	1 (4%)
33	H2U	DA	2449	33	18,21,22	0.78	0	19,30,33	0.44	0
1	2MG	BA	1207	1	23,26,27	0.29	0	33,38,41	0.42	0
1	MA6	BA	1519	1	23,26,27	0.53	0	33,38,41	1.07	4 (12%)
31	PSU	CA	1917	31	18,21,22	0.32	0	21,30,33	0.42	0
1	2MG	BA	1516	1	23,26,27	0.29	0	33,38,41	0.42	0
33	PSU	DA	1911	33	18,21,22	0.32	0	21,30,33	0.42	0
1	MA6	AA	1518	1	23,26,27	0.41	0	33,38,41	1.09	4 (12%)
33	6MZ	DA	2030	33	22,25,26	0.53	0	29,36,39	0.58	0
31	PSU	CA	746	31,56	18,21,22	0.69	1 (5%)	21,30,33	0.59	0
33	PSU	DA	746	56,33	18,21,22	0.98	2 (11%)	21,30,33	0.38	0
31	OMC	CA	2498	31,56	19,22,23	0.37	0	25,31,34	0.35	0
31	OMG	CA	2251	31	23,26,27	0.40	0	32,38,41	0.51	0
1	G7M	BA	527	1	23,26,27	0.67	0	34,39,42	2.06	5 (14%)
33	PSU	DA	955	33	18,21,22	0.49	0	21,30,33	0.44	0
31	PSU	CA	955	31	18,21,22	0.32	0	21,30,33	0.46	0
1	PSU	AA	516	56,1	18,21,22	0.31	0	21,30,33	0.42	0
12	D2T	AL	89	12	8,9,10	0.92	0	6,11,13	0.98	0
1	2MG	BA	966	1	23,26,27	0.31	0	33,38,41	0.40	0
31	PSU	CA	1911	31	18,21,22	0.32	0	21,30,33	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	6MZ	DA	1618	33	22,25,26	0.36	0	29,36,39	0.47	0
1	4OC	AA	1402	1	20,23,24	0.31	0	25,32,35	0.57	1 (4%)
33	5MU	DA	747	33	19,22,23	0.31	0	27,32,35	0.37	0
33	PSU	DA	2604	33	18,21,22	0.44	0	21,30,33	0.48	0
31	6MZ	CA	1618	31	22,25,26	0.48	0	29,36,39	0.81	1 (3%)

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	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
33	2MG	DA	2445	33	-	2/9/27/28	0/3/3/3
42	4D4	CN	81	42	-	1/11/12/14	-
33	PSU	DA	2457	33	-	0/7/25/26	0/2/2/2
33	G7M	DA	2069	33	-	1/7/25/26	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
33	PSU	DA	2605	33	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
42	4D4	DN	81[A]	-	-	1/11/12/14	-
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
33	2MG	DA	1835	33	-	1/9/27/28	0/3/3/3
33	OMU	DA	2552	33	-	0/9/27/28	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	1/7/25/26	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
33	2MA	DA	2503	56,33	-	1/7/25/26	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
33	5MU	DA	1939	33	-	1/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	1/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
33	OMC	DA	2498	56,33	-	0/9/27/28	0/2/2/2
12	D2T	BL	89	12	-	6/7/12/14	-
31	2MG	CA	2445	31	-	1/9/27/28	0/3/3/3
31	G7M	CA	2069	31	-	1/7/25/26	0/3/3/3
33	OMG	DA	2251	33	-	1/9/27/28	0/3/3/3
42	4D4	DN	81[B]	-	-	3/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	2/9/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
33	PSU	DA	2504	33	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
33	PSU	DA	2580	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	1917	33	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
33	5MC	DA	1962	33	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
33	1MG	DA	745	33	-	0/7/25/26	0/3/3/3
33	3TD	DA	1915	33	-	0/7/25/26	0/2/2/2
33	H2U	DA	2449	33	-	0/7/38/39	0/2/2/2
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
33	PSU	DA	1911	33	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
33	6MZ	DA	2030	33	-	0/9/27/28	0/3/3/3
31	PSU	CA	746	31,56	-	1/7/25/26	0/2/2/2
33	PSU	DA	746	56,33	-	1/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	2/9/27/28	0/2/2/2
31	OMG	CA	2251	31	-	1/9/27/28	0/3/3/3
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
33	PSU	DA	955	33	-	0/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	6MZ	DA	1618	33	-	0/9/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
33	5MU	DA	747	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	2604	33	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	CN	81	4D4	CZ-NE	5.77	1.44	1.33
33	DA	745	1MG	C2-N1	5.48	1.47	1.37
42	DN	81[B]	4D4	CZ-NE	4.76	1.42	1.33
31	CA	745	1MG	C2-N1	4.44	1.45	1.37
42	DN	81[A]	4D4	CZ-NE	3.99	1.41	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2069	G7M	C6-C5-N7	-8.72	121.24	132.17
33	DA	2503	2MA	N6-C6-N1	8.36	128.31	117.03
31	CA	2503	2MA	N6-C6-N1	7.92	127.71	117.03
33	DA	2069	G7M	C6-C5-N7	-7.86	122.32	132.17
1	AA	527	G7M	C6-C5-N7	-7.79	122.40	132.17

There are no chirality outliers.

5 of 50 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
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
12	BL	89	D2T	O-C-CA-CB

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	DD	150[B]	MEQ	1	0
31	CA	2503	2MA	1	0
33	DA	2503	2MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	CA	1835	2MG	1	0
12	BL	89	D2T	1	0
1	AA	1519	MA6	1	0
31	CA	2030	6MZ	1	0
31	CA	2552	OMU	1	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
1	AA	1518	MA6	1	0
33	DA	2030	6MZ	1	0
31	CA	2251	OMG	1	0
12	AL	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	DA	3207	-	7,7,7	0.67	0	9,10,10	0.43	0
64	SPD	DA	3185	-	9,9,9	0.12	0	8,8,8	0.15	0
62	EDO	DA	3227	-	3,3,3	0.53	0	2,2,2	0.36	0
57	PG4	BA	1642	-	12,12,12	0.17	0	11,11,11	0.16	0
58	MPD	DA	3204	-	7,7,7	0.54	0	9,10,10	0.53	0
63	PGE	DS	201	-	9,9,9	0.29	0	8,8,8	0.21	0
58	MPD	AA	1676	-	7,7,7	0.54	0	9,10,10	0.57	0
65	1PE	DA	3200	-	15,15,15	0.30	0	14,14,14	0.38	0
62	EDO	DA	3196	-	3,3,3	0.56	0	2,2,2	0.17	0
62	EDO	DA	3205	-	3,3,3	0.72	0	2,2,2	0.10	0
62	EDO	D1	101	-	3,3,3	0.58	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	1PE	DA	3183	-	15,15,15	0.18	0	14,14,14	0.15	0
57	PG4	DA	3213	-	12,12,12	0.14	0	11,11,11	0.16	0
59	PUT	AA	1673	-	5,5,5	0.09	0	4,4,4	0.09	0
66	ACY	DA	3194	-	3,3,3	2.36	1 (33%)	3,3,3	2.16	2 (66%)
59	PUT	DA	3202	-	5,5,5	0.09	0	4,4,4	0.09	0
58	MPD	DT	202	-	7,7,7	0.57	0	9,10,10	0.40	0
62	EDO	DA	3212	-	3,3,3	0.57	0	2,2,2	0.39	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.11	0
63	PGE	DA	3184	-	9,9,9	0.25	0	8,8,8	0.32	0
58	MPD	DN	201	-	7,7,7	0.81	0	9,10,10	0.49	0
58	MPD	DS	203	-	7,7,7	0.26	0	9,10,10	0.41	0
59	PUT	DA	3216	-	5,5,5	0.20	0	4,4,4	0.18	0
64	SPD	DA	3181	-	9,9,9	0.07	0	8,8,8	0.14	0
61	PEG	DP	201	-	6,6,6	0.12	0	5,5,5	0.04	0
59	PUT	DA	3186	-	5,5,5	0.30	0	4,4,4	0.20	0
62	EDO	DA	3206	-	3,3,3	0.58	0	2,2,2	0.28	0
61	PEG	AL	201	-	6,6,6	0.20	0	5,5,5	0.10	0
62	EDO	DA	3001	-	3,3,3	0.52	0	2,2,2	0.45	0
59	PUT	DA	3209	-	5,5,5	0.19	0	4,4,4	0.09	0
61	PEG	DA	3223	-	6,6,6	0.20	0	5,5,5	0.06	0
61	PEG	DA	3197	-	6,6,6	0.16	0	5,5,5	0.08	0
57	PG4	DS	202	-	12,12,12	0.29	0	11,11,11	0.23	0
58	MPD	DA	3201	-	7,7,7	0.54	0	9,10,10	0.51	0
59	PUT	DA	3226	-	5,5,5	0.10	0	4,4,4	0.08	0
61	PEG	DQ	201	-	6,6,6	0.11	0	5,5,5	0.07	0
63	PGE	DD	302	-	9,9,9	0.16	0	8,8,8	0.11	0
58	MPD	DE	301	-	7,7,7	0.70	0	9,10,10	0.49	0
59	PUT	DA	3220	-	5,5,5	0.14	0	4,4,4	0.07	0
59	PUT	AA	1674	-	5,5,5	0.14	0	4,4,4	0.06	0
58	MPD	DK	201	-	7,7,7	0.75	0	9,10,10	0.33	0
59	PUT	AA	1672	-	5,5,5	0.18	0	4,4,4	0.12	0
63	PGE	DT	201	-	9,9,9	0.14	0	8,8,8	0.12	0
61	PEG	DA	3198	-	6,6,6	0.21	0	5,5,5	0.15	0
68	TRS	DA	3217	-	7,7,7	0.27	0	9,9,9	0.28	0
63	PGE	DA	3211	-	9,9,9	0.10	0	8,8,8	0.08	0
63	PGE	D3	101	-	9,9,9	0.17	0	8,8,8	0.09	0
58	MPD	DA	3188	-	7,7,7	0.51	0	9,10,10	0.53	0
61	PEG	DA	3224	-	6,6,6	0.28	0	5,5,5	0.19	0
59	PUT	DA	3187	-	5,5,5	0.26	0	4,4,4	0.11	0
57	PG4	DA	3191	-	12,12,12	0.19	0	11,11,11	0.21	0
61	PEG	D3	102	-	6,6,6	0.25	0	5,5,5	0.17	0
59	PUT	DA	3210	-	5,5,5	0.19	0	4,4,4	0.08	0
57	PG4	AA	1670	-	12,12,12	0.25	0	11,11,11	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	DA	3222	-	9,9,9	0.15	0	8,8,8	0.27	0
58	MPD	DA	3190	-	7,7,7	0.51	0	9,10,10	0.64	0
66	ACY	DA	3189	-	3,3,3	0.60	0	3,3,3	0.98	0
58	MPD	DA	3228	-	7,7,7	0.54	0	9,10,10	0.34	0
66	ACY	DA	3199	-	3,3,3	0.66	0	3,3,3	0.97	0
62	EDO	D0	101	-	3,3,3	0.58	0	2,2,2	0.30	0
59	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.28	0
61	PEG	DL	201	-	6,6,6	0.17	0	5,5,5	0.08	0
58	MPD	AA	1671	-	7,7,7	0.60	0	9,10,10	0.44	0
59	PUT	DA	3218	-	5,5,5	0.16	0	4,4,4	0.13	0
61	PEG	D1	102	-	6,6,6	0.24	0	5,5,5	0.08	0
57	PG4	DQ	202	-	12,12,12	0.18	0	11,11,11	0.13	0
64	SPD	DA	3203	-	9,9,9	0.18	0	8,8,8	0.23	0
63	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.18	0
62	EDO	DA	3192	-	3,3,3	0.50	0	2,2,2	0.34	0
62	EDO	DB	211	-	3,3,3	0.53	0	2,2,2	0.31	0
57	PG4	DR	203	-	12,12,12	0.20	0	11,11,11	0.22	0
63	PGE	DA	3214	-	9,9,9	0.16	0	8,8,8	0.14	0
62	EDO	DA	3195	-	3,3,3	0.57	0	2,2,2	0.32	0
67	GUN	DA	3208	-	12,12,12	0.37	0	15,17,17	0.28	0
59	PUT	DA	3193	-	5,5,5	0.33	0	4,4,4	0.38	0
62	EDO	DB	210	-	3,3,3	0.54	0	2,2,2	0.25	0
58	MPD	DE	302	-	7,7,7	0.62	0	9,10,10	0.52	0
59	PUT	DA	3182	-	5,5,5	0.13	0	4,4,4	0.13	0
64	SPD	DA	3221	-	9,9,9	0.10	0	8,8,8	0.33	0
61	PEG	DA	3215	-	6,6,6	0.15	0	5,5,5	0.04	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	DA	3207	-	-	0/5/5/5	-
64	SPD	DA	3185	-	-	1/7/7/7	-
62	EDO	DA	3227	-	-	0/1/1/1	-
57	PG4	BA	1642	-	-	1/10/10/10	-
58	MPD	DA	3204	-	-	2/5/5/5	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	MPD	AA	1676	-	-	1/5/5/5	-
65	1PE	DA	3200	-	-	5/13/13/13	-
62	EDO	DA	3196	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	EDO	DA	3205	-	-	0/1/1/1	-
62	EDO	D1	101	-	-	0/1/1/1	-
65	1PE	DA	3183	-	-	5/13/13/13	-
57	PG4	DA	3213	-	-	4/10/10/10	-
59	PUT	AA	1673	-	-	0/3/3/3	-
59	PUT	DA	3202	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	1/5/5/5	-
62	EDO	DA	3212	-	-	0/1/1/1	-
59	PUT	AA	1675	-	-	1/3/3/3	-
63	PGE	DA	3184	-	-	3/7/7/7	-
58	MPD	DN	201	-	-	3/5/5/5	-
58	MPD	DS	203	-	-	0/5/5/5	-
59	PUT	DA	3216	-	-	0/3/3/3	-
64	SPD	DA	3181	-	-	4/7/7/7	-
61	PEG	DP	201	-	-	2/4/4/4	-
59	PUT	DA	3186	-	-	0/3/3/3	-
62	EDO	DA	3206	-	-	0/1/1/1	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	EDO	DA	3001	-	-	0/1/1/1	-
59	PUT	DA	3209	-	-	0/3/3/3	-
61	PEG	DA	3223	-	-	2/4/4/4	-
61	PEG	DA	3197	-	-	1/4/4/4	-
57	PG4	DS	202	-	-	2/10/10/10	-
58	MPD	DA	3201	-	-	4/5/5/5	-
59	PUT	DA	3226	-	-	0/3/3/3	-
61	PEG	DQ	201	-	-	1/4/4/4	-
63	PGE	DD	302	-	-	4/7/7/7	-
58	MPD	DE	301	-	-	1/5/5/5	-
59	PUT	DA	3220	-	-	1/3/3/3	-
59	PUT	AA	1674	-	-	1/3/3/3	-
58	MPD	DK	201	-	-	1/5/5/5	-
59	PUT	AA	1672	-	-	0/3/3/3	-
63	PGE	DT	201	-	-	4/7/7/7	-
61	PEG	DA	3198	-	-	1/4/4/4	-
68	TRS	DA	3217	-	-	0/9/9/9	-
63	PGE	DA	3211	-	-	3/7/7/7	-
63	PGE	D3	101	-	-	2/7/7/7	-
58	MPD	DA	3188	-	-	2/5/5/5	-
61	PEG	DA	3224	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3187	-	-	0/3/3/3	-
57	PG4	DA	3191	-	-	5/10/10/10	-
61	PEG	D3	102	-	-	1/4/4/4	-
59	PUT	DA	3210	-	-	0/3/3/3	-
57	PG4	AA	1670	-	-	5/10/10/10	-
63	PGE	DA	3222	-	-	3/7/7/7	-
58	MPD	DA	3190	-	-	2/5/5/5	-
58	MPD	DA	3228	-	-	2/5/5/5	-
62	EDO	D0	101	-	-	1/1/1/1	-
59	PUT	DA	3219	-	-	1/3/3/3	-
61	PEG	DL	201	-	-	1/4/4/4	-
58	MPD	AA	1671	-	-	0/5/5/5	-
59	PUT	DA	3218	-	-	0/3/3/3	-
61	PEG	D1	102	-	-	2/4/4/4	-
57	PG4	DQ	202	-	-	3/10/10/10	-
64	SPD	DA	3203	-	-	1/7/7/7	-
63	PGE	DU	101	-	-	3/7/7/7	-
62	EDO	DA	3192	-	-	0/1/1/1	-
62	EDO	DB	211	-	-	0/1/1/1	-
57	PG4	DR	203	-	-	5/10/10/10	-
63	PGE	DA	3214	-	-	3/7/7/7	-
62	EDO	DA	3195	-	-	0/1/1/1	-
67	GUN	DA	3208	-	-	-	0/2/2/2
59	PUT	DA	3193	-	-	0/3/3/3	-
62	EDO	DB	210	-	-	0/1/1/1	-
58	MPD	DE	302	-	-	2/5/5/5	-
59	PUT	DA	3182	-	-	0/3/3/3	-
64	SPD	DA	3221	-	-	2/7/7/7	-
61	PEG	DA	3215	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3194	ACY	O-C	3.75	1.38	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3194	ACY	OXT-C-CH3	2.93	127.32	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3194	ACY	O-C-CH3	-2.18	113.59	122.53

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-O4
58	DA	3201	MPD	C2-C3-C4-O4
58	DA	3201	MPD	C2-C3-C4-C5
58	DE	302	MPD	C2-C3-C4-O4
64	DA	3181	SPD	C3-C4-C5-N6

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	1642	PG4	1	0
63	DS	201	PGE	2	0
65	DA	3183	1PE	1	0
62	DA	3206	EDO	1	0
57	DS	202	PG4	1	0
58	DE	301	MPD	1	0
68	DA	3217	TRS	1	0
57	DA	3191	PG4	1	0
59	DA	3210	PUT	1	0
57	AA	1670	PG4	1	0
63	DA	3222	PGE	2	0
58	DA	3190	MPD	1	0
58	AA	1671	MPD	1	0
61	D1	102	PEG	2	0
57	DR	203	PG4	3	0
59	DA	3193	PUT	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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	-0.26	11 (0%) 84 68	40, 90, 219, 296	0
1	BA	1522/1534 (99%)	0.39	82 (5%) 31 17	46, 131, 271, 279	0
2	AB	224/224 (100%)	0.42	7 (3%) 51 31	65, 116, 194, 247	0
2	BB	224/224 (100%)	0.56	10 (4%) 38 21	91, 129, 190, 236	0
3	AC	206/206 (100%)	-0.04	1 (0%) 87 73	67, 95, 126, 146	0
3	BC	206/206 (100%)	0.48	5 (2%) 59 38	86, 134, 172, 196	0
4	AD	205/205 (100%)	0.17	0 100 100	63, 99, 125, 146	0
4	BD	205/205 (100%)	-0.19	0 100 100	42, 72, 104, 134	0
5	AE	155/155 (100%)	-0.00	1 (0%) 85 70	48, 82, 118, 155	0
5	BE	150/155 (96%)	0.16	0 100 100	60, 83, 132, 206	0
6	AF	106/106 (100%)	0.12	0 100 100	68, 94, 118, 143	0
6	BF	100/106 (94%)	0.34	2 (2%) 65 44	79, 114, 141, 155	0
7	AG	151/151 (100%)	0.41	8 (5%) 32 17	81, 116, 143, 156	0
7	BG	151/151 (100%)	1.01	22 (14%) 6 3	125, 189, 206, 220	0
8	AH	129/129 (100%)	0.02	2 (1%) 70 49	54, 84, 111, 121	0
8	BH	129/129 (100%)	0.45	4 (3%) 51 31	76, 108, 142, 160	0
9	AI	127/127 (100%)	0.51	5 (3%) 43 24	76, 114, 149, 158	0
9	BI	127/127 (100%)	0.96	20 (15%) 5 2	125, 158, 188, 202	0
10	AJ	99/99 (100%)	0.63	2 (2%) 65 44	70, 106, 135, 146	0
10	BJ	98/99 (98%)	1.15	14 (14%) 6 3	121, 165, 189, 199	0
11	AK	117/117 (100%)	0.35	1 (0%) 81 63	54, 106, 141, 153	0
11	BK	117/117 (100%)	0.39	4 (3%) 48 28	80, 117, 144, 170	0
12	AL	122/123 (99%)	-0.00	1 (0%) 82 64	49, 69, 99, 124	0
12	BL	122/123 (99%)	0.50	4 (3%) 49 29	62, 90, 116, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.61	3 (2%) 57 36	89, 118, 154, 171	0
13	BM	114/114 (100%)	0.92	9 (7%) 18 10	195, 227, 238, 248	0
14	AN	100/100 (100%)	0.66	3 (3%) 52 32	71, 104, 179, 192	0
14	BN	100/100 (100%)	1.13	16 (16%) 5 2	114, 173, 217, 228	0
15	AO	88/88 (100%)	0.03	0 100 100	58, 81, 108, 136	0
15	BO	88/88 (100%)	0.38	0 100 100	70, 111, 132, 159	0
16	AP	82/82 (100%)	0.27	2 (2%) 59 38	62, 82, 127, 146	0
16	BP	82/82 (100%)	1.31	13 (15%) 5 2	95, 114, 151, 162	0
17	AQ	80/80 (100%)	0.24	2 (2%) 58 37	54, 79, 116, 139	0
17	BQ	80/80 (100%)	0.84	5 (6%) 26 14	82, 125, 147, 160	0
18	AR	55/55 (100%)	0.04	0 100 100	53, 87, 117, 153	0
18	BR	55/55 (100%)	0.32	2 (3%) 46 26	60, 88, 124, 154	0
19	AS	79/79 (100%)	0.60	4 (5%) 33 18	90, 114, 145, 152	0
19	BS	79/79 (100%)	1.05	13 (16%) 4 2	200, 222, 234, 239	0
20	AT	86/86 (100%)	0.42	1 (1%) 76 58	64, 83, 113, 136	0
20	BT	85/86 (98%)	1.36	16 (18%) 3 2	108, 138, 167, 180	0
21	AU	56/56 (100%)	0.87	9 (16%) 4 2	93, 124, 166, 180	0
21	BU	56/56 (100%)	0.53	2 (3%) 46 26	81, 107, 154, 167	0
22	C1	56/56 (100%)	1.84	24 (42%) 0 0	124, 162, 181, 184	0
22	D1	56/56 (100%)	-0.59	0 100 100	14, 39, 71, 99	0
23	C2	50/51 (98%)	1.15	9 (18%) 3 2	139, 161, 173, 186	0
23	D2	51/51 (100%)	-0.23	0 100 100	54, 67, 101, 110	0
24	C3	46/46 (100%)	2.36	25 (54%) 0 0	119, 143, 157, 165	0
24	D3	46/46 (100%)	-0.36	1 (2%) 62 41	29, 40, 64, 112	0
25	C4	64/64 (100%)	2.23	33 (51%) 0 0	116, 138, 155, 161	0
25	D4	64/64 (100%)	-0.46	0 100 100	26, 41, 53, 73	0
26	C5	38/38 (100%)	1.68	14 (36%) 1 1	108, 126, 139, 143	0
26	D5	38/38 (100%)	-0.36	0 100 100	33, 45, 69, 87	0
27	C0	58/58 (100%)	1.47	16 (27%) 1 1	115, 135, 151, 156	0
27	D0	58/58 (100%)	-0.42	2 (3%) 48 28	17, 32, 59, 94	2 (3%)
28	CB	118/120 (98%)	0.66	0 100 100	135, 190, 241, 251	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.84	0 100 100	28, 57, 87, 143	0
29	CC	271/271 (100%)	0.91	42 (15%) 5 2	80, 113, 143, 167	0
29	DC	271/271 (100%)	-0.35	2 (0%) 84 68	23, 53, 84, 113	0
30	CD	209/209 (100%)	1.42	59 (28%) 1 1	102, 136, 165, 177	0
31	CA	2876/2904 (99%)	1.17	465 (16%) 4 2	69, 185, 272, 290	0
32	DD	208/209 (99%)	-0.63	0 100 100	15, 40, 73, 98	0
33	DA	2873/2903 (98%)	-0.82	44 (1%) 72 52	13, 46, 203, 298	11 (0%)
34	CE	201/201 (100%)	1.62	71 (35%) 1 1	121, 176, 206, 224	0
34	DE	201/201 (100%)	-0.39	0 100 100	17, 57, 103, 139	0
35	CF	177/177 (100%)	0.88	10 (5%) 30 16	194, 215, 226, 232	0
35	DF	177/177 (100%)	-0.02	0 100 100	52, 80, 120, 145	0
36	CG	176/176 (100%)	0.91	13 (7%) 20 11	146, 178, 208, 222	0
36	DG	176/176 (100%)	-0.19	1 (0%) 85 70	33, 70, 99, 136	0
37	CH	149/149 (100%)	0.44	4 (2%) 56 35	89, 149, 170, 178	0
37	DH	149/149 (100%)	0.38	1 (0%) 84 68	73, 154, 190, 203	0
38	CJ	134/134 (100%)	1.27	25 (18%) 3 2	236, 254, 265, 273	0
38	DJ	134/134 (100%)	1.31	25 (18%) 3 2	193, 222, 235, 242	0
39	CK	142/142 (100%)	1.54	47 (33%) 1 1	106, 132, 169, 195	0
39	DK	142/142 (100%)	-0.57	0 100 100	18, 35, 66, 88	0
40	CL	122/123 (99%)	1.01	10 (8%) 17 9	96, 118, 151, 168	0
40	DL	123/123 (100%)	-0.55	0 100 100	26, 44, 70, 112	0
41	CM	144/144 (100%)	1.80	57 (39%) 1 0	117, 169, 227, 247	0
41	DM	144/144 (100%)	-0.39	0 100 100	14, 54, 87, 128	0
42	CN	135/136 (99%)	1.14	20 (14%) 5 3	92, 125, 151, 178	0
42	DN	135/136 (99%)	-0.62	0 100 100	20, 41, 73, 89	1 (0%)
43	CO	120/125 (96%)	1.89	43 (35%) 1 1	110, 141, 163, 197	0
43	DO	125/125 (100%)	-0.64	0 100 100	18, 36, 84, 137	0
44	CP	116/117 (99%)	1.11	19 (16%) 4 2	140, 171, 187, 195	0
44	DP	117/117 (100%)	-0.34	0 100 100	34, 55, 88, 95	0
45	CQ	114/114 (100%)	1.17	19 (16%) 4 2	113, 131, 157, 180	0
45	DQ	114/114 (100%)	-0.46	0 100 100	29, 51, 80, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	CR	117/117 (100%)	1.96	51 (43%) 0 0	108, 137, 166, 175	0
46	DR	117/117 (100%)	-0.67	0 100 100	14, 30, 50, 80	0
47	CS	103/103 (100%)	1.72	32 (31%) 1 1	124, 149, 173, 187	0
47	DS	103/103 (100%)	-0.64	0 100 100	19, 43, 76, 103	0
48	CT	110/110 (100%)	1.91	45 (40%) 0 0	123, 155, 177, 188	0
48	DT	110/110 (100%)	-0.62	0 100 100	19, 33, 66, 126	0
49	CU	93/93 (100%)	1.63	29 (31%) 1 1	136, 168, 193, 201	0
49	DU	93/93 (100%)	-0.07	0 100 100	26, 55, 126, 141	0
50	CV	102/102 (100%)	2.08	41 (40%) 0 0	147, 176, 207, 219	0
50	DV	102/102 (100%)	-0.30	0 100 100	41, 62, 104, 139	0
51	CW	94/94 (100%)	0.80	6 (6%) 25 14	128, 153, 165, 173	0
51	DW	94/94 (100%)	-0.43	2 (2%) 63 42	29, 54, 86, 99	0
52	CX	75/76 (98%)	1.29	13 (17%) 4 2	109, 140, 152, 186	0
52	DX	76/76 (100%)	-0.43	0 100 100	16, 40, 74, 114	1 (1%)
53	CY	77/77 (100%)	1.35	20 (25%) 1 1	108, 123, 156, 170	0
53	DY	77/77 (100%)	-0.28	0 100 100	32, 55, 88, 98	0
54	CZ	62/62 (100%)	1.85	22 (35%) 1 1	161, 179, 190, 196	0
54	DZ	62/62 (100%)	-0.07	0 100 100	44, 74, 108, 140	0
55	DI	135/135 (100%)	0.77	12 (8%) 15 8	78, 153, 204, 224	1 (0%)
All	All	20634/20744 (99%)	0.34	1680 (8%) 18 10	13, 111, 241, 298	16 (0%)

The worst 5 of 1680 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	CM	27	LEU	6.8
48	CT	47	VAL	6.7
46	CR	8	VAL	6.6
43	CO	46	ARG	6.5
43	CO	25	ALA	6.5

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
31	PSU	CA	1917	20/21	0.62	0.12	120,122,127,127	0
31	6MZ	CA	1618	23/24	0.72	0.17	165,167,172,173	0
31	PSU	CA	1911	20/21	0.74	0.08	128,136,137,138	0
1	2MG	BA	966	24/25	0.75	0.14	140,144,153,153	0
31	3TD	CA	1915	21/22	0.78	0.08	139,145,147,148	0
31	PSU	CA	955	20/21	0.78	0.14	108,113,117,117	0
31	2MA	CA	2503	23/24	0.79	0.17	101,104,114,114	0
1	2MG	BA	1207	24/25	0.81	0.11	154,155,158,161	0
31	PSU	CA	2580	20/21	0.81	0.15	105,112,116,117	0
31	PSU	CA	2504	20/21	0.82	0.16	91,98,101,102	0
31	6MZ	CA	2030	23/24	0.82	0.15	117,125,129,130	0
1	5MC	BA	967	21/22	0.83	0.12	135,141,145,145	0
31	PSU	CA	2457	20/21	0.84	0.14	109,112,117,118	0
31	PSU	CA	746	20/21	0.85	0.16	127,129,130,130	0
42	4D4	CN	81	12/13	0.85	0.12	99,103,115,116	0
12	D2T	BL	89	10/11	0.88	0.14	79,85,97,98	0
31	2MG	CA	2445	24/25	0.89	0.15	79,94,103,104	0
31	OMU	CA	2552	21/22	0.89	0.15	100,103,113,115	0
1	PSU	BA	516	20/21	0.89	0.11	78,85,90,91	0
31	G7M	CA	2069	24/25	0.89	0.16	105,111,117,118	0
31	1MG	CA	745	24/25	0.90	0.17	117,123,124,126	0
1	5MC	BA	1407	21/22	0.90	0.11	93,96,104,107	0
31	OMG	CA	2251	24/25	0.90	0.14	95,101,105,106	0
31	5MU	CA	747	21/22	0.90	0.11	129,137,142,144	0
31	PSU	CA	2605	20/21	0.90	0.12	81,87,95,96	0
33	PSU	DA	1917	20/21	0.90	0.08	83,86,95,95	0
12	D2T	AL	89	10/11	0.90	0.13	59,63,78,81	0
31	2MG	CA	1835	24/25	0.91	0.11	76,80,82,83	0
31	5MU	CA	1939	21/22	0.91	0.12	79,86,88,89	0
1	2MG	BA	1516	24/25	0.92	0.10	82,87,93,93	0
33	3TD	DA	1915	21/22	0.92	0.09	110,116,120,122	0
1	2MG	AA	966	24/25	0.92	0.09	83,86,88,88	0
1	2MG	AA	1207	24/25	0.92	0.08	90,100,107,107	0
31	5MC	CA	1962	21/22	0.93	0.10	76,79,80,85	0
1	MA6	BA	1518	24/25	0.93	0.11	71,77,85,86	0
1	5MC	AA	967	21/22	0.93	0.10	84,88,89,89	0
31	OMC	CA	2498	21/22	0.93	0.11	98,104,108,109	0
1	UR3	BA	1498	21/22	0.94	0.09	83,84,89,89	0
1	PSU	AA	516	20/21	0.94	0.08	77,81,84,85	0
33	PSU	DA	1911	20/21	0.94	0.07	86,90,91,92	0
1	MA6	BA	1519	24/25	0.95	0.10	78,82,85,85	0
1	UR3	AA	1498	21/22	0.95	0.09	54,58,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	G7M	BA	527	24/25	0.95	0.09	69,73,78,78	0
33	PSU	DA	2604	20/21	0.95	0.08	31,43,54,56	0
1	G7M	AA	527	24/25	0.95	0.09	57,62,67,70	0
1	4OC	BA	1402	22/23	0.96	0.07	72,74,77,78	0
1	MA6	AA	1519	24/25	0.97	0.08	46,51,55,59	0
1	5MC	AA	1407	21/22	0.97	0.06	54,55,57,58	0
1	4OC	AA	1402	22/23	0.97	0.07	60,63,64,65	0
33	5MU	DA	1939	21/22	0.97	0.09	38,40,48,50	0
1	MA6	AA	1518	24/25	0.97	0.07	45,48,54,54	0
33	2MG	DA	1835	24/25	0.97	0.08	44,48,54,61	0
42	4D4	DN	81[A]	12/13	0.97	0.08	29,36,47,49	9
42	4D4	DN	81[B]	12/13	0.97	0.08	13,22,30,31	9
33	2MA	DA	2503	23/24	0.98	0.07	16,28,36,40	0
33	PSU	DA	2504	20/21	0.98	0.06	29,34,37,41	0
33	5MU	DA	747	21/22	0.98	0.06	26,28,35,37	0
33	PSU	DA	2605	20/21	0.98	0.05	33,40,41,41	0
1	2MG	AA	1516	24/25	0.98	0.06	51,53,55,57	0
33	5MC	DA	1962	21/22	0.98	0.06	40,46,48,48	0
33	G7M	DA	2069	24/25	0.98	0.07	34,37,43,45	0
33	OMG	DA	2251	24/25	0.99	0.04	28,30,40,44	0
33	2MG	DA	2445	24/25	0.99	0.05	16,25,30,31	0
33	H2U	DA	2449	20/21	0.99	0.06	12,22,32,33	0
33	PSU	DA	2457	20/21	0.99	0.04	24,25,30,32	0
33	OMC	DA	2498	21/22	0.99	0.05	15,20,26,33	0
33	1MG	DA	745	24/25	0.99	0.05	26,32,36,38	0
33	PSU	DA	746	20/21	0.99	0.04	16,22,31,32	0
33	OMU	DA	2552	21/22	0.99	0.06	25,30,35,42	0
33	PSU	DA	2580	20/21	0.99	0.05	18,26,29,31	0
32	MEQ	DD	150[A]	10/11	0.99	0.09	9,14,29,29	10
33	PSU	DA	955	20/21	0.99	0.05	17,22,24,25	0
33	6MZ	DA	1618	23/24	0.99	0.04	17,28,32,32	0
33	6MZ	DA	2030	23/24	0.99	0.04	16,20,26,27	0
32	MEQ	DD	150[B]	10/11	0.99	0.09	26,31,38,40	10

6.3 Carbohydrates i

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	CA	3110	1/1	0.06	0.41	168,168,168,168	0
56	MG	CA	3124	1/1	0.11	0.25	165,165,165,165	0
56	MG	CA	3146	1/1	0.11	0.25	220,220,220,220	0
56	MG	CA	3007	1/1	0.31	0.13	256,256,256,256	0
56	MG	CA	3038	1/1	0.37	0.10	250,250,250,250	0
56	MG	CA	3115	1/1	0.38	0.44	85,85,85,85	0
56	MG	CA	3123	1/1	0.44	0.26	200,200,200,200	0
56	MG	CA	3003	1/1	0.52	0.31	280,280,280,280	0
56	MG	CA	3132	1/1	0.53	0.19	116,116,116,116	0
56	MG	AA	1628	1/1	0.57	0.22	177,177,177,177	0
56	MG	AA	1606	1/1	0.57	0.46	106,106,106,106	0
56	MG	CA	3002	1/1	0.58	0.20	273,273,273,273	0
56	MG	DA	3166	1/1	0.59	0.27	141,141,141,141	0
56	MG	CA	3092	1/1	0.61	0.14	210,210,210,210	0
56	MG	BA	1624	1/1	0.61	0.27	274,274,274,274	0
56	MG	CA	3139	1/1	0.62	0.28	100,100,100,100	0
56	MG	CA	3075	1/1	0.63	0.24	241,241,241,241	0
56	MG	BA	1604	1/1	0.64	0.15	218,218,218,218	0
56	MG	CA	3104	1/1	0.64	0.13	234,234,234,234	0
56	MG	CA	3111	1/1	0.65	0.24	121,121,121,121	0
56	MG	CA	3077	1/1	0.65	0.09	240,240,240,240	0
56	MG	CA	3061	1/1	0.66	0.15	264,264,264,264	0
56	MG	CA	3034	1/1	0.66	0.19	239,239,239,239	0
56	MG	AA	1619	1/1	0.67	0.21	98,98,98,98	0
56	MG	CA	3032	1/1	0.67	0.15	257,257,257,257	0
56	MG	CA	3005	1/1	0.67	0.18	250,250,250,250	0
56	MG	CA	3154	1/1	0.68	0.23	132,132,132,132	0
56	MG	CA	3067	1/1	0.68	0.17	283,283,283,283	0
56	MG	BA	1625	1/1	0.69	0.15	269,269,269,269	0
56	MG	CA	3060	1/1	0.70	0.13	259,259,259,259	0
56	MG	CA	3152	1/1	0.71	0.15	167,167,167,167	0
56	MG	CA	3014	1/1	0.71	0.16	256,256,256,256	0
56	MG	CA	3026	1/1	0.71	0.12	201,201,201,201	0
56	MG	CA	3083	1/1	0.73	0.17	263,263,263,263	0
56	MG	CA	3021	1/1	0.74	0.38	272,272,272,272	0
56	MG	CA	3028	1/1	0.74	0.12	263,263,263,263	0
56	MG	CA	3155	1/1	0.76	0.19	196,196,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	CA	3135	1/1	0.76	0.30	96,96,96,96	0
56	MG	CA	3156	1/1	0.77	0.11	252,252,252,252	0
61	PEG	DP	201	7/7	0.77	0.24	136,137,140,141	0
56	MG	CA	3047	1/1	0.78	0.35	230,230,230,230	0
56	MG	CA	3009	1/1	0.78	0.13	271,271,271,271	0
56	MG	CA	3008	1/1	0.78	0.17	251,251,251,251	0
56	MG	BA	1606	1/1	0.79	0.18	249,249,249,249	0
56	MG	CA	3140	1/1	0.79	0.16	112,112,112,112	0
58	MPD	DK	201	8/8	0.79	0.20	138,140,140,141	0
56	MG	CA	3122	1/1	0.79	0.19	81,81,81,81	0
56	MG	CA	3141	1/1	0.80	0.24	72,72,72,72	0
58	MPD	DE	301	8/8	0.80	0.22	151,152,153,153	0
56	MG	CA	3151	1/1	0.81	0.28	81,81,81,81	0
56	MG	CA	3129	1/1	0.81	0.19	109,109,109,109	0
56	MG	AA	1605	1/1	0.81	0.36	98,98,98,98	0
56	MG	CA	3133	1/1	0.81	0.15	112,112,112,112	0
56	MG	BA	1640	1/1	0.81	0.21	131,131,131,131	0
56	MG	DA	3159	1/1	0.81	0.33	60,60,60,60	0
56	MG	AA	1609	1/1	0.81	0.19	72,72,72,72	0
56	MG	CA	3071	1/1	0.81	0.10	230,230,230,230	0
56	MG	AA	1661	1/1	0.81	0.11	166,166,166,166	0
59	PUT	AA	1673	6/6	0.81	0.12	91,92,94,95	0
56	MG	CA	3126	1/1	0.81	0.08	74,74,74,74	0
56	MG	CA	3073	1/1	0.82	0.20	212,212,212,212	0
56	MG	CA	3023	1/1	0.82	0.24	206,206,206,206	0
56	MG	DA	3157	1/1	0.82	0.12	67,67,67,67	0
56	MG	CA	3039	1/1	0.82	0.17	203,203,203,203	0
56	MG	BA	1639	1/1	0.82	0.11	70,70,70,70	0
56	MG	CA	3019	1/1	0.82	0.12	71,71,71,71	0
56	MG	BA	1603	1/1	0.82	0.10	254,254,254,254	0
56	MG	CA	3022	1/1	0.82	0.21	235,235,235,235	0
59	PUT	AA	1675	6/6	0.82	0.27	111,112,113,113	0
56	MG	CA	3037	1/1	0.82	0.19	206,206,206,206	0
56	MG	DA	3169	1/1	0.83	0.11	86,86,86,86	0
56	MG	DA	3171	1/1	0.83	0.31	106,106,106,106	0
56	MG	AA	1624	1/1	0.83	0.23	85,85,85,85	0
56	MG	CA	3072	1/1	0.83	0.11	273,273,273,273	0
56	MG	CA	3064	1/1	0.83	0.16	283,283,283,283	0
59	PUT	AA	1674	6/6	0.83	0.29	108,109,110,110	0
56	MG	CA	3010	1/1	0.83	0.13	250,250,250,250	0
56	MG	CA	3131	1/1	0.83	0.16	75,75,75,75	0
56	MG	AA	1623	1/1	0.84	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	BA	1607	1/1	0.84	0.13	203,203,203,203	0
56	MG	CA	3006	1/1	0.84	0.10	240,240,240,240	0
56	MG	BA	1636	1/1	0.84	0.28	91,91,91,91	0
62	EDO	DA	3001	4/4	0.84	0.23	95,95,95,96	0
56	MG	CA	3112	1/1	0.85	0.23	85,85,85,85	0
56	MG	DA	3170	1/1	0.85	0.31	79,79,79,79	0
56	MG	CA	3036	1/1	0.85	0.21	194,194,194,194	0
58	MPD	DA	3188	8/8	0.85	0.20	91,94,96,98	0
56	MG	CA	3120	1/1	0.85	0.15	135,135,135,135	0
56	MG	CA	3091	1/1	0.85	0.10	137,137,137,137	0
56	MG	AA	1660	1/1	0.85	0.15	278,278,278,278	0
56	MG	CA	3076	1/1	0.85	0.12	214,214,214,214	0
56	MG	CA	3065	1/1	0.85	0.12	151,151,151,151	0
59	PUT	DA	3218	6/6	0.85	0.24	122,122,123,123	0
61	PEG	DA	3197	7/7	0.85	0.22	91,99,102,102	0
56	MG	DA	3160	1/1	0.85	0.15	87,87,87,87	0
61	PEG	DQ	201	7/7	0.85	0.15	118,119,121,121	0
56	MG	CA	3082	1/1	0.85	0.16	152,152,152,152	0
58	MPD	DA	3201	8/8	0.86	0.26	125,126,127,128	0
56	MG	CA	3121	1/1	0.86	0.17	63,63,63,63	0
56	MG	AA	1615	1/1	0.86	0.56	110,110,110,110	0
56	MG	AA	1608	1/1	0.86	0.20	83,83,83,83	0
56	MG	CA	3105	1/1	0.86	0.19	254,254,254,254	0
56	MG	BA	1629	1/1	0.86	0.16	195,195,195,195	0
56	MG	CA	3004	1/1	0.86	0.14	203,203,203,203	0
59	PUT	DA	3219	6/6	0.86	0.18	55,57,61,62	0
56	MG	AA	1622	1/1	0.86	0.17	70,70,70,70	0
56	MG	AA	1602	1/1	0.86	0.13	80,80,80,80	0
56	MG	DA	3178	1/1	0.86	0.11	105,105,105,105	0
56	MG	CA	3051	1/1	0.86	0.15	183,183,183,183	0
56	MG	CA	3094	1/1	0.87	0.15	139,139,139,139	0
58	MPD	DN	201	8/8	0.87	0.18	90,95,96,96	0
56	MG	AA	1603	1/1	0.87	0.19	91,91,91,91	0
56	MG	CA	3068	1/1	0.87	0.21	266,266,266,266	0
56	MG	CA	3134	1/1	0.87	0.13	134,134,134,134	0
56	MG	CA	3125	1/1	0.87	0.11	85,85,85,85	0
56	MG	CA	3109	1/1	0.87	0.18	80,80,80,80	0
57	PG4	DQ	202	13/13	0.87	0.14	65,68,81,81	0
56	MG	DA	3129	1/1	0.87	0.09	46,46,46,46	0
56	MG	CA	3127	1/1	0.87	0.17	71,71,71,71	0
56	MG	BA	1617	1/1	0.87	0.10	160,160,160,160	0
59	PUT	AA	1672	6/6	0.88	0.27	88,89,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	PG4	BA	1642	13/13	0.88	0.14	94,97,106,107	0
57	PG4	DA	3213	13/13	0.88	0.18	101,107,112,112	0
56	MG	DA	3122	1/1	0.88	0.31	86,86,86,86	0
59	PUT	DA	3182	6/6	0.88	0.23	77,78,80,80	0
56	MG	AA	1664	1/1	0.88	0.08	147,147,147,147	0
56	MG	DA	3137	1/1	0.88	0.51	29,29,29,29	1
58	MPD	DA	3204	8/8	0.88	0.18	93,94,97,97	0
56	MG	DA	3146	1/1	0.88	0.16	117,117,117,117	0
56	MG	CA	3054	1/1	0.88	0.12	180,180,180,180	0
56	MG	CA	3063	1/1	0.88	0.21	181,181,181,181	0
63	PGE	DS	201	10/10	0.88	0.12	68,74,77,77	0
66	ACY	DA	3194	4/4	0.88	0.18	52,56,56,58	0
56	MG	CA	3084	1/1	0.89	0.12	196,196,196,196	0
56	MG	CA	3107	1/1	0.89	0.26	67,67,67,67	0
56	MG	CA	3057	1/1	0.89	0.07	143,143,143,143	0
56	MG	DA	3176	1/1	0.89	0.11	59,59,59,59	0
61	PEG	AL	201	7/7	0.89	0.11	78,79,84,85	0
61	PEG	D3	102	7/7	0.89	0.26	105,109,110,111	0
58	MPD	DE	302	8/8	0.89	0.26	116,118,121,121	0
56	MG	CA	3137	1/1	0.89	0.06	137,137,137,137	0
57	PG4	AA	1670	13/13	0.89	0.12	77,84,91,92	0
56	MG	BA	1623	1/1	0.89	0.16	193,193,193,193	0
62	EDO	DA	3212	4/4	0.89	0.14	72,73,74,75	0
56	MG	CA	3074	1/1	0.89	0.11	142,142,142,142	0
63	PGE	DT	201	10/10	0.89	0.21	137,138,140,140	0
56	MG	BA	1619	1/1	0.89	0.19	198,198,198,198	0
56	MG	DA	3136	1/1	0.90	0.12	91,91,91,91	0
56	MG	CA	3087	1/1	0.90	0.11	196,196,196,196	0
59	PUT	DA	3193	6/6	0.90	0.30	88,90,92,92	0
59	PUT	DA	3210	6/6	0.90	0.32	108,110,112,113	0
56	MG	CA	3090	1/1	0.90	0.25	222,222,222,222	0
56	MG	DA	3155	1/1	0.90	0.09	47,47,47,47	0
56	MG	DA	3156	1/1	0.90	0.10	45,45,45,45	0
56	MG	CA	3145	1/1	0.90	0.13	50,50,50,50	0
56	MG	AA	1626	1/1	0.90	0.08	77,77,77,77	0
56	MG	CA	3001	1/1	0.90	0.17	294,294,294,294	0
56	MG	CA	3093	1/1	0.90	0.07	140,140,140,140	0
56	MG	AA	1612	1/1	0.90	0.14	59,59,59,59	0
56	MG	CA	3012	1/1	0.90	0.12	130,130,130,130	0
56	MG	AA	1635	1/1	0.90	0.23	209,209,209,209	0
56	MG	CA	3055	1/1	0.90	0.05	145,145,145,145	0
56	MG	CA	3085	1/1	0.90	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
68	TRS	DA	3217	8/8	0.90	0.15	149,150,153,155	0
56	MG	DA	3174	1/1	0.91	0.16	99,99,99,99	0
56	MG	CA	3142	1/1	0.91	0.13	73,73,73,73	0
56	MG	DA	3131	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3180	1/1	0.91	0.14	72,72,72,72	0
56	MG	CA	3099	1/1	0.91	0.15	189,189,189,189	0
59	PUT	DA	3216	6/6	0.91	0.19	71,72,72,72	0
56	MG	CA	3102	1/1	0.91	0.11	92,92,92,92	0
57	PG4	DA	3191	13/13	0.91	0.18	76,87,103,103	0
56	MG	CA	3029	1/1	0.91	0.16	181,181,181,181	0
56	MG	DA	3151	1/1	0.91	0.25	82,82,82,82	0
56	MG	BA	1612	1/1	0.91	0.21	200,200,200,200	0
61	PEG	DA	3198	7/7	0.91	0.29	118,120,124,124	0
56	MG	CA	3153	1/1	0.91	0.10	49,49,49,49	0
56	MG	CA	3106	1/1	0.91	0.10	81,81,81,81	0
62	EDO	DB	210	4/4	0.91	0.18	87,88,89,90	0
56	MG	CA	3119	1/1	0.91	0.08	68,68,68,68	0
62	EDO	DA	3206	4/4	0.91	0.25	104,104,105,105	0
56	MG	AA	1647	1/1	0.91	0.14	217,217,217,217	0
56	MG	DA	3061	1/1	0.91	0.07	209,209,209,209	0
56	MG	DA	3118	1/1	0.91	0.09	62,62,62,62	0
56	MG	CA	3108	1/1	0.91	0.17	74,74,74,74	0
56	MG	DA	3125	1/1	0.91	0.19	48,48,48,48	0
56	MG	CA	3138	1/1	0.92	0.12	67,67,67,67	0
56	MG	CA	3059	1/1	0.92	0.09	120,120,120,120	0
56	MG	CA	3116	1/1	0.92	0.25	62,62,62,62	0
56	MG	DB	207	1/1	0.92	0.16	74,74,74,74	0
57	PG4	DR	203	13/13	0.92	0.28	151,153,155,155	0
57	PG4	DS	202	13/13	0.92	0.12	73,75,77,77	0
56	MG	DA	3006	1/1	0.92	0.08	118,118,118,118	0
56	MG	CA	3048	1/1	0.92	0.10	112,112,112,112	0
56	MG	AA	1630	1/1	0.92	0.08	124,124,124,124	0
58	MPD	DA	3228	8/8	0.92	0.23	92,96,99,99	0
56	MG	DA	3167	1/1	0.92	0.08	23,23,23,23	0
56	MG	CA	3062	1/1	0.92	0.09	191,191,191,191	0
56	MG	DA	3124	1/1	0.92	0.18	59,59,59,59	0
56	MG	AA	1654	1/1	0.92	0.13	200,200,200,200	0
56	MG	CA	3148	1/1	0.92	0.30	27,27,27,27	1
56	MG	CA	3149	1/1	0.92	0.28	52,52,52,52	0
56	MG	AA	1617	1/1	0.92	0.18	63,63,63,63	0
56	MG	BA	1609	1/1	0.92	0.11	203,203,203,203	0
67	GUN	DA	3208	11/11	0.92	0.19	111,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3088	1/1	0.92	0.10	75,75,75,75	0
58	MPD	AA	1676	8/8	0.93	0.21	96,98,102,102	0
56	MG	DA	3130	1/1	0.93	0.21	76,76,76,76	0
56	MG	CA	3130	1/1	0.93	0.11	75,75,75,75	0
56	MG	BA	1616	1/1	0.93	0.08	169,169,169,169	0
56	MG	AA	1614	1/1	0.93	0.24	81,81,81,81	0
56	MG	DA	3142	1/1	0.93	0.13	58,58,58,58	0
56	MG	DB	208	1/1	0.93	0.22	60,60,60,60	0
61	PEG	DA	3224	7/7	0.93	0.18	75,76,78,79	0
61	PEG	DL	201	7/7	0.93	0.09	78,80,83,84	0
56	MG	CA	3086	1/1	0.93	0.07	67,67,67,67	0
56	MG	BA	1627	1/1	0.93	0.12	109,109,109,109	0
56	MG	DA	3110	1/1	0.93	0.19	273,273,273,273	0
56	MG	CA	3044	1/1	0.93	0.15	102,102,102,102	0
56	MG	CA	3113	1/1	0.93	0.16	50,50,50,50	0
56	MG	AA	1601	1/1	0.93	0.20	48,48,48,48	0
62	EDO	DA	3227	4/4	0.93	0.27	123,124,125,126	0
63	PGE	D3	101	10/10	0.93	0.16	93,97,100,100	0
56	MG	BA	1634	1/1	0.93	0.09	133,133,133,133	0
56	MG	AA	1677	1/1	0.93	0.11	121,121,121,121	0
64	SPD	DA	3203	10/10	0.93	0.21	93,98,105,106	0
65	1PE	DA	3183	16/16	0.93	0.13	46,56,86,87	0
59	PUT	DA	3202	6/6	0.93	0.21	95,96,96,96	0
66	ACY	DA	3199	4/4	0.93	0.19	83,84,85,85	0
59	PUT	DA	3209	6/6	0.93	0.15	80,83,87,88	0
58	MPD	AA	1671	8/8	0.93	0.15	110,112,114,115	0
56	MG	CA	3033	1/1	0.94	0.19	154,154,154,154	0
56	MG	DA	3165	1/1	0.94	0.28	118,118,118,118	0
58	MPD	DA	3190	8/8	0.94	0.17	99,100,101,101	0
56	MG	BA	1633	1/1	0.94	0.11	248,248,248,248	0
56	MG	CA	3035	1/1	0.94	0.17	102,102,102,102	0
61	PEG	DA	3215	7/7	0.94	0.25	126,128,134,135	0
56	MG	DA	3168	1/1	0.94	0.21	47,47,47,47	0
56	MG	CA	3128	1/1	0.94	0.08	65,65,65,65	0
56	MG	CA	3018	1/1	0.94	0.08	131,131,131,131	0
56	MG	AA	1642	1/1	0.94	0.12	173,173,173,173	0
62	EDO	D1	101	4/4	0.94	0.08	53,53,53,54	0
56	MG	AA	1616	1/1	0.94	0.29	55,55,55,55	0
58	MPD	DT	202	8/8	0.94	0.23	117,118,119,119	0
56	MG	CA	3096	1/1	0.94	0.11	105,105,105,105	0
56	MG	CA	3098	1/1	0.94	0.07	101,101,101,101	0
56	MG	BA	1637	1/1	0.94	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1638	1/1	0.94	0.23	64,64,64,64	0
63	PGE	DD	302	10/10	0.94	0.24	75,77,78,79	0
56	MG	DA	3143	1/1	0.94	0.13	111,111,111,111	0
59	PUT	DA	3187	6/6	0.94	0.09	36,42,42,42	0
56	MG	CA	3136	1/1	0.94	0.14	66,66,66,66	0
64	SPD	DA	3221	10/10	0.94	0.15	47,58,65,68	0
56	MG	DB	206	1/1	0.94	0.05	61,61,61,61	0
65	1PE	DA	3200	16/16	0.94	0.18	62,67,77,77	0
56	MG	AA	1665	1/1	0.94	0.10	153,153,153,153	0
56	MG	AA	1621	1/1	0.94	0.20	59,59,59,59	0
56	MG	AA	1656	1/1	0.94	0.09	132,132,132,132	0
56	MG	AA	1610	1/1	0.94	0.10	76,76,76,76	0
56	MG	CA	3013	1/1	0.95	0.07	91,91,91,91	0
56	MG	DA	3097	1/1	0.95	0.15	187,187,187,187	0
56	MG	BA	1608	1/1	0.95	0.07	122,122,122,122	0
56	MG	DA	3173	1/1	0.95	0.13	73,73,73,73	0
56	MG	DA	3112	1/1	0.95	0.09	94,94,94,94	0
56	MG	AA	1669	1/1	0.95	0.09	91,91,91,91	0
56	MG	DA	3177	1/1	0.95	0.18	118,118,118,118	0
56	MG	CA	3078	1/1	0.95	0.08	128,128,128,128	0
60	ZN	C5	101	1/1	0.95	0.07	149,149,149,149	0
56	MG	CA	3101	1/1	0.95	0.07	164,164,164,164	0
61	PEG	D1	102	7/7	0.95	0.12	61,65,68,69	0
56	MG	DR	202	1/1	0.95	0.08	29,29,29,29	0
56	MG	CA	3079	1/1	0.95	0.10	156,156,156,156	0
56	MG	DA	3126	1/1	0.95	0.22	55,55,55,55	0
56	MG	AA	1657	1/1	0.95	0.07	152,152,152,152	0
61	PEG	DA	3223	7/7	0.95	0.16	82,82,84,85	0
56	MG	CA	3147	1/1	0.95	0.32	50,50,50,50	1
56	MG	BA	1614	1/1	0.95	0.11	127,127,127,127	0
56	MG	BA	1601	1/1	0.95	0.08	140,140,140,140	0
56	MG	CA	3150	1/1	0.95	0.05	50,50,50,50	0
56	MG	DA	3141	1/1	0.95	0.25	46,46,46,46	0
56	MG	AA	1613	1/1	0.95	0.11	52,52,52,52	0
56	MG	AA	1650	1/1	0.95	0.09	149,149,149,149	0
62	EDO	DA	3196	4/4	0.95	0.28	86,88,89,89	0
62	EDO	DA	3205	4/4	0.95	0.17	79,82,83,83	0
56	MG	DA	3145	1/1	0.95	0.17	58,58,58,58	0
56	MG	BA	1622	1/1	0.95	0.07	150,150,150,150	0
56	MG	AA	1618	1/1	0.95	0.18	57,57,57,57	0
56	MG	CA	3089	1/1	0.95	0.12	69,69,69,69	0
56	MG	CA	3053	1/1	0.95	0.06	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
63	PGE	DA	3184	10/10	0.95	0.11	39,51,60,63	0
63	PGE	DA	3211	10/10	0.95	0.14	81,82,90,93	0
63	PGE	DA	3214	10/10	0.95	0.12	81,82,84,85	0
63	PGE	DA	3222	10/10	0.95	0.17	79,90,99,99	0
56	MG	DB	205	1/1	0.95	0.12	64,64,64,64	0
56	MG	AA	1644	1/1	0.95	0.08	123,123,123,123	0
63	PGE	DU	101	10/10	0.95	0.11	79,83,88,88	0
64	SPD	DA	3181	10/10	0.95	0.11	66,69,73,73	0
56	MG	BA	1641	1/1	0.95	0.09	72,72,72,72	0
56	MG	DA	3163	1/1	0.95	0.33	70,70,70,70	0
56	MG	DA	3164	1/1	0.95	0.17	78,78,78,78	0
56	MG	CA	3056	1/1	0.95	0.22	48,48,48,48	0
56	MG	DB	209	1/1	0.95	0.21	105,105,105,105	0
56	MG	DD	301	1/1	0.95	0.12	53,53,53,53	0
56	MG	CA	3117	1/1	0.95	0.16	64,64,64,64	0
59	PUT	DA	3186	6/6	0.95	0.12	44,49,50,51	0
56	MG	AA	1627	1/1	0.96	0.07	55,55,55,55	0
56	MG	CA	3046	1/1	0.96	0.11	123,123,123,123	0
56	MG	CA	3030	1/1	0.96	0.04	76,76,76,76	0
56	MG	CA	3031	1/1	0.96	0.04	102,102,102,102	0
56	MG	DA	3138	1/1	0.96	0.11	43,43,43,43	0
62	EDO	DB	211	4/4	0.96	0.14	96,96,96,96	0
56	MG	DA	3140	1/1	0.96	0.09	54,54,54,54	0
62	EDO	DA	3192	4/4	0.96	0.17	92,92,93,94	0
62	EDO	DA	3195	4/4	0.96	0.14	71,73,74,75	0
56	MG	BA	1630	1/1	0.96	0.07	165,165,165,165	0
56	MG	BA	1632	1/1	0.96	0.08	72,72,72,72	0
56	MG	DA	3004	1/1	0.96	0.09	107,107,107,107	0
56	MG	DA	3179	1/1	0.96	0.27	56,56,56,56	0
56	MG	DA	3144	1/1	0.96	0.09	65,65,65,65	0
56	MG	DR	201	1/1	0.96	0.17	228,228,228,228	0
56	MG	AA	1607	1/1	0.96	0.15	52,52,52,52	0
56	MG	AA	1638	1/1	0.96	0.06	105,105,105,105	0
56	MG	CB	201	1/1	0.96	0.06	169,169,169,169	0
56	MG	DA	3152	1/1	0.96	0.40	59,59,59,59	0
56	MG	DA	3153	1/1	0.96	0.13	47,47,47,47	0
56	MG	CB	203	1/1	0.96	0.05	106,106,106,106	0
56	MG	BA	1635	1/1	0.96	0.06	96,96,96,96	0
59	PUT	DA	3220	6/6	0.96	0.23	77,80,81,81	0
56	MG	BA	1628	1/1	0.96	0.05	80,80,80,80	0
56	MG	CA	3040	1/1	0.96	0.06	134,134,134,134	0
56	MG	DA	3123	1/1	0.96	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3042	1/1	0.96	0.07	93,93,93,93	0
56	MG	CA	3097	1/1	0.96	0.10	123,123,123,123	0
56	MG	CA	3080	1/1	0.96	0.18	160,160,160,160	0
56	MG	DA	3128	1/1	0.96	0.20	52,52,52,52	0
58	MPD	DA	3207	8/8	0.96	0.15	64,70,73,78	0
56	MG	CA	3081	1/1	0.96	0.07	117,117,117,117	0
56	MG	BA	1613	1/1	0.97	0.07	86,86,86,86	0
56	MG	AA	1636	1/1	0.97	0.07	89,89,89,89	0
56	MG	AA	1658	1/1	0.97	0.05	58,58,58,58	0
56	MG	AA	1611	1/1	0.97	0.09	50,50,50,50	0
62	EDO	D0	101	4/4	0.97	0.13	67,67,68,69	0
56	MG	DA	3132	1/1	0.97	0.07	57,57,57,57	0
56	MG	DA	3133	1/1	0.97	0.10	55,55,55,55	0
56	MG	CA	3058	1/1	0.97	0.10	203,203,203,203	0
56	MG	CA	3114	1/1	0.97	0.05	40,40,40,40	0
56	MG	CA	3024	1/1	0.97	0.07	153,153,153,153	0
56	MG	CA	3025	1/1	0.97	0.11	109,109,109,109	0
56	MG	CA	3011	1/1	0.97	0.05	68,68,68,68	0
56	MG	CA	3118	1/1	0.97	0.10	52,52,52,52	0
56	MG	CA	3027	1/1	0.97	0.06	118,118,118,118	0
56	MG	BA	1618	1/1	0.97	0.09	91,91,91,91	0
56	MG	CA	3100	1/1	0.97	0.09	104,104,104,104	0
56	MG	CA	3144	1/1	0.97	0.04	54,54,54,54	0
56	MG	DA	3148	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3150	1/1	0.97	0.10	41,41,41,41	0
56	MG	AA	1634	1/1	0.97	0.06	141,141,141,141	0
56	MG	BA	1602	1/1	0.97	0.04	79,79,79,79	0
56	MG	CA	3103	1/1	0.97	0.04	93,93,93,93	0
59	PUT	DA	3226	6/6	0.97	0.15	74,74,75,75	0
60	ZN	AB	301	1/1	0.97	0.04	125,125,125,125	0
56	MG	DA	3120	1/1	0.97	0.09	64,64,64,64	0
56	MG	DA	3121	1/1	0.97	0.25	51,51,51,51	0
56	MG	CA	3066	1/1	0.97	0.07	133,133,133,133	0
56	MG	CA	3016	1/1	0.97	0.07	107,107,107,107	0
56	MG	CA	3017	1/1	0.97	0.08	87,87,87,87	0
66	ACY	DA	3189	4/4	0.97	0.11	65,66,66,67	0
56	MG	DA	3161	1/1	0.97	0.14	48,48,48,48	0
56	MG	DA	3162	1/1	0.97	0.16	50,50,50,50	0
56	MG	CA	3070	1/1	0.97	0.04	94,94,94,94	0
56	MG	AA	1604	1/1	0.97	0.24	57,57,57,57	0
56	MG	DA	3135	1/1	0.98	0.07	25,25,25,25	0
56	MG	DA	3036	1/1	0.98	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MPD	DS	203	8/8	0.98	0.09	59,60,62,64	0
56	MG	AA	1640	1/1	0.98	0.04	80,80,80,80	0
56	MG	DA	3070	1/1	0.98	0.08	58,58,58,58	0
56	MG	DA	3071	1/1	0.98	0.07	102,102,102,102	0
56	MG	DA	3081	1/1	0.98	0.04	80,80,80,80	0
56	MG	DA	3175	1/1	0.98	0.09	47,47,47,47	0
56	MG	CB	202	1/1	0.98	0.08	123,123,123,123	0
56	MG	DA	3098	1/1	0.98	0.05	19,19,19,19	0
56	MG	AA	1659	1/1	0.98	0.04	94,94,94,94	0
56	MG	CA	3052	1/1	0.98	0.05	80,80,80,80	0
56	MG	DA	3116	1/1	0.98	0.11	33,33,33,33	0
56	MG	DA	3147	1/1	0.98	0.17	46,46,46,46	0
56	MG	AA	1629	1/1	0.98	0.05	100,100,100,100	0
56	MG	DA	3119	1/1	0.98	0.12	56,56,56,56	0
56	MG	AA	1643	1/1	0.98	0.03	65,65,65,65	0
56	MG	BA	1626	1/1	0.98	0.08	138,138,138,138	0
56	MG	AA	1655	1/1	0.98	0.05	101,101,101,101	0
56	MG	DA	3154	1/1	0.98	0.09	62,62,62,62	0
56	MG	CA	3143	1/1	0.98	0.05	54,54,54,54	0
56	MG	AA	1620	1/1	0.98	0.05	79,79,79,79	0
56	MG	AA	1667	1/1	0.98	0.05	33,33,33,33	0
64	SPD	DA	3185	10/10	0.98	0.11	52,53,57,58	0
56	MG	CA	3043	1/1	0.98	0.04	72,72,72,72	0
56	MG	DA	3127	1/1	0.98	0.24	24,24,24,24	0
56	MG	AA	1645	1/1	0.98	0.09	54,54,54,54	0
56	MG	DA	3003	1/1	0.98	0.05	93,93,93,93	0
56	MG	CA	3045	1/1	0.98	0.08	78,78,78,78	0
56	MG	BA	1631	1/1	0.98	0.04	42,42,42,42	0
56	MG	DA	3010	1/1	0.98	0.06	145,145,145,145	0
56	MG	DA	3029	1/1	0.98	0.05	68,68,68,68	0
56	MG	DA	3134	1/1	0.98	0.05	120,120,120,120	0
56	MG	CA	3015	1/1	0.99	0.13	59,59,59,59	0
56	MG	DA	3078	1/1	0.99	0.04	127,127,127,127	0
56	MG	DA	3079	1/1	0.99	0.02	44,44,44,44	0
56	MG	DA	3158	1/1	0.99	0.09	61,61,61,61	0
56	MG	CA	3049	1/1	0.99	0.05	53,53,53,53	0
56	MG	DA	3083	1/1	0.99	0.02	23,23,23,23	0
56	MG	DA	3084	1/1	0.99	0.04	56,56,56,56	0
56	MG	DA	3088	1/1	0.99	0.03	13,13,13,13	0
56	MG	DA	3093	1/1	0.99	0.06	17,17,17,17	0
56	MG	DA	3094	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3069	1/1	0.99	0.03	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3050	1/1	0.99	0.04	58,58,58,58	0
56	MG	DA	3107	1/1	0.99	0.02	26,26,26,26	0
56	MG	AA	1649	1/1	0.99	0.03	62,62,62,62	0
56	MG	AA	1641	1/1	0.99	0.03	44,44,44,44	0
56	MG	AA	1651	1/1	0.99	0.03	61,61,61,61	0
56	MG	DB	201	1/1	0.99	0.03	66,66,66,66	0
56	MG	DA	3172	1/1	0.99	0.05	48,48,48,48	0
56	MG	DB	204	1/1	0.99	0.03	56,56,56,56	0
56	MG	AA	1663	1/1	0.99	0.05	65,65,65,65	0
56	MG	CA	3095	1/1	0.99	0.04	80,80,80,80	0
56	MG	CA	3020	1/1	0.99	0.03	73,73,73,73	0
56	MG	BA	1620	1/1	0.99	0.04	90,90,90,90	0
56	MG	BA	1605	1/1	0.99	0.05	58,58,58,58	0
56	MG	AA	1631	1/1	0.99	0.05	42,42,42,42	0
56	MG	DA	3002	1/1	0.99	0.05	77,77,77,77	0
56	MG	DA	3230	1/1	0.99	0.03	60,60,60,60	0
56	MG	DA	3231	1/1	0.99	0.05	43,43,43,43	0
56	MG	AA	1632	1/1	0.99	0.04	88,88,88,88	0
56	MG	CA	3041	1/1	0.99	0.06	47,47,47,47	0
56	MG	DA	3005	1/1	0.99	0.04	78,78,78,78	0
56	MG	AA	1666	1/1	0.99	0.05	56,56,56,56	0
56	MG	AA	1633	1/1	0.99	0.03	76,76,76,76	0
56	MG	DA	3013	1/1	0.99	0.05	92,92,92,92	0
56	MG	DA	3014	1/1	0.99	0.05	56,56,56,56	0
56	MG	DA	3017	1/1	0.99	0.03	53,53,53,53	0
56	MG	DA	3026	1/1	0.99	0.03	39,39,39,39	0
56	MG	DA	3027	1/1	0.99	0.05	136,136,136,136	0
56	MG	BA	1610	1/1	0.99	0.03	97,97,97,97	0
56	MG	AA	1668	1/1	0.99	0.07	62,62,62,62	0
56	MG	DA	3139	1/1	0.99	0.10	73,73,73,73	0
56	MG	DA	3042	1/1	0.99	0.06	24,24,24,24	0
56	MG	DA	3043	1/1	0.99	0.05	84,84,84,84	0
56	MG	DA	3044	1/1	0.99	0.04	73,73,73,73	0
56	MG	DA	3045	1/1	0.99	0.03	25,25,25,25	0
56	MG	DA	3046	1/1	0.99	0.05	46,46,46,46	0
56	MG	DA	3050	1/1	0.99	0.03	44,44,44,44	0
56	MG	DA	3051	1/1	0.99	0.04	52,52,52,52	0
56	MG	DA	3053	1/1	0.99	0.03	68,68,68,68	0
56	MG	AA	1639	1/1	0.99	0.03	82,82,82,82	0
56	MG	DA	3149	1/1	0.99	0.02	38,38,38,38	0
56	MG	DA	3062	1/1	0.99	0.04	110,110,110,110	0
56	MG	DA	3063	1/1	0.99	0.06	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3067	1/1	0.99	0.05	43,43,43,43	0
56	MG	DA	3069	1/1	0.99	0.06	65,65,65,65	0
56	MG	AA	1625	1/1	0.99	0.05	61,61,61,61	0
56	MG	DA	3225	1/1	1.00	0.03	14,14,14,14	0
56	MG	DA	3229	1/1	1.00	0.02	45,45,45,45	0
56	MG	DA	3095	1/1	1.00	0.03	14,14,14,14	0
56	MG	DA	3096	1/1	1.00	0.02	36,36,36,36	0
56	MG	AA	1662	1/1	1.00	0.03	66,66,66,66	0
56	MG	BA	1611	1/1	1.00	0.02	31,31,31,31	0
56	MG	DA	3099	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3100	1/1	1.00	0.06	53,53,53,53	0
56	MG	DA	3101	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3102	1/1	1.00	0.03	38,38,38,38	0
56	MG	DA	3103	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3104	1/1	1.00	0.04	20,20,20,20	0
56	MG	DA	3105	1/1	1.00	0.03	11,11,11,11	0
56	MG	DA	3106	1/1	1.00	0.03	32,32,32,32	0
56	MG	DA	3028	1/1	1.00	0.06	21,21,21,21	0
56	MG	DA	3108	1/1	1.00	0.01	36,36,36,36	0
56	MG	DA	3109	1/1	1.00	0.02	13,13,13,13	0
56	MG	DD	303	1/1	1.00	0.04	37,37,37,37	0
56	MG	DA	3111	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3030	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3113	1/1	1.00	0.03	30,30,30,30	0
56	MG	DA	3114	1/1	1.00	0.01	7,7,7,7	0
56	MG	DA	3115	1/1	1.00	0.01	32,32,32,32	0
56	MG	DA	3031	1/1	1.00	0.04	16,16,16,16	0
56	MG	DA	3117	1/1	1.00	0.02	43,43,43,43	0
56	MG	DA	3032	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3033	1/1	1.00	0.01	10,10,10,10	0
56	MG	DA	3034	1/1	1.00	0.05	28,28,28,28	0
56	MG	DA	3035	1/1	1.00	0.04	15,15,15,15	0
56	MG	AA	1652	1/1	1.00	0.11	18,18,18,18	0
56	MG	DA	3037	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3038	1/1	1.00	0.01	29,29,29,29	0
56	MG	DA	3039	1/1	1.00	0.02	43,43,43,43	0
56	MG	DA	3040	1/1	1.00	0.12	10,10,10,10	0
56	MG	DA	3041	1/1	1.00	0.01	25,25,25,25	0
56	MG	BA	1621	1/1	1.00	0.09	13,13,13,13	0
56	MG	DB	202	1/1	1.00	0.05	60,60,60,60	0
56	MG	DB	203	1/1	1.00	0.02	27,27,27,27	0
56	MG	AA	1653	1/1	1.00	0.03	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	DA	3007	1/1	1.00	0.02	19,19,19,19	0
56	MG	DA	3047	1/1	1.00	0.03	47,47,47,47	0
56	MG	DA	3048	1/1	1.00	0.04	67,67,67,67	0
56	MG	DA	3049	1/1	1.00	0.02	10,10,10,10	0
56	MG	DA	3008	1/1	1.00	0.01	15,15,15,15	0
56	MG	DA	3009	1/1	1.00	0.03	29,29,29,29	0
60	ZN	D5	101	1/1	1.00	0.02	55,55,55,55	0
56	MG	DA	3052	1/1	1.00	0.01	53,53,53,53	0
56	MG	AA	1646	1/1	1.00	0.02	50,50,50,50	0
56	MG	DA	3054	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3055	1/1	1.00	0.02	19,19,19,19	0
56	MG	DA	3056	1/1	1.00	0.01	7,7,7,7	0
56	MG	DA	3057	1/1	1.00	0.02	33,33,33,33	0
56	MG	DA	3058	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3059	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3060	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3011	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3012	1/1	1.00	0.01	18,18,18,18	0
56	MG	BA	1615	1/1	1.00	0.02	44,44,44,44	0
56	MG	DA	3064	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3065	1/1	1.00	0.02	24,24,24,24	0
56	MG	DA	3066	1/1	1.00	0.04	49,49,49,49	0
56	MG	AA	1637	1/1	1.00	0.03	47,47,47,47	0
56	MG	DA	3068	1/1	1.00	0.05	52,52,52,52	0
56	MG	DA	3015	1/1	1.00	0.02	28,28,28,28	0
56	MG	DA	3016	1/1	1.00	0.02	32,32,32,32	0
56	MG	AA	1648	1/1	1.00	0.03	55,55,55,55	0
56	MG	DA	3072	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3073	1/1	1.00	0.03	37,37,37,37	0
56	MG	DA	3074	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3075	1/1	1.00	0.04	26,26,26,26	0
56	MG	DA	3076	1/1	1.00	0.03	34,34,34,34	0
56	MG	DA	3077	1/1	1.00	0.02	34,34,34,34	0
56	MG	DA	3018	1/1	1.00	0.15	10,10,10,10	0
56	MG	DA	3019	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3080	1/1	1.00	0.03	28,28,28,28	0
56	MG	DA	3020	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3082	1/1	1.00	0.04	64,64,64,64	0
56	MG	DA	3021	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3022	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3085	1/1	1.00	0.01	27,27,27,27	0
56	MG	DA	3086	1/1	1.00	0.03	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3087	1/1	1.00	0.02	58,58,58,58	0
56	MG	DA	3023	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3089	1/1	1.00	0.03	16,16,16,16	0
56	MG	DA	3090	1/1	1.00	0.01	11,11,11,11	0
56	MG	DA	3091	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3092	1/1	1.00	0.02	11,11,11,11	0
56	MG	DA	3024	1/1	1.00	0.01	45,45,45,45	0
56	MG	DA	3025	1/1	1.00	0.06	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.