wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2025 – 03:54 AM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

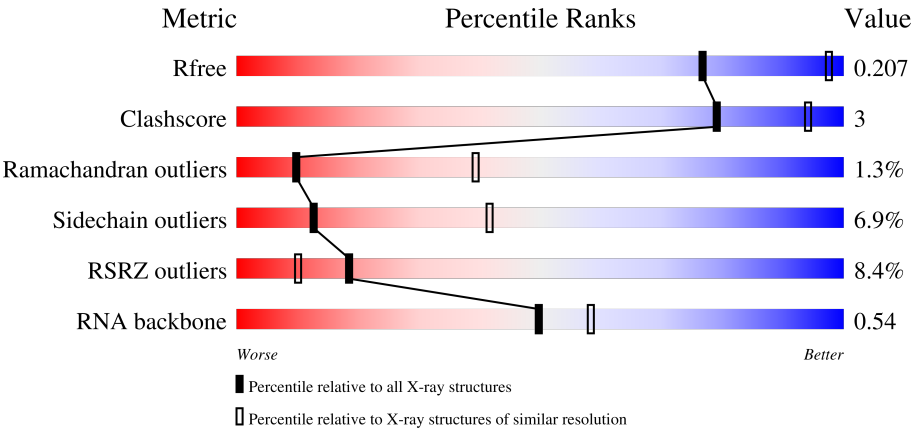
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	5% 74% 22%
1	BA	1534	7% 74% 23%
2	AB	224	4% 88% 12%
2	BB	224	8% 88% 10%

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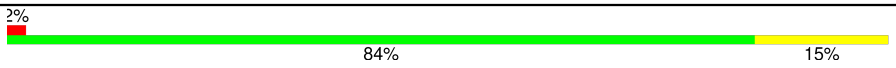
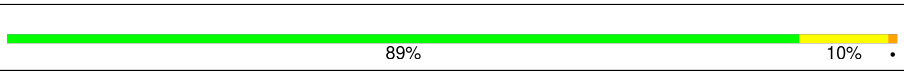
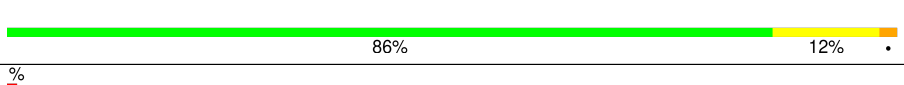
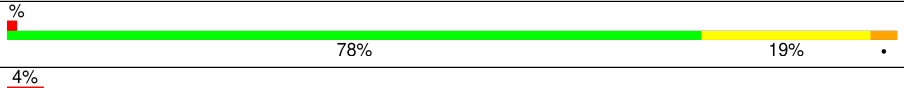
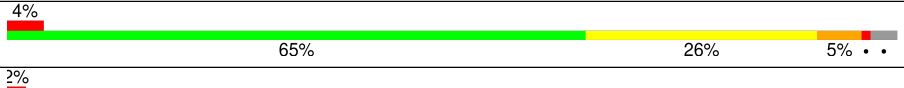
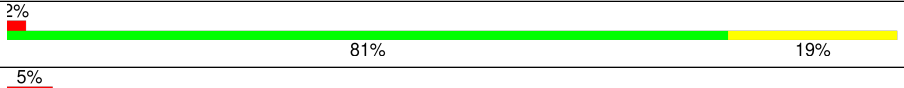
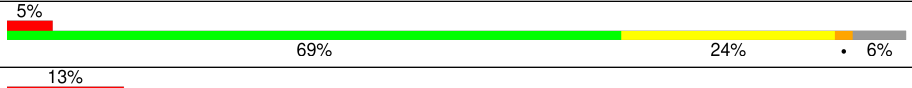
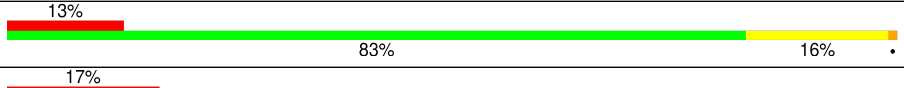
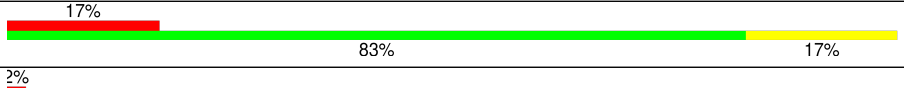
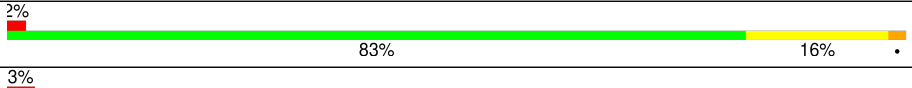
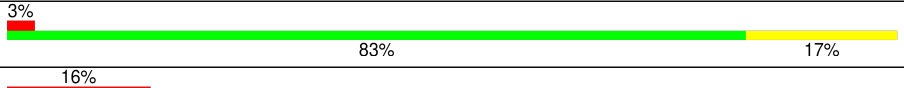
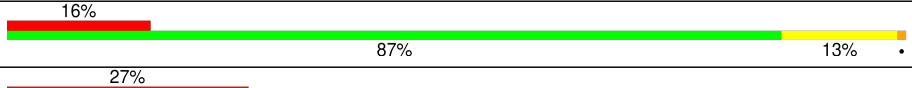
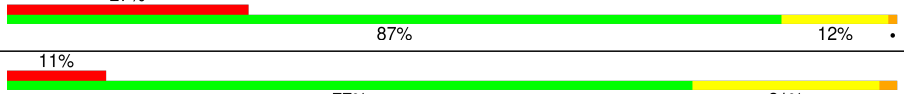
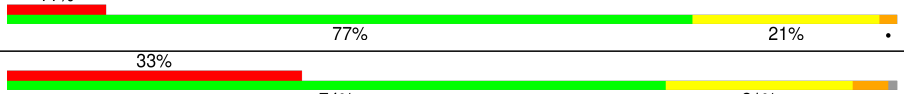
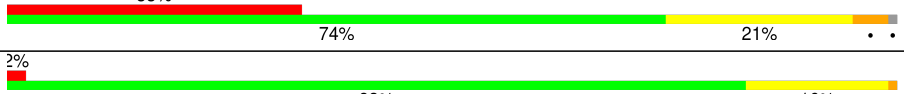
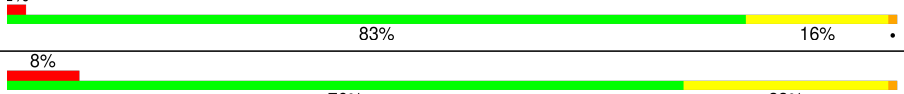
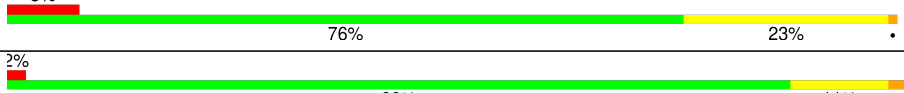
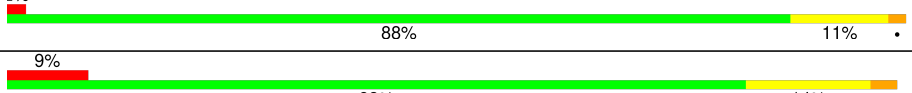
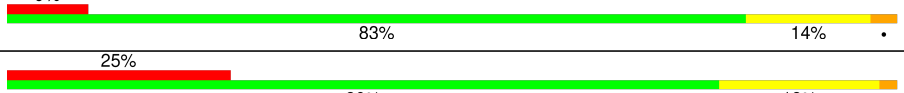
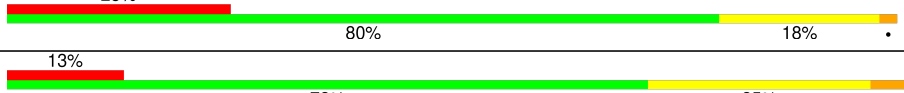
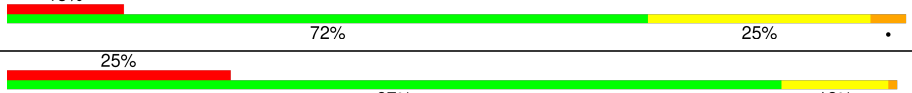
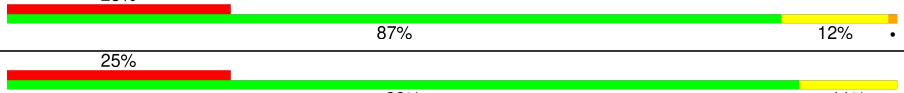
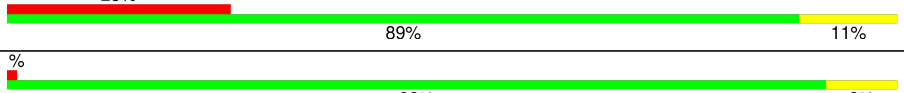
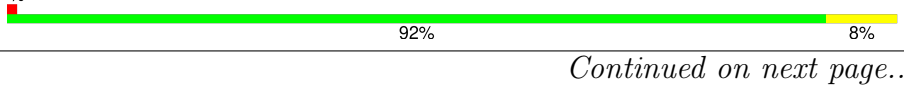
Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	2% 91% 8%
16	AP	82	2% 90% 10%
16	BP	82	18% 82% 17%
17	AQ	80	% 78% 21%
17	BQ	80	9% 61% 31% 6%
18	AR	55	2% 87% 13%
18	BR	55	9% 93% 7%
19	AS	79	25% 82% 16%
19	BS	79	23% 84% 14%
20	AT	86	2% 90% 7%
20	BT	86	22% 79% 15% 5%
21	AU	56	5% 88% 12%
21	BU	56	4% 88% 12%
22	C1	56	39% 84% 12%
22	D1	56	84% 16%
23	C2	51	31% 69% 27%
23	D2	51	2% 73% 25%
24	C3	46	54% 85% 15%
24	D3	46	2% 89% 11%
25	C4	64	75% 84% 16%
25	D4	64	91% 9%
26	C5	38	26% 79% 18%
26	D5	38	87% 13%
27	C0	58	17% 76% 22%
27	D0	58	83% 16%

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Mol	Chain	Length	Quality of chain
28	CB	120	2% 85% 11%
28	DB	120	91% 8%
29	CC	271	15% 82% 16%
29	DC	271	% 90% 8%
30	CD	209	13% 88% 11%
30	DD	209	90% 10%
31	CA	2904	10% 73% 23%
32	CE	201	23% 83% 14%
32	DE	201	91% 8%
33	CF	177	7% 83% 15%
33	DF	177	% 81% 18%
34	CG	176	3% 89% 11%
34	DG	176	% 90% 10%
35	CH	149	3% 79% 20%
35	DH	149	3% 82% 18%
36	CJ	134	25% 88% 11%
36	DJ	134	30% 88% 11%
37	CK	142	7% 92% 7%
37	DK	142	94% 6%
38	CL	123	8% 85% 11%
38	DL	123	87% 11%
39	CM	144	33% 79% 19%
39	DM	144	% 92% 8%
40	CN	136	6% 85% 15%
40	DN	136	84% 15%

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Mol	Chain	Length	Quality of chain
41	CO	125	28% 82% 12%
41	DO	125	91% 6%
42	CP	117	13% 87% 10%
42	DP	117	% 85% 12%
43	CQ	114	10% 90% 8%
43	DQ	114	% 90% 9%
44	CR	117	21% 87% 13%
44	DR	117	89% 11%
45	CS	103	22% 80% 17%
45	DS	103	2% 90% 10%
46	CT	110	28% 82% 16%
46	DT	110	% 85% 15%
47	CU	93	31% 80% 16%
47	DU	93	5% 87% 13%
48	CV	102	51% 80% 19%
48	DV	102	% 85% 14%
49	CW	94	4% 86% 14%
49	DW	94	89% 11%
50	CX	76	16% 88% 11%
50	DX	76	87% 9%
51	CY	77	19% 82% 18%
51	DY	77	% 91% 9%
52	CZ	62	27% 82% 18%
52	DZ	62	2% 92% 8%
53	DI	135	19% 75% 22%

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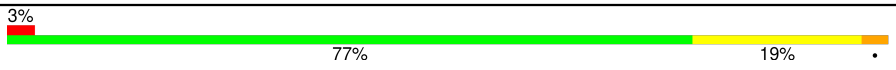
Mol	Chain	Length	Quality of chain
54	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1617	-	-	-	X
55	MG	AA	1622	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3135	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3148	-	-	-	X
58	PUT	AA	1674	-	-	-	X
66	ACY	DA	3196	-	X	-	-

2 Entry composition (i)

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 5S rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

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

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

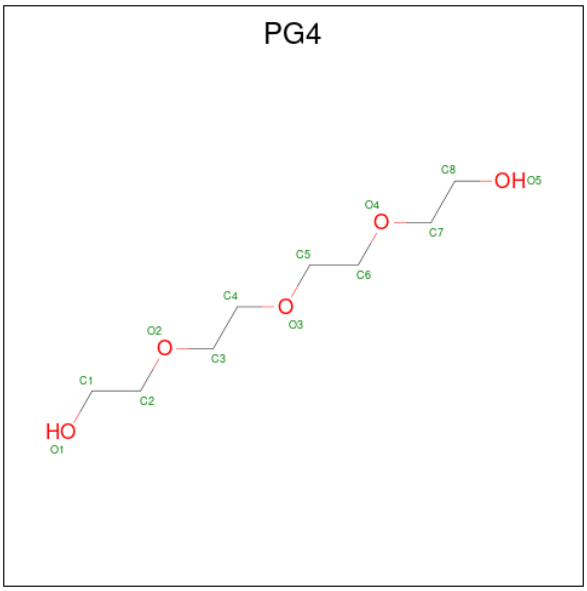
- Molecule 54 is a RNA chain called 23S rRNA.

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).

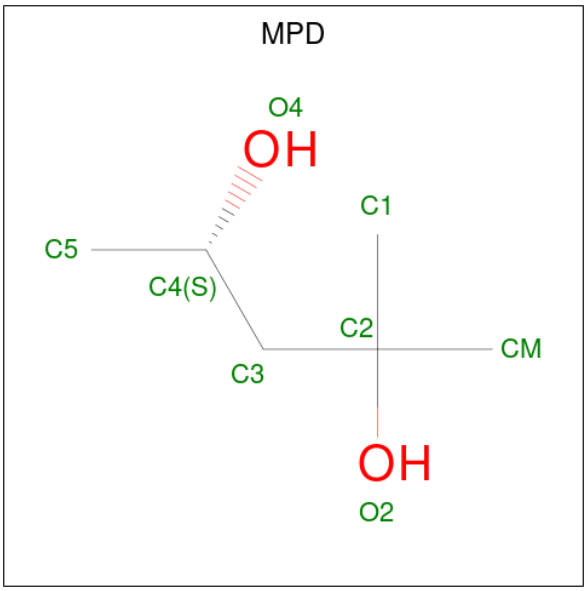
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total	Mg	0	0
			72	72		
55	BA	45	Total	Mg	0	0
			45	45		
55	CB	3	Total	Mg	0	0
			3	3		
55	CA	156	Total	Mg	0	0
			156	156		
55	DD	1	Total	Mg	0	0
			1	1		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	DB	9	Total	Mg	0	0
			9	9		
55	DA	183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

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



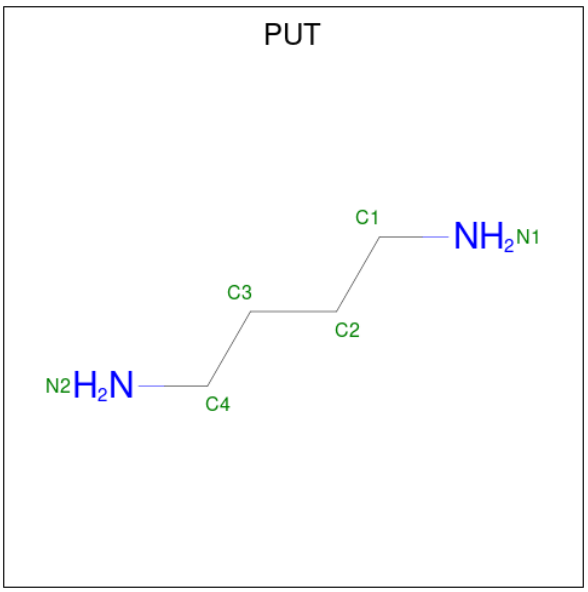
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	1	Total C O 13 8 5	0	0
56	BA	1	Total C O 13 8 5	0	0
56	DQ	1	Total C O 13 8 5	0	0
56	DR	1	Total C O 13 8 5	0	0
56	DS	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0

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

- 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

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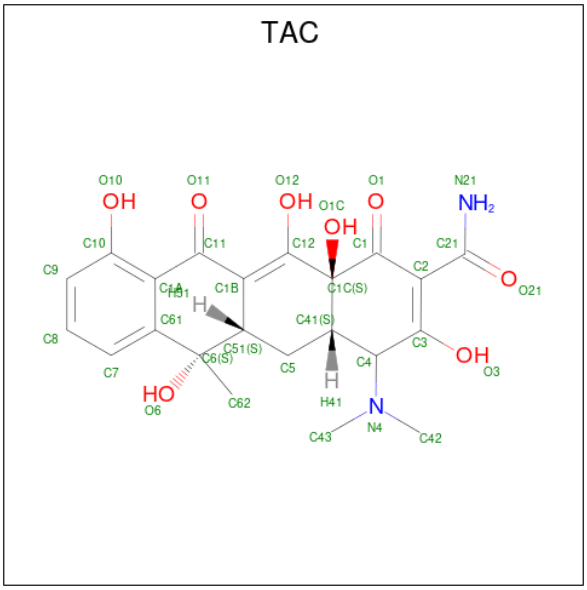
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0

- 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	AB	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

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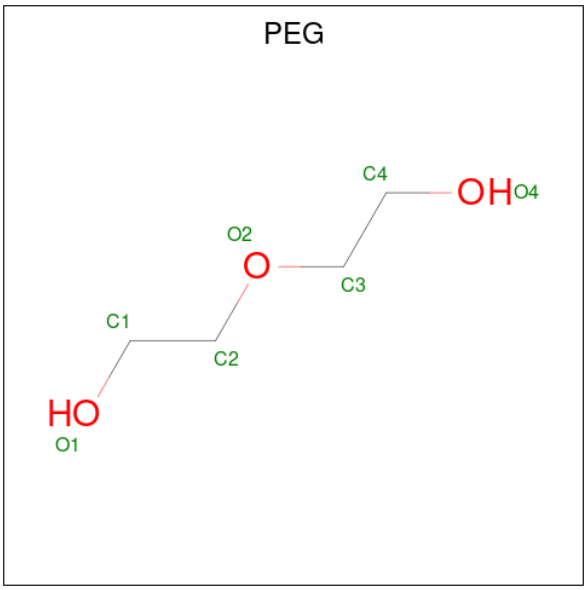
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	D5	1	Total Zn 1 1	0	0

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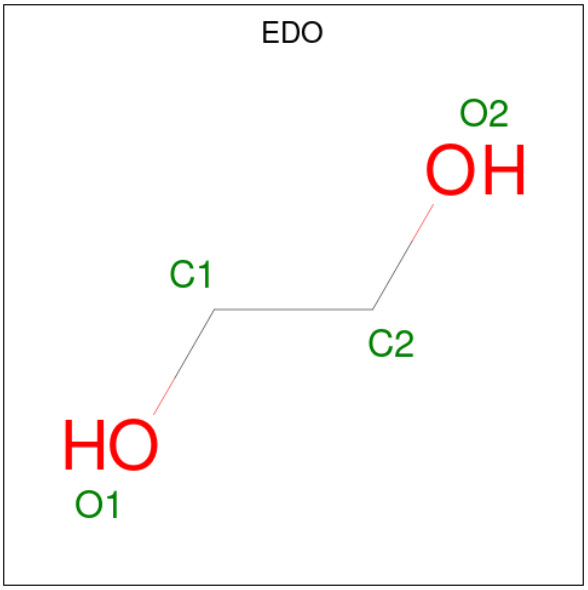
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DA	1	Total C O 7 4 3	0	0

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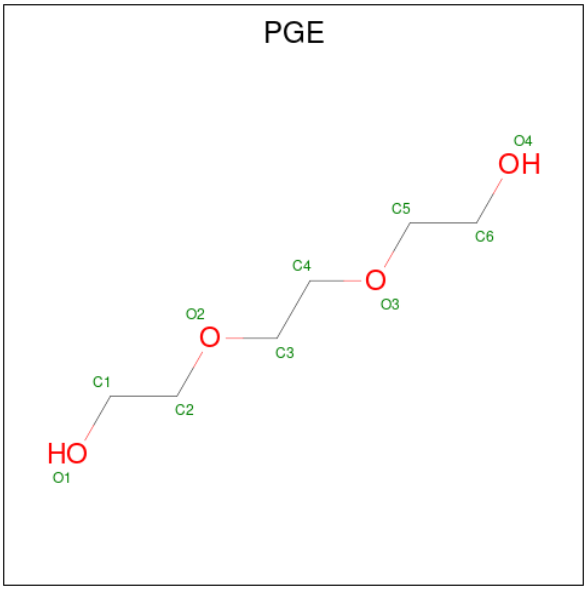
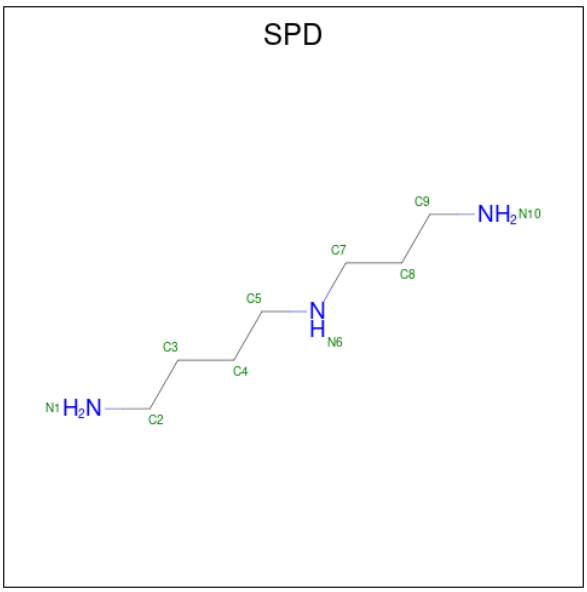
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0

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



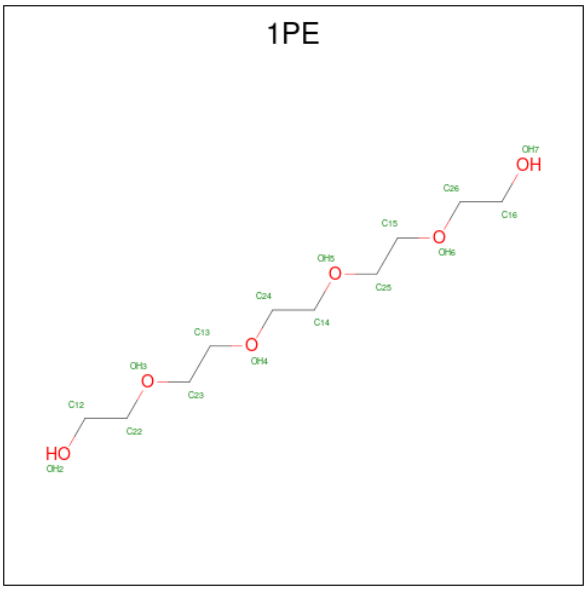
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	D1	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0

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



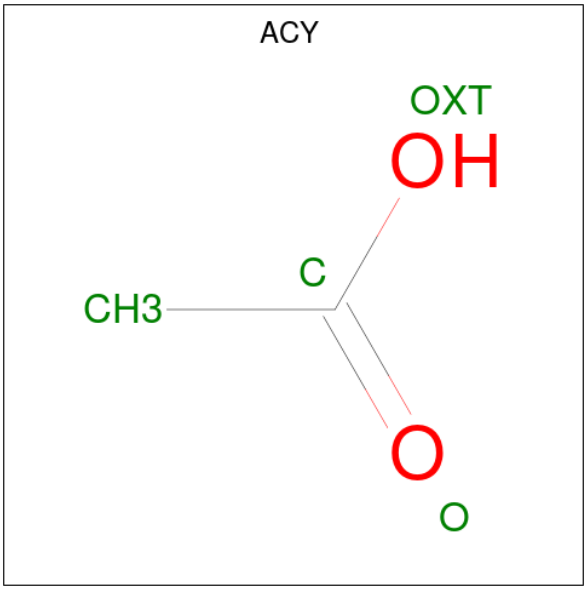
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

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



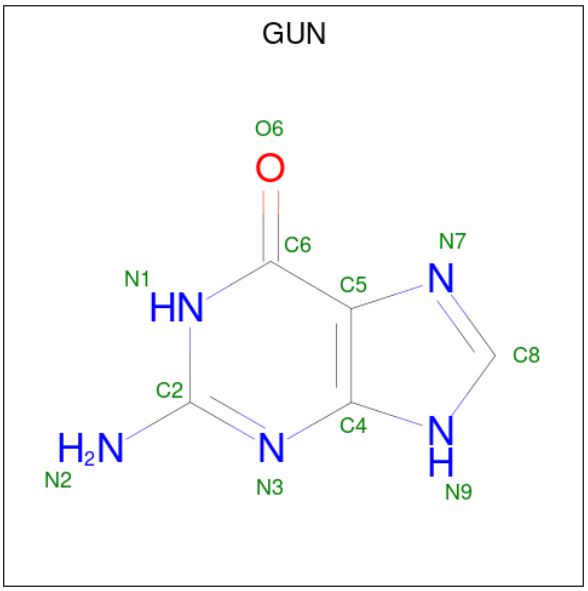
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C O 16 10 6	0	0
65	DA	1	Total C O 16 10 6	0	0

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



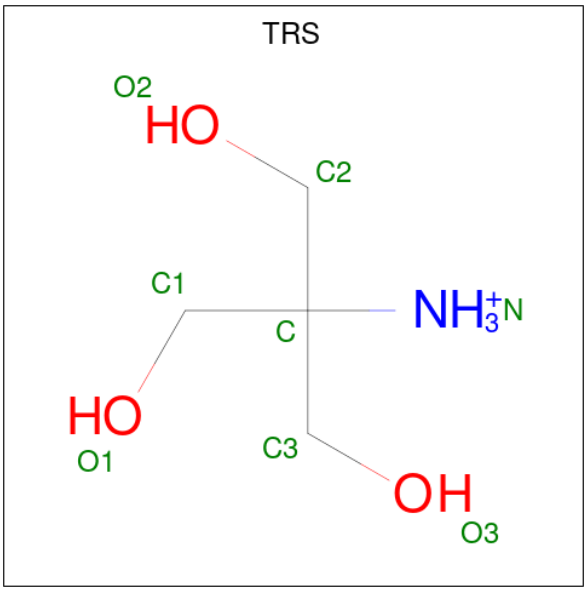
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0

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



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

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



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

- Molecule 69 is water.

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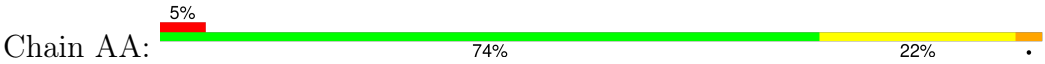
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DV	20	Total O 20 20	0	0
69	DW	31	Total O 31 31	0	0
69	DX	25	Total O 25 25	0	0
69	DY	9	Total O 9 9	0	0
69	DZ	8	Total O 8 8	0	0
69	DB	209	Total O 209 209	0	0
69	DA	4840	Total O 4840 4840	0	0

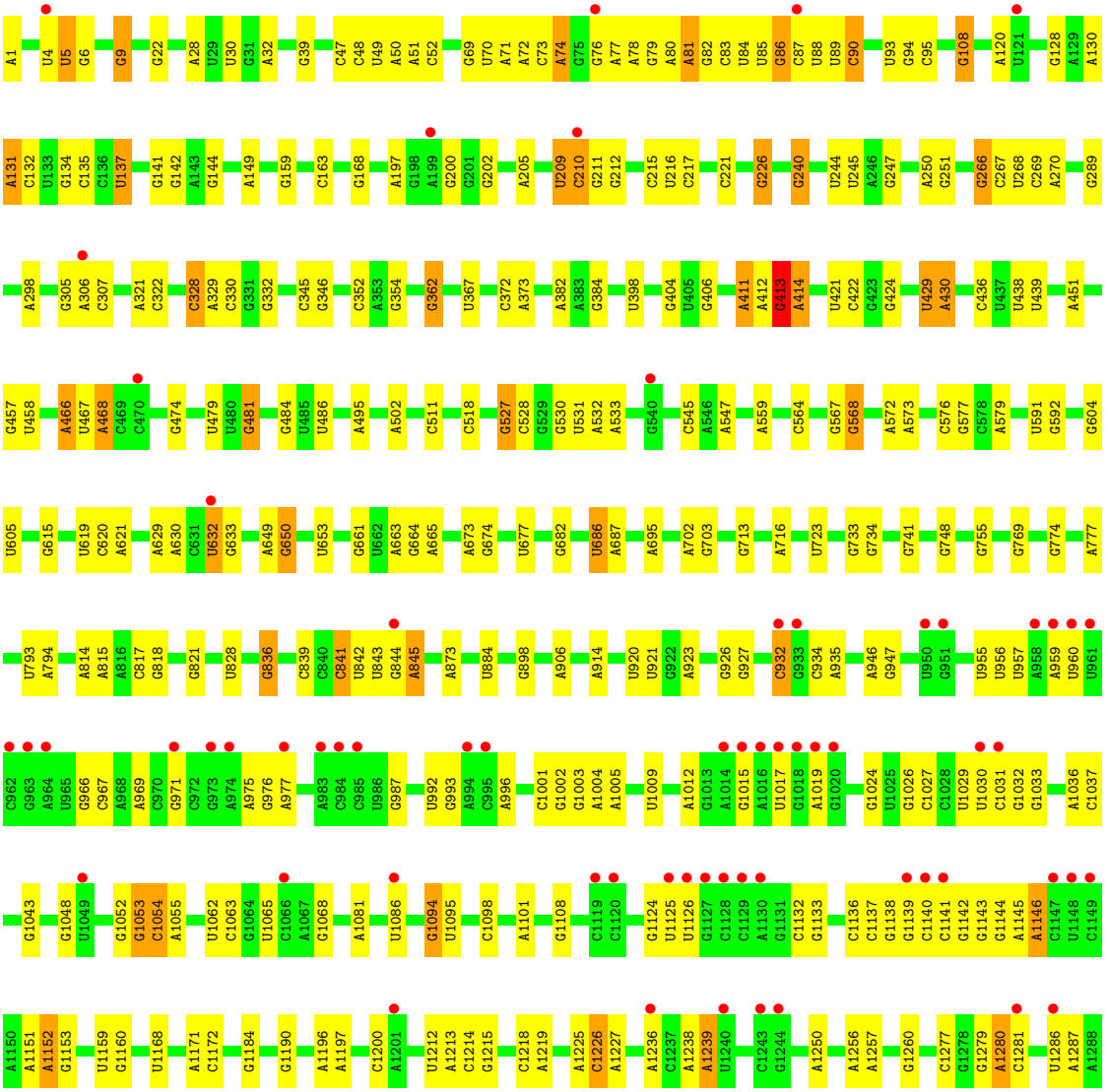
3 Residue-property plots (i)

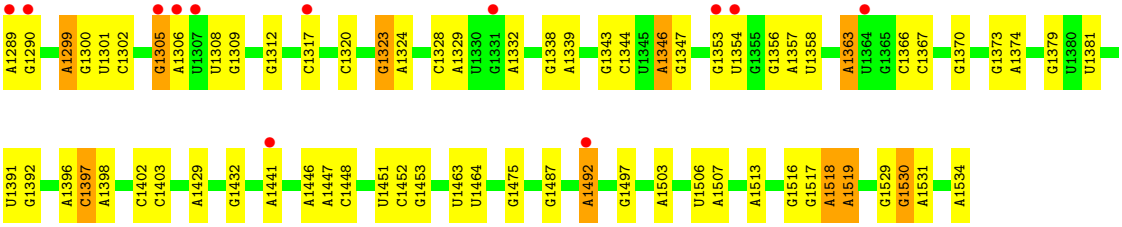
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

Chain AA:

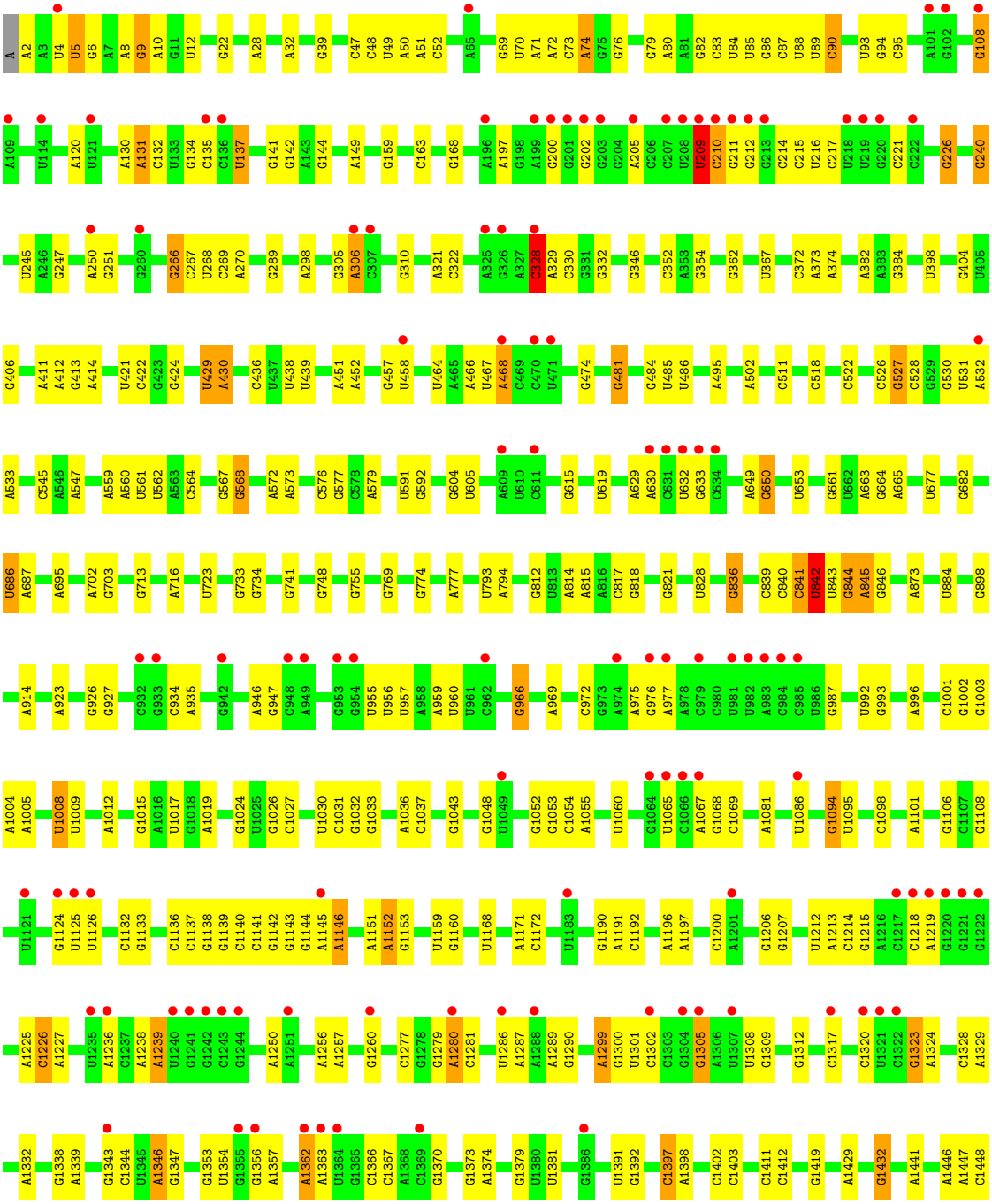






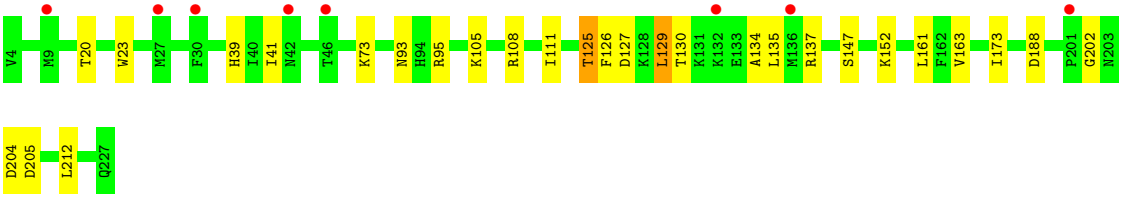
• Molecule 1: 16S rRNA

Chain BA:



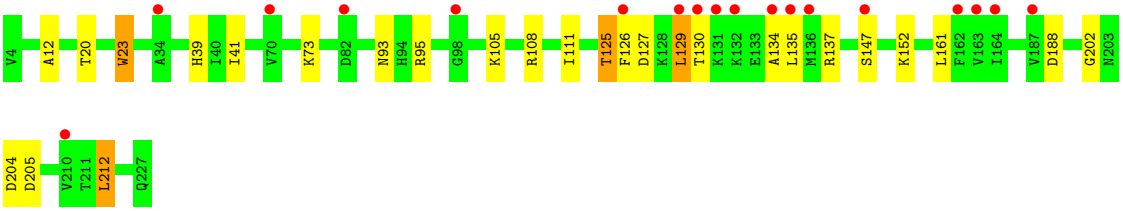
• Molecule 2: 30S ribosomal protein S2

Chain AB:



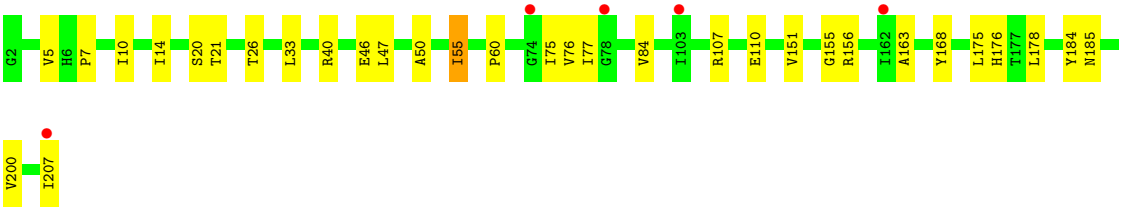
• Molecule 2: 30S ribosomal protein S2

Chain BB:



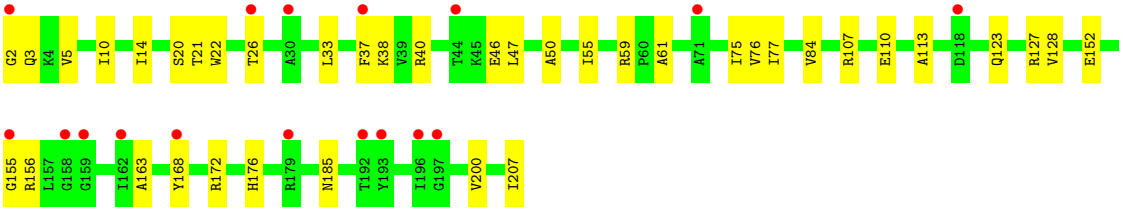
• Molecule 3: 30S ribosomal protein S3

Chain AC:



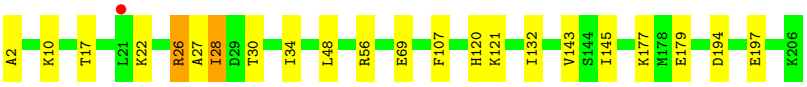
• Molecule 3: 30S ribosomal protein S3

Chain BC:



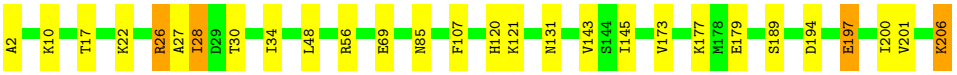
• Molecule 4: 30S ribosomal protein S4

Chain AD:



• Molecule 4: 30S ribosomal protein S4

Chain BD:

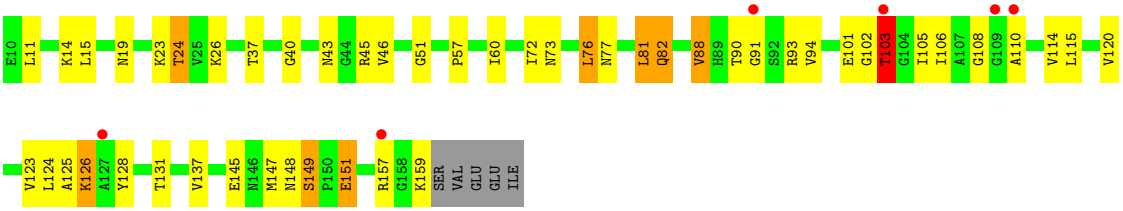


• Molecule 5: 30S ribosomal protein S5

Chain AE:

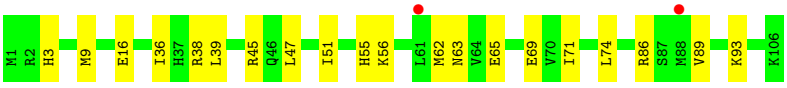
• Molecule 5: 30S ribosomal protein S5

Chain BE:



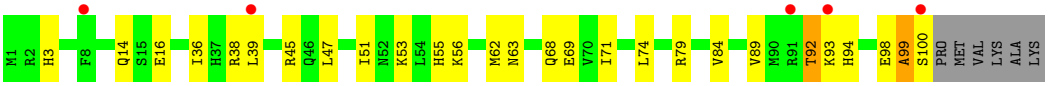
• Molecule 6: 30S ribosomal protein S6

Chain AF:



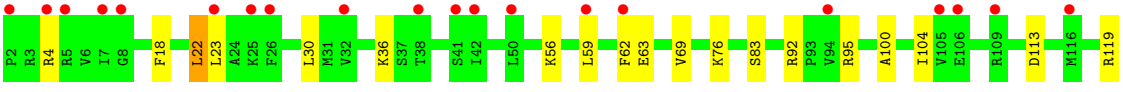
• Molecule 6: 30S ribosomal protein S6

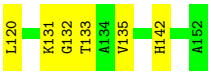
Chain BF:



• Molecule 7: 30S ribosomal protein S7

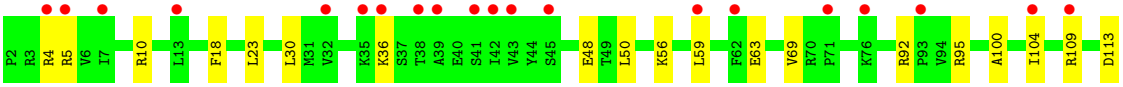
Chain AG:

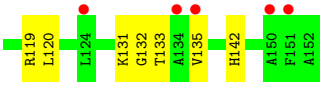




• Molecule 7: 30S ribosomal protein S7

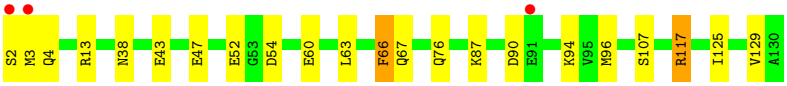
Chain BG:





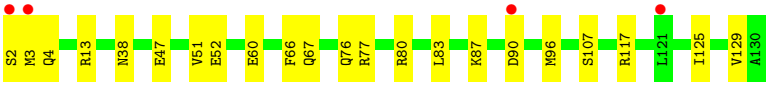
• Molecule 8: 30S ribosomal protein S8

Chain AH:



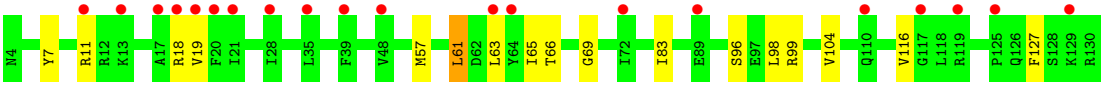
• Molecule 8: 30S ribosomal protein S8

Chain BH:



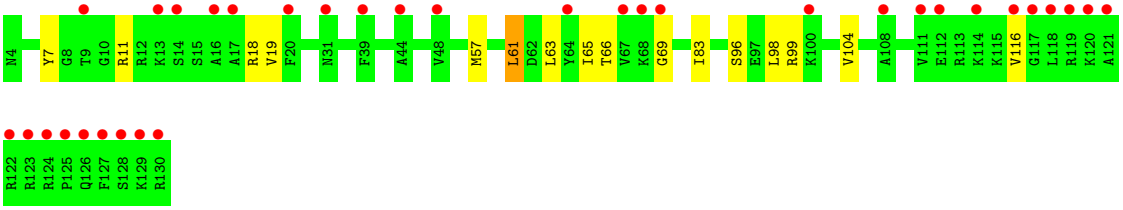
• Molecule 9: 30S ribosomal protein S9

Chain AI:



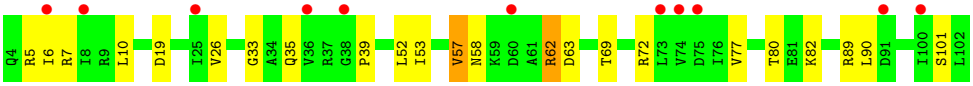
• Molecule 9: 30S ribosomal protein S9

Chain BI:



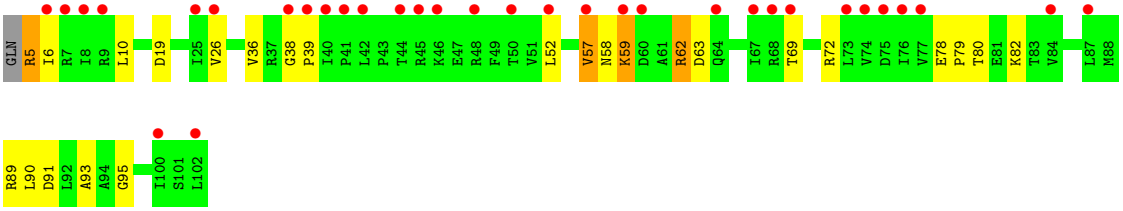
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



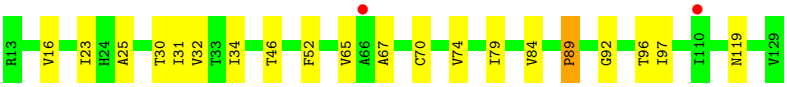
• Molecule 10: 30S ribosomal protein S10

Chain BJ:



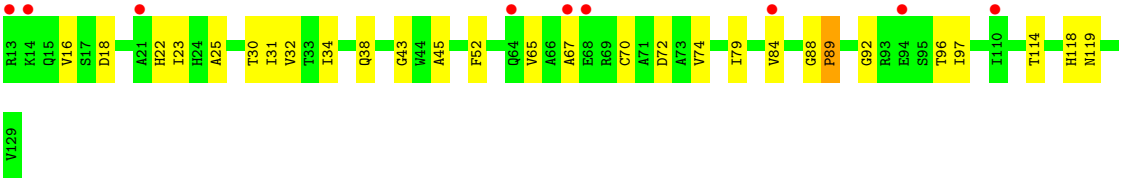
• Molecule 11: 30S ribosomal protein S11

Chain AK:



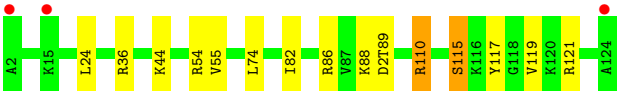
• Molecule 11: 30S ribosomal protein S11

Chain BK:



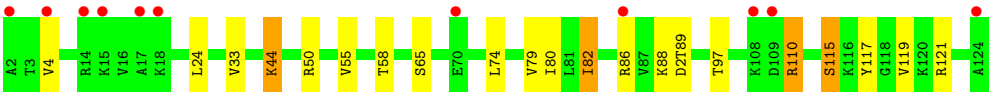
• Molecule 12: 30S ribosomal protein S12

Chain AL:



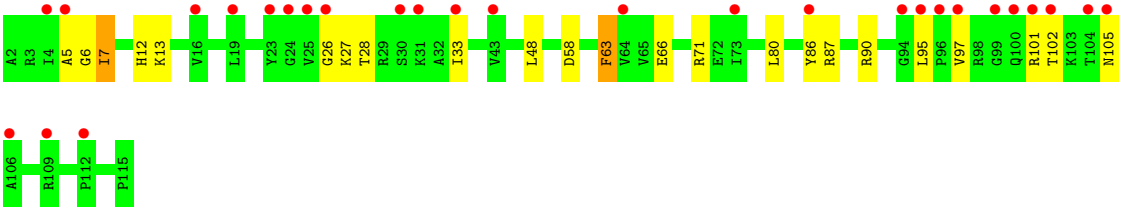
• Molecule 12: 30S ribosomal protein S12

Chain BL:

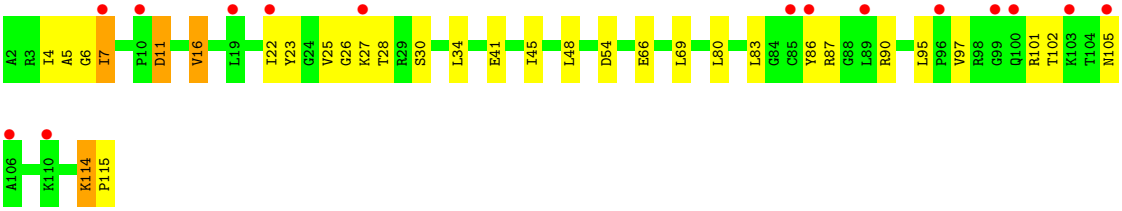


• Molecule 13: 30S ribosomal protein S13

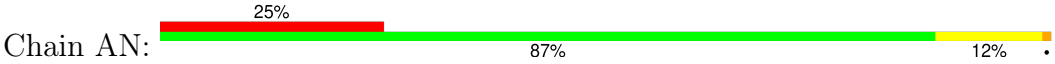
Chain AM:

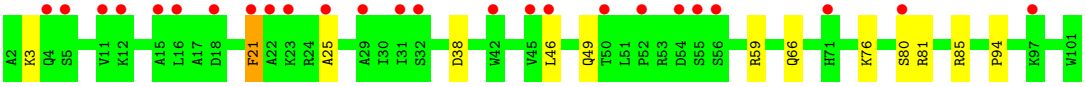


• Molecule 13: 30S ribosomal protein S13

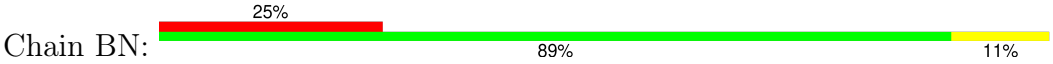


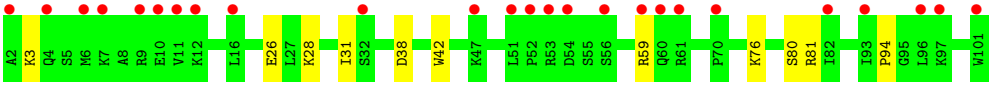
• Molecule 14: 30S ribosomal protein S14



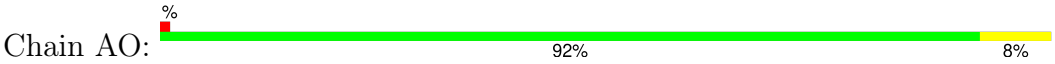


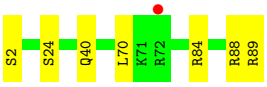
• Molecule 14: 30S ribosomal protein S14



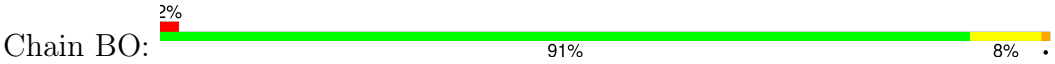


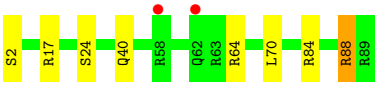
• Molecule 15: 30S ribosomal protein S15





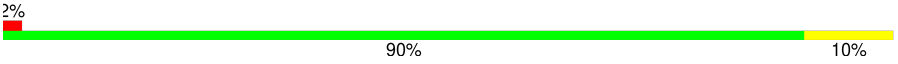
• Molecule 15: 30S ribosomal protein S15

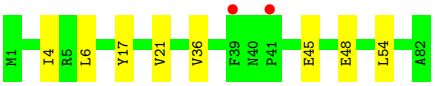




• Molecule 16: 30S ribosomal protein S16

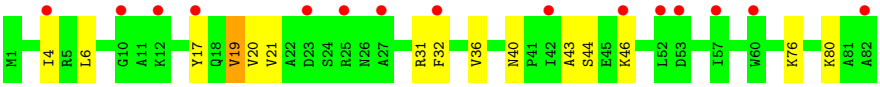
Chain AP:





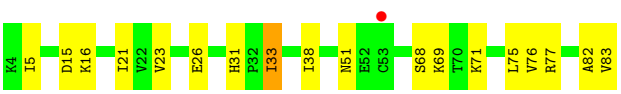
• Molecule 16: 30S ribosomal protein S16

Chain BP:



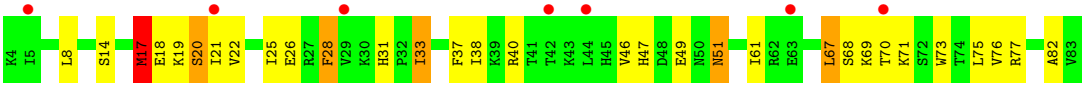
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



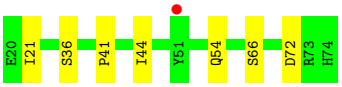
• Molecule 17: 30S ribosomal protein S17

Chain BQ:



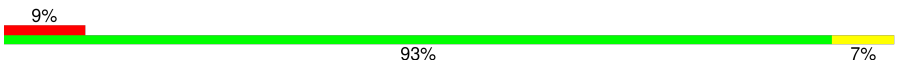
• Molecule 18: 30S ribosomal protein S18

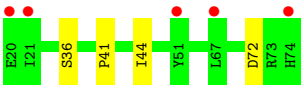
Chain AR:



• Molecule 18: 30S ribosomal protein S18

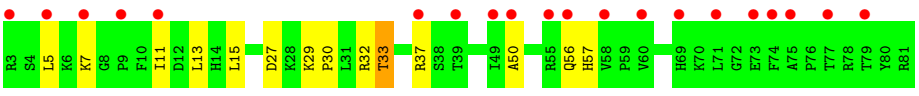
Chain BR:





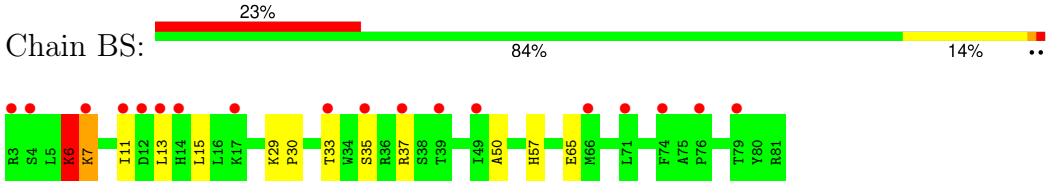
• Molecule 19: 30S ribosomal protein S19

Chain AS:



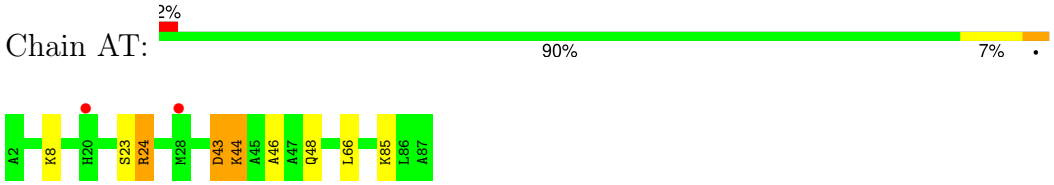
• Molecule 19: 30S ribosomal protein S19

Chain BS:



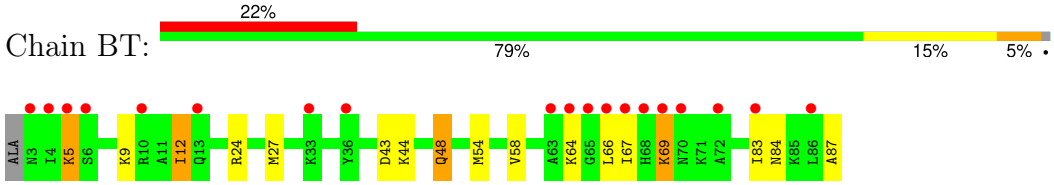
• Molecule 20: 30S ribosomal protein S20

Chain AT:



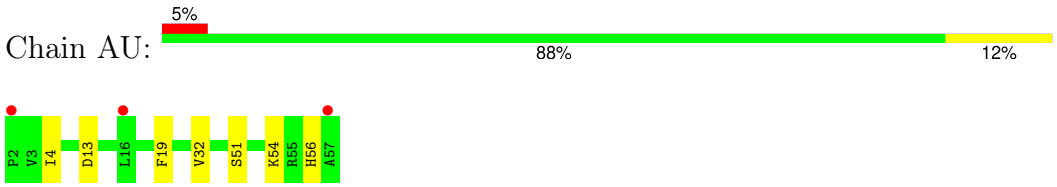
• Molecule 20: 30S ribosomal protein S20

Chain BT:



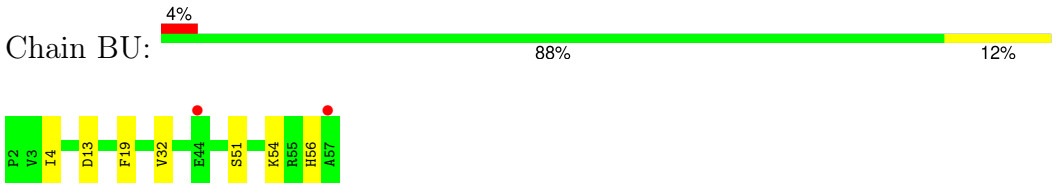
• Molecule 21: 30S ribosomal protein S21

Chain AU:



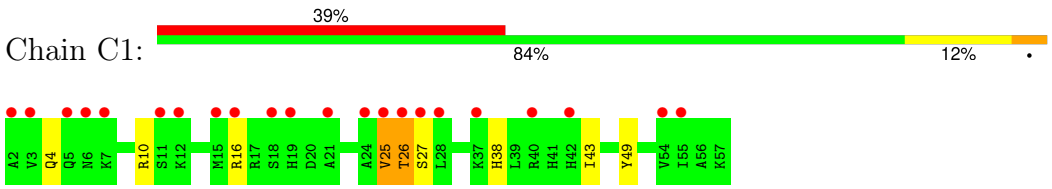
• Molecule 21: 30S ribosomal protein S21

Chain BU:



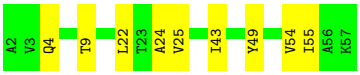
• Molecule 22: 50S ribosomal protein L32

Chain C1:



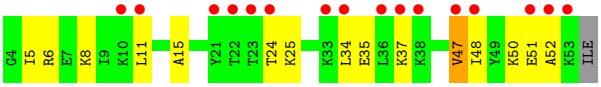
• Molecule 22: 50S ribosomal protein L32

Chain D1:



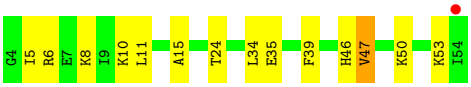
• Molecule 23: 50S ribosomal protein L33

Chain C2:



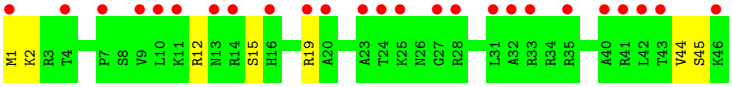
• Molecule 23: 50S ribosomal protein L33

Chain D2:



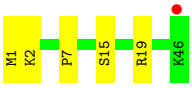
• Molecule 24: 50S ribosomal protein L34

Chain C3:



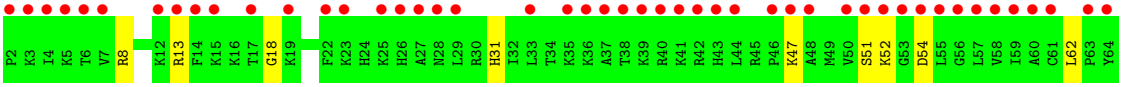
• Molecule 24: 50S ribosomal protein L34

Chain D3:



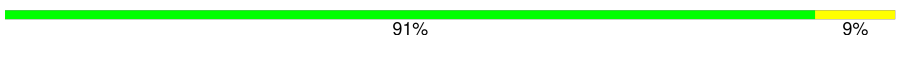
• Molecule 25: 50S ribosomal protein L35

Chain C4:



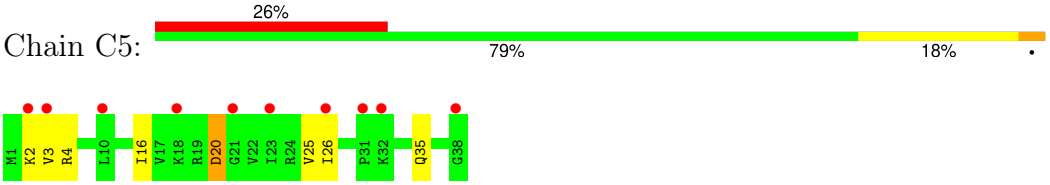
• Molecule 25: 50S ribosomal protein L35

Chain D4:



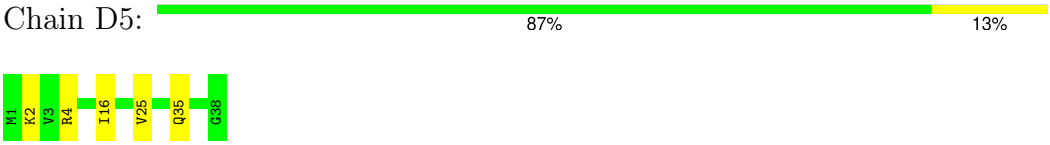
• Molecule 26: 50S ribosomal protein L36

Chain C5:



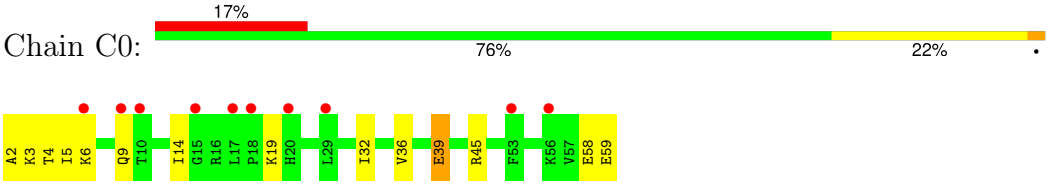
• Molecule 26: 50S ribosomal protein L36

Chain D5:



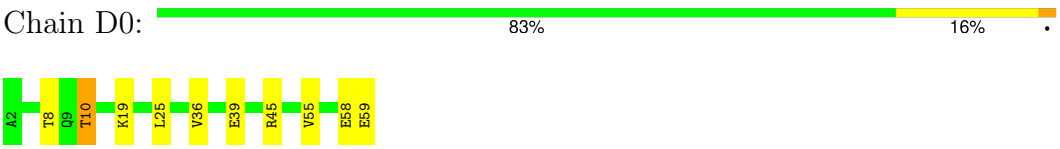
• Molecule 27: 50S ribosomal protein L30

Chain C0:



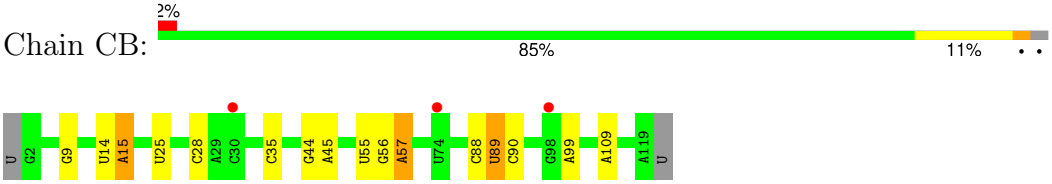
• Molecule 27: 50S ribosomal protein L30

Chain D0:



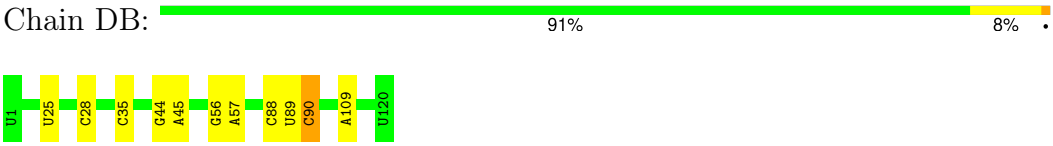
• Molecule 28: 5S rRNA

Chain CB:



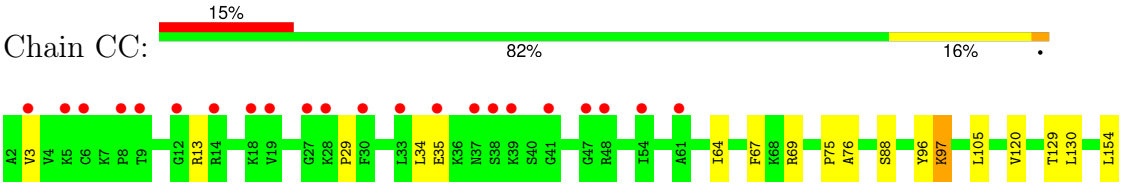
• Molecule 28: 5S rRNA

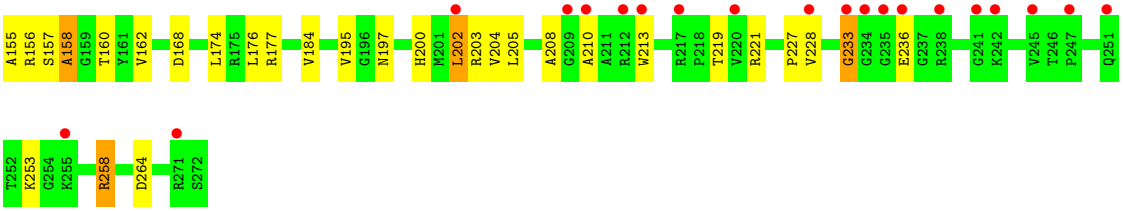
Chain DB:



• Molecule 29: 50S ribosomal protein L2

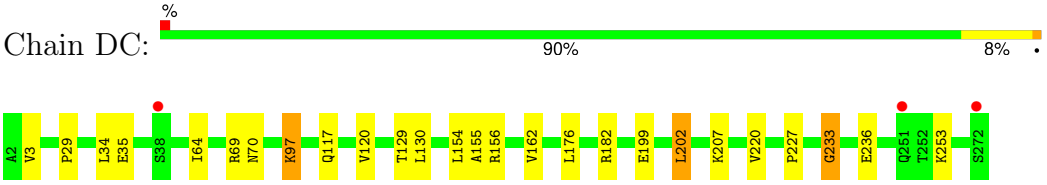
Chain CC:





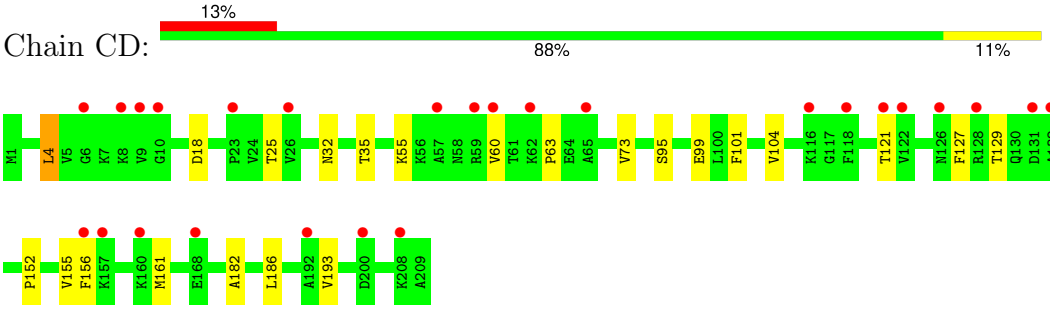
• Molecule 29: 50S ribosomal protein L2

Chain DC:



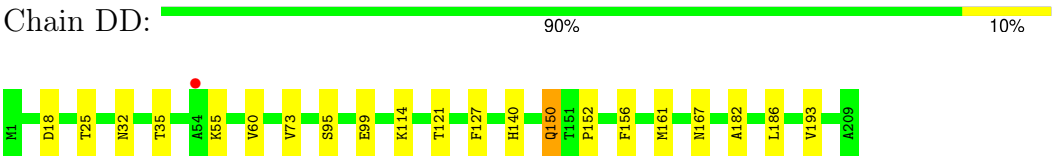
• Molecule 30: 50S ribosomal protein L3

Chain CD:



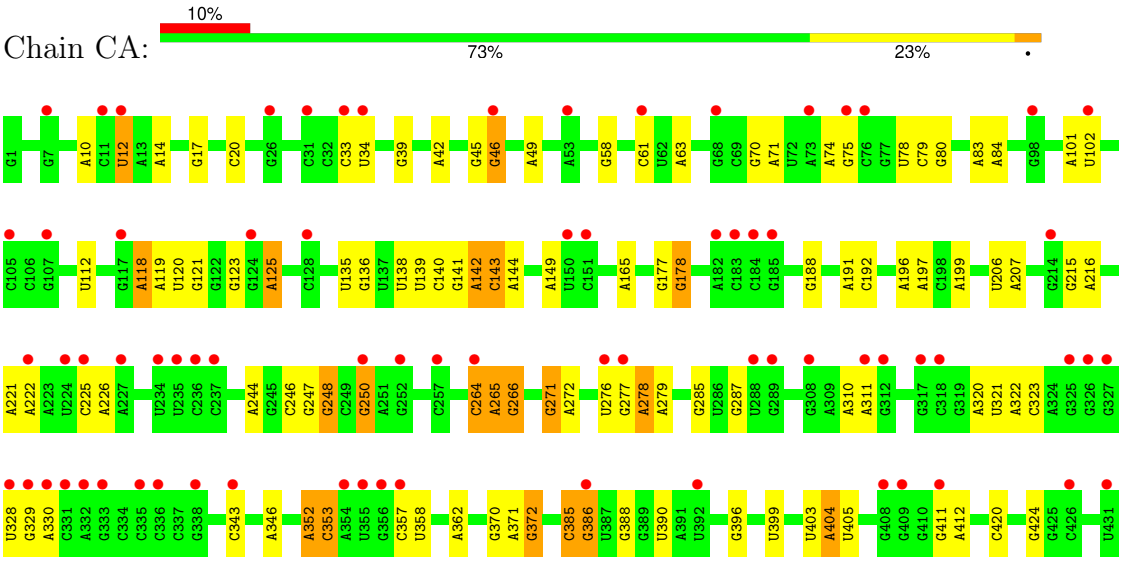
• Molecule 30: 50S ribosomal protein L3

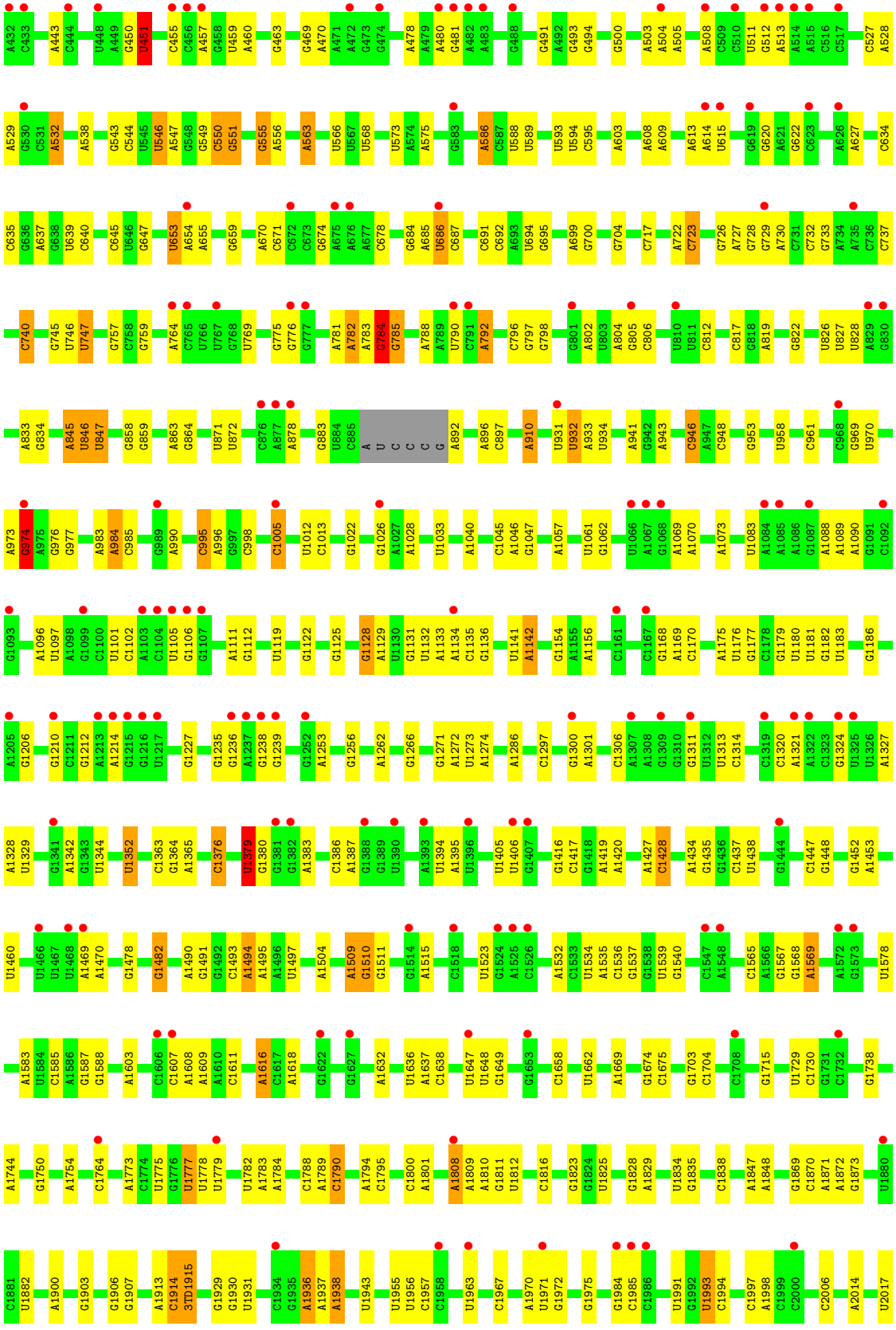
Chain DD:



• Molecule 31: 23S rRNA

Chain CA:

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A529 G530 C531 A532 A538 G543 C544 U545 U546 A547 G548 G549 C550 G551 G555 A556 A563 U566 U567 U568 U573 A574 A575 G583 A586 C587 U588 U589 U593 U594 C595 A603 A608 A609 A613 A614 U615 G619 G620 A621 G622 C623 A626 A627 C634
C635 G636 A637 G638 U639 C640 C645 U646 G647 U653 A654 A655 G659 A670 C671 C672 C673 G674 A675 A676 A677 C678 G684 A685 U686 C687 C691 C692 A693 U694 G695 A699 G700 G704 C717 A722 C723 G726 A727 G728 G729 A730 C731 C732 G733 A734 A735 C736 C737
C740 G745 U746 U747 G757 C758 G759 A764 C765 U766 U767 G768 U769 G775 G776 G777 A781 A782 A783 G784 G785 A788 A789 U790 C791 A792 C796 G797 G798 G801 A802 U803 A804 G805 C806 U810 U811 C812 C817 G818 A819 G822 U826 U827 U828 A829 G830
A833 C834 A845 U846 U847 C858 G859 A863 G864 U871 U872 C876 A877 A878 G883 U884 C885 A U C C C G A892 A896 C897 A910 U931 U932 A933 U934 A941 G942 A943 C946 A947 C948 G953 U958 C961 G968 G969 U970
A973 G974 A975 G976 G977 A983 A984 C985 G989 A990 C995 A996 G997 C998 C1005 U1012 C1013 G1022 G1026 A1027 A1028 U1033 A1040 C1045 A1046 G1047 A1057 U1061 G1062 U1066 A1067 G1068 A1069 A1070 A1073 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092
G1093 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 A1111 G1112 U1119 G1122 G1125 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 U1141 A1142 G1154 A1155 A1156 C1161 C1167 G1168 A1169 C1170 A1175 U1176 C1177 C1178 G1179 U1180 U1181 G1182 U1183 G1186
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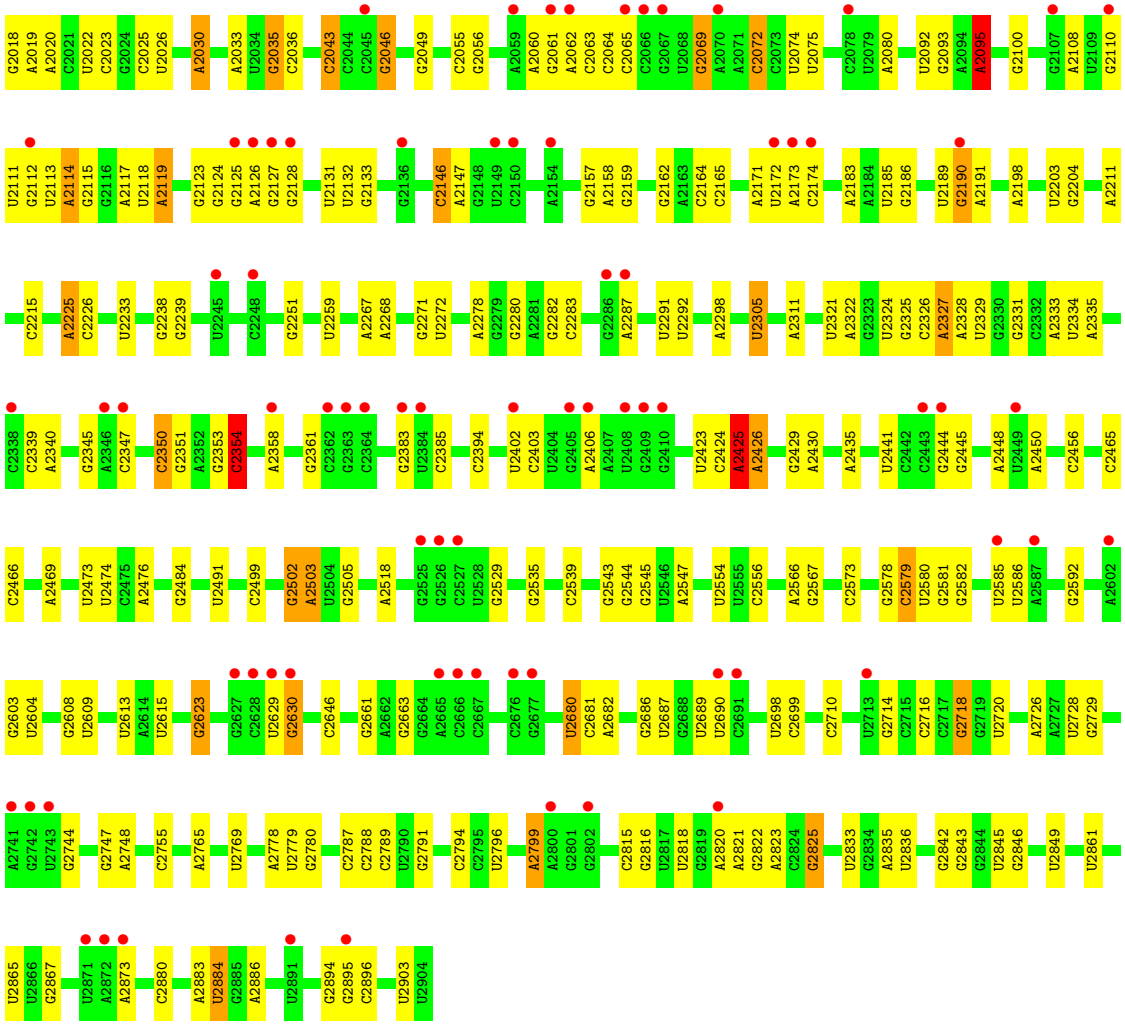
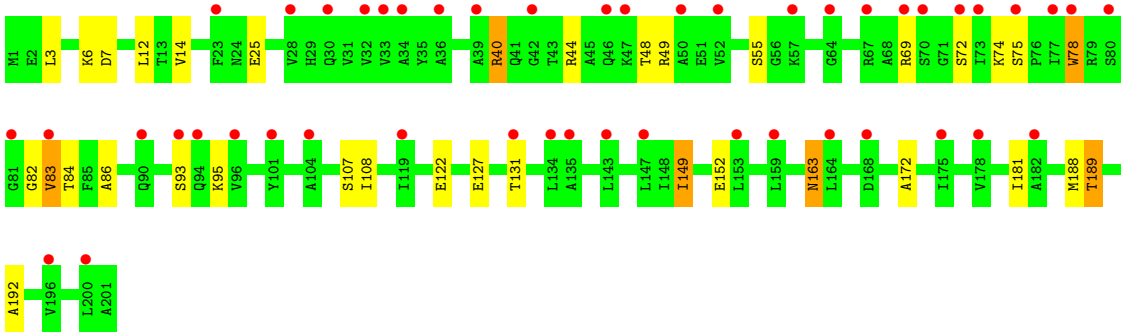
U1460 U1466 U1467 U1468 A1469 A1470 G1478 G1482 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1504 A1509 G1510 G1511 G1514 A1515 C1518 U1523 G1524 A1525 C1526 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1547 A1548 C1565 A1566 G1567 G1568 A1569 A1572 G1573 U1578
A1583 U1584 C1585 A1586 G1587 G1588 A1603 C1606 C1607 A1608 A1609 A1610 C1611 A1616 C1617 A1618 G1622 G1627 A1632 U1636 A1637 C1638 U1647 U1648 G1649 G1653 C1658 U1662 A1669 G1674 C1675 G1703 C1704 C1708 G1715 U1729 C1730 G1731 C1732 G1738
A1744 G1750 A1754 C1764 A1773 C1774 U1775 G1776 U1777 U1778 U1779 U1782 A1783 A1784 C1788 A1789 C1790 A1794 C1795 C1800 A1801 A1808 A1809 A1810 G1811 U1812 C1816 G1823 G1824 U1825 G1828 A1829 U1834 G1835 C1838 A1847 A1848 G1869 C1870 A1871 A1872 G1873 U1880
C1881 U1882 A1900 G1903 G1906 G1907 A1913 C1914 3TD1915 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1943 U1955 U1956 C1957 C1958 U1963 C1967 A1970 U1971 G1972 G1975 G1984 C1985 C1986 U1991 G1992 U1993 C1994 C1997 A1998 C1999 C2000 C2006 A2014 U2017



• Molecule 32: 50S ribosomal protein L4

Chain CE:

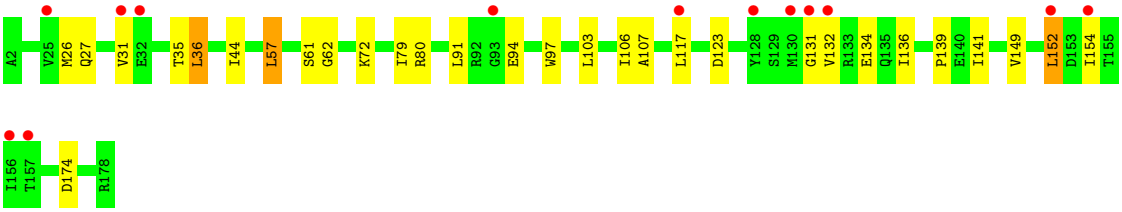


• Molecule 32: 50S ribosomal protein L4

Chain DE:

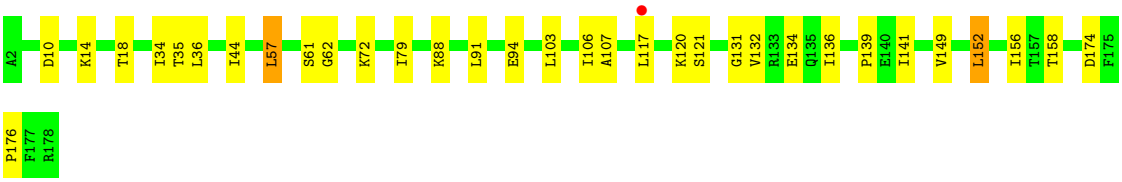
• Molecule 33: 50S ribosomal protein L5

Chain CF:



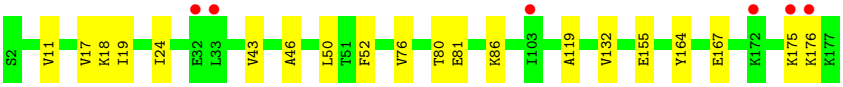
• Molecule 33: 50S ribosomal protein L5

Chain DF:



• Molecule 34: 50S ribosomal protein L6

Chain CG:



• Molecule 34: 50S ribosomal protein L6

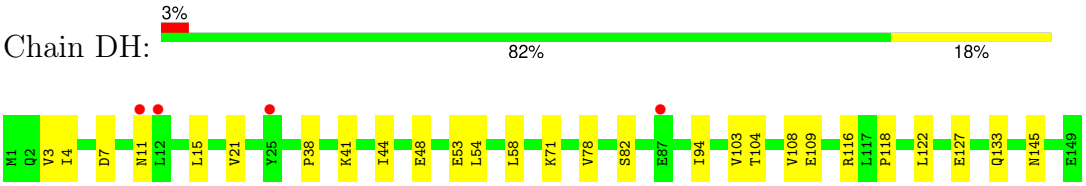
Chain DG:

• Molecule 35: 50S ribosomal protein L9

Chain CH:

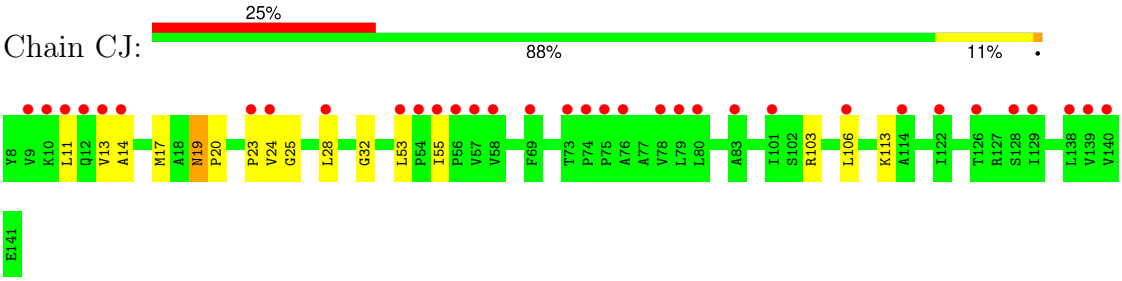
• Molecule 35: 50S ribosomal protein L9

Chain DH:



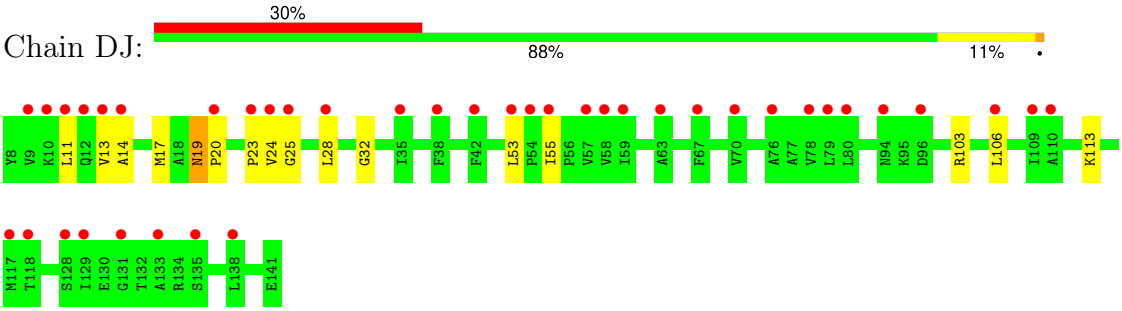
• Molecule 36: 50S ribosomal protein L11

Chain CJ:



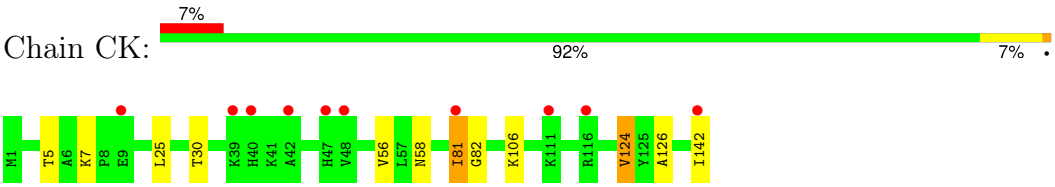
• Molecule 36: 50S ribosomal protein L11

Chain DJ:



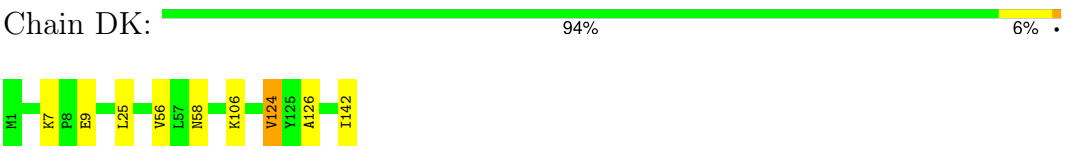
• Molecule 37: 50S ribosomal protein L13

Chain CK:



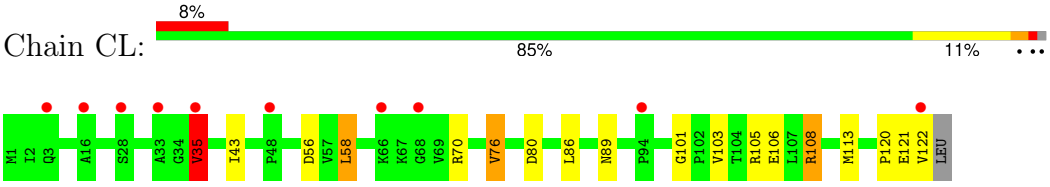
• Molecule 37: 50S ribosomal protein L13

Chain DK:



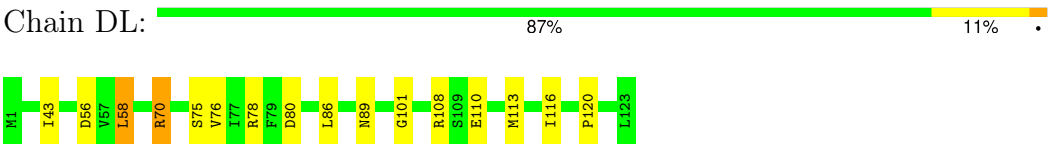
• Molecule 38: 50S ribosomal protein L14

Chain CL:



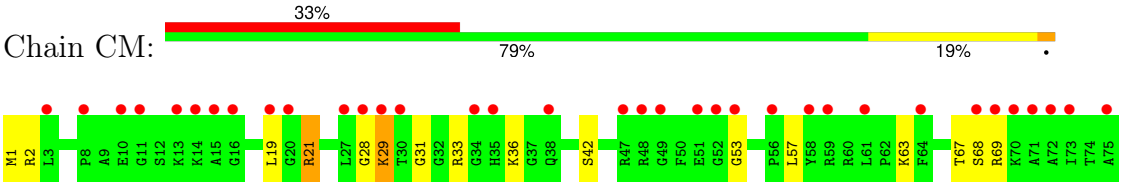
• Molecule 38: 50S ribosomal protein L14

Chain DL:



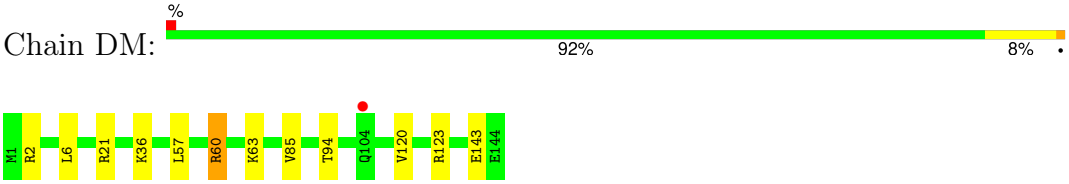
• Molecule 39: 50S ribosomal protein L15

Chain CM:



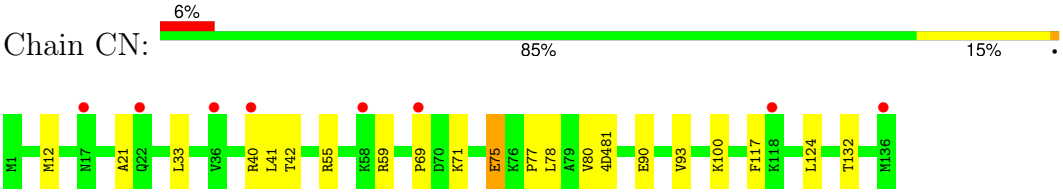
• Molecule 39: 50S ribosomal protein L15

Chain DM:



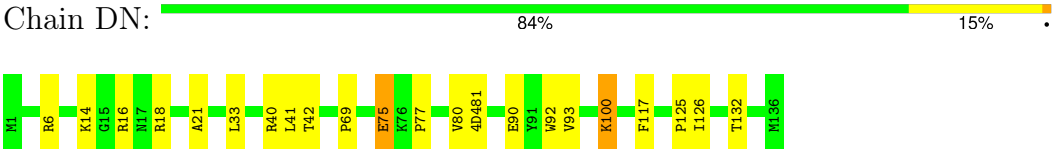
• Molecule 40: 50S ribosomal protein L16

Chain CN:



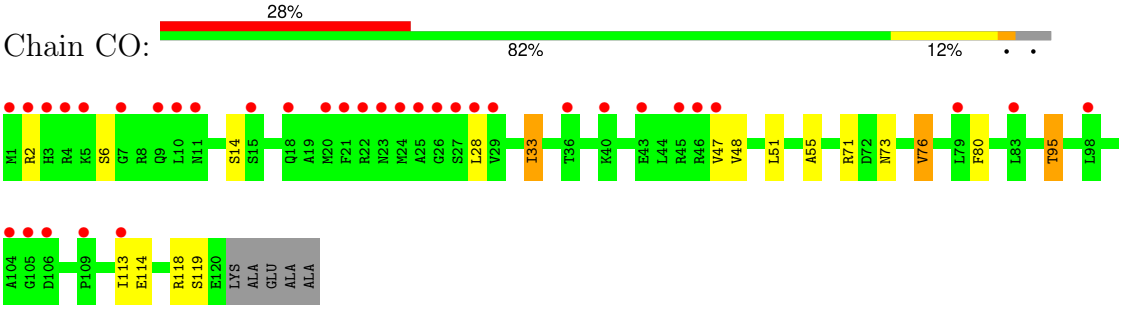
• Molecule 40: 50S ribosomal protein L16

Chain DN:



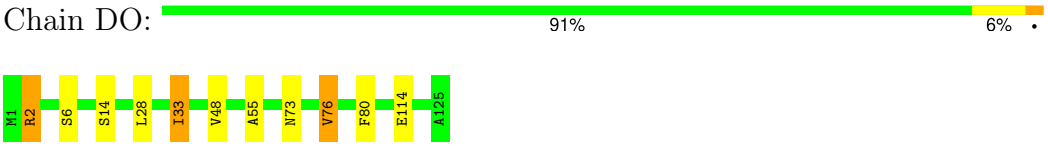
• Molecule 41: 50S ribosomal protein L17

Chain CO:



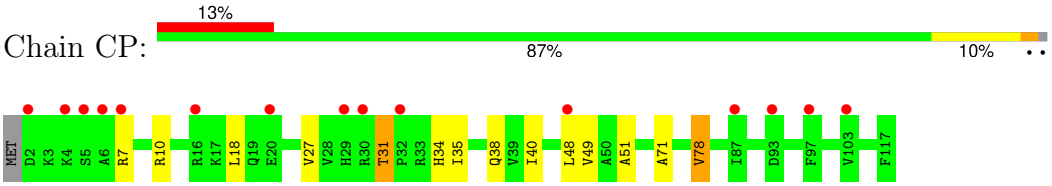
• Molecule 41: 50S ribosomal protein L17

Chain DO:



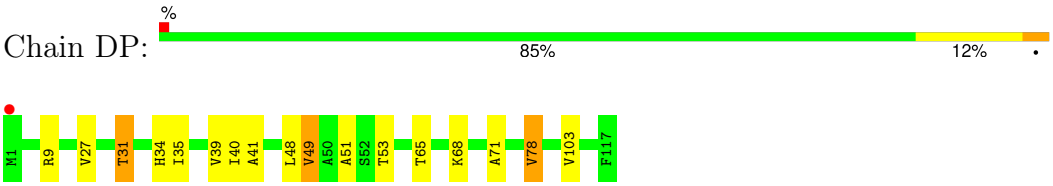
• Molecule 42: 50S ribosomal protein L18

Chain CP:



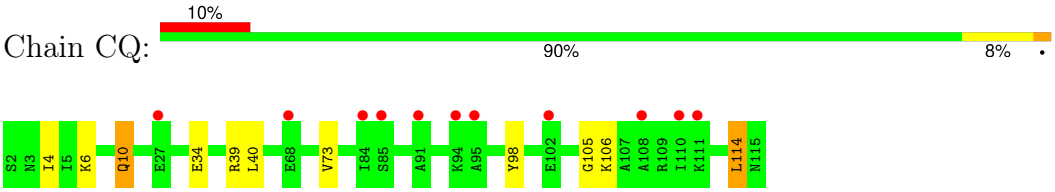
• Molecule 42: 50S ribosomal protein L18

Chain DP:



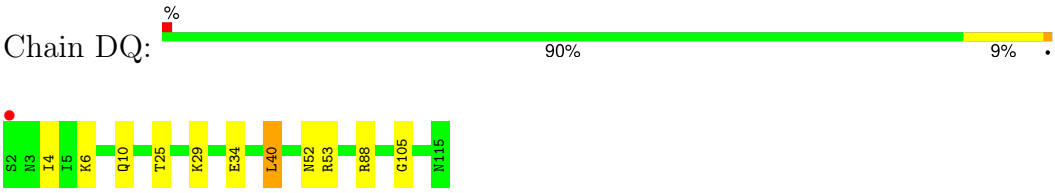
• Molecule 43: 50S ribosomal protein L19

Chain CQ:



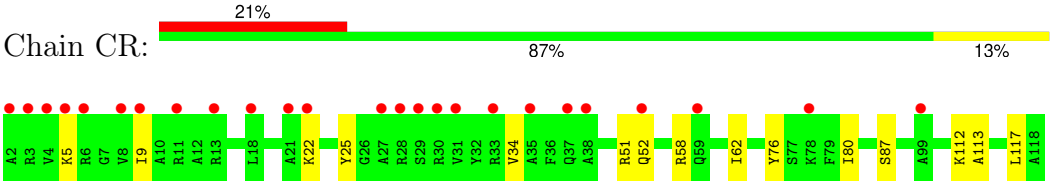
• Molecule 43: 50S ribosomal protein L19

Chain DQ:



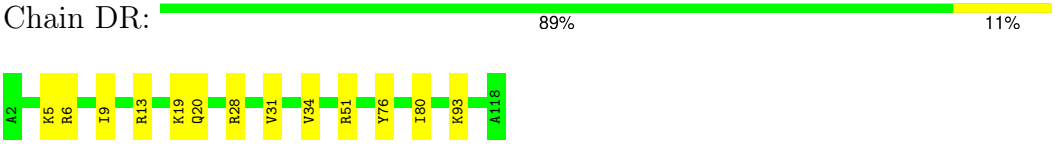
• Molecule 44: 50S ribosomal protein L20

Chain CR:



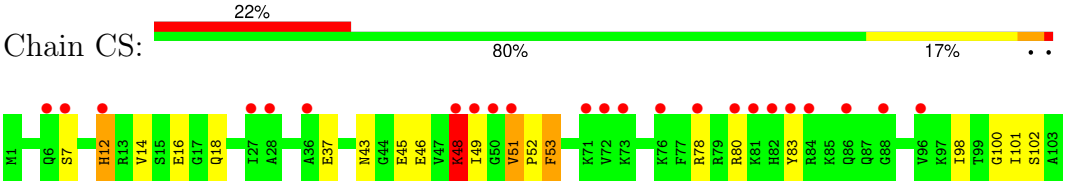
• Molecule 44: 50S ribosomal protein L20

Chain DR:



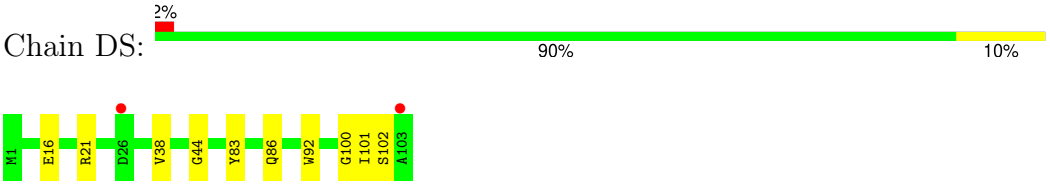
• Molecule 45: 50S ribosomal protein L21

Chain CS:



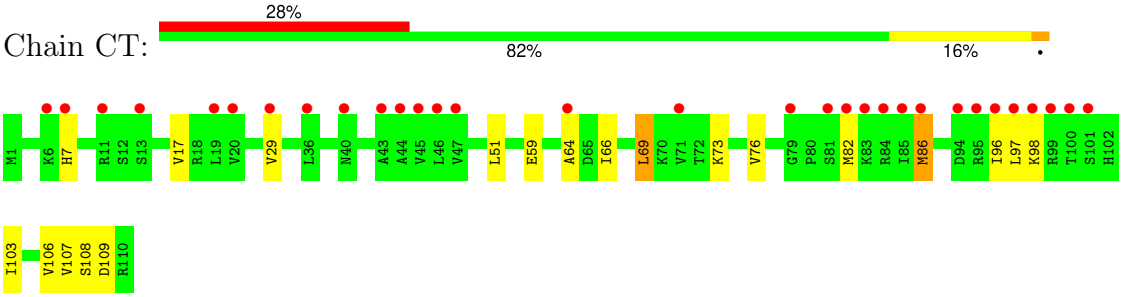
• Molecule 45: 50S ribosomal protein L21

Chain DS:



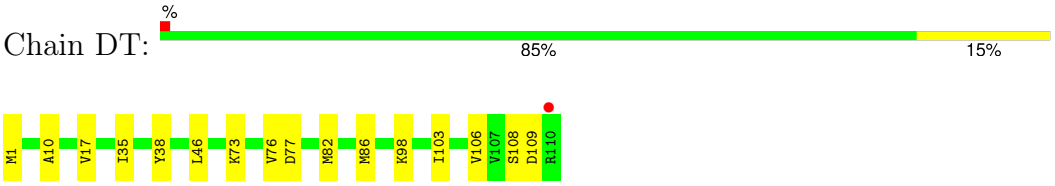
• Molecule 46: 50S ribosomal protein L22

Chain CT:



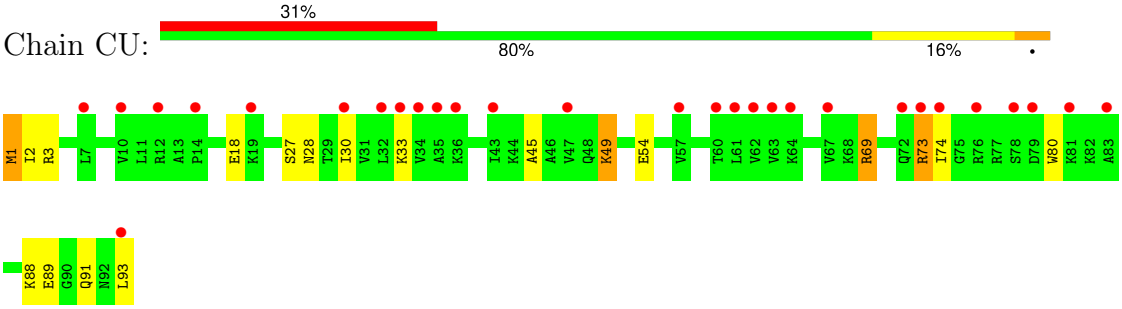
• Molecule 46: 50S ribosomal protein L22

Chain DT:



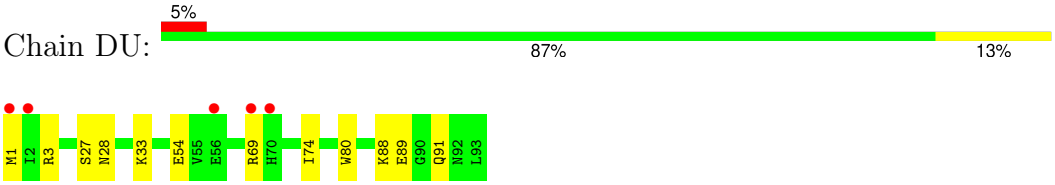
• Molecule 47: 50S ribosomal protein L23

Chain CU:



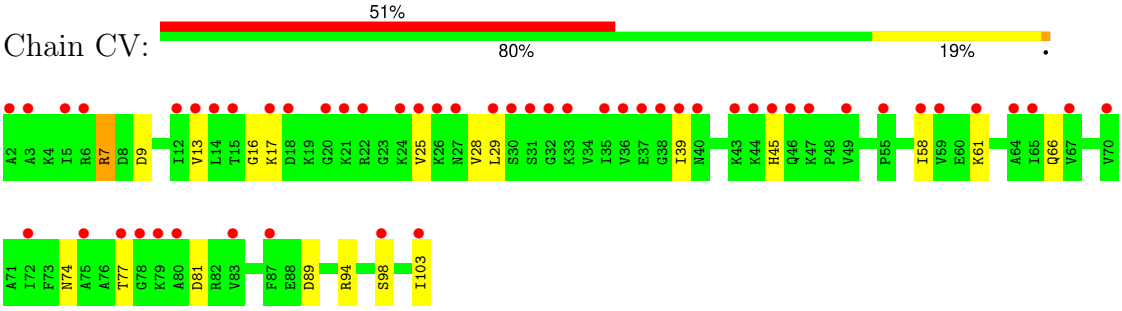
• Molecule 47: 50S ribosomal protein L23

Chain DU:



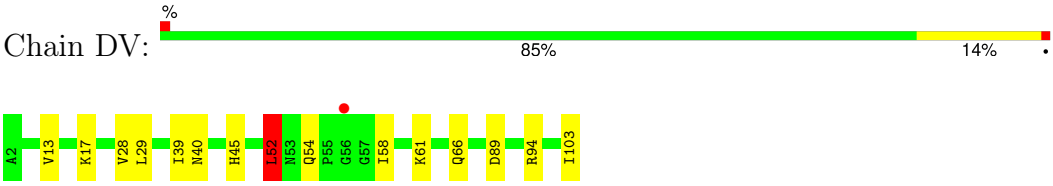
• Molecule 48: 50S ribosomal protein L24

Chain CV:



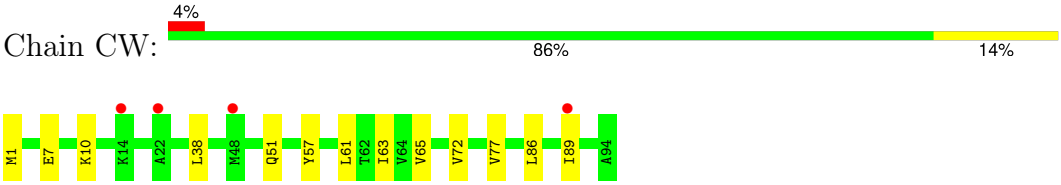
• Molecule 48: 50S ribosomal protein L24

Chain DV:



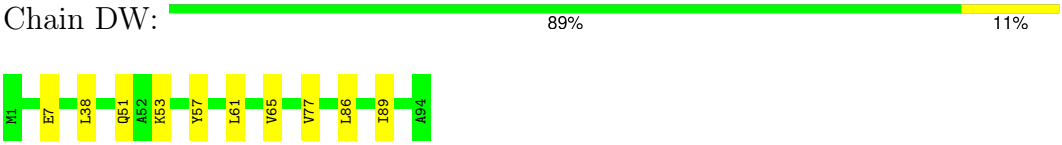
• Molecule 49: 50S ribosomal protein L25

Chain CW:



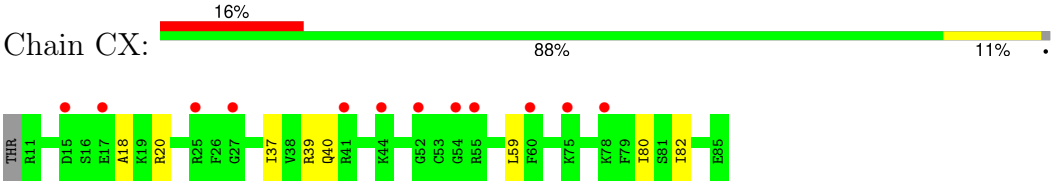
• Molecule 49: 50S ribosomal protein L25

Chain DW:



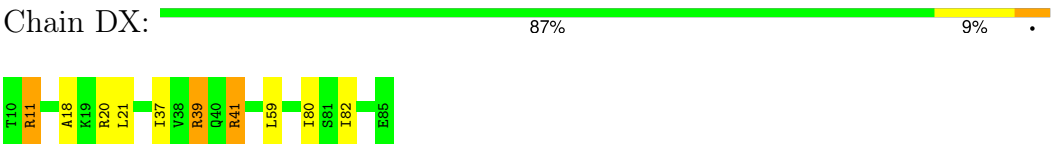
• Molecule 50: 50S ribosomal protein L27

Chain CX:



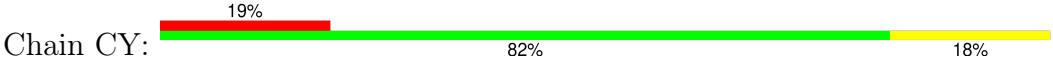
• Molecule 50: 50S ribosomal protein L27

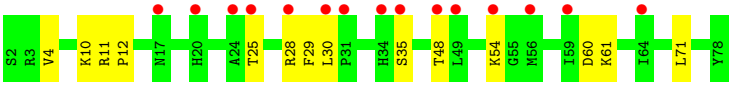
Chain DX:



• Molecule 51: 50S ribosomal protein L28

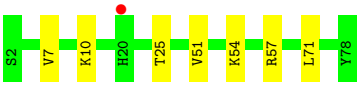
Chain CY:





• Molecule 51: 50S ribosomal protein L28

Chain DY:

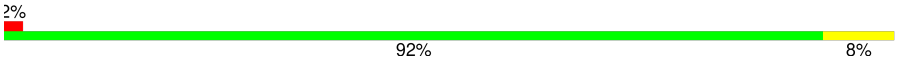


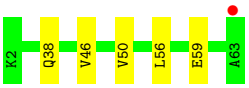
• Molecule 52: 50S ribosomal protein L29

Chain CZ:

• Molecule 52: 50S ribosomal protein L29

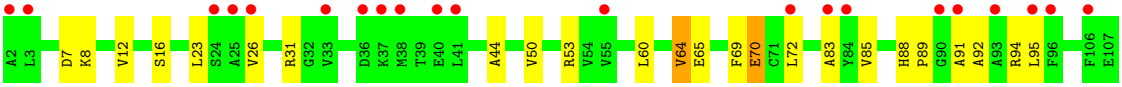
Chain DZ:

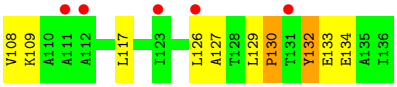




• Molecule 53: 50S ribosomal protein L10

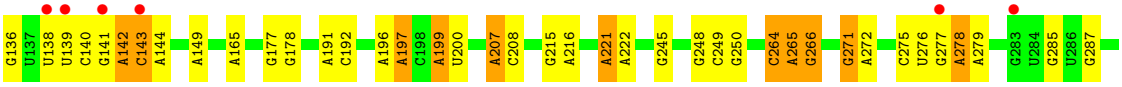
Chain DI:

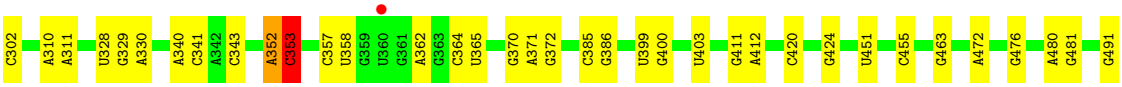


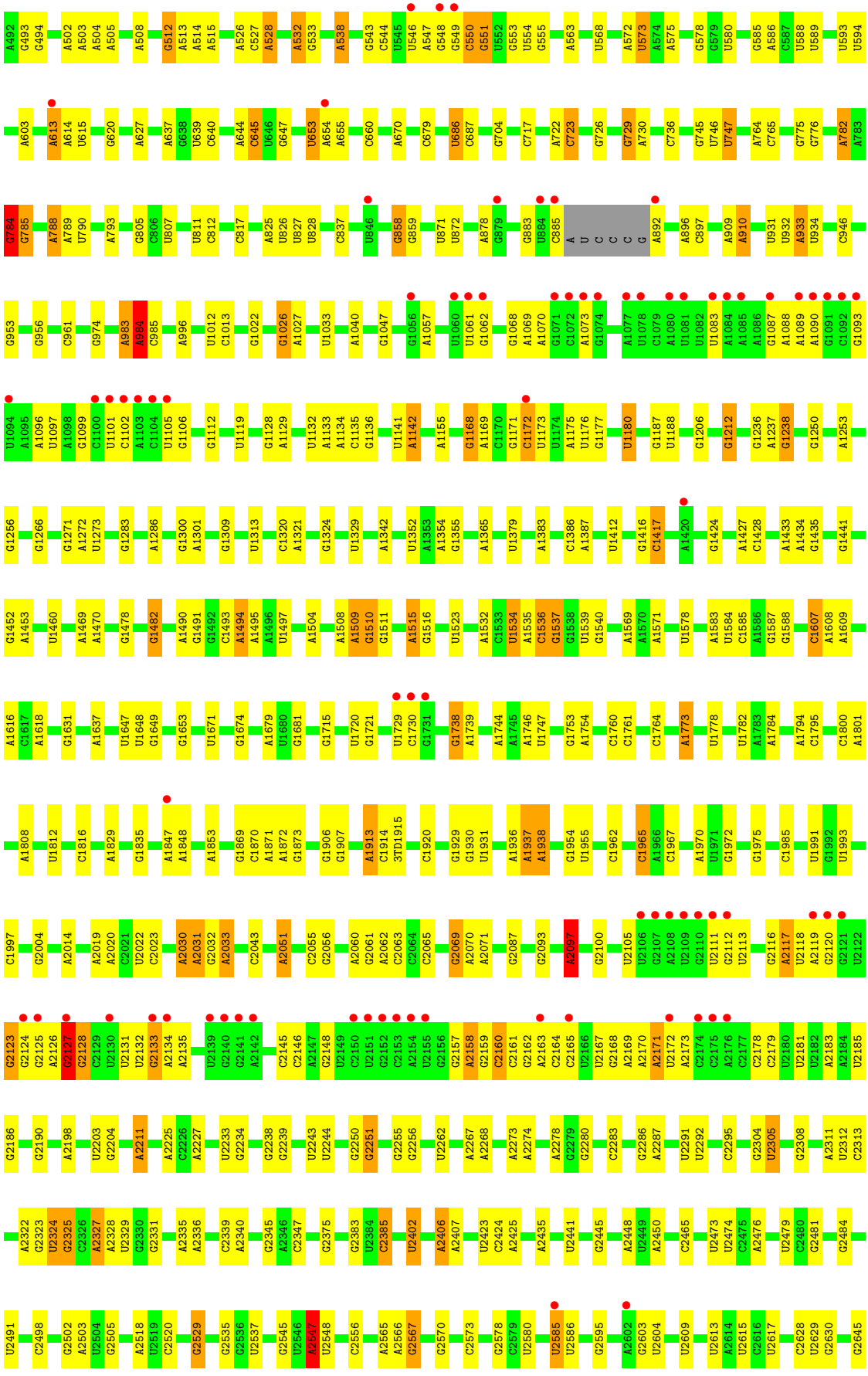


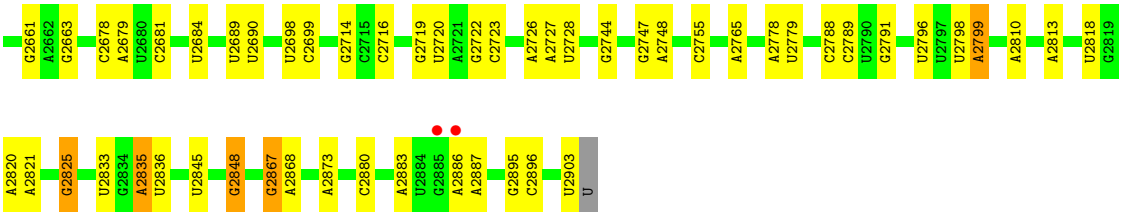
• Molecule 54: 23S rRNA

Chain DA:






A492 G493 G494 A502 A503 A504 A505 A508 G512 A513 A514 A515 A526 C527 A528 A532 G533 A538 G543 C544 U545 U546 A547 G548 G549 C550 G551 U552 G553 U554 G555 A563 U568 A572 U573 A574 A575 G578 G579 U580 G585 A586 C587 U588 U589 U593 U594
A603 A613 A614 U615 G620 A627 A637 G638 U639 C640 A644 C645 U646 G647 U653 A654 A655 C660 A670 C679 U686 C687 G704 C717 A722 C723 G726 G729 A730 C736 G745 U746 U747 A764 C765 G775 G776 A782 A783
G784 G785 A788 A789 U790 A793 G805 C806 U807 U811 C812 C817 A825 U826 U827 U828 C837 U846 G858 G859 U871 U872 A878 G879 G883 U884 C885 A U C C C G A892 A896 C897 A909 A910 U931 U932 A933 U934 C946
G953 G956 C961 G974 A983 A984 C985 A996 U1012 C1013 G1022 G1026 A1027 U1033 A1040 G1047 G1056 A1057 U1060 U1061 G1062 G1068 A1069 A1070 G1071 C1072 A1073 G1074 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093
U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1112 U1119 G1128 A1129 U1132 A1133 A1134 C1135 G1136 U1141 A1142 A1155 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 U1180 G1187 U1188 G1206 G1212 G1236 A1237 G1238 G1250 A1253
G1256 G1266 G1271 A1272 U1273 G1283 A1286 G1300 A1301 G1309 U1313 C1320 A1321 G1324 U1329 A1342 U1352 A1353 A1354 G1355 A1365 U1379 A1383 C1386 A1387 U1412 G1416 C1417 A1420 G1424 A1427 C1428 A1433 A1434 G1435 G1441
G1452 A1453 U1460 A1469 A1470 G1478 G1482 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1504 A1508 A1509 G1510 G1511 A1515 G1516 U1523 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 A1569 A1570 A1571 U1578 A1583 U1584 C1585 A1586 G1587 G1588 C1607 A1608 A1609
A1616 C1617 A1618 G1631 A1637 U1647 U1648 G1649 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 G1835 A1847 A1848 A1853 A1869 C1870 A1871 A1872 G1873 G1906 G1907 A1913 C1914 3TD1915 C1920 G1929 G1930 U1931 A1936 A1937 A1938 G1954 U1955 C1962 C1965 A1966 C1967 A1970 U1971 G1972 G1975 C1985 U1991 G1992 U1993
C1997 G2004 A2014 A2019 A2020 C2021 U2022 C2023 A2030 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 G2116 A2117 U2118 A2119 G2120 G2121 U2122
G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 U2139 G2140 G2141 A2142 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 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 G2445 A2448 U2449 A2450 C2465 U2473 U2474 C2475 A2476 U2479 C2480 G2481 G2484
U2491 C2498 G2502 A2503 U2504 G2505 A2518 U2519 C2520 G2529 G2535 G2536 U2537 G2545 U2546 A2547 U2548 C2556 A2565 A2566 G2567 G2570 C2573 G2578 C2579 U2580 U2585 U2586 G2595 A2602 G2603 U2604 U2609 U2613 A2614 U2615 C2616 U2617 C2628 U2629 C2630 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
U2884
G2885
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) 99.1 (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 2.11.6	Depositor
R, R_{free}	0.172 , 0.193 0.184 , 0.207	Depositor DCC
R_{free} test set	4504 reflections (0.40%)	wwPDB-VP
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 , 90.1	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 (i)

5.1 Standard geometry (i)

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

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	31318	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	194494	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%)	7 32
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	7 32
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	25 61
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	8 36
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	25 61
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	25 61
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	19 54
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	2 13
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100 100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	2 13
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	19 54
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	19 54
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16 51
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	8 34
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%)	5 28
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1 6
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14 49
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	14 49
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100 100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16 51
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	4 22
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2 12
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	6 29
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	13 46
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100 100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	11 41
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10 39
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4 24
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	10 39
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1 10

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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%)	10 39
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	11 41
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	5 25
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%)	1 8
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2 13
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5 26
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	8 34
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	8 34
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4 21
26	D5	36/38 (95%)	36 (100%)	0	0	100 100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3 16
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100 100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	8 36
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	19 54
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%)	8 36
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	25 61
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	22 57
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	12 44
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	5 26
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	22 57
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9 37
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3 20
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3 20
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	9 37
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	19 54
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7 33
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	7 33
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5 28
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19 54
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%)	7 33
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%)	14 49
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14 49
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%)	3 20
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	13 46
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%)	12 44
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	12 44
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	2 14
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	6 29
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%)	7 33
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	2 12
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	10 39

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%)	11 38
2	BB	186/186 (100%)	172 (92%)	14 (8%)	11 38
3	AC	170/170 (100%)	156 (92%)	14 (8%)	9 34
3	BC	170/170 (100%)	156 (92%)	14 (8%)	9 34
4	AD	172/172 (100%)	165 (96%)	7 (4%)	26 60
4	BD	172/172 (100%)	163 (95%)	9 (5%)	19 52
5	AE	118/118 (100%)	103 (87%)	15 (13%)	3 17
5	BE	113/118 (96%)	91 (80%)	22 (20%)	1 6
6	AF	92/92 (100%)	84 (91%)	8 (9%)	8 32
6	BF	87/92 (95%)	73 (84%)	14 (16%)	2 10
7	AG	124/124 (100%)	109 (88%)	15 (12%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	BG	124/124 (100%)	106 (86%)	18 (14%)	2 13
8	AH	104/104 (100%)	90 (86%)	14 (14%)	3 14
8	BH	104/104 (100%)	88 (85%)	16 (15%)	2 11
9	AI	105/105 (100%)	99 (94%)	6 (6%)	17 49
9	BI	105/105 (100%)	99 (94%)	6 (6%)	17 49
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	10 35
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	4 20
11	AK	90/90 (100%)	90 (100%)	0	100 100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	13 43
12	AL	102/102 (100%)	93 (91%)	9 (9%)	8 31
12	BL	102/102 (100%)	90 (88%)	12 (12%)	4 19
13	AM	92/92 (100%)	84 (91%)	8 (9%)	8 32
13	BM	92/92 (100%)	84 (91%)	8 (9%)	8 32
14	AN	83/83 (100%)	81 (98%)	2 (2%)	44 74
14	BN	83/83 (100%)	80 (96%)	3 (4%)	30 64
15	AO	76/76 (100%)	69 (91%)	7 (9%)	7 29
15	BO	76/76 (100%)	68 (90%)	8 (10%)	5 23
16	AP	65/65 (100%)	62 (95%)	3 (5%)	23 56
16	BP	65/65 (100%)	61 (94%)	4 (6%)	15 45
17	AQ	74/74 (100%)	66 (89%)	8 (11%)	5 22
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	2 12
18	AR	48/48 (100%)	47 (98%)	1 (2%)	48 77
18	BR	48/48 (100%)	48 (100%)	0	100 100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	4 20
19	BS	70/70 (100%)	65 (93%)	5 (7%)	12 40
20	AT	65/65 (100%)	58 (89%)	7 (11%)	5 22
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1 7
21	AU	48/48 (100%)	46 (96%)	2 (4%)	25 59
21	BU	48/48 (100%)	46 (96%)	2 (4%)	25 59
22	C1	47/47 (100%)	46 (98%)	1 (2%)	48 77
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%)	24 58
23	D2	45/46 (98%)	42 (93%)	3 (7%)	13 43
24	C3	38/38 (100%)	36 (95%)	2 (5%)	19 51
24	D3	38/38 (100%)	36 (95%)	2 (5%)	19 51
25	C4	51/51 (100%)	45 (88%)	6 (12%)	4 19
25	D4	51/51 (100%)	48 (94%)	3 (6%)	16 47
26	C5	34/34 (100%)	31 (91%)	3 (9%)	8 31
26	D5	34/34 (100%)	33 (97%)	1 (3%)	37 70
27	C0	48/48 (100%)	41 (85%)	7 (15%)	2 12
27	D0	49/48 (102%)	43 (88%)	6 (12%)	4 18
29	CC	216/216 (100%)	203 (94%)	13 (6%)	16 47
29	DC	216/216 (100%)	208 (96%)	8 (4%)	29 63
30	CD	163/163 (100%)	159 (98%)	4 (2%)	42 73
30	DD	163/163 (100%)	160 (98%)	3 (2%)	54 80
32	CE	165/165 (100%)	149 (90%)	16 (10%)	6 27
32	DE	165/165 (100%)	159 (96%)	6 (4%)	30 64
33	CF	148/148 (100%)	134 (90%)	14 (10%)	7 28
33	DF	148/148 (100%)	134 (90%)	14 (10%)	7 28
34	CG	137/137 (100%)	134 (98%)	3 (2%)	47 76
34	DG	137/137 (100%)	133 (97%)	4 (3%)	37 70
35	CH	114/114 (100%)	102 (90%)	12 (10%)	5 23
35	DH	114/114 (100%)	105 (92%)	9 (8%)	10 35
36	CJ	104/104 (100%)	99 (95%)	5 (5%)	21 55
36	DJ	104/104 (100%)	99 (95%)	5 (5%)	21 55
37	CK	116/116 (100%)	112 (97%)	4 (3%)	32 66
37	DK	116/116 (100%)	113 (97%)	3 (3%)	41 72
38	CL	103/104 (99%)	95 (92%)	8 (8%)	10 36
38	DL	104/104 (100%)	99 (95%)	5 (5%)	21 55
39	CM	103/103 (100%)	95 (92%)	8 (8%)	10 36
39	DM	103/103 (100%)	100 (97%)	3 (3%)	37 70
40	CN	108/108 (100%)	103 (95%)	5 (5%)	23 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	DN	109/108 (101%)	104 (95%)	5 (5%)	23 56
41	CO	100/102 (98%)	93 (93%)	7 (7%)	12 41
41	DO	102/102 (100%)	97 (95%)	5 (5%)	21 54
42	CP	86/87 (99%)	80 (93%)	6 (7%)	12 41
42	DP	87/87 (100%)	84 (97%)	3 (3%)	32 66
43	CQ	99/99 (100%)	95 (96%)	4 (4%)	27 61
43	DQ	99/99 (100%)	98 (99%)	1 (1%)	73 88
44	CR	89/89 (100%)	85 (96%)	4 (4%)	23 57
44	DR	89/89 (100%)	85 (96%)	4 (4%)	23 57
45	CS	84/84 (100%)	77 (92%)	7 (8%)	9 34
45	DS	84/84 (100%)	82 (98%)	2 (2%)	44 74
46	CT	93/93 (100%)	87 (94%)	6 (6%)	14 43
46	DT	93/93 (100%)	89 (96%)	4 (4%)	25 58
47	CU	80/80 (100%)	71 (89%)	9 (11%)	4 21
47	DU	80/80 (100%)	77 (96%)	3 (4%)	28 62
48	CV	83/83 (100%)	77 (93%)	6 (7%)	12 39
48	DV	83/83 (100%)	79 (95%)	4 (5%)	21 55
49	CW	78/78 (100%)	74 (95%)	4 (5%)	20 53
49	DW	78/78 (100%)	75 (96%)	3 (4%)	28 62
50	CX	56/58 (97%)	53 (95%)	3 (5%)	18 50
50	DX	58/58 (100%)	53 (91%)	5 (9%)	8 32
51	CY	67/67 (100%)	63 (94%)	4 (6%)	16 47
51	DY	67/67 (100%)	65 (97%)	2 (3%)	36 69
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	11 38
52	DZ	54/54 (100%)	53 (98%)	1 (2%)	52 79
53	DI	103/103 (100%)	96 (93%)	7 (7%)	13 42
All	All	9460/9477 (100%)	8810 (93%)	650 (7%)	13 42

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

Mol	Chain	Res	Type
37	CK	5	THR
34	DG	18	LYS

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Mol	Chain	Res	Type
39	CM	21	ARG
36	CJ	113	LYS
46	CT	108	SER

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

Mol	Chain	Res	Type
20	BT	48	GLN
48	CV	74	ASN
20	BT	52	ASN
34	CG	38	ASN
52	CZ	45	GLN

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	1535	A
31	CA	2778	A
54	DA	2311	A
31	CA	1609	A

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Mol	Chain	Res	Type
31	CA	2146	C

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	$\#\|Z\| > 2$
31	PSU	CA	1917	31	18,21,22	0.32	0	21,30,33	0.50	0
1	2MG	AA	1207	1	18,26,27	0.91	0	16,38,41	0.60	0
1	2MG	BA	1207	1	18,26,27	0.83	1 (5%)	16,38,41	0.57	0
40	4D4	DN	81[B]	-	9,11,12	1.62	2 (22%)	7,13,15	2.83	2 (28%)
54	3TD	DA	1915	54	19,22,23	0.46	0	23,32,35	0.85	1 (4%)
1	5MC	BA	1407	1	19,22,23	0.48	0	26,32,35	0.47	0
31	6MZ	CA	1618	31	17,25,26	1.08	0	15,36,39	0.92	1 (6%)
31	5MC	CA	1962	31	19,22,23	0.28	0	26,32,35	0.42	0
31	3TD	CA	1915	31	19,22,23	0.48	0	23,32,35	0.83	1 (4%)
54	6MZ	DA	1618	54	17,25,26	0.97	1 (5%)	15,36,39	0.86	0
31	PSU	CA	2604	31	18,21,22	1.81	2 (11%)	21,30,33	1.48	3 (14%)
54	G7M	DA	2069	54	20,26,27	0.93	1 (5%)	16,39,42	1.43	1 (6%)
1	G7M	AA	527	1	20,26,27	0.77	0	16,39,42	1.95	1 (6%)
31	OMG	CA	2251	31	19,26,27	0.83	1 (5%)	21,38,41	0.66	0
40	4D4	DN	81[A]	-	9,11,12	2.22	2 (22%)	7,13,15	2.66	2 (28%)
54	2MA	DA	2503	55,54	17,25,26	0.98	2 (11%)	16,37,40	2.30	1 (6%)
1	MA6	BA	1519	1	19,26,27	0.91	0	18,38,41	1.31	2 (11%)
54	PSU	DA	2457	54	18,21,22	0.52	0	21,30,33	0.48	0
1	2MG	BA	1516	1	18,26,27	0.85	0	16,38,41	0.64	0
31	OMU	CA	2552	31	19,22,23	0.30	0	25,31,34	0.29	0
54	1MG	DA	745	54	19,26,27	1.17	2 (10%)	18,39,42	0.85	1 (5%)
1	MA6	AA	1519	1	19,26,27	0.92	0	18,38,41	1.38	2 (11%)
54	5MC	DA	1962	54	19,22,23	0.63	1 (5%)	26,32,35	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	DA	1917	54	18,21,22	0.44	0	21,30,33	0.56	0
1	5MC	BA	967	1	19,22,23	0.26	0	26,32,35	0.37	0
31	PSU	CA	2580	31	18,21,22	0.47	0	21,30,33	0.63	0
12	D2T	BL	89	12	8,9,10	1.09	1 (12%)	6,11,13	1.23	0
40	4D4	CN	81	40	9,11,12	2.18	2 (22%)	7,13,15	2.57	2 (28%)
31	2MG	CA	1835	31	18,26,27	1.02	2 (11%)	16,38,41	0.53	0
1	2MG	AA	1516	1	18,26,27	0.89	1 (5%)	16,38,41	0.68	0
54	PSU	DA	2580	54	18,21,22	0.81	1 (5%)	21,30,33	0.76	1 (4%)
54	2MG	DA	1835	54	18,26,27	1.04	2 (11%)	16,38,41	0.59	0
31	PSU	CA	1911	31	18,21,22	0.26	0	21,30,33	0.39	0
31	5MU	CA	1939	31	19,22,23	0.52	0	27,32,35	0.36	0
1	G7M	BA	527	1	20,26,27	0.78	1 (5%)	16,39,42	1.90	1 (6%)
1	5MC	AA	1407	1	19,22,23	0.52	0	26,32,35	0.49	0
12	D2T	AL	89	12	8,9,10	1.43	2 (25%)	6,11,13	1.29	0
54	PSU	DA	955	54	18,21,22	0.54	0	21,30,33	0.66	0
1	4OC	BA	1402	1	20,23,24	0.38	0	25,32,35	0.44	0
31	PSU	CA	955	31	18,21,22	0.34	0	21,30,33	0.55	0
31	PSU	CA	2457	31	18,21,22	0.62	0	21,30,33	0.44	0
31	5MU	CA	747	31	19,22,23	0.31	0	27,32,35	0.31	0
54	2MG	DA	2445	54	18,26,27	1.04	1 (5%)	16,38,41	0.80	0
54	5MU	DA	1939	54	19,22,23	0.63	0	27,32,35	0.48	0
30	MEQ	DD	150[B]	30	8,9,10	1.35	1 (12%)	5,10,12	0.84	0
1	PSU	BA	516	1	18,21,22	0.42	0	21,30,33	0.46	0
54	PSU	DA	2504	54	18,21,22	0.47	0	21,30,33	0.41	0
54	PSU	DA	2605	54	18,21,22	0.62	0	21,30,33	0.67	0
31	PSU	CA	2504	31	18,21,22	0.38	0	21,30,33	0.43	0
1	PSU	AA	516	55,1	18,21,22	0.36	0	21,30,33	0.48	0
54	5MU	DA	747	54	19,22,23	0.39	0	27,32,35	0.39	0
31	PSU	CA	2605	31	18,21,22	0.40	0	21,30,33	0.61	0
31	2MA	CA	2503	31	17,25,26	0.90	0	16,37,40	2.31	1 (6%)
54	PSU	DA	1911	54	18,21,22	0.31	0	21,30,33	0.37	0
1	2MG	BA	966	1	18,26,27	0.85	1 (5%)	16,38,41	0.55	0
54	PSU	DA	2604	54	18,21,22	0.94	1 (5%)	21,30,33	0.67	0
31	PSU	CA	746	55,31	18,21,22	0.58	1 (5%)	21,30,33	0.39	0
30	MEQ	DD	150[A]	30	8,9,10	0.47	0	5,10,12	0.48	0
1	2MG	AA	966	1	18,26,27	0.76	0	16,38,41	0.66	0
31	G7M	CA	2069	31	20,26,27	0.92	1 (5%)	16,39,42	1.49	1 (6%)
54	OMG	DA	2251	54	19,26,27	1.07	2 (10%)	21,38,41	0.64	0
54	6MZ	DA	2030	54	17,25,26	1.26	3 (17%)	15,36,39	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	MEQ	CD	150	30	7,8,10	0.44	0	4,9,12	0.41	0
54	OMU	DA	2552	54	19,22,23	0.52	0	25,31,34	0.31	0
1	UR3	BA	1498	1	19,22,23	0.41	0	26,32,35	0.39	0
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.42	0
31	1MG	CA	745	31	19,26,27	1.17	2 (10%)	18,39,42	0.88	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.91	0	15,36,39	1.01	1 (6%)
1	UR3	AA	1498	1	19,22,23	0.69	0	26,32,35	0.46	0
31	OMC	CA	2498	55,31	19,22,23	0.41	0	25,31,34	0.50	0
54	PSU	DA	746	55,54	18,21,22	0.98	2 (11%)	21,30,33	0.34	0
1	MA6	BA	1518	1	19,26,27	0.83	0	18,38,41	1.23	2 (11%)
54	OMC	DA	2498	55,54	19,22,23	0.54	0	25,31,34	0.54	0
1	MA6	AA	1518	1	19,26,27	0.90	0	18,38,41	1.24	2 (11%)
1	5MC	AA	967	1	19,22,23	0.28	0	26,32,35	0.37	0
54	H2U	DA	2449	54	18,21,22	0.58	0	19,30,33	0.53	0
31	2MG	CA	2445	31	18,26,27	0.93	2 (11%)	16,38,41	0.69	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
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
40	4D4	DN	81[B]	-	-	6/11/12/14	-
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
31	PSU	CA	2604	31	-	0/7/25/26	0/2/2/2
54	G7M	DA	2069	54	-	0/3/25/26	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
40	4D4	DN	81[A]	-	-	2/11/12/14	-
54	2MA	DA	2503	55,54	-	0/3/25/26	0/3/3/3
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
54	5MC	DA	1962	54	-	2/7/25/26	0/2/2/2
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
40	4D4	CN	81	40	-	2/11/12/14	-
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	1/7/25/26	0/2/2/2
54	2MG	DA	2445	54	-	2/5/27/28	0/3/3/3
54	5MU	DA	1939	54	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[B]	30	-	3/8/9/11	-
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	55,1	-	0/7/25/26	0/2/2/2
54	5MU	DA	747	54	-	2/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
31	PSU	CA	746	55,31	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	MEQ	DD	150[A]	30	-	4/8/9/11	-
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
54	OMG	DA	2251	54	-	0/5/27/28	0/3/3/3
54	6MZ	DA	2030	54	-	1/5/27/28	0/3/3/3
30	MEQ	CD	150	30	-	3/6/7/11	-
54	OMU	DA	2552	54	-	0/9/27/28	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	55,31	-	0/9/27/28	0/2/2/2
54	PSU	DA	746	55,54	-	2/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	1/7/29/30	0/3/3/3
54	OMC	DA	2498	55,54	-	0/9/27/28	0/2/2/2
1	MA6	AA	1518	1	-	1/7/29/30	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2604	PSU	C2-N1	6.14	1.44	1.36
40	CN	81	4D4	CZ-NE	5.94	1.44	1.33
40	DN	81[A]	4D4	CZ-NE	5.93	1.44	1.33
40	DN	81[B]	4D4	CZ-NE	4.08	1.41	1.33
31	CA	745	1MG	C2-N1	3.78	1.44	1.37

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	CA	2503	2MA	C4-N3-C2	-8.99	116.40	123.30
54	DA	2503	2MA	C4-N3-C2	-8.97	116.42	123.30
1	AA	527	G7M	O4'-C1'-N9	7.26	118.38	108.75
1	BA	527	G7M	O4'-C1'-N9	7.23	118.33	108.75
40	DN	81[B]	4D4	NE-CZ-NH2	6.09	131.13	120.67

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C5-C6-N6-C9
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	1519	MA6	C5-C6-N6-C9
40	DN	81[B]	4D4	C-CA-CB-OB

There are no ring outliers.

18 monomers are involved in 22 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
57	MPD	DS	203	-	7,7,7	0.23	0	9,10,10	0.39	0
58	PUT	AA	1672	-	5,5,5	0.25	0	4,4,4	0.30	0
62	EDO	DA	3003	-	3,3,3	0.56	0	2,2,2	0.26	0
56	PG4	AA	1670	-	12,12,12	0.33	0	11,11,11	0.41	0
56	PG4	DA	3216	-	12,12,12	0.18	0	11,11,11	0.23	0
66	ACY	DA	3191	-	3,3,3	0.96	0	3,3,3	0.99	0
68	TRS	DA	3220	-	7,7,7	0.34	0	9,9,9	0.37	0
66	ACY	DA	3201	-	3,3,3	0.66	0	3,3,3	1.03	0
61	PEG	DA	3218	-	6,6,6	0.25	0	5,5,5	0.09	0
58	PUT	DA	3184	-	5,5,5	0.44	0	4,4,4	0.29	0
57	MPD	DA	3204	-	7,7,7	0.76	0	9,10,10	0.67	0
59	TAC	AA	1681	55	34,35,35	0.56	0	43,58,58	0.94	3 (6%)
58	PUT	AA	1675	-	5,5,5	0.18	0	4,4,4	0.10	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.16	0
61	PEG	AL	201	-	6,6,6	0.32	0	5,5,5	0.17	0
57	MPD	DT	202	-	7,7,7	0.73	0	9,10,10	0.38	0
58	PUT	DA	3213	-	5,5,5	0.20	0	4,4,4	0.25	0
57	MPD	DN	201	-	7,7,7	0.88	0	9,10,10	0.54	0
57	MPD	AA	1676	-	7,7,7	0.71	0	9,10,10	0.76	0
64	SPD	DA	3187	-	9,9,9	0.19	0	8,8,8	0.33	0
61	PEG	DA	3200	-	6,6,6	0.39	0	5,5,5	0.22	0
63	PGE	DU	101	-	9,9,9	0.21	0	8,8,8	0.13	0
61	PEG	DQ	201	-	6,6,6	0.18	0	5,5,5	0.17	0
59	TAC	BA	1644	55	34,35,35	0.58	0	43,58,58	0.92	2 (4%)
56	PG4	DQ	202	-	12,12,12	0.21	0	11,11,11	0.16	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.36	0
58	PUT	DA	3221	-	5,5,5	0.21	0	4,4,4	0.17	0
57	MPD	DE	301	-	7,7,7	0.73	0	9,10,10	0.56	0
56	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.17	0
62	EDO	DA	3197	-	3,3,3	0.70	0	2,2,2	0.13	0
58	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.12	0
58	PUT	AA	1674	-	5,5,5	0.16	0	4,4,4	0.12	0
63	PGE	DA	3225	-	9,9,9	0.17	0	8,8,8	0.15	0
59	TAC	AA	1680	55	34,35,35	0.53	0	43,58,58	1.12	2 (4%)
62	EDO	DA	3198	-	3,3,3	0.54	0	2,2,2	0.41	0
63	PGE	DA	3203	-	9,9,9	0.31	0	8,8,8	0.27	0
63	PGE	DA	3217	-	9,9,9	0.19	0	8,8,8	0.25	0
57	MPD	DA	3190	-	7,7,7	0.33	0	9,10,10	0.44	0
57	MPD	DK	201	-	7,7,7	0.48	0	9,10,10	0.25	0
58	PUT	DA	3189	-	5,5,5	0.25	0	4,4,4	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	EDO	DA	3209	-	3,3,3	0.59	0	2,2,2	0.31	0
57	MPD	AA	1671	-	7,7,7	0.60	0	9,10,10	0.56	0
58	PUT	DA	3222	-	5,5,5	0.53	0	4,4,4	0.74	0
63	PGE	DA	3001	-	9,9,9	0.32	0	8,8,8	0.32	0
61	PEG	DA	3199	-	6,6,6	0.23	0	5,5,5	0.16	0
58	PUT	DM	201	-	5,5,5	0.14	0	4,4,4	0.06	0
64	SPD	DA	3183	-	9,9,9	0.10	0	8,8,8	0.14	0
57	MPD	DA	3207	-	7,7,7	0.75	0	9,10,10	0.51	0
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.14	0
64	SPD	DA	3206	-	9,9,9	0.25	0	8,8,8	0.26	0
62	EDO	DB	212	-	3,3,3	0.71	0	2,2,2	0.13	0
57	MPD	DT	201	-	7,7,7	0.48	0	9,10,10	0.25	0
61	PEG	D3	101	-	6,6,6	0.29	0	5,5,5	0.29	0
62	EDO	D1	101	-	3,3,3	0.67	0	2,2,2	0.08	0
62	EDO	DB	211	-	3,3,3	0.60	0	2,2,2	0.22	0
63	PGE	DA	3214	-	9,9,9	0.30	0	8,8,8	0.41	0
57	MPD	DE	302	-	7,7,7	0.85	0	9,10,10	0.59	0
59	TAC	BA	1643	55	34,35,35	0.47	0	43,58,58	0.99	3 (6%)
62	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.29	0
58	PUT	DA	3212	-	5,5,5	0.25	0	4,4,4	0.07	0
62	EDO	DA	3215	-	3,3,3	0.71	0	2,2,2	0.17	0
56	PG4	DR	202	-	12,12,12	0.29	0	11,11,11	0.38	0
58	PUT	DA	3188	-	5,5,5	0.24	0	4,4,4	0.12	0
56	PG4	DA	3193	-	12,12,12	0.41	0	11,11,11	0.34	0
61	PEG	D1	103	-	6,6,6	0.38	0	5,5,5	0.19	0
62	EDO	DA	3002	-	3,3,3	0.56	0	2,2,2	0.39	0
64	SPD	DA	3224	-	9,9,9	0.24	0	8,8,8	0.48	0
66	ACY	DA	3196	-	3,3,3	2.46	1 (33%)	3,3,3	2.20	2 (66%)
58	PUT	DA	3223	-	5,5,5	0.24	0	4,4,4	0.16	0
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.34	0
65	1PE	DA	3202	-	15,15,15	0.36	0	14,14,14	0.36	0
57	MPD	DA	3192	-	7,7,7	0.38	0	9,10,10	0.70	0
58	PUT	AA	1673	-	5,5,5	0.13	0	4,4,4	0.09	0
63	PGE	DA	3186	-	9,9,9	0.38	0	8,8,8	0.44	0
62	EDO	DB	201	-	3,3,3	0.62	0	2,2,2	0.20	0
63	PGE	D1	102	-	9,9,9	0.24	0	8,8,8	0.22	0
58	PUT	DA	3205	-	5,5,5	0.20	0	4,4,4	0.21	0
62	EDO	DA	3194	-	3,3,3	0.88	0	2,2,2	0.12	0
57	MPD	DA	3210	-	7,7,7	0.72	0	9,10,10	0.32	0
58	PUT	DA	3195	-	5,5,5	0.39	0	4,4,4	0.65	0
63	PGE	DS	201	-	9,9,9	0.40	0	8,8,8	0.31	0
61	PEG	DA	3226	-	6,6,6	0.45	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
61	PEG	DA	3227	-	6,6,6	0.27	0	5,5,5	0.17	0
67	GUN	DA	3211	-	7,12,12	0.40	0	8,17,17	0.69	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
57	MPD	DS	203	-	-	0/5/5/5	-
58	PUT	AA	1672	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-
56	PG4	AA	1670	-	-	4/10/10/10	-
56	PG4	DA	3216	-	-	4/10/10/10	-
68	TRS	DA	3220	-	-	0/9/9/9	-
61	PEG	DA	3218	-	-	2/4/4/4	-
58	PUT	DA	3184	-	-	0/3/3/3	-
57	MPD	DA	3204	-	-	4/5/5/5	-
59	TAC	AA	1681	55	-	6/8/74/74	0/4/4/4
58	PUT	AA	1675	-	-	1/3/3/3	-
61	PEG	DP	201	-	-	3/4/4/4	-
61	PEG	AL	201	-	-	2/4/4/4	-
57	MPD	DT	202	-	-	3/5/5/5	-
58	PUT	DA	3213	-	-	0/3/3/3	-
57	MPD	DN	201	-	-	3/5/5/5	-
57	MPD	AA	1676	-	-	2/5/5/5	-
64	SPD	DA	3187	-	-	2/7/7/7	-
61	PEG	DA	3200	-	-	2/4/4/4	-
63	PGE	DU	101	-	-	3/7/7/7	-
61	PEG	DQ	201	-	-	1/4/4/4	-
59	TAC	BA	1644	55	-	6/8/74/74	0/4/4/4
56	PG4	DQ	202	-	-	3/10/10/10	-
65	1PE	DA	3185	-	-	5/13/13/13	-
58	PUT	DA	3221	-	-	0/3/3/3	-
57	MPD	DE	301	-	-	3/5/5/5	-
56	PG4	BA	1642	-	-	0/10/10/10	-
62	EDO	DA	3197	-	-	1/1/1/1	-
58	PUT	DA	3219	-	-	0/3/3/3	-
58	PUT	AA	1674	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DA	3225	-	-	5/7/7/7	-
59	TAC	AA	1680	55	-	1/8/74/74	0/4/4/4
62	EDO	DA	3198	-	-	0/1/1/1	-
63	PGE	DA	3203	-	-	4/7/7/7	-
63	PGE	DA	3217	-	-	2/7/7/7	-
57	MPD	DA	3190	-	-	1/5/5/5	-
57	MPD	DK	201	-	-	3/5/5/5	-
58	PUT	DA	3189	-	-	0/3/3/3	-
62	EDO	DA	3209	-	-	0/1/1/1	-
57	MPD	AA	1671	-	-	1/5/5/5	-
58	PUT	DA	3222	-	-	0/3/3/3	-
63	PGE	DA	3001	-	-	4/7/7/7	-
61	PEG	DA	3199	-	-	1/4/4/4	-
58	PUT	DM	201	-	-	0/3/3/3	-
64	SPD	DA	3183	-	-	1/7/7/7	-
57	MPD	DA	3207	-	-	3/5/5/5	-
61	PEG	DL	201	-	-	1/4/4/4	-
64	SPD	DA	3206	-	-	2/7/7/7	-
62	EDO	DB	212	-	-	1/1/1/1	-
57	MPD	DT	201	-	-	3/5/5/5	-
61	PEG	D3	101	-	-	2/4/4/4	-
62	EDO	D1	101	-	-	0/1/1/1	-
62	EDO	DB	211	-	-	0/1/1/1	-
63	PGE	DA	3214	-	-	3/7/7/7	-
57	MPD	DE	302	-	-	2/5/5/5	-
59	TAC	BA	1643	55	-	8/8/74/74	0/4/4/4
62	EDO	DA	3208	-	-	1/1/1/1	-
58	PUT	DA	3212	-	-	1/3/3/3	-
62	EDO	DA	3215	-	-	0/1/1/1	-
56	PG4	DR	202	-	-	5/10/10/10	-
58	PUT	DA	3188	-	-	0/3/3/3	-
56	PG4	DA	3193	-	-	7/10/10/10	-
61	PEG	D1	103	-	-	1/4/4/4	-
62	EDO	DA	3002	-	-	1/1/1/1	-
64	SPD	DA	3224	-	-	3/7/7/7	-
58	PUT	DA	3223	-	-	1/3/3/3	-
56	PG4	DS	202	-	-	4/10/10/10	-
65	1PE	DA	3202	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DA	3192	-	-	2/5/5/5	-
58	PUT	AA	1673	-	-	0/3/3/3	-
63	PGE	DA	3186	-	-	2/7/7/7	-
62	EDO	DB	201	-	-	0/1/1/1	-
63	PGE	D1	102	-	-	5/7/7/7	-
58	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3194	-	-	0/1/1/1	-
57	MPD	DA	3210	-	-	0/5/5/5	-
58	PUT	DA	3195	-	-	0/3/3/3	-
63	PGE	DS	201	-	-	2/7/7/7	-
61	PEG	DA	3226	-	-	3/4/4/4	-
61	PEG	DA	3227	-	-	0/4/4/4	-
67	GUN	DA	3211	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.09	1.40	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	AA	1680	TAC	C5-C41-C4	-5.44	105.87	113.73
59	BA	1643	TAC	C5-C41-C4	-3.96	108.01	113.73
59	AA	1681	TAC	C5-C41-C4	-3.29	108.98	113.73
59	BA	1644	TAC	O3-C3-C2	-3.13	117.69	122.93
59	BA	1644	TAC	C5-C41-C4	-2.96	109.46	113.73

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1676	MPD	C2-C3-C4-C5
59	AA	1681	TAC	C1-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-N21
59	AA	1681	TAC	C41-C4-N4-C42

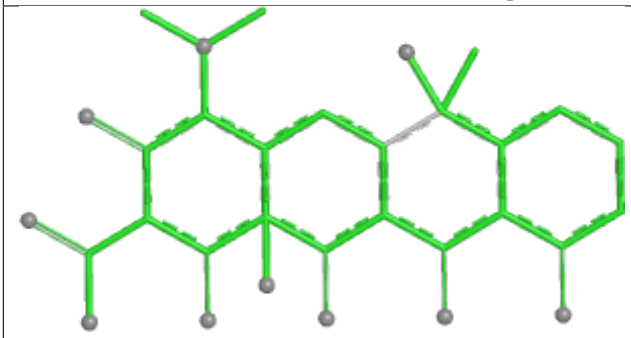
There are no ring outliers.

27 monomers are involved in 46 short contacts:

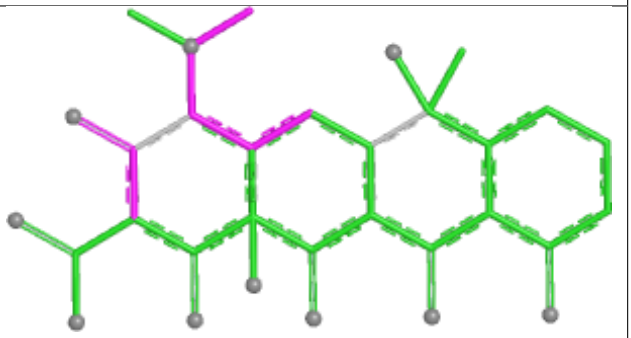
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	1670	PG4	1	0
56	DA	3216	PG4	1	0
68	DA	3220	TRS	1	0
57	DA	3204	MPD	1	0
59	AA	1681	TAC	2	0
61	DP	201	PEG	1	0
57	DN	201	MPD	1	0
57	AA	1676	MPD	3	0
63	DU	101	PGE	3	0
56	BA	1642	PG4	1	0
63	DA	3225	PGE	2	0
62	DA	3198	EDO	1	0
58	DA	3189	PUT	1	0
58	DA	3222	PUT	3	0
63	DA	3001	PGE	1	0
57	DA	3207	MPD	1	0
63	DA	3214	PGE	1	0
56	DR	202	PG4	5	0
56	DA	3193	PG4	2	0
61	D1	103	PEG	1	0
64	DA	3224	SPD	2	0
56	DS	202	PG4	3	0
65	DA	3202	1PE	1	0
57	DA	3192	MPD	1	0
63	D1	102	PGE	2	0
58	DA	3195	PUT	3	0
63	DS	201	PGE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

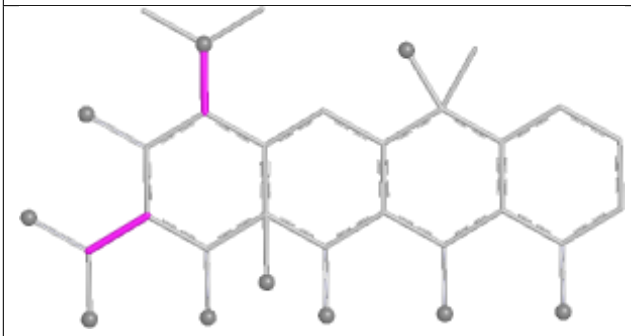
Ligand TAC AA 1681



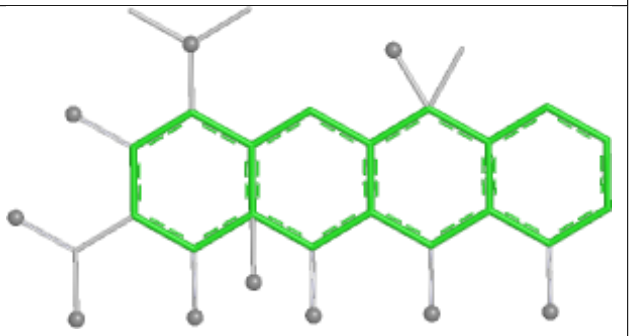
Bond lengths



Bond angles

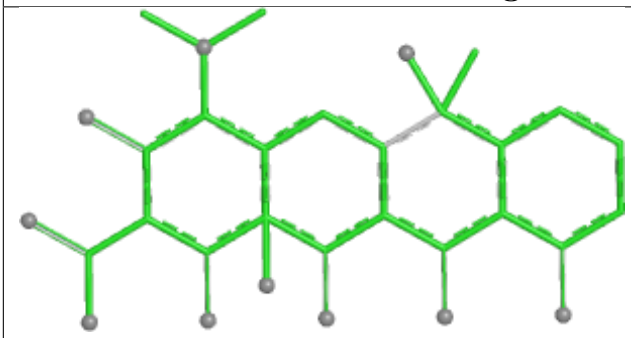


Torsions

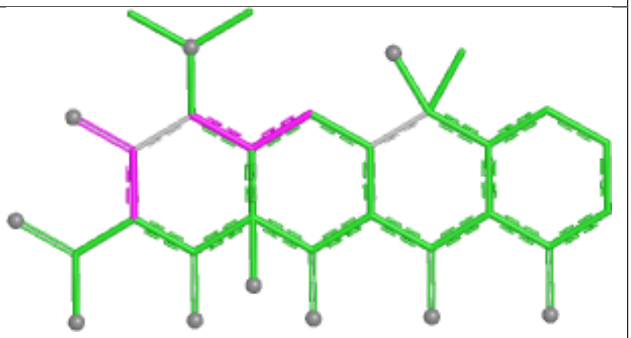


Rings

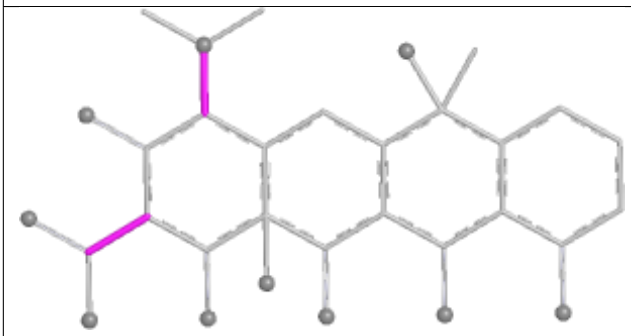
Ligand TAC BA 1644



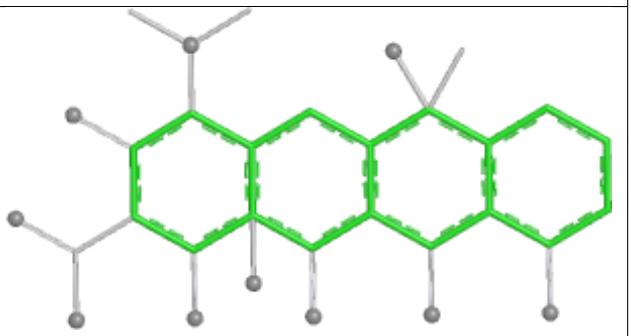
Bond lengths



Bond angles

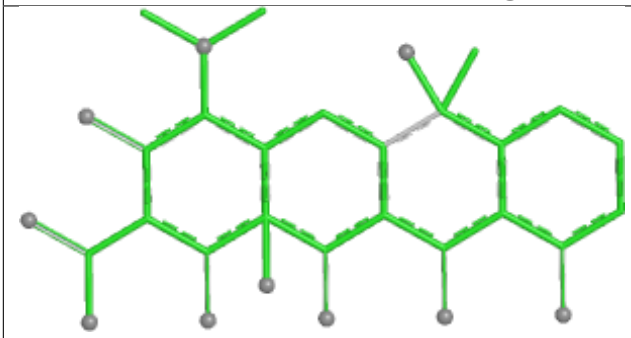


Torsions

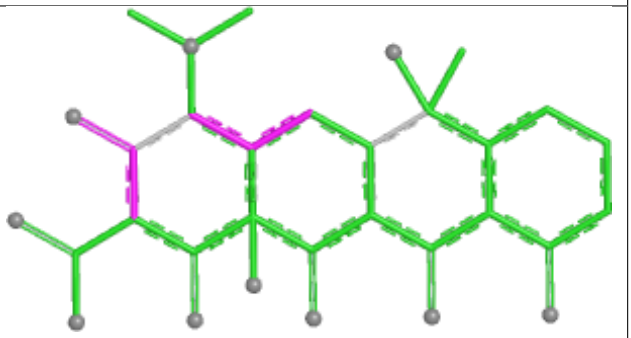


Rings

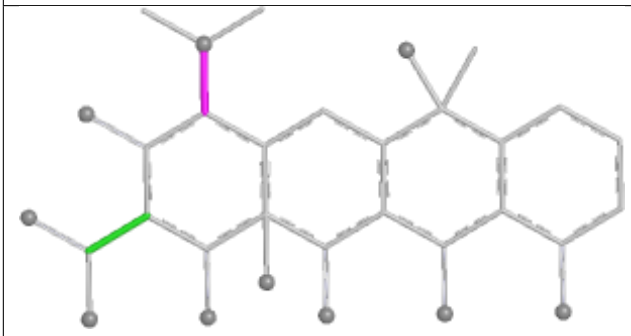
Ligand TAC AA 1680



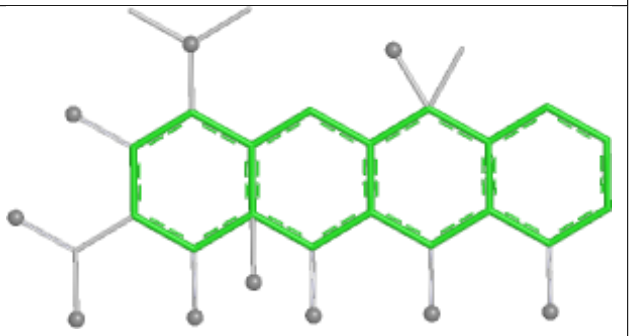
Bond lengths



Bond angles

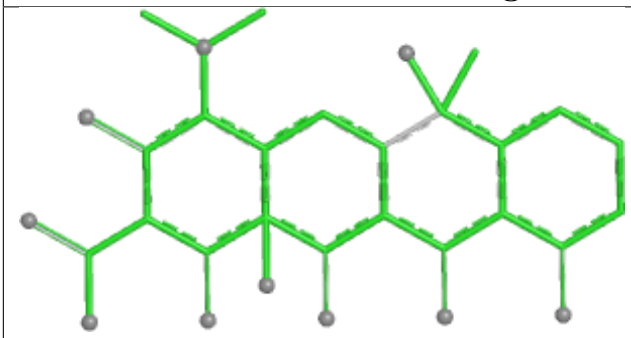


Torsions

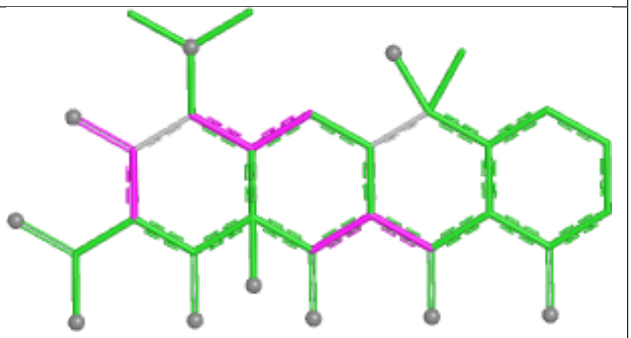


Rings

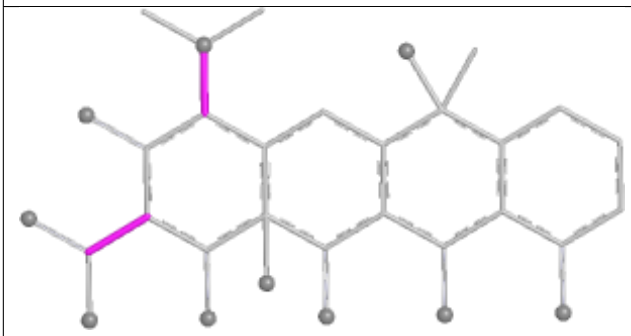
Ligand TAC BA 1643



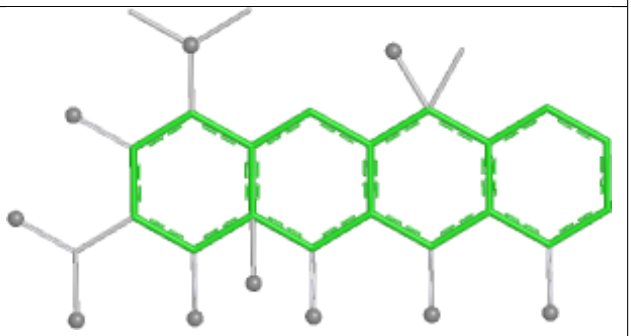
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1523/1534 (99%)	0.09	76 (4%) 35 20	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.55	111 (7%) 22 12	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.38	8 (3%) 46 27	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.74	18 (8%) 20 11	89, 139, 197, 228	0
3	AC	206/206 (100%)	0.12	5 (2%) 59 37	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.64	17 (8%) 19 10	90, 138, 170, 184	0
4	AD	205/205 (100%)	0.07	1 (0%) 87 75	63, 92, 129, 160	0
4	BD	205/205 (100%)	-0.13	0 100 100	53, 77, 106, 132	0
5	AE	155/155 (100%)	-0.11	1 (0%) 85 71	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.45	6 (4%) 43 25	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.18	2 (1%) 66 44	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.40	5 (5%) 35 20	77, 117, 140, 153	0
7	AG	151/151 (100%)	1.13	20 (13%) 8 5	95, 136, 160, 174	0
7	BG	151/151 (100%)	1.14	25 (16%) 5 3	136, 196, 213, 220	0
8	AH	129/129 (100%)	0.03	3 (2%) 61 39	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.50	4 (3%) 51 30	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.14	20 (15%) 6 4	74, 135, 164, 171	0
9	BI	127/127 (100%)	1.45	34 (26%) 2 2	133, 164, 201, 210	0
10	AJ	99/99 (100%)	0.94	11 (11%) 12 7	83, 118, 141, 147	0
10	BJ	98/99 (98%)	1.70	33 (33%) 1 1	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.28	2 (1%) 69 47	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.51	9 (7%) 21 12	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.16	3 (2%) 58 36	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.74	11 (9%) 17 9	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%)	1.41	28 (24%) 2 2	108, 130, 165, 171	0
13	BM	114/114 (100%)	1.15	15 (13%) 8 5	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.40	25 (25%) 2 2	77, 117, 178, 184	0
14	BN	100/100 (100%)	1.54	25 (25%) 2 2	124, 178, 216, 222	0
15	AO	88/88 (100%)	0.06	1 (1%) 77 58	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.42	2 (2%) 61 39	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.30	2 (2%) 59 37	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.29	15 (18%) 4 3	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.08	1 (1%) 74 54	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.02	7 (8%) 17 9	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.18	1 (1%) 67 45	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.38	5 (9%) 16 9	65, 86, 129, 168	0
19	AS	79/79 (100%)	1.49	20 (25%) 2 2	114, 135, 155, 163	0
19	BS	79/79 (100%)	1.30	18 (22%) 2 2	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.27	2 (2%) 61 39	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.44	19 (22%) 3 2	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.36	3 (5%) 32 18	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.42	2 (3%) 46 27	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.76	22 (39%) 1 1	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.77	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	1.73	16 (32%) 1 1	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.23	1 (1%) 64 43	46, 60, 87, 104	0
24	C3	46/46 (100%)	2.23	25 (54%) 0 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.61	1 (2%) 62 40	23, 31, 48, 112	0
25	C4	64/64 (100%)	2.78	48 (75%) 0 0	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.68	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.67	10 (26%) 2 2	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.49	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	1.11	10 (17%) 5 3	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.63	0 100 100	21, 29, 53, 80	2 (3%)
28	CB	118/120 (98%)	0.61	3 (2%) 58 36	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%)	-0.75	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.82	42 (15%) 6 4	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.53	3 (1%) 77 58	22, 49, 76, 92	0
30	CD	208/209 (99%)	0.99	27 (12%) 9 5	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.73	1 (0%) 87 75	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	0.93	285 (9%) 14 8	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.44	47 (23%) 2 2	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.54	0 100 100	19, 50, 96, 132	0
33	CF	177/177 (100%)	0.86	13 (7%) 22 12	193, 211, 219, 227	0
33	DF	177/177 (100%)	-0.06	1 (0%) 85 71	44, 75, 117, 142	0
34	CG	176/176 (100%)	0.67	6 (3%) 48 28	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.22	1 (0%) 85 71	38, 66, 97, 123	0
35	CH	149/149 (100%)	0.55	5 (3%) 48 28	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.56	4 (2%) 56 34	55, 142, 179, 198	0
36	CJ	134/134 (100%)	1.46	34 (25%) 2 2	235, 251, 263, 270	0
36	DJ	134/134 (100%)	1.60	40 (29%) 1 1	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.83	10 (7%) 24 13	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.81	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	0.87	10 (8%) 19 10	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.73	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	1.53	48 (33%) 1 1	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.51	1 (0%) 84 68	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.66	8 (5%) 29 16	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.79	0 100 100	13, 34, 63, 95	1 (0%)
41	CO	120/125 (96%)	1.56	35 (29%) 1 1	94, 117, 139, 180	0
41	DO	125/125 (100%)	-0.69	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	0.75	15 (12%) 9 5	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.43	1 (0%) 81 63	34, 52, 82, 94	0
43	CQ	114/114 (100%)	0.99	11 (9%) 15 8	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.53	1 (0%) 81 63	26, 43, 75, 116	0
44	CR	117/117 (100%)	1.23	25 (21%) 3 2	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%)	-0.88	0 100 100	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.25	23 (22%) 3 2	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.72	2 (1%) 66 44	15, 39, 68, 94	0
46	CT	110/110 (100%)	1.60	31 (28%) 1 2	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.72	1 (0%) 81 63	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.70	29 (31%) 1 1	124, 146, 173, 182	0
47	DU	93/93 (100%)	-0.05	5 (5%) 32 18	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.00	52 (50%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.32	1 (0%) 79 60	36, 56, 101, 131	0
49	CW	94/94 (100%)	0.64	4 (4%) 40 23	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.51	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.08	12 (16%) 6 4	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.55	0 100 100	16, 36, 62, 104	1 (1%)
51	CY	77/77 (100%)	1.34	15 (19%) 4 2	78, 113, 143, 160	0
51	DY	77/77 (100%)	-0.45	1 (1%) 74 54	24, 50, 85, 112	0
52	CZ	62/62 (100%)	1.55	17 (27%) 2 2	123, 162, 179, 190	0
52	DZ	62/62 (100%)	-0.03	1 (1%) 70 49	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.26	26 (19%) 4 2	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.76	89 (3%) 51 30	15, 39, 206, 298	11 (0%)
All	All	20632/20745 (99%)	0.35	1735 (8%) 18 10	10, 100, 227, 298	16 (0%)

The worst 5 of 1735 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	11.1
1	AA	121	U	8.8
10	BJ	74	VAL	8.4
54	DA	1731	G	7.7
54	DA	2120	G	7.2

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	2MG	BA	1207	24/25	0.63	0.12	158,159,162,165	0
1	2MG	BA	966	24/25	0.66	0.15	149,153,160,161	0
1	5MC	BA	967	21/22	0.74	0.15	148,154,156,157	0
31	PSU	CA	1917	20/21	0.76	0.11	118,126,134,134	0
31	2MA	CA	2503	23/24	0.84	0.18	90,96,102,102	0
1	2MG	AA	1207	24/25	0.85	0.12	113,117,120,122	0
31	3TD	CA	1915	21/22	0.85	0.09	146,150,155,155	0
31	PSU	CA	1911	20/21	0.86	0.08	111,128,131,132	0
31	PSU	CA	746	20/21	0.86	0.12	93,99,101,102	0
31	PSU	CA	2504	20/21	0.86	0.16	78,86,90,91	0
31	PSU	CA	2457	20/21	0.87	0.12	79,83,85,85	0
31	6MZ	CA	1618	23/24	0.87	0.13	98,107,108,109	0
31	PSU	CA	955	20/21	0.87	0.12	84,89,90,90	0
31	PSU	CA	2580	20/21	0.87	0.11	77,86,88,89	0
1	PSU	BA	516	20/21	0.88	0.10	91,96,99,102	0
31	6MZ	CA	2030	23/24	0.88	0.14	78,86,97,99	0
12	D2T	BL	89	10/11	0.89	0.16	81,86,96,96	0
54	3TD	DA	1915	21/22	0.89	0.10	86,90,102,103	0
30	MEQ	CD	150	9/11	0.89	0.19	81,87,117,120	0
1	2MG	AA	966	24/25	0.90	0.11	78,87,97,97	0
54	PSU	DA	1917	20/21	0.91	0.09	63,73,79,79	0
31	5MC	CA	1962	21/22	0.91	0.14	67,72,76,76	0
31	5MU	CA	1939	21/22	0.92	0.12	69,74,80,82	0
31	1MG	CA	745	24/25	0.92	0.12	85,87,90,93	0
12	D2T	AL	89	10/11	0.92	0.12	47,53,67,70	0
40	4D4	CN	81	12/13	0.92	0.12	83,89,102,103	0
31	G7M	CA	2069	24/25	0.92	0.16	78,83,88,88	0
31	2MG	CA	2445	24/25	0.92	0.17	66,75,80,83	0
31	2MG	CA	1835	24/25	0.92	0.11	60,73,76,78	0
1	UR3	BA	1498	21/22	0.93	0.10	78,80,84,84	0
31	5MU	CA	747	21/22	0.93	0.10	93,100,102,105	0
31	OMC	CA	2498	21/22	0.93	0.12	77,80,86,87	0
1	PSU	AA	516	20/21	0.93	0.08	68,72,78,78	0
1	5MC	BA	1407	21/22	0.93	0.11	81,95,99,100	0
1	G7M	BA	527	24/25	0.94	0.09	80,85,91,93	0
1	5MC	AA	967	21/22	0.94	0.10	76,93,96,97	0
31	OMG	CA	2251	24/25	0.94	0.13	67,73,75,77	0
1	2MG	BA	1516	24/25	0.94	0.09	61,67,78,80	0
31	OMU	CA	2552	21/22	0.94	0.17	78,81,85,89	0
1	MA6	BA	1518	24/25	0.95	0.09	67,74,79,79	0
31	PSU	CA	2605	20/21	0.95	0.09	74,75,78,80	0
31	PSU	CA	2604	20/21	0.95	0.08	65,71,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	DA	1911	20/21	0.96	0.06	67,74,75,75	0
1	UR3	AA	1498	21/22	0.96	0.08	51,53,57,59	0
1	4OC	BA	1402	22/23	0.96	0.07	74,79,81,82	0
1	G7M	AA	527	24/25	0.96	0.08	53,59,62,65	0
1	MA6	BA	1519	24/25	0.96	0.09	68,73,77,78	0
40	4D4	DN	81[A]	12/13	0.97	0.10	26,33,49,50	9
40	4D4	DN	81[B]	12/13	0.97	0.10	11,21,28,29	9
54	2MG	DA	1835	24/25	0.97	0.07	31,42,47,48	0
1	4OC	AA	1402	22/23	0.97	0.07	48,55,61,62	0
1	2MG	AA	1516	24/25	0.97	0.08	44,49,52,53	0
1	MA6	AA	1518	24/25	0.97	0.08	44,46,50,53	0
54	PSU	DA	2604	20/21	0.97	0.08	32,36,47,47	0
1	MA6	AA	1519	24/25	0.97	0.08	46,48,50,54	0
1	5MC	AA	1407	21/22	0.97	0.06	43,47,52,53	0
54	2MA	DA	2503	23/24	0.98	0.06	15,28,32,41	0
54	PSU	DA	2504	20/21	0.98	0.06	31,33,36,38	0
54	OMU	DA	2552	21/22	0.98	0.07	22,26,30,35	0
54	5MU	DA	747	21/22	0.98	0.06	20,25,31,38	0
54	PSU	DA	2605	20/21	0.98	0.07	26,34,37,38	0
54	5MU	DA	1939	21/22	0.98	0.07	25,30,36,40	0
30	MEQ	DD	150[A]	10/11	0.98	0.07	11,18,25,27	10
30	MEQ	DD	150[B]	10/11	0.98	0.07	19,28,34,35	10
54	5MC	DA	1962	21/22	0.98	0.07	28,37,39,42	0
54	PSU	DA	2457	20/21	0.99	0.05	22,25,26,29	0
54	OMC	DA	2498	21/22	0.99	0.05	18,21,24,27	0
54	PSU	DA	955	20/21	0.99	0.06	20,23,26,26	0
54	6MZ	DA	1618	23/24	0.99	0.05	17,24,27,28	0
54	PSU	DA	746	20/21	0.99	0.06	18,23,26,30	0
54	PSU	DA	2580	20/21	0.99	0.06	17,21,28,29	0
54	1MG	DA	745	24/25	0.99	0.05	16,22,28,30	0
54	6MZ	DA	2030	23/24	0.99	0.05	15,20,26,28	0
54	G7M	DA	2069	24/25	0.99	0.06	20,28,31,33	0
54	OMG	DA	2251	24/25	0.99	0.05	21,25,34,42	0
54	2MG	DA	2445	24/25	0.99	0.06	16,22,24,25	0
54	H2U	DA	2449	20/21	0.99	0.05	19,22,24,26	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1622	1/1	0.29	0.42	116,116,116,116	0
55	MG	BA	1646	1/1	0.31	0.34	141,141,141,141	0
55	MG	CA	3154	1/1	0.31	0.34	136,136,136,136	0
55	MG	CA	3075	1/1	0.33	0.35	221,221,221,221	0
55	MG	CA	3005	1/1	0.46	0.23	239,239,239,239	0
55	MG	BA	1641	1/1	0.48	0.30	121,121,121,121	0
55	MG	CA	3122	1/1	0.52	0.58	106,106,106,106	0
55	MG	CA	3038	1/1	0.55	0.12	258,258,258,258	0
55	MG	BA	1603	1/1	0.55	0.12	279,279,279,279	0
55	MG	CA	3155	1/1	0.55	0.24	152,152,152,152	0
55	MG	CA	3067	1/1	0.56	0.19	277,277,277,277	0
55	MG	DA	3168	1/1	0.56	0.32	106,106,106,106	0
55	MG	CA	3146	1/1	0.59	0.25	164,164,164,164	0
55	MG	CA	3124	1/1	0.60	0.21	124,124,124,124	0
55	MG	CA	3034	1/1	0.62	0.26	244,244,244,244	0
55	MG	AA	1628	1/1	0.62	0.22	110,110,110,110	0
55	MG	BA	1607	1/1	0.64	0.27	203,203,203,203	0
55	MG	BA	1638	1/1	0.65	0.52	107,107,107,107	0
55	MG	CA	3135	1/1	0.65	0.50	107,107,107,107	0
55	MG	AA	1677	1/1	0.66	0.15	138,138,138,138	0
55	MG	BA	1606	1/1	0.66	0.25	251,251,251,251	0
55	MG	CA	3077	1/1	0.67	0.21	232,232,232,232	0
55	MG	AA	1678	1/1	0.68	0.28	76,76,76,76	0
55	MG	CA	3060	1/1	0.69	0.17	234,234,234,234	0
55	MG	CA	3061	1/1	0.69	0.11	225,225,225,225	0
55	MG	BA	1624	1/1	0.69	0.13	249,249,249,249	0
55	MG	CA	3148	1/1	0.70	0.44	46,46,46,46	1
55	MG	CA	3139	1/1	0.70	0.20	83,83,83,83	0
55	MG	CA	3132	1/1	0.71	0.24	97,97,97,97	0
55	MG	CA	3110	1/1	0.72	0.23	102,102,102,102	0
55	MG	CA	3002	1/1	0.73	0.15	258,258,258,258	0
55	MG	CA	3104	1/1	0.73	0.21	254,254,254,254	0
55	MG	CA	3123	1/1	0.73	0.14	115,115,115,115	0
57	MPD	DE	301	8/8	0.73	0.25	123,126,129,129	0
59	TAC	BA	1644	32/32	0.73	0.22	139,152,159,159	0
55	MG	DA	3144	1/1	0.74	0.26	107,107,107,107	0
55	MG	CA	3152	1/1	0.74	0.14	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	3147	1/1	0.74	0.51	51,51,51,51	1
55	MG	BA	1639	1/1	0.74	0.27	93,93,93,93	0
61	PEG	DQ	201	7/7	0.74	0.24	104,108,109,109	0
55	MG	BA	1636	1/1	0.75	0.38	91,91,91,91	0
55	MG	AA	1660	1/1	0.75	0.18	281,281,281,281	0
55	MG	CA	3003	1/1	0.75	0.32	270,270,270,270	0
55	MG	CA	3125	1/1	0.76	0.28	98,98,98,98	0
55	MG	AA	1624	1/1	0.76	0.31	93,93,93,93	0
55	MG	CA	3047	1/1	0.76	0.38	238,238,238,238	0
55	MG	CA	3009	1/1	0.76	0.26	240,240,240,240	0
55	MG	AA	1617	1/1	0.76	0.71	147,147,147,147	0
62	EDO	DA	3003	4/4	0.76	0.29	89,89,89,89	0
66	ACY	DA	3196	4/4	0.76	0.28	72,76,77,77	0
55	MG	CA	3111	1/1	0.77	0.19	76,76,76,76	0
58	PUT	AA	1673	6/6	0.77	0.17	92,93,93,94	0
55	MG	AA	1654	1/1	0.77	0.40	259,259,259,259	0
55	MG	CA	3156	1/1	0.77	0.16	218,218,218,218	0
55	MG	CA	3032	1/1	0.77	0.12	244,244,244,244	0
55	MG	AA	1616	1/1	0.77	0.34	87,87,87,87	0
55	MG	CA	3129	1/1	0.78	0.20	89,89,89,89	0
55	MG	BA	1625	1/1	0.78	0.19	251,251,251,251	0
57	MPD	DK	201	8/8	0.78	0.21	96,98,100,100	0
55	MG	DA	3147	1/1	0.78	0.22	104,104,104,104	0
55	MG	CA	3134	1/1	0.79	0.28	126,126,126,126	0
55	MG	CA	3073	1/1	0.79	0.19	229,229,229,229	0
61	PEG	DP	201	7/7	0.79	0.20	90,91,93,95	0
55	MG	CA	3001	1/1	0.79	0.29	296,296,296,296	0
55	MG	CA	3021	1/1	0.79	0.39	261,261,261,261	0
55	MG	AA	1626	1/1	0.79	0.21	113,113,113,113	0
55	MG	BA	1647	1/1	0.80	0.19	86,86,86,86	0
55	MG	CA	3137	1/1	0.80	0.18	123,123,123,123	0
55	MG	BA	1640	1/1	0.80	0.35	94,94,94,94	0
55	MG	CA	3014	1/1	0.80	0.16	200,200,200,200	0
58	PUT	AA	1674	6/6	0.80	0.44	128,131,132,133	0
55	MG	BA	1604	1/1	0.81	0.12	187,187,187,187	0
57	MPD	DN	201	8/8	0.81	0.22	84,91,101,101	0
55	MG	CA	3007	1/1	0.81	0.11	214,214,214,214	0
55	MG	CA	3133	1/1	0.81	0.26	83,83,83,83	0
58	PUT	AA	1675	6/6	0.81	0.29	106,107,108,109	0
57	MPD	AA	1676	8/8	0.82	0.35	102,115,118,121	0
55	MG	DA	3111	1/1	0.82	0.38	292,292,292,292	0
55	MG	DA	3133	1/1	0.82	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	3115	1/1	0.82	0.27	72,72,72,72	0
55	MG	CA	3150	1/1	0.82	0.15	74,74,74,74	0
55	MG	CA	3028	1/1	0.82	0.13	274,274,274,274	0
55	MG	CA	3068	1/1	0.83	0.14	205,205,205,205	0
55	MG	AA	1601	1/1	0.83	0.55	76,76,76,76	0
55	MG	CA	3113	1/1	0.83	0.54	79,79,79,79	0
55	MG	DA	3130	1/1	0.83	0.38	99,99,99,99	0
55	MG	CA	3131	1/1	0.83	0.17	83,83,83,83	0
55	MG	AA	1608	1/1	0.83	0.32	78,78,78,78	0
55	MG	CA	3120	1/1	0.83	0.19	137,137,137,137	0
55	MG	BA	1623	1/1	0.83	0.24	254,254,254,254	0
55	MG	DA	3176	1/1	0.83	0.29	97,97,97,97	0
55	MG	DA	3180	1/1	0.83	0.22	95,95,95,95	0
55	MG	BA	1648	1/1	0.83	0.25	68,68,68,68	0
67	GUN	DA	3211	11/11	0.83	0.18	82,84,86,86	0
55	MG	CA	3151	1/1	0.84	0.31	81,81,81,81	0
58	PUT	AA	1672	6/6	0.84	0.37	90,93,95,95	0
55	MG	CA	3094	1/1	0.84	0.19	126,126,126,126	0
55	MG	CA	3142	1/1	0.84	0.12	71,71,71,71	0
55	MG	CA	3026	1/1	0.84	0.17	111,111,111,111	0
59	TAC	BA	1643	32/32	0.84	0.14	146,150,152,152	0
58	PUT	DA	3205	6/6	0.85	0.35	77,82,89,91	0
55	MG	DA	3163	1/1	0.85	0.24	84,84,84,84	0
55	MG	CA	3116	1/1	0.85	0.33	75,75,75,75	0
57	MPD	DT	201	8/8	0.85	0.30	84,87,99,100	0
55	MG	CA	3119	1/1	0.85	0.30	86,86,86,86	0
55	MG	BA	1633	1/1	0.85	0.17	241,241,241,241	0
55	MG	AA	1661	1/1	0.85	0.12	139,139,139,139	0
55	MG	AA	1609	1/1	0.85	0.35	88,88,88,88	0
55	MG	CA	3105	1/1	0.86	0.28	260,260,260,260	0
55	MG	DA	3121	1/1	0.86	0.35	70,70,70,70	0
57	MPD	DA	3190	8/8	0.86	0.17	78,82,85,89	0
55	MG	CA	3109	1/1	0.86	0.15	62,62,62,62	0
55	MG	AA	1611	1/1	0.86	0.30	94,94,94,94	0
55	MG	AA	1655	1/1	0.86	0.08	151,151,151,151	0
55	MG	CA	3128	1/1	0.86	0.12	82,82,82,82	0
55	MG	CA	3062	1/1	0.86	0.10	190,190,190,190	0
58	PUT	DA	3222	6/6	0.86	0.22	41,43,47,47	0
55	MG	CA	3130	1/1	0.86	0.28	76,76,76,76	0
55	MG	CA	3083	1/1	0.86	0.15	203,203,203,203	0
55	MG	CA	3090	1/1	0.86	0.13	170,170,170,170	0
56	PG4	AA	1670	13/13	0.86	0.12	64,79,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	3117	1/1	0.86	0.28	69,69,69,69	0
63	PGE	D1	102	10/10	0.86	0.26	107,117,119,119	0
55	MG	CA	3008	1/1	0.86	0.20	147,147,147,147	0
55	MG	BA	1612	1/1	0.86	0.23	159,159,159,159	0
58	PUT	DA	3195	6/6	0.87	0.30	76,81,86,87	0
55	MG	BA	1630	1/1	0.87	0.14	160,160,160,160	0
57	MPD	DE	302	8/8	0.87	0.31	71,76,83,85	0
55	MG	CA	3093	1/1	0.87	0.10	84,84,84,84	0
55	MG	DA	3062	1/1	0.87	0.14	211,211,211,211	0
55	MG	CA	3138	1/1	0.87	0.20	84,84,84,84	0
55	MG	DA	3173	1/1	0.87	0.32	100,100,100,100	0
55	MG	DA	3120	1/1	0.87	0.30	81,81,81,81	0
55	MG	BA	1616	1/1	0.87	0.19	162,162,162,162	0
55	MG	CA	3010	1/1	0.87	0.19	245,245,245,245	0
55	MG	AA	1605	1/1	0.87	0.45	80,80,80,80	0
55	MG	CA	3080	1/1	0.88	0.16	119,119,119,119	0
55	MG	AA	1604	1/1	0.88	0.23	50,50,50,50	0
55	MG	CA	3108	1/1	0.88	0.21	73,73,73,73	0
55	MG	AA	1618	1/1	0.88	0.57	86,86,86,86	0
61	PEG	D3	101	7/7	0.88	0.53	83,89,94,95	0
57	MPD	DA	3204	8/8	0.88	0.29	117,118,124,125	0
55	MG	DA	3127	1/1	0.88	0.35	71,71,71,71	0
55	MG	CA	3118	1/1	0.88	0.29	64,64,64,64	0
62	EDO	DA	3198	4/4	0.88	0.26	76,79,79,79	0
55	MG	AA	1606	1/1	0.88	0.33	83,83,83,83	0
55	MG	AA	1623	1/1	0.88	0.11	62,62,62,62	0
66	ACY	DA	3201	4/4	0.88	0.20	66,68,68,69	0
55	MG	CA	3112	1/1	0.88	0.08	62,62,62,62	0
55	MG	CA	3107	1/1	0.89	0.28	65,65,65,65	0
55	MG	AA	1603	1/1	0.89	0.24	81,81,81,81	0
55	MG	AA	1619	1/1	0.89	0.31	93,93,93,93	0
55	MG	CA	3136	1/1	0.89	0.37	87,87,87,87	0
55	MG	CA	3064	1/1	0.89	0.19	260,260,260,260	0
55	MG	AA	1621	1/1	0.89	0.69	97,97,97,97	0
55	MG	BA	1629	1/1	0.89	0.24	184,184,184,184	0
56	PG4	DQ	202	13/13	0.89	0.10	53,59,69,71	0
56	PG4	DR	202	13/13	0.89	0.29	97,109,121,121	0
55	MG	CA	3141	1/1	0.89	0.32	66,66,66,66	0
55	MG	CA	3072	1/1	0.89	0.12	249,249,249,249	0
55	MG	CA	3099	1/1	0.89	0.11	156,156,156,156	0
61	PEG	DA	3226	7/7	0.89	0.20	57,62,74,75	0
55	MG	CA	3022	1/1	0.89	0.24	206,206,206,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1615	1/1	0.89	0.48	84,84,84,84	0
55	MG	DA	3138	1/1	0.89	0.56	38,38,38,38	1
63	PGE	DS	201	10/10	0.89	0.14	65,78,83,83	0
63	PGE	DA	3001	10/10	0.89	0.18	75,85,99,101	0
55	MG	DA	3142	1/1	0.89	0.42	84,84,84,84	0
55	MG	CA	3106	1/1	0.89	0.22	75,75,75,75	0
57	MPD	DA	3210	8/8	0.89	0.24	87,89,92,94	0
61	PEG	D1	103	7/7	0.90	0.29	76,77,78,78	0
56	PG4	DA	3193	13/13	0.90	0.21	65,77,93,94	0
55	MG	CA	3126	1/1	0.90	0.29	85,85,85,85	0
55	MG	DA	3171	1/1	0.90	0.09	74,74,74,74	0
55	MG	DA	3141	1/1	0.90	0.12	40,40,40,40	0
62	EDO	DB	211	4/4	0.90	0.31	88,88,90,90	0
62	EDO	DA	3002	4/4	0.90	0.40	71,74,79,82	0
55	MG	CA	3016	1/1	0.90	0.22	164,164,164,164	0
55	MG	CA	3071	1/1	0.90	0.09	152,152,152,152	0
55	MG	DA	3146	1/1	0.90	0.20	70,70,70,70	0
55	MG	CA	3145	1/1	0.90	0.19	62,62,62,62	0
63	PGE	DU	101	10/10	0.90	0.17	79,84,91,92	0
59	TAC	AA	1681	32/32	0.90	0.13	94,106,109,110	0
66	ACY	DA	3191	4/4	0.90	0.21	80,82,82,82	0
55	MG	DA	3137	1/1	0.90	0.35	80,80,80,80	0
57	MPD	DA	3207	8/8	0.90	0.17	86,86,88,89	0
61	PEG	AL	201	7/7	0.90	0.15	79,79,85,86	0
68	TRS	DA	3220	8/8	0.90	0.16	94,100,107,109	0
55	MG	CA	3076	1/1	0.91	0.08	132,132,132,132	0
55	MG	BA	1614	1/1	0.91	0.12	137,137,137,137	0
55	MG	CA	3153	1/1	0.91	0.17	59,59,59,59	0
57	MPD	DT	202	8/8	0.91	0.26	105,107,109,109	0
55	MG	AA	1636	1/1	0.91	0.12	113,113,113,113	0
57	MPD	DA	3192	8/8	0.91	0.23	69,77,79,80	0
55	MG	AA	1664	1/1	0.91	0.10	199,199,199,199	0
55	MG	AA	1625	1/1	0.91	0.16	68,68,68,68	0
56	PG4	DA	3216	13/13	0.91	0.15	77,89,96,96	0
55	MG	DA	3170	1/1	0.91	0.27	90,90,90,90	0
61	PEG	DL	201	7/7	0.91	0.12	66,69,70,71	0
55	MG	CA	3149	1/1	0.91	0.22	63,63,63,63	0
55	MG	CA	3012	1/1	0.91	0.08	84,84,84,84	0
61	PEG	DA	3199	7/7	0.91	0.19	79,84,92,93	0
55	MG	CA	3121	1/1	0.92	0.16	65,65,65,65	0
55	MG	CA	3056	1/1	0.92	0.63	78,78,78,78	0
55	MG	DA	3169	1/1	0.92	0.36	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3123	1/1	0.92	0.31	81,81,81,81	0
55	MG	CA	3140	1/1	0.92	0.11	75,75,75,75	0
55	MG	DA	3172	1/1	0.92	0.40	81,81,81,81	0
55	MG	AA	1602	1/1	0.92	0.23	75,75,75,75	0
55	MG	BA	1637	1/1	0.92	0.19	86,86,86,86	0
61	PEG	DA	3227	7/7	0.92	0.21	75,79,86,87	0
55	MG	CA	3143	1/1	0.92	0.07	67,67,67,67	0
55	MG	CA	3037	1/1	0.92	0.21	146,146,146,146	0
56	PG4	BA	1642	13/13	0.92	0.11	84,86,94,96	0
55	MG	AA	1614	1/1	0.92	0.22	79,79,79,79	0
62	EDO	DA	3209	4/4	0.92	0.26	93,94,95,95	0
55	MG	DA	3012	1/1	0.92	0.13	153,153,153,153	0
56	PG4	DS	202	13/13	0.92	0.11	52,54,63,64	0
55	MG	DA	3037	1/1	0.92	0.18	22,22,22,22	0
58	PUT	DA	3212	6/6	0.92	0.19	54,63,66,70	0
63	PGE	DA	3203	10/10	0.92	0.17	68,72,76,76	0
63	PGE	DA	3225	10/10	0.92	0.17	73,81,92,92	0
65	1PE	DA	3202	16/16	0.92	0.17	55,64,72,72	0
55	MG	CA	3039	1/1	0.92	0.10	158,158,158,158	0
59	TAC	AA	1680	32/32	0.92	0.13	70,81,96,96	0
55	MG	BA	1609	1/1	0.92	0.09	168,168,168,168	0
55	MG	DA	3152	1/1	0.92	0.42	94,94,94,94	0
55	MG	DA	3158	1/1	0.92	0.18	63,63,63,63	0
55	MG	DA	3129	1/1	0.93	0.34	67,67,67,67	0
55	MG	AA	1630	1/1	0.93	0.11	105,105,105,105	0
55	MG	DA	3131	1/1	0.93	0.26	63,63,63,63	0
62	EDO	DA	3208	4/4	0.93	0.23	69,71,72,72	0
55	MG	AA	1665	1/1	0.93	0.12	136,136,136,136	0
62	EDO	DA	3215	4/4	0.93	0.15	67,71,74,74	0
55	MG	CA	3035	1/1	0.93	0.21	89,89,89,89	0
55	MG	CA	3054	1/1	0.93	0.07	118,118,118,118	0
55	MG	DA	3119	1/1	0.93	0.17	69,69,69,69	0
55	MG	CA	3036	1/1	0.93	0.10	133,133,133,133	0
55	MG	CA	3102	1/1	0.93	0.08	104,104,104,104	0
58	PUT	DA	3188	6/6	0.93	0.13	43,50,50,51	0
64	SPD	DA	3183	10/10	0.93	0.16	60,70,74,75	0
64	SPD	DA	3206	10/10	0.93	0.25	86,93,96,96	0
58	PUT	DA	3189	6/6	0.93	0.14	40,44,47,47	0
55	MG	CA	3078	1/1	0.93	0.10	153,153,153,153	0
61	PEG	DA	3200	7/7	0.93	0.33	65,68,77,77	0
55	MG	DA	3124	1/1	0.93	0.35	76,76,76,76	0
55	MG	AA	1642	1/1	0.93	0.10	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	PUT	DA	3213	6/6	0.93	0.23	83,85,91,93	0
55	MG	DA	3160	1/1	0.94	0.51	81,81,81,81	0
55	MG	AA	1610	1/1	0.94	0.22	95,95,95,95	0
55	MG	DA	3164	1/1	0.94	0.20	59,59,59,59	0
55	MG	DA	3167	1/1	0.94	0.30	90,90,90,90	0
55	MG	AA	1607	1/1	0.94	0.26	70,70,70,70	0
55	MG	CA	3019	1/1	0.94	0.09	58,58,58,58	0
55	MG	BA	1634	1/1	0.94	0.12	129,129,129,129	0
55	MG	CA	3084	1/1	0.94	0.10	167,167,167,167	0
62	EDO	D1	101	4/4	0.94	0.08	56,57,60,60	0
55	MG	AA	1669	1/1	0.94	0.10	172,172,172,172	0
62	EDO	DB	212	4/4	0.94	0.14	70,72,73,73	0
55	MG	CA	3023	1/1	0.94	0.12	159,159,159,159	0
55	MG	AA	1612	1/1	0.94	0.18	57,57,57,57	0
55	MG	DA	3177	1/1	0.94	0.26	67,67,67,67	0
55	MG	DA	3178	1/1	0.94	0.25	69,69,69,69	0
55	MG	DA	3179	1/1	0.94	0.19	101,101,101,101	0
55	MG	CA	3127	1/1	0.94	0.24	65,65,65,65	0
55	MG	DB	207	1/1	0.94	0.11	80,80,80,80	0
55	MG	DB	209	1/1	0.94	0.20	65,65,65,65	0
55	MG	DB	210	1/1	0.94	0.15	76,76,76,76	0
55	MG	CA	3114	1/1	0.94	0.14	57,57,57,57	0
58	PUT	DA	3219	6/6	0.94	0.14	63,64,65,66	0
63	PGE	DA	3214	10/10	0.94	0.14	56,58,66,66	0
58	PUT	DA	3221	6/6	0.94	0.20	113,116,117,118	0
55	MG	CA	3048	1/1	0.94	0.08	91,91,91,91	0
58	PUT	DA	3223	6/6	0.94	0.17	54,55,62,64	0
64	SPD	DA	3224	10/10	0.94	0.14	30,40,57,60	0
55	MG	AA	1627	1/1	0.94	0.28	72,72,72,72	0
55	MG	DA	3080	1/1	0.94	0.11	149,149,149,149	0
57	MPD	AA	1671	8/8	0.94	0.21	83,86,89,90	0
55	MG	DA	3149	1/1	0.94	0.06	47,47,47,47	0
55	MG	AA	1679	1/1	0.94	0.24	62,62,62,62	0
55	MG	CA	3058	1/1	0.94	0.21	138,138,138,138	0
62	EDO	DA	3194	4/4	0.95	0.16	61,63,64,65	0
55	MG	DA	3153	1/1	0.95	0.25	53,53,53,53	0
55	MG	DA	3154	1/1	0.95	0.21	62,62,62,62	0
55	MG	BA	1627	1/1	0.95	0.13	126,126,126,126	0
55	MG	CA	3063	1/1	0.95	0.14	118,118,118,118	0
55	MG	DA	3161	1/1	0.95	0.21	62,62,62,62	0
55	MG	CA	3079	1/1	0.95	0.06	116,116,116,116	0
55	MG	DA	3132	1/1	0.95	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3165	1/1	0.95	0.17	47,47,47,47	0
58	PUT	DA	3184	6/6	0.95	0.15	53,55,60,60	0
55	MG	AA	1634	1/1	0.95	0.09	144,144,144,144	0
55	MG	CA	3082	1/1	0.95	0.16	112,112,112,112	0
55	MG	BA	1617	1/1	0.95	0.06	105,105,105,105	0
61	PEG	DA	3218	7/7	0.95	0.21	99,105,110,112	0
55	MG	AA	1656	1/1	0.95	0.08	140,140,140,140	0
65	1PE	DA	3185	16/16	0.95	0.11	37,52,80,82	0
55	MG	CA	3055	1/1	0.95	0.07	135,135,135,135	0
55	MG	AA	1663	1/1	0.95	0.06	94,94,94,94	0
55	MG	BA	1645	1/1	0.95	0.10	94,94,94,94	0
55	MG	CA	3074	1/1	0.95	0.07	101,101,101,101	0
55	MG	BA	1635	1/1	0.95	0.09	113,113,113,113	0
55	MG	AA	1658	1/1	0.95	0.12	101,101,101,101	0
62	EDO	DB	201	4/4	0.96	0.16	72,75,76,76	0
55	MG	CB	202	1/1	0.96	0.11	113,113,113,113	0
55	MG	CB	203	1/1	0.96	0.07	133,133,133,133	0
55	MG	DA	3117	1/1	0.96	0.27	62,62,62,62	0
55	MG	BA	1619	1/1	0.96	0.07	79,79,79,79	0
55	MG	CA	3088	1/1	0.96	0.06	67,67,67,67	0
62	EDO	DA	3197	4/4	0.96	0.09	51,51,53,53	0
55	MG	CA	3046	1/1	0.96	0.10	117,117,117,117	0
55	MG	CA	3092	1/1	0.96	0.06	125,125,125,125	0
55	MG	CA	3024	1/1	0.96	0.10	81,81,81,81	0
55	MG	DA	3125	1/1	0.96	0.30	58,58,58,58	0
55	MG	DA	3126	1/1	0.96	0.32	57,57,57,57	0
55	MG	CA	3011	1/1	0.96	0.06	70,70,70,70	0
55	MG	CA	3049	1/1	0.96	0.05	57,57,57,57	0
55	MG	CA	3053	1/1	0.96	0.10	81,81,81,81	0
63	PGE	DA	3186	10/10	0.96	0.09	33,40,41,41	0
60	ZN	C5	101	1/1	0.96	0.07	149,149,149,149	0
55	MG	AA	1633	1/1	0.96	0.06	128,128,128,128	0
63	PGE	DA	3217	10/10	0.96	0.15	67,71,76,76	0
55	MG	DR	203	1/1	0.96	0.13	140,140,140,140	0
55	MG	CA	3031	1/1	0.96	0.06	73,73,73,73	0
55	MG	DB	208	1/1	0.96	0.09	77,77,77,77	0
55	MG	AA	1657	1/1	0.96	0.10	105,105,105,105	0
55	MG	DA	3175	1/1	0.96	0.14	68,68,68,68	0
55	MG	DA	3140	1/1	0.96	0.17	68,68,68,68	0
55	MG	CA	3057	1/1	0.96	0.07	106,106,106,106	0
55	MG	AA	1647	1/1	0.96	0.09	149,149,149,149	0
55	MG	DA	3143	1/1	0.96	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	3018	1/1	0.96	0.07	90,90,90,90	0
55	MG	CB	201	1/1	0.96	0.06	159,159,159,159	0
55	MG	DA	3095	1/1	0.97	0.09	74,74,74,74	0
55	MG	AA	1613	1/1	0.97	0.35	59,59,59,59	0
55	MG	CA	3051	1/1	0.97	0.04	73,73,73,73	0
55	MG	CA	3066	1/1	0.97	0.08	110,110,110,110	0
55	MG	DA	3145	1/1	0.97	0.11	78,78,78,78	0
55	MG	CA	3025	1/1	0.97	0.05	87,87,87,87	0
55	MG	CA	3006	1/1	0.97	0.07	143,143,143,143	0
55	MG	DA	3181	1/1	0.97	0.21	70,70,70,70	0
55	MG	DA	3148	1/1	0.97	0.30	62,62,62,62	0
55	MG	CA	3069	1/1	0.97	0.09	110,110,110,110	0
55	MG	DA	3151	1/1	0.97	0.14	30,30,30,30	0
55	MG	CA	3070	1/1	0.97	0.04	87,87,87,87	0
55	MG	DB	206	1/1	0.97	0.16	64,64,64,64	0
55	MG	CA	3089	1/1	0.97	0.13	54,54,54,54	0
55	MG	DA	3155	1/1	0.97	0.27	60,60,60,60	0
55	MG	DA	3156	1/1	0.97	0.25	72,72,72,72	0
55	MG	DA	3157	1/1	0.97	0.21	54,54,54,54	0
55	MG	CA	3020	1/1	0.97	0.07	86,86,86,86	0
55	MG	DA	3128	1/1	0.97	0.52	62,62,62,62	0
55	MG	CA	3029	1/1	0.97	0.17	114,114,114,114	0
55	MG	DA	3162	1/1	0.97	0.11	57,57,57,57	0
55	MG	CA	3042	1/1	0.97	0.06	82,82,82,82	0
55	MG	CA	3043	1/1	0.97	0.07	86,86,86,86	0
55	MG	AA	1620	1/1	0.97	0.16	63,63,63,63	0
55	MG	DA	3043	1/1	0.97	0.09	32,32,32,32	0
55	MG	DA	3134	1/1	0.97	0.15	95,95,95,95	0
55	MG	DA	3044	1/1	0.97	0.06	70,70,70,70	0
55	MG	BA	1605	1/1	0.97	0.05	146,146,146,146	0
55	MG	DA	3139	1/1	0.97	0.08	55,55,55,55	0
55	MG	BA	1601	1/1	0.97	0.09	130,130,130,130	0
55	MG	CA	3065	1/1	0.98	0.07	72,72,72,72	0
55	MG	DA	3079	1/1	0.98	0.04	124,124,124,124	0
55	MG	CA	3085	1/1	0.98	0.04	69,69,69,69	0
55	MG	DA	3082	1/1	0.98	0.05	72,72,72,72	0
55	MG	CA	3086	1/1	0.98	0.06	59,59,59,59	0
55	MG	AA	1651	1/1	0.98	0.05	69,69,69,69	0
55	MG	CA	3144	1/1	0.98	0.03	63,63,63,63	0
55	MG	CA	3027	1/1	0.98	0.06	68,68,68,68	0
55	MG	AA	1635	1/1	0.98	0.09	104,104,104,104	0
55	MG	CA	3091	1/1	0.98	0.06	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MPD	DS	203	8/8	0.98	0.14	47,50,57,58	0
55	MG	DA	3122	1/1	0.98	0.27	46,46,46,46	0
55	MG	CA	3013	1/1	0.98	0.06	99,99,99,99	0
55	MG	CA	3030	1/1	0.98	0.05	64,64,64,64	0
55	MG	CA	3052	1/1	0.98	0.06	71,71,71,71	0
55	MG	CA	3095	1/1	0.98	0.04	69,69,69,69	0
55	MG	CA	3098	1/1	0.98	0.04	78,78,78,78	0
55	MG	BA	1608	1/1	0.98	0.05	86,86,86,86	0
55	MG	DA	3166	1/1	0.98	0.11	88,88,88,88	0
55	MG	CA	3101	1/1	0.98	0.04	97,97,97,97	0
55	MG	AA	1659	1/1	0.98	0.05	74,74,74,74	0
55	MG	CA	3103	1/1	0.98	0.04	90,90,90,90	0
58	PUT	DM	201	6/6	0.98	0.10	40,48,52,56	0
55	MG	BA	1610	1/1	0.98	0.06	93,93,93,93	0
55	MG	BA	1626	1/1	0.98	0.04	85,85,85,85	0
55	MG	AA	1668	1/1	0.98	0.10	59,59,59,59	0
55	MG	DA	3136	1/1	0.98	0.09	43,43,43,43	0
55	MG	BA	1628	1/1	0.98	0.04	92,92,92,92	0
55	MG	BA	1613	1/1	0.98	0.10	79,79,79,79	0
55	MG	AA	1644	1/1	0.98	0.15	87,87,87,87	0
55	MG	DA	3008	1/1	0.98	0.07	87,87,87,87	0
55	MG	BA	1632	1/1	0.98	0.10	78,78,78,78	0
64	SPD	DA	3187	10/10	0.98	0.09	30,41,47,48	0
55	MG	DA	3015	1/1	0.98	0.05	40,40,40,40	0
55	MG	DA	3026	1/1	0.98	0.06	92,92,92,92	0
55	MG	DA	3182	1/1	0.98	0.22	52,52,52,52	0
55	MG	DA	3230	1/1	0.98	0.06	48,48,48,48	0
55	MG	DA	3231	1/1	0.98	0.13	36,36,36,36	0
55	MG	CA	3081	1/1	0.98	0.04	84,84,84,84	0
60	ZN	AB	301	1/1	0.98	0.06	150,150,150,150	0
55	MG	AA	1641	1/1	0.98	0.06	65,65,65,65	0
55	MG	CA	3045	1/1	0.98	0.07	107,107,107,107	0
55	MG	DA	3064	1/1	0.99	0.11	49,49,49,49	0
55	MG	DA	3070	1/1	0.99	0.04	62,62,62,62	0
55	MG	DA	3072	1/1	0.99	0.07	55,55,55,55	0
55	MG	DA	3159	1/1	0.99	0.06	76,76,76,76	0
55	MG	DA	3074	1/1	0.99	0.05	47,47,47,47	0
55	MG	DA	3078	1/1	0.99	0.05	52,52,52,52	0
55	MG	BA	1602	1/1	0.99	0.05	84,84,84,84	0
55	MG	CA	3040	1/1	0.99	0.04	83,83,83,83	0
55	MG	BA	1631	1/1	0.99	0.03	45,45,45,45	0
55	MG	DA	3083	1/1	0.99	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3085	1/1	0.99	0.03	50,50,50,50	0
55	MG	BA	1615	1/1	0.99	0.04	65,65,65,65	0
55	MG	DA	3098	1/1	0.99	0.06	87,87,87,87	0
55	MG	DA	3101	1/1	0.99	0.03	45,45,45,45	0
55	MG	CA	3044	1/1	0.99	0.07	59,59,59,59	0
60	ZN	D5	101	1/1	0.99	0.02	55,55,55,55	0
55	MG	DA	3113	1/1	0.99	0.06	52,52,52,52	0
55	MG	DA	3114	1/1	0.99	0.04	39,39,39,39	0
55	MG	AA	1639	1/1	0.99	0.04	89,89,89,89	0
55	MG	DA	3174	1/1	0.99	0.07	70,70,70,70	0
55	MG	DA	3118	1/1	0.99	0.07	36,36,36,36	0
55	MG	AA	1645	1/1	0.99	0.04	46,46,46,46	0
55	MG	CA	3096	1/1	0.99	0.02	64,64,64,64	0
55	MG	CA	3004	1/1	0.99	0.06	106,106,106,106	0
55	MG	BA	1618	1/1	0.99	0.03	69,69,69,69	0
55	MG	CA	3100	1/1	0.99	0.07	73,73,73,73	0
55	MG	AA	1629	1/1	0.99	0.04	71,71,71,71	0
55	MG	CA	3050	1/1	0.99	0.03	54,54,54,54	0
55	MG	DA	3228	1/1	0.99	0.07	36,36,36,36	0
55	MG	DR	201	1/1	0.99	0.08	32,32,32,32	0
55	MG	BA	1620	1/1	0.99	0.04	113,113,113,113	0
55	MG	DB	202	1/1	0.99	0.07	52,52,52,52	0
55	MG	DB	204	1/1	0.99	0.04	37,37,37,37	0
55	MG	BA	1621	1/1	0.99	0.14	36,36,36,36	0
55	MG	BA	1622	1/1	0.99	0.06	99,99,99,99	0
55	MG	AA	1667	1/1	0.99	0.07	41,41,41,41	0
55	MG	AA	1648	1/1	0.99	0.04	60,60,60,60	0
55	MG	AA	1649	1/1	0.99	0.04	57,57,57,57	0
55	MG	DA	3135	1/1	0.99	0.04	78,78,78,78	0
55	MG	DA	3006	1/1	0.99	0.04	75,75,75,75	0
55	MG	DA	3007	1/1	0.99	0.06	88,88,88,88	0
55	MG	CA	3033	1/1	0.99	0.11	91,91,91,91	0
55	MG	AA	1650	1/1	0.99	0.03	79,79,79,79	0
55	MG	CA	3059	1/1	0.99	0.03	74,74,74,74	0
55	MG	DA	3016	1/1	0.99	0.05	43,43,43,43	0
55	MG	AA	1638	1/1	0.99	0.04	86,86,86,86	0
55	MG	DA	3028	1/1	0.99	0.04	56,56,56,56	0
55	MG	DA	3030	1/1	0.99	0.04	42,42,42,42	0
55	MG	DA	3035	1/1	0.99	0.08	32,32,32,32	0
55	MG	AA	1653	1/1	0.99	0.05	61,61,61,61	0
55	MG	CA	3017	1/1	0.99	0.07	75,75,75,75	0
55	MG	CA	3087	1/1	0.99	0.03	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3047	1/1	0.99	0.06	58,58,58,58	0
55	MG	DA	3150	1/1	0.99	0.05	50,50,50,50	0
55	MG	DA	3049	1/1	0.99	0.03	39,39,39,39	0
55	MG	DA	3052	1/1	0.99	0.03	70,70,70,70	0
55	MG	DA	3054	1/1	0.99	0.05	70,70,70,70	0
55	MG	AA	1662	1/1	0.99	0.04	73,73,73,73	0
55	MG	DA	3063	1/1	0.99	0.04	85,85,85,85	0
55	MG	CA	3097	1/1	1.00	0.05	83,83,83,83	0
55	MG	DA	3086	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3087	1/1	1.00	0.01	34,34,34,34	0
55	MG	DA	3088	1/1	1.00	0.02	42,42,42,42	0
55	MG	DA	3089	1/1	1.00	0.04	23,23,23,23	0
55	MG	DA	3229	1/1	1.00	0.04	36,36,36,36	0
55	MG	DA	3090	1/1	1.00	0.04	30,30,30,30	0
55	MG	DA	3091	1/1	1.00	0.05	17,17,17,17	0
55	MG	DA	3092	1/1	1.00	0.02	21,21,21,21	0
55	MG	DA	3093	1/1	1.00	0.07	23,23,23,23	0
55	MG	DA	3094	1/1	1.00	0.07	20,20,20,20	0
55	MG	DA	3017	1/1	1.00	0.01	20,20,20,20	0
55	MG	DA	3096	1/1	1.00	0.05	36,36,36,36	0
55	MG	DA	3097	1/1	1.00	0.03	26,26,26,26	0
55	MG	DA	3018	1/1	1.00	0.02	43,43,43,43	0
55	MG	DA	3099	1/1	1.00	0.04	23,23,23,23	0
55	MG	DA	3100	1/1	1.00	0.02	26,26,26,26	0
55	MG	DA	3019	1/1	1.00	0.15	8,8,8,8	0
55	MG	DA	3102	1/1	1.00	0.02	30,30,30,30	0
55	MG	DA	3103	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3104	1/1	1.00	0.05	34,34,34,34	0
55	MG	DA	3105	1/1	1.00	0.07	31,31,31,31	0
55	MG	DA	3106	1/1	1.00	0.10	41,41,41,41	0
55	MG	DA	3107	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3108	1/1	1.00	0.05	30,30,30,30	0
55	MG	DA	3109	1/1	1.00	0.02	23,23,23,23	0
55	MG	DA	3110	1/1	1.00	0.05	35,35,35,35	0
55	MG	DA	3020	1/1	1.00	0.04	45,45,45,45	0
55	MG	DA	3112	1/1	1.00	0.04	24,24,24,24	0
55	MG	DA	3021	1/1	1.00	0.04	27,27,27,27	0
55	MG	DA	3022	1/1	1.00	0.07	21,21,21,21	0
55	MG	DA	3115	1/1	1.00	0.02	37,37,37,37	0
55	MG	DA	3116	1/1	1.00	0.02	34,34,34,34	0
55	MG	DA	3023	1/1	1.00	0.04	20,20,20,20	0
55	MG	DA	3024	1/1	1.00	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3025	1/1	1.00	0.02	31,31,31,31	0
55	MG	AA	1637	1/1	1.00	0.04	53,53,53,53	0
55	MG	DA	3027	1/1	1.00	0.03	33,33,33,33	0
55	MG	AA	1631	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3029	1/1	1.00	0.10	29,29,29,29	0
55	MG	DB	203	1/1	1.00	0.03	30,30,30,30	0
55	MG	DA	3031	1/1	1.00	0.02	27,27,27,27	0
55	MG	DA	3032	1/1	1.00	0.06	23,23,23,23	0
55	MG	DA	3033	1/1	1.00	0.05	26,26,26,26	0
55	MG	DA	3034	1/1	1.00	0.02	16,16,16,16	0
55	MG	AA	1643	1/1	1.00	0.02	53,53,53,53	0
55	MG	DA	3036	1/1	1.00	0.06	25,25,25,25	0
55	MG	DB	205	1/1	1.00	0.03	46,46,46,46	0
55	MG	DA	3038	1/1	1.00	0.01	19,19,19,19	0
55	MG	DA	3039	1/1	1.00	0.05	23,23,23,23	0
55	MG	DA	3040	1/1	1.00	0.04	36,36,36,36	0
55	MG	DA	3041	1/1	1.00	0.12	11,11,11,11	0
55	MG	DA	3042	1/1	1.00	0.03	29,29,29,29	0
55	MG	AA	1632	1/1	1.00	0.02	65,65,65,65	0
55	MG	CA	3015	1/1	1.00	0.13	57,57,57,57	0
55	MG	DA	3045	1/1	1.00	0.04	49,49,49,49	0
55	MG	DA	3046	1/1	1.00	0.03	31,31,31,31	0
55	MG	AA	1640	1/1	1.00	0.05	52,52,52,52	0
55	MG	DA	3048	1/1	1.00	0.03	26,26,26,26	0
55	MG	AA	1666	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3050	1/1	1.00	0.02	18,18,18,18	0
55	MG	DA	3051	1/1	1.00	0.02	14,14,14,14	0
55	MG	BA	1611	1/1	1.00	0.04	56,56,56,56	0
55	MG	DA	3053	1/1	1.00	0.04	44,44,44,44	0
55	MG	DA	3004	1/1	1.00	0.03	60,60,60,60	0
55	MG	DA	3055	1/1	1.00	0.06	24,24,24,24	0
55	MG	DA	3056	1/1	1.00	0.03	42,42,42,42	0
55	MG	DA	3057	1/1	1.00	0.03	13,13,13,13	0
55	MG	DA	3058	1/1	1.00	0.02	32,32,32,32	0
55	MG	DA	3059	1/1	1.00	0.01	23,23,23,23	0
55	MG	DA	3060	1/1	1.00	0.04	21,21,21,21	0
55	MG	DA	3061	1/1	1.00	0.03	30,30,30,30	0
55	MG	DA	3005	1/1	1.00	0.07	60,60,60,60	0
55	MG	AA	1652	1/1	1.00	0.14	21,21,21,21	0
55	MG	AA	1646	1/1	1.00	0.02	49,49,49,49	0
55	MG	DA	3065	1/1	1.00	0.03	19,19,19,19	0
55	MG	DA	3066	1/1	1.00	0.07	40,40,40,40	0

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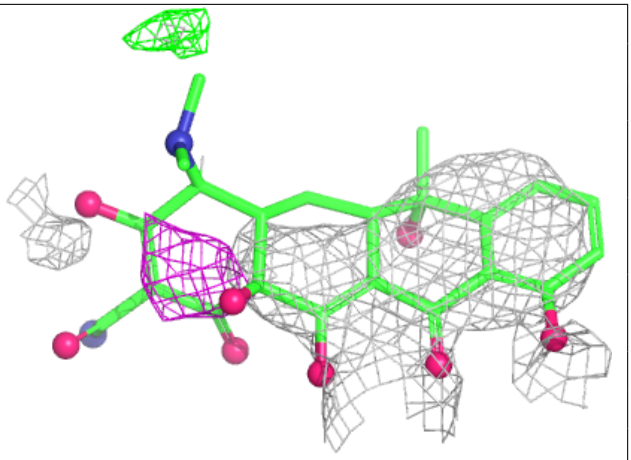
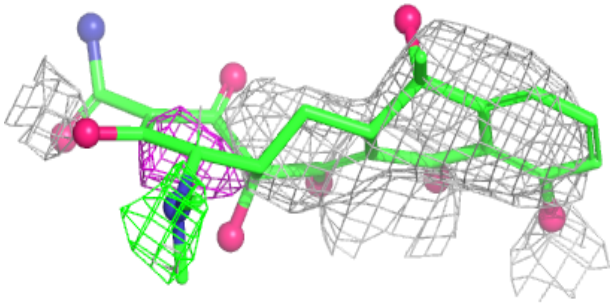
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3067	1/1	1.00	0.03	36,36,36,36	0
55	MG	DA	3068	1/1	1.00	0.05	35,35,35,35	0
55	MG	DA	3069	1/1	1.00	0.09	46,46,46,46	0
55	MG	CA	3041	1/1	1.00	0.04	50,50,50,50	0
55	MG	DA	3071	1/1	1.00	0.07	34,34,34,34	0
55	MG	DA	3009	1/1	1.00	0.03	23,23,23,23	0
55	MG	DA	3073	1/1	1.00	0.01	31,31,31,31	0
55	MG	DA	3010	1/1	1.00	0.04	17,17,17,17	0
55	MG	DA	3075	1/1	1.00	0.04	37,37,37,37	0
55	MG	DA	3076	1/1	1.00	0.02	23,23,23,23	0
55	MG	DA	3077	1/1	1.00	0.01	30,30,30,30	0
55	MG	DA	3011	1/1	1.00	0.02	33,33,33,33	0
55	MG	DD	301	1/1	1.00	0.04	40,40,40,40	0
55	MG	DA	3013	1/1	1.00	0.04	19,19,19,19	0
55	MG	DA	3081	1/1	1.00	0.04	45,45,45,45	0
55	MG	DA	3014	1/1	1.00	0.02	14,14,14,14	0
55	MG	DM	202	1/1	1.00	0.05	34,34,34,34	0
55	MG	DA	3084	1/1	1.00	0.06	35,35,35,35	0

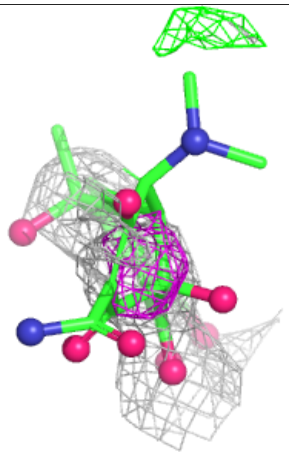
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TAC BA 1644:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

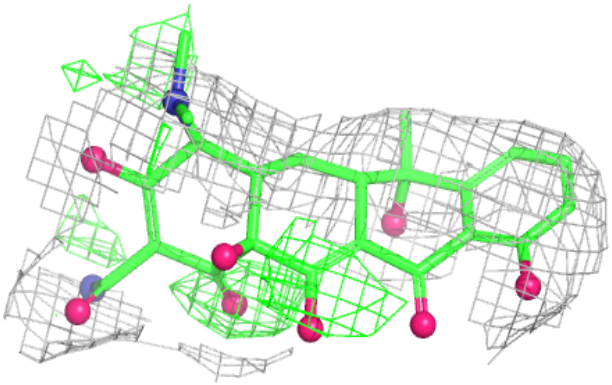


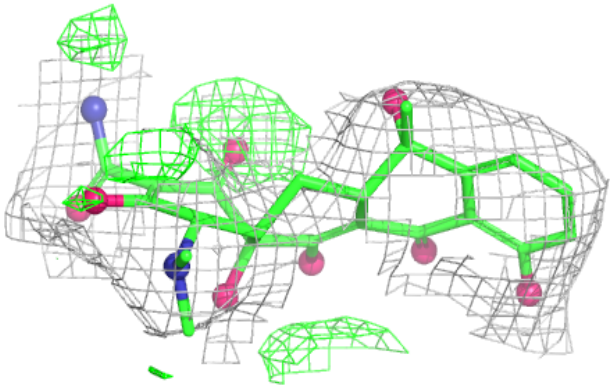


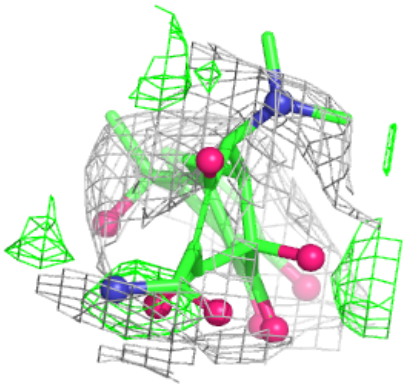


Electron density around TAC BA 1643:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

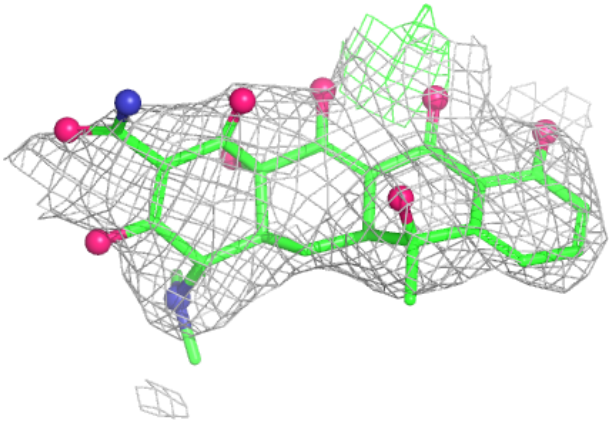


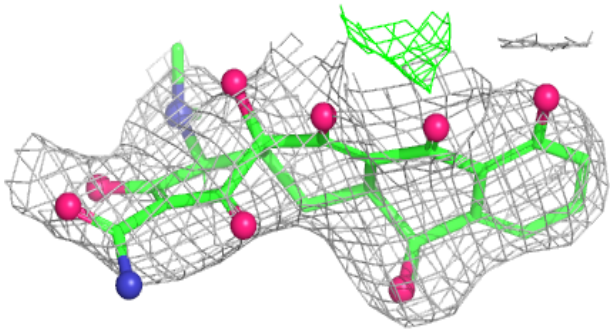


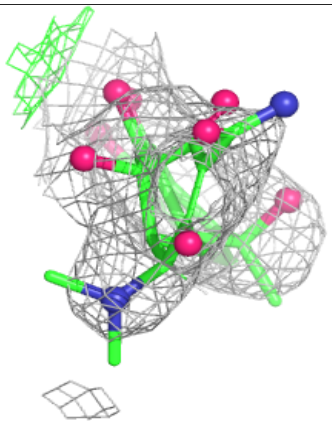


Electron density around TAC AA 1681:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

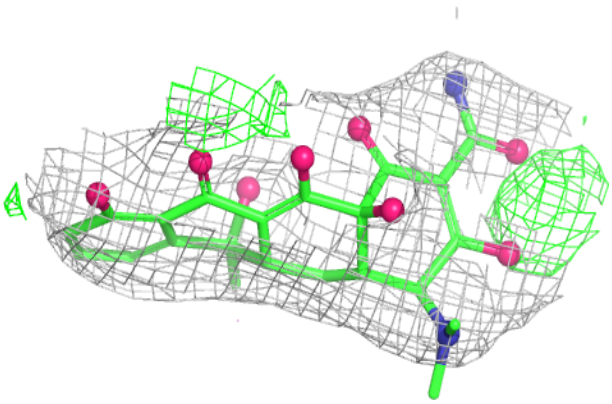


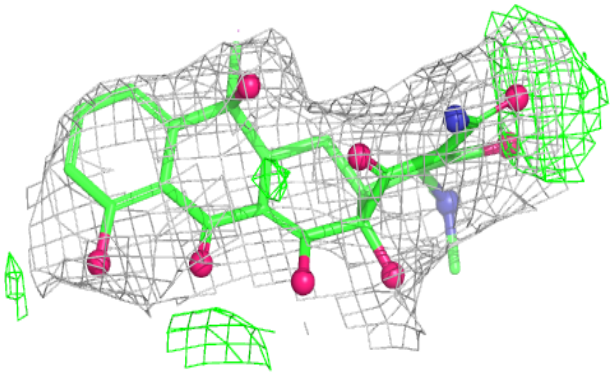


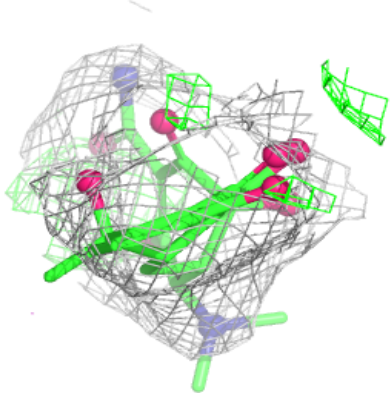


Electron density around TAC AA 1680:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.