wwPDB X-ray Structure Validation Summary Report (i)

Jul 27, 2016 – 09:06 AM EDT

PDB ID	:	5J7L
Title	:	Structure of the 70S E coli ribosome with the U1052G mutation in the 16S rRNA bound to tetracycline
Authors	:	Cocozaki, A.; Ferguson, A.
Deposited on	:	2016-04-06
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

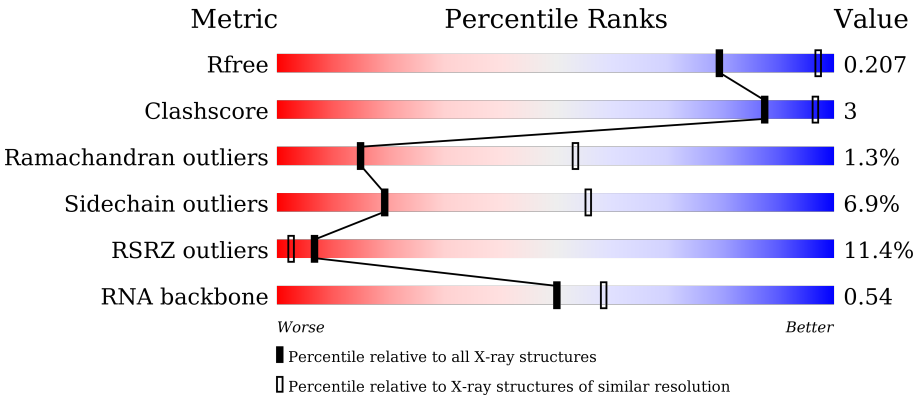
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	2%, 75%, 22%, ·
1	BA	1534	11%, 74%, 23%, ·
2	AB	224	13%, 88%, 12%, ·
2	BB	224	16%, 88%, 10%, ·

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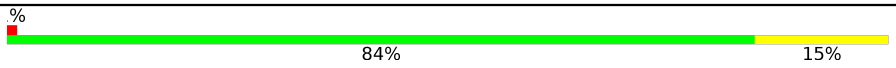
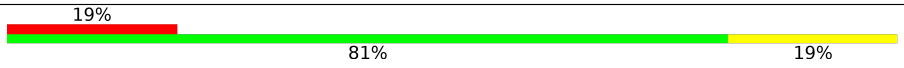
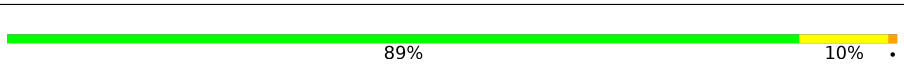
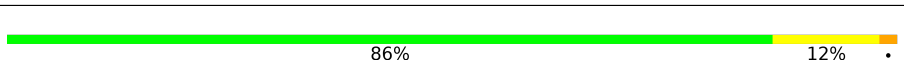
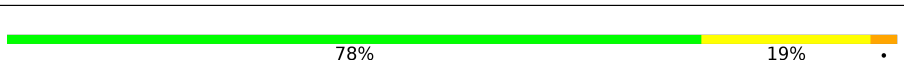
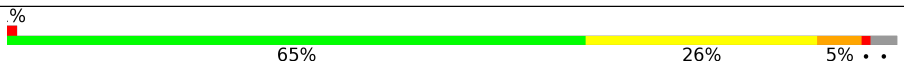
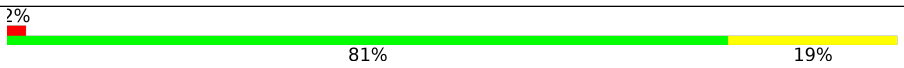
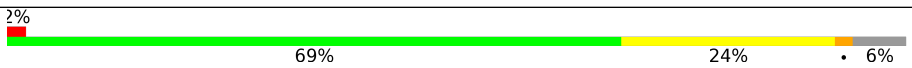
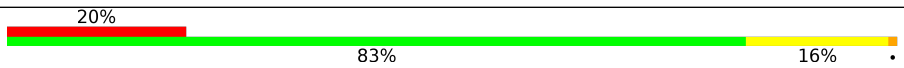
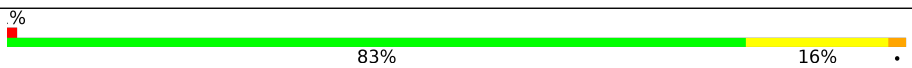
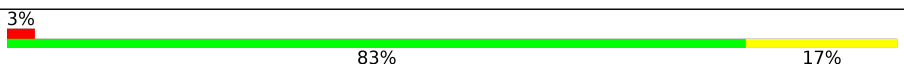
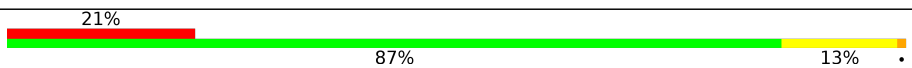
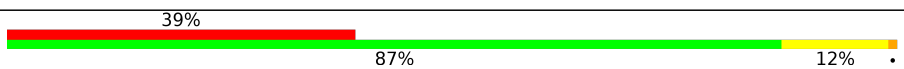
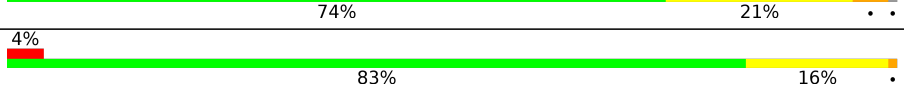
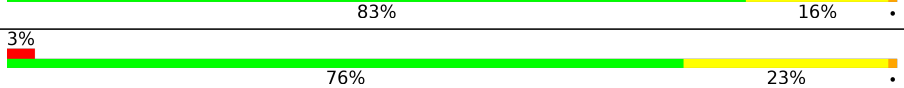
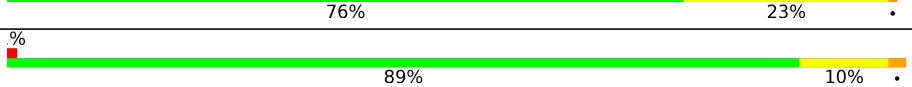
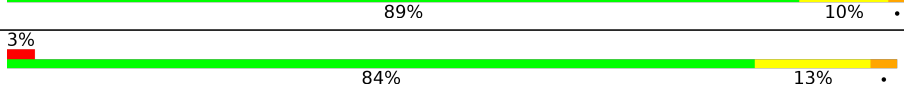
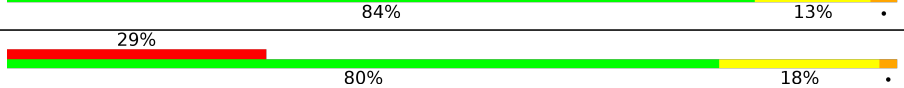
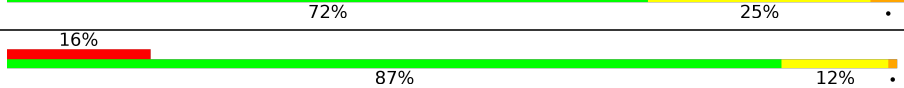
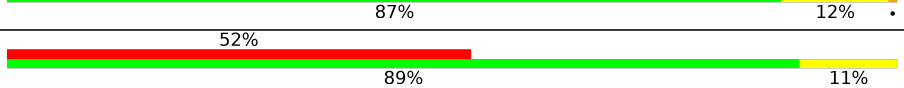
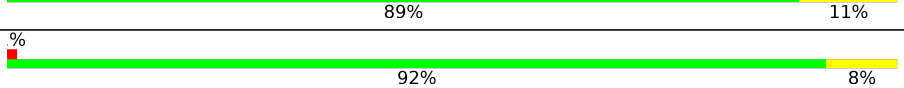
Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	7% 91% 8%
16	AP	82	4% 90% 10%
16	BP	82	23% 82% 17%
17	AQ	80	3% 78% 21%
17	BQ	80	21% 61% 31% 6%
18	AR	55	2% 87% 13%
18	BR	55	5% 93% 7%
19	AS	79	13% 82% 16%
19	BS	79	76% 84% 14%
20	AT	86	90% 7%
20	BT	86	26% 79% 15% 5%
21	AU	56	4% 88% 13%
21	BU	56	2% 88% 13%
22	C1	56	21% 84% 13%
22	D1	56	84% 16%
23	C2	51	67% 69% 27%
23	D2	51	73% 25%
24	C3	46	28% 85% 15%
24	D3	46	89% 11%
25	C4	64	14% 84% 16%
25	D4	64	91% 9%
26	C5	38	24% 79% 18%
26	D5	38	87% 13%
27	C0	58	14% 76% 22%
27	D0	58	83% 16%

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Mol	Chain	Length	Quality of chain
28	CB	120	8% 85% 11%
28	DB	120	91% 8%
29	CC	271	6% 82% 16%
29	DC	271	90% 8%
30	CD	209	15% 88% 11%
30	DD	209	90% 10%
31	CA	2904	9% 74% 23%
32	CE	201	23% 83% 14%
32	DE	201	91% 8%
33	CF	177	63% 83% 15%
33	DF	177	% 81% 18%
34	CG	176	44% 89% 11%
34	DG	176	% 90% 10%
35	CH	149	26% 79% 20%
35	DH	149	18% 82% 18%
36	CJ	134	90% 88% 11%
36	DJ	134	61% 88% 11%
37	CK	142	3% 92% 7%
37	DK	142	94% 6%
38	CL	123	4% 85% 11%
38	DL	123	87% 11%
39	CM	144	38% 79% 19%
39	DM	144	92% 8%
40	CN	136	4% 85% 14%
40	DN	136	85% 14%

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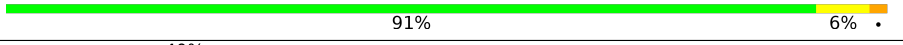
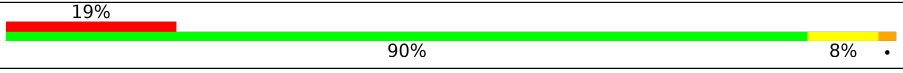
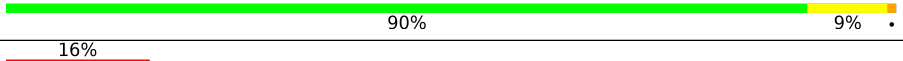
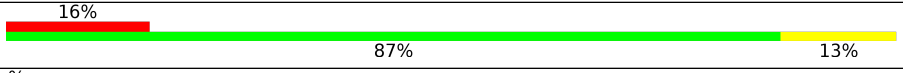
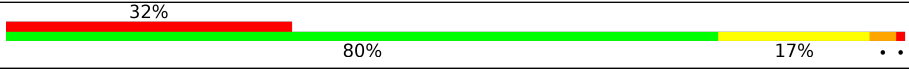
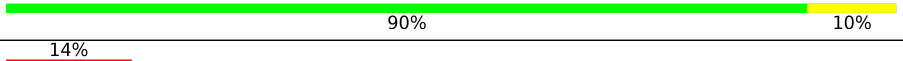
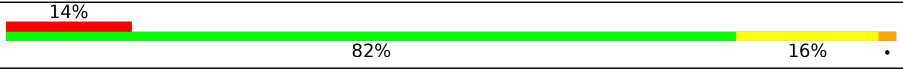
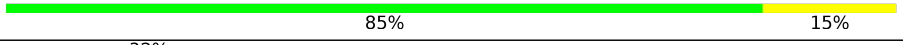
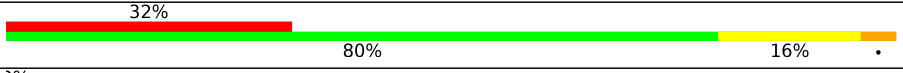
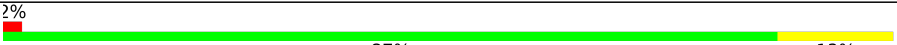
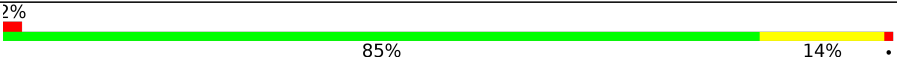
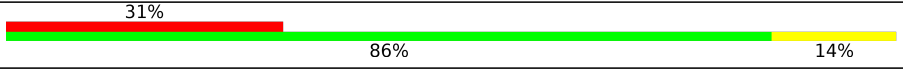
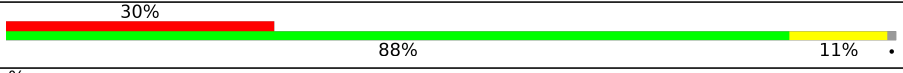
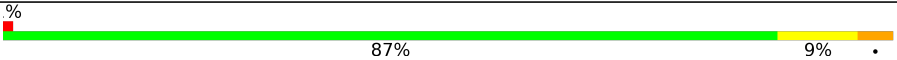
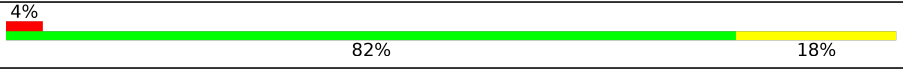
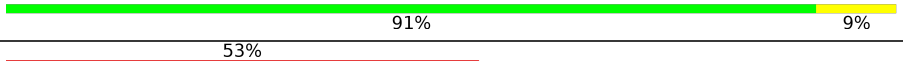
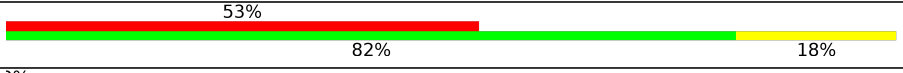
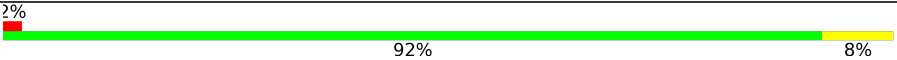
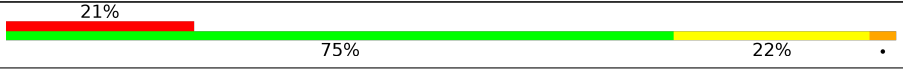
Mol	Chain	Length	Quality of chain
41	CO	125	
41	DO	125	
42	CP	117	
42	DP	117	
43	CQ	114	
43	DQ	114	
44	CR	117	
44	DR	117	
45	CS	103	
45	DS	103	
46	CT	110	
46	DT	110	
47	CU	93	
47	DU	93	
48	CV	102	
48	DV	102	
49	CW	94	
49	DW	94	
50	CX	76	
50	DX	76	
51	CY	77	
51	DY	77	
52	CZ	62	
52	DZ	62	
53	DI	135	

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Mol	Chain	Length	Quality of chain
54	DA	2904	3% 77% 19%

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
55	MG	AA	1608	-	-	-	X
55	MG	AA	1612	-	-	-	X
55	MG	BA	1601	-	-	-	X
55	MG	BA	1612	-	-	-	X
55	MG	BA	1646	-	-	-	X
55	MG	CA	3003	-	-	-	X
55	MG	CA	3026	-	-	-	X
55	MG	CA	3105	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3123	-	-	-	X
55	MG	CA	3130	-	-	-	X
55	MG	CA	3133	-	-	-	X
55	MG	CA	3137	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3151	-	-	-	X
55	MG	DA	3037	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3126	-	-	-	X
55	MG	DA	3127	-	-	-	X
55	MG	DA	3172	-	-	-	X
56	PG4	AA	1670	-	-	-	X
56	PG4	BA	1642	-	-	-	X
56	PG4	DA	3193	-	-	-	X
56	PG4	DA	3216	-	-	-	X
56	PG4	DS	202	-	-	-	X
57	MPD	AA	1671	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DA	3192	-	-	-	X
57	MPD	DA	3204	-	-	-	X
57	MPD	DA	3207	-	-	-	X
57	MPD	DE	301	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1673	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	DA	3184	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	PUT	DA	3189	-	-	-	X
58	PUT	DA	3195	-	-	-	X
58	PUT	DA	3205	-	-	-	X
58	PUT	DA	3213	-	-	-	X
58	PUT	DA	3219	-	-	-	X
58	PUT	DA	3222	-	-	-	X
59	TAC	BA	1644	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	101	-	-	-	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3218	-	-	-	X
61	PEG	DA	3226	-	-	-	X
61	PEG	DL	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	D1	101	-	-	-	X
62	EDO	DA	3197	-	-	-	X
62	EDO	DA	3198	-	-	-	X
62	EDO	DA	3209	-	-	-	X
62	EDO	DB	201	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	DA	3001	-	-	-	X
63	PGE	DA	3203	-	-	-	X
63	PGE	DA	3214	-	-	-	X
63	PGE	DA	3217	-	-	-	X
63	PGE	DA	3225	-	-	-	X
63	PGE	DS	201	-	-	-	X
63	PGE	DU	101	-	-	-	X
64	SPD	DA	3183	-	-	-	X
64	SPD	DA	3187	-	-	-	X
64	SPD	DA	3206	-	-	-	X
64	SPD	DA	3224	-	-	-	X
65	1PE	DA	3185	-	-	-	X
65	1PE	DA	3202	-	-	-	X
66	ACY	DA	3201	-	-	-	X
67	GUN	DA	3211	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295261 atoms, of which 2 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 595593103
BA	1052	G	U	engineered mutation	GB 595593103

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 28 is a RNA chain called 50S ribosomal protein L1.

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			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	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 L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	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

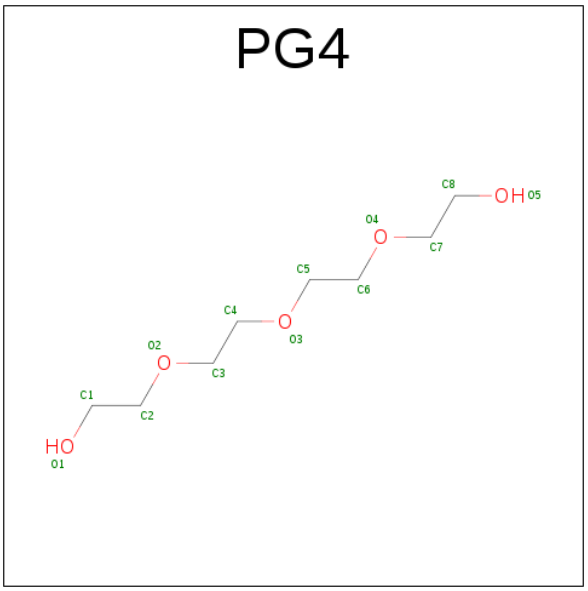
- Molecule 54 is a RNA chain called 23S rRNA.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

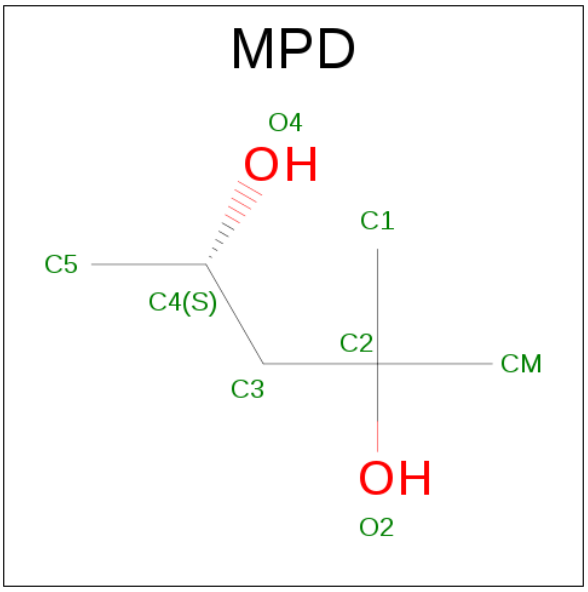
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	45	Total	Mg	0	0
			45	45		
55	CA	156	Total	Mg	0	0
			156	156		
55	CB	3	Total	Mg	0	0
			3	3		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	AA	72	Total	Mg	0	0
			72	72		
55	DA	183	Total	Mg	0	0
			183	183		
55	DB	9	Total	Mg	0	0
			9	9		
55	DD	1	Total	Mg	0	0
			1	1		

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



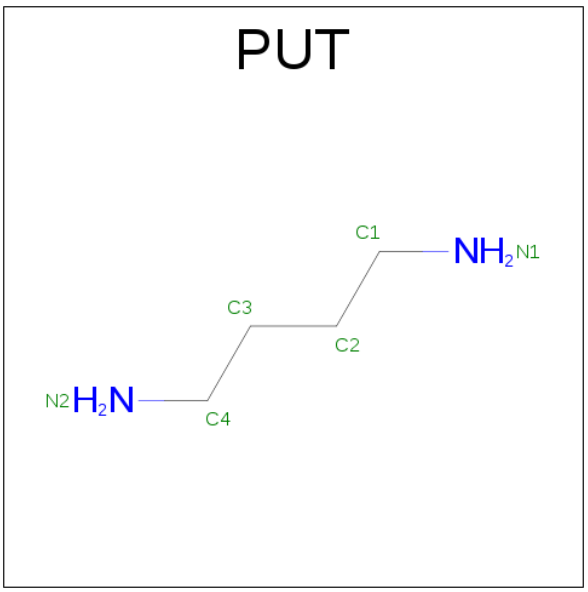
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	1	Total C O 13 8 5	0	0
56	BA	1	Total C O 13 8 5	0	0
56	DQ	1	Total C O 13 8 5	0	0
56	DR	1	Total C O 13 8 5	0	0
56	DS	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 58 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



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

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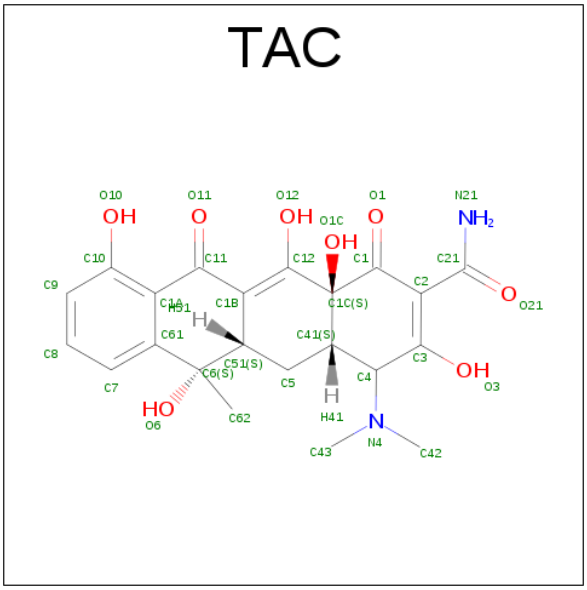
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0

- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total C N O 32 22 2 8	0	0
59	AA	1	Total C H N O 33 22 1 2 8	0	0
59	BA	1	Total C N O 32 22 2 8	0	0
59	BA	1	Total C H N O 33 22 1 2 8	0	0

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

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

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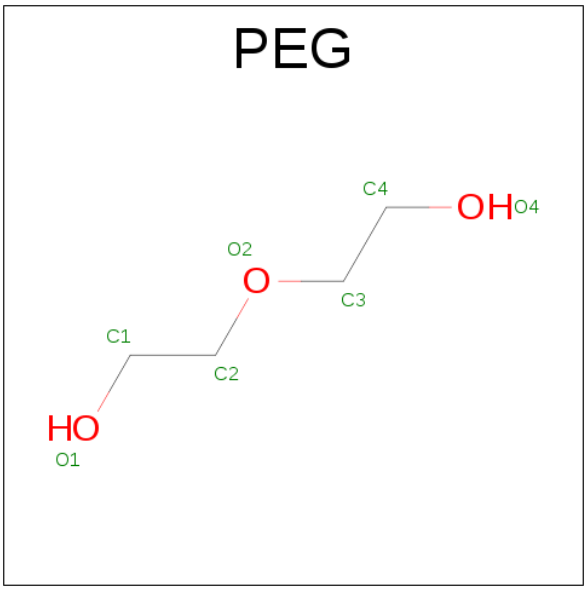
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	D5	1	Total Zn 1 1	0	0

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



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

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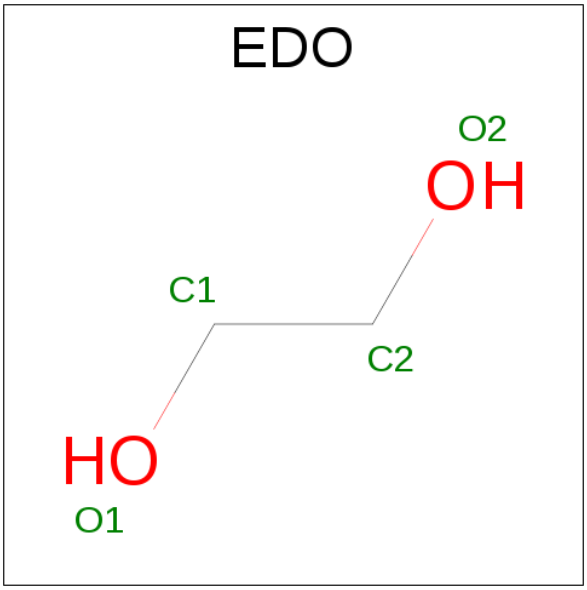
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DA	1	Total C O 7 4 3	0	0

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



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

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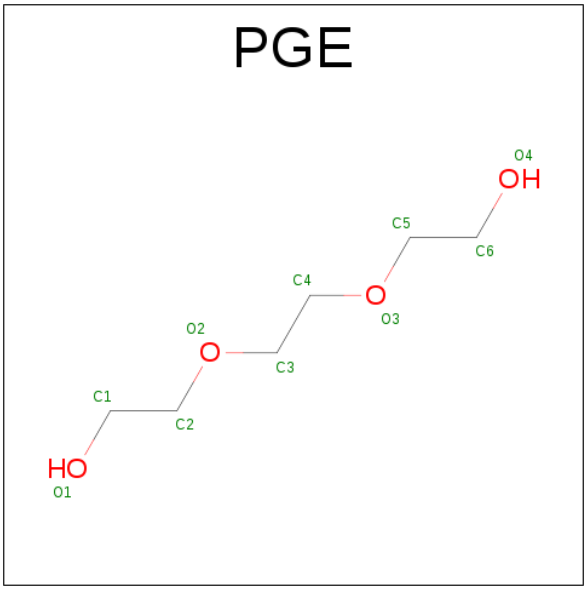
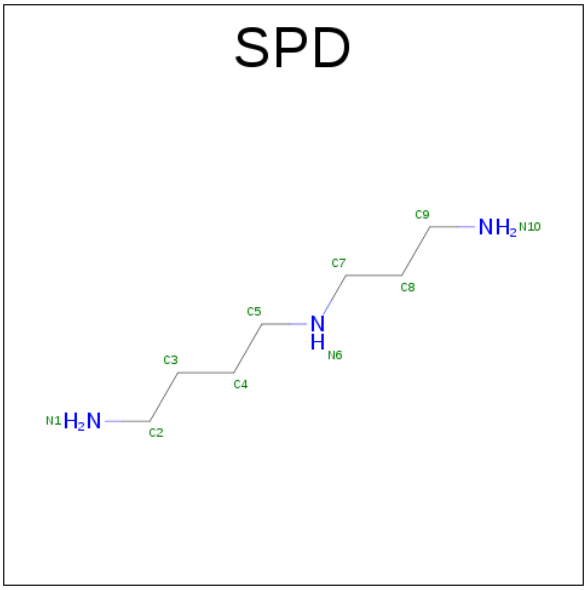
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0

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



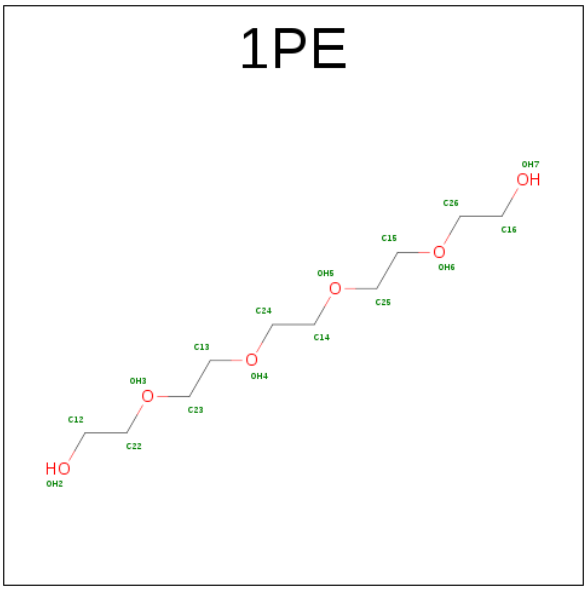
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	D1	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0

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



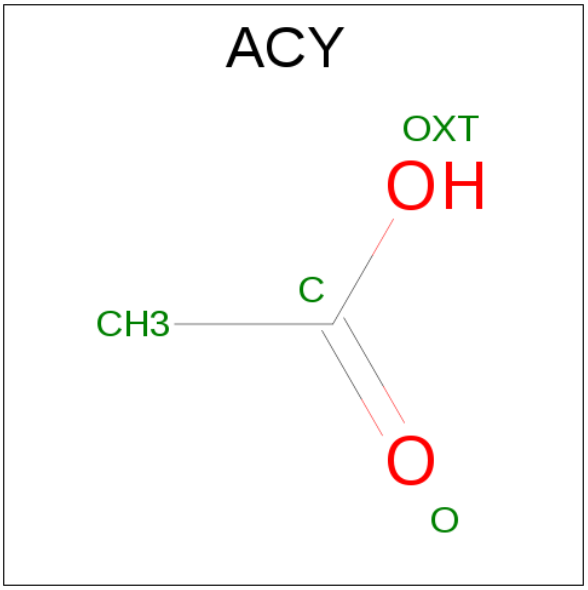
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

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



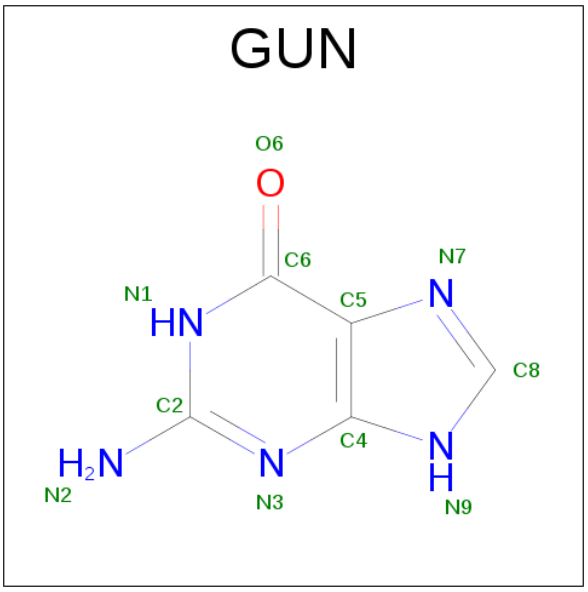
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C O 16 10 6	0	0
65	DA	1	Total C O 16 10 6	0	0

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



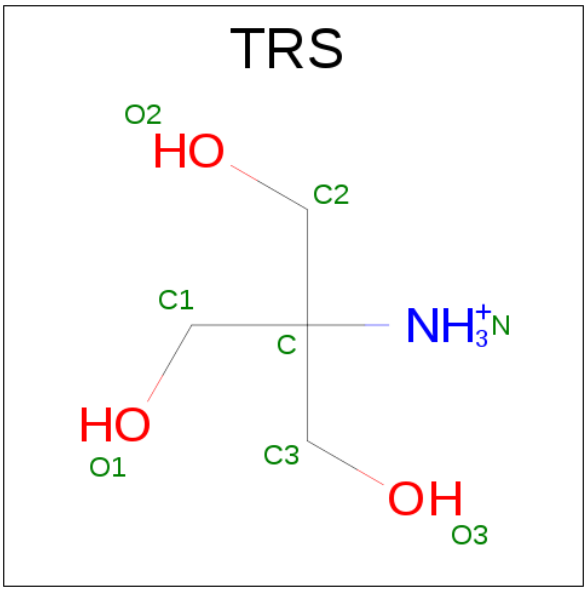
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0

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



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	AA	501	Total O 501 501	0	0
69	AC	4	Total O 4 4	0	0
69	AD	2	Total O 2 2	0	0
69	AE	5	Total O 5 5	0	0
69	AG	1	Total O 1 1	0	0
69	AH	1	Total O 1 1	0	0
69	AJ	2	Total O 2 2	0	0
69	AK	6	Total O 6 6	0	0
69	AL	10	Total O 10 10	0	0
69	AM	5	Total O 5 5	0	0
69	AN	6	Total O 6 6	0	0
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	AT	3	Total O 3 3	0	0
69	AU	3	Total O 3 3	0	0
69	C3	4	Total O 4 4	0	0
69	C4	1	Total O 1 1	0	0
69	BA	287	Total O 287 287	0	0
69	BD	13	Total O 13 13	0	0
69	BE	1	Total O 1 1	0	0
69	BF	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	BK	2	Total O 2 2	0	0
69	BL	4	Total O 4 4	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	BT	2	Total O 2 2	0	0
69	BU	2	Total O 2 2	0	0
69	D1	43	Total O 43 43	0	0
69	D2	6	Total O 6 6	0	0
69	D3	22	Total O 22 22	0	0
69	D4	39	Total O 39 39	0	0
69	D5	8	Total O 8 8	0	0
69	D0	24	Total O 24 24	0	0
69	CB	13	Total O 13 13	0	0
69	CC	10	Total O 10 10	0	0
69	CD	6	Total O 6 6	0	0
69	CA	691	Total O 691 691	0	0
69	DC	100	Total O 100 100	0	0
69	DD	98	Total O 98 98	0	0
69	CE	5	Total O 5 5	0	0
69	CL	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	CM	4	Total O 4 4	0	0
69	CO	2	Total O 2 2	0	0
69	CU	3	Total O 3 3	0	0
69	CV	1	Total O 1 1	0	0
69	CW	1	Total O 1 1	0	0
69	CY	1	Total O 1 1	0	0
69	DE	61	Total O 61 61	0	0
69	DF	15	Total O 15 15	0	0
69	DG	6	Total O 6 6	0	0
69	DH	2	Total O 2 2	0	0
69	DK	65	Total O 65 65	0	0
69	DL	52	Total O 52 52	0	0
69	DM	63	Total O 63 63	0	0
69	DN	72	Total O 72 72	0	0
69	DO	44	Total O 44 44	0	0
69	DP	38	Total O 38 38	0	0
69	DQ	33	Total O 33 33	0	0
69	DR	62	Total O 62 62	0	0
69	DS	46	Total O 46 46	0	0
69	DT	69	Total O 69 69	0	0
69	DU	18	Total O 18 18	0	0

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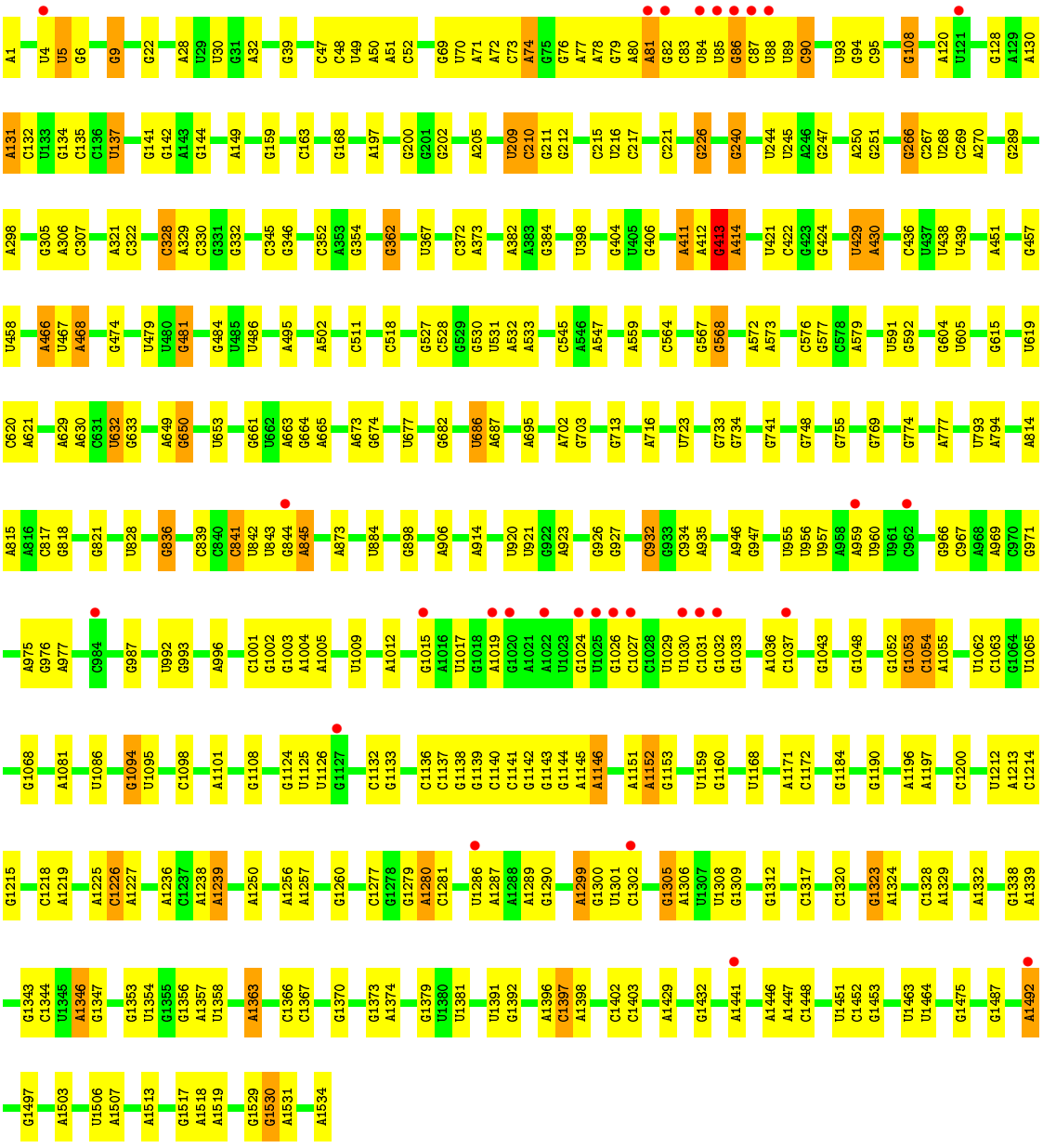
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DV	20	Total O 20 20	0	0
69	DW	31	Total O 31 31	0	0
69	DX	25	Total O 25 25	0	0
69	DY	9	Total O 9 9	0	0
69	DZ	8	Total O 8 8	0	0
69	DB	209	Total O 209 209	0	0
69	DA	4840	Total O 4840 4840	0	0

3 Residue-property plots (i)

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

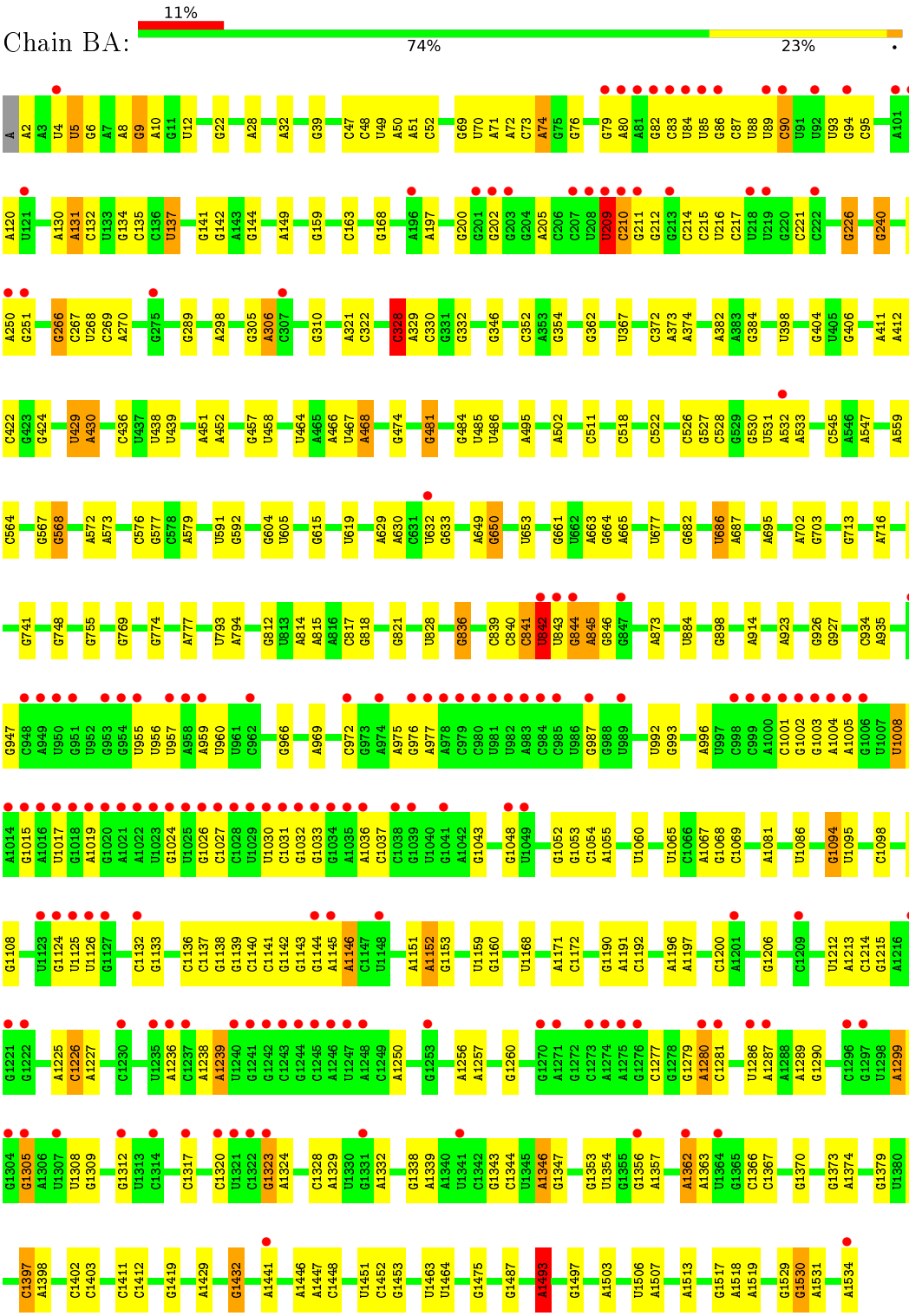
- Molecule 1: 16S rRNA

Chain AA: 



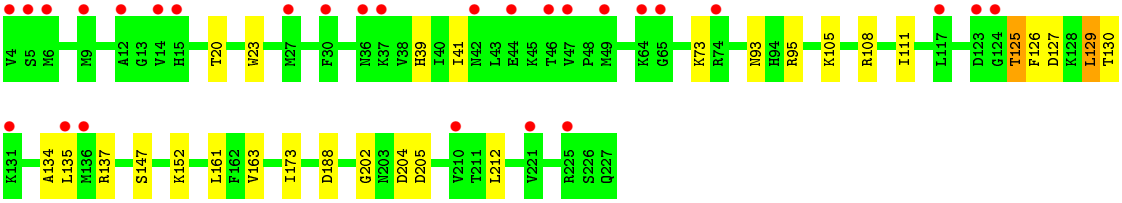
• Molecule 1: 16S rRNA

Chain BA:



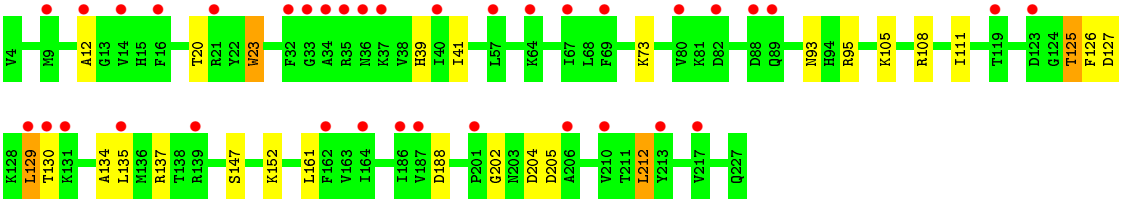
• Molecule 2: 30S ribosomal protein S2

Chain AB:



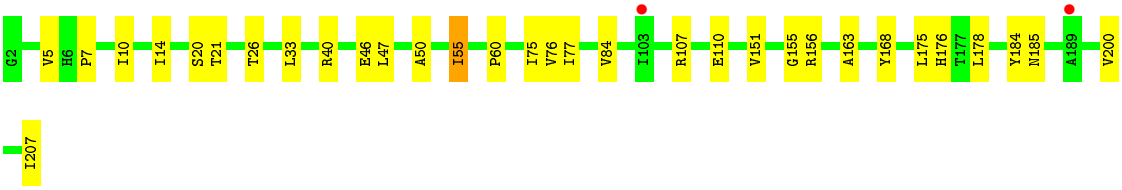
• Molecule 2: 30S ribosomal protein S2

Chain BB:



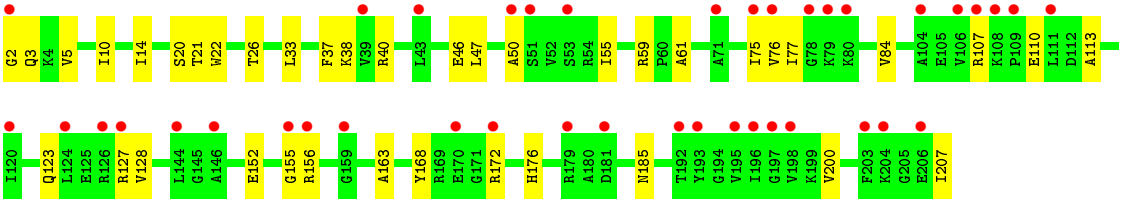
• Molecule 3: 30S ribosomal protein S3

Chain AC:



• Molecule 3: 30S ribosomal protein S3

Chain BC:



• Molecule 4: 30S ribosomal protein S4

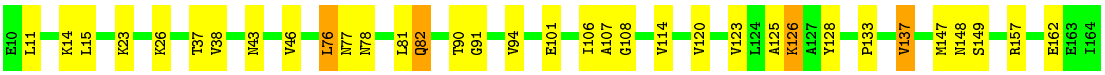
Chain AD:

• Molecule 4: 30S ribosomal protein S4

Chain BD:

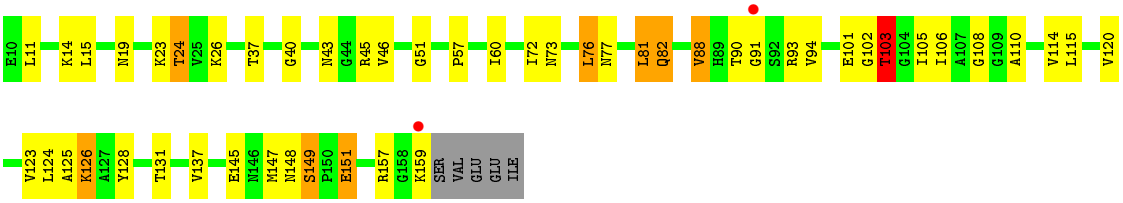
• Molecule 5: 30S ribosomal protein S5

Chain AE:



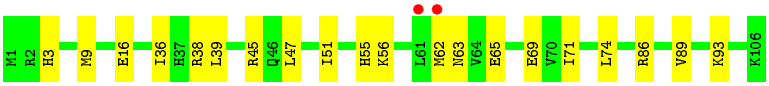
• Molecule 5: 30S ribosomal protein S5

Chain BE:



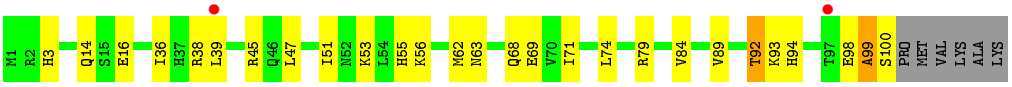
• Molecule 6: 30S ribosomal protein S6

Chain AF:



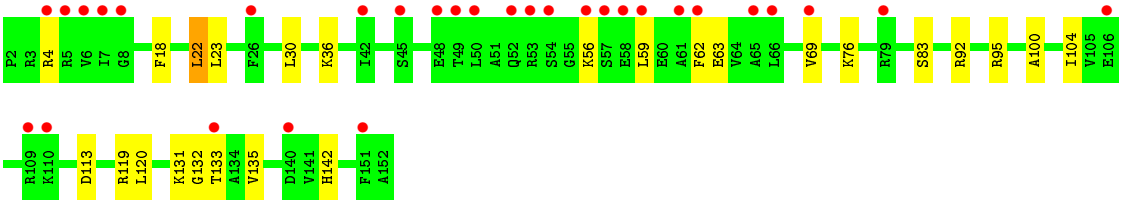
• Molecule 6: 30S ribosomal protein S6

Chain BF:



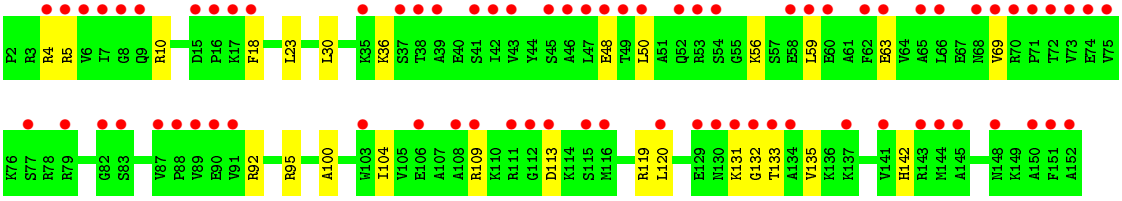
• Molecule 7: 30S ribosomal protein S7

Chain AG:

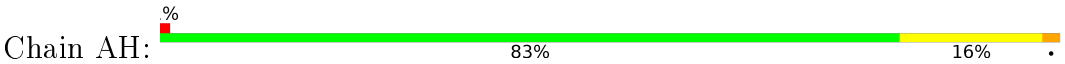


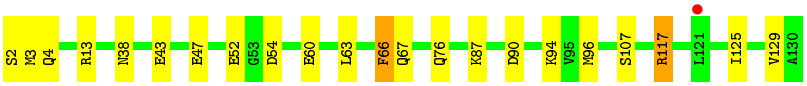
• Molecule 7: 30S ribosomal protein S7

Chain BG:

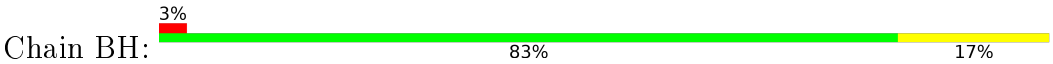


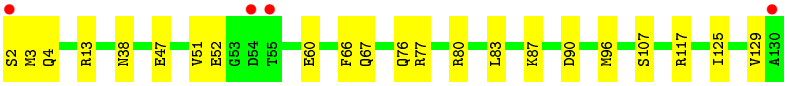
• Molecule 8: 30S ribosomal protein S8



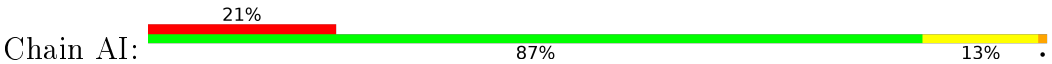


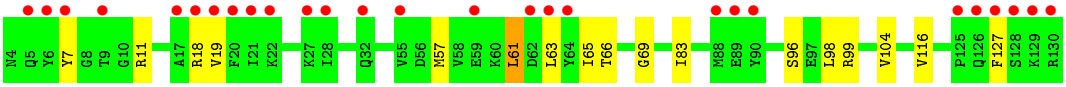
• Molecule 8: 30S ribosomal protein S8



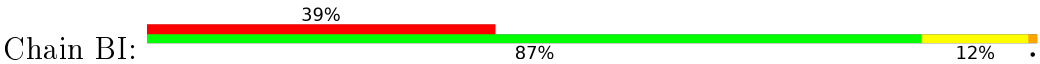


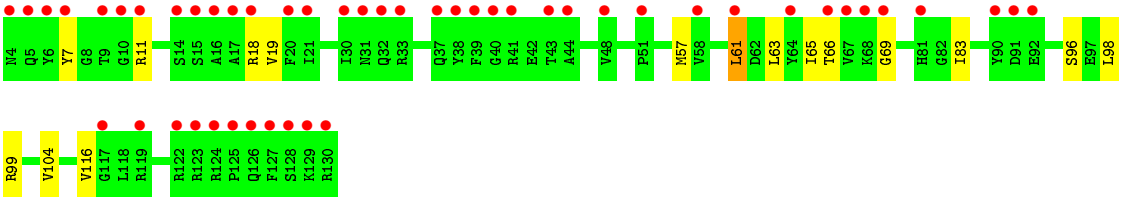
• Molecule 9: 30S ribosomal protein S9



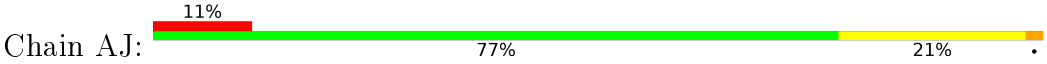


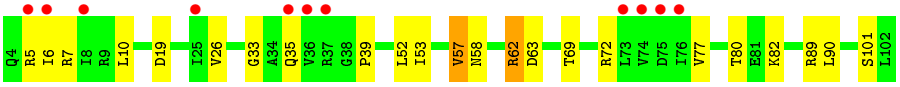
• Molecule 9: 30S ribosomal protein S9



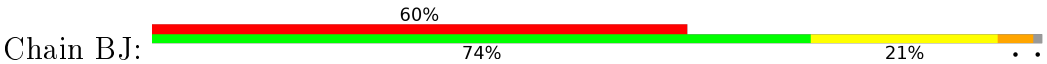


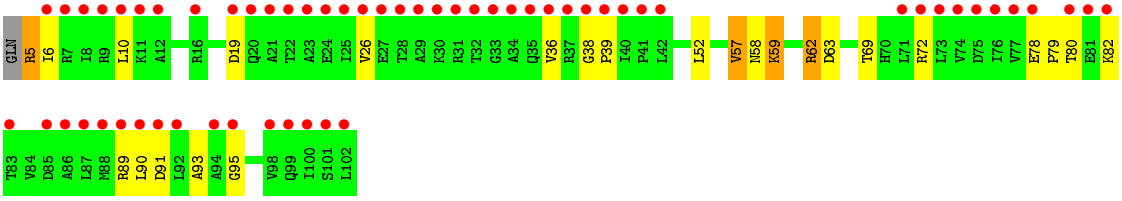
• Molecule 10: 30S ribosomal protein S10



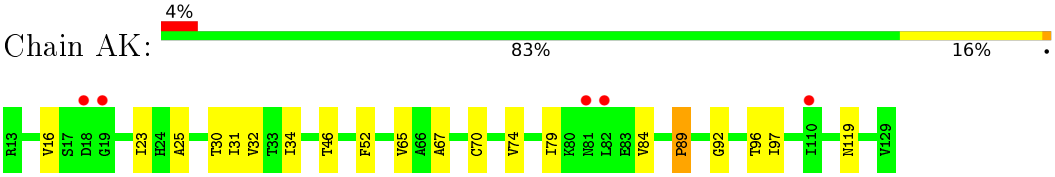


• Molecule 10: 30S ribosomal protein S10

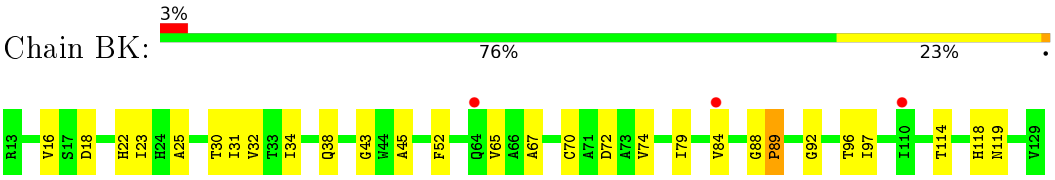




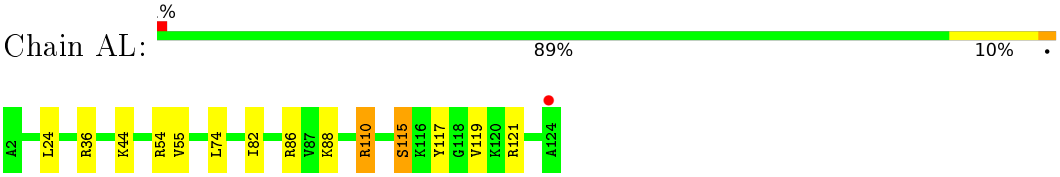
• Molecule 11: 30S ribosomal protein S11



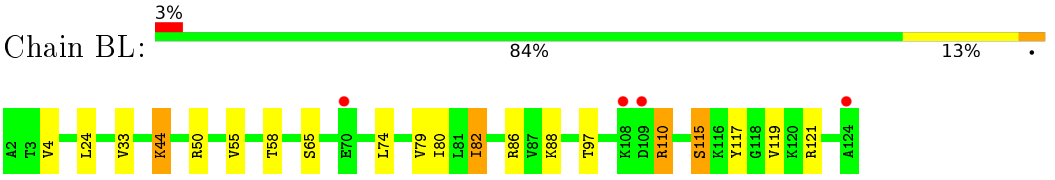
• Molecule 11: 30S ribosomal protein S11



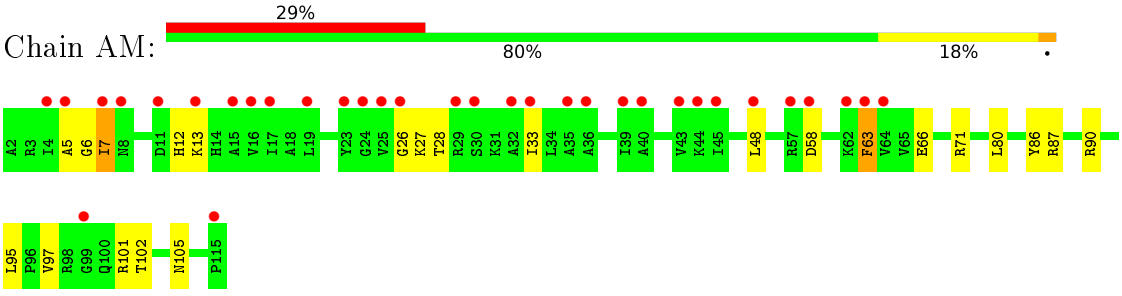
• Molecule 12: 30S ribosomal protein S12



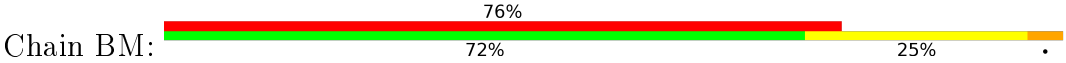
• Molecule 12: 30S ribosomal protein S12

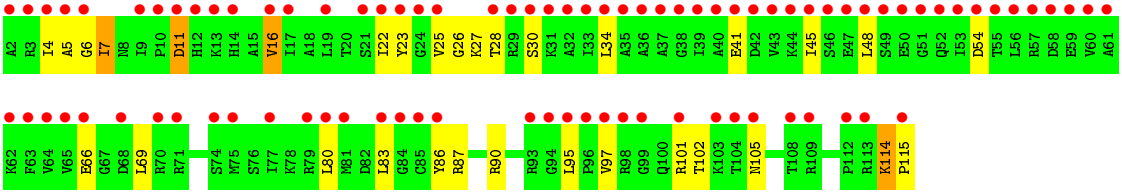


• Molecule 13: 30S ribosomal protein S13

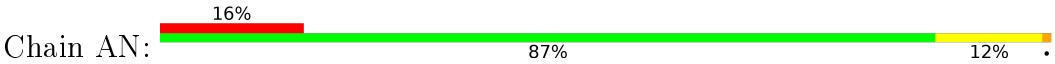


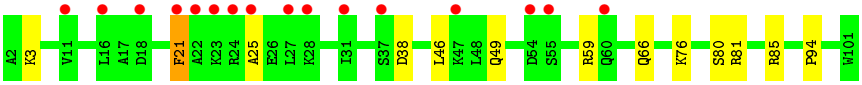
• Molecule 13: 30S ribosomal protein S13



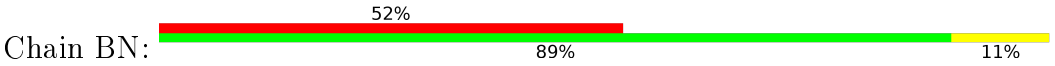


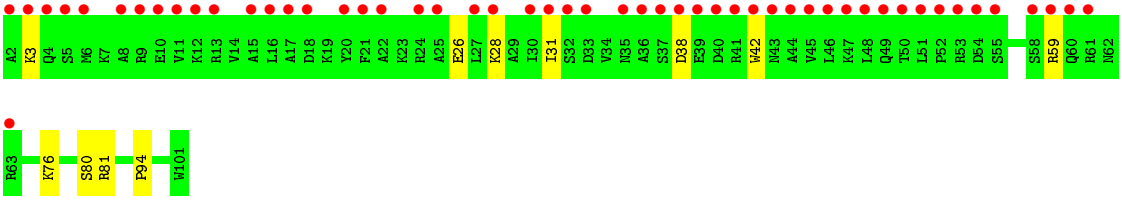
• Molecule 14: 30S ribosomal protein S14



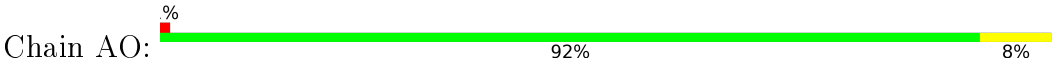


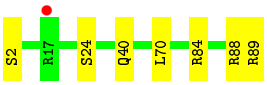
• Molecule 14: 30S ribosomal protein S14



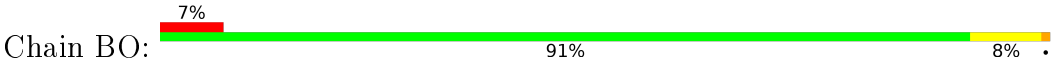


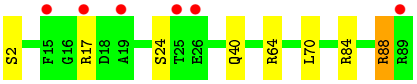
• Molecule 15: 30S ribosomal protein S15



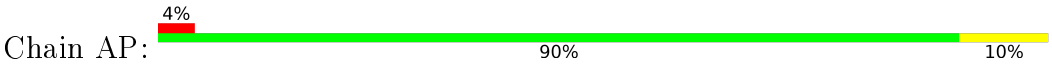


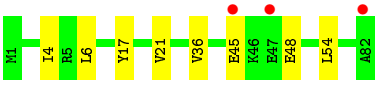
• Molecule 15: 30S ribosomal protein S15



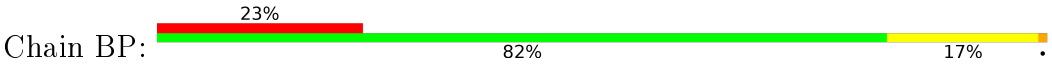


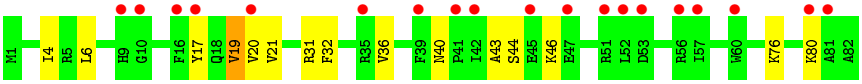
• Molecule 16: 30S ribosomal protein S16



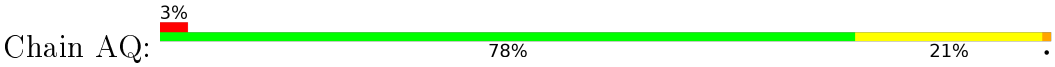


• Molecule 16: 30S ribosomal protein S16

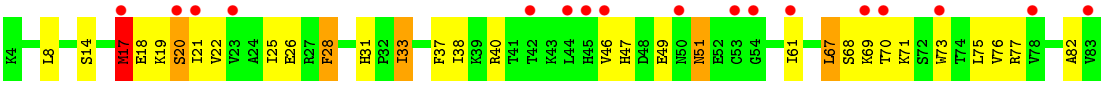




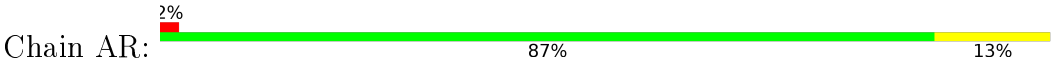
• Molecule 17: 30S ribosomal protein S17

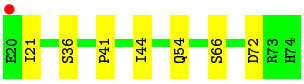


• Molecule 17: 30S ribosomal protein S17

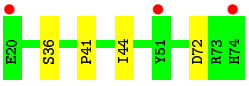


• Molecule 18: 30S ribosomal protein S18

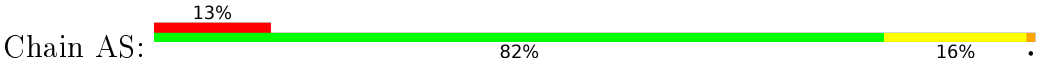


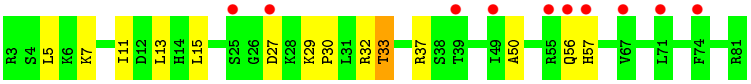


• Molecule 18: 30S ribosomal protein S18

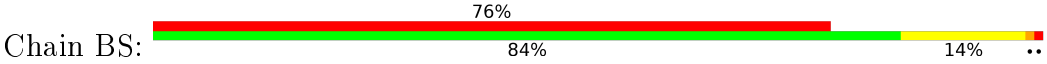


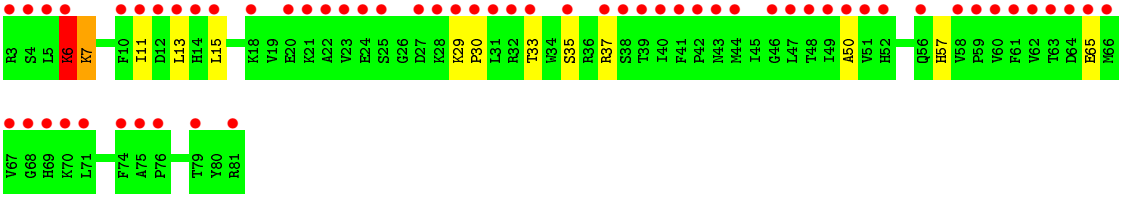
• Molecule 19: 30S ribosomal protein S19





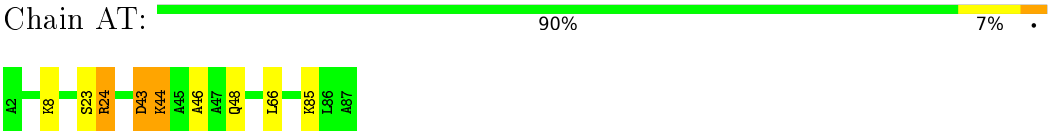
• Molecule 19: 30S ribosomal protein S19





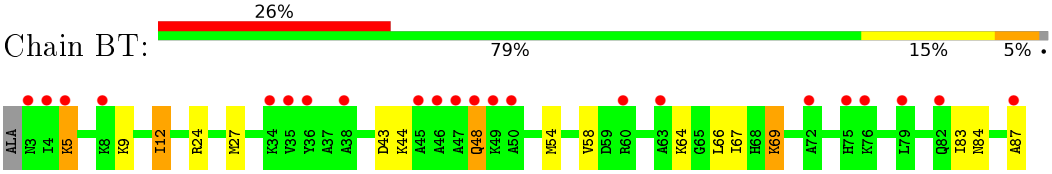
• Molecule 20: 30S ribosomal protein S20

Chain AT:



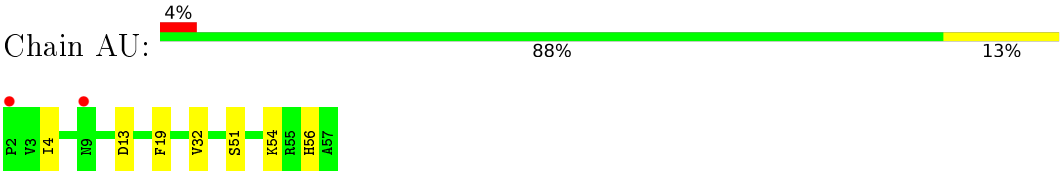
• Molecule 20: 30S ribosomal protein S20

Chain BT:



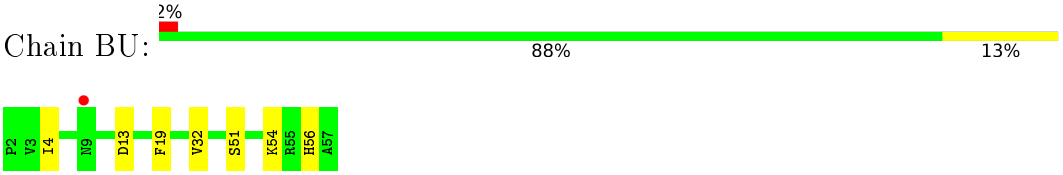
• Molecule 21: 30S ribosomal protein S21

Chain AU:



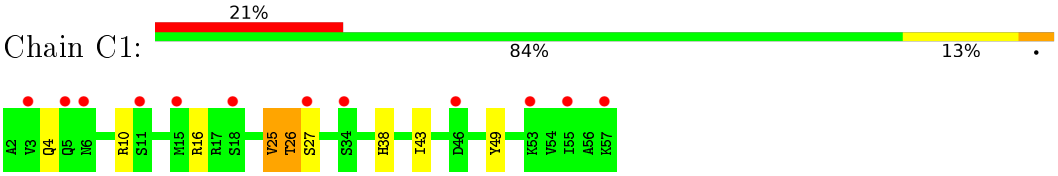
• Molecule 21: 30S ribosomal protein S21

Chain BU:



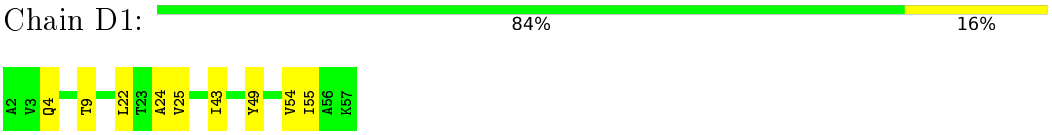
• Molecule 22: 50S ribosomal protein L32

Chain C1:



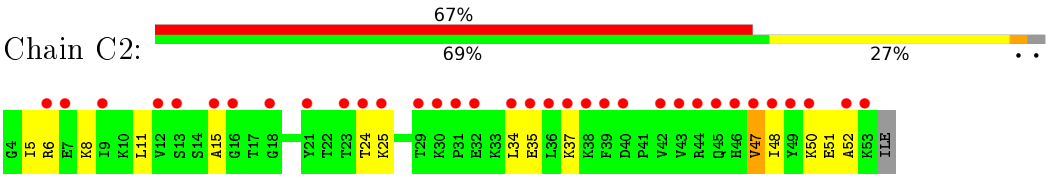
• Molecule 22: 50S ribosomal protein L32

Chain D1:



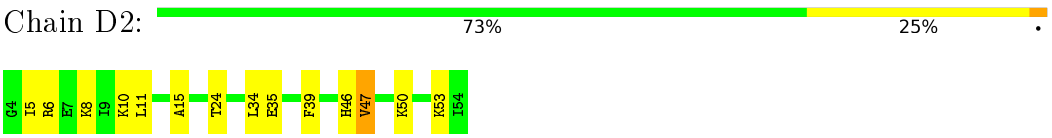
• Molecule 23: 50S ribosomal protein L33

Chain C2:



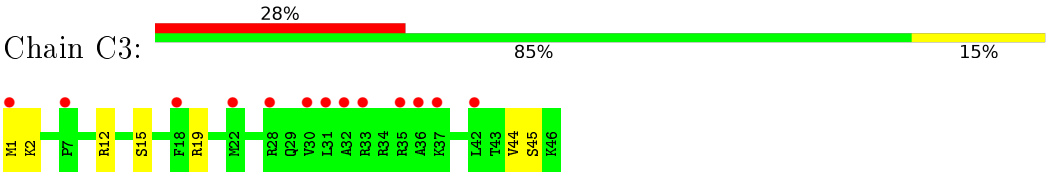
• Molecule 23: 50S ribosomal protein L33

Chain D2:



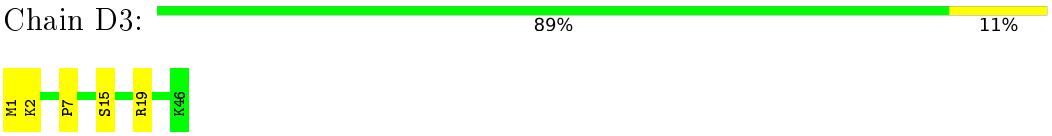
• Molecule 24: 50S ribosomal protein L34

Chain C3:



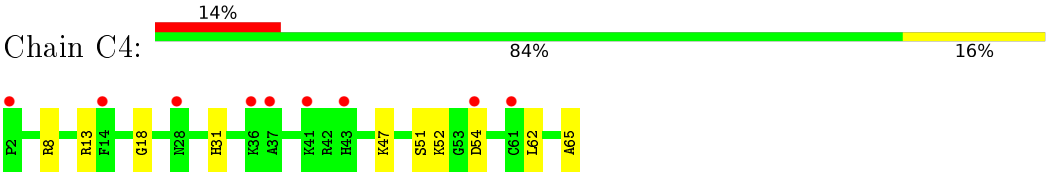
• Molecule 24: 50S ribosomal protein L34

Chain D3:



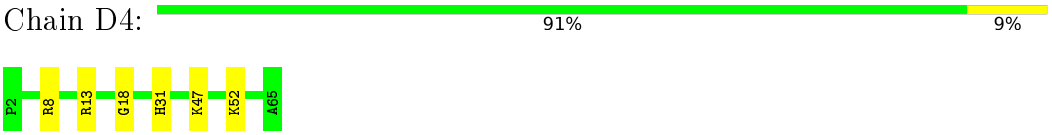
• Molecule 25: 50S ribosomal protein L35

Chain C4:



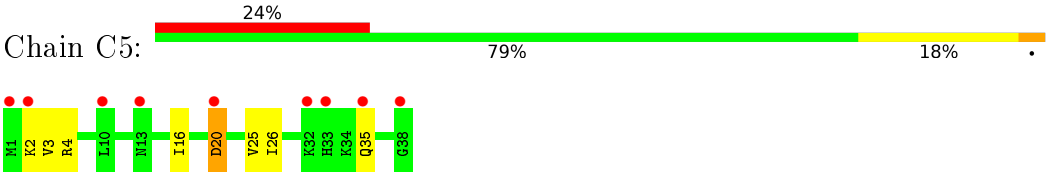
• Molecule 25: 50S ribosomal protein L35

Chain D4:



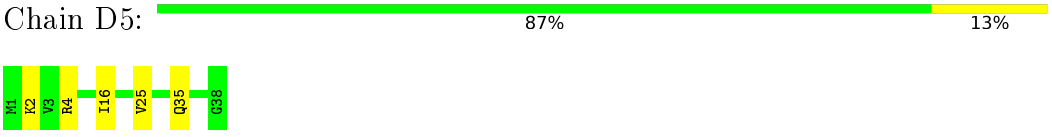
• Molecule 26: 50S ribosomal protein L36

Chain C5:



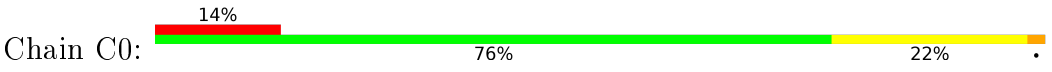
• Molecule 26: 50S ribosomal protein L36

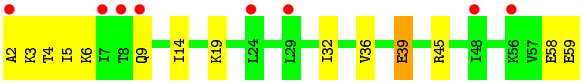
Chain D5:



• Molecule 27: 50S ribosomal protein L30

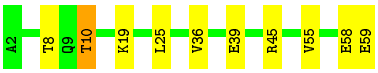
Chain C0:





• Molecule 27: 50S ribosomal protein L30

Chain D0:

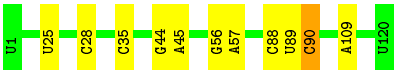


• Molecule 28: 50S ribosomal protein L1

Chain CB:

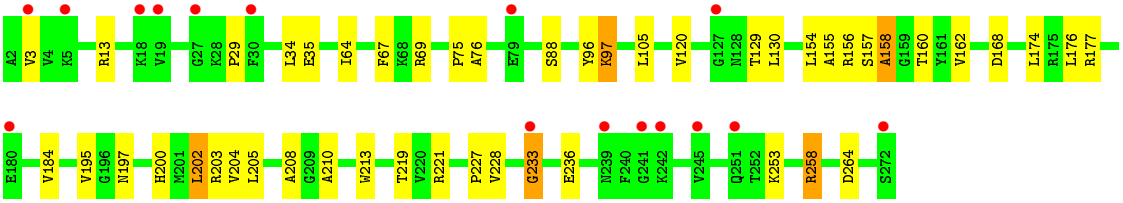
• Molecule 28: 50S ribosomal protein L1

Chain DB:



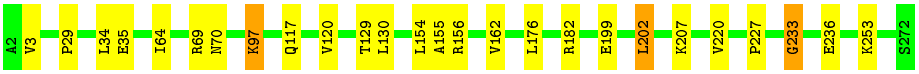
• Molecule 29: 50S ribosomal protein L2

Chain CC:



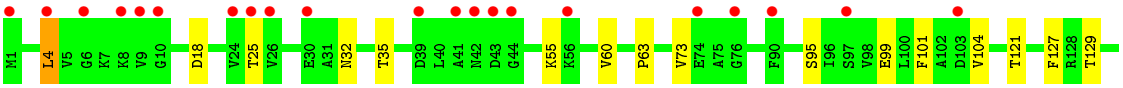
• Molecule 29: 50S ribosomal protein L2

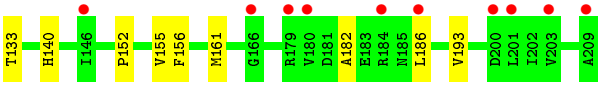
Chain DC:



• Molecule 30: 50S ribosomal protein L3

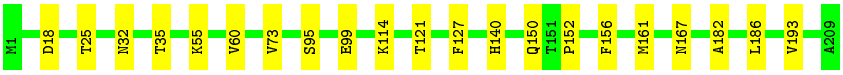
Chain CD:





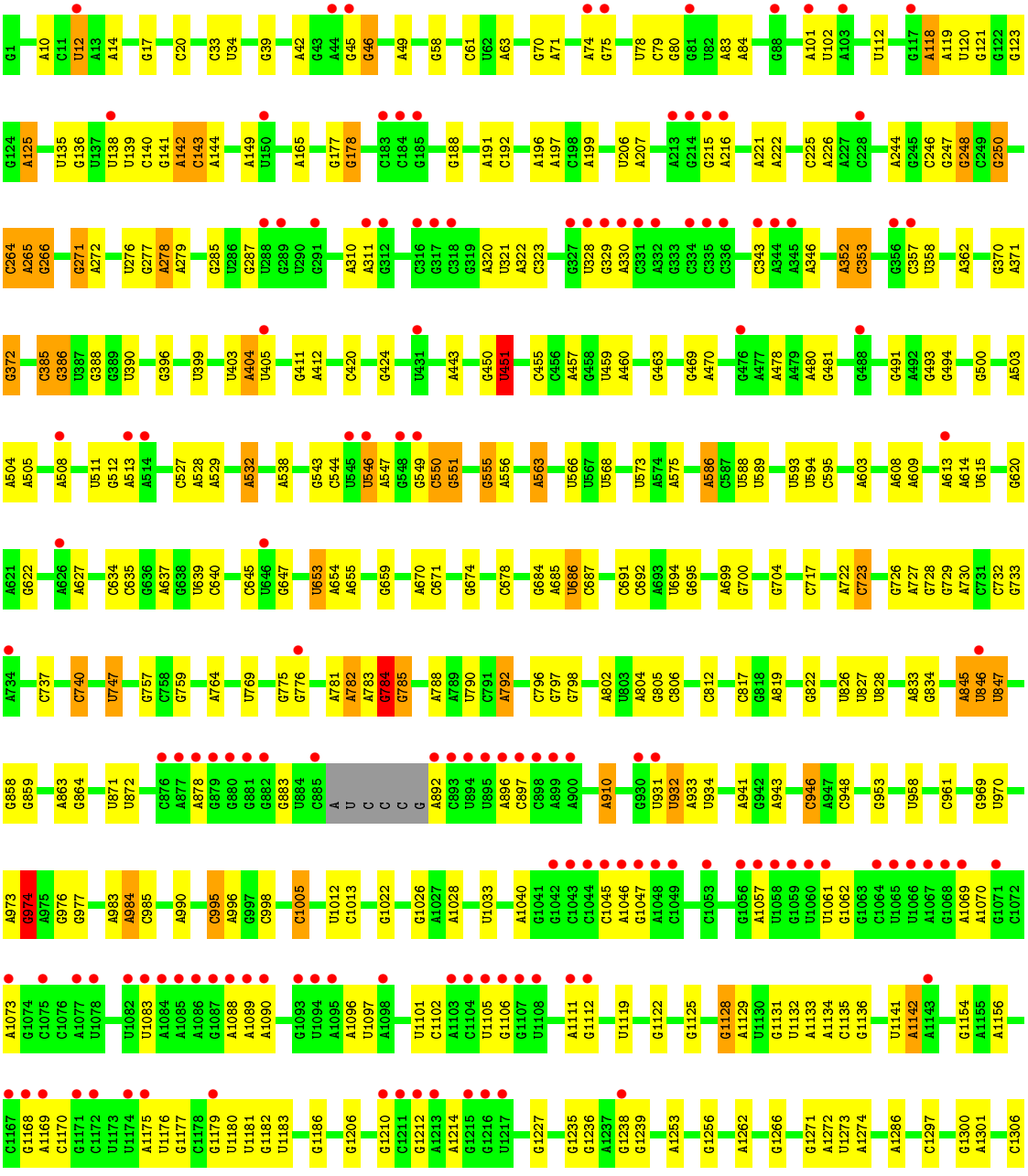
• Molecule 30: 50S ribosomal protein L3

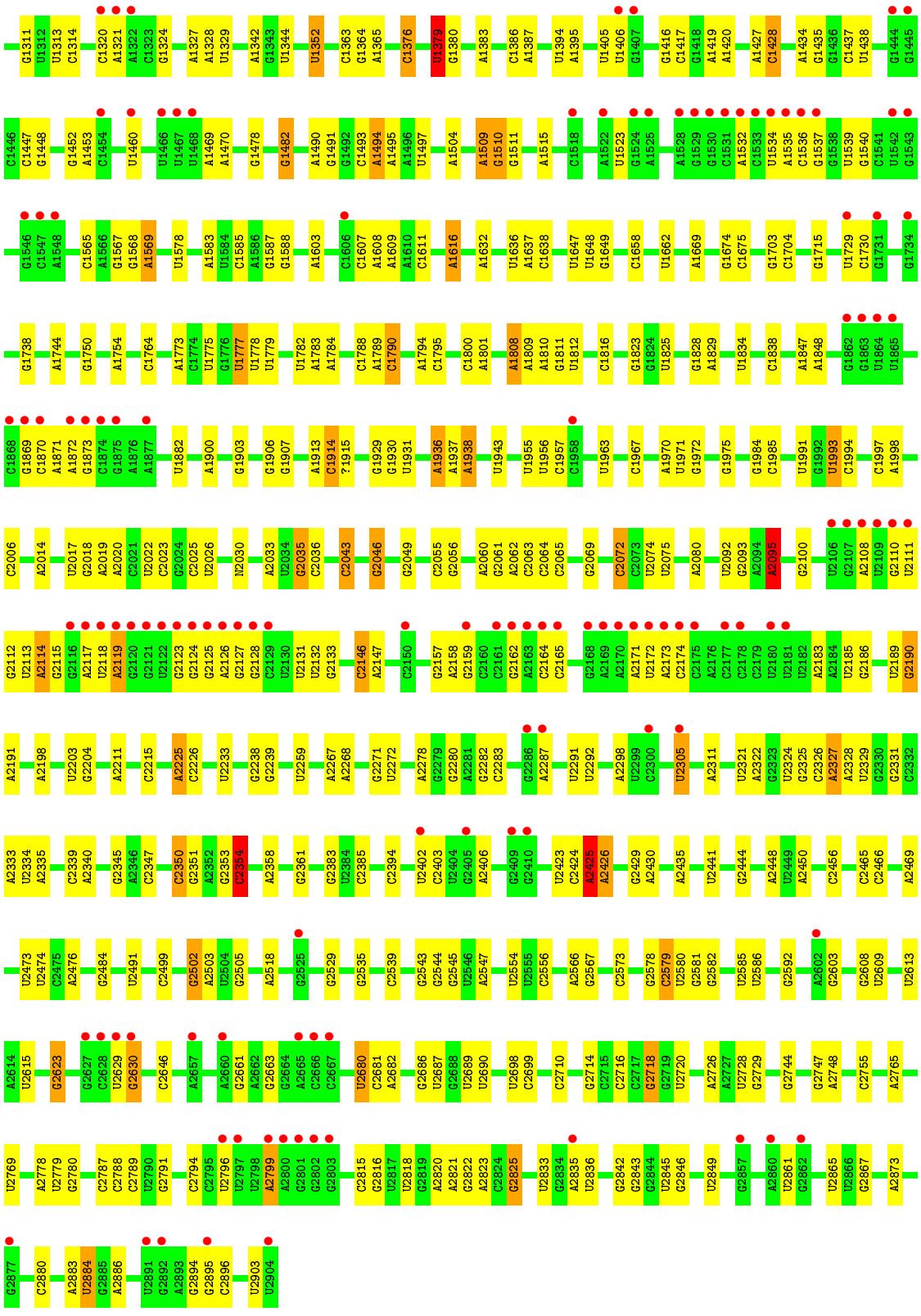
Chain DD:



• Molecule 31: 23S rRNA

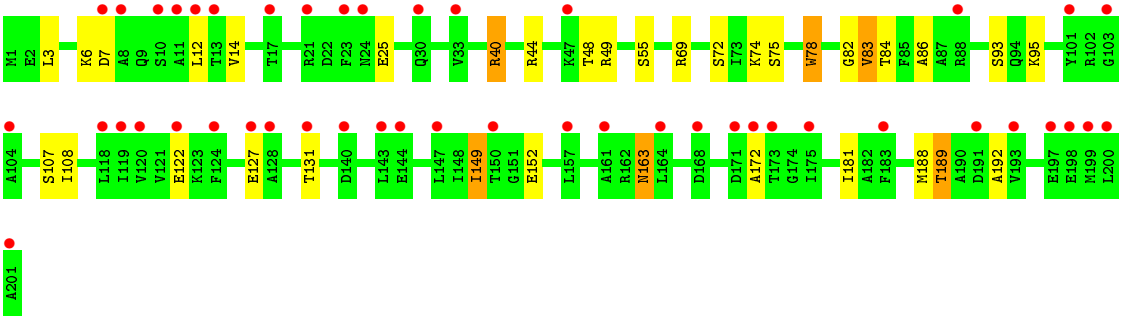
Chain CA:





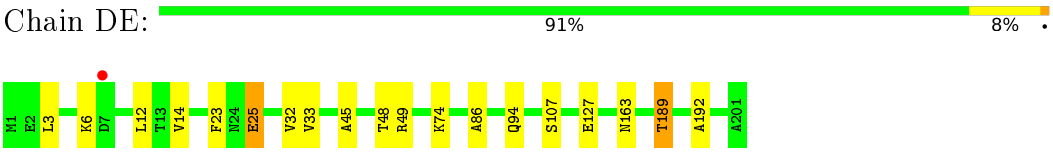
• Molecule 32: 50S ribosomal protein L4

Chain CE:



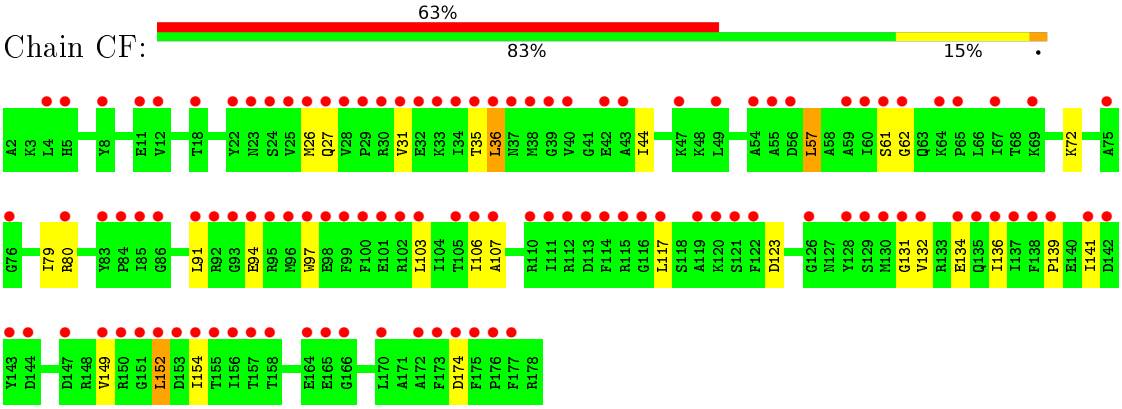
- Molecule 32: 50S ribosomal protein L4

Chain DE:



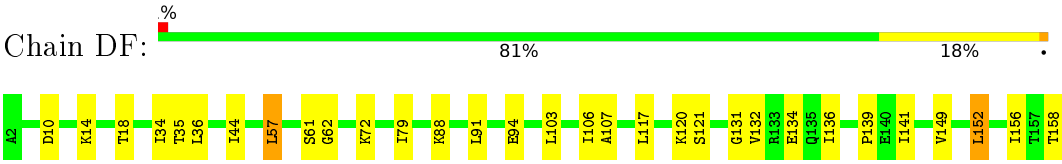
- Molecule 33: 50S ribosomal protein L5

Chain CF:



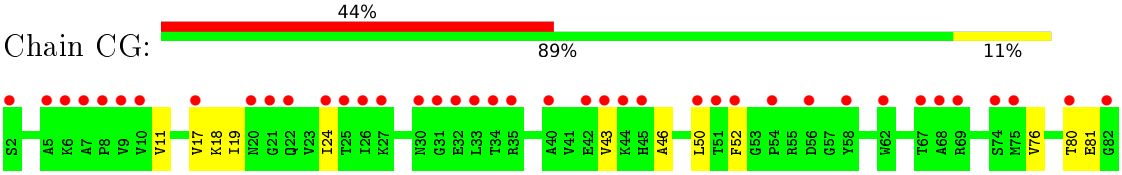
- Molecule 33: 50S ribosomal protein L5

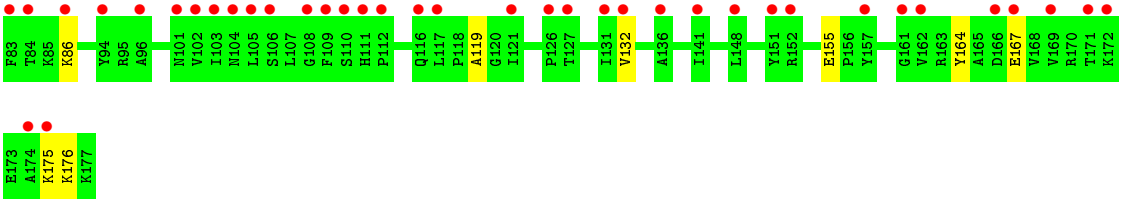
Chain DF:



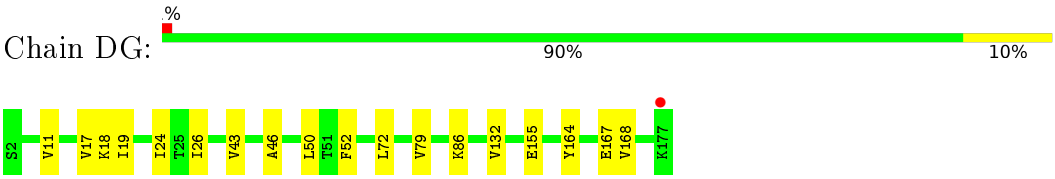
- Molecule 34: 50S ribosomal protein L6

Chain CG:

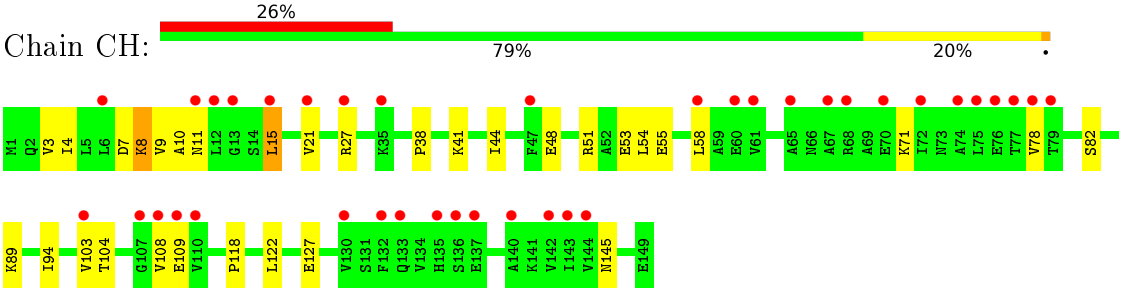




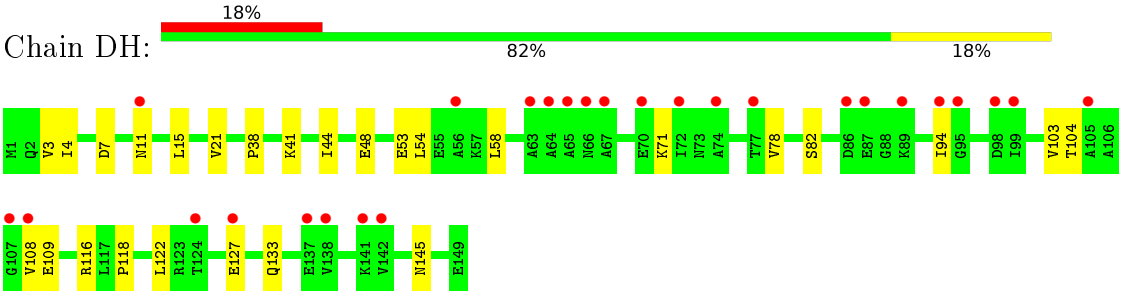
• Molecule 34: 50S ribosomal protein L6



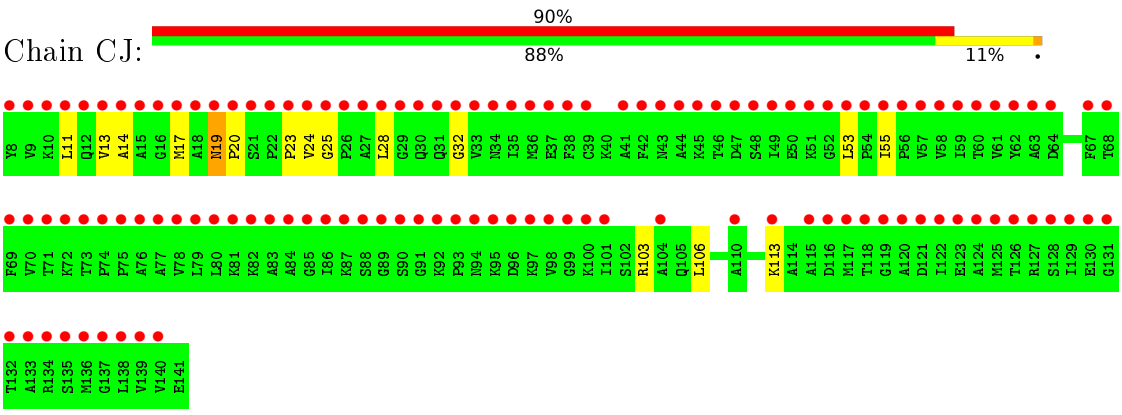
• Molecule 35: 50S ribosomal protein L9



• Molecule 35: 50S ribosomal protein L9

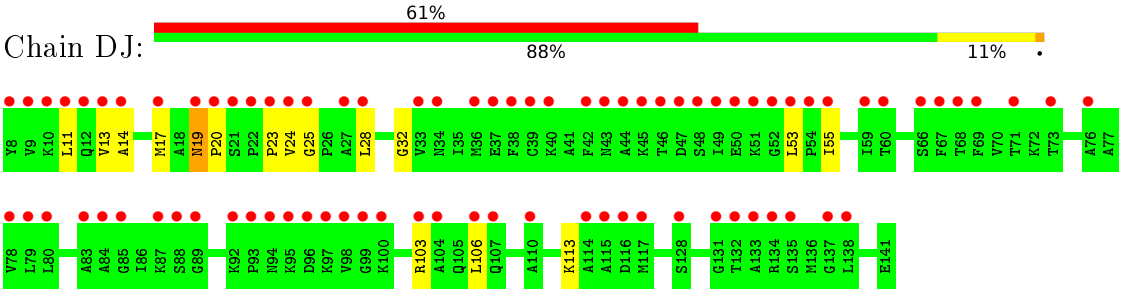


• Molecule 36: 50S ribosomal protein L11



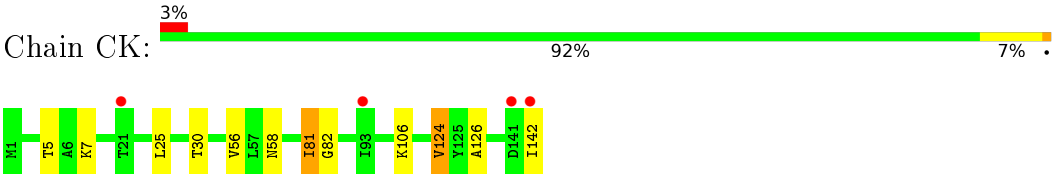
• Molecule 36: 50S ribosomal protein L11

Chain DJ:



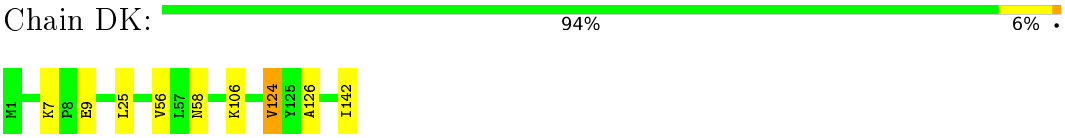
• Molecule 37: 50S ribosomal protein L13

Chain CK:



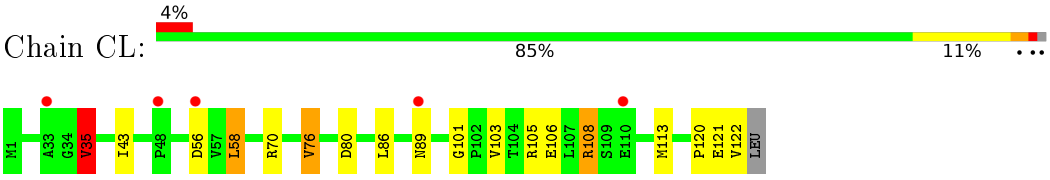
• Molecule 37: 50S ribosomal protein L13

Chain DK:



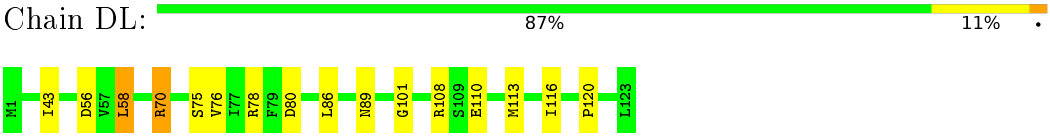
• Molecule 38: 50S ribosomal protein L14

Chain CL:



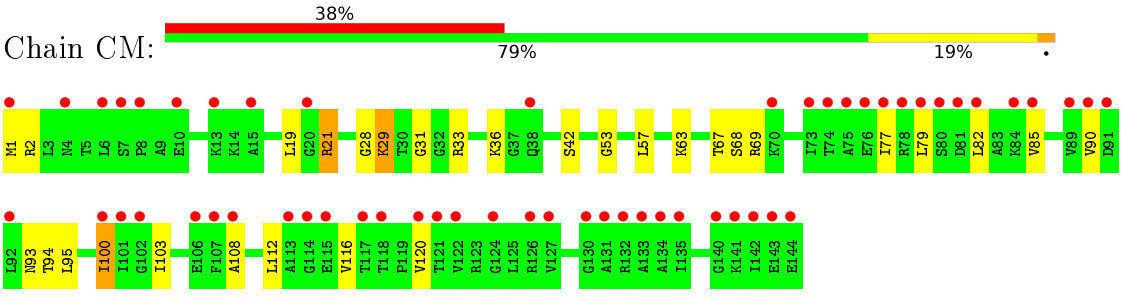
• Molecule 38: 50S ribosomal protein L14

Chain DL:



• Molecule 39: 50S ribosomal protein L15

Chain CM:

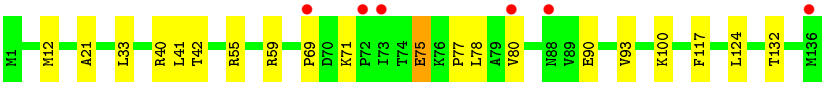


• Molecule 39: 50S ribosomal protein L15

Chain DM:

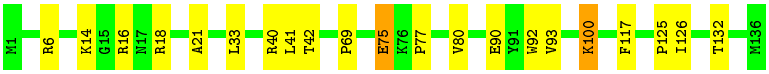
• Molecule 40: 50S ribosomal protein L16

Chain CN:



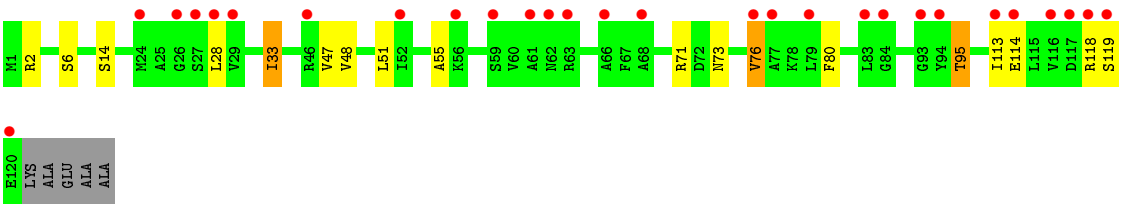
• Molecule 40: 50S ribosomal protein L16

Chain DN:



• Molecule 41: 50S ribosomal protein L17

Chain CO:

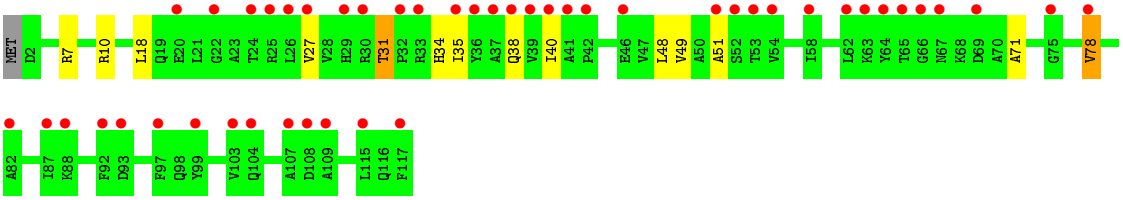


• Molecule 41: 50S ribosomal protein L17

Chain DO:

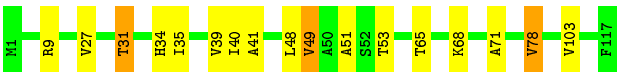
• Molecule 42: 50S ribosomal protein L18

Chain CP:



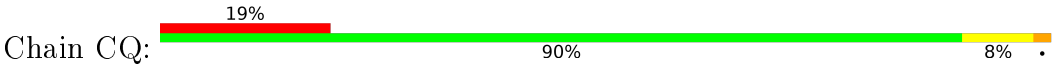
• Molecule 42: 50S ribosomal protein L18

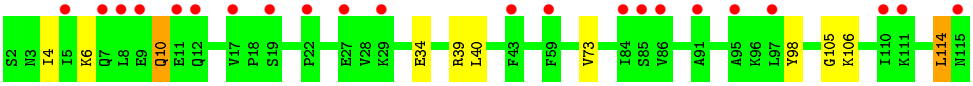
Chain DP:



• Molecule 43: 50S ribosomal protein L19

Chain CQ:



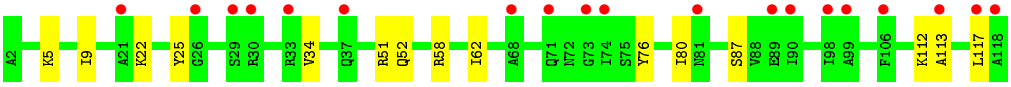


• Molecule 43: 50S ribosomal protein L19

Chain DQ:

• Molecule 44: 50S ribosomal protein L20

Chain CR:



• Molecule 44: 50S ribosomal protein L20

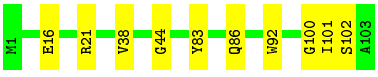
Chain DR:

• Molecule 45: 50S ribosomal protein L21

Chain CS:

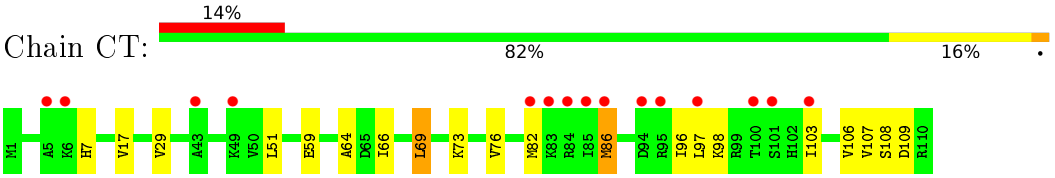
• Molecule 45: 50S ribosomal protein L21

Chain DS:



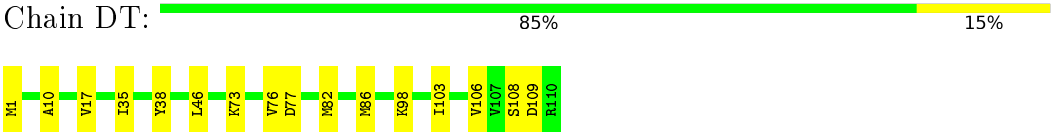
• Molecule 46: 50S ribosomal protein L22

Chain CT:



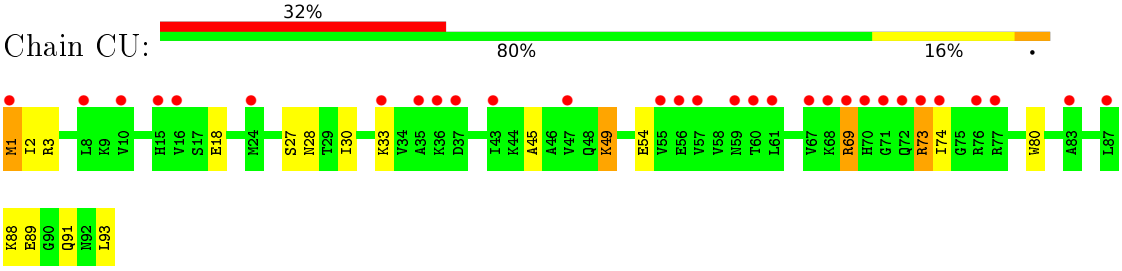
• Molecule 46: 50S ribosomal protein L22

Chain DT:



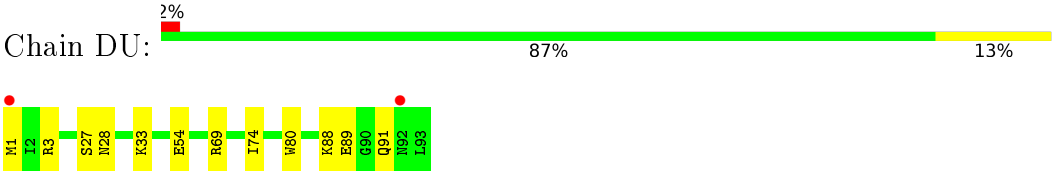
• Molecule 47: 50S ribosomal protein L23

Chain CU:



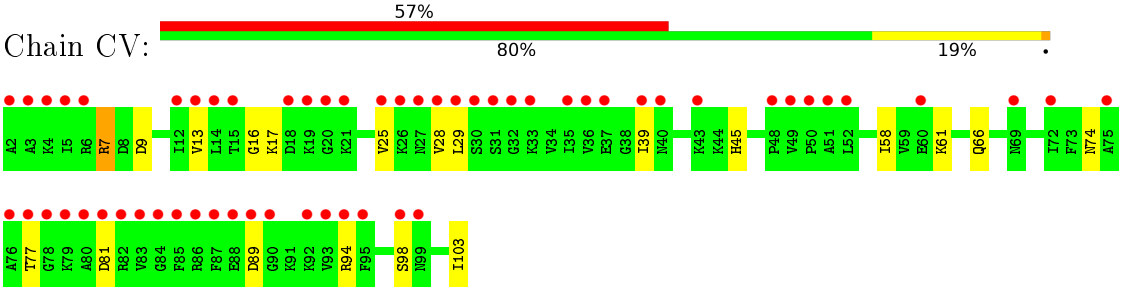
• Molecule 47: 50S ribosomal protein L23

Chain DU:



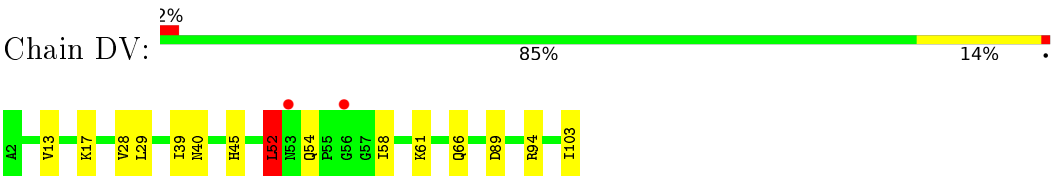
• Molecule 48: 50S ribosomal protein L24

Chain CV:



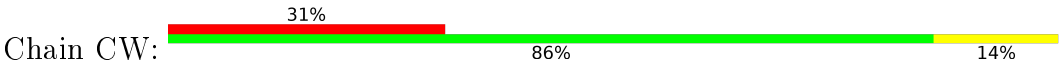
• Molecule 48: 50S ribosomal protein L24

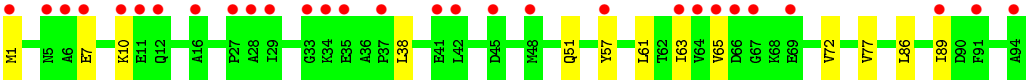
Chain DV:



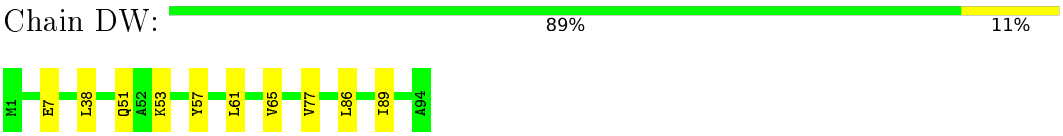
• Molecule 49: 50S ribosomal protein L25

Chain CW:

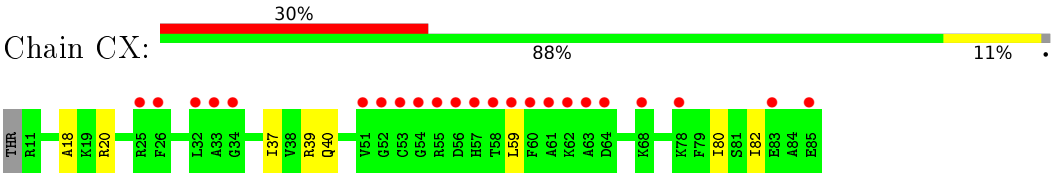




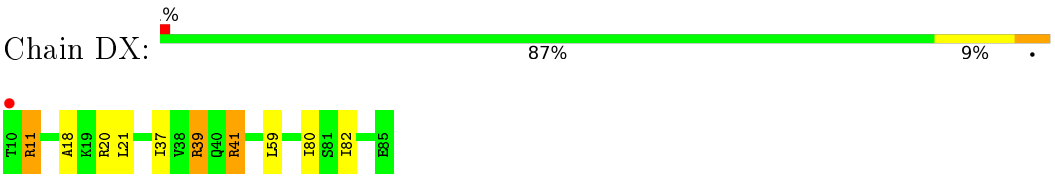
• Molecule 49: 50S ribosomal protein L25



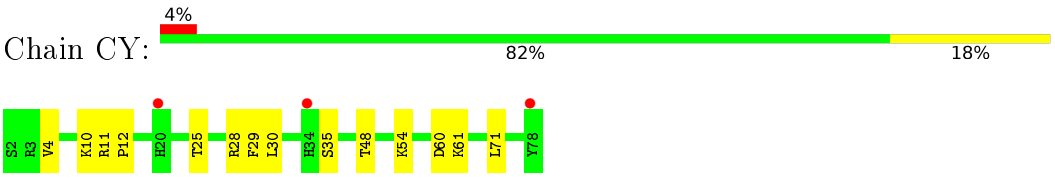
• Molecule 50: 50S ribosomal protein L27



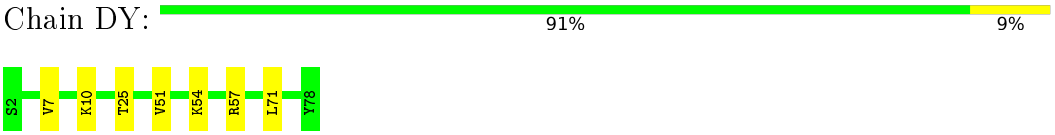
• Molecule 50: 50S ribosomal protein L27



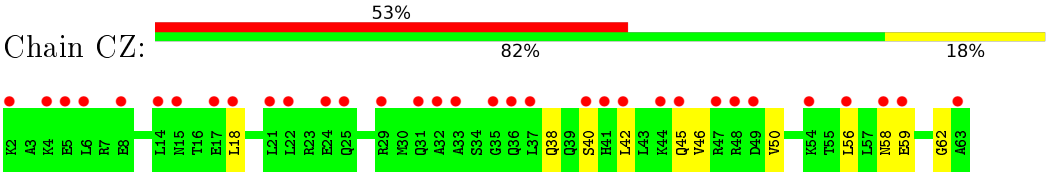
• Molecule 51: 50S ribosomal protein L28



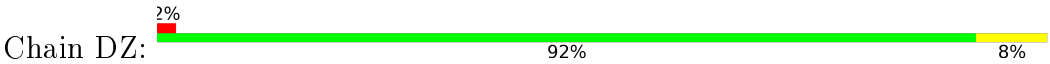
• Molecule 51: 50S ribosomal protein L28

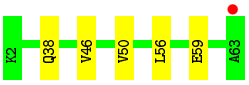


• Molecule 52: 50S ribosomal protein L29



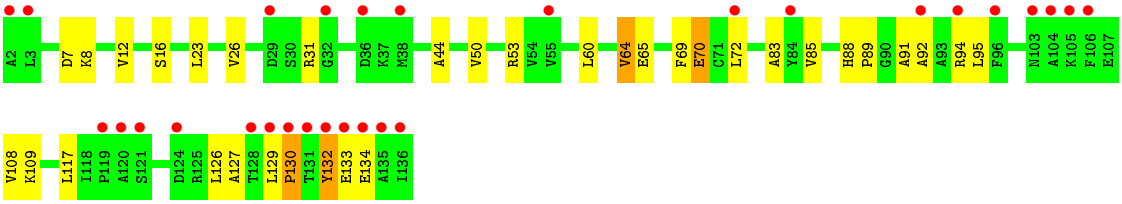
• Molecule 52: 50S ribosomal protein L29





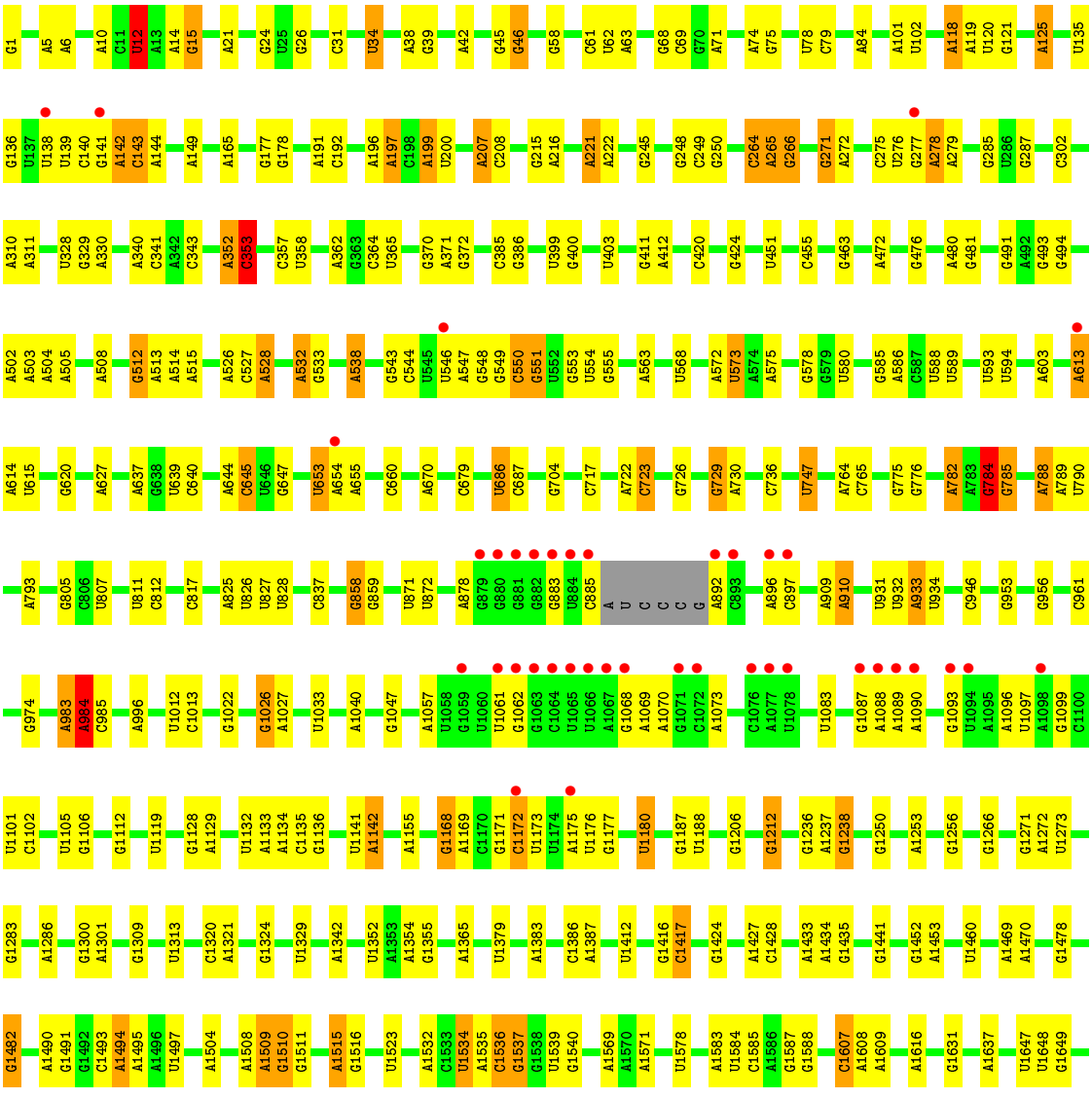
• Molecule 53: 50S ribosomal protein L10

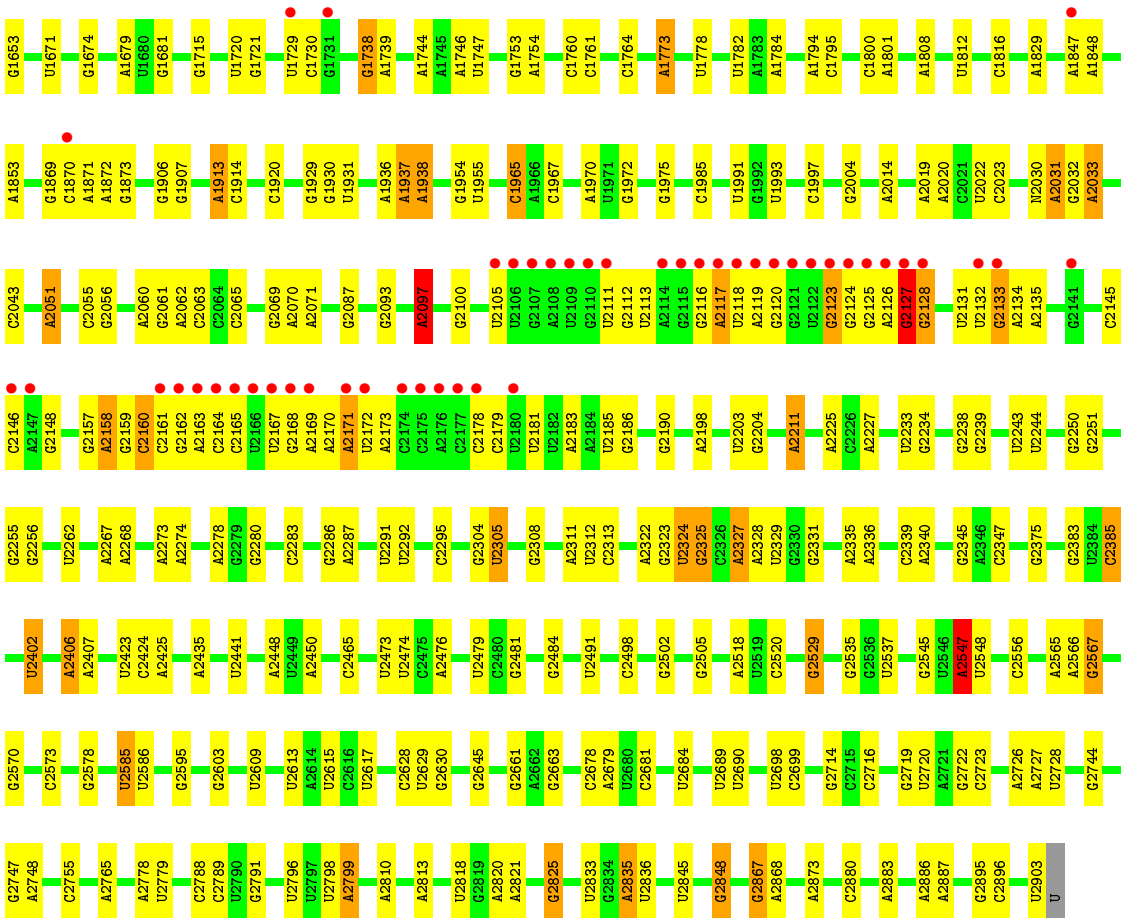
Chain DI:



• Molecule 54: 23S rRNA

Chain DA:




G1653 U1671 G1674 A1679 U1680 G1681 G1715 U1720 G1721 U1729 C1730 G1731 G1738 A1739 A1744 A1745 A1746 U1747 G1753 A1754 C1760 C1761 C1764 A1773 U1778 U1782 A1783 A1784 A1794 C1795 C1800 A1801 A1808 U1812 C1816 A1829 A1847 A1848
A1853 G1869 C1870 A1871 A1872 G1873 G1906 G1907 A1913 C1914 C1920 G1929 G1930 U1931 A1936 A1937 A1938 G1954 U1955 C1965 A1966 C1967 A1970 U1971 G1972 G1975 C1985 U1991 G1992 U1993 C1997 G2004 A2014 A2019 A2020 C2021 U2022 C2023 M2030 A2031 G2032 A2033
C2043 A2051 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 G2069 A2070 A2071 G2087 G2093 A2097 G2100 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 U2131 U2132 G2133 A2134 A2135 G2141 C2145
C2146 A2147 G2148 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 G2190 A2198 U2203 G2204 A2211 A2225 C2226 A2227 U2233 G2234 G2238 G2239 U2243 U2244 G2250 G2251
G2255 G2256 U2262 A2267 A2268 A2273 A2274 A2278 G2279 G2280 C2283 G2286 A2287 U2291 U2292 C2295 G2304 U2305 G2308 A2311 U2312 C2313 A2322 G2323 U2324 G2325 C2326 A2327 A2328 U2329 G2330 G2331 A2335 A2336 C2339 A2340 G2345 A2346 C2347 G2375 G2383 U2384 C2385
U2402 A2406 A2407 U2423 C2424 A2425 A2435 U2441 A2448 U2449 A2450 C2465 U2473 U2474 C2475 A2476 U2479 C2480 G2481 G2484 U2491 C2498 G2502 G2505 A2518 U2519 C2520 G2529 G2535 G2536 U2537 G2545 U2546 A2547 U2548 C2556 A2565 A2566 G2567
G2570 C2573 G2578 U2585 U2586 G2595 G2603 U2609 U2613 A2614 U2615 C2616 U2617 C2628 U2629 G2630 G2645 G2661 A2662 G2663 C2678 A2679 U2680 C2681 U2684 U2689 U2690 U2698 C2699 G2714 C2715 C2716 G2719 U2720 A2721 G2722 C2723 A2726 A2727 U2728 G2744
G2747 A2748 C2755 A2765 A2778 U2779 C2788 C2789 U2790 G2791 U2796 U2797 U2798 A2799 A2810 A2813 U2818 G2819 A2820 A2821 G2825 U2833 G2834 A2835 U2836 U2845 G2848 G2867 A2868 A2873 C2880 A2883 A2886 A2887 G2895 C2896 U2903 U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.41Å 435.70Å 625.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.00 48.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-3.00) 99.2 (48.61-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.172 , 0.193 0.184 , 0.207	Depositor DCC
R_{free} test set	4504 reflections (0.40%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	295261	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.97	8/36597 (0.0%)	0.86	4/57088 (0.0%)
1	BA	0.99	13/36572 (0.0%)	0.86	7/57049 (0.0%)
2	AB	0.45	0/1784	0.64	0/2403
2	BB	0.44	0/1784	0.64	0/2403
3	AC	0.46	0/1652	0.66	0/2225
3	BC	0.45	0/1652	0.68	0/2225
4	AD	0.43	0/1665	0.66	0/2227
4	BD	0.44	0/1665	0.67	0/2227
5	AE	0.47	0/1157	0.75	0/1557
5	BE	0.50	0/1118	0.80	0/1504
6	AF	0.45	0/881	0.70	1/1189 (0.1%)
6	BF	0.46	0/835	0.79	1/1128 (0.1%)
7	AG	0.45	0/1196	0.62	0/1602
7	BG	0.45	0/1196	0.62	0/1602
8	AH	0.43	0/989	0.70	0/1326
8	BH	0.42	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.65	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.42	0/806	0.66	0/1089
10	BJ	0.48	0/797	0.70	0/1077
11	AK	0.43	0/893	0.63	0/1205
11	BK	0.42	0/893	0.67	0/1205
12	AL	0.44	0/960	0.72	0/1286
12	BL	0.44	0/960	0.73	0/1286
13	AM	0.50	0/893	0.73	0/1193
13	BM	0.49	0/893	0.72	0/1193
14	AN	0.45	0/817	0.64	0/1088
14	BN	0.43	0/817	0.63	0/1088
15	AO	0.45	0/722	0.61	0/964
15	BO	0.43	0/722	0.61	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	AP	0.45	0/659	0.69	0/884
16	BP	0.48	0/659	0.76	0/884
17	AQ	0.46	0/658	0.72	0/881
17	BQ	0.50	0/658	0.76	0/881
18	AR	0.47	0/463	0.65	0/621
18	BR	0.48	0/463	0.65	0/621
19	AS	0.46	0/653	0.60	0/877
19	BS	0.46	0/653	0.61	0/877
20	AT	0.48	0/676	0.67	0/895
20	BT	0.53	0/671	0.69	0/888
21	AU	0.40	0/472	0.61	0/627
21	BU	0.38	0/472	0.62	0/627
22	C1	0.48	0/450	0.67	0/599
22	D1	0.58	0/450	0.72	0/599
23	C2	0.48	0/416	0.70	0/554
23	D2	0.47	0/421	0.69	0/561
24	C3	0.45	0/380	0.68	0/498
24	D3	0.56	0/380	0.76	0/498
25	C4	0.43	0/513	0.65	0/676
25	D4	0.50	0/513	0.68	0/676
26	C5	0.41	0/303	0.79	0/397
26	D5	0.50	0/303	0.78	0/397
27	C0	0.48	0/453	0.77	0/605
27	D0	0.62	0/467	0.79	1/623 (0.2%)
28	CB	0.91	0/2828	0.88	1/4410 (0.0%)
28	DB	1.01	0/2872	0.88	0/4478
29	CC	0.43	0/2122	0.73	0/2852
29	DC	0.48	0/2122	0.74	1/2852 (0.0%)
30	CD	0.42	0/1576	0.67	0/2119
30	DD	0.51	0/1576	0.68	0/2119
31	CA	1.02	39/69143 (0.1%)	0.87	11/107862 (0.0%)
32	CE	0.43	0/1571	0.70	0/2113
32	DE	0.49	0/1571	0.68	0/2113
33	CF	0.41	0/1435	0.67	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.39	0/1343	0.66	0/1816
34	DG	0.43	0/1343	0.64	0/1816
35	CH	0.46	0/1121	0.68	1/1515 (0.1%)
35	DH	0.46	0/1121	0.67	0/1515
36	CJ	0.49	0/993	0.62	0/1341
36	DJ	0.49	0/993	0.62	0/1341
37	CK	0.41	0/1152	0.68	0/1551
37	DK	0.53	0/1152	0.71	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	CL	0.45	0/947	0.71	0/1268
38	DL	0.51	0/955	0.72	0/1279
39	CM	0.45	0/1062	0.73	1/1413 (0.1%)
39	DM	0.47	0/1062	0.70	0/1413
40	CN	0.45	0/1081	0.72	0/1443
40	DN	0.54	0/1092	0.76	0/1457
41	CO	0.44	0/973	0.68	0/1301
41	DO	0.54	0/1006	0.74	0/1345
42	CP	0.42	0/902	0.71	0/1209
42	DP	0.49	0/910	0.71	0/1219
43	CQ	0.40	0/929	0.69	1/1242 (0.1%)
43	DQ	0.45	0/929	0.69	0/1242
44	CR	0.43	0/960	0.65	0/1278
44	DR	0.54	0/960	0.68	0/1278
45	CS	0.42	0/829	0.73	0/1107
45	DS	0.51	0/829	0.74	0/1107
46	CT	0.41	0/864	0.70	0/1156
46	DT	0.53	0/864	0.69	0/1156
47	CU	0.44	0/745	0.71	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.44	0/788	0.75	0/1051
48	DV	0.47	0/788	0.75	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.49	0/766	0.68	0/1025
50	CX	0.40	0/576	0.65	0/762
50	DX	0.55	0/598	0.74	0/790
51	CY	0.41	0/635	0.70	0/848
51	DY	0.46	0/635	0.70	0/848
52	CZ	0.42	0/502	0.59	0/667
52	DZ	0.45	0/502	0.59	0/667
53	DI	0.50	0/1037	0.76	1/1402 (0.1%)
54	DA	1.14	49/69364 (0.1%)	0.91	15/108207 (0.0%)
All	All	0.91	109/309249 (0.0%)	0.84	46/462175 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	8
40	CN	0	1
40	DN	0	1
54	DA	0	41
All	All	0	56

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.26	1.28	1.42
54	DA	12	U	C1'-N1	8.76	1.61	1.48
31	CA	1936	A	N9-C4	-8.51	1.32	1.37
54	DA	2097	A	O5'-C5'	-8.36	1.29	1.42
31	CA	2425	A	C3'-O3'	8.30	1.53	1.42

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	CB	15	A	O4'-C1'-N9	10.03	116.22	108.20
54	DA	1936	A	O4'-C1'-N9	8.20	114.76	108.20
1	BA	1362	A	C1'-O4'-C4'	-7.38	104.00	109.90
1	AA	1	A	OP1-P-OP2	-7.19	108.81	119.60
31	CA	271	G	P-O3'-C3'	7.11	128.24	119.70

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
1	BA	1432	G	Sidechain
1	BA	898	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	32933	0	16592	113	0
1	BA	32911	0	16581	115	0
2	AB	1753	0	1780	7	0
2	BB	1753	0	1780	9	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	11	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	14	0
5	BE	1105	0	1148	25	0
6	AF	862	0	864	7	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	6	0
8	BH	979	0	1031	3	0
9	AI	1022	0	1070	8	0
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	13	0
11	BK	877	0	887	15	0
12	AL	957	0	1017	5	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	13	0
13	BM	884	0	941	18	0
14	AN	805	0	844	8	0
14	BN	805	0	844	7	0
15	AO	714	0	734	0	0
15	BO	714	0	734	0	0
16	AP	649	0	666	2	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	13	0
18	AR	456	0	478	3	0
18	BR	456	0	478	2	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	3	0
20	BT	665	0	714	4	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	9	0
23	C2	409	0	440	6	0
23	D2	414	0	442	6	0
24	C3	377	0	418	3	0
24	D3	377	0	418	3	0
25	C4	504	0	572	2	0
25	D4	504	0	572	2	0
26	C5	302	0	340	6	0
26	D5	302	0	340	2	0
27	C0	449	0	488	3	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	6	0
28	DB	2569	0	1301	3	0
29	CC	2083	0	2154	24	0
29	DC	2083	0	2154	12	0
30	CD	1565	0	1614	15	0
30	DD	1576	0	1627	15	0
31	CA	62229	0	31317	224	0
32	CE	1552	0	1619	18	0
32	DE	1552	0	1619	9	0
33	CF	1411	0	1444	14	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	8	0
34	DG	1323	0	1371	8	0
35	CH	1110	0	1148	10	0
35	DH	1110	0	1148	9	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	5	0
37	CK	1129	0	1162	8	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	7	0
39	CM	1053	0	1129	19	0
39	DM	1053	0	1129	6	0
40	CN	1075	0	1154	9	0
40	DN	1092	0	1177	13	0
41	CO	960	0	1000	6	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	11	0
43	CQ	917	0	962	6	0
43	DQ	917	0	962	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	CR	947	0	1019	11	0
44	DR	947	0	1019	13	0
45	CS	816	0	839	12	0
45	DS	816	0	839	7	0
46	CT	857	0	922	9	0
46	DT	857	0	922	9	0
47	CU	739	0	807	8	0
47	DU	739	0	807	7	0
48	CV	780	0	831	7	0
48	DV	780	0	831	6	0
49	CW	753	0	780	5	0
49	DW	753	0	780	4	0
50	CX	569	0	581	3	0
50	DX	591	0	606	10	0
51	CY	625	0	652	8	0
51	DY	625	0	652	3	0
52	CZ	501	0	531	3	0
52	DZ	501	0	531	2	0
53	DI	1023	0	1052	15	0
54	DA	62423	0	31411	176	0
55	AA	72	0	0	0	0
55	BA	45	0	0	0	0
55	CA	156	0	0	0	0
55	CB	3	0	0	0	0
55	DA	183	0	0	0	0
55	DB	9	0	0	0	0
55	DD	1	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	1	0
56	DA	26	0	36	3	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	3	0
57	AA	16	0	28	3	0
57	DA	40	0	70	3	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AA	24	0	48	0	0
58	DA	66	0	132	7	0
58	DM	6	0	12	0	0
59	AA	64	1	42	2	0
59	BA	64	1	42	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
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	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	1	0
62	DB	12	0	18	0	0
63	D1	10	0	14	2	0
63	DA	60	0	84	4	0
63	DS	10	0	14	1	0
63	DU	10	0	14	3	0
64	DA	40	0	76	2	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	501	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	5	0	0	2	0
69	AN	6	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BK	2	0	0	0	0
69	BL	4	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BT	2	0	0	0	0
69	BU	2	0	0	0	0
69	C3	4	0	0	0	0
69	C4	1	0	0	0	0
69	CA	691	0	0	3	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0
69	CO	2	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	0	0
69	D1	43	0	0	0	0
69	D2	6	0	0	0	0
69	D3	22	0	0	0	0
69	D4	39	0	0	0	0
69	D5	8	0	0	0	0
69	DA	4840	0	0	15	0
69	DB	209	0	0	1	0
69	DC	100	0	0	1	0
69	DD	98	0	0	2	0
69	DE	61	0	0	0	0
69	DF	15	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DM	63	0	0	0	0
69	DN	72	0	0	0	0
69	DO	44	0	0	0	0
69	DP	38	0	0	0	0
69	DQ	33	0	0	0	0
69	DR	62	0	0	1	0
69	DS	46	0	0	2	0
69	DT	69	0	0	1	0
69	DU	18	0	0	0	0
69	DV	20	0	0	0	0
69	DW	31	0	0	0	0
69	DX	25	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	8	0	0	0	0
All	All	295259	2	194493	1263	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 1263 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)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.27	1.10
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.61	1.00
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.46	0.97
31:CA:1847:A:HO2'	31:CA:1848:A:H8	0.98	0.95
31:CA:528:A:C2	31:CA:2043:C:H4'	2.00	0.95

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%)	207 (93%)	11 (5%)	4 (2%)	11 45
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	11 45
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34 76
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	13 50
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	34 76
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	34 76
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	26 70
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	3 20
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100 100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	3 20
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	26 70
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	26 70
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	24 66
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	12 48
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%)	6 (6%)	2 (2%)	9 40
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	2 9
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21 64
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	21 64
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100 100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	24 66
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	6 32
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	3 18
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	9 41
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	19 61
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100 100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	16 56
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	15 53
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7 34
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	15 53
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	AR	53/55 (96%)	51 (96%)	2 (4%)	0	100 100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
19	AS	77/79 (98%)	68 (88%)	9 (12%)	0	100 100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	15 53
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	16 56
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	7 35
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2 13
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3 20
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8 36
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	12 48
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	12 48
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	6 30
26	D5	36/38 (95%)	36 (100%)	0	0	100 100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4 24
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100 100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	13 50
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	26 70
30	CD	206/209 (99%)	195 (95%)	11 (5%)	0	100 100
30	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
32	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	13 50
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	34 76
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	30 72
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	17 58
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	8 36
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	30 72
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	5 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	14 51
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5 29
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5 29
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	14 51
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26 70
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11 46
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	11 46
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	9 40
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	26 70
40	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100 100
40	DN	134/136 (98%)	131 (98%)	3 (2%)	0	100 100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	11 46
41	DO	123/125 (98%)	117 (95%)	6 (5%)	0	100 100
42	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100 100
42	DP	115/117 (98%)	113 (98%)	2 (2%)	0	100 100
43	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21 64
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21 64
44	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
45	CS	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	5 29
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	19 61
46	CT	108/110 (98%)	102 (94%)	6 (6%)	0	100 100
46	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100 100
47	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	17 58
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	17 58
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	4 21
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	9 41
49	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100 100
49	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100 100
50	CX	73/76 (96%)	71 (97%)	2 (3%)	0	100 100
50	DX	75/76 (99%)	73 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	CY	75/77 (97%)	73 (97%)	2 (3%)	0	100 100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11 46
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	3 18
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	15 53

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
10	AJ	57	VAL
13	AM	5	ALA
17	AQ	82	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	186/186 (100%)	172 (92%)	14 (8%)	17 51
2	BB	186/186 (100%)	172 (92%)	14 (8%)	17 51
3	AC	170/170 (100%)	156 (92%)	14 (8%)	14 46
3	BC	170/170 (100%)	156 (92%)	14 (8%)	14 46
4	AD	172/172 (100%)	165 (96%)	7 (4%)	37 76
4	BD	172/172 (100%)	163 (95%)	9 (5%)	29 68
5	AE	118/118 (100%)	103 (87%)	15 (13%)	5 23
5	BE	113/118 (96%)	91 (80%)	22 (20%)	2 9
6	AF	92/92 (100%)	84 (91%)	8 (9%)	13 43
6	BF	87/92 (95%)	73 (84%)	14 (16%)	3 14
7	AG	124/124 (100%)	109 (88%)	15 (12%)	6 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	BG	124/124 (100%)	106 (86%)	18 (14%)	4 18
8	AH	104/104 (100%)	90 (86%)	14 (14%)	5 20
8	BH	104/104 (100%)	88 (85%)	16 (15%)	3 16
9	AI	105/105 (100%)	99 (94%)	6 (6%)	25 64
9	BI	105/105 (100%)	99 (94%)	6 (6%)	25 64
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	15 47
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	7 27
11	AK	90/90 (100%)	90 (100%)	0	100 100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	20 57
12	AL	102/102 (100%)	93 (91%)	9 (9%)	12 42
12	BL	102/102 (100%)	90 (88%)	12 (12%)	6 26
13	AM	92/92 (100%)	84 (91%)	8 (9%)	13 43
13	BM	92/92 (100%)	84 (91%)	8 (9%)	13 43
14	AN	83/83 (100%)	81 (98%)	2 (2%)	57 87
14	BN	83/83 (100%)	80 (96%)	3 (4%)	42 79
15	AO	76/76 (100%)	69 (91%)	7 (9%)	11 40
15	BO	76/76 (100%)	68 (90%)	8 (10%)	8 32
16	AP	65/65 (100%)	62 (95%)	3 (5%)	33 73
16	BP	65/65 (100%)	61 (94%)	4 (6%)	23 60
17	AQ	74/74 (100%)	66 (89%)	8 (11%)	8 30
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	4 17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	61 89
18	BR	48/48 (100%)	48 (100%)	0	100 100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	7 28
19	BS	70/70 (100%)	65 (93%)	5 (7%)	18 54
20	AT	65/65 (100%)	58 (89%)	7 (11%)	8 30
20	BT	65/65 (100%)	53 (82%)	12 (18%)	2 10
21	AU	48/48 (100%)	46 (96%)	2 (4%)	36 76
21	BU	48/48 (100%)	46 (96%)	2 (4%)	36 76
22	C1	47/47 (100%)	46 (98%)	1 (2%)	61 89
22	D1	47/47 (100%)	47 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	C2	45/46 (98%)	43 (96%)	2 (4%)	35 74
23	D2	45/46 (98%)	42 (93%)	3 (7%)	20 57
24	C3	38/38 (100%)	36 (95%)	2 (5%)	28 67
24	D3	38/38 (100%)	36 (95%)	2 (5%)	28 67
25	C4	51/51 (100%)	45 (88%)	6 (12%)	6 26
25	D4	51/51 (100%)	48 (94%)	3 (6%)	24 63
26	C5	34/34 (100%)	31 (91%)	3 (9%)	12 42
26	D5	34/34 (100%)	33 (97%)	1 (3%)	50 84
27	C0	48/48 (100%)	41 (85%)	7 (15%)	4 18
27	D0	49/48 (102%)	43 (88%)	6 (12%)	6 25
29	CC	216/216 (100%)	203 (94%)	13 (6%)	24 62
29	DC	216/216 (100%)	208 (96%)	8 (4%)	41 79
30	CD	163/163 (100%)	159 (98%)	4 (2%)	55 86
30	DD	163/163 (100%)	160 (98%)	3 (2%)	66 91
32	CE	165/165 (100%)	149 (90%)	16 (10%)	10 37
32	DE	165/165 (100%)	159 (96%)	6 (4%)	42 79
33	CF	148/148 (100%)	134 (90%)	14 (10%)	11 38
33	DF	148/148 (100%)	134 (90%)	14 (10%)	11 38
34	CG	137/137 (100%)	134 (98%)	3 (2%)	60 88
34	DG	137/137 (100%)	133 (97%)	4 (3%)	50 84
35	CH	114/114 (100%)	102 (90%)	12 (10%)	8 32
35	DH	114/114 (100%)	105 (92%)	9 (8%)	15 48
36	CJ	104/104 (100%)	99 (95%)	5 (5%)	31 71
36	DJ	104/104 (100%)	99 (95%)	5 (5%)	31 71
37	CK	116/116 (100%)	112 (97%)	4 (3%)	44 81
37	DK	116/116 (100%)	113 (97%)	3 (3%)	54 85
38	CL	103/104 (99%)	95 (92%)	8 (8%)	16 49
38	DL	104/104 (100%)	99 (95%)	5 (5%)	31 71
39	CM	103/103 (100%)	95 (92%)	8 (8%)	16 49
39	DM	103/103 (100%)	100 (97%)	3 (3%)	50 84
40	CN	108/108 (100%)	103 (95%)	5 (5%)	33 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	DN	109/108 (101%)	104 (95%)	5 (5%)	33 73
41	CO	100/102 (98%)	93 (93%)	7 (7%)	19 55
41	DO	102/102 (100%)	97 (95%)	5 (5%)	31 71
42	CP	86/87 (99%)	80 (93%)	6 (7%)	19 55
42	DP	87/87 (100%)	84 (97%)	3 (3%)	44 81
43	CQ	99/99 (100%)	95 (96%)	4 (4%)	38 77
43	DQ	99/99 (100%)	98 (99%)	1 (1%)	82 95
44	CR	89/89 (100%)	85 (96%)	4 (4%)	34 74
44	DR	89/89 (100%)	85 (96%)	4 (4%)	34 74
45	CS	84/84 (100%)	77 (92%)	7 (8%)	14 46
45	DS	84/84 (100%)	82 (98%)	2 (2%)	57 87
46	CT	93/93 (100%)	87 (94%)	6 (6%)	21 58
46	DT	93/93 (100%)	89 (96%)	4 (4%)	35 75
47	CU	80/80 (100%)	71 (89%)	9 (11%)	7 28
47	DU	80/80 (100%)	77 (96%)	3 (4%)	40 78
48	CV	83/83 (100%)	77 (93%)	6 (7%)	18 53
48	DV	83/83 (100%)	79 (95%)	4 (5%)	31 71
49	CW	78/78 (100%)	74 (95%)	4 (5%)	29 69
49	DW	78/78 (100%)	75 (96%)	3 (4%)	40 78
50	CX	56/58 (97%)	53 (95%)	3 (5%)	27 66
50	DX	58/58 (100%)	53 (91%)	5 (9%)	13 44
51	CY	67/67 (100%)	63 (94%)	4 (6%)	24 62
51	DY	67/67 (100%)	65 (97%)	2 (3%)	48 83
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	17 52
52	DZ	54/54 (100%)	53 (98%)	1 (2%)	65 90
53	DI	103/103 (100%)	96 (93%)	7 (7%)	20 56
All	All	9460/9477 (100%)	8810 (93%)	650 (7%)	19 56

5 of 650 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	BJ	63	ASP
20	BT	64	LYS

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Mol	Chain	Res	Type
39	DM	120	VAL
11	BK	38	GLN
15	BO	24	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
3	BC	3	GLN
8	BH	4	GLN
36	DJ	43	ASN
5	BE	70	ASN
5	BE	89	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	255 (16%)	32 (2%)
1	BA	1529/1534 (99%)	255 (16%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	1 (0%)
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2892/2904 (99%)	468 (16%)	79 (2%)
54	DA	2880/2904 (99%)	397 (13%)	60 (2%)
All	All	9067/9116 (99%)	1397 (15%)	208 (2%)

5 of 1397 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	984	A
31	CA	1536	C
54	DA	2127	G
31	CA	1046	A

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Mol	Chain	Res	Type
31	CA	1253	A

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

77 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	2MG	AA	1207	1	18,26,27	1.02	1 (5%)	21,38,41	2.53	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.79	0	21,32,35	1.22	2 (9%)
1	5MC	AA	1407	1	14,22,23	0.93	1 (7%)	17,32,35	0.74	1 (5%)
1	UR3	AA	1498	1	13,22,23	1.12	2 (15%)	18,32,35	0.69	0
1	2MG	AA	1516	1	18,26,27	1.28	2 (11%)	21,38,41	2.44	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.67	0	15,38,41	0.59	0
1	MA6	AA	1519	1	18,26,27	0.75	0	15,38,41	0.60	0
1	PSU	AA	516	1,55	15,21,22	1.19	2 (13%)	16,30,33	3.49	2 (12%)
1	G7M	AA	527	1	18,26,27	1.12	2 (11%)	21,39,42	3.53	6 (28%)
1	2MG	AA	966	1	18,26,27	1.14	2 (11%)	21,38,41	2.50	3 (14%)
1	5MC	AA	967	1	14,22,23	0.81	1 (7%)	17,32,35	0.66	1 (5%)
12	D2T	AL	89	12	4,9,10	0.58	0	4,11,13	1.66	2 (50%)
1	2MG	BA	1207	1	18,26,27	1.12	2 (11%)	21,38,41	2.54	4 (19%)
1	4OC	BA	1402	1	15,23,24	0.79	0	21,32,35	1.23	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.95	1 (7%)	17,32,35	0.72	1 (5%)
1	UR3	BA	1498	1	13,22,23	0.96	1 (7%)	18,32,35	0.53	0
1	2MG	BA	1516	1	18,26,27	1.19	2 (11%)	21,38,41	2.42	3 (14%)
1	MA6	BA	1518	1	18,26,27	0.61	0	15,38,41	0.58	0
1	MA6	BA	1519	1	18,26,27	0.69	0	15,38,41	0.60	0
1	PSU	BA	516	1	15,21,22	1.20	2 (13%)	16,30,33	3.48	2 (12%)
1	G7M	BA	527	1	18,26,27	0.94	1 (5%)	21,39,42	3.53	5 (23%)
1	2MG	BA	966	1	18,26,27	1.08	1 (5%)	21,38,41	2.55	4 (19%)
1	5MC	BA	967	1	14,22,23	0.79	1 (7%)	17,32,35	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	D2T	BL	89	12	4,9,10	0.49	0	4,11,13	1.71	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.83	0	15,36,39	0.87	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.14	1 (5%)	21,38,41	2.36	3 (14%)
31	PSU	CA	1911	31	15,21,22	1.12	2 (13%)	16,30,33	3.46	1 (6%)
31	3TD	CA	1915	31	15,22,23	1.01	2 (13%)	17,32,35	0.99	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.16	2 (13%)	16,30,33	3.54	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.19	1 (7%)	16,32,35	4.77	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.82	1 (7%)	17,32,35	0.65	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.89	0	15,36,39	0.88	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.93	1 (5%)	21,39,42	3.68	6 (28%)
31	OMG	CA	2251	31	18,26,27	1.14	2 (11%)	21,38,41	2.77	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.30	2 (11%)	21,38,41	2.62	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.21	2 (13%)	16,30,33	3.50	1 (6%)
31	OMC	CA	2498	55,31	15,22,23	0.87	1 (6%)	20,31,34	0.57	0
31	2MA	CA	2503	31	17,25,26	0.89	0	18,37,40	1.04	1 (5%)
31	PSU	CA	2504	31	15,21,22	1.15	2 (13%)	16,30,33	3.47	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.22	2 (14%)	19,31,34	2.93	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.26	2 (13%)	16,30,33	3.57	3 (18%)
31	PSU	CA	2604	31	15,21,22	17.92	2 (13%)	16,30,33	9.22	2 (12%)
31	PSU	CA	2605	31	15,21,22	1.21	2 (13%)	16,30,33	3.51	1 (6%)
31	1MG	CA	745	31	17,26,27	1.20	1 (5%)	19,39,42	1.18	2 (10%)
31	PSU	CA	746	55,31	15,21,22	1.35	3 (20%)	16,30,33	3.47	2 (12%)
31	5MU	CA	747	31	13,22,23	1.09	1 (7%)	16,32,35	4.77	3 (18%)
31	PSU	CA	955	31	15,21,22	1.14	2 (13%)	16,30,33	3.44	1 (6%)
30	MEQ	CD	150	30	6,8,10	0.43	0	7,9,12	0.98	1 (14%)
40	4D4	CN	81	40	7,11,12	0.59	0	5,13,15	0.93	0
54	6MZ	DA	1618	54	17,25,26	0.91	0	15,36,39	0.61	0
54	2MG	DA	1835	54	18,26,27	1.08	1 (5%)	21,38,41	2.38	3 (14%)
54	PSU	DA	1911	54	15,21,22	1.15	2 (13%)	16,30,33	3.43	1 (6%)
54	3TD	DA	1915	54	15,22,23	0.93	1 (6%)	17,32,35	1.04	1 (5%)
54	PSU	DA	1917	54	15,21,22	1.27	2 (13%)	16,30,33	3.53	1 (6%)
54	5MU	DA	1939	54	13,22,23	1.48	3 (23%)	16,32,35	4.72	3 (18%)
54	5MC	DA	1962	54	14,22,23	0.88	1 (7%)	17,32,35	0.76	1 (5%)
54	6MZ	DA	2030	54	17,25,26	1.24	2 (11%)	15,36,39	0.98	1 (6%)
54	G7M	DA	2069	54	18,26,27	1.00	1 (5%)	21,39,42	3.16	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	OMG	DA	2251	54	18,26,27	0.92	1 (5%)	21,38,41	2.59	4 (19%)
54	2MG	DA	2445	54	18,26,27	1.42	4 (22%)	21,38,41	2.74	4 (19%)
54	H2U	DA	2449	54	17,21,22	0.50	0	23,30,33	0.52	0
54	PSU	DA	2457	54	15,21,22	1.37	2 (13%)	16,30,33	3.48	2 (12%)
54	OMC	DA	2498	55,54	15,22,23	1.00	0	20,31,34	0.57	0
54	2MA	DA	2503	55,54	17,25,26	0.80	0	18,37,40	1.09	2 (11%)
54	PSU	DA	2504	54	15,21,22	1.19	2 (13%)	16,30,33	3.47	1 (6%)
54	OMU	DA	2552	54	14,22,23	1.13	1 (7%)	19,31,34	2.91	2 (10%)
54	PSU	DA	2580	54	15,21,22	1.61	5 (33%)	16,30,33	3.53	2 (12%)
54	PSU	DA	2604	54	15,21,22	1.63	5 (33%)	16,30,33	3.53	1 (6%)
54	PSU	DA	2605	54	15,21,22	1.33	3 (20%)	16,30,33	3.54	2 (12%)
54	1MG	DA	745	54	17,26,27	1.24	2 (11%)	19,39,42	1.21	2 (10%)
54	PSU	DA	746	55,54	15,21,22	1.72	5 (33%)	16,30,33	3.57	2 (12%)
54	5MU	DA	747	54	13,22,23	1.15	2 (15%)	16,32,35	4.72	3 (18%)
54	PSU	DA	955	54	15,21,22	1.37	3 (20%)	16,30,33	3.47	1 (6%)
30	MEQ	DD	150[A]	30	7,9,10	0.40	0	8,10,12	1.36	2 (25%)
30	MEQ	DD	150[B]	30	7,9,10	1.55	1 (14%)	8,10,12	1.67	2 (25%)
40	4D4	DN	81[A]	-	7,11,12	0.56	0	5,13,15	0.99	0
40	4D4	DN	81[B]	-	7,11,12	0.91	1 (14%)	5,13,15	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,55	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	AL	89	12	-	0/2/12/14	0/0/0/0
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	BA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	BA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	BA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	55,31	-	0/5/27/28	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/5/27/28	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2604	31	-	0/7/25/26	1/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	55,31	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
30	MEQ	CD	150	30	-	0/5/7/11	0/0/0/0
40	4D4	CN	81	40	-	0/8/12/14	0/0/0/0
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
54	2MG	DA	1835	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	5MU	DA	1939	54	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MC	DA	1962	54	-	0/3/25/26	0/2/2/2
54	6MZ	DA	2030	54	-	0/5/27/28	0/3/3/3
54	G7M	DA	2069	54	-	0/3/25/26	0/3/3/3
54	OMG	DA	2251	54	-	0/5/27/28	0/3/3/3
54	2MG	DA	2445	54	-	0/5/27/28	0/3/3/3
54	H2U	DA	2449	54	-	0/7/38/39	0/2/2/2
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	OMC	DA	2498	55,54	-	0/5/27/28	0/2/2/2
54	2MA	DA	2503	55,54	-	0/3/25/26	0/3/3/3
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
54	OMU	DA	2552	54	-	0/5/27/28	0/2/2/2
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
54	PSU	DA	746	55,54	-	0/7/25/26	0/2/2/2
54	5MU	DA	747	54	-	0/3/25/26	0/2/2/2
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[A]	30	-	0/7/9/11	0/0/0/0
30	MEQ	DD	150[B]	30	-	0/7/9/11	0/0/0/0
40	4D4	DN	81[A]	-	-	0/8/12/14	0/0/0/0
40	4D4	DN	81[B]	-	-	0/8/12/14	0/0/0/0

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	746	PSU	C2'-C1'	-3.45	1.50	1.53
54	DA	1939	5MU	C2'-C1'	-3.29	1.48	1.53
54	DA	746	PSU	O4'-C1'	-3.13	1.39	1.44
54	DA	2030	6MZ	C2'-C1'	-2.98	1.48	1.53
54	DA	2580	PSU	C5-C1'	-2.94	1.49	1.52

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	DA	747	5MU	C5-C4-N3	-12.16	115.14	125.35
31	CA	747	5MU	C5-C4-N3	-12.15	115.15	125.35
31	CA	1939	5MU	C5-C4-N3	-12.04	115.25	125.35
54	DA	1939	5MU	C5-C4-N3	-12.00	115.27	125.35
1	BA	527	G7M	C5-C6-N1	-10.03	110.41	123.52

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	CA	2604	PSU	C2-C4-C5-C6-N1-N3

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1402	4OC	1	0
1	AA	1518	MA6	2	0
1	AA	1519	MA6	2	0
1	AA	967	5MC	1	0
1	BA	1402	4OC	1	0
1	BA	1518	MA6	2	0
1	BA	1519	MA6	2	0
31	CA	1915	3TD	1	0
31	CA	2030	6MZ	3	0
31	CA	2503	2MA	1	0
31	CA	2580	PSU	1	0
31	CA	747	5MU	1	0
54	DA	2030	6MZ	1	0
54	DA	2251	OMG	1	0
54	DA	2498	OMC	1	0
54	DA	747	5MU	1	0
30	DD	150[A]	MEQ	2	0
30	DD	150[B]	MEQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 559 ligands modelled in this entry, 475 are monoatomic - leaving 84 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	$\#\|Z\|>2$
56	PG4	AA	1670	-	12,12,12	0.35	0	11,11,11	0.41	0
57	MPD	AA	1671	-	6,7,7	0.38	0	6,10,10	0.40	0
58	PUT	AA	1672	-	5,5,5	0.29	0	4,4,4	0.30	0
58	PUT	AA	1673	-	5,5,5	0.18	0	4,4,4	0.18	0
58	PUT	AA	1674	-	5,5,5	0.21	0	4,4,4	0.17	0
58	PUT	AA	1675	-	5,5,5	0.23	0	4,4,4	0.12	0
57	MPD	AA	1676	-	6,7,7	0.52	0	6,10,10	0.39	0
59	TAC	AA	1680	55	33,35,35	0.52	0	42,58,58	0.64	0
59	TAC	AA	1681	55	33,35,35	0.55	0	42,58,58	0.71	1 (2%)
61	PEG	AL	201	-	6,6,6	0.33	0	5,5,5	0.13	0
56	PG4	BA	1642	-	12,12,12	0.25	0	11,11,11	0.16	0
59	TAC	BA	1643	55	33,35,35	0.46	0	42,58,58	0.82	0
59	TAC	BA	1644	55	33,35,35	0.58	0	42,58,58	0.68	0
62	EDO	D1	101	-	3,3,3	0.70	0	2,2,2	0.10	0
63	PGE	D1	102	-	9,9,9	0.26	0	8,8,8	0.21	0
61	PEG	D1	103	-	6,6,6	0.39	0	5,5,5	0.17	0
61	PEG	D3	101	-	6,6,6	0.30	0	5,5,5	0.28	0
63	PGE	DA	3001	-	9,9,9	0.33	0	8,8,8	0.32	0
62	EDO	DA	3002	-	3,3,3	0.59	0	2,2,2	0.41	0
62	EDO	DA	3003	-	3,3,3	0.59	0	2,2,2	0.27	0
64	SPD	DA	3183	-	9,9,9	0.13	0	8,8,8	0.17	0
58	PUT	DA	3184	-	5,5,5	0.46	0	4,4,4	0.25	0
65	1PE	DA	3185	-	15,15,15	0.21	0	14,14,14	0.37	0
63	PGE	DA	3186	-	9,9,9	0.39	0	8,8,8	0.44	0
64	SPD	DA	3187	-	9,9,9	0.22	0	8,8,8	0.35	0
58	PUT	DA	3188	-	5,5,5	0.28	0	4,4,4	0.15	0
58	PUT	DA	3189	-	5,5,5	0.30	0	4,4,4	0.38	0
57	MPD	DA	3190	-	6,7,7	0.32	0	6,10,10	0.36	0
66	ACY	DA	3191	-	0,3,3	0.00	-	0,3,3	0.00	-
57	MPD	DA	3192	-	6,7,7	0.35	0	6,10,10	0.39	0
56	PG4	DA	3193	-	12,12,12	0.42	0	11,11,11	0.33	0
62	EDO	DA	3194	-	3,3,3	0.92	0	2,2,2	0.15	0
58	PUT	DA	3195	-	5,5,5	0.42	0	4,4,4	0.56	0
66	ACY	DA	3196	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3197	-	3,3,3	0.74	0	2,2,2	0.12	0
62	EDO	DA	3198	-	3,3,3	0.58	0	2,2,2	0.44	0
61	PEG	DA	3199	-	6,6,6	0.24	0	5,5,5	0.15	0
61	PEG	DA	3200	-	6,6,6	0.40	0	5,5,5	0.21	0
66	ACY	DA	3201	-	0,3,3	0.00	-	0,3,3	0.00	-
65	1PE	DA	3202	-	15,15,15	0.37	0	14,14,14	0.36	0
63	PGE	DA	3203	-	9,9,9	0.33	0	8,8,8	0.25	0
57	MPD	DA	3204	-	6,7,7	0.58	0	6,10,10	0.62	0
58	PUT	DA	3205	-	5,5,5	0.25	0	4,4,4	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
64	SPD	DA	3206	-	9,9,9	0.27	0	8,8,8	0.23	0
57	MPD	DA	3207	-	6,7,7	0.55	0	6,10,10	0.47	0
62	EDO	DA	3208	-	3,3,3	0.62	0	2,2,2	0.30	0
62	EDO	DA	3209	-	3,3,3	0.63	0	2,2,2	0.33	0
57	MPD	DA	3210	-	6,7,7	0.48	0	6,10,10	0.31	0
67	GUN	DA	3211	-	9,12,12	1.71	2 (22%)	7,17,17	4.69	5 (71%)
58	PUT	DA	3212	-	5,5,5	0.30	0	4,4,4	0.03	0
58	PUT	DA	3213	-	5,5,5	0.25	0	4,4,4	0.24	0
63	PGE	DA	3214	-	9,9,9	0.31	0	8,8,8	0.41	0
62	EDO	DA	3215	-	3,3,3	0.75	0	2,2,2	0.18	0
56	PG4	DA	3216	-	12,12,12	0.19	0	11,11,11	0.23	0
63	PGE	DA	3217	-	9,9,9	0.20	0	8,8,8	0.24	0
61	PEG	DA	3218	-	6,6,6	0.27	0	5,5,5	0.06	0
58	PUT	DA	3219	-	5,5,5	0.24	0	4,4,4	0.15	0
68	TRS	DA	3220	-	7,7,7	0.51	0	9,9,9	0.42	0
58	PUT	DA	3221	-	5,5,5	0.26	0	4,4,4	0.15	0
58	PUT	DA	3222	-	5,5,5	0.54	0	4,4,4	0.66	0
58	PUT	DA	3223	-	5,5,5	0.27	0	4,4,4	0.21	0
64	SPD	DA	3224	-	9,9,9	0.26	0	8,8,8	0.44	0
63	PGE	DA	3225	-	9,9,9	0.18	0	8,8,8	0.15	0
61	PEG	DA	3226	-	6,6,6	0.47	0	5,5,5	0.16	0
61	PEG	DA	3227	-	6,6,6	0.28	0	5,5,5	0.14	0
62	EDO	DB	201	-	3,3,3	0.66	0	2,2,2	0.20	0
62	EDO	DB	211	-	3,3,3	0.63	0	2,2,2	0.23	0
62	EDO	DB	212	-	3,3,3	0.75	0	2,2,2	0.15	0
57	MPD	DE	301	-	6,7,7	0.46	0	6,10,10	0.50	0
57	MPD	DE	302	-	6,7,7	0.53	0	6,10,10	0.31	0
57	MPD	DK	201	-	6,7,7	0.39	0	6,10,10	0.20	0
61	PEG	DL	201	-	6,6,6	0.11	0	5,5,5	0.16	0
58	PUT	DM	201	-	5,5,5	0.17	0	4,4,4	0.14	0
57	MPD	DN	201	-	6,7,7	0.67	0	6,10,10	0.38	0
61	PEG	DP	201	-	6,6,6	0.31	0	5,5,5	0.13	0
61	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.17	0
56	PG4	DQ	202	-	12,12,12	0.23	0	11,11,11	0.15	0
56	PG4	DR	202	-	12,12,12	0.30	0	11,11,11	0.38	0
63	PGE	DS	201	-	9,9,9	0.42	0	8,8,8	0.31	0
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.33	0
57	MPD	DS	203	-	6,7,7	0.23	0	6,10,10	0.27	0
57	MPD	DT	201	-	6,7,7	0.43	0	6,10,10	0.21	0
57	MPD	DT	202	-	6,7,7	0.47	0	6,10,10	0.40	0
63	PGE	DU	101	-	9,9,9	0.23	0	8,8,8	0.11	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
56	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
57	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
58	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
57	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
59	TAC	AA	1680	55	-	0/8/74/74	0/4/4/4
59	TAC	AA	1681	55	-	0/8/74/74	0/4/4/4
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
56	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
59	TAC	BA	1643	55	-	0/8/74/74	0/4/4/4
59	TAC	BA	1644	55	-	0/8/74/74	0/4/4/4
62	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
63	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
61	PEG	D1	103	-	-	0/4/4/4	0/0/0/0
61	PEG	D3	101	-	-	0/4/4/4	0/0/0/0
63	PGE	DA	3001	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3002	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
64	SPD	DA	3183	-	-	0/7/7/7	0/0/0/0
58	PUT	DA	3184	-	-	0/3/3/3	0/0/0/0
65	1PE	DA	3185	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3186	-	-	0/7/7/7	0/0/0/0
64	SPD	DA	3187	-	-	0/7/7/7	0/0/0/0
58	PUT	DA	3188	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3189	-	-	0/3/3/3	0/0/0/0
57	MPD	DA	3190	-	-	0/5/5/5	0/0/0/0
66	ACY	DA	3191	-	-	0/0/0/0	0/0/0/0
57	MPD	DA	3192	-	-	0/5/5/5	0/0/0/0
56	PG4	DA	3193	-	-	0/10/10/10	0/0/0/0
62	EDO	DA	3194	-	-	0/1/1/1	0/0/0/0
58	PUT	DA	3195	-	-	0/3/3/3	0/0/0/0
66	ACY	DA	3196	-	-	0/0/0/0	0/0/0/0
62	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3198	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3200	-	-	0/4/4/4	0/0/0/0
66	ACY	DA	3201	-	-	0/0/0/0	0/0/0/0
65	1PE	DA	3202	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DA	3203	-	-	0/7/7/7	0/0/0/0
57	MPD	DA	3204	-	-	0/5/5/5	0/0/0/0
58	PUT	DA	3205	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3206	-	-	0/7/7/7	0/0/0/0
57	MPD	DA	3207	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3208	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3209	-	-	0/1/1/1	0/0/0/0
57	MPD	DA	3210	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3211	-	-	0/0/0/0	0/2/2/2
58	PUT	DA	3212	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3213	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3214	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3215	-	-	0/1/1/1	0/0/0/0
56	PG4	DA	3216	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3217	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3218	-	-	0/4/4/4	0/0/0/0
58	PUT	DA	3219	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3220	-	-	0/9/9/9	0/0/0/0
58	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3222	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3223	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3224	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3225	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3226	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3227	-	-	0/4/4/4	0/0/0/0
62	EDO	DB	201	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	212	-	-	0/1/1/1	0/0/0/0
57	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
57	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
57	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
58	PUT	DM	201	-	-	0/3/3/3	0/0/0/0
57	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
56	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
56	PG4	DR	202	-	-	0/10/10/10	0/0/0/0
63	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
56	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
57	MPD	DS	203	-	-	0/5/5/5	0/0/0/0
57	MPD	DT	201	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DT	202	-	-	0/5/5/5	0/0/0/0
63	PGE	DU	101	-	-	0/7/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3211	GUN	C6-C5	3.17	1.47	1.41
67	DA	3211	GUN	C6-N1	3.29	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	DA	3211	GUN	C5-C6-N1	-8.21	112.79	123.52
67	DA	3211	GUN	C5-C4-N9	-3.15	105.53	111.12
67	DA	3211	GUN	C6-C5-C4	-3.08	117.34	120.86
67	DA	3211	GUN	N3-C2-N1	-2.94	123.56	127.56
59	AA	1681	TAC	C42-N4-C4	2.12	119.17	114.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	1670	PG4	1	0
57	AA	1676	MPD	3	0
59	AA	1681	TAC	2	0
56	BA	1642	PG4	1	0
63	D1	102	PGE	2	0
61	D1	103	PEG	1	0
63	DA	3001	PGE	1	0
58	DA	3189	PUT	1	0
57	DA	3192	MPD	1	0
56	DA	3193	PG4	2	0
58	DA	3195	PUT	3	0
62	DA	3198	EDO	1	0
65	DA	3202	1PE	1	0
57	DA	3204	MPD	1	0
57	DA	3207	MPD	1	0
63	DA	3214	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	3216	PG4	1	0
68	DA	3220	TRS	1	0
58	DA	3222	PUT	3	0
64	DA	3224	SPD	2	0
63	DA	3225	PGE	2	0
57	DN	201	MPD	1	0
61	DP	201	PEG	1	0
56	DR	202	PG4	5	0
63	DS	201	PGE	1	0
56	DS	202	PG4	3	0
63	DU	101	PGE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1523/1534 (99%)	-0.06	30 (1%) 68 39	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.47	167 (10%) 7 3	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.64	28 (12%) 5 2	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.89	36 (16%) 3 1	89, 139, 197, 228	0
3	AC	206/206 (100%)	-0.11	2 (0%) 84 60	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.97	40 (19%) 1 1	90, 138, 170, 184	0
4	AD	205/205 (100%)	-0.31	0 100 100	63, 92, 129, 160	0
4	BD	205/205 (100%)	-0.45	0 100 100	53, 77, 106, 132	0
5	AE	155/155 (100%)	-0.10	0 100 100	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.07	2 (1%) 79 53	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.01	2 (1%) 70 41	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.44	2 (2%) 68 39	77, 117, 140, 153	0
7	AG	151/151 (100%)	0.87	30 (19%) 1 1	95, 136, 160, 174	0
7	BG	151/151 (100%)	2.32	75 (49%) 0 0	136, 196, 213, 220	0
8	AH	129/129 (100%)	-0.08	1 (0%) 87 67	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.03	4 (3%) 52 24	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.12	27 (21%) 1 1	75, 135, 164, 171	0
9	BI	127/127 (100%)	1.90	49 (38%) 0 0	133, 164, 201, 210	0
10	AJ	99/99 (100%)	0.62	11 (11%) 7 3	83, 118, 141, 147	0
10	BJ	98/99 (98%)	3.09	59 (60%) 0 0	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.24	5 (4%) 39 16	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.24	3 (2%) 59 29	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.28	1 (0%) 87 67	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.33	4 (3%) 50 22	65, 86, 114, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/114 (100%)	1.42	33 (28%) 1 0	108, 130, 165, 171	0
13	BM	114/114 (100%)	3.34	87 (76%) 0 0	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.01	16 (16%) 3 1	77, 117, 178, 184	0
14	BN	100/100 (100%)	2.55	52 (52%) 0 0	124, 178, 216, 222	0
15	AO	88/88 (100%)	-0.07	1 (1%) 82 58	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.45	6 (6%) 20 7	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.40	3 (3%) 45 19	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.16	19 (23%) 1 1	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.01	2 (2%) 61 30	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.10	17 (21%) 1 1	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.15	1 (1%) 71 43	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.26	3 (5%) 29 11	65, 86, 129, 168	0
19	AS	79/79 (100%)	0.82	10 (12%) 5 2	114, 135, 155, 163	0
19	BS	79/79 (100%)	3.80	60 (75%) 0 0	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.01	0 100 100	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.28	22 (25%) 1 1	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.26	2 (3%) 46 20	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.29	1 (1%) 71 43	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.10	12 (21%) 1 1	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.56	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	2.98	34 (68%) 0 0	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.01	0 100 100	46, 60, 87, 104	0
24	C3	46/46 (100%)	1.49	13 (28%) 1 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.38	0 100 100	23, 31, 48, 112	0
25	C4	64/64 (100%)	0.89	9 (14%) 4 1	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.46	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.23	9 (23%) 1 1	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.33	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	0.79	8 (13%) 4 1	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.53	0 100 100	21, 30, 53, 80	0
28	CB	118/120 (98%)	0.64	9 (7%) 17 6	102, 170, 229, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DB	120/120 (100%)	-0.35	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.36	16 (5%) 26 10	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.47	0 100 100	22, 49, 76, 92	0
30	CD	208/209 (99%)	0.91	31 (14%) 3 1	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.51	0 100 100	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	0.61	264 (9%) 11 4	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.29	46 (22%) 1 1	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.40	1 (0%) 91 76	19, 50, 97, 132	0
33	CF	177/177 (100%)	3.03	112 (63%) 0 0	193, 211, 219, 227	0
33	DF	177/177 (100%)	-0.17	1 (0%) 90 73	44, 75, 117, 142	0
34	CG	176/176 (100%)	1.95	78 (44%) 0 0	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.16	1 (0%) 90 73	38, 66, 97, 123	0
35	CH	149/149 (100%)	1.38	38 (25%) 1 1	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.85	27 (18%) 2 1	55, 142, 179, 198	0
36	CJ	134/134 (100%)	6.11	120 (89%) 0 0	235, 251, 263, 270	0
36	DJ	134/134 (100%)	3.48	82 (61%) 0 0	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.34	4 (2%) 56 27	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.57	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	0.28	5 (4%) 41 16	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.52	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	2.01	55 (38%) 0 0	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.53	0 100 100	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.34	6 (4%) 38 16	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.65	0 100 100	21, 34, 63, 95	0
41	CO	120/125 (96%)	1.29	28 (23%) 1 1	94, 117, 139, 181	0
41	DO	125/125 (100%)	-0.48	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	1.93	47 (40%) 0 0	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.36	0 100 100	34, 52, 82, 94	0
43	CQ	114/114 (100%)	1.18	22 (19%) 2 1	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.49	0 100 100	26, 43, 75, 116	0
44	CR	117/117 (100%)	0.95	19 (16%) 3 1	81, 103, 125, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	DR	117/117 (100%)	-0.46	1 (0%) 85 64	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.66	33 (32%) 1 0	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.53	0 100 100	15, 39, 68, 94	0
46	CT	110/110 (100%)	0.84	15 (13%) 4 1	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.59	0 100 100	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.59	30 (32%) 1 0	124, 146, 173, 182	0
47	DU	93/93 (100%)	-0.00	2 (2%) 65 35	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.59	58 (56%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.26	2 (1%) 68 39	36, 56, 101, 131	0
49	CW	94/94 (100%)	1.46	29 (30%) 1 0	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.52	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.41	23 (30%) 1 0	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.52	1 (1%) 79 53	25, 36, 62, 104	0
51	CY	77/77 (100%)	0.43	3 (3%) 43 18	78, 113, 143, 161	0
51	DY	77/77 (100%)	-0.43	0 100 100	24, 50, 85, 112	0
52	CZ	62/62 (100%)	2.35	33 (53%) 0 0	123, 162, 179, 190	0
52	DZ	62/62 (100%)	-0.03	1 (1%) 74 47	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.22	29 (21%) 1 1	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.09	88 (3%) 52 24	16, 39, 206, 298	0
All	All	20632/20745 (99%)	0.49	2358 (11%) 7 2	10, 100, 227, 298	1 (0%)

The worst 5 of 2358 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	CJ	13	VAL	23.0
36	DJ	54	PRO	22.7
36	CJ	54	PRO	20.7
36	CJ	14	ALA	17.1
36	CJ	87	LYS	16.7

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	1MG	DA	745	24/25	0.99	0.18	-	16,22,28,30	0
31	G7M	CA	2069	24/25	0.93	0.20	-	78,83,88,88	0
30	MEQ	CD	150	9/11	0.89	0.25	-	81,87,117,120	0
1	5MC	AA	967	21/22	0.95	0.16	-	76,93,96,97	0
31	PSU	CA	955	20/21	0.93	0.17	-	84,89,90,90	0
1	PSU	AA	516	20/21	0.98	0.13	-	68,72,78,78	0
1	MA6	AA	1518	24/25	0.98	0.17	-	44,46,50,53	0
30	MEQ	DD	150[B]	10/11	0.98	0.21	-	19,28,34,35	10
31	PSU	CA	746	20/21	0.93	0.15	-	93,99,101,102	0
30	MEQ	DD	150[A]	10/11	0.98	0.21	-	11,18,25,27	10
1	G7M	BA	527	24/25	0.96	0.16	-	80,85,91,93	0
1	MA6	AA	1519	24/25	0.97	0.18	-	46,48,50,54	0
1	2MG	BA	966	24/25	0.84	0.34	-	149,153,160,161	0
31	PSU	CA	2580	20/21	0.94	0.19	-	77,86,88,89	0
54	6MZ	DA	1618	23/24	0.99	0.16	-	17,24,27,28	0
1	2MG	AA	1516	24/25	0.97	0.15	-	44,49,52,53	0
54	5MU	DA	747	21/22	0.99	0.18	-	20,25,31,38	0
1	2MG	BA	1207	24/25	0.84	0.21	-	158,159,162,165	0
54	PSU	DA	2580	20/21	0.99	0.17	-	17,21,28,29	0
54	6MZ	DA	2030	23/24	0.99	0.18	-	15,20,26,28	0
31	3TD	CA	1915	21/22	0.88	0.18	-	146,150,155,155	0
54	PSU	DA	2605	20/21	0.99	0.16	-	26,34,37,38	0
1	UR3	AA	1498	21/22	0.97	0.14	-	51,53,57,59	0
31	PSU	CA	2504	20/21	0.92	0.20	-	78,86,90,91	0
1	4OC	AA	1402	22/23	0.98	0.16	-	48,55,61,62	0
1	2MG	AA	1207	24/25	0.92	0.13	-	113,117,120,122	0
31	2MG	CA	2445	24/25	0.94	0.26	-	66,75,80,83	0
1	5MC	AA	1407	21/22	0.98	0.14	-	43,47,52,53	0
31	PSU	CA	2604	20/21	0.97	0.14	-	65,71,84,84	0
54	PSU	DA	1911	20/21	0.97	0.17	-	67,74,75,75	0
31	OMC	CA	2498	21/22	0.96	0.18	-	77,80,86,87	0
1	PSU	BA	516	20/21	0.89	0.16	-	91,96,99,102	0
31	5MU	CA	747	21/22	0.94	0.17	-	93,100,102,105	0
31	PSU	CA	2605	20/21	0.96	0.15	-	74,75,78,80	0
31	6MZ	CA	1618	23/24	0.94	0.23	-	98,107,108,109	0
31	PSU	CA	2457	20/21	0.95	0.16	-	79,83,85,85	0
1	UR3	BA	1498	21/22	0.96	0.13	-	78,80,84,84	0
31	2MA	CA	2503	23/24	0.90	0.21	-	90,96,102,102	0
54	PSU	DA	955	20/21	0.99	0.19	-	20,23,26,26	0
54	5MU	DA	1939	21/22	0.99	0.18	-	25,30,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	D2T	BL	89	10/11	0.93	0.26	-	81,86,96,96	0
54	OMC	DA	2498	21/22	0.99	0.18	-	18,21,24,27	0
31	PSU	CA	1911	20/21	0.92	0.18	-	111,128,131,132	0
12	D2T	AL	89	10/11	0.94	0.20	-	47,53,67,70	0
1	MA6	BA	1519	24/25	0.96	0.21	-	68,73,77,78	0
1	5MC	BA	1407	21/22	0.93	0.17	-	81,95,99,100	0
40	4D4	DN	81[B]	12/13	0.98	0.21	-	11,21,28,29	9
31	6MZ	CA	2030	23/24	0.92	0.20	-	78,86,97,99	0
54	PSU	DA	746	20/21	0.99	0.17	-	18,23,26,30	0
54	2MA	DA	2503	23/24	0.99	0.18	-	15,28,32,41	0
31	1MG	CA	745	24/25	0.95	0.21	-	85,87,90,93	0
54	5MC	DA	1962	21/22	0.98	0.18	-	28,37,39,42	0
31	2MG	CA	1835	24/25	0.95	0.16	-	60,73,76,78	0
40	4D4	DN	81[A]	12/13	0.98	0.21	-	26,33,49,50	9
54	PSU	DA	1917	20/21	0.96	0.15	-	63,73,79,79	0
54	OMU	DA	2552	21/22	0.99	0.17	-	22,26,30,35	0
1	2MG	BA	1516	24/25	0.95	0.15	-	61,67,78,80	0
54	G7M	DA	2069	24/25	0.99	0.16	-	20,28,31,33	0
31	PSU	CA	1917	20/21	0.87	0.19	-	118,126,134,134	0
31	OMG	CA	2251	24/25	0.95	0.24	-	67,73,75,77	0
31	5MU	CA	1939	21/22	0.97	0.14	-	69,74,80,82	0
54	OMG	DA	2251	24/25	0.99	0.17	-	21,25,34,42	0
1	5MC	BA	967	21/22	0.82	0.31	-	148,154,156,157	0
54	2MG	DA	2445	24/25	0.99	0.18	-	16,22,24,25	0
1	2MG	AA	966	24/25	0.95	0.15	-	78,87,97,97	0
54	PSU	DA	2504	20/21	0.99	0.16	-	31,33,36,38	0
31	OMU	CA	2552	21/22	0.94	0.34	-	78,81,85,89	0
54	2MG	DA	1835	24/25	0.97	0.18	-	31,42,47,48	0
31	5MC	CA	1962	21/22	0.97	0.22	-	67,72,76,76	0
1	G7M	AA	527	24/25	0.98	0.14	-	53,59,62,65	0
54	PSU	DA	2457	20/21	0.99	0.17	-	22,25,26,29	0
54	3TD	DA	1915	21/22	0.94	0.20	-	86,90,102,103	0
1	MA6	BA	1518	24/25	0.95	0.20	-	67,74,79,79	0
54	H2U	DA	2449	20/21	0.99	0.17	-	19,22,24,26	0
1	4OC	BA	1402	22/23	0.96	0.15	-	74,79,81,82	0
54	PSU	DA	2604	20/21	0.99	0.16	-	32,36,47,47	0
40	4D4	CN	81	12/13	0.93	0.27	-	83,89,102,103	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	PUT	AA	1674	6/6	0.70	0.73	68.80	128,131,132,133	0
58	PUT	DA	3195	6/6	0.73	0.60	54.59	76,81,86,87	0
58	PUT	DA	3213	6/6	0.86	0.50	32.99	83,85,91,93	0
55	MG	CA	3003	1/1	0.54	1.52	32.28	270,270,270,270	0
61	PEG	D1	103	7/7	0.74	0.46	31.21	76,77,78,78	0
61	PEG	DA	3200	7/7	0.83	0.68	31.07	65,68,77,77	0
64	SPD	DA	3183	10/10	0.93	0.43	30.06	60,70,74,75	0
61	PEG	D3	101	7/7	0.75	1.12	27.39	83,89,94,95	0
57	MPD	DA	3204	8/8	0.81	0.43	22.93	117,118,124,125	0
64	SPD	DA	3206	10/10	0.76	0.32	18.34	86,93,96,96	0
57	MPD	AA	1676	8/8	0.62	0.68	17.63	102,115,118,121	0
55	MG	CA	3133	1/1	0.66	0.50	17.30	83,83,83,83	0
58	PUT	DA	3222	6/6	0.83	0.33	17.07	41,43,47,47	0
63	PGE	DA	3214	10/10	0.93	0.36	16.79	56,58,66,66	0
61	PEG	DA	3218	7/7	0.85	0.33	16.56	99,105,110,112	0
61	PEG	DA	3226	7/7	0.83	0.30	16.12	57,62,74,75	0
63	PGE	DA	3001	10/10	0.79	0.58	15.96	75,85,99,101	0
58	PUT	DA	3184	6/6	0.89	0.29	15.87	53,55,60,60	0
65	1PE	DA	3202	16/16	0.90	0.36	15.22	55,64,72,72	0
63	PGE	DA	3203	10/10	0.91	0.31	14.16	68,72,76,76	0
56	PG4	BA	1642	13/13	0.91	0.42	14.02	84,86,94,96	0
63	PGE	DA	3217	10/10	0.93	0.34	13.91	67,71,76,76	0
63	PGE	D1	102	10/10	0.75	0.65	13.72	107,117,119,119	0
58	PUT	DA	3189	6/6	0.92	0.32	12.25	40,44,47,47	0
56	PG4	DA	3193	13/13	0.85	0.73	11.51	65,77,93,94	0
58	PUT	DA	3219	6/6	0.89	0.29	10.99	63,64,65,66	0
63	PGE	DA	3225	10/10	0.91	0.29	10.77	73,81,92,92	0
62	EDO	DA	3198	4/4	0.90	0.28	10.75	76,79,79,79	0
55	MG	CA	3122	1/1	0.75	0.57	10.68	106,106,106,106	0
61	PEG	DQ	201	7/7	0.58	0.98	10.12	104,108,109,109	0
56	PG4	DA	3216	13/13	0.89	0.27	10.11	77,89,96,96	0
55	MG	AA	1608	1/1	0.87	0.41	9.85	78,78,78,78	0
55	MG	AA	1612	1/1	0.84	0.34	9.39	57,57,57,57	0
57	MPD	DE	301	8/8	0.77	0.81	9.31	123,126,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	3127	1/1	0.95	0.37	9.00	71,71,71,71	0
55	MG	DA	3037	1/1	0.95	0.24	8.75	22,22,22,22	0
55	MG	CA	3147	1/1	0.93	0.38	8.64	51,51,51,51	1
62	EDO	DA	3209	4/4	0.84	0.42	8.43	93,94,95,95	0
55	MG	DA	3172	1/1	0.83	0.29	8.42	81,81,81,81	0
58	PUT	AA	1672	6/6	0.70	0.51	7.83	90,93,95,95	0
55	MG	DA	3126	1/1	0.95	0.28	7.70	57,57,57,57	0
57	MPD	DA	3207	8/8	0.90	0.32	7.58	86,86,88,89	0
57	MPD	DA	3192	8/8	0.89	0.43	7.29	69,77,79,80	0
59	TAC	BA	1644	32/32	0.74	0.45	7.28	139,152,159,159	0
55	MG	CA	3105	1/1	0.90	0.61	7.25	260,260,260,260	0
58	PUT	AA	1673	6/6	0.89	0.29	6.97	92,93,93,94	0
64	SPD	DA	3224	10/10	0.93	0.23	6.71	30,40,57,60	0
56	PG4	DS	202	13/13	0.92	0.30	6.55	52,54,63,64	0
56	PG4	AA	1670	13/13	0.88	0.25	6.04	64,79,91,92	0
55	MG	DA	3124	1/1	0.93	0.24	6.01	76,76,76,76	0
55	MG	CA	3123	1/1	0.60	0.62	5.62	115,115,115,115	0
66	ACY	DA	3201	4/4	0.95	0.21	5.59	66,68,68,69	0
58	PUT	DA	3205	6/6	0.86	0.33	5.33	77,82,89,91	0
63	PGE	DU	101	10/10	0.92	0.41	5.17	79,84,91,92	0
67	GUN	DA	3211	11/11	0.88	0.36	5.06	82,84,86,86	0
55	MG	BA	1646	1/1	0.88	0.35	4.86	141,141,141,141	0
55	MG	CA	3130	1/1	0.81	0.29	4.65	76,76,76,76	0
62	EDO	D1	101	4/4	0.87	0.24	4.05	56,57,60,60	0
55	MG	BA	1612	1/1	0.75	0.29	3.72	159,159,159,159	0
55	MG	CA	3137	1/1	0.91	0.28	3.55	123,123,123,123	0
63	PGE	DS	201	10/10	0.82	0.39	3.50	65,78,83,83	0
57	MPD	AA	1671	8/8	0.93	0.46	3.45	83,86,89,90	0
61	PEG	DL	201	7/7	0.92	0.25	3.33	66,69,70,71	0
65	1PE	DA	3185	16/16	0.94	0.18	3.31	37,52,80,82	0
55	MG	CA	3151	1/1	0.79	0.30	3.25	81,81,81,81	0
55	MG	CA	3026	1/1	0.95	0.35	2.88	111,111,111,111	0
64	SPD	DA	3187	10/10	0.97	0.20	2.84	30,41,47,48	0
55	MG	BA	1601	1/1	0.98	0.25	2.65	130,130,130,130	0
62	EDO	DA	3197	4/4	0.95	0.22	2.39	51,51,53,53	0
62	EDO	DB	201	4/4	0.94	0.19	2.30	72,75,76,76	0
55	MG	AA	1642	1/1	0.97	0.22	1.96	89,89,89,89	0
55	MG	DA	3093	1/1	0.99	0.18	1.84	23,23,23,23	0
55	MG	CA	3009	1/1	0.84	0.23	1.50	240,240,240,240	0
61	PEG	AL	201	7/7	0.84	0.22	1.49	79,79,85,86	0
55	MG	CA	3037	1/1	0.93	0.30	1.36	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	3177	1/1	0.96	0.18	1.14	67,67,67,67	0
55	MG	AA	1644	1/1	0.95	0.17	1.11	87,87,87,87	0
55	MG	DD	301	1/1	0.97	0.18	0.62	40,40,40,40	0
55	MG	CA	3136	1/1	0.90	0.22	0.56	87,87,87,87	0
59	TAC	AA	1680	32/32	0.93	0.19	0.44	70,81,96,96	0
55	MG	CA	3155	1/1	0.90	0.22	0.40	152,152,152,152	0
56	PG4	DQ	202	13/13	0.92	0.20	0.39	53,59,69,71	0
55	MG	AA	1661	1/1	0.79	0.20	0.20	139,139,139,139	0
55	MG	DA	3112	1/1	0.99	0.18	0.19	24,24,24,24	0
59	TAC	AA	1681	32/32	0.92	0.21	0.09	94,106,109,110	0
57	MPD	DS	203	8/8	0.98	0.20	-0.01	47,50,57,58	0
55	MG	DA	3024	1/1	0.99	0.18	-0.13	36,36,36,36	0
55	MG	DA	3132	1/1	0.88	0.15	-0.14	54,54,54,54	0
55	MG	AA	1678	1/1	0.64	0.22	-0.18	76,76,76,76	0
55	MG	BA	1614	1/1	0.94	0.15	-0.19	137,137,137,137	0
63	PGE	DA	3186	10/10	0.95	0.16	-0.24	33,40,41,41	0
55	MG	DA	3147	1/1	0.93	0.16	-0.36	104,104,104,104	0
55	MG	CA	3099	1/1	0.93	0.22	-0.47	156,156,156,156	0
55	MG	DA	3013	1/1	0.99	0.19	-0.49	19,19,19,19	0
55	MG	CA	3089	1/1	0.93	0.18	-0.51	54,54,54,54	0
55	MG	DA	3023	1/1	0.99	0.18	-0.51	20,20,20,20	0
55	MG	CA	3094	1/1	0.77	0.23	-0.57	126,126,126,126	0
55	MG	CA	3018	1/1	0.98	0.17	-0.64	90,90,90,90	0
58	PUT	DM	201	6/6	0.97	0.17	-0.69	40,48,52,56	0
55	MG	BA	1624	1/1	0.79	0.29	-0.75	249,249,249,249	0
55	MG	BA	1613	1/1	0.99	0.17	-0.79	79,79,79,79	0
55	MG	DA	3029	1/1	0.99	0.18	-0.83	29,29,29,29	0
55	MG	CA	3019	1/1	0.83	0.18	-0.86	58,58,58,58	0
55	MG	DA	3066	1/1	0.99	0.17	-0.90	40,40,40,40	0
55	MG	CA	3100	1/1	0.97	0.18	-1.04	73,73,73,73	0
55	MG	AA	1657	1/1	0.89	0.20	-1.06	105,105,105,105	0
55	MG	CA	3153	1/1	0.92	0.16	-1.13	59,59,59,59	0
55	MG	AA	1677	1/1	0.93	0.15	-1.20	138,138,138,138	0
55	MG	CA	3102	1/1	0.93	0.10	-1.24	104,104,104,104	0
55	MG	AA	1668	1/1	0.99	0.13	-1.25	59,59,59,59	0
55	MG	AA	1656	1/1	0.98	0.13	-1.35	140,140,140,140	0
55	MG	CA	3061	1/1	0.56	0.07	-1.36	225,225,225,225	0
59	TAC	BA	1643	32/32	0.86	0.16	-1.43	146,150,152,152	0
55	MG	CB	202	1/1	0.94	0.12	-1.45	113,113,113,113	0
55	MG	AA	1611	1/1	0.94	0.15	-1.52	94,94,94,94	0
55	MG	DA	3094	1/1	0.97	0.15	-1.61	20,20,20,20	0
60	ZN	D5	101	1/1	1.00	0.12	-1.61	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3011	1/1	0.88	0.16	-1.73	70,70,70,70	0
60	ZN	C5	101	1/1	0.89	0.05	-1.85	149,149,149,149	0
55	MG	CA	3103	1/1	0.97	0.11	-2.19	90,90,90,90	0
55	MG	DA	3110	1/1	0.99	0.16	-2.31	35,35,35,35	0
60	ZN	AB	301	1/1	0.97	0.12	-2.34	150,150,150,150	0
55	MG	DA	3022	1/1	0.99	0.15	-2.34	21,21,21,21	0
55	MG	DA	3228	1/1	0.99	0.16	-2.36	36,36,36,36	0
55	MG	CB	201	1/1	0.96	0.06	-2.43	159,159,159,159	0
55	MG	DA	3014	1/1	0.99	0.15	-2.46	14,14,14,14	0
55	MG	BA	1617	1/1	0.91	0.12	-2.63	105,105,105,105	0
55	MG	BA	1632	1/1	0.93	0.11	-2.67	78,78,78,78	0
55	MG	CA	3079	1/1	0.96	0.10	-2.72	116,116,116,116	0
55	MG	CA	3054	1/1	0.83	0.12	-2.76	118,118,118,118	0
55	MG	DA	3018	1/1	0.99	0.07	-2.80	43,43,43,43	0
55	MG	BA	1620	1/1	0.98	0.09	-2.81	113,113,113,113	0
55	MG	AA	1663	1/1	0.96	0.09	-2.81	94,94,94,94	0
55	MG	CA	3024	1/1	0.96	0.12	-2.91	81,81,81,81	0
55	MG	CA	3020	1/1	0.98	0.13	-3.00	86,86,86,86	0
55	MG	DA	3017	1/1	1.00	0.14	-3.01	20,20,20,20	0
55	MG	DA	3009	1/1	0.99	0.12	-3.01	23,23,23,23	0
55	MG	DA	3031	1/1	0.98	0.17	-3.20	27,27,27,27	0
55	MG	DA	3043	1/1	0.97	0.14	-3.25	32,32,32,32	0
55	MG	CA	3101	1/1	0.98	0.08	-3.30	97,97,97,97	0
55	MG	CA	3051	1/1	0.97	0.10	-3.41	73,73,73,73	0
55	MG	CA	3006	1/1	0.92	0.11	-3.41	143,143,143,143	0
55	MG	CA	3041	1/1	0.99	0.05	-3.60	50,50,50,50	0
55	MG	CA	3033	1/1	0.96	0.11	-3.67	91,91,91,91	0
55	MG	CA	3063	1/1	0.93	0.17	-3.73	118,118,118,118	0
55	MG	CA	3088	1/1	0.97	0.08	-3.79	67,67,67,67	0
55	MG	DA	3090	1/1	0.98	0.14	-3.84	30,30,30,30	0
55	MG	CA	3144	1/1	0.92	0.07	-3.98	63,63,63,63	0
55	MG	DA	3095	1/1	0.97	0.12	-4.00	74,74,74,74	0
55	MG	BA	1622	1/1	0.99	0.07	-4.13	99,99,99,99	0
55	MG	BA	1608	1/1	0.93	0.08	-4.16	86,86,86,86	0
55	MG	DA	3064	1/1	0.99	0.12	-4.22	49,49,49,49	0
55	MG	DB	202	1/1	0.96	0.09	-4.27	52,52,52,52	0
55	MG	BA	1626	1/1	0.95	0.10	-4.29	85,85,85,85	0
55	MG	BA	1605	1/1	0.97	0.07	-4.45	146,146,146,146	0
55	MG	AA	1637	1/1	0.99	0.07	-4.49	53,53,53,53	0
55	MG	DA	3097	1/1	0.96	0.07	-4.68	26,26,26,26	0
55	MG	DA	3159	1/1	0.93	0.10	-4.88	76,76,76,76	0
55	MG	AA	1639	1/1	0.99	0.08	-4.88	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	1659	1/1	0.96	0.07	-4.97	74,74,74,74	0
55	MG	AA	1648	1/1	0.98	0.08	-5.00	60,60,60,60	0
55	MG	DA	3050	1/1	0.99	0.13	-5.16	18,18,18,18	0
55	MG	CA	3013	1/1	0.86	0.15	-5.29	99,99,99,99	0
55	MG	BA	1615	1/1	0.98	0.06	-5.37	65,65,65,65	0
55	MG	BA	1602	1/1	0.91	0.06	-5.42	84,84,84,84	0
55	MG	DA	3084	1/1	0.99	0.11	-5.67	35,35,35,35	0
55	MG	CA	3052	1/1	0.82	0.07	-5.73	71,71,71,71	0
55	MG	DA	3135	1/1	0.96	0.04	-5.86	78,78,78,78	0
55	MG	DA	3109	1/1	1.00	0.16	-6.04	23,23,23,23	0
55	MG	CA	3086	1/1	0.98	0.08	-6.16	59,59,59,59	0
55	MG	DA	3026	1/1	0.95	0.09	-6.19	92,92,92,92	0
55	MG	DA	3092	1/1	0.97	0.10	-6.24	21,21,21,21	0
55	MG	DA	3058	1/1	1.00	0.09	-6.33	32,32,32,32	0
55	MG	AA	1631	1/1	0.96	0.08	-6.54	47,47,47,47	0
55	MG	DA	3150	1/1	0.99	0.10	-6.69	50,50,50,50	0
55	MG	DA	3047	1/1	0.97	0.12	-6.76	58,58,58,58	0
55	MG	DA	3004	1/1	0.99	0.09	-6.85	60,60,60,60	0
55	MG	DA	3071	1/1	0.99	0.10	-7.02	34,34,34,34	0
55	MG	BA	1610	1/1	0.96	0.04	-7.69	93,93,93,93	0
55	MG	CA	3044	1/1	0.96	0.09	-7.84	59,59,59,59	0
55	MG	CA	3040	1/1	0.98	0.07	-7.89	83,83,83,83	0
55	MG	DA	3099	1/1	0.99	0.14	-8.16	23,23,23,23	0
55	MG	DA	3027	1/1	0.98	0.13	-8.36	33,33,33,33	0
55	MG	DA	3046	1/1	1.00	0.13	-9.26	31,31,31,31	0
55	MG	CA	3030	1/1	0.94	0.06	-9.95	64,64,64,64	0
55	MG	DA	3007	1/1	0.95	0.06	-10.03	88,88,88,88	0
55	MG	AA	1653	1/1	0.98	0.07	-10.75	61,61,61,61	0
55	MG	DA	3102	1/1	0.99	0.09	-12.91	30,30,30,30	0
55	MG	AA	1646	1/1	0.99	0.06	-13.53	49,49,49,49	0
55	MG	DA	3063	1/1	0.98	0.07	-14.35	85,85,85,85	0
55	MG	DA	3169	1/1	0.97	0.27	-	66,66,66,66	0
55	MG	DA	3028	1/1	0.98	0.12	-	56,56,56,56	0
55	MG	CA	3115	1/1	0.73	0.23	-	72,72,72,72	0
55	MG	CA	3093	1/1	0.69	0.14	-	84,84,84,84	0
55	MG	DA	3021	1/1	0.98	0.13	-	27,27,27,27	0
55	MG	CA	3124	1/1	0.83	0.20	-	124,124,124,124	0
55	MG	CA	3131	1/1	0.48	0.59	-	83,83,83,83	0
55	MG	BA	1616	1/1	0.95	0.17	-	162,162,162,162	0
55	MG	DA	3152	1/1	0.77	0.30	-	94,94,94,94	0
57	MPD	DN	201	8/8	0.80	0.45	-	84,91,101,101	0
55	MG	DA	3091	1/1	0.99	0.16	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3095	1/1	0.97	0.07	-	69,69,69,69	0
55	MG	DA	3033	1/1	0.97	0.16	-	26,26,26,26	0
55	MG	DA	3088	1/1	0.99	0.10	-	42,42,42,42	0
55	MG	CA	3150	1/1	0.85	0.55	-	74,74,74,74	0
55	MG	DA	3041	1/1	0.99	0.20	-	11,11,11,11	0
68	TRS	DA	3220	8/8	0.83	0.54	-	94,100,107,109	0
57	MPD	DK	201	8/8	0.84	0.32	-	96,98,100,100	0
55	MG	AA	1636	1/1	0.94	0.26	-	113,113,113,113	0
55	MG	DA	3068	1/1	0.99	0.16	-	35,35,35,35	0
55	MG	DA	3154	1/1	0.89	0.34	-	62,62,62,62	0
55	MG	DA	3016	1/1	0.98	0.09	-	43,43,43,43	0
55	MG	CA	3073	1/1	0.96	0.33	-	229,229,229,229	0
55	MG	AA	1604	1/1	0.94	0.29	-	50,50,50,50	0
55	MG	DA	3111	1/1	0.92	0.29	-	292,292,292,292	0
55	MG	DA	3156	1/1	0.91	0.35	-	72,72,72,72	0
55	MG	DA	3180	1/1	0.93	1.60	-	95,95,95,95	0
55	MG	DA	3048	1/1	0.99	0.13	-	26,26,26,26	0
55	MG	DA	3122	1/1	0.97	0.45	-	46,46,46,46	0
55	MG	CA	3043	1/1	0.84	0.08	-	86,86,86,86	0
61	PEG	DA	3227	7/7	0.90	0.33	-	75,79,86,87	0
55	MG	CA	3068	1/1	0.84	0.24	-	205,205,205,205	0
57	MPD	DA	3210	8/8	0.85	0.34	-	87,89,92,94	0
55	MG	CA	3126	1/1	0.90	0.13	-	85,85,85,85	0
55	MG	DA	3065	1/1	0.96	0.15	-	19,19,19,19	0
55	MG	CA	3066	1/1	0.85	0.12	-	110,110,110,110	0
55	MG	DB	208	1/1	0.86	0.80	-	77,77,77,77	0
55	MG	CA	3025	1/1	0.95	0.08	-	87,87,87,87	0
55	MG	DA	3128	1/1	0.92	0.98	-	62,62,62,62	0
55	MG	BA	1633	1/1	0.96	0.13	-	241,241,241,241	0
55	MG	DA	3006	1/1	0.98	0.06	-	75,75,75,75	0
55	MG	AA	1613	1/1	0.90	0.82	-	59,59,59,59	0
55	MG	CA	3135	1/1	0.58	0.57	-	107,107,107,107	0
55	MG	DA	3167	1/1	0.86	0.35	-	90,90,90,90	0
55	MG	CA	3014	1/1	0.67	0.16	-	200,200,200,200	0
55	MG	CA	3156	1/1	0.63	0.17	-	218,218,218,218	0
55	MG	CA	3039	1/1	0.82	0.59	-	158,158,158,158	0
55	MG	AA	1665	1/1	0.94	0.37	-	136,136,136,136	0
55	MG	BA	1637	1/1	0.23	1.04	-	86,86,86,86	0
55	MG	DA	3101	1/1	0.98	0.09	-	45,45,45,45	0
55	MG	CA	3049	1/1	0.96	0.12	-	57,57,57,57	0
55	MG	AA	1655	1/1	0.89	0.14	-	151,151,151,151	0
55	MG	CA	3120	1/1	0.93	0.15	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	1635	1/1	0.99	0.08	-	104,104,104,104	0
55	MG	AA	1602	1/1	0.90	0.19	-	75,75,75,75	0
55	MG	DA	3082	1/1	0.98	0.12	-	72,72,72,72	0
55	MG	DA	3067	1/1	0.99	0.06	-	36,36,36,36	0
55	MG	CA	3114	1/1	0.84	0.31	-	57,57,57,57	0
55	MG	CA	3080	1/1	0.90	0.23	-	119,119,119,119	0
55	MG	DA	3077	1/1	0.99	0.07	-	30,30,30,30	0
55	MG	AA	1651	1/1	0.96	0.09	-	69,69,69,69	0
55	MG	DA	3118	1/1	0.98	0.08	-	36,36,36,36	0
55	MG	AA	1669	1/1	0.98	0.14	-	172,172,172,172	0
55	MG	AA	1614	1/1	0.87	0.10	-	79,79,79,79	0
55	MG	CA	3082	1/1	0.96	0.25	-	112,112,112,112	0
55	MG	DA	3079	1/1	0.98	0.16	-	124,124,124,124	0
55	MG	BA	1623	1/1	0.89	0.58	-	254,254,254,254	0
55	MG	DB	206	1/1	0.92	0.59	-	64,64,64,64	0
62	EDO	DA	3002	4/4	0.91	0.59	-	71,74,79,82	0
55	MG	CA	3008	1/1	0.63	0.10	-	147,147,147,147	0
57	MPD	DA	3190	8/8	0.91	0.30	-	78,82,85,89	0
55	MG	CA	3121	1/1	0.97	0.14	-	65,65,65,65	0
55	MG	CA	3023	1/1	0.93	0.16	-	159,159,159,159	0
55	MG	CA	3092	1/1	0.93	0.06	-	125,125,125,125	0
55	MG	CA	3048	1/1	0.89	0.13	-	91,91,91,91	0
55	MG	AA	1603	1/1	0.76	0.36	-	81,81,81,81	0
55	MG	DA	3040	1/1	0.99	0.08	-	36,36,36,36	0
55	MG	DB	210	1/1	0.90	0.44	-	76,76,76,76	0
55	MG	DR	201	1/1	0.95	0.33	-	32,32,32,32	0
55	MG	DA	3045	1/1	0.99	0.05	-	49,49,49,49	0
55	MG	DB	204	1/1	0.96	0.06	-	37,37,37,37	0
55	MG	CA	3032	1/1	0.92	0.54	-	244,244,244,244	0
55	MG	AA	1622	1/1	0.44	1.00	-	116,116,116,116	0
55	MG	CA	3096	1/1	0.97	0.05	-	64,64,64,64	0
58	PUT	DA	3188	6/6	0.93	0.22	-	43,50,50,51	0
55	MG	CA	3149	1/1	0.87	0.42	-	63,63,63,63	0
62	EDO	DA	3208	4/4	0.91	0.25	-	69,71,72,72	0
55	MG	AA	1623	1/1	0.88	0.27	-	62,62,62,62	0
55	MG	DA	3053	1/1	0.98	0.11	-	44,44,44,44	0
55	MG	CA	3074	1/1	0.88	0.09	-	101,101,101,101	0
55	MG	DA	3019	1/1	0.99	0.28	-	8,8,8,8	0
55	MG	DA	3160	1/1	0.90	0.68	-	81,81,81,81	0
55	MG	DA	3059	1/1	0.99	0.08	-	23,23,23,23	0
55	MG	DA	3130	1/1	0.72	0.39	-	99,99,99,99	0
61	PEG	DP	201	7/7	0.79	0.82	-	90,91,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	3174	1/1	0.94	0.27	-	70,70,70,70	0
55	MG	CA	3001	1/1	0.25	0.27	-	296,296,296,296	0
55	MG	CA	3129	1/1	0.79	0.21	-	89,89,89,89	0
55	MG	CA	3069	1/1	0.92	0.23	-	110,110,110,110	0
55	MG	DA	3025	1/1	0.99	0.10	-	31,31,31,31	0
55	MG	AA	1620	1/1	0.92	0.27	-	63,63,63,63	0
55	MG	DA	3012	1/1	0.95	0.22	-	153,153,153,153	0
55	MG	CA	3047	1/1	0.70	0.18	-	238,238,238,238	0
55	MG	CA	3083	1/1	0.93	0.13	-	203,203,203,203	0
55	MG	DA	3044	1/1	0.96	0.10	-	70,70,70,70	0
55	MG	DA	3131	1/1	0.85	0.22	-	63,63,63,63	0
55	MG	DA	3105	1/1	0.98	0.19	-	31,31,31,31	0
55	MG	DA	3039	1/1	1.00	0.13	-	23,23,23,23	0
62	EDO	DB	211	4/4	0.89	0.32	-	88,88,90,90	0
55	MG	AA	1667	1/1	0.95	0.10	-	41,41,41,41	0
55	MG	CA	3035	1/1	0.85	0.23	-	89,89,89,89	0
55	MG	DA	3137	1/1	0.67	0.30	-	80,80,80,80	0
55	MG	DA	3175	1/1	0.94	0.21	-	68,68,68,68	0
55	MG	CA	3145	1/1	0.91	0.24	-	62,62,62,62	0
55	MG	BA	1634	1/1	0.92	0.09	-	129,129,129,129	0
55	MG	DA	3134	1/1	0.86	0.28	-	95,95,95,95	0
55	MG	CA	3075	1/1	0.45	2.16	-	221,221,221,221	0
55	MG	DA	3075	1/1	0.99	0.15	-	37,37,37,37	0
55	MG	CA	3038	1/1	0.65	0.14	-	258,258,258,258	0
55	MG	CA	3050	1/1	0.98	0.09	-	54,54,54,54	0
55	MG	CA	3128	1/1	0.80	0.43	-	82,82,82,82	0
55	MG	DA	3171	1/1	0.88	0.55	-	74,74,74,74	0
55	MG	DA	3138	1/1	0.81	0.53	-	38,38,38,38	1
55	MG	DA	3081	1/1	0.98	0.09	-	45,45,45,45	0
56	PG4	DR	202	13/13	0.82	0.37	-	97,109,121,121	0
55	MG	CA	3072	1/1	0.94	0.54	-	249,249,249,249	0
55	MG	BA	1638	1/1	0.64	0.65	-	107,107,107,107	0
55	MG	CA	3087	1/1	0.99	0.05	-	59,59,59,59	0
55	MG	DA	3030	1/1	0.95	0.18	-	42,42,42,42	0
55	MG	DA	3073	1/1	1.00	0.13	-	31,31,31,31	0
55	MG	CA	3084	1/1	0.95	0.26	-	167,167,167,167	0
55	MG	AA	1658	1/1	0.76	0.13	-	101,101,101,101	0
55	MG	DA	3141	1/1	0.92	0.23	-	40,40,40,40	0
55	MG	CA	3031	1/1	0.93	0.07	-	73,73,73,73	0
55	MG	DA	3139	1/1	0.97	0.10	-	55,55,55,55	0
55	MG	DA	3085	1/1	0.98	0.12	-	50,50,50,50	0
55	MG	DA	3170	1/1	0.54	0.43	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	1605	1/1	0.86	0.52	-	80,80,80,80	0
55	MG	CA	3015	1/1	0.98	0.18	-	57,57,57,57	0
55	MG	CA	3012	1/1	0.87	0.12	-	84,84,84,84	0
55	MG	DA	3173	1/1	0.94	0.44	-	100,100,100,100	0
55	MG	BA	1607	1/1	0.94	0.46	-	203,203,203,203	0
55	MG	DA	3114	1/1	0.99	0.12	-	39,39,39,39	0
55	MG	CA	3004	1/1	0.91	0.07	-	106,106,106,106	0
55	MG	AA	1619	1/1	0.88	0.32	-	93,93,93,93	0
55	MG	CA	3148	1/1	0.95	0.60	-	46,46,46,46	1
55	MG	DA	3121	1/1	0.87	0.16	-	70,70,70,70	0
55	MG	DA	3120	1/1	0.94	0.34	-	81,81,81,81	0
55	MG	CA	3060	1/1	0.20	0.45	-	234,234,234,234	0
55	MG	DA	3060	1/1	1.00	0.14	-	21,21,21,21	0
58	PUT	DA	3223	6/6	0.95	0.20	-	54,55,62,64	0
55	MG	BA	1604	1/1	0.73	0.18	-	187,187,187,187	0
55	MG	BA	1647	1/1	0.83	0.11	-	86,86,86,86	0
55	MG	CA	3117	1/1	0.91	0.43	-	69,69,69,69	0
55	MG	DA	3011	1/1	1.00	0.08	-	33,33,33,33	0
55	MG	AA	1641	1/1	0.95	0.07	-	65,65,65,65	0
55	MG	DA	3231	1/1	0.99	0.24	-	36,36,36,36	0
55	MG	DA	3100	1/1	0.98	0.15	-	26,26,26,26	0
55	MG	DA	3106	1/1	0.99	0.17	-	41,41,41,41	0
55	MG	CA	3152	1/1	0.94	0.44	-	145,145,145,145	0
55	MG	DA	3164	1/1	0.96	0.29	-	59,59,59,59	0
55	MG	AA	1664	1/1	0.88	0.18	-	199,199,199,199	0
55	MG	CA	3077	1/1	0.73	0.57	-	232,232,232,232	0
55	MG	BA	1635	1/1	0.92	0.07	-	113,113,113,113	0
55	MG	CA	3116	1/1	0.80	0.45	-	75,75,75,75	0
55	MG	CA	3017	1/1	0.93	0.07	-	75,75,75,75	0
62	EDO	DA	3003	4/4	0.86	0.32	-	89,89,89,89	0
55	MG	BA	1645	1/1	0.91	0.12	-	94,94,94,94	0
55	MG	CA	3127	1/1	0.91	0.08	-	65,65,65,65	0
55	MG	DA	3168	1/1	0.88	0.48	-	106,106,106,106	0
55	MG	AA	1666	1/1	0.96	0.05	-	47,47,47,47	0
55	MG	DA	3162	1/1	0.93	0.12	-	57,57,57,57	0
55	MG	BA	1630	1/1	0.81	0.10	-	160,160,160,160	0
55	MG	BA	1631	1/1	0.93	0.06	-	45,45,45,45	0
55	MG	BA	1629	1/1	0.81	0.38	-	184,184,184,184	0
55	MG	AA	1638	1/1	0.98	0.07	-	86,86,86,86	0
55	MG	DA	3074	1/1	0.97	0.04	-	47,47,47,47	0
55	MG	DA	3005	1/1	0.99	0.12	-	60,60,60,60	0
55	MG	DA	3096	1/1	0.99	0.12	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3002	1/1	0.83	0.19	-	258,258,258,258	0
55	MG	DA	3020	1/1	1.00	0.05	-	45,45,45,45	0
55	MG	DA	3161	1/1	0.91	0.28	-	62,62,62,62	0
55	MG	CA	3036	1/1	0.95	0.14	-	133,133,133,133	0
55	MG	CA	3021	1/1	0.94	0.82	-	261,261,261,261	0
55	MG	DA	3115	1/1	0.99	0.16	-	37,37,37,37	0
55	MG	DA	3038	1/1	0.99	0.09	-	19,19,19,19	0
55	MG	CA	3065	1/1	0.93	0.11	-	72,72,72,72	0
55	MG	DA	3107	1/1	0.98	0.14	-	35,35,35,35	0
55	MG	CA	3125	1/1	0.86	0.25	-	98,98,98,98	0
55	MG	CA	3104	1/1	0.84	0.21	-	254,254,254,254	0
55	MG	CA	3113	1/1	0.76	0.57	-	79,79,79,79	0
55	MG	CA	3071	1/1	0.85	0.09	-	152,152,152,152	0
55	MG	DA	3103	1/1	0.99	0.12	-	35,35,35,35	0
55	MG	BA	1639	1/1	0.38	0.49	-	93,93,93,93	0
55	MG	DA	3148	1/1	0.93	0.20	-	62,62,62,62	0
55	MG	AA	1621	1/1	0.78	0.61	-	97,97,97,97	0
55	MG	CA	3016	1/1	0.96	0.50	-	164,164,164,164	0
55	MG	CA	3142	1/1	0.95	0.10	-	71,71,71,71	0
55	MG	AA	1628	1/1	0.78	0.22	-	110,110,110,110	0
55	MG	CA	3059	1/1	0.99	0.09	-	74,74,74,74	0
55	MG	DA	3015	1/1	0.98	0.10	-	40,40,40,40	0
55	MG	CA	3042	1/1	0.98	0.10	-	82,82,82,82	0
55	MG	DA	3104	1/1	0.99	0.19	-	34,34,34,34	0
55	MG	CA	3005	1/1	0.45	0.72	-	239,239,239,239	0
55	MG	DA	3032	1/1	0.99	0.18	-	23,23,23,23	0
55	MG	AA	1649	1/1	0.95	0.07	-	57,57,57,57	0
55	MG	BA	1619	1/1	0.96	0.19	-	79,79,79,79	0
55	MG	CA	3110	1/1	0.78	0.23	-	102,102,102,102	0
57	MPD	DT	201	8/8	0.79	0.37	-	84,87,99,100	0
55	MG	AA	1634	1/1	0.90	0.18	-	144,144,144,144	0
55	MG	BA	1603	1/1	0.81	0.50	-	279,279,279,279	0
55	MG	AA	1607	1/1	0.96	0.48	-	70,70,70,70	0
55	MG	AA	1632	1/1	0.95	0.04	-	65,65,65,65	0
55	MG	CA	3028	1/1	0.70	0.23	-	274,274,274,274	0
55	MG	DA	3061	1/1	0.99	0.14	-	30,30,30,30	0
55	MG	CA	3143	1/1	0.94	0.14	-	67,67,67,67	0
55	MG	DA	3098	1/1	0.97	0.10	-	87,87,87,87	0
55	MG	CA	3055	1/1	0.97	0.07	-	135,135,135,135	0
55	MG	CA	3010	1/1	0.94	0.34	-	245,245,245,245	0
55	MG	DA	3145	1/1	0.99	0.11	-	78,78,78,78	0
55	MG	DA	3036	1/1	0.99	0.19	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	1624	1/1	0.64	0.49	-	93,93,93,93	0
55	MG	DA	3166	1/1	0.82	0.65	-	88,88,88,88	0
55	MG	DA	3076	1/1	1.00	0.13	-	23,23,23,23	0
55	MG	AA	1626	1/1	0.36	1.73	-	113,113,113,113	0
55	MG	BA	1648	1/1	0.97	0.35	-	68,68,68,68	0
55	MG	AA	1647	1/1	0.96	0.09	-	149,149,149,149	0
55	MG	DA	3056	1/1	0.99	0.17	-	42,42,42,42	0
55	MG	DA	3153	1/1	0.90	0.23	-	53,53,53,53	0
55	MG	BA	1628	1/1	0.93	0.12	-	92,92,92,92	0
55	MG	DA	3083	1/1	0.97	0.05	-	45,45,45,45	0
55	MG	CA	3112	1/1	0.89	0.17	-	62,62,62,62	0
55	MG	CA	3132	1/1	0.92	0.46	-	97,97,97,97	0
55	MG	DB	207	1/1	0.89	0.57	-	80,80,80,80	0
55	MG	DA	3052	1/1	0.97	0.10	-	70,70,70,70	0
55	MG	DA	3057	1/1	0.99	0.08	-	13,13,13,13	0
55	MG	CA	3111	1/1	0.83	0.24	-	76,76,76,76	0
55	MG	DA	3176	1/1	0.93	0.32	-	97,97,97,97	0
55	MG	CA	3057	1/1	0.91	0.10	-	106,106,106,106	0
55	MG	DA	3179	1/1	0.83	0.36	-	101,101,101,101	0
55	MG	DA	3034	1/1	0.99	0.13	-	16,16,16,16	0
55	MG	CA	3034	1/1	0.50	0.16	-	244,244,244,244	0
55	MG	DA	3151	1/1	0.97	0.25	-	30,30,30,30	0
55	MG	AA	1610	1/1	0.93	0.44	-	95,95,95,95	0
55	MG	CA	3106	1/1	0.91	0.17	-	75,75,75,75	0
55	MG	CB	203	1/1	0.73	0.09	-	133,133,133,133	0
55	MG	AA	1643	1/1	0.99	0.13	-	53,53,53,53	0
55	MG	DA	3049	1/1	0.97	0.10	-	39,39,39,39	0
55	MG	BA	1625	1/1	0.91	0.23	-	251,251,251,251	0
55	MG	DR	203	1/1	0.96	0.12	-	140,140,140,140	0
57	MPD	DE	302	8/8	0.88	0.57	-	71,76,83,85	0
55	MG	AA	1616	1/1	0.55	0.50	-	87,87,87,87	0
55	MG	CA	3119	1/1	0.81	0.35	-	86,86,86,86	0
55	MG	CA	3022	1/1	0.93	0.84	-	206,206,206,206	0
55	MG	DA	3163	1/1	0.60	0.34	-	84,84,84,84	0
55	MG	DA	3157	1/1	0.98	0.14	-	54,54,54,54	0
55	MG	CA	3108	1/1	0.95	0.21	-	73,73,73,73	0
55	MG	CA	3062	1/1	0.89	0.11	-	190,190,190,190	0
55	MG	DA	3010	1/1	1.00	0.11	-	17,17,17,17	0
55	MG	AA	1633	1/1	0.98	0.23	-	128,128,128,128	0
55	MG	CA	3081	1/1	0.98	0.06	-	84,84,84,84	0
55	MG	DA	3119	1/1	0.99	0.31	-	69,69,69,69	0
55	MG	CA	3139	1/1	0.56	0.37	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3107	1/1	0.95	0.37	-	65,65,65,65	0
55	MG	DA	3146	1/1	0.87	0.24	-	70,70,70,70	0
55	MG	CA	3134	1/1	0.65	0.46	-	126,126,126,126	0
55	MG	DA	3144	1/1	0.70	1.09	-	107,107,107,107	0
55	MG	AA	1618	1/1	0.85	1.19	-	86,86,86,86	0
55	MG	DA	3165	1/1	0.85	0.19	-	47,47,47,47	0
55	MG	DA	3070	1/1	0.98	0.07	-	62,62,62,62	0
55	MG	CA	3029	1/1	0.92	0.27	-	114,114,114,114	0
55	MG	CA	3141	1/1	0.89	0.28	-	66,66,66,66	0
55	MG	DA	3062	1/1	0.80	0.10	-	211,211,211,211	0
55	MG	CA	3076	1/1	0.85	0.18	-	132,132,132,132	0
55	MG	DA	3129	1/1	0.89	0.16	-	67,67,67,67	0
55	MG	DA	3078	1/1	0.98	0.07	-	52,52,52,52	0
55	MG	AA	1630	1/1	0.91	0.15	-	105,105,105,105	0
55	MG	AA	1654	1/1	0.82	0.35	-	259,259,259,259	0
55	MG	CA	3067	1/1	0.88	0.46	-	277,277,277,277	0
55	MG	CA	3085	1/1	0.91	0.08	-	69,69,69,69	0
55	MG	AA	1617	1/1	0.08	0.29	-	147,147,147,147	0
55	MG	BA	1640	1/1	0.91	0.22	-	94,94,94,94	0
55	MG	CA	3070	1/1	0.86	0.09	-	87,87,87,87	0
55	MG	DA	3089	1/1	0.98	0.18	-	23,23,23,23	0
66	ACY	DA	3196	4/4	0.78	0.31	-	72,76,77,77	0
55	MG	DA	3182	1/1	0.87	0.28	-	52,52,52,52	0
55	MG	BA	1627	1/1	0.90	0.30	-	126,126,126,126	0
55	MG	AA	1609	1/1	0.90	0.20	-	88,88,88,88	0
55	MG	AA	1640	1/1	0.97	0.09	-	52,52,52,52	0
55	MG	CA	3090	1/1	0.90	0.40	-	170,170,170,170	0
55	MG	CA	3078	1/1	0.90	0.06	-	153,153,153,153	0
55	MG	CA	3146	1/1	0.87	0.16	-	164,164,164,164	0
55	MG	BA	1618	1/1	0.98	0.07	-	69,69,69,69	0
55	MG	DA	3080	1/1	0.98	0.14	-	149,149,149,149	0
55	MG	CA	3109	1/1	0.92	0.24	-	62,62,62,62	0
55	MG	CA	3138	1/1	0.86	0.11	-	84,84,84,84	0
55	MG	CA	3097	1/1	0.96	0.08	-	83,83,83,83	0
55	MG	CA	3140	1/1	0.88	0.22	-	75,75,75,75	0
55	MG	AA	1662	1/1	0.98	0.15	-	73,73,73,73	0
55	MG	AA	1627	1/1	0.80	0.22	-	72,72,72,72	0
55	MG	CA	3058	1/1	0.95	0.22	-	138,138,138,138	0
55	MG	AA	1660	1/1	0.92	0.27	-	281,281,281,281	0
55	MG	DA	3054	1/1	0.98	0.10	-	70,70,70,70	0
55	MG	DA	3008	1/1	0.95	0.09	-	87,87,87,87	0
55	MG	DB	205	1/1	0.99	0.13	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	3123	1/1	0.90	0.32	-	81,81,81,81	0
55	MG	DA	3158	1/1	0.91	0.38	-	63,63,63,63	0
55	MG	DA	3181	1/1	0.94	0.31	-	70,70,70,70	0
55	MG	DA	3035	1/1	0.99	0.20	-	32,32,32,32	0
55	MG	DA	3178	1/1	0.95	0.21	-	69,69,69,69	0
55	MG	CA	3118	1/1	0.91	0.30	-	64,64,64,64	0
55	MG	AA	1601	1/1	0.83	0.87	-	76,76,76,76	0
55	MG	DA	3087	1/1	0.98	0.14	-	34,34,34,34	0
55	MG	DB	203	1/1	1.00	0.10	-	30,30,30,30	0
55	MG	DA	3155	1/1	0.97	0.19	-	60,60,60,60	0
55	MG	AA	1629	1/1	0.98	0.10	-	71,71,71,71	0
62	EDO	DA	3194	4/4	0.88	0.24	-	61,63,64,65	0
55	MG	CA	3056	1/1	0.86	0.36	-	78,78,78,78	0
55	MG	DM	202	1/1	0.99	0.04	-	34,34,34,34	0
55	MG	CA	3045	1/1	0.94	0.11	-	107,107,107,107	0
55	MG	DA	3042	1/1	0.99	0.10	-	29,29,29,29	0
57	MPD	DT	202	8/8	0.80	0.35	-	105,107,109,109	0
62	EDO	DA	3215	4/4	0.90	0.24	-	67,71,74,74	0
55	MG	DA	3136	1/1	0.94	0.20	-	43,43,43,43	0
55	MG	DA	3149	1/1	0.94	0.11	-	47,47,47,47	0
55	MG	AA	1606	1/1	0.88	0.23	-	83,83,83,83	0
58	PUT	AA	1675	6/6	0.76	0.47	-	106,107,108,109	0
55	MG	DA	3086	1/1	1.00	0.11	-	29,29,29,29	0
55	MG	CA	3154	1/1	-0.24	1.40	-	136,136,136,136	0
55	MG	DB	209	1/1	0.97	0.23	-	65,65,65,65	0
55	MG	DA	3117	1/1	0.97	0.20	-	62,62,62,62	0
55	MG	DA	3108	1/1	0.99	0.09	-	30,30,30,30	0
55	MG	CA	3046	1/1	0.81	0.12	-	117,117,117,117	0
58	PUT	DA	3212	6/6	0.85	0.28	-	54,63,66,70	0
55	MG	BA	1609	1/1	0.88	0.16	-	168,168,168,168	0
55	MG	AA	1625	1/1	0.91	0.38	-	68,68,68,68	0
55	MG	DA	3055	1/1	0.99	0.21	-	24,24,24,24	0
55	MG	DA	3072	1/1	0.98	0.19	-	55,55,55,55	0
55	MG	BA	1636	1/1	0.95	0.45	-	91,91,91,91	0
55	MG	DA	3143	1/1	0.94	0.18	-	50,50,50,50	0
55	MG	BA	1606	1/1	0.85	0.18	-	251,251,251,251	0
55	MG	CA	3064	1/1	0.96	0.28	-	260,260,260,260	0
55	MG	DA	3051	1/1	0.99	0.09	-	14,14,14,14	0
55	MG	DA	3142	1/1	0.95	0.38	-	84,84,84,84	0
55	MG	DA	3113	1/1	0.98	0.09	-	52,52,52,52	0
55	MG	BA	1641	1/1	0.66	0.27	-	121,121,121,121	0
66	ACY	DA	3191	4/4	0.91	0.28	-	80,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
61	PEG	DA	3199	7/7	0.87	0.41	-	79,84,92,93	0
55	MG	CA	3053	1/1	0.95	0.15	-	81,81,81,81	0
55	MG	BA	1621	1/1	0.98	0.22	-	36,36,36,36	0
55	MG	DA	3125	1/1	0.98	0.19	-	58,58,58,58	0
55	MG	AA	1645	1/1	0.97	0.07	-	46,46,46,46	0
55	MG	CA	3091	1/1	0.96	0.09	-	80,80,80,80	0
55	MG	DA	3229	1/1	0.99	0.07	-	36,36,36,36	0
55	MG	CA	3027	1/1	0.95	0.14	-	68,68,68,68	0
58	PUT	DA	3221	6/6	0.86	0.40	-	113,116,117,118	0
55	MG	AA	1615	1/1	0.86	0.48	-	84,84,84,84	0
55	MG	AA	1679	1/1	0.98	0.21	-	62,62,62,62	0
55	MG	DA	3069	1/1	0.99	0.15	-	46,46,46,46	0
55	MG	BA	1611	1/1	0.99	0.10	-	56,56,56,56	0
55	MG	AA	1652	1/1	0.98	0.25	-	21,21,21,21	0
55	MG	CA	3007	1/1	0.72	0.40	-	214,214,214,214	0
55	MG	DA	3140	1/1	0.96	0.20	-	68,68,68,68	0
55	MG	DA	3230	1/1	0.98	0.07	-	48,48,48,48	0
55	MG	CA	3098	1/1	0.96	0.07	-	78,78,78,78	0
55	MG	DA	3116	1/1	0.97	0.13	-	34,34,34,34	0
55	MG	AA	1650	1/1	0.97	0.07	-	79,79,79,79	0
62	EDO	DB	212	4/4	0.95	0.24	-	70,72,73,73	0
55	MG	DA	3133	1/1	0.62	0.23	-	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.