



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:05 am BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

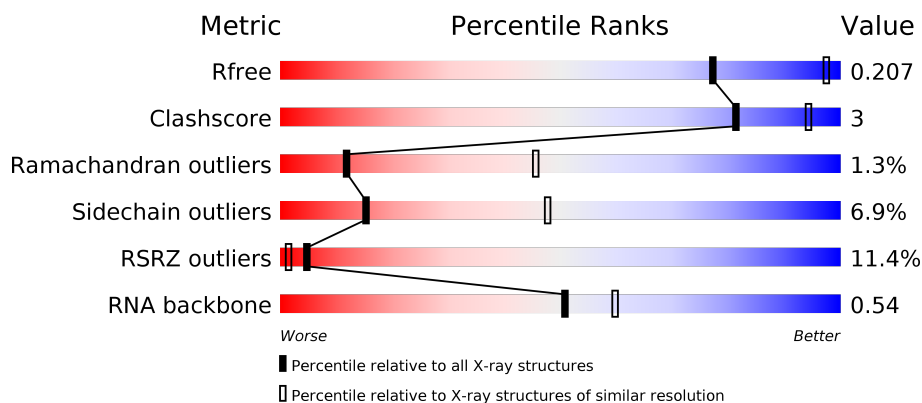
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	BA	1534	<div> <div>11%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
2	AB	224	<div> <div>13%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
2	BB	224	<div> <div>16%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	% 84% 15%
3	BC	206	19% 81% 19%
4	AD	205	89% 10% .
4	BD	205	86% 12% .
5	AE	155	78% 19% .
5	BE	155	% 65% 26% 5% . .
6	AF	106	% 81% 19%
6	BF	106	2% 69% 24% . 6%
7	AG	151	20% 83% 16% .
7	BG	151	51% 83% 17%
8	AH	129	% 83% 16% .
8	BH	129	3% 83% 17%
9	AI	127	21% 87% 13% .
9	BI	127	39% 87% 12% .
10	AJ	99	11% 77% 21% .
10	BJ	99	60% 74% 21% . .
11	AK	117	4% 83% 16% .
11	BK	117	3% 76% 23% .
12	AL	123	% 89% 10% .
12	BL	123	3% 84% 13% .
13	AM	114	30% 80% 18% .
13	BM	114	76% 72% 25% .
14	AN	100	17% 87% 12% .
14	BN	100	52% 89% 11%
15	AO	88	% 92% 8%

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

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
30	DD	209	
31	CA	2904	
32	CE	201	
32	DE	201	
33	CF	177	
33	DF	177	
34	CG	176	
34	DG	176	
35	CH	149	
35	DH	149	
36	CJ	134	
36	DJ	134	
37	CK	142	
37	DK	142	
38	CL	123	
38	DL	123	
39	CM	144	
39	DM	144	
40	CN	136	
40	DN	136	

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

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Mol	Chain	Length	Quality of chain
54	DA	2904	

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	1616	-	-	-	X
55	MG	AA	1621	-	-	-	X
55	MG	AA	1622	-	-	-	X
55	MG	AA	1624	-	-	-	X
55	MG	AA	1626	-	-	-	X
55	MG	BA	1637	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	BA	1639	-	-	-	X
55	MG	CA	3003	-	-	-	X
55	MG	CA	3005	-	-	-	X
55	MG	CA	3060	-	-	-	X
55	MG	CA	3075	-	-	-	X
55	MG	CA	3077	-	-	-	X
55	MG	CA	3113	-	-	-	X
55	MG	CA	3116	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3123	-	-	-	X
55	MG	CA	3131	-	-	-	X
55	MG	CA	3133	-	-	-	X
55	MG	CA	3134	-	-	-	X
55	MG	CA	3135	-	-	-	X
55	MG	CA	3154	-	-	-	X
55	MG	DA	3144	-	-	-	X
55	MG	DA	3170	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DE	301	-	-	-	X
57	MPD	DN	201	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	AA	1675	-	-	-	X
58	PUT	DA	3195	-	-	-	X
59	TAC	BA	1644	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	101	-	-	-	X
61	PEG	DP	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PEG	DQ	201	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	DA	3001	-	-	-	X

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 28 is a RNA chain called 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	0	0	0
			892	552	178	162			
42	DP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- 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	0	0
			917	574	179	163	1		
43	DQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

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

- 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	0	0
			816	516	153	145	2		
45	DS	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- 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	0	0
			857	532	166	156	3		
46	DT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- 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	0	0
			739	466	139	132	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

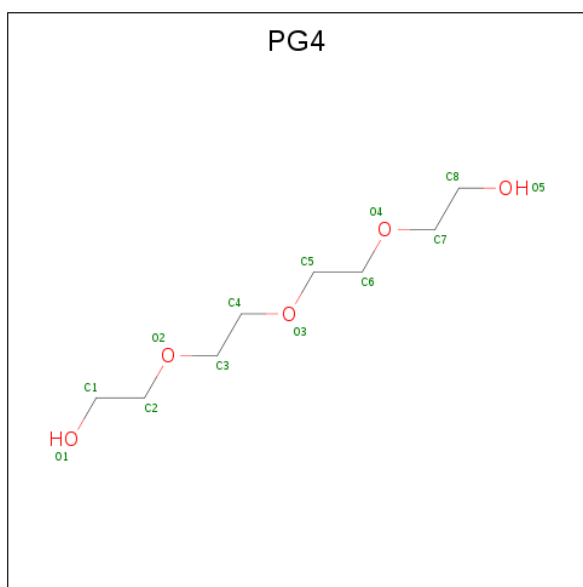
- Molecule 54 is a RNA chain called 23S rRNA.

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

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

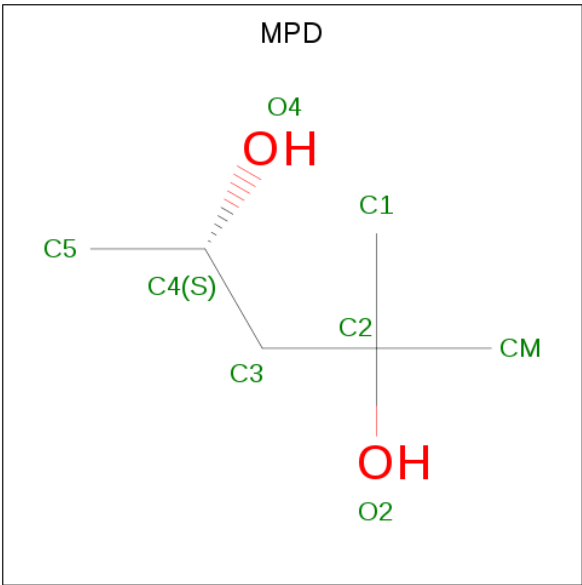
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	45	Total	Mg	0	0
			45	45		
55	CA	156	Total	Mg	0	0
			156	156		
55	CB	3	Total	Mg	0	0
			3	3		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	AA	72	Total	Mg	0	0
			72	72		
55	DA	183	Total	Mg	0	0
			183	183		
55	DB	9	Total	Mg	0	0
			9	9		
55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

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



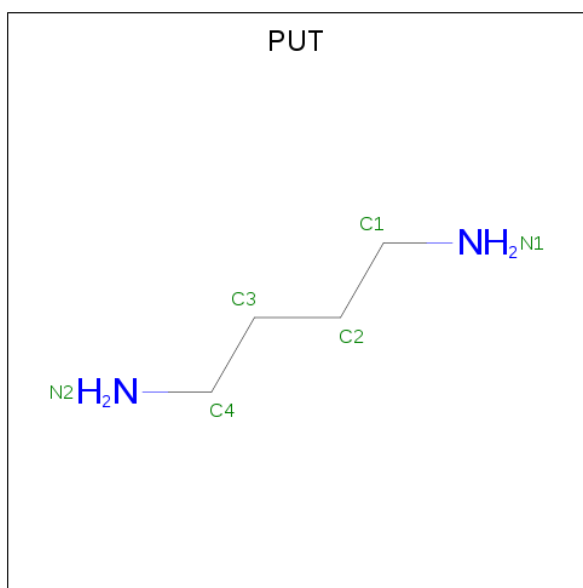
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		
56	DQ	1	Total	C	O	0	0
			13	8	5		
56	DR	1	Total	C	O	0	0
			13	8	5		
56	DS	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		

- 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		

- Molecule 58 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



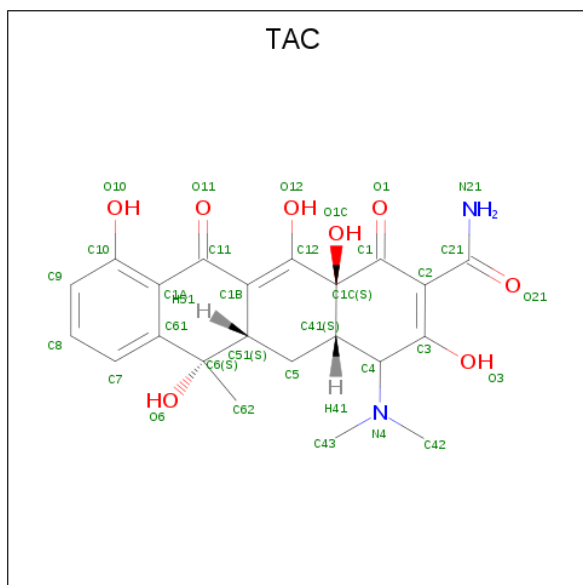
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	DM	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6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

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

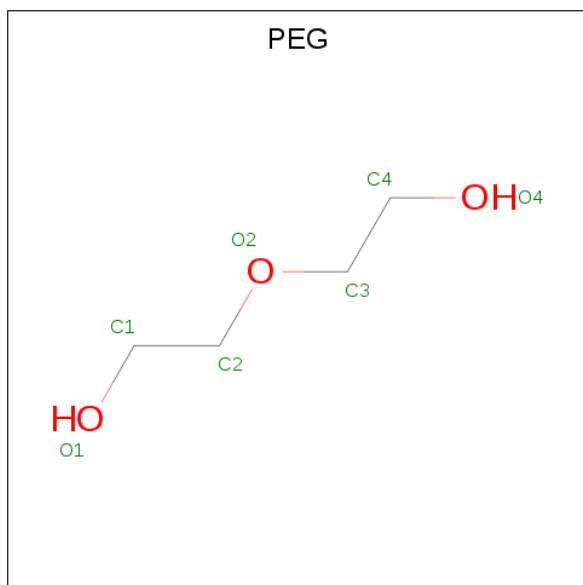
- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula:  $C_{22}H_{24}N_2O_8$ ).



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

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



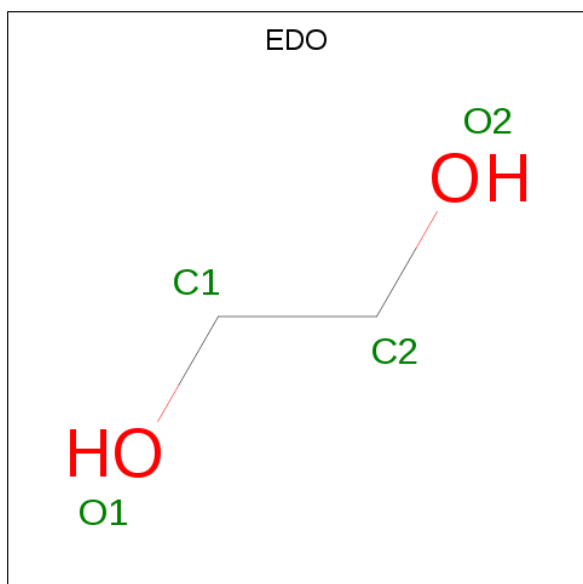
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7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

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

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



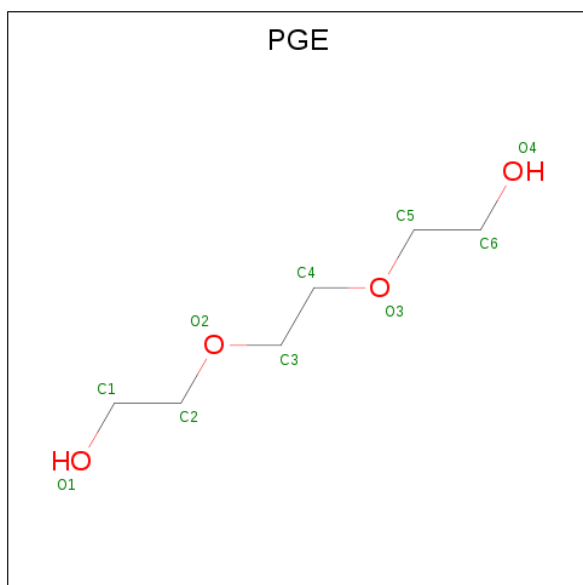
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

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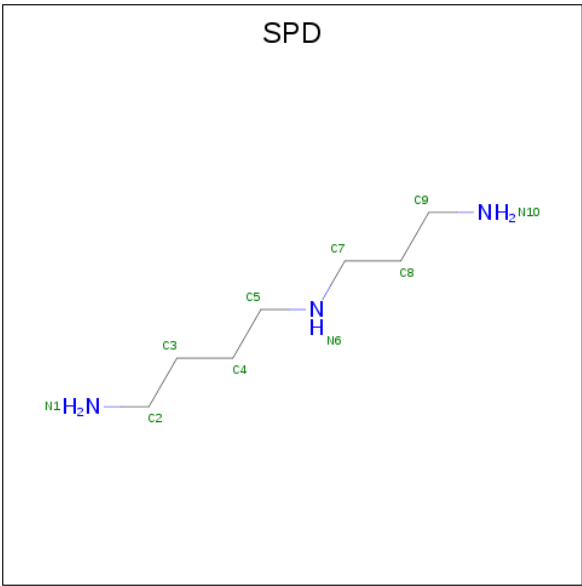
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

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



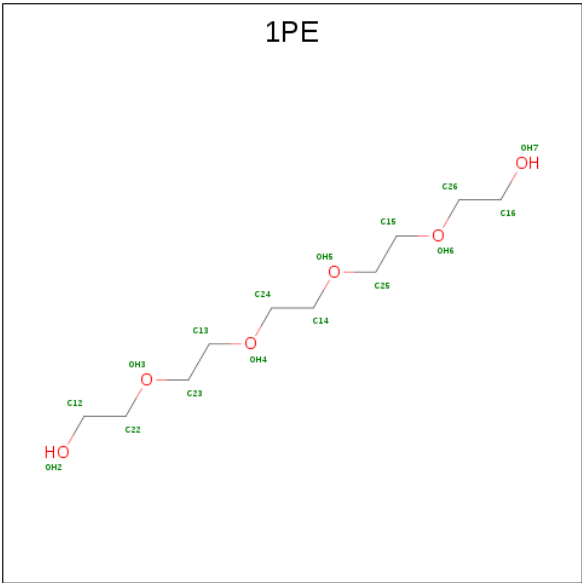
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0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

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



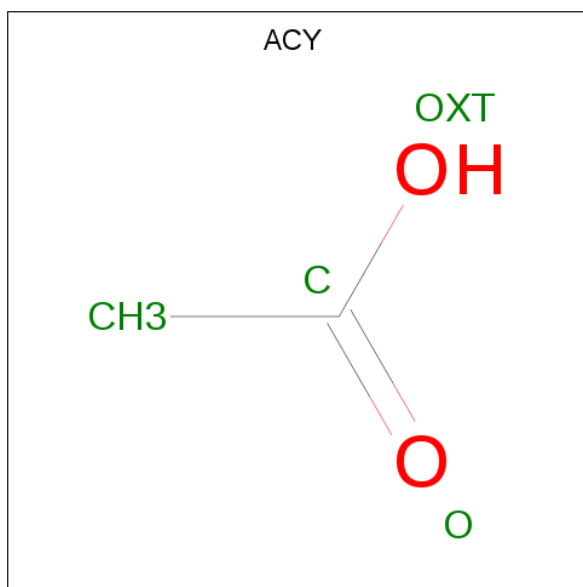
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



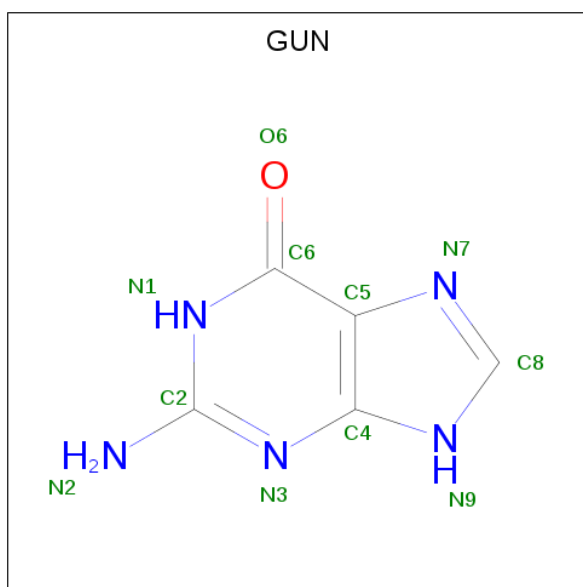
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

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



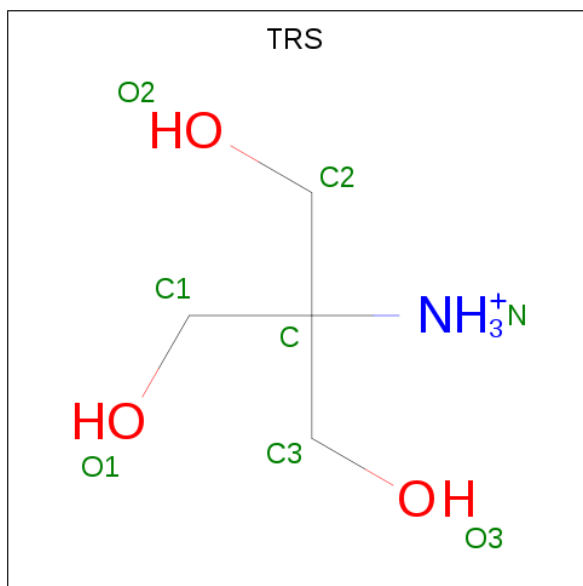
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

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



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

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



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

- Molecule 69 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BK	2	Total 2	O 2	0	0
69	BL	4	Total 4	O 4	0	0
69	BN	2	Total 2	O 2	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BT	2	Total 2	O 2	0	0
69	BU	2	Total 2	O 2	0	0
69	D1	43	Total 43	O 43	0	0
69	D2	6	Total 6	O 6	0	0
69	D3	22	Total 22	O 22	0	0
69	D4	39	Total 39	O 39	0	0
69	D5	8	Total 8	O 8	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	6	Total 6	O 6	0	0
69	CA	691	Total 691	O 691	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	98	Total 98	O 98	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0

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

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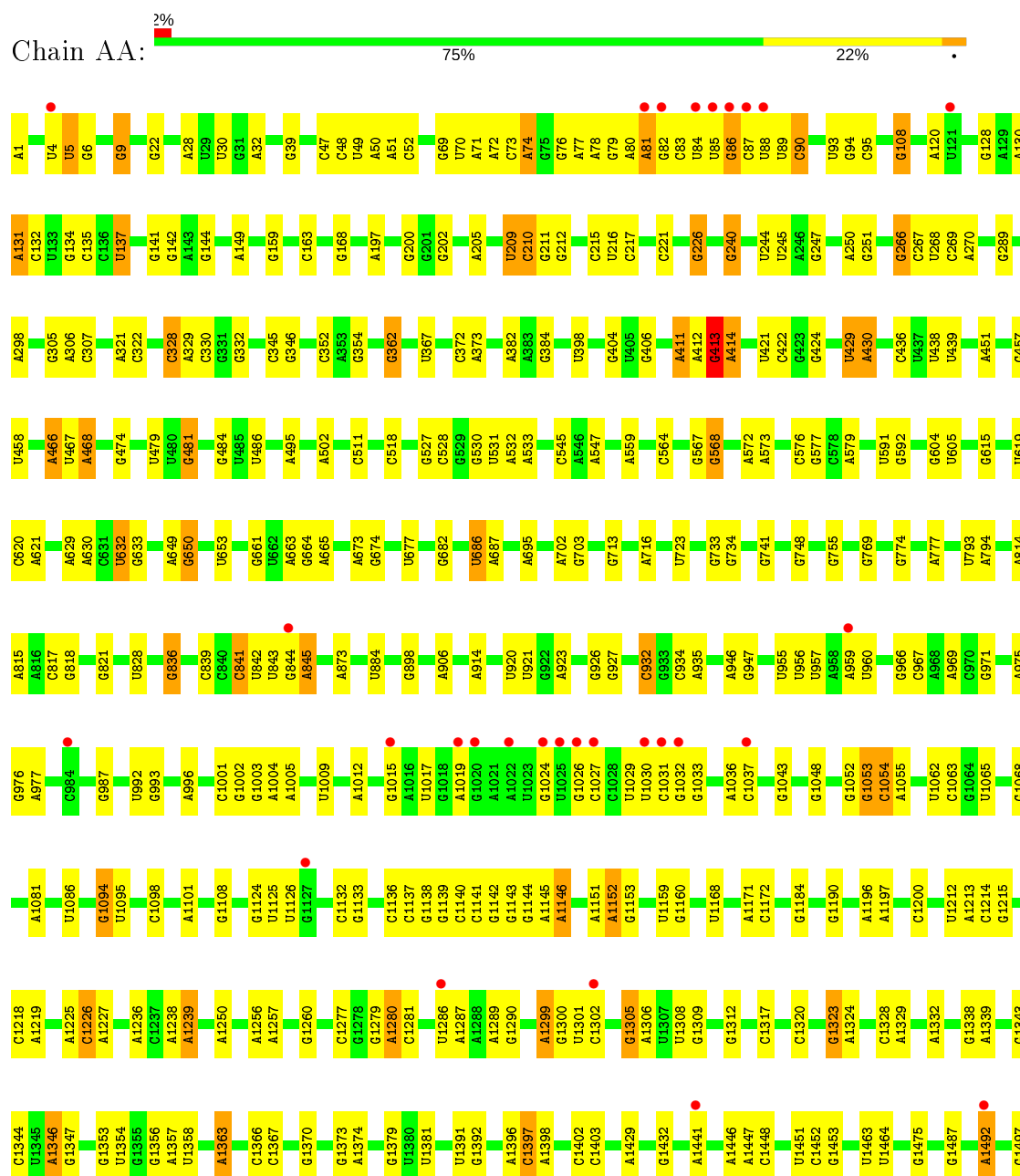
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DV	20	Total 20	O 20	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	25	Total 25	O 25	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	8	Total 8	O 8	0	0
69	DB	209	Total 209	O 209	0	0
69	DA	4840	Total 4840	O 4840	0	0

### 3 Residue-property plots [i](#)

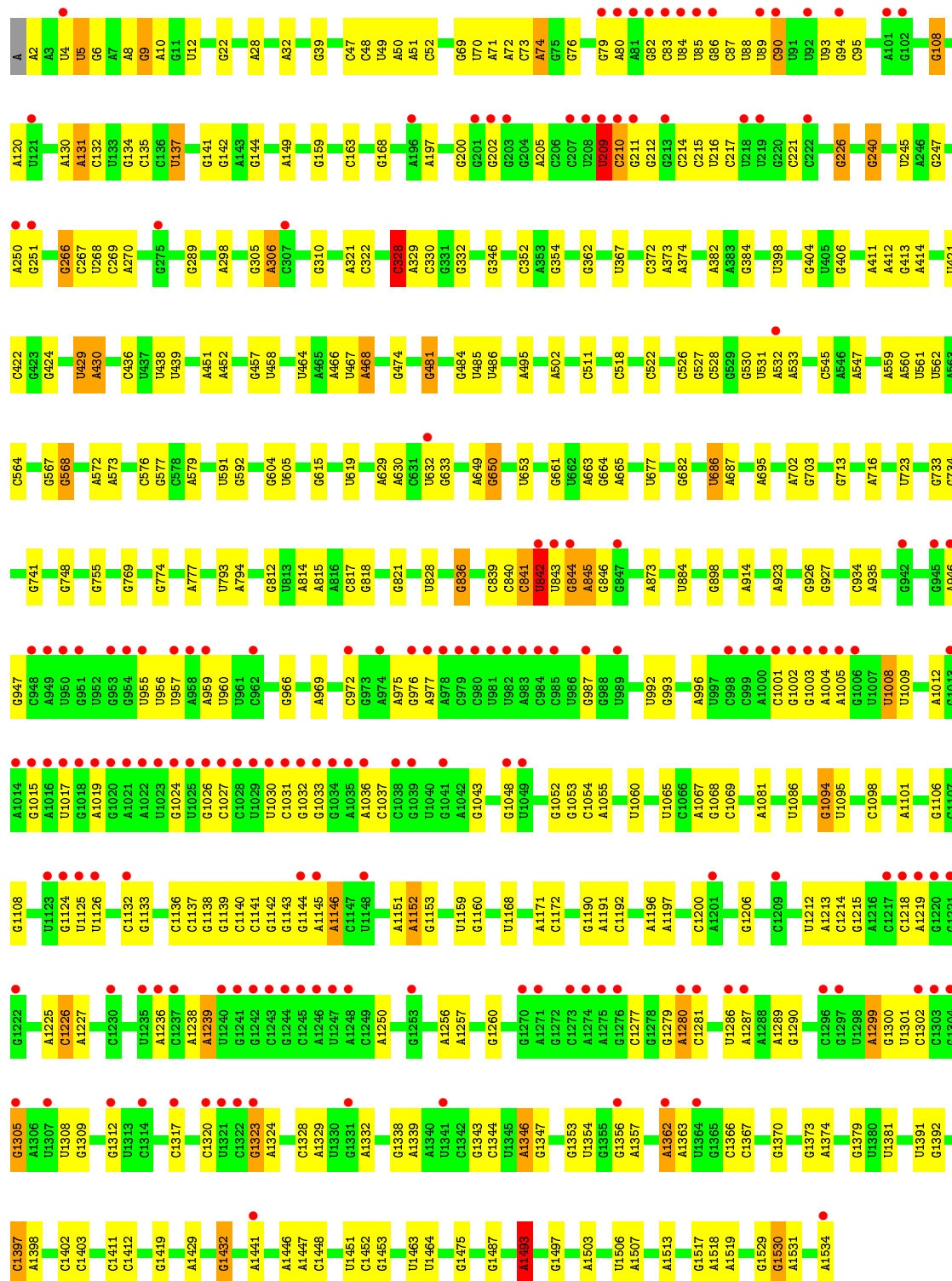
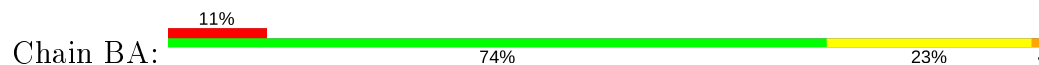
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA

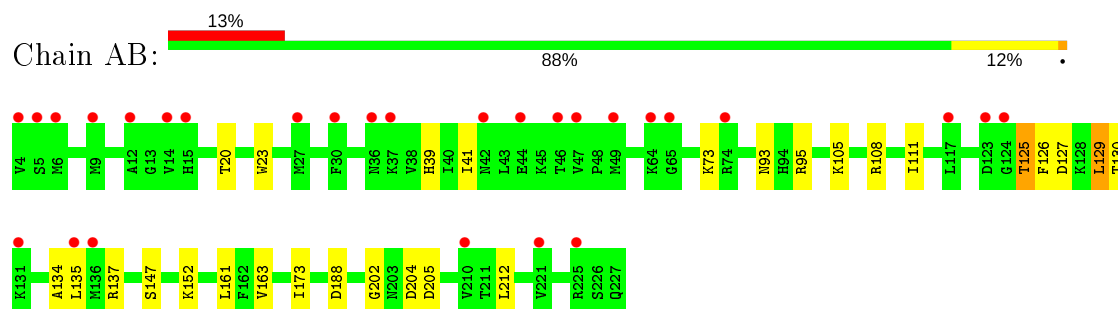




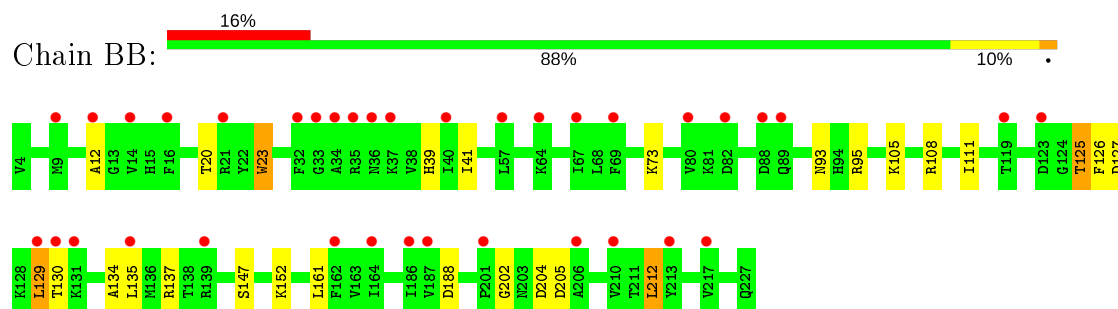
● Molecule 1: 16S rRNA



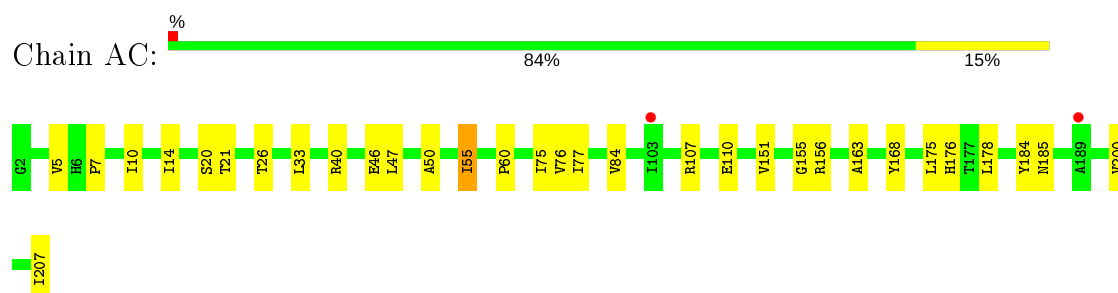
- Molecule 2: 30S ribosomal protein S2



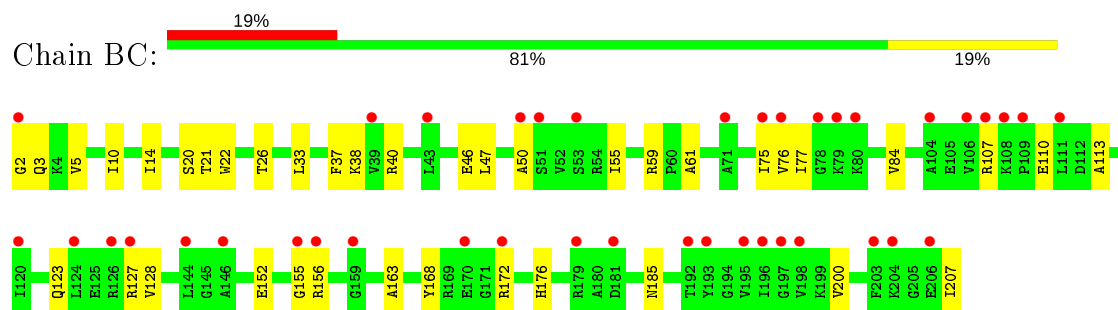
- Molecule 2: 30S ribosomal protein S2



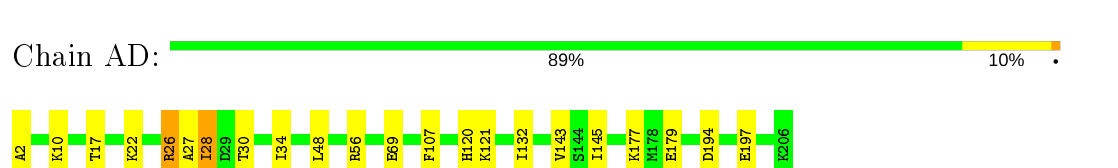
- Molecule 3: 30S ribosomal protein S3




- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4




- Molecule 4: 30S ribosomal protein S4

Chain BD:  86% 12% .



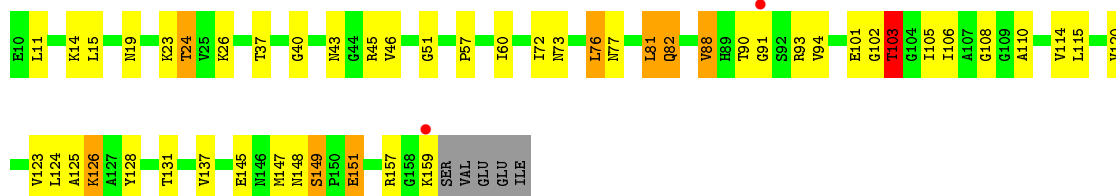
- Molecule 5: 30S ribosomal protein S5

Chain AE:  78% 19% .




- Molecule 5: 30S ribosomal protein S5

Chain BE:  65% 26% 5% . .



- Molecule 6: 30S ribosomal protein S6

Chain AF:  81% 19%




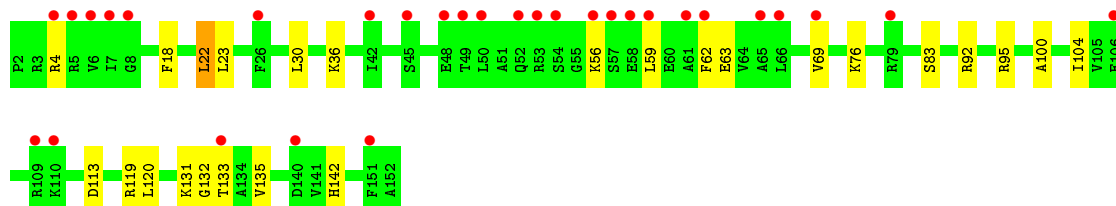
- Molecule 6: 30S ribosomal protein S6

Chain BF:  69% 24% 6%



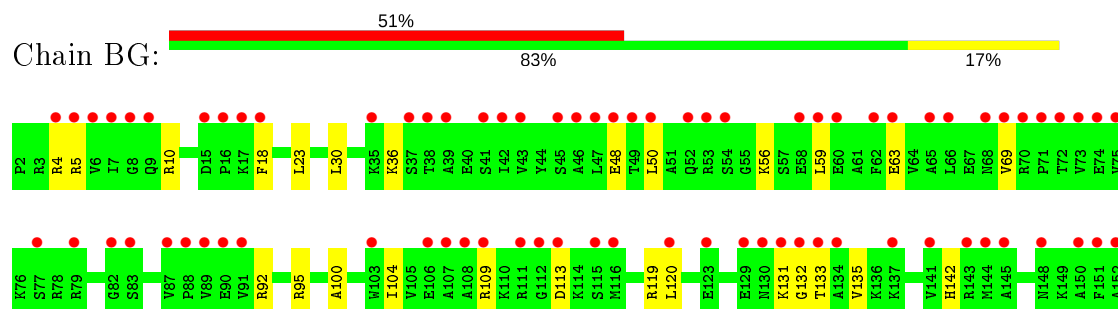
- Molecule 7: 30S ribosomal protein S7

Chain AG:  20% 83% 16% .



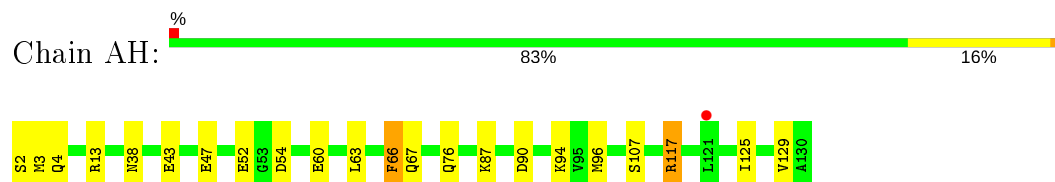
- Molecule 7: 30S ribosomal protein S7

Chain BG:



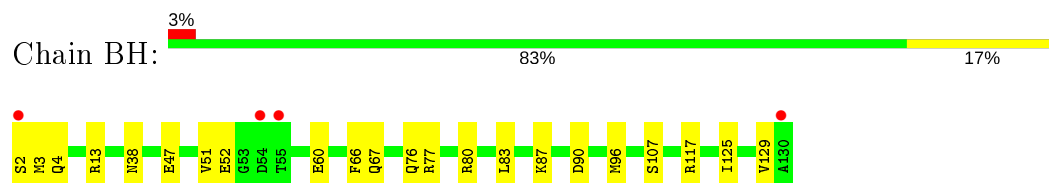
- Molecule 8: 30S ribosomal protein S8

Chain AH:



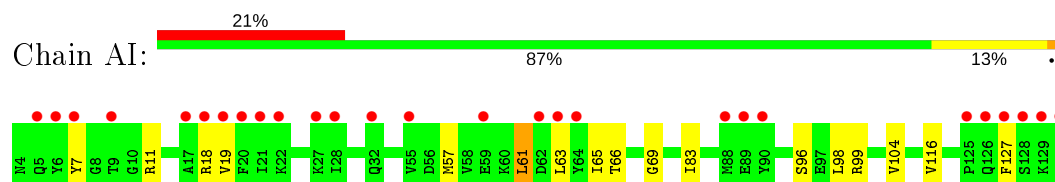
- Molecule 8: 30S ribosomal protein S8

Chain BH:



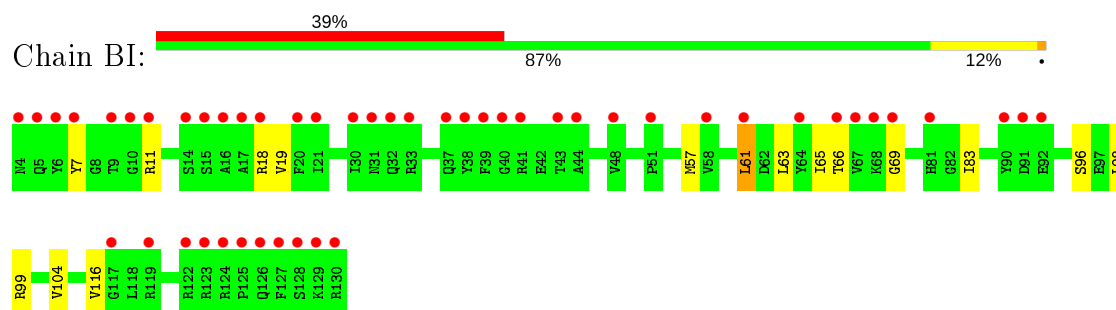
- Molecule 9: 30S ribosomal protein S9

Chain AI:



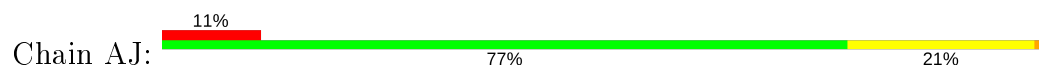
- Molecule 9: 30S ribosomal protein S9

Chain BI:



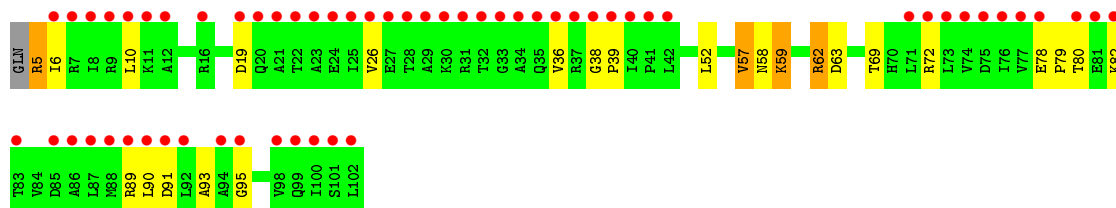
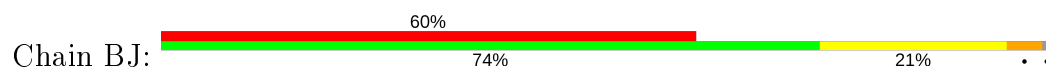
- Molecule 10: 30S ribosomal protein S10

Chain AJ:

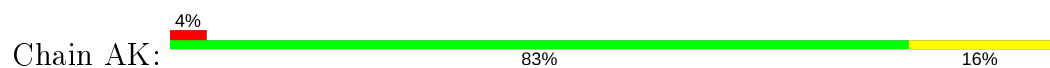




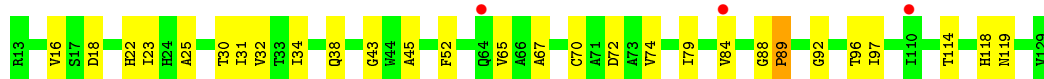
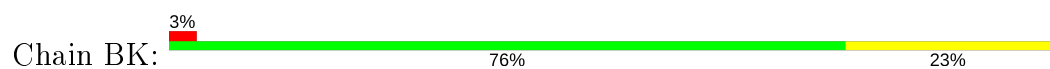
- Molecule 10: 30S ribosomal protein S10



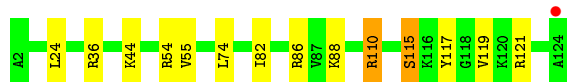
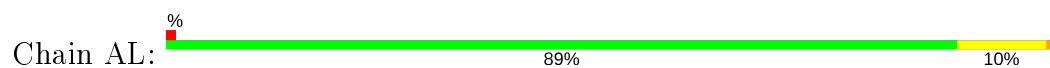
- Molecule 11: 30S ribosomal protein S11



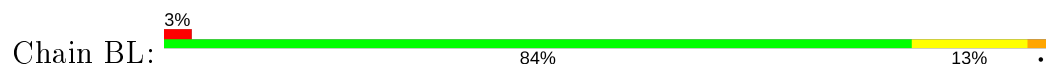
- Molecule 11: 30S ribosomal protein S11



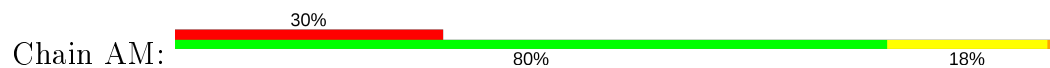
- Molecule 12: 30S ribosomal protein S12

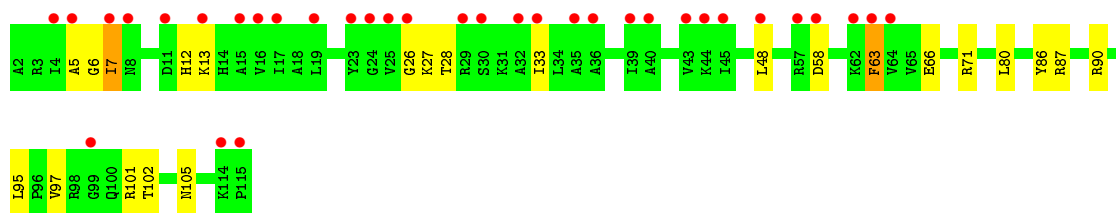


- Molecule 12: 30S ribosomal protein S12

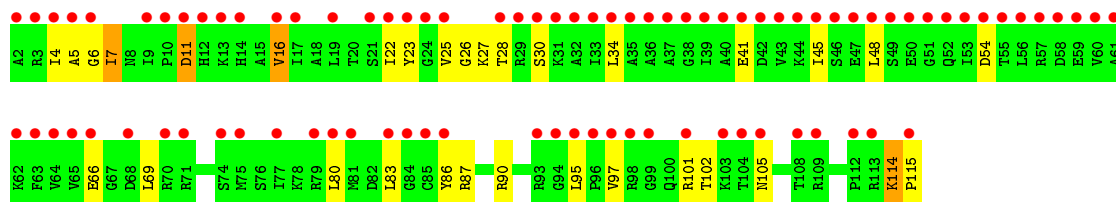
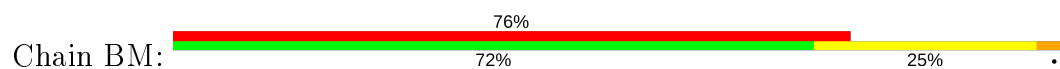


- Molecule 13: 30S ribosomal protein S13

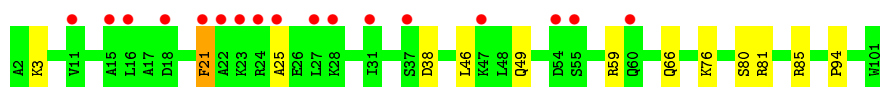
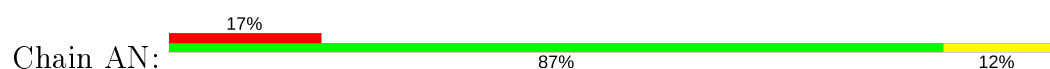




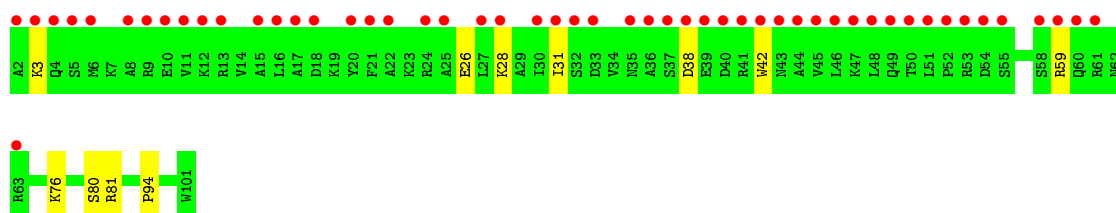
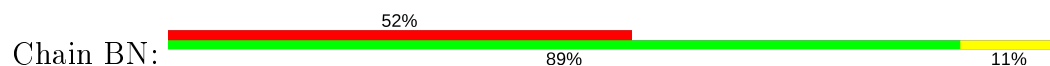
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14



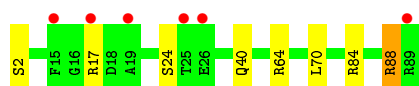
• Molecule 14: 30S ribosomal protein S14



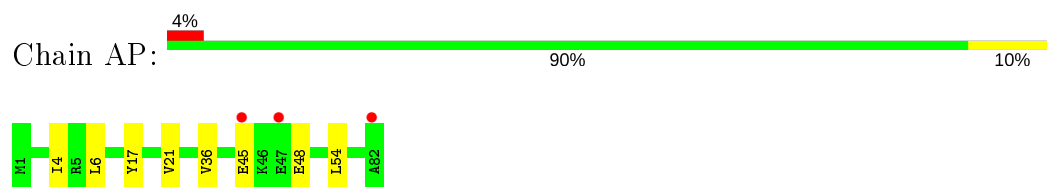
• Molecule 15: 30S ribosomal protein S15



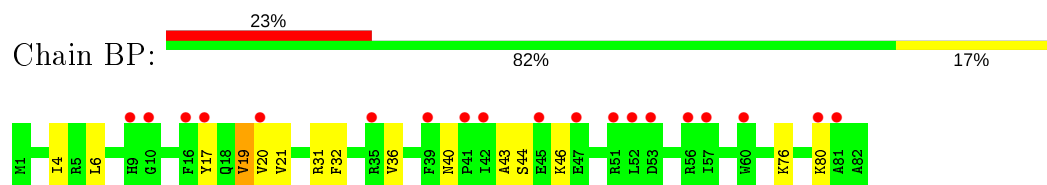
• Molecule 15: 30S ribosomal protein S15



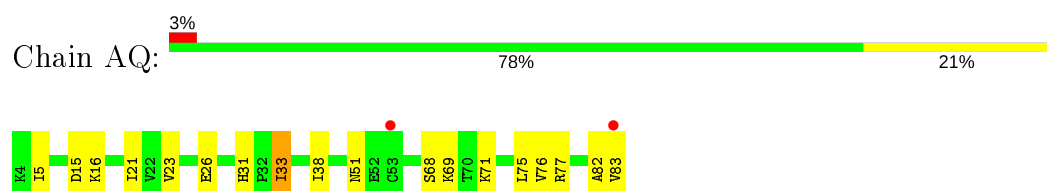
## ● Molecule 16: 30S ribosomal protein S16



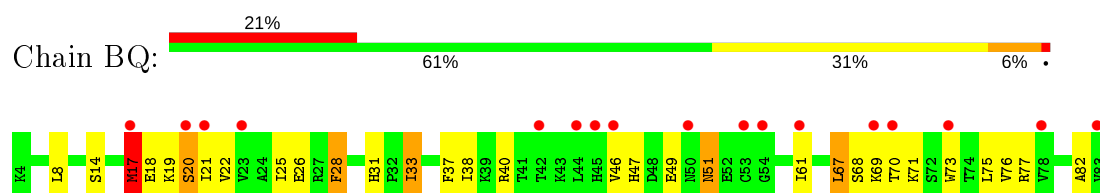
## ● Molecule 16: 30S ribosomal protein S16



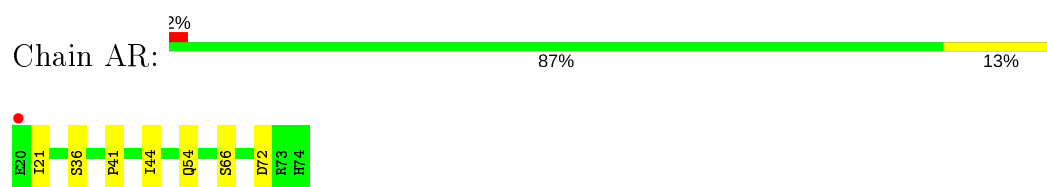
## ● Molecule 17: 30S ribosomal protein S17



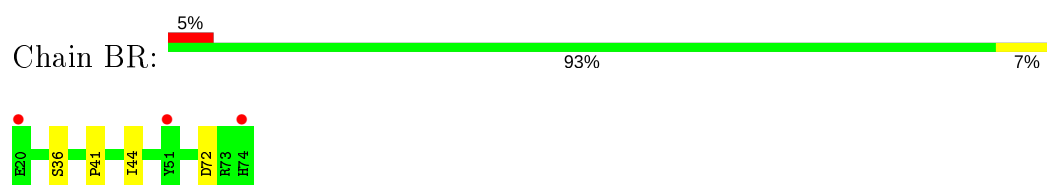
## ● Molecule 17: 30S ribosomal protein S17



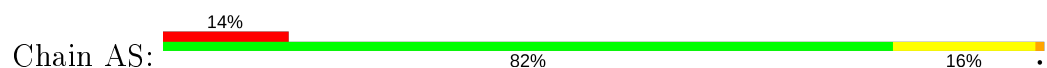
## ● Molecule 18: 30S ribosomal protein S18

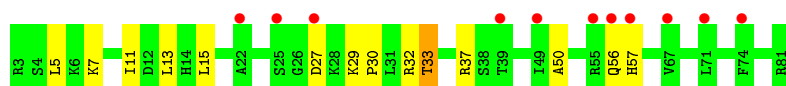


## ● Molecule 18: 30S ribosomal protein S18

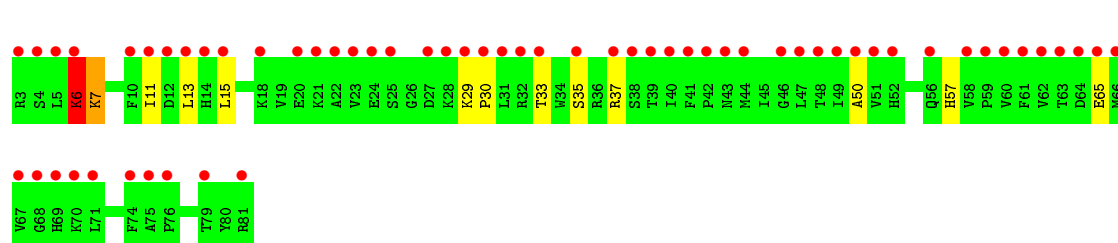
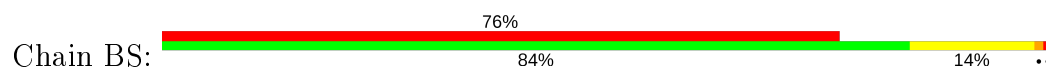


## ● Molecule 19: 30S ribosomal protein S19

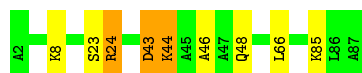




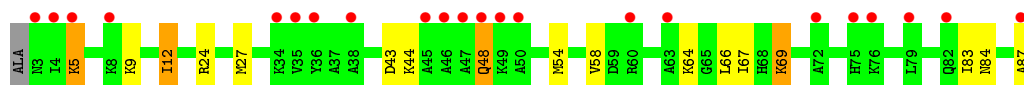
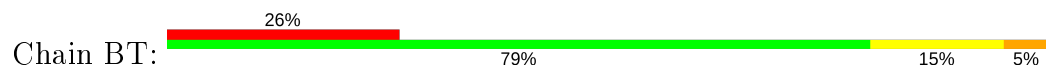
- Molecule 19: 30S ribosomal protein S19



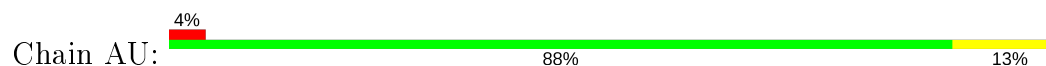
- Molecule 20: 30S ribosomal protein S20



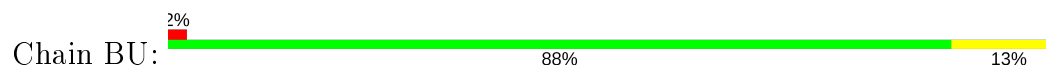
- Molecule 20: 30S ribosomal protein S20



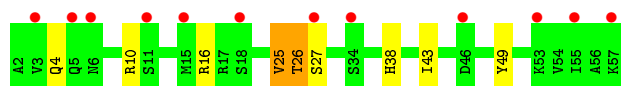
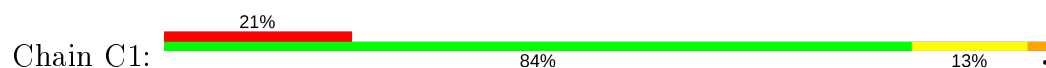
- Molecule 21: 30S ribosomal protein S21




- Molecule 21: 30S ribosomal protein S21

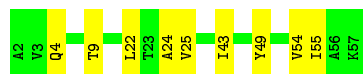


- Molecule 22: 50S ribosomal protein L32



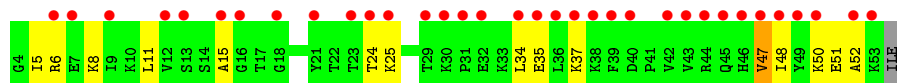
- Molecule 22: 50S ribosomal protein L32

Chain D1:  84% 16%



- Molecule 23: 50S ribosomal protein L33

Chain C2:  67% 69% 27% ..




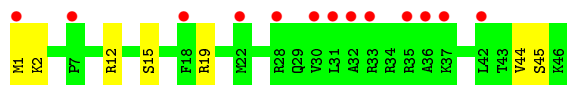
- Molecule 23: 50S ribosomal protein L33

Chain D2:  73% 25% .



- Molecule 24: 50S ribosomal protein L34

Chain C3:  28% 85% 15%




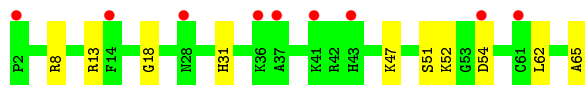
- Molecule 24: 50S ribosomal protein L34

Chain D3:  89% 11%



- Molecule 25: 50S ribosomal protein L35

Chain C4:  14% 84% 16%

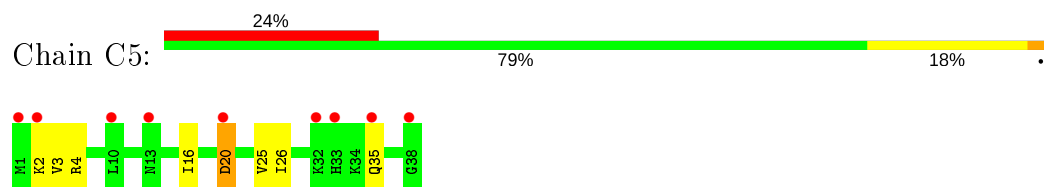


- Molecule 25: 50S ribosomal protein L35

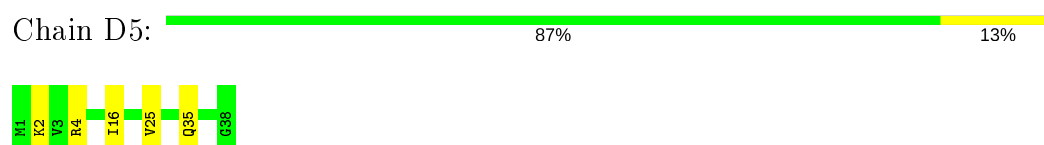
Chain D4:  91% 9%



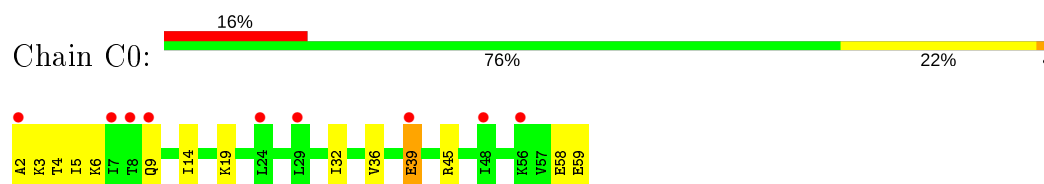
- Molecule 26: 50S ribosomal protein L36



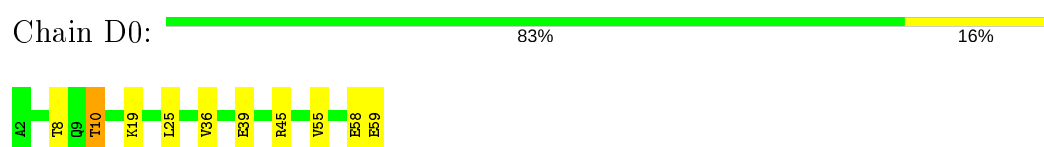
- Molecule 26: 50S ribosomal protein L36



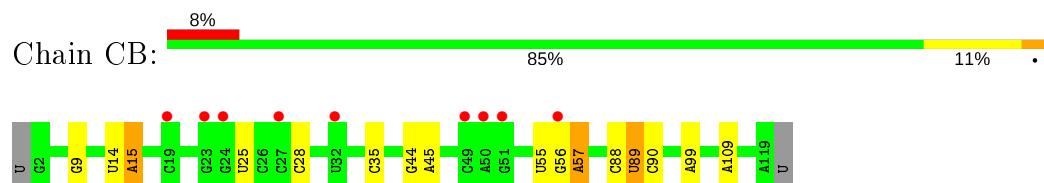
- Molecule 27: 50S ribosomal protein L30



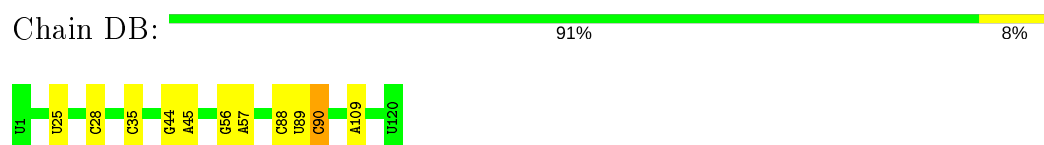
- Molecule 27: 50S ribosomal protein L30



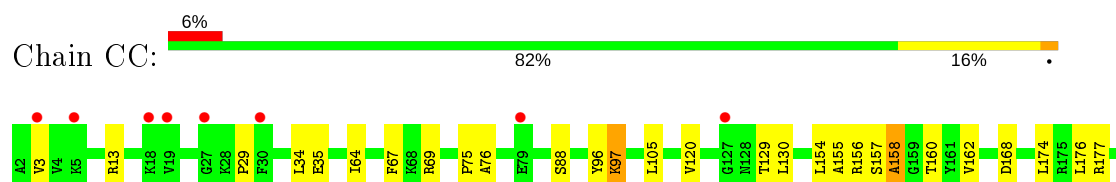
- Molecule 28: 5S rRNA



- Molecule 28: 5S rRNA

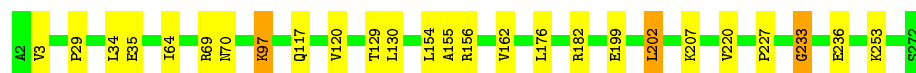


- Molecule 29: 50S ribosomal protein L2

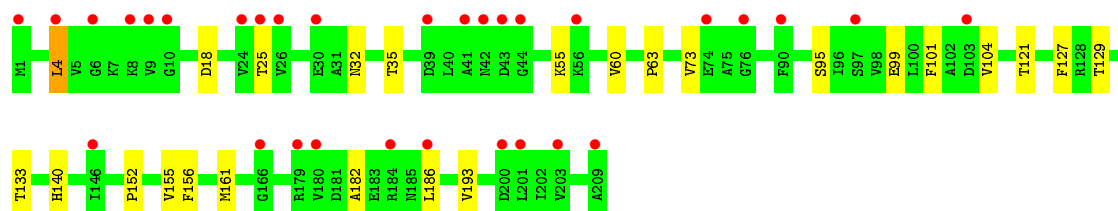
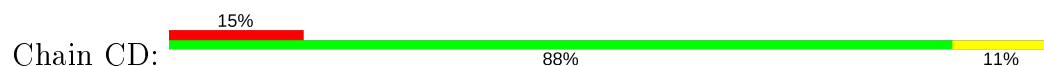




- Molecule 29: 50S ribosomal protein L2



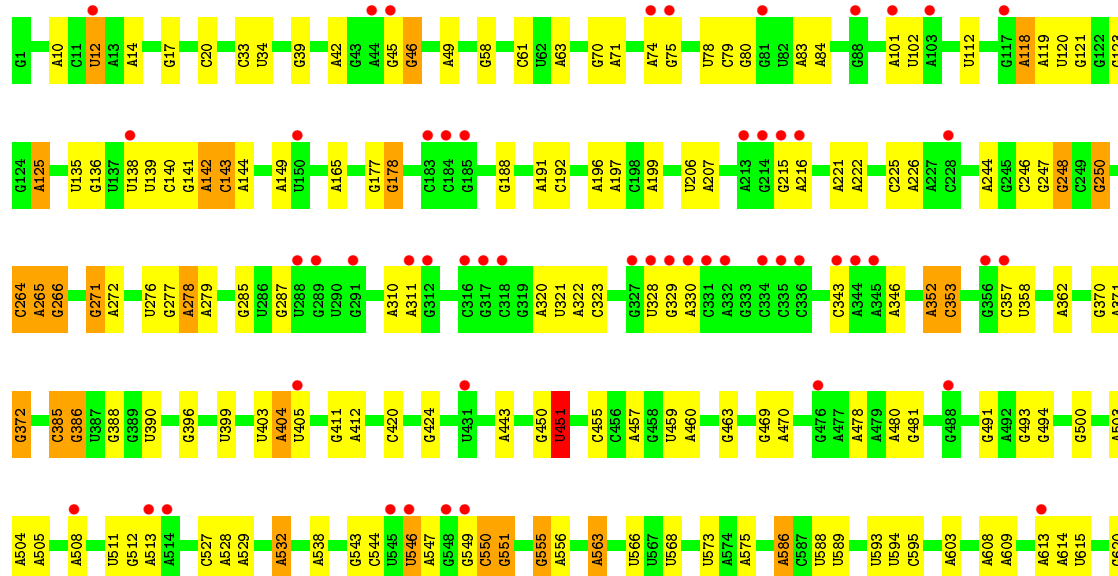
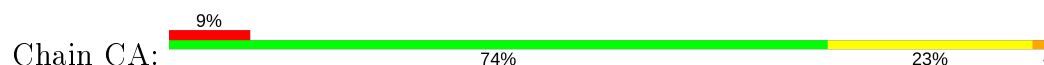
- Molecule 30: 50S ribosomal protein L3

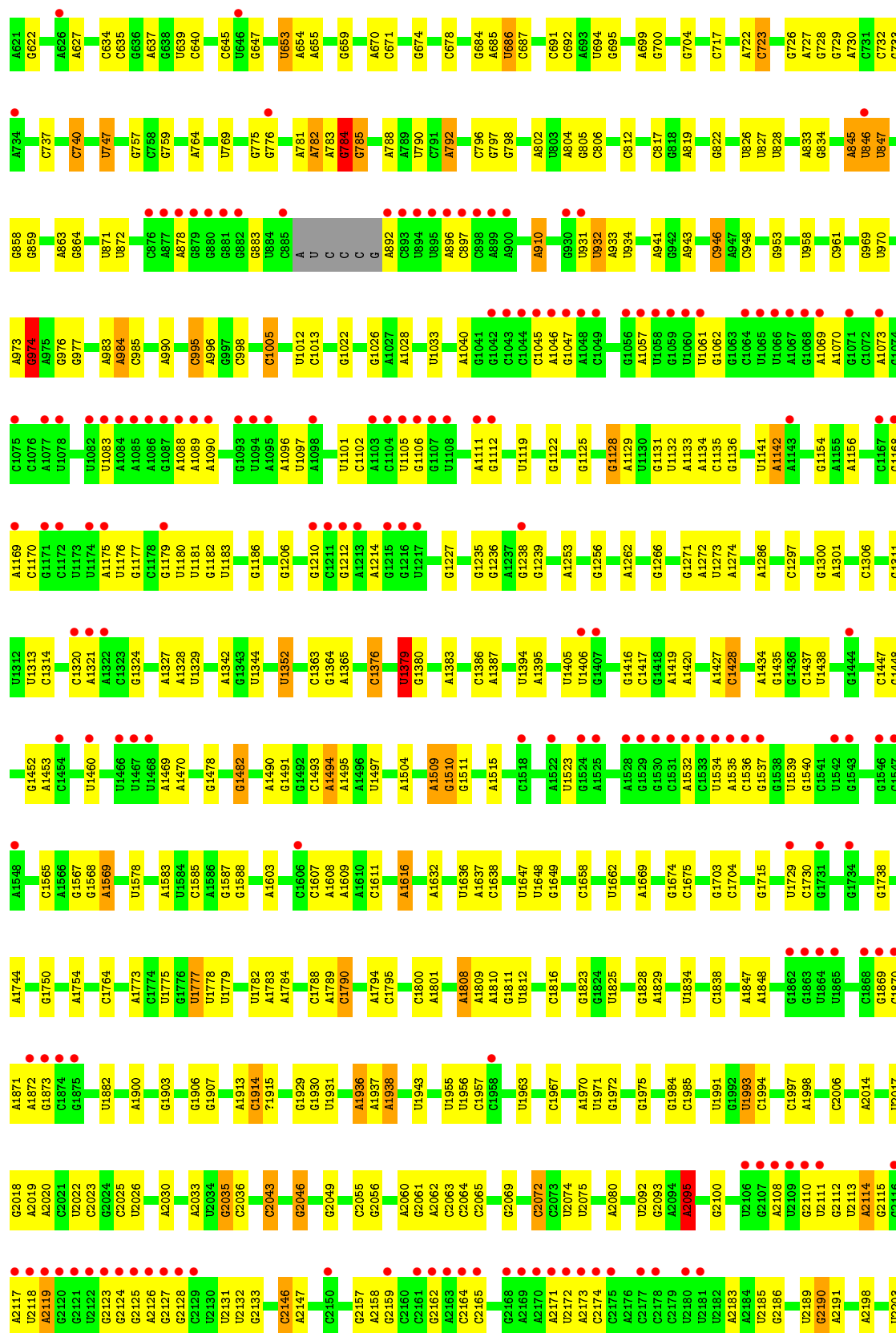


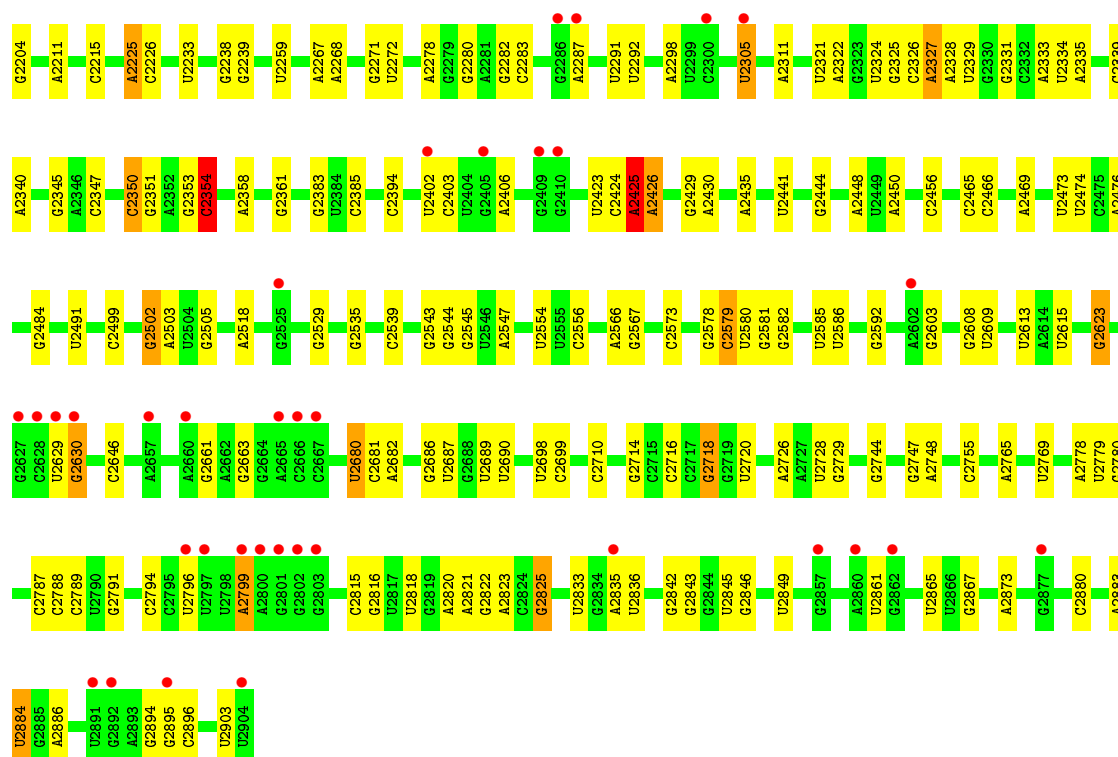
- Molecule 30: 50S ribosomal protein L3



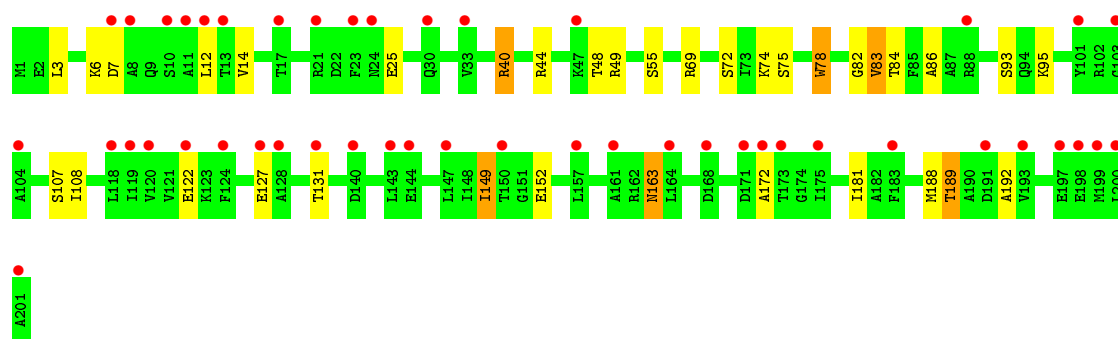
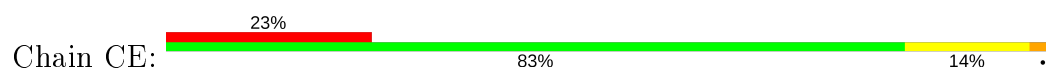
- Molecule 31: 23S rRNA







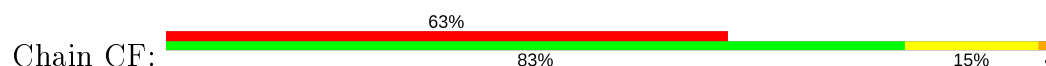
• Molecule 32: 50S ribosomal protein L4

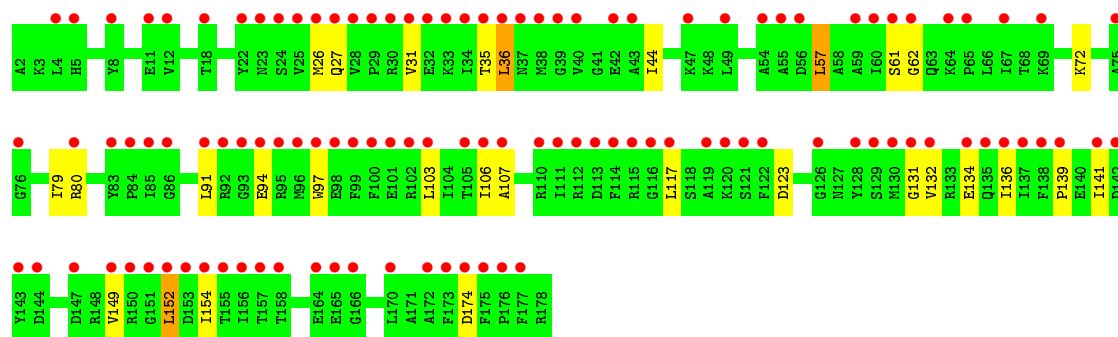


• Molecule 32: 50S ribosomal protein L4

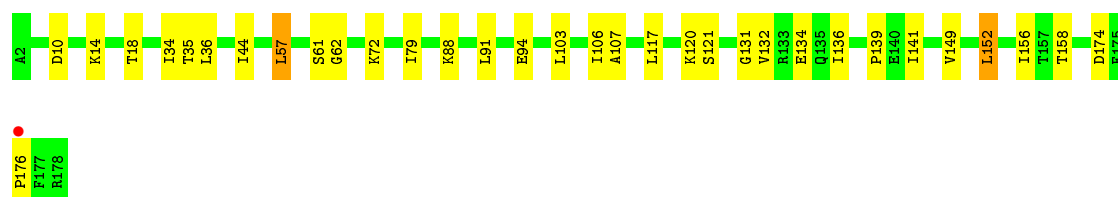
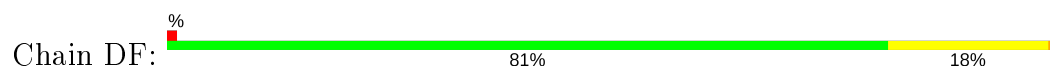


• Molecule 33: 50S ribosomal protein L5

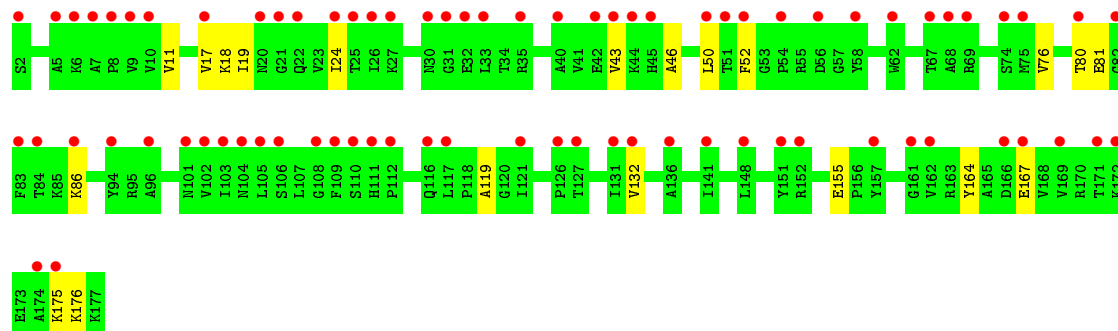
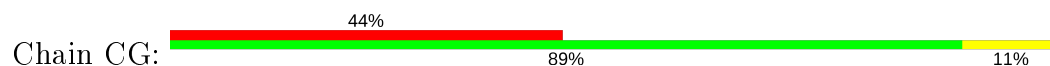




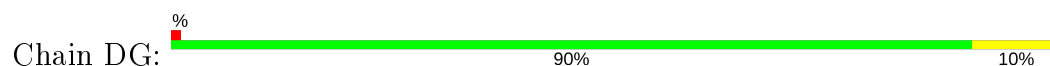
- Molecule 33: 50S ribosomal protein L5



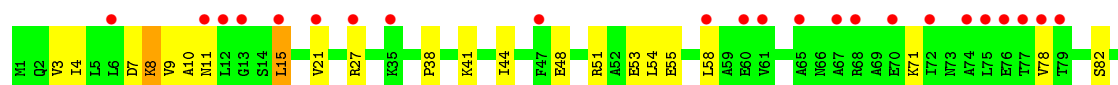
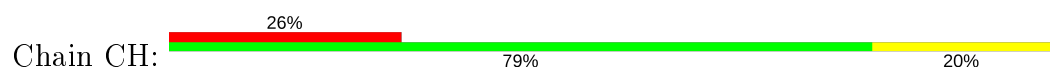
- Molecule 34: 50S ribosomal protein L6

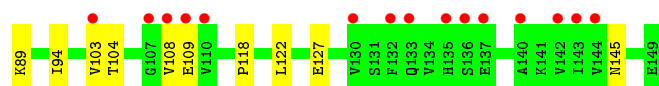


- Molecule 34: 50S ribosomal protein L6

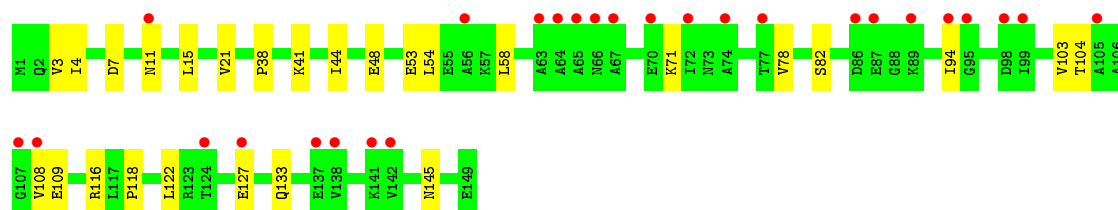
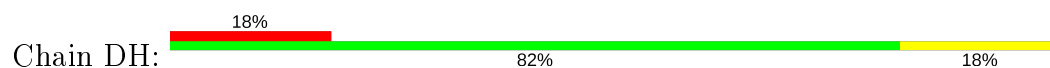


- Molecule 35: 50S ribosomal protein L9

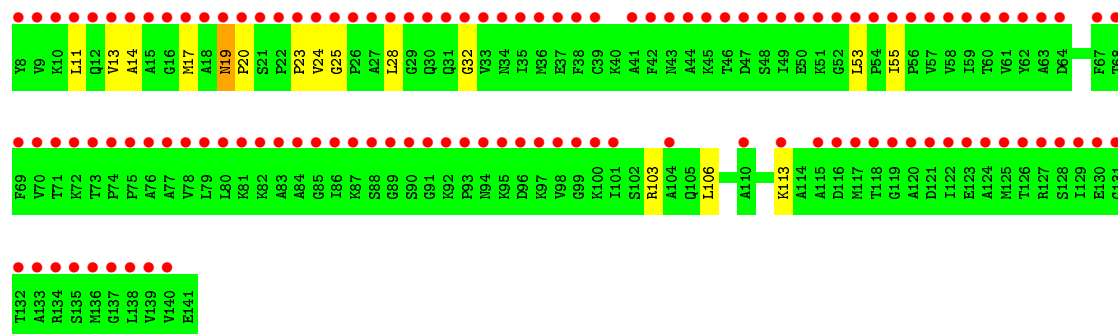
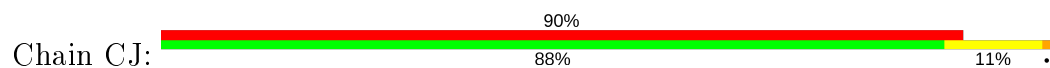




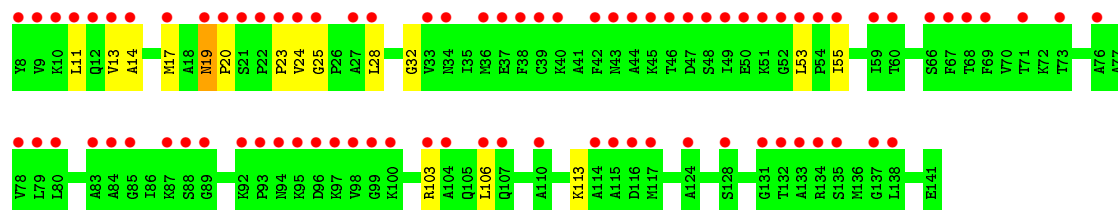
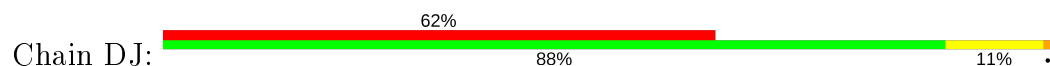
- Molecule 35: 50S ribosomal protein L9



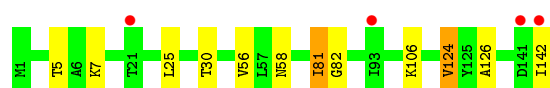
- Molecule 36: 50S ribosomal protein L11



- Molecule 36: 50S ribosomal protein L11

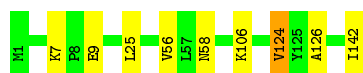


- Molecule 37: 50S ribosomal protein L13

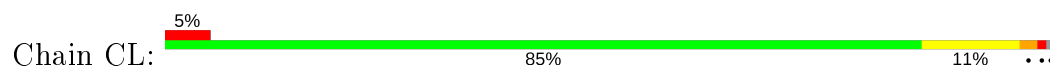


- Molecule 37: 50S ribosomal protein L13





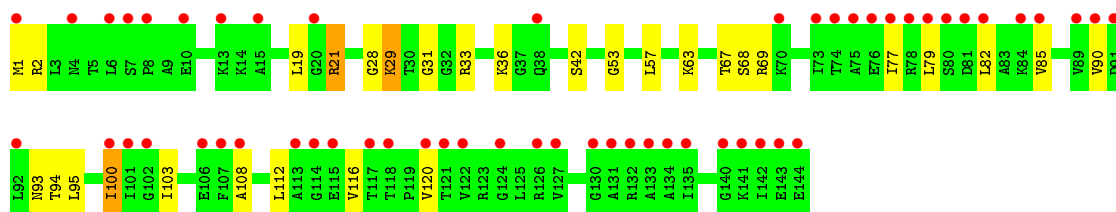
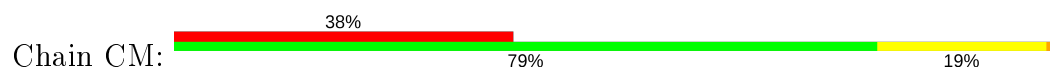
- Molecule 38: 50S ribosomal protein L14



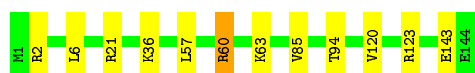
- Molecule 38: 50S ribosomal protein L14



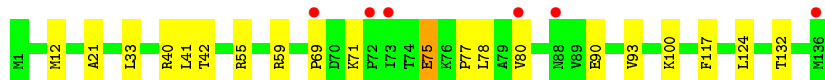
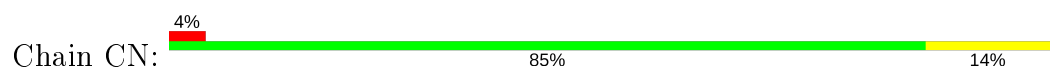
- Molecule 39: 50S ribosomal protein L15



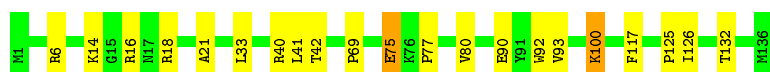
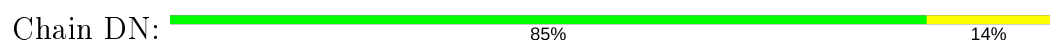
- Molecule 39: 50S ribosomal protein L15



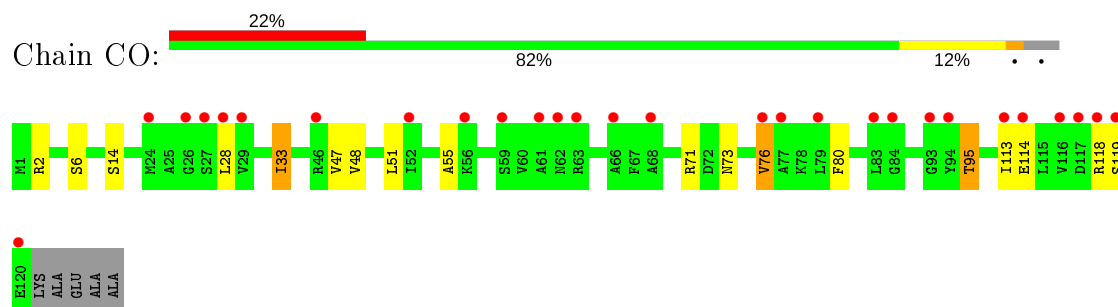
- Molecule 40: 50S ribosomal protein L16



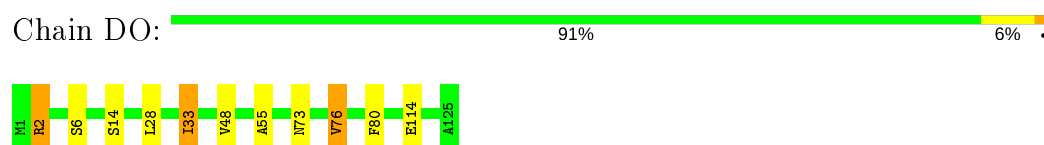
- Molecule 40: 50S ribosomal protein L16



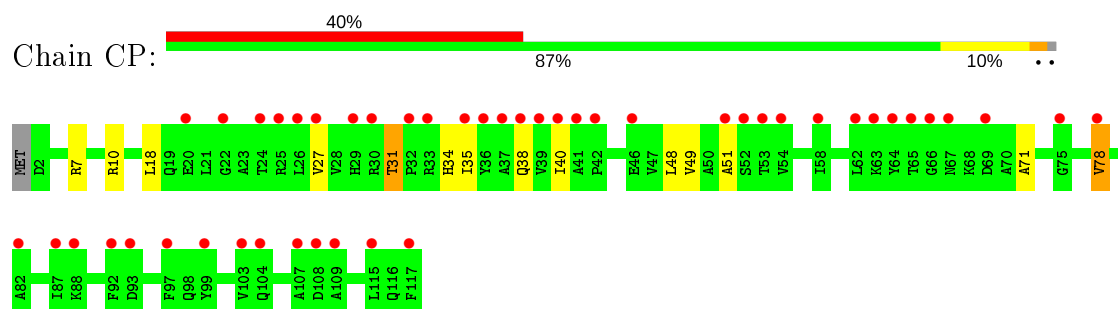
- Molecule 41: 50S ribosomal protein L17



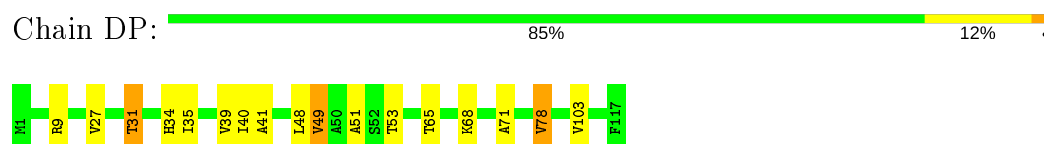
- Molecule 41: 50S ribosomal protein L17



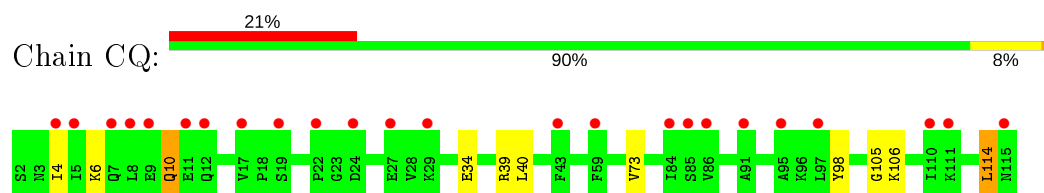
- Molecule 42: 50S ribosomal protein L18



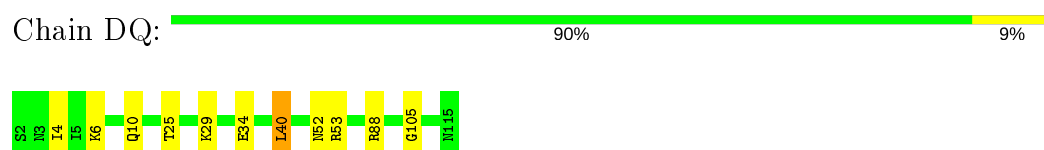
- Molecule 42: 50S ribosomal protein L18



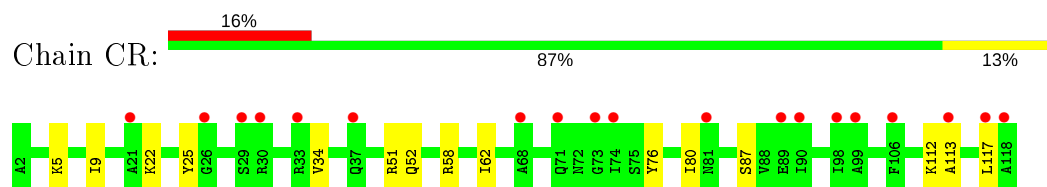
- Molecule 43: 50S ribosomal protein L19



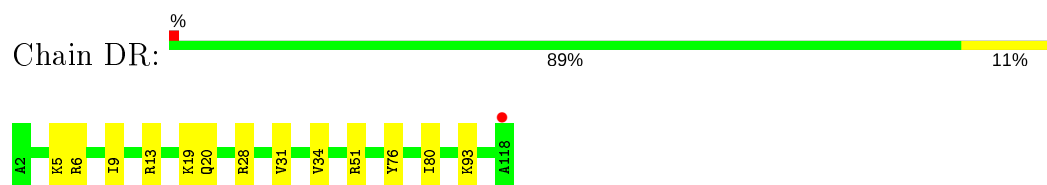
- Molecule 43: 50S ribosomal protein L19



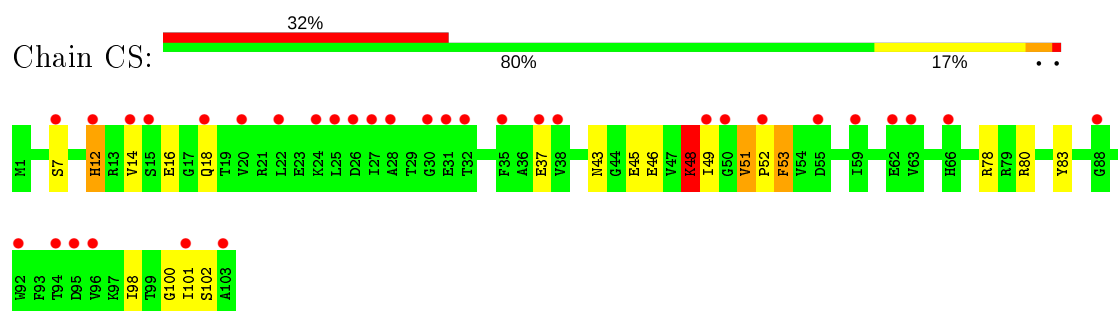
- Molecule 44: 50S ribosomal protein L20



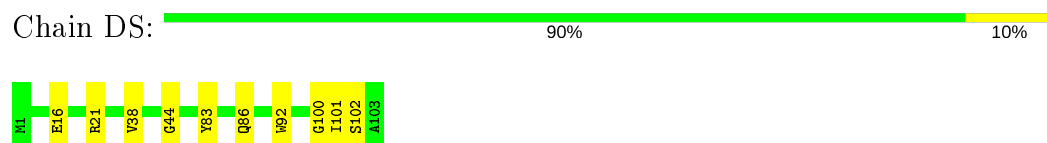
- Molecule 44: 50S ribosomal protein L20



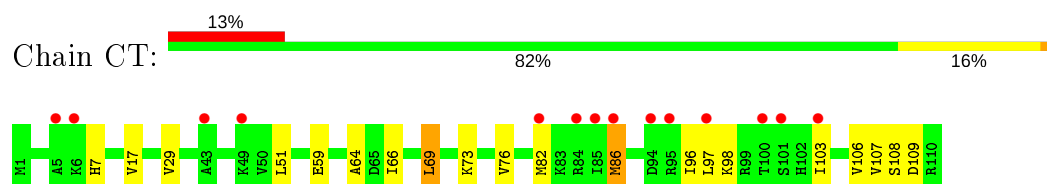
- Molecule 45: 50S ribosomal protein L21



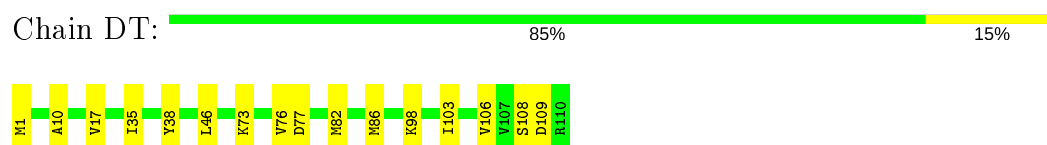
- Molecule 45: 50S ribosomal protein L21



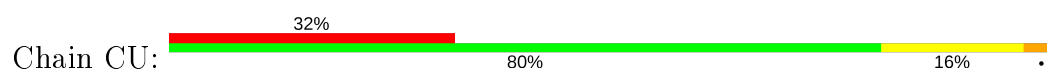
- Molecule 46: 50S ribosomal protein L22

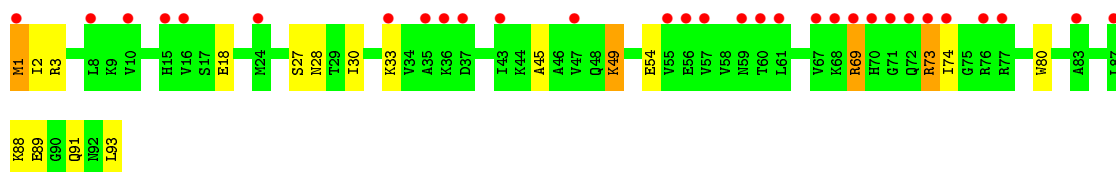


- Molecule 46: 50S ribosomal protein L22

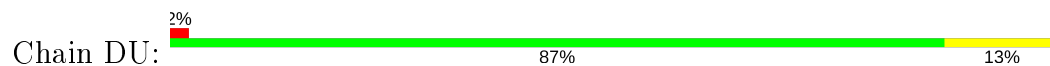


- Molecule 47: 50S ribosomal protein L23

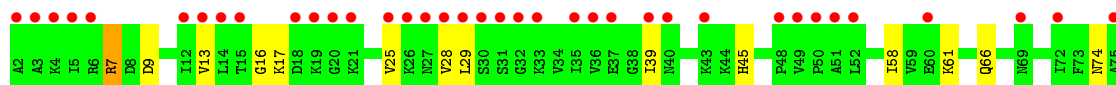
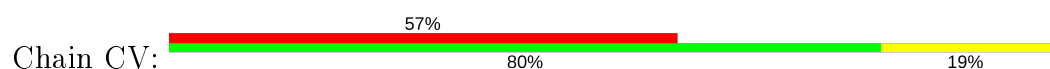




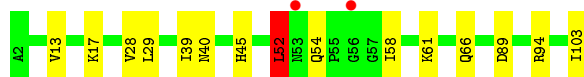
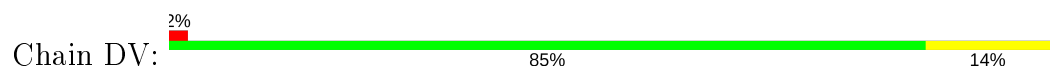
- Molecule 47: 50S ribosomal protein L23



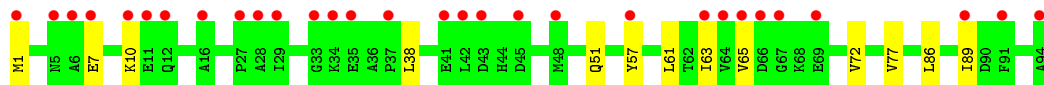
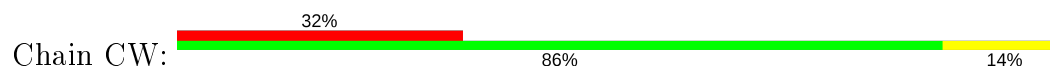
- Molecule 48: 50S ribosomal protein L24



- Molecule 48: 50S ribosomal protein L24



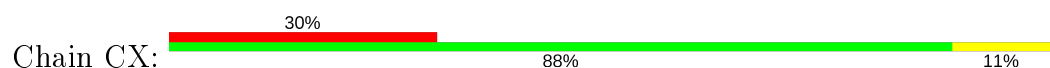
- Molecule 49: 50S ribosomal protein L25

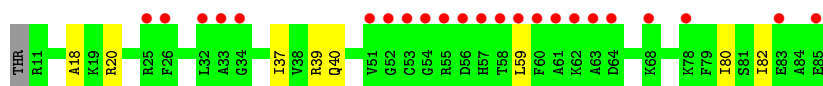


- Molecule 49: 50S ribosomal protein L25

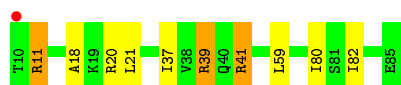
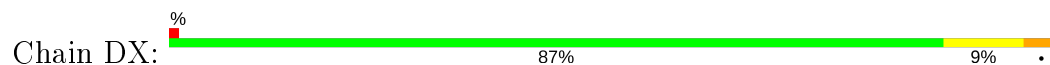


- Molecule 50: 50S ribosomal protein L27

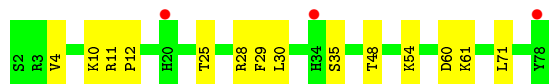
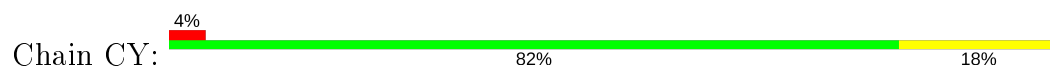




- Molecule 50: 50S ribosomal protein L27



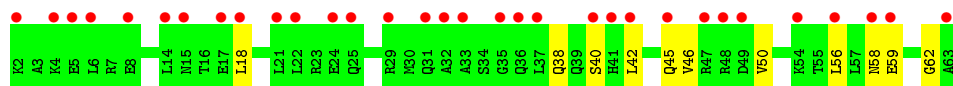
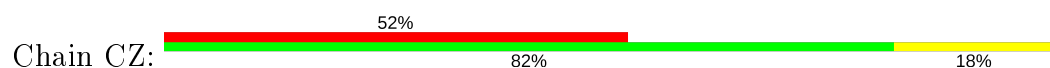
- Molecule 51: 50S ribosomal protein L28



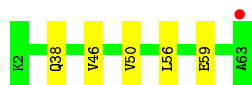
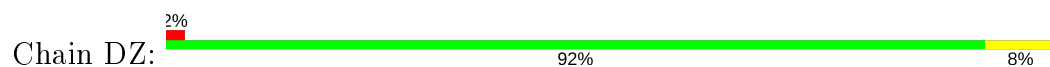
- Molecule 51: 50S ribosomal protein L28



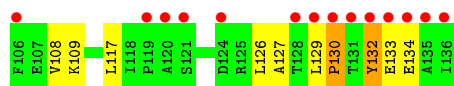
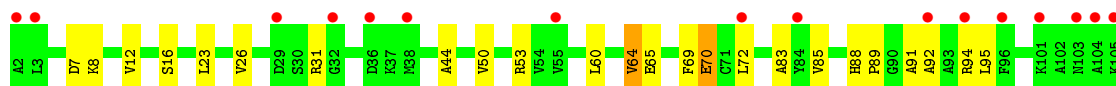
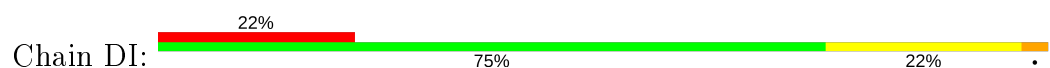
- Molecule 52: 50S ribosomal protein L29



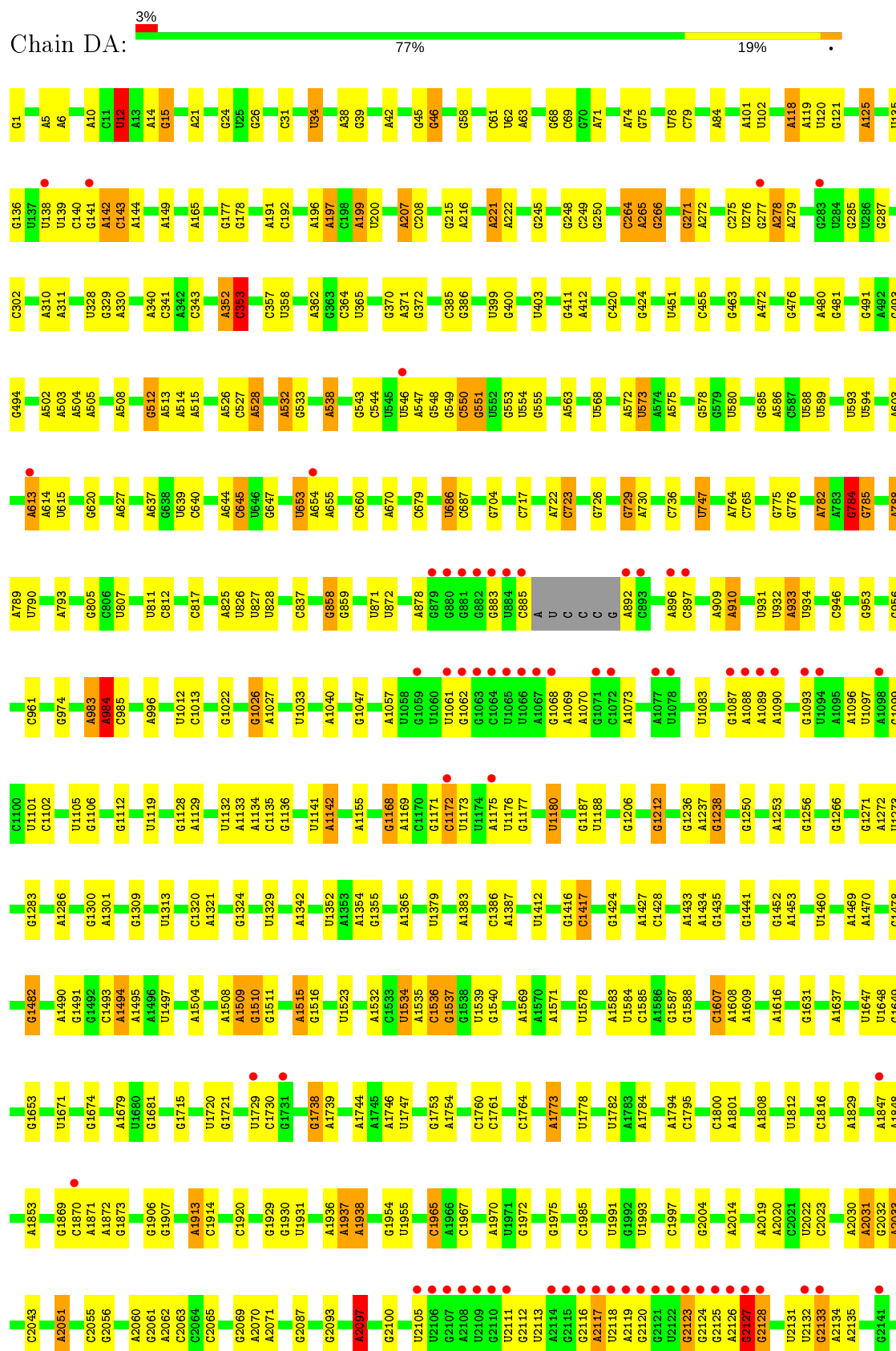
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L10



• Molecule 54: 23S rRNA



C2145	C2146	A2147	G2148	G2157	A2158	G2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	A2171	U2172	U2173	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	U2267	A2268	A2273	A2274	A2278	G2279	G2280	C2283	G2286	A2287	U2291	U2292	C2295	G2304	U2305	G2308	A2311	U2312	C2313	A2322	G2323	U2324	C2325	C2326	A2327	A2328	U2329	G2330	G2331	A2335	A2336	C2339	A2340	G2345	A2346	C2347	G2375	G2383	U2384								
C2385	U2402	A2406	A2407	U2423	C2424	A2425	A2435	U2441	A2448	U2449	A2450	C2465	U2473	U2474	C2475	A2476	U2479	C2480	G2481	G2484	U2491	C2498	G2502	G2505	A2518	U2519	C2520	G2529	G2535	G2536	U2537	G2545	U2546	A2547	U2548	C2556	A2565	A2566	G2567										
G2570	C2573	G2578	U2585	U2586	G2595	G2603	U2609	U2613	A2614	U2615	G2616	U2617	C2628	U2629	G2630	G2645	G2661	A2662	G2663	C2678	A2679	U2680	C2681	U2684	U2689	U2690	U2698	C2699	G2714	C2715	C2716	G2719	U2720	A2721	G2722	C2723	A2726	A2727	U2728	G2744									
G2747	A2748	C2755	A2765	A2778	U2779	C2788	C2789	U2790	G2791	U2796	U2797	U2798	A2799	A2810	A2813	U2818	G2819	A2820	A2821	G2825	U2833	G2834	A2835	U2836	U2845	G2848	G2867	A2868	A2873	C2880	A2883	A2886	A2887	G2895	C2896	U2903	U												

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.41Å 435.70Å 625.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.00 48.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-3.00) 99.2 (48.61-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 84.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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(°)	Ideal(°)
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 ⓘ

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%)	8	37
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	8	37
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	29	68
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	10	42
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	68
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	68
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	22	60
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	3	16
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	3	16
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	22	60
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	22	60
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	57
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	40
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%)	7	33
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1	7
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	55
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	17	55
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	19	57
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	5	26
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	14
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	7	34
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	53
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	48
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12	45
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5	28
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	12	45
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2	12

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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%)	12	45
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	13	48
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	6	29
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	10
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	16
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6	30
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	40
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	40
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	25
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3	19
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	10	42
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	22	60
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%)	10	42
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	29	68
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	25	64
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	14	50
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	6	30
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	25	64
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	43
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	24
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	24
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	11	43
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	22	60
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9	39
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	9	39
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	33
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	22	60
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%)	9	39
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%)	17	55
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17	55
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%)	4	24
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	15	53
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%)	14	50
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	14	50
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	3	17
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	7	34
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%)	9	39
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	2	14
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	12	45

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 ⓘ

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%)	13	43
2	BB	186/186 (100%)	172 (92%)	14 (8%)	13	43
3	AC	170/170 (100%)	156 (92%)	14 (8%)	11	39
3	BC	170/170 (100%)	156 (92%)	14 (8%)	11	39
4	AD	172/172 (100%)	165 (96%)	7 (4%)	30	67
4	BD	172/172 (100%)	163 (95%)	9 (5%)	23	59
5	AE	118/118 (100%)	103 (87%)	15 (13%)	4	19
5	BE	113/118 (96%)	91 (80%)	22 (20%)	1	7
6	AF	92/92 (100%)	84 (91%)	8 (9%)	10	37
6	BF	87/92 (95%)	73 (84%)	14 (16%)	2	12
7	AG	124/124 (100%)	109 (88%)	15 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BG	124/124 (100%)	106 (86%)	18 (14%)	3	15
8	AH	104/104 (100%)	90 (86%)	14 (14%)	4	17
8	BH	104/104 (100%)	88 (85%)	16 (15%)	2	13
9	AI	105/105 (100%)	99 (94%)	6 (6%)	20	56
9	BI	105/105 (100%)	99 (94%)	6 (6%)	20	56
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	12	40
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5	23
11	AK	90/90 (100%)	90 (100%)	0	100	100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	16	49
12	AL	102/102 (100%)	93 (91%)	9 (9%)	10	36
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	22
13	AM	92/92 (100%)	84 (91%)	8 (9%)	10	37
13	BM	92/92 (100%)	84 (91%)	8 (9%)	10	37
14	AN	83/83 (100%)	81 (98%)	2 (2%)	49	79
14	BN	83/83 (100%)	80 (96%)	3 (4%)	35	70
15	AO	76/76 (100%)	69 (91%)	7 (9%)	9	34
15	BO	76/76 (100%)	68 (90%)	8 (10%)	7	27
16	AP	65/65 (100%)	62 (95%)	3 (5%)	27	64
16	BP	65/65 (100%)	61 (94%)	4 (6%)	18	52
17	AQ	74/74 (100%)	66 (89%)	8 (11%)	6	26
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	3	14
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	82
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	5	24
19	BS	70/70 (100%)	65 (93%)	5 (7%)	14	46
20	AT	65/65 (100%)	58 (89%)	7 (11%)	6	26
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	48/48 (100%)	46 (96%)	2 (4%)	30	66
21	BU	48/48 (100%)	46 (96%)	2 (4%)	30	66
22	C1	47/47 (100%)	46 (98%)	1 (2%)	53	82
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%)	28	65
23	D2	45/46 (98%)	42 (93%)	3 (7%)	16	49
24	C3	38/38 (100%)	36 (95%)	2 (5%)	22	58
24	D3	38/38 (100%)	36 (95%)	2 (5%)	22	58
25	C4	51/51 (100%)	45 (88%)	6 (12%)	5	22
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19	54
26	C5	34/34 (100%)	31 (91%)	3 (9%)	10	36
26	D5	34/34 (100%)	33 (97%)	1 (3%)	42	76
27	C0	48/48 (100%)	41 (85%)	7 (15%)	3	15
27	D0	49/48 (102%)	43 (88%)	6 (12%)	5	21
29	CC	216/216 (100%)	203 (94%)	13 (6%)	19	53
29	DC	216/216 (100%)	208 (96%)	8 (4%)	34	70
30	CD	163/163 (100%)	159 (98%)	4 (2%)	47	79
30	DD	163/163 (100%)	160 (98%)	3 (2%)	59	85
32	CE	165/165 (100%)	149 (90%)	16 (10%)	8	31
32	DE	165/165 (100%)	159 (96%)	6 (4%)	35	70
33	CF	148/148 (100%)	134 (90%)	14 (10%)	8	32
33	DF	148/148 (100%)	134 (90%)	14 (10%)	8	32
34	CG	137/137 (100%)	134 (98%)	3 (2%)	52	81
34	DG	137/137 (100%)	133 (97%)	4 (3%)	42	76
35	CH	114/114 (100%)	102 (90%)	12 (10%)	7	27
35	DH	114/114 (100%)	105 (92%)	9 (8%)	12	41
36	CJ	104/104 (100%)	99 (95%)	5 (5%)	25	62
36	DJ	104/104 (100%)	99 (95%)	5 (5%)	25	62
37	CK	116/116 (100%)	112 (97%)	4 (3%)	37	72
37	DK	116/116 (100%)	113 (97%)	3 (3%)	46	78
38	CL	103/104 (99%)	95 (92%)	8 (8%)	12	42
38	DL	104/104 (100%)	99 (95%)	5 (5%)	25	62
39	CM	103/103 (100%)	95 (92%)	8 (8%)	12	42
39	DM	103/103 (100%)	100 (97%)	3 (3%)	42	76
40	CN	108/108 (100%)	103 (95%)	5 (5%)	27	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DN	109/108 (101%)	104 (95%)	5 (5%)	27	64
41	CO	100/102 (98%)	93 (93%)	7 (7%)	15	47
41	DO	102/102 (100%)	97 (95%)	5 (5%)	25	61
42	CP	86/87 (99%)	80 (93%)	6 (7%)	15	47
42	DP	87/87 (100%)	84 (97%)	3 (3%)	37	72
43	CQ	99/99 (100%)	95 (96%)	4 (4%)	31	68
43	DQ	99/99 (100%)	98 (99%)	1 (1%)	76	91
44	CR	89/89 (100%)	85 (96%)	4 (4%)	27	64
44	DR	89/89 (100%)	85 (96%)	4 (4%)	27	64
45	CS	84/84 (100%)	77 (92%)	7 (8%)	11	39
45	DS	84/84 (100%)	82 (98%)	2 (2%)	49	79
46	CT	93/93 (100%)	87 (94%)	6 (6%)	17	50
46	DT	93/93 (100%)	89 (96%)	4 (4%)	29	66
47	CU	80/80 (100%)	71 (89%)	9 (11%)	6	24
47	DU	80/80 (100%)	77 (96%)	3 (4%)	33	69
48	CV	83/83 (100%)	77 (93%)	6 (7%)	14	45
48	DV	83/83 (100%)	79 (95%)	4 (5%)	25	62
49	CW	78/78 (100%)	74 (95%)	4 (5%)	24	60
49	DW	78/78 (100%)	75 (96%)	3 (4%)	33	69
50	CX	56/58 (97%)	53 (95%)	3 (5%)	22	57
50	DX	58/58 (100%)	53 (91%)	5 (9%)	10	37
51	CY	67/67 (100%)	63 (94%)	4 (6%)	19	53
51	DY	67/67 (100%)	65 (97%)	2 (3%)	41	75
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	44
52	DZ	54/54 (100%)	53 (98%)	1 (2%)	57	84
53	DI	103/103 (100%)	96 (93%)	7 (7%)	16	48
All	All	9460/9477 (100%)	8810 (93%)	650 (7%)	15	48

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

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 1397 RNA backbone outliers are listed below:

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

5 of 208 RNA pucker outliers are listed below:

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

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Mol	Chain	Res	Type
31	CA	1253	A

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

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
54	1MG	DA	745	54	18,26,27	1.30	2 (11%)	19,39,42	1.35	2 (10%)
31	G7M	CA	2069	31	20,26,27	1.06	2 (10%)	20,39,42	3.74	5 (25%)
30	MEQ	CD	150	30	7,8,10	0.43	0	4,9,12	0.42	0
1	5MC	AA	967	1	15,22,23	0.80	0	19,32,35	1.14	2 (10%)
31	PSU	CA	955	31	17,21,22	1.20	2 (11%)	20,30,33	5.29	4 (20%)
1	PSU	AA	516	1,55	17,21,22	1.28	2 (11%)	20,30,33	5.32	4 (20%)
1	MA6	AA	1518	1	19,26,27	0.88	0	18,38,41	1.21	1 (5%)
30	MEQ	DD	150[B]	30	8,9,10	1.52	1 (12%)	5,10,12	0.84	0
31	PSU	CA	746	55,31	17,21,22	1.41	3 (17%)	20,30,33	5.30	5 (25%)
30	MEQ	DD	150[A]	30	8,9,10	0.47	0	5,10,12	0.50	0
1	G7M	BA	527	1	20,26,27	1.05	1 (5%)	20,39,42	3.46	5 (25%)
1	MA6	AA	1519	1	19,26,27	0.89	0	18,38,41	1.37	1 (5%)
1	2MG	BA	966	1	19,26,27	1.14	2 (10%)	21,38,41	2.39	4 (19%)
1	2MG	BA	1207	1	19,26,27	1.19	2 (10%)	21,38,41	2.38	4 (19%)
54	6MZ	DA	1618	54	18,25,26	0.95	1 (5%)	16,36,39	0.67	0
1	2MG	AA	1516	1	19,26,27	1.37	2 (10%)	21,38,41	2.29	4 (19%)
54	5MU	DA	747	54	15,22,23	1.24	2 (13%)	16,32,35	3.60	1 (6%)
31	PSU	CA	2580	31	17,21,22	1.33	3 (17%)	20,30,33	5.32	4 (20%)
54	PSU	DA	2580	54	17,21,22	1.67	5 (29%)	20,30,33	5.30	5 (25%)
54	6MZ	DA	2030	54	18,25,26	1.29	2 (11%)	16,36,39	1.13	3 (18%)
31	3TD	CA	1915	31	17,22,23	1.24	3 (17%)	19,32,35	1.50	2 (10%)
54	PSU	DA	2605	54	17,21,22	1.41	3 (17%)	20,30,33	5.32	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UR3	AA	1498	1	14,22,23	1.12	2 (14%)	15,32,35	0.51	0
31	PSU	CA	2504	31	17,21,22	1.24	3 (17%)	20,30,33	5.29	4 (20%)
1	4OC	AA	1402	1	16,23,24	0.80	0	17,32,35	0.78	1 (5%)
1	2MG	AA	1207	1	19,26,27	1.06	1 (5%)	21,38,41	2.36	4 (19%)
31	2MG	CA	2445	31	19,26,27	1.42	2 (10%)	21,38,41	2.45	4 (19%)
1	5MC	AA	1407	1	15,22,23	0.98	1 (6%)	19,32,35	1.23	2 (10%)
31	PSU	CA	2604	31	17,21,22	1.36	3 (17%)	20,30,33	5.36	4 (20%)
54	PSU	DA	1911	54	17,21,22	1.22	3 (17%)	20,30,33	5.25	4 (20%)
31	OMC	CA	2498	55,31	15,22,23	0.94	1 (6%)	17,31,34	1.19	1 (5%)
1	PSU	BA	516	1	17,21,22	1.28	2 (11%)	20,30,33	5.31	4 (20%)
31	5MU	CA	747	31	15,22,23	1.19	1 (6%)	16,32,35	3.67	2 (12%)
31	PSU	CA	2605	31	17,21,22	1.27	2 (11%)	20,30,33	5.32	4 (20%)
31	6MZ	CA	1618	31	18,25,26	0.92	0	16,36,39	0.89	2 (12%)
31	PSU	CA	2457	31	17,21,22	1.37	3 (17%)	20,30,33	5.29	4 (20%)
1	UR3	BA	1498	1	14,22,23	0.96	1 (7%)	15,32,35	0.40	0
31	2MA	CA	2503	31	17,25,26	0.88	0	19,37,40	2.02	2 (10%)
54	PSU	DA	955	54	17,21,22	1.39	3 (17%)	20,30,33	5.28	4 (20%)
54	5MU	DA	1939	54	15,22,23	1.55	2 (13%)	16,32,35	3.67	3 (18%)
12	D2T	BL	89	12	4,9,10	0.53	0	3,11,13	1.08	0
54	OMC	DA	2498	55,54	15,22,23	1.04	0	17,31,34	1.20	1 (5%)
1	2MG	BA	1516	1	19,26,27	1.25	2 (10%)	21,38,41	2.25	4 (19%)
31	PSU	CA	1911	31	17,21,22	1.20	2 (11%)	20,30,33	5.28	4 (20%)
1	MA6	BA	1519	1	19,26,27	0.87	0	18,38,41	1.29	1 (5%)
40	4D4	CN	81	40	9,11,12	2.09	2 (22%)	8,13,15	2.37	2 (25%)
40	4D4	DN	81[B]	-	9,11,12	1.53	1 (11%)	8,13,15	2.60	2 (25%)
31	6MZ	CA	2030	31	18,25,26	0.92	0	16,36,39	0.88	1 (6%)
54	PSU	DA	746	55,54	17,21,22	1.69	5 (29%)	20,30,33	5.36	5 (25%)
54	2MA	DA	2503	55,54	17,25,26	0.87	0	19,37,40	1.95	3 (15%)
31	1MG	CA	745	31	18,26,27	1.29	2 (11%)	19,39,42	1.32	2 (10%)
54	5MC	DA	1962	54	15,22,23	1.13	2 (13%)	19,32,35	1.17	2 (10%)
31	2MG	CA	1835	31	19,26,27	1.18	1 (5%)	21,38,41	2.20	4 (19%)
40	4D4	DN	81[A]	-	9,11,12	2.12	2 (22%)	8,13,15	2.51	2 (25%)
54	PSU	DA	1917	54	17,21,22	1.33	2 (11%)	20,30,33	5.34	4 (20%)
54	OMU	DA	2552	54	14,22,23	1.26	1 (7%)	14,31,34	1.08	1 (7%)
12	D2T	AL	89	12	4,9,10	0.63	0	3,11,13	1.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	G7M	DA	2069	54	20,26,27	1.13	2 (10%)	20,39,42	2.94	5 (25%)
31	PSU	CA	1917	31	17,21,22	1.21	2 (11%)	20,30,33	5.35	4 (20%)
31	OMG	CA	2251	31	18,26,27	1.23	2 (11%)	20,38,41	2.55	4 (20%)
31	5MU	CA	1939	31	15,22,23	1.26	1 (6%)	16,32,35	3.70	2 (12%)
54	OMG	DA	2251	54	18,26,27	0.99	1 (5%)	20,38,41	2.40	5 (25%)
1	5MC	BA	967	1	15,22,23	0.77	0	19,32,35	1.16	2 (10%)
54	2MG	DA	2445	54	19,26,27	1.53	4 (21%)	21,38,41	2.54	4 (19%)
1	2MG	AA	966	1	19,26,27	1.21	2 (10%)	21,38,41	2.32	3 (14%)
54	PSU	DA	2504	54	17,21,22	1.23	2 (11%)	20,30,33	5.34	4 (20%)
31	OMU	CA	2552	31	14,22,23	1.28	2 (14%)	14,31,34	1.10	1 (7%)
54	2MG	DA	1835	54	19,26,27	1.11	1 (5%)	21,38,41	2.22	4 (19%)
31	5MC	CA	1962	31	15,22,23	0.85	1 (6%)	19,32,35	1.15	2 (10%)
1	G7M	AA	527	1	20,26,27	1.21	2 (10%)	20,39,42	3.35	7 (35%)
54	PSU	DA	2457	54	17,21,22	1.41	3 (17%)	20,30,33	5.26	4 (20%)
54	3TD	DA	1915	54	17,22,23	1.27	2 (11%)	19,32,35	1.49	2 (10%)
1	MA6	BA	1518	1	19,26,27	0.82	0	18,38,41	1.19	1 (5%)
54	H2U	DA	2449	54	18,21,22	0.57	0	21,30,33	0.55	0
1	4OC	BA	1402	1	16,23,24	0.79	0	17,32,35	0.78	1 (5%)
54	PSU	DA	2604	54	17,21,22	1.69	5 (29%)	20,30,33	5.34	4 (20%)
1	5MC	BA	1407	1	15,22,23	1.00	1 (6%)	19,32,35	1.19	2 (10%)

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
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
31	G7M	CA	2069	31	-	1/3/25/26	0/3/3/3
30	MEQ	CD	150	30	-	3/6/7/11	-
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1,55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
30	MEQ	DD	150[B]	30	-	3/8/9/11	-
31	PSU	CA	746	55,31	-	3/7/25/26	0/2/2/2
30	MEQ	DD	150[A]	30	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
54	5MU	DA	747	54	-	2/5/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
54	6MZ	DA	2030	54	-	1/5/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	2604	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	55,31	-	0/7/27/28	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	1/5/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/5/25/26	0/2/2/2
31	2MA	CA	2503	31	-	1/3/25/26	0/3/3/3
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
54	5MU	DA	1939	54	-	0/5/25/26	0/2/2/2
12	D2T	BL	89	12	-	1/3/12/14	-
54	OMC	DA	2498	55,54	-	0/7/27/28	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	2/7/29/30	0/3/3/3
40	4D4	CN	81	40	-	1/11/12/14	-
40	4D4	DN	81[B]	-	-	6/11/12/14	-
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
54	PSU	DA	746	55,54	-	3/7/25/26	0/2/2/2
54	2MA	DA	2503	55,54	-	1/3/25/26	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MC	DA	1962	54	-	2/5/25/26	0/2/2/2
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
40	4D4	DN	81[A]	-	-	2/11/12/14	-
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	OMU	DA	2552	54	-	0/7/27/28	0/2/2/2
12	D2T	AL	89	12	-	1/3/12/14	-
54	G7M	DA	2069	54	-	1/3/25/26	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/5/25/26	0/2/2/2
54	OMG	DA	2251	54	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/5/25/26	0/2/2/2
54	2MG	DA	2445	54	-	2/5/27/28	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/7/27/28	0/2/2/2
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	2/5/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/5/25/26	0/2/2/2

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	CN	81	4D4	CZ-NE	5.79	1.44	1.33
40	DN	81[A]	4D4	CZ-NE	5.79	1.44	1.33
31	CA	745	1MG	C6-C5	4.33	1.48	1.41
30	DD	150[B]	MEQ	CB-CA	4.13	1.59	1.53
40	DN	81[B]	4D4	CZ-NE	3.98	1.41	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	2504	PSU	N1-C2-N3	-17.27	114.70	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	746	PSU	N1-C2-N3	-17.22	114.74	128.43
31	CA	1917	PSU	N1-C2-N3	-17.17	114.78	128.43
54	DA	2604	PSU	N1-C2-N3	-17.15	114.80	128.43
1	AA	516	PSU	N1-C2-N3	-17.14	114.80	128.43

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	CD	150	MEQ	C-CA-CB-CG
30	DD	150[B]	MEQ	N-CA-CB-CG
31	CA	746	PSU	O4'-C1'-C5-C4
31	CA	746	PSU	O4'-C1'-C5-C6
30	DD	150[A]	MEQ	C-CA-CB-CG

There are no ring outliers.

18 monomers are involved in 22 short contacts:

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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
59	TAC	AA	1681	55	33,35,35	0.53	0	42,58,58	0.81	2 (4%)
57	MPD	DT	201	-	7,7,7	0.53	0	9,10,10	0.22	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.36	0
58	PUT	DA	3212	-	5,5,5	0.26	0	4,4,4	0.03	0
56	PG4	DQ	202	-	12,12,12	0.21	0	11,11,11	0.16	0
57	MPD	DA	3192	-	7,7,7	0.43	0	9,10,10	0.67	0
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.14	0
57	MPD	AA	1671	-	7,7,7	0.69	0	9,10,10	0.51	0
64	SPD	DA	3187	-	9,9,9	0.20	0	8,8,8	0.31	0
62	EDO	DB	201	-	3,3,3	0.70	0	2,2,2	0.15	0
57	MPD	DA	3207	-	7,7,7	0.84	0	9,10,10	0.48	0
64	SPD	DA	3183	-	9,9,9	0.11	0	8,8,8	0.14	0
61	PEG	DQ	201	-	6,6,6	0.18	0	5,5,5	0.17	0
63	PGE	DA	3203	-	9,9,9	0.31	0	8,8,8	0.27	0
59	TAC	BA	1644	55	33,35,35	0.53	0	42,58,58	0.80	1 (2%)
62	EDO	DA	3209	-	3,3,3	0.66	0	2,2,2	0.27	0
58	PUT	DA	3223	-	5,5,5	0.24	0	4,4,4	0.16	0
59	TAC	AA	1680	55	33,35,35	0.51	0	42,58,58	0.75	1 (2%)
58	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.13	0
62	EDO	DA	3208	-	3,3,3	0.66	0	2,2,2	0.24	0
58	PUT	DA	3221	-	5,5,5	0.22	0	4,4,4	0.15	0
62	EDO	DA	3003	-	3,3,3	0.62	0	2,2,2	0.22	0
63	PGE	DA	3001	-	9,9,9	0.31	0	8,8,8	0.32	0
63	PGE	DU	101	-	9,9,9	0.21	0	8,8,8	0.13	0
66	ACY	DA	3196	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
61	PEG	D1	103	-	6,6,6	0.37	0	5,5,5	0.20	0
58	PUT	DA	3189	-	5,5,5	0.26	0	4,4,4	0.37	0
63	PGE	DS	201	-	9,9,9	0.40	0	8,8,8	0.31	0
62	EDO	DA	3002	-	3,3,3	0.62	0	2,2,2	0.35	0
62	EDO	DB	211	-	3,3,3	0.67	0	2,2,2	0.19	0
58	PUT	DA	3184	-	5,5,5	0.44	0	4,4,4	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PUT	DM	201	-	5,5,5	0.14	0	4,4,4	0.09	0
63	PGE	D1	102	-	9,9,9	0.24	0	8,8,8	0.22	0
63	PGE	DA	3217	-	9,9,9	0.19	0	8,8,8	0.26	0
62	EDO	DA	3198	-	3,3,3	0.61	0	2,2,2	0.38	0
66	ACY	DA	3191	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
57	MPD	AA	1676	-	7,7,7	0.79	0	9,10,10	0.71	0
57	MPD	DT	202	-	7,7,7	0.82	0	9,10,10	0.39	0
58	PUT	DA	3195	-	5,5,5	0.39	0	4,4,4	0.60	0
58	PUT	DA	3213	-	5,5,5	0.21	0	4,4,4	0.23	0
62	EDO	D1	101	-	3,3,3	0.74	0	2,2,2	0.12	0
59	TAC	BA	1643	55	33,35,35	0.42	0	42,58,58	0.80	2 (4%)
57	MPD	DS	203	-	7,7,7	0.28	0	9,10,10	0.36	0
58	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.11	0
61	PEG	DA	3199	-	6,6,6	0.22	0	5,5,5	0.16	0
62	EDO	DA	3194	-	3,3,3	0.97	0	2,2,2	0.18	0
57	MPD	DA	3204	-	7,7,7	0.84	0	9,10,10	0.67	0
56	PG4	DR	202	-	12,12,12	0.29	0	11,11,11	0.38	0
68	TRS	DA	3220	-	7,7,7	0.28	0	9,9,9	0.29	0
57	MPD	DK	201	-	7,7,7	0.53	0	9,10,10	0.28	0
58	PUT	DA	3205	-	5,5,5	0.21	0	4,4,4	0.20	0
63	PGE	DA	3186	-	9,9,9	0.38	0	8,8,8	0.44	0
64	SPD	DA	3224	-	9,9,9	0.24	0	8,8,8	0.45	0
61	PEG	DA	3226	-	6,6,6	0.45	0	5,5,5	0.19	0
61	PEG	D3	101	-	6,6,6	0.28	0	5,5,5	0.30	0
57	MPD	DN	201	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
65	1PE	DA	3202	-	15,15,15	0.36	0	14,14,14	0.36	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.17	0
63	PGE	DA	3214	-	9,9,9	0.30	0	8,8,8	0.41	0
56	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.17	0
56	PG4	DA	3193	-	12,12,12	0.40	0	11,11,11	0.34	0
58	PUT	DA	3188	-	5,5,5	0.25	0	4,4,4	0.12	0
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.34	0
61	PEG	AL	201	-	6,6,6	0.32	0	5,5,5	0.17	0
56	PG4	DA	3216	-	12,12,12	0.18	0	11,11,11	0.23	0
61	PEG	DA	3218	-	6,6,6	0.25	0	5,5,5	0.09	0
58	PUT	AA	1674	-	5,5,5	0.17	0	4,4,4	0.13	0
57	MPD	DE	302	-	7,7,7	0.95	1 (14%)	9,10,10	0.54	0
67	GUN	DA	3211	-	9,12,12	1.83	2 (22%)	8,17,17	3.80	4 (50%)
63	PGE	DA	3225	-	9,9,9	0.17	0	8,8,8	0.16	0
58	PUT	AA	1672	-	5,5,5	0.26	0	4,4,4	0.28	0
58	PUT	AA	1675	-	5,5,5	0.19	0	4,4,4	0.09	0
62	EDO	DA	3197	-	3,3,3	0.78	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PUT	DA	3222	-	5,5,5	0.52	0	4,4,4	0.70	0
56	PG4	AA	1670	-	12,12,12	0.34	0	11,11,11	0.41	0
57	MPD	DE	301	-	7,7,7	0.82	0	9,10,10	0.52	0
62	EDO	DB	212	-	3,3,3	0.79	0	2,2,2	0.17	0
57	MPD	DA	3190	-	7,7,7	0.36	0	9,10,10	0.41	0
61	PEG	DA	3200	-	6,6,6	0.38	0	5,5,5	0.23	0
66	ACY	DA	3201	-	1,3,3	1.64	0	0,3,3	0.00	-
57	MPD	DA	3210	-	7,7,7	0.81	0	9,10,10	0.31	0
61	PEG	DA	3227	-	6,6,6	0.26	0	5,5,5	0.18	0
64	SPD	DA	3206	-	9,9,9	0.25	0	8,8,8	0.23	0
62	EDO	DA	3215	-	3,3,3	0.79	0	2,2,2	0.15	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
59	TAC	AA	1681	55	-	6/8/74/74	0/4/4/4
57	MPD	DT	201	-	-	3/5/5/5	-
65	1PE	DA	3185	-	-	5/13/13/13	-
58	PUT	DA	3212	-	-	1/3/3/3	-
56	PG4	DQ	202	-	-	3/10/10/10	-
57	MPD	DA	3192	-	-	2/5/5/5	-
61	PEG	DL	201	-	-	1/4/4/4	-
57	MPD	AA	1671	-	-	1/5/5/5	-
64	SPD	DA	3187	-	-	2/7/7/7	-
62	EDO	DB	201	-	-	0/1/1/1	-
57	MPD	DA	3207	-	-	3/5/5/5	-
64	SPD	DA	3183	-	-	1/7/7/7	-
61	PEG	DQ	201	-	-	1/4/4/4	-
63	PGE	DA	3203	-	-	4/7/7/7	-
59	TAC	BA	1644	55	-	6/8/74/74	0/4/4/4
62	EDO	DA	3209	-	-	0/1/1/1	-
58	PUT	DA	3223	-	-	1/3/3/3	-
59	TAC	AA	1680	55	-	1/8/74/74	0/4/4/4
58	PUT	DA	3219	-	-	0/3/3/3	-
62	EDO	DA	3208	-	-	1/1/1/1	-
58	PUT	DA	3221	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DA	3001	-	-	4/7/7/7	-
58	PUT	DA	3188	-	-	0/3/3/3	-
61	PEG	D1	103	-	-	1/4/4/4	-
58	PUT	DA	3189	-	-	0/3/3/3	-
63	PGE	DS	201	-	-	3/7/7/7	-
62	EDO	DA	3002	-	-	1/1/1/1	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	PUT	DA	3184	-	-	0/3/3/3	-
58	PUT	DM	201	-	-	0/3/3/3	-
63	PGE	D1	102	-	-	5/7/7/7	-
63	PGE	DA	3217	-	-	2/7/7/7	-
62	EDO	DA	3198	-	-	0/1/1/1	-
67	GUN	DA	3211	-	-	-	0/2/2/2
57	MPD	AA	1676	-	-	0/5/5/5	-
65	1PE	DA	3202	-	-	7/13/13/13	-
58	PUT	DA	3195	-	-	0/3/3/3	-
58	PUT	DA	3213	-	-	0/3/3/3	-
62	EDO	D1	101	-	-	0/1/1/1	-
59	TAC	BA	1643	55	-	8/8/74/74	0/4/4/4
57	MPD	DS	203	-	-	0/5/5/5	-
58	PUT	AA	1673	-	-	0/3/3/3	-
61	PEG	DA	3199	-	-	1/4/4/4	-
62	EDO	DA	3194	-	-	0/1/1/1	-
57	MPD	DA	3204	-	-	2/5/5/5	-
56	PG4	DR	202	-	-	5/10/10/10	-
68	TRS	DA	3220	-	-	0/9/9/9	-
57	MPD	DK	201	-	-	2/5/5/5	-
58	PUT	DA	3205	-	-	0/3/3/3	-
63	PGE	DA	3186	-	-	2/7/7/7	-
64	SPD	DA	3224	-	-	3/7/7/7	-
61	PEG	DA	3226	-	-	3/4/4/4	-
57	MPD	DN	201	-	-	2/5/5/5	-
57	MPD	DT	202	-	-	2/5/5/5	-
61	PEG	DP	201	-	-	3/4/4/4	-
63	PGE	DA	3214	-	-	3/7/7/7	-
56	PG4	BA	1642	-	-	0/10/10/10	-
56	PG4	DA	3193	-	-	6/10/10/10	-
56	PG4	DS	202	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PEG	AL	201	-	-	2/4/4/4	-
56	PG4	DA	3216	-	-	4/10/10/10	-
61	PEG	DA	3218	-	-	1/4/4/4	-
58	PUT	AA	1674	-	-	0/3/3/3	-
57	MPD	DE	302	-	-	3/5/5/5	-
63	PGE	DU	101	-	-	3/7/7/7	-
63	PGE	DA	3225	-	-	5/7/7/7	-
58	PUT	AA	1672	-	-	0/3/3/3	-
58	PUT	AA	1675	-	-	1/3/3/3	-
62	EDO	DA	3197	-	-	1/1/1/1	-
58	PUT	DA	3222	-	-	0/3/3/3	-
56	PG4	AA	1670	-	-	4/10/10/10	-
57	MPD	DE	301	-	-	2/5/5/5	-
62	EDO	DB	212	-	-	1/1/1/1	-
57	MPD	DA	3190	-	-	1/5/5/5	-
61	PEG	DA	3200	-	-	2/4/4/4	-
61	PEG	D3	101	-	-	2/4/4/4	-
57	MPD	DA	3210	-	-	0/5/5/5	-
61	PEG	DA	3227	-	-	0/4/4/4	-
64	SPD	DA	3206	-	-	2/7/7/7	-
62	EDO	DA	3215	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3211	GUN	C6-C5	3.69	1.47	1.41
67	DA	3211	GUN	C6-N1	3.41	1.39	1.33
66	DA	3196	ACY	CH3-C	3.13	1.52	1.48
66	DA	3191	ACY	CH3-C	2.73	1.52	1.48
57	DE	302	MPD	C3-C2	2.22	1.59	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3211	GUN	C5-C6-N1	-7.78	112.79	123.43
67	DA	3211	GUN	C6-N1-C2	5.55	124.74	115.93
67	DA	3211	GUN	C6-C5-C4	-3.62	117.34	120.80
59	BA	1644	TAC	O3-C3-C2	-3.00	117.69	122.96
67	DA	3211	GUN	N3-C2-N1	-2.75	123.56	127.22

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BA	1644	TAC	C1-C2-C21-O21
59	BA	1644	TAC	C1-C2-C21-N21
59	BA	1644	TAC	C3-C4-N4-C43
59	BA	1644	TAC	C41-C4-N4-C42
59	AA	1681	TAC	C1-C2-C21-O21

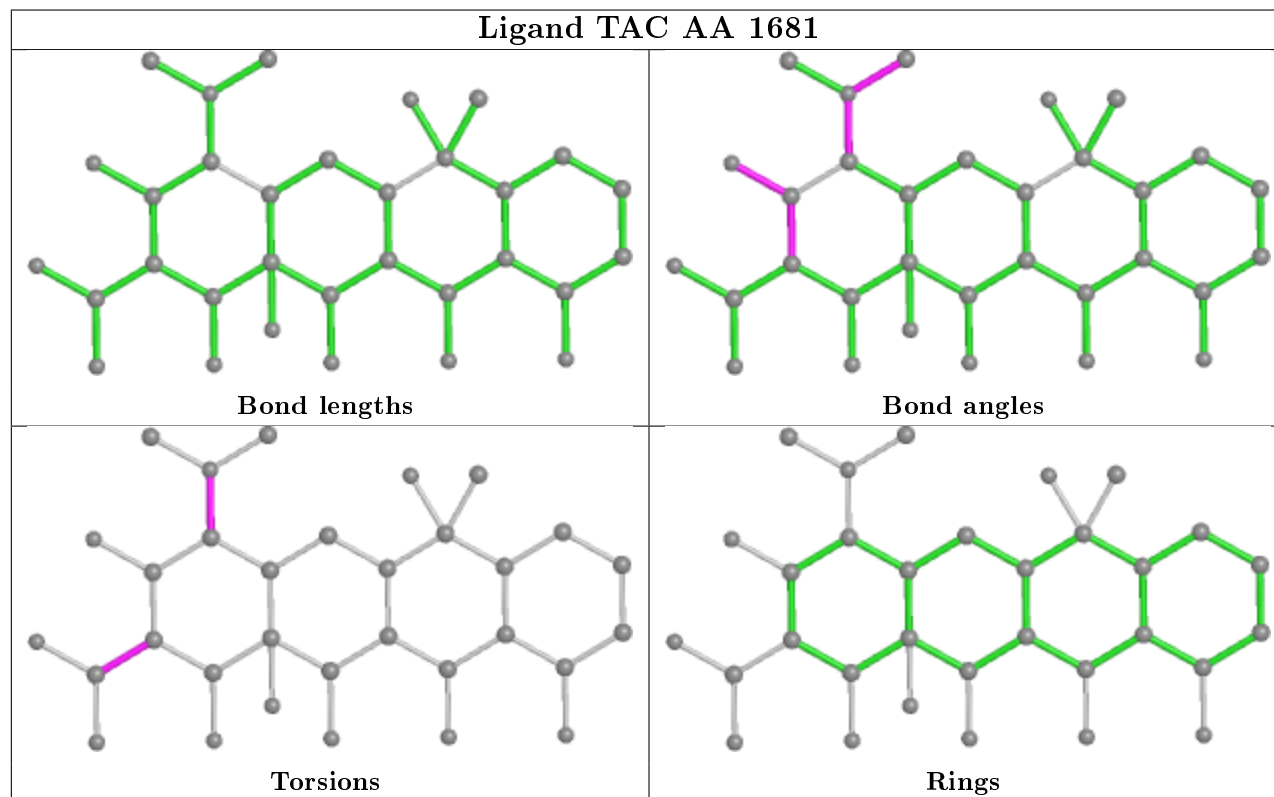
There are no ring outliers.

27 monomers are involved in 46 short contacts:

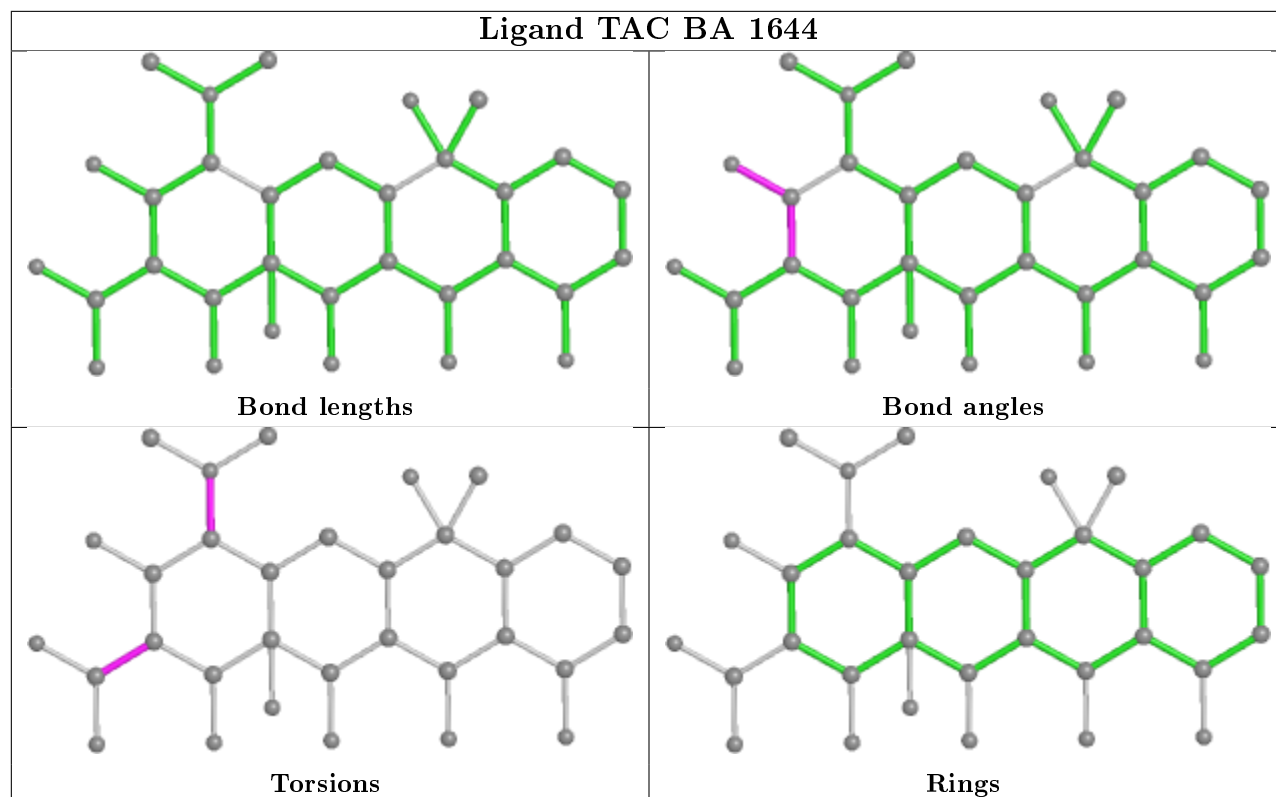
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AA	1681	TAC	2	0
57	DA	3192	MPD	1	0
57	DA	3207	MPD	1	0
63	DA	3001	PGE	1	0
63	DU	101	PGE	3	0
61	D1	103	PEG	1	0
58	DA	3189	PUT	1	0
63	DS	201	PGE	1	0
63	D1	102	PGE	2	0
62	DA	3198	EDO	1	0
57	AA	1676	MPD	3	0
58	DA	3195	PUT	3	0
57	DA	3204	MPD	1	0
56	DR	202	PG4	5	0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

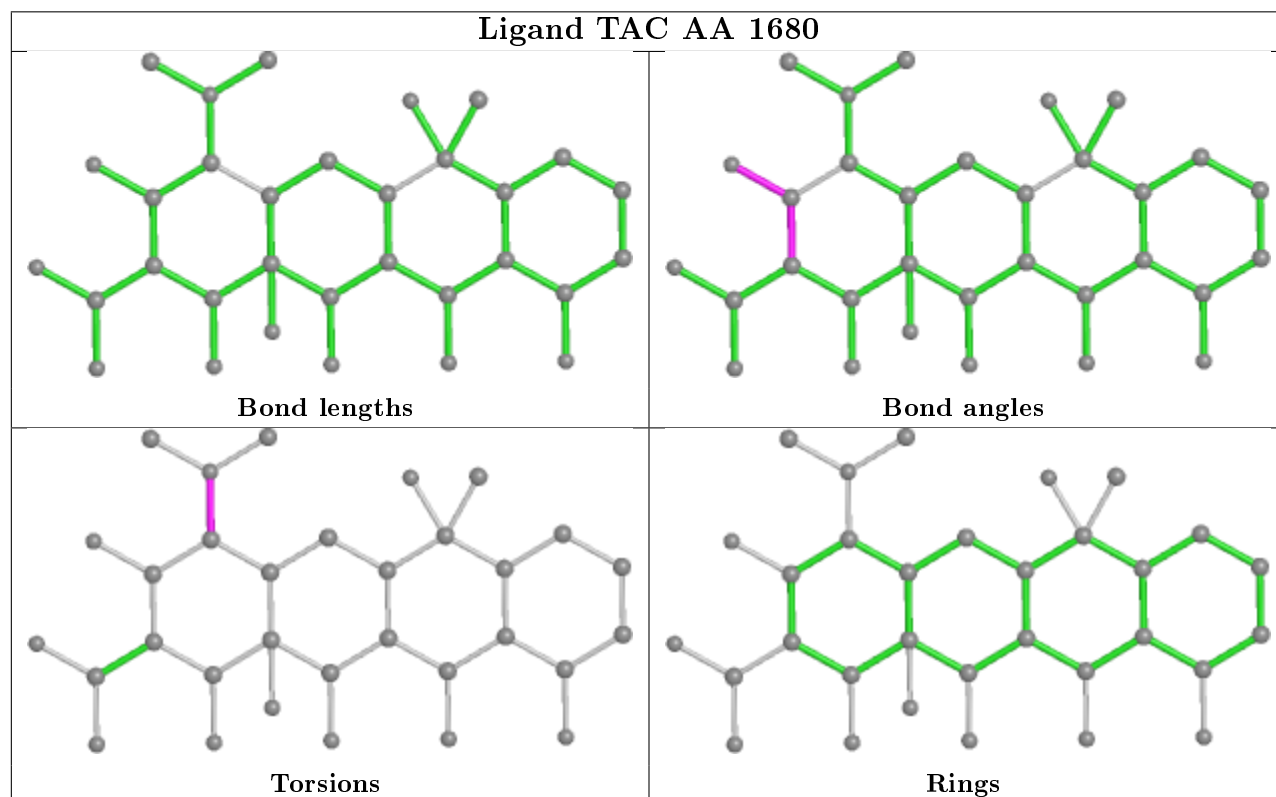
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

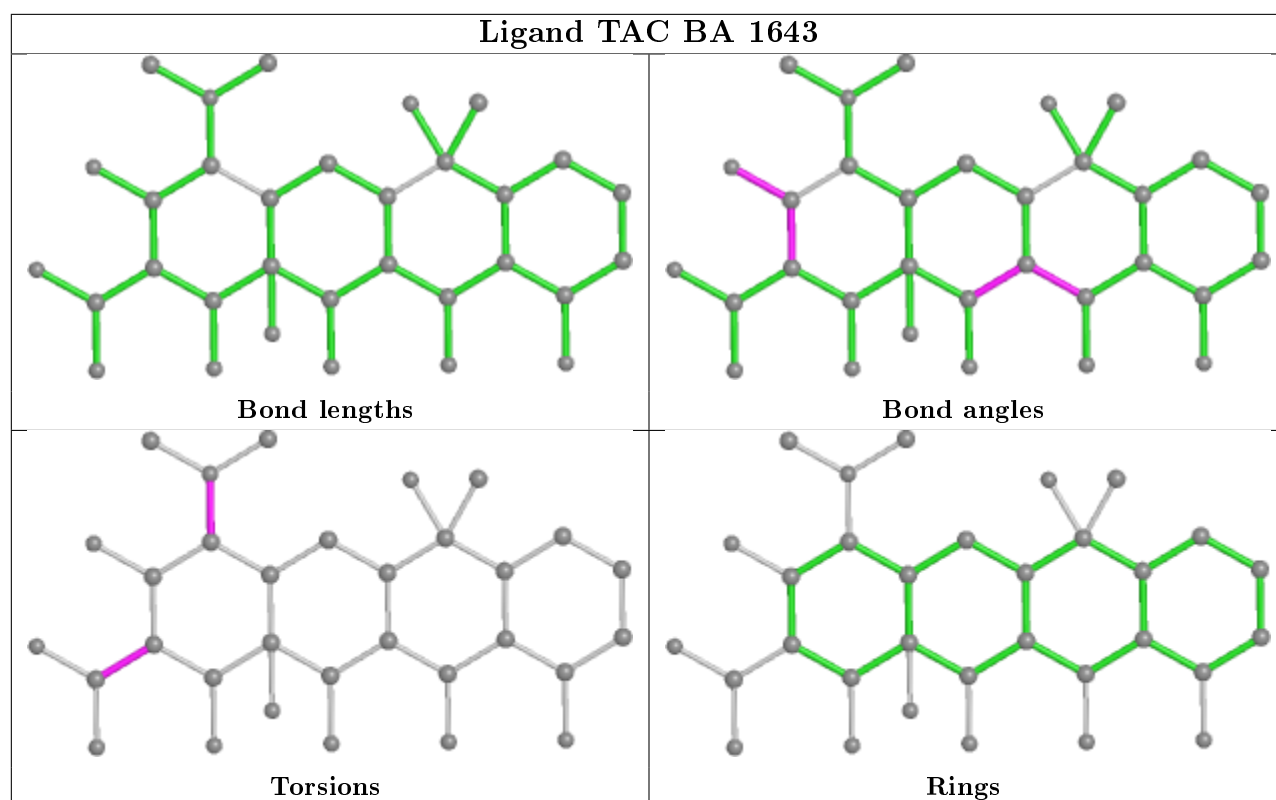


## Ligand TAC BA 1644



## Ligand TAC AA 1680





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	-0.06	29 (1%) 66 37	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.47	166 (10%) 5 2	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.63	28 (12%) 3 1	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.89	36 (16%) 1 0	89, 139, 197, 228	0
3	AC	206/206 (100%)	-0.11	2 (0%) 82 59	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.98	40 (19%) 1 0	90, 138, 170, 184	0
4	AD	205/205 (100%)	-0.31	0 100 100	63, 92, 129, 160	0
4	BD	205/205 (100%)	-0.45	0 100 100	53, 77, 106, 132	0
5	AE	155/155 (100%)	-0.10	0 100 100	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.07	2 (1%) 77 51	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.00	1 (0%) 84 63	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.43	2 (2%) 65 36	77, 117, 140, 153	0
7	AG	151/151 (100%)	0.88	30 (19%) 1 0	95, 136, 160, 174	0
7	BG	151/151 (100%)	2.32	77 (50%) 0 0	136, 196, 213, 220	0
8	AH	129/129 (100%)	-0.09	1 (0%) 86 65	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.03	4 (3%) 49 21	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.11	27 (21%) 0 0	75, 135, 164, 171	0
9	BI	127/127 (100%)	1.89	49 (38%) 0 0	133, 164, 201, 210	0
10	AJ	99/99 (100%)	0.62	11 (11%) 5 1	83, 118, 141, 147	0
10	BJ	98/99 (98%)	3.08	59 (60%) 0 0	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.24	5 (4%) 35 13	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.23	3 (2%) 56 27	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.28	1 (0%) 86 65	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.32	4 (3%) 46 20	65, 86, 114, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	1.42	34 (29%) 0 0	108, 130, 165, 171	0
13	BM	114/114 (100%)	3.36	87 (76%) 0 0	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.02	17 (17%) 1 0	77, 117, 178, 184	0
14	BN	100/100 (100%)	2.56	52 (52%) 0 0	124, 178, 216, 222	0
15	AO	88/88 (100%)	-0.07	1 (1%) 80 56	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.45	6 (6%) 17 5	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.40	3 (3%) 41 17	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.17	19 (23%) 0 0	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.02	2 (2%) 57 29	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.11	17 (21%) 0 0	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.14	1 (1%) 68 40	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.26	3 (5%) 25 9	65, 86, 129, 168	0
19	AS	79/79 (100%)	0.83	11 (13%) 2 1	114, 135, 155, 163	0
19	BS	79/79 (100%)	3.80	60 (75%) 0 0	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.01	0 100 100	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.29	22 (25%) 0 0	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.26	2 (3%) 42 17	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.30	1 (1%) 68 40	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.10	12 (21%) 0 0	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.56	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	3.00	34 (68%) 0 0	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.00	0 100 100	46, 60, 87, 104	0
24	C3	46/46 (100%)	1.49	13 (28%) 0 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.38	0 100 100	23, 31, 48, 112	0
25	C4	64/64 (100%)	0.89	9 (14%) 2 1	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.46	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.23	9 (23%) 0 0	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.33	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	0.80	9 (15%) 2 1	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.52	0 100 100	21, 30, 53, 80	0
28	CB	118/120 (98%)	0.65	9 (7%) 13 4	102, 170, 229, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	-0.35	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.36	16 (5%) 22 7	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.47	0 100 100	22, 49, 76, 92	0
30	CD	208/209 (99%)	0.91	31 (14%) 2 1	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.51	0 100 100	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	0.61	261 (9%) 9 3	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.30	46 (22%) 0 0	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.40	1 (0%) 91 75	19, 50, 97, 132	0
33	CF	177/177 (100%)	3.04	112 (63%) 0 0	193, 211, 219, 227	0
33	DF	177/177 (100%)	-0.17	1 (0%) 89 72	44, 75, 117, 142	0
34	CG	176/176 (100%)	1.95	77 (43%) 0 0	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.16	1 (0%) 89 72	38, 66, 97, 123	0
35	CH	149/149 (100%)	1.37	38 (25%) 0 0	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.85	27 (18%) 1 0	55, 142, 179, 198	0
36	CJ	134/134 (100%)	6.11	120 (89%) 0 0	235, 251, 263, 270	0
36	DJ	134/134 (100%)	3.49	83 (61%) 0 0	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.34	4 (2%) 53 25	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.57	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	0.29	6 (4%) 29 11	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.52	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	2.01	55 (38%) 0 0	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.53	0 100 100	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.34	6 (4%) 34 13	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.64	0 100 100	21, 34, 63, 95	0
41	CO	120/125 (96%)	1.28	28 (23%) 0 0	94, 117, 139, 181	0
41	DO	125/125 (100%)	-0.48	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	1.91	47 (40%) 0 0	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.36	0 100 100	34, 52, 82, 94	0
43	CQ	114/114 (100%)	1.18	24 (21%) 1 0	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.49	0 100 100	26, 43, 75, 116	0
44	CR	117/117 (100%)	0.95	19 (16%) 1 0	81, 103, 125, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DR	117/117 (100%)	-0.46	1 (0%) 84 63	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.66	33 (32%) 0 0	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.53	0 100 100	15, 39, 68, 94	0
46	CT	110/110 (100%)	0.85	14 (12%) 3 1	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.59	0 100 100	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.60	30 (32%) 0 0	124, 146, 173, 182	0
47	DU	93/93 (100%)	-0.01	2 (2%) 62 33	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.59	58 (56%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.25	2 (1%) 65 36	36, 56, 101, 131	0
49	CW	94/94 (100%)	1.45	30 (31%) 0 0	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.52	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.42	23 (30%) 0 0	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.52	1 (1%) 77 51	25, 36, 62, 104	0
51	CY	77/77 (100%)	0.44	3 (3%) 39 15	78, 113, 143, 161	0
51	DY	77/77 (100%)	-0.42	0 100 100	24, 50, 85, 112	0
52	CZ	62/62 (100%)	2.37	32 (51%) 0 0	123, 162, 179, 190	0
52	DZ	62/62 (100%)	-0.03	1 (1%) 72 44	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.23	30 (22%) 0 0	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.09	88 (3%) 49 21	16, 39, 206, 298	0
All	All	20632/20745 (99%)	0.49	2361 (11%) 5 1	10, 100, 227, 298	1 (0%)

The worst 5 of 2361 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	CJ	13	VAL	22.9
36	DJ	54	PRO	22.9
36	CJ	54	PRO	20.6
36	CJ	14	ALA	17.1
36	CJ	87	LYS	16.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	5MC	BA	967	21/22	0.82	0.31	148,154,156,157	0
1	2MG	BA	1207	24/25	0.84	0.21	158,159,162,165	0
1	2MG	BA	966	24/25	0.84	0.34	149,153,160,161	0
31	PSU	CA	1917	20/21	0.87	0.19	118,126,134,134	0
31	3TD	CA	1915	21/22	0.88	0.18	146,150,155,155	0
30	MEQ	CD	150	9/11	0.89	0.25	81,87,117,120	0
1	PSU	BA	516	20/21	0.89	0.16	91,96,99,102	0
31	2MA	CA	2503	23/24	0.90	0.21	90,96,102,102	0
31	PSU	CA	1911	20/21	0.92	0.18	111,128,131,132	0
31	6MZ	CA	2030	23/24	0.92	0.20	78,86,97,99	0
31	PSU	CA	2504	20/21	0.92	0.20	78,86,90,91	0
1	2MG	AA	1207	24/25	0.92	0.13	113,117,120,122	0
31	PSU	CA	955	20/21	0.93	0.17	84,89,90,90	0
1	5MC	BA	1407	21/22	0.93	0.17	81,95,99,100	0
31	PSU	CA	746	20/21	0.93	0.15	93,99,101,102	0
31	G7M	CA	2069	24/25	0.93	0.20	78,83,88,88	0
12	D2T	BL	89	10/11	0.93	0.26	81,86,96,96	0
40	4D4	CN	81	12/13	0.93	0.27	83,89,102,103	0
31	6MZ	CA	1618	23/24	0.94	0.23	98,107,108,109	0
31	2MG	CA	2445	24/25	0.94	0.25	66,75,80,83	0
31	PSU	CA	2580	20/21	0.94	0.19	77,86,88,89	0
31	5MU	CA	747	21/22	0.94	0.17	93,100,102,105	0
31	OMU	CA	2552	21/22	0.94	0.34	78,81,85,89	0
54	3TD	DA	1915	21/22	0.94	0.20	86,90,102,103	0
12	D2T	AL	89	10/11	0.94	0.20	47,53,67,70	0
1	5MC	AA	967	21/22	0.95	0.16	76,93,96,97	0
31	OMG	CA	2251	24/25	0.95	0.24	67,73,75,77	0
31	PSU	CA	2457	20/21	0.95	0.16	79,83,85,85	0
1	2MG	AA	966	24/25	0.95	0.15	78,87,97,97	0
31	1MG	CA	745	24/25	0.95	0.21	85,87,90,93	0
31	2MG	CA	1835	24/25	0.95	0.16	60,73,76,78	0
1	MA6	BA	1518	24/25	0.95	0.20	67,74,79,79	0
1	2MG	BA	1516	24/25	0.95	0.15	61,67,78,80	0
31	OMC	CA	2498	21/22	0.96	0.18	77,80,86,87	0
1	UR3	BA	1498	21/22	0.96	0.13	78,80,84,84	0
54	PSU	DA	1917	20/21	0.96	0.15	63,73,79,79	0
1	MA6	BA	1519	24/25	0.96	0.21	68,73,77,78	0
31	PSU	CA	2605	20/21	0.96	0.16	74,75,78,80	0
1	4OC	BA	1402	22/23	0.96	0.15	74,79,81,82	0
1	G7M	BA	527	24/25	0.96	0.16	80,85,91,93	0
1	2MG	AA	1516	24/25	0.97	0.15	44,49,52,53	0
1	UR3	AA	1498	21/22	0.97	0.14	51,53,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	2MG	DA	1835	24/25	0.97	0.18	31,42,47,48	0
31	5MC	CA	1962	21/22	0.97	0.22	67,72,76,76	0
31	PSU	CA	2604	20/21	0.97	0.14	65,71,84,84	0
54	PSU	DA	1911	20/21	0.97	0.17	67,74,75,75	0
31	5MU	CA	1939	21/22	0.97	0.14	69,74,80,82	0
1	MA6	AA	1519	24/25	0.97	0.18	46,48,50,54	0
1	PSU	AA	516	20/21	0.98	0.13	68,72,78,78	0
54	5MC	DA	1962	21/22	0.98	0.18	28,37,39,42	0
1	5MC	AA	1407	21/22	0.98	0.14	43,47,52,53	0
40	4D4	DN	81[A]	12/13	0.98	0.21	26,33,49,50	9
30	MEQ	DD	150[A]	10/11	0.98	0.21	11,18,25,27	10
1	G7M	AA	527	24/25	0.98	0.14	53,59,62,65	0
1	MA6	AA	1518	24/25	0.98	0.17	44,46,50,53	0
1	4OC	AA	1402	22/23	0.98	0.16	48,55,61,62	0
40	4D4	DN	81[B]	12/13	0.98	0.21	11,21,28,29	9
30	MEQ	DD	150[B]	10/11	0.98	0.21	19,28,34,35	10
54	PSU	DA	2580	20/21	0.99	0.17	17,21,28,29	0
54	6MZ	DA	2030	23/24	0.99	0.18	15,20,26,28	0
54	PSU	DA	955	20/21	0.99	0.19	20,23,26,26	0
54	OMG	DA	2251	24/25	0.99	0.17	21,25,34,42	0
54	PSU	DA	746	20/21	0.99	0.17	18,23,26,30	0
54	2MG	DA	2445	24/25	0.99	0.18	16,22,24,25	0
54	2MA	DA	2503	23/24	0.99	0.18	15,28,32,41	0
54	PSU	DA	2504	20/21	0.99	0.17	31,33,36,38	0
54	5MU	DA	1939	21/22	0.99	0.18	25,30,36,40	0
54	1MG	DA	745	24/25	0.99	0.18	16,22,28,30	0
54	OMC	DA	2498	21/22	0.99	0.18	18,21,24,27	0
54	PSU	DA	2605	20/21	0.99	0.16	26,34,37,38	0
54	PSU	DA	2457	20/21	0.99	0.17	22,25,26,29	0
54	5MU	DA	747	21/22	0.99	0.18	20,25,31,38	0
54	OMU	DA	2552	21/22	0.99	0.17	22,26,30,35	0
54	H2U	DA	2449	20/21	0.99	0.17	19,22,24,26	0
54	6MZ	DA	1618	23/24	0.99	0.16	17,24,27,28	0
54	PSU	DA	2604	20/21	0.99	0.16	32,36,47,47	0
54	G7M	DA	2069	24/25	0.99	0.16	20,28,31,33	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	MG	CA	3154	1/1	-0.24	1.38	136,136,136,136	0
55	MG	AA	1617	1/1	0.09	0.29	147,147,147,147	0
55	MG	CA	3060	1/1	0.20	0.45	234,234,234,234	0
55	MG	BA	1637	1/1	0.23	1.04	86,86,86,86	0
55	MG	CA	3001	1/1	0.25	0.27	296,296,296,296	0
55	MG	AA	1626	1/1	0.36	1.72	113,113,113,113	0
55	MG	BA	1639	1/1	0.39	0.49	93,93,93,93	0
55	MG	AA	1622	1/1	0.45	1.00	116,116,116,116	0
55	MG	CA	3005	1/1	0.45	0.72	239,239,239,239	0
55	MG	CA	3075	1/1	0.45	2.17	221,221,221,221	0
55	MG	CA	3131	1/1	0.48	0.59	83,83,83,83	0
55	MG	CA	3034	1/1	0.49	0.16	244,244,244,244	0
55	MG	DA	3170	1/1	0.53	0.43	90,90,90,90	0
55	MG	CA	3003	1/1	0.54	1.52	270,270,270,270	0
55	MG	CA	3061	1/1	0.55	0.07	225,225,225,225	0
55	MG	AA	1616	1/1	0.55	0.50	87,87,87,87	0
55	MG	CA	3139	1/1	0.56	0.37	83,83,83,83	0
61	PEG	DQ	201	7/7	0.58	0.98	104,108,109,109	0
55	MG	CA	3135	1/1	0.58	0.57	107,107,107,107	0
55	MG	DA	3163	1/1	0.60	0.34	84,84,84,84	0
55	MG	CA	3123	1/1	0.60	0.62	115,115,115,115	0
55	MG	DA	3133	1/1	0.62	0.23	78,78,78,78	0
57	MPD	AA	1676	8/8	0.62	0.68	102,115,118,121	0
55	MG	CA	3156	1/1	0.63	0.17	218,218,218,218	0
55	MG	CA	3008	1/1	0.63	0.10	147,147,147,147	0
55	MG	BA	1638	1/1	0.64	0.65	107,107,107,107	0
55	MG	AA	1678	1/1	0.64	0.22	76,76,76,76	0
55	MG	AA	1624	1/1	0.64	0.49	93,93,93,93	0
55	MG	CA	3134	1/1	0.65	0.46	126,126,126,126	0
55	MG	CA	3038	1/1	0.65	0.14	258,258,258,258	0
55	MG	CA	3133	1/1	0.66	0.50	83,83,83,83	0
55	MG	BA	1641	1/1	0.66	0.28	121,121,121,121	0
55	MG	DA	3137	1/1	0.67	0.30	80,80,80,80	0
55	MG	CA	3014	1/1	0.68	0.16	200,200,200,200	0
55	MG	CA	3093	1/1	0.69	0.14	84,84,84,84	0
58	PUT	AA	1674	6/6	0.70	0.72	128,131,132,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	PUT	AA	1672	6/6	0.70	0.50	90,93,95,95	0
55	MG	CA	3028	1/1	0.70	0.23	274,274,274,274	0
55	MG	DA	3144	1/1	0.70	1.10	107,107,107,107	0
55	MG	CA	3047	1/1	0.71	0.18	238,238,238,238	0
55	MG	DA	3130	1/1	0.71	0.39	99,99,99,99	0
55	MG	CA	3007	1/1	0.72	0.40	214,214,214,214	0
55	MG	CA	3077	1/1	0.73	0.59	232,232,232,232	0
55	MG	CA	3115	1/1	0.73	0.23	72,72,72,72	0
55	MG	BA	1604	1/1	0.73	0.18	187,187,187,187	0
55	MG	CB	203	1/1	0.73	0.09	133,133,133,133	0
58	PUT	DA	3195	6/6	0.73	0.60	76,81,86,87	0
59	TAC	BA	1644	32/32	0.74	0.45	139,152,159,159	0
61	PEG	D1	103	7/7	0.74	0.46	76,77,78,78	0
55	MG	BA	1612	1/1	0.75	0.28	159,159,159,159	0
55	MG	CA	3122	1/1	0.75	0.57	106,106,106,106	0
61	PEG	D3	101	7/7	0.75	1.12	83,89,94,95	0
63	PGE	D1	102	10/10	0.75	0.65	107,117,119,119	0
64	SPD	DA	3206	10/10	0.76	0.32	86,93,96,96	0
55	MG	AA	1658	1/1	0.76	0.13	101,101,101,101	0
58	PUT	AA	1675	6/6	0.76	0.47	106,107,108,109	0
55	MG	CA	3094	1/1	0.77	0.23	126,126,126,126	0
55	MG	AA	1603	1/1	0.77	0.36	81,81,81,81	0
57	MPD	DE	301	8/8	0.77	0.82	123,126,129,129	0
55	MG	CA	3113	1/1	0.77	0.57	79,79,79,79	0
55	MG	DA	3152	1/1	0.77	0.30	94,94,94,94	0
66	ACY	DA	3196	4/4	0.78	0.31	72,76,77,77	0
55	MG	AA	1621	1/1	0.78	0.61	97,97,97,97	0
55	MG	AA	1628	1/1	0.78	0.23	110,110,110,110	0
55	MG	CA	3110	1/1	0.78	0.24	102,102,102,102	0
55	MG	CA	3129	1/1	0.79	0.20	89,89,89,89	0
55	MG	CA	3151	1/1	0.79	0.29	81,81,81,81	0
57	MPD	DT	201	8/8	0.79	0.37	84,87,99,100	0
63	PGE	DA	3001	10/10	0.79	0.58	75,85,99,101	0
61	PEG	DP	201	7/7	0.79	0.82	90,91,93,95	0
57	MPD	DT	202	8/8	0.80	0.35	105,107,109,109	0
55	MG	AA	1661	1/1	0.80	0.20	139,139,139,139	0
55	MG	AA	1627	1/1	0.80	0.22	72,72,72,72	0
55	MG	DA	3062	1/1	0.80	0.10	211,211,211,211	0
55	MG	CA	3116	1/1	0.80	0.45	75,75,75,75	0
55	MG	CA	3128	1/1	0.80	0.44	82,82,82,82	0
55	MG	BA	1624	1/1	0.80	0.29	249,249,249,249	0
57	MPD	DN	201	8/8	0.80	0.46	84,91,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MPD	DA	3204	8/8	0.81	0.43	117,118,124,125	0
55	MG	CA	3130	1/1	0.81	0.29	76,76,76,76	0
55	MG	BA	1603	1/1	0.81	0.50	279,279,279,279	0
55	MG	DA	3138	1/1	0.81	0.52	38,38,38,38	1
55	MG	CA	3046	1/1	0.81	0.12	117,117,117,117	0
55	MG	CA	3119	1/1	0.81	0.35	86,86,86,86	0
55	MG	BA	1629	1/1	0.81	0.37	184,184,184,184	0
55	MG	BA	1630	1/1	0.81	0.10	160,160,160,160	0
55	MG	DA	3179	1/1	0.82	0.36	101,101,101,101	0
55	MG	CA	3039	1/1	0.82	0.59	158,158,158,158	0
55	MG	AA	1654	1/1	0.82	0.35	259,259,259,259	0
56	PG4	DR	202	13/13	0.82	0.37	97,109,121,121	0
55	MG	CA	3052	1/1	0.82	0.07	71,71,71,71	0
63	PGE	DS	201	10/10	0.82	0.39	65,78,83,83	0
55	MG	DA	3166	1/1	0.82	0.65	88,88,88,88	0
55	MG	CA	3111	1/1	0.83	0.24	76,76,76,76	0
68	TRS	DA	3220	8/8	0.83	0.54	94,100,107,109	0
55	MG	CA	3124	1/1	0.83	0.20	124,124,124,124	0
55	MG	AA	1601	1/1	0.83	0.87	76,76,76,76	0
61	PEG	DA	3226	7/7	0.83	0.29	57,62,74,75	0
55	MG	CA	3054	1/1	0.83	0.12	118,118,118,118	0
58	PUT	DA	3222	6/6	0.83	0.33	41,43,47,47	0
55	MG	CA	3019	1/1	0.83	0.18	58,58,58,58	0
61	PEG	DA	3200	7/7	0.83	0.68	65,68,77,77	0
55	MG	CA	3002	1/1	0.83	0.19	258,258,258,258	0
55	MG	DA	3172	1/1	0.83	0.29	81,81,81,81	0
55	MG	BA	1647	1/1	0.83	0.11	86,86,86,86	0
62	EDO	DA	3209	4/4	0.84	0.43	93,94,95,95	0
55	MG	AA	1612	1/1	0.84	0.34	57,57,57,57	0
55	MG	CA	3114	1/1	0.84	0.31	57,57,57,57	0
55	MG	CA	3009	1/1	0.84	0.23	240,240,240,240	0
55	MG	CA	3104	1/1	0.84	0.21	254,254,254,254	0
57	MPD	DK	201	8/8	0.84	0.32	96,98,100,100	0
55	MG	CA	3043	1/1	0.84	0.08	86,86,86,86	0
55	MG	CA	3068	1/1	0.84	0.24	205,205,205,205	0
61	PEG	AL	201	7/7	0.84	0.22	79,79,85,86	0
56	PG4	DA	3193	13/13	0.85	0.72	65,77,93,94	0
55	MG	DA	3131	1/1	0.85	0.22	63,63,63,63	0
55	MG	AA	1618	1/1	0.85	1.19	86,86,86,86	0
55	MG	DA	3165	1/1	0.85	0.19	47,47,47,47	0
55	MG	CA	3035	1/1	0.85	0.23	89,89,89,89	0
55	MG	CA	3071	1/1	0.85	0.09	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3076	1/1	0.85	0.18	132,132,132,132	0
58	PUT	DA	3212	6/6	0.85	0.28	54,63,66,70	0
55	MG	BA	1606	1/1	0.85	0.18	251,251,251,251	0
55	MG	CA	3150	1/1	0.85	0.54	74,74,74,74	0
57	MPD	DA	3210	8/8	0.85	0.34	87,89,92,94	0
58	PUT	DA	3221	6/6	0.85	0.40	113,116,117,118	0
61	PEG	DA	3218	7/7	0.85	0.33	99,105,110,112	0
55	MG	CA	3066	1/1	0.85	0.12	110,110,110,110	0
62	EDO	DA	3003	4/4	0.86	0.31	89,89,89,89	0
55	MG	DB	208	1/1	0.86	0.79	77,77,77,77	0
55	MG	CA	3138	1/1	0.86	0.11	84,84,84,84	0
55	MG	DA	3167	1/1	0.86	0.35	90,90,90,90	0
55	MG	CA	3013	1/1	0.86	0.15	99,99,99,99	0
55	MG	CA	3125	1/1	0.86	0.25	98,98,98,98	0
58	PUT	DA	3205	6/6	0.86	0.33	77,82,89,91	0
55	MG	CA	3070	1/1	0.86	0.09	87,87,87,87	0
59	TAC	BA	1643	32/32	0.86	0.16	146,150,152,152	0
58	PUT	DA	3213	6/6	0.86	0.50	83,85,91,93	0
55	MG	AA	1615	1/1	0.86	0.48	84,84,84,84	0
55	MG	CA	3056	1/1	0.86	0.36	78,78,78,78	0
55	MG	DA	3134	1/1	0.86	0.28	95,95,95,95	0
55	MG	AA	1605	1/1	0.87	0.52	80,80,80,80	0
55	MG	CA	3012	1/1	0.87	0.12	84,84,84,84	0
55	MG	DA	3182	1/1	0.87	0.28	52,52,52,52	0
55	MG	DA	3121	1/1	0.87	0.16	70,70,70,70	0
55	MG	AA	1614	1/1	0.87	0.10	79,79,79,79	0
61	PEG	DA	3199	7/7	0.87	0.41	79,84,92,93	0
55	MG	DA	3146	1/1	0.87	0.24	70,70,70,70	0
62	EDO	D1	101	4/4	0.87	0.24	56,57,60,60	0
55	MG	CA	3146	1/1	0.87	0.16	164,164,164,164	0
55	MG	CA	3149	1/1	0.87	0.42	63,63,63,63	0
55	MG	AA	1664	1/1	0.88	0.18	199,199,199,199	0
55	MG	CA	3074	1/1	0.88	0.09	101,101,101,101	0
55	MG	AA	1606	1/1	0.88	0.23	83,83,83,83	0
55	MG	DA	3168	1/1	0.88	0.48	106,106,106,106	0
55	MG	DA	3132	1/1	0.88	0.15	54,54,54,54	0
55	MG	BA	1646	1/1	0.88	0.36	141,141,141,141	0
55	MG	AA	1619	1/1	0.88	0.31	93,93,93,93	0
56	PG4	AA	1670	13/13	0.88	0.25	64,79,91,92	0
55	MG	BA	1609	1/1	0.88	0.16	168,168,168,168	0
55	MG	CA	3067	1/1	0.88	0.46	277,277,277,277	0
55	MG	DA	3171	1/1	0.88	0.54	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MPD	DE	302	8/8	0.88	0.57	71,76,83,85	0
55	MG	CA	3140	1/1	0.88	0.22	75,75,75,75	0
62	EDO	DA	3194	4/4	0.88	0.24	61,63,64,65	0
55	MG	AA	1608	1/1	0.88	0.41	78,78,78,78	0
67	GUN	DA	3211	11/11	0.88	0.36	82,84,86,86	0
55	MG	AA	1623	1/1	0.88	0.27	62,62,62,62	0
55	MG	AA	1655	1/1	0.89	0.14	151,151,151,151	0
57	MPD	DA	3192	8/8	0.89	0.43	69,77,79,80	0
55	MG	CA	3112	1/1	0.89	0.17	62,62,62,62	0
62	EDO	DB	211	4/4	0.89	0.31	88,88,90,90	0
55	MG	CA	3062	1/1	0.89	0.11	190,190,190,190	0
58	PUT	AA	1673	6/6	0.89	0.29	92,93,93,94	0
55	MG	DA	3154	1/1	0.89	0.34	62,62,62,62	0
55	MG	AA	1657	1/1	0.89	0.20	105,105,105,105	0
57	MPD	DA	3207	8/8	0.89	0.32	86,86,88,89	0
55	MG	BA	1623	1/1	0.89	0.57	254,254,254,254	0
55	MG	CA	3011	1/1	0.89	0.16	70,70,70,70	0
55	MG	CA	3048	1/1	0.89	0.13	91,91,91,91	0
55	MG	CA	3126	1/1	0.89	0.13	85,85,85,85	0
56	PG4	DA	3216	13/13	0.89	0.27	77,89,96,96	0
58	PUT	DA	3184	6/6	0.89	0.29	53,55,60,60	0
58	PUT	DA	3219	6/6	0.89	0.29	63,64,65,66	0
55	MG	DB	207	1/1	0.89	0.57	80,80,80,80	0
55	MG	CA	3141	1/1	0.89	0.28	66,66,66,66	0
60	ZN	C5	101	1/1	0.89	0.05	149,149,149,149	0
55	MG	DA	3129	1/1	0.89	0.16	67,67,67,67	0
55	MG	CA	3080	1/1	0.90	0.24	119,119,119,119	0
55	MG	CA	3105	1/1	0.90	0.60	260,260,260,260	0
62	EDO	DA	3198	4/4	0.90	0.28	76,79,79,79	0
55	MG	DA	3161	1/1	0.90	0.28	62,62,62,62	0
55	MG	DA	3153	1/1	0.90	0.23	53,53,53,53	0
65	1PE	DA	3202	16/16	0.90	0.36	55,64,72,72	0
55	MG	AA	1613	1/1	0.90	0.82	59,59,59,59	0
55	MG	DB	210	1/1	0.90	0.43	76,76,76,76	0
55	MG	DA	3160	1/1	0.90	0.68	81,81,81,81	0
55	MG	BA	1627	1/1	0.90	0.30	126,126,126,126	0
62	EDO	DA	3215	4/4	0.90	0.24	67,71,74,74	0
55	MG	AA	1609	1/1	0.90	0.20	88,88,88,88	0
55	MG	CA	3078	1/1	0.90	0.06	153,153,153,153	0
61	PEG	DA	3227	7/7	0.90	0.32	75,79,86,87	0
55	MG	AA	1634	1/1	0.90	0.18	144,144,144,144	0
55	MG	CA	3136	1/1	0.90	0.23	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3123	1/1	0.90	0.31	81,81,81,81	0
55	MG	AA	1602	1/1	0.90	0.19	75,75,75,75	0
55	MG	CA	3090	1/1	0.90	0.40	170,170,170,170	0
55	MG	CA	3155	1/1	0.90	0.22	152,152,152,152	0
55	MG	BA	1640	1/1	0.91	0.22	94,94,94,94	0
55	MG	CA	3106	1/1	0.91	0.18	75,75,75,75	0
55	MG	CA	3118	1/1	0.91	0.30	64,64,64,64	0
55	MG	BA	1645	1/1	0.91	0.12	94,94,94,94	0
55	MG	BA	1602	1/1	0.91	0.06	84,84,84,84	0
57	MPD	DA	3190	8/8	0.91	0.30	78,82,85,89	0
55	MG	DA	3156	1/1	0.91	0.35	72,72,72,72	0
55	MG	CA	3145	1/1	0.91	0.23	62,62,62,62	0
55	MG	CA	3004	1/1	0.91	0.07	106,106,106,106	0
55	MG	CA	3117	1/1	0.91	0.43	69,69,69,69	0
55	MG	AA	1630	1/1	0.91	0.15	105,105,105,105	0
62	EDO	DA	3208	4/4	0.91	0.25	69,71,72,72	0
55	MG	AA	1625	1/1	0.91	0.38	68,68,68,68	0
62	EDO	DA	3002	4/4	0.91	0.59	71,74,79,82	0
55	MG	CA	3085	1/1	0.91	0.08	69,69,69,69	0
56	PG4	DS	202	13/13	0.91	0.30	52,54,63,64	0
55	MG	CA	3057	1/1	0.91	0.10	106,106,106,106	0
63	PGE	DA	3203	10/10	0.91	0.31	68,72,76,76	0
55	MG	CA	3137	1/1	0.91	0.29	123,123,123,123	0
55	MG	BA	1617	1/1	0.91	0.12	105,105,105,105	0
63	PGE	DA	3225	10/10	0.91	0.29	73,81,92,92	0
55	MG	BA	1625	1/1	0.91	0.24	251,251,251,251	0
55	MG	CA	3127	1/1	0.91	0.09	65,65,65,65	0
66	ACY	DA	3191	4/4	0.91	0.28	80,82,82,82	0
55	MG	DA	3158	1/1	0.91	0.37	63,63,63,63	0
55	MG	CA	3029	1/1	0.92	0.27	114,114,114,114	0
55	MG	BA	1634	1/1	0.92	0.09	129,129,129,129	0
55	MG	CA	3069	1/1	0.92	0.23	110,110,110,110	0
55	MG	CA	3132	1/1	0.92	0.47	97,97,97,97	0
55	MG	CA	3144	1/1	0.92	0.07	63,63,63,63	0
55	MG	DA	3111	1/1	0.92	0.29	292,292,292,292	0
55	MG	DA	3141	1/1	0.92	0.23	40,40,40,40	0
55	MG	DB	206	1/1	0.92	0.58	64,64,64,64	0
61	PEG	DL	201	7/7	0.92	0.25	66,69,70,71	0
56	PG4	DQ	202	13/13	0.92	0.20	53,59,69,71	0
55	MG	AA	1660	1/1	0.92	0.27	281,281,281,281	0
55	MG	CA	3153	1/1	0.92	0.16	59,59,59,59	0
55	MG	BA	1635	1/1	0.92	0.07	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	PG4	BA	1642	13/13	0.92	0.42	84,86,94,96	0
63	PGE	DU	101	10/10	0.92	0.41	79,84,91,92	0
55	MG	CA	3032	1/1	0.92	0.54	244,244,244,244	0
55	MG	CA	3109	1/1	0.92	0.24	62,62,62,62	0
55	MG	AA	1620	1/1	0.92	0.27	63,63,63,63	0
59	TAC	AA	1681	32/32	0.92	0.21	94,106,109,110	0
55	MG	DA	3124	1/1	0.92	0.24	76,76,76,76	0
55	MG	DA	3128	1/1	0.92	0.98	62,62,62,62	0
55	MG	CA	3006	1/1	0.92	0.10	143,143,143,143	0
58	PUT	DA	3189	6/6	0.92	0.32	40,44,47,47	0
55	MG	CA	3099	1/1	0.93	0.22	156,156,156,156	0
55	MG	BA	1631	1/1	0.93	0.06	45,45,45,45	0
55	MG	DA	3176	1/1	0.93	0.32	97,97,97,97	0
58	PUT	DA	3188	6/6	0.93	0.22	43,50,50,51	0
55	MG	BA	1628	1/1	0.93	0.12	92,92,92,92	0
64	SPD	DA	3224	10/10	0.93	0.23	30,40,57,60	0
64	SPD	DA	3183	10/10	0.93	0.43	60,70,74,75	0
55	MG	AA	1610	1/1	0.93	0.44	95,95,95,95	0
55	MG	CA	3065	1/1	0.93	0.11	72,72,72,72	0
55	MG	CA	3031	1/1	0.93	0.07	73,73,73,73	0
55	MG	CA	3089	1/1	0.93	0.18	54,54,54,54	0
55	MG	CA	3022	1/1	0.93	0.83	206,206,206,206	0
55	MG	CA	3083	1/1	0.93	0.13	203,203,203,203	0
63	PGE	DA	3217	10/10	0.93	0.34	67,71,76,76	0
55	MG	DA	3148	1/1	0.93	0.20	62,62,62,62	0
55	MG	CA	3063	1/1	0.93	0.16	118,118,118,118	0
59	TAC	AA	1680	32/32	0.93	0.19	70,81,96,96	0
55	MG	CA	3147	1/1	0.93	0.39	51,51,51,51	1
55	MG	BA	1632	1/1	0.93	0.11	78,78,78,78	0
55	MG	DA	3159	1/1	0.93	0.10	76,76,76,76	0
55	MG	CA	3023	1/1	0.93	0.15	159,159,159,159	0
55	MG	CA	3092	1/1	0.93	0.06	125,125,125,125	0
55	MG	CA	3102	1/1	0.93	0.10	104,104,104,104	0
55	MG	CA	3120	1/1	0.93	0.15	137,137,137,137	0
55	MG	BA	1608	1/1	0.93	0.08	86,86,86,86	0
55	MG	CA	3017	1/1	0.93	0.07	75,75,75,75	0
57	MPD	AA	1671	8/8	0.93	0.45	83,86,89,90	0
63	PGE	DA	3214	10/10	0.93	0.36	56,58,66,66	0
55	MG	DA	3147	1/1	0.93	0.16	104,104,104,104	0
55	MG	DA	3180	1/1	0.93	1.60	95,95,95,95	0
55	MG	CA	3037	1/1	0.93	0.30	146,146,146,146	0
55	MG	AA	1677	1/1	0.93	0.15	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3162	1/1	0.93	0.12	57,57,57,57	0
55	MG	DA	3175	1/1	0.94	0.21	68,68,68,68	0
55	MG	BA	1614	1/1	0.94	0.15	137,137,137,137	0
62	EDO	DB	201	4/4	0.94	0.19	72,75,76,76	0
55	MG	AA	1665	1/1	0.94	0.36	136,136,136,136	0
55	MG	DA	3173	1/1	0.94	0.45	100,100,100,100	0
55	MG	BA	1607	1/1	0.94	0.46	203,203,203,203	0
55	MG	CA	3030	1/1	0.94	0.06	64,64,64,64	0
55	MG	AA	1636	1/1	0.94	0.26	113,113,113,113	0
55	MG	DA	3120	1/1	0.94	0.34	81,81,81,81	0
55	MG	DA	3143	1/1	0.94	0.18	50,50,50,50	0
55	MG	CB	202	1/1	0.94	0.12	113,113,113,113	0
55	MG	AA	1604	1/1	0.94	0.29	50,50,50,50	0
55	MG	CA	3143	1/1	0.94	0.14	67,67,67,67	0
55	MG	CA	3010	1/1	0.94	0.34	245,245,245,245	0
55	MG	AA	1611	1/1	0.94	0.15	94,94,94,94	0
55	MG	CA	3021	1/1	0.94	0.82	261,261,261,261	0
65	1PE	DA	3185	16/16	0.94	0.18	37,52,80,82	0
55	MG	CA	3072	1/1	0.94	0.54	249,249,249,249	0
55	MG	CA	3152	1/1	0.94	0.44	145,145,145,145	0
55	MG	DA	3181	1/1	0.94	0.31	70,70,70,70	0
55	MG	DA	3149	1/1	0.94	0.11	47,47,47,47	0
55	MG	DA	3174	1/1	0.94	0.27	70,70,70,70	0
55	MG	DA	3136	1/1	0.94	0.20	43,43,43,43	0
55	MG	DA	3008	1/1	0.95	0.09	87,87,87,87	0
55	MG	AA	1649	1/1	0.95	0.07	57,57,57,57	0
55	MG	DR	201	1/1	0.95	0.34	32,32,32,32	0
55	MG	DA	3007	1/1	0.95	0.06	88,88,88,88	0
55	MG	DA	3178	1/1	0.95	0.21	69,69,69,69	0
55	MG	CA	3108	1/1	0.95	0.21	73,73,73,73	0
55	MG	AA	1667	1/1	0.95	0.10	41,41,41,41	0
55	MG	CA	3045	1/1	0.95	0.11	107,107,107,107	0
55	MG	CA	3026	1/1	0.95	0.34	111,111,111,111	0
55	MG	DA	3127	1/1	0.95	0.37	71,71,71,71	0
55	MG	DA	3012	1/1	0.95	0.22	153,153,153,153	0
55	MG	AA	1632	1/1	0.95	0.04	65,65,65,65	0
55	MG	BA	1616	1/1	0.95	0.17	162,162,162,162	0
55	MG	DA	3037	1/1	0.95	0.24	22,22,22,22	0
55	MG	DA	3126	1/1	0.95	0.28	57,57,57,57	0
55	MG	CA	3148	1/1	0.95	0.60	46,46,46,46	1
55	MG	CA	3142	1/1	0.95	0.10	71,71,71,71	0
55	MG	BA	1636	1/1	0.95	0.45	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3036	1/1	0.95	0.14	133,133,133,133	0
55	MG	DA	3026	1/1	0.95	0.09	92,92,92,92	0
58	PUT	DA	3223	6/6	0.95	0.20	54,55,62,64	0
62	EDO	DA	3197	4/4	0.95	0.22	51,51,53,53	0
55	MG	CA	3025	1/1	0.95	0.08	87,87,87,87	0
55	MG	DA	3142	1/1	0.95	0.38	84,84,84,84	0
55	MG	CA	3027	1/1	0.95	0.14	68,68,68,68	0
63	PGE	DA	3186	10/10	0.95	0.16	33,40,41,41	0
55	MG	AA	1641	1/1	0.95	0.07	65,65,65,65	0
55	MG	CA	3053	1/1	0.95	0.15	81,81,81,81	0
55	MG	BA	1626	1/1	0.95	0.10	85,85,85,85	0
55	MG	DA	3030	1/1	0.95	0.19	42,42,42,42	0
55	MG	CA	3084	1/1	0.95	0.26	167,167,167,167	0
62	EDO	DB	212	4/4	0.95	0.24	70,72,73,73	0
55	MG	CA	3107	1/1	0.95	0.37	65,65,65,65	0
55	MG	AA	1644	1/1	0.95	0.17	87,87,87,87	0
55	MG	CA	3058	1/1	0.95	0.22	138,138,138,138	0
66	ACY	DA	3201	4/4	0.95	0.21	66,68,68,69	0
55	MG	DA	3177	1/1	0.96	0.17	67,67,67,67	0
55	MG	DA	3044	1/1	0.96	0.10	70,70,70,70	0
55	MG	CB	201	1/1	0.96	0.06	159,159,159,159	0
55	MG	DA	3097	1/1	0.96	0.07	26,26,26,26	0
55	MG	CA	3098	1/1	0.96	0.07	78,78,78,78	0
55	MG	CA	3049	1/1	0.96	0.12	57,57,57,57	0
55	MG	CA	3044	1/1	0.96	0.09	59,59,59,59	0
55	MG	AA	1659	1/1	0.96	0.07	74,74,74,74	0
55	MG	DA	3065	1/1	0.96	0.15	19,19,19,19	0
55	MG	DA	3164	1/1	0.96	0.29	59,59,59,59	0
55	MG	CA	3097	1/1	0.96	0.08	83,83,83,83	0
55	MG	BA	1619	1/1	0.96	0.19	79,79,79,79	0
55	MG	DB	204	1/1	0.96	0.06	37,37,37,37	0
55	MG	CA	3016	1/1	0.96	0.50	164,164,164,164	0
55	MG	CA	3024	1/1	0.96	0.12	81,81,81,81	0
55	MG	AA	1651	1/1	0.96	0.09	69,69,69,69	0
55	MG	DR	203	1/1	0.96	0.12	140,140,140,140	0
55	MG	CA	3064	1/1	0.96	0.28	260,260,260,260	0
55	MG	BA	1633	1/1	0.96	0.13	241,241,241,241	0
55	MG	DA	3135	1/1	0.96	0.04	78,78,78,78	0
55	MG	CA	3082	1/1	0.96	0.25	112,112,112,112	0
55	MG	AA	1631	1/1	0.96	0.08	47,47,47,47	0
55	MG	DA	3092	1/1	0.96	0.10	21,21,21,21	0
55	MG	CA	3079	1/1	0.96	0.10	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3055	1/1	0.96	0.07	135,135,135,135	0
55	MG	CA	3091	1/1	0.96	0.09	80,80,80,80	0
55	MG	AA	1666	1/1	0.96	0.05	47,47,47,47	0
55	MG	AA	1607	1/1	0.96	0.48	70,70,70,70	0
55	MG	AA	1663	1/1	0.96	0.09	94,94,94,94	0
55	MG	DA	3140	1/1	0.96	0.20	68,68,68,68	0
55	MG	BA	1610	1/1	0.96	0.04	93,93,93,93	0
55	MG	DB	202	1/1	0.96	0.09	52,52,52,52	0
55	MG	AA	1647	1/1	0.96	0.09	149,149,149,149	0
55	MG	CA	3033	1/1	0.96	0.11	91,91,91,91	0
55	MG	DA	3052	1/1	0.97	0.10	70,70,70,70	0
55	MG	DA	3116	1/1	0.97	0.13	34,34,34,34	0
55	MG	CA	3096	1/1	0.97	0.05	64,64,64,64	0
64	SPD	DA	3187	10/10	0.97	0.20	30,41,47,48	0
58	PUT	DM	201	6/6	0.97	0.17	40,48,52,56	0
55	MG	DD	301	1/1	0.97	0.18	40,40,40,40	0
55	MG	CA	3103	1/1	0.97	0.11	90,90,90,90	0
55	MG	DB	209	1/1	0.97	0.23	65,65,65,65	0
55	MG	DA	3117	1/1	0.97	0.20	62,62,62,62	0
55	MG	CA	3073	1/1	0.97	0.33	229,229,229,229	0
55	MG	DA	3049	1/1	0.97	0.10	39,39,39,39	0
55	MG	DA	3074	1/1	0.97	0.04	47,47,47,47	0
55	MG	CA	3100	1/1	0.97	0.17	73,73,73,73	0
55	MG	DA	3095	1/1	0.97	0.12	74,74,74,74	0
55	MG	CA	3121	1/1	0.97	0.14	65,65,65,65	0
55	MG	DA	3047	1/1	0.97	0.12	58,58,58,58	0
55	MG	DA	3098	1/1	0.97	0.10	87,87,87,87	0
55	MG	AA	1640	1/1	0.97	0.09	52,52,52,52	0
55	MG	DA	3122	1/1	0.97	0.45	46,46,46,46	0
55	MG	BA	1605	1/1	0.97	0.07	146,146,146,146	0
60	ZN	AB	301	1/1	0.97	0.12	150,150,150,150	0
55	MG	DA	3043	1/1	0.97	0.14	32,32,32,32	0
55	MG	DA	3151	1/1	0.97	0.25	30,30,30,30	0
55	MG	BA	1648	1/1	0.97	0.35	68,68,68,68	0
55	MG	AA	1645	1/1	0.97	0.07	46,46,46,46	0
55	MG	DA	3094	1/1	0.97	0.15	20,20,20,20	0
55	MG	CA	3051	1/1	0.97	0.10	73,73,73,73	0
55	MG	CA	3095	1/1	0.97	0.07	69,69,69,69	0
55	MG	DA	3139	1/1	0.97	0.10	55,55,55,55	0
55	MG	DA	3033	1/1	0.97	0.16	26,26,26,26	0
55	MG	DA	3155	1/1	0.97	0.19	60,60,60,60	0
55	MG	DA	3083	1/1	0.97	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3169	1/1	0.97	0.27	66,66,66,66	0
55	MG	AA	1642	1/1	0.97	0.21	89,89,89,89	0
55	MG	AA	1650	1/1	0.97	0.07	79,79,79,79	0
55	MG	CA	3088	1/1	0.97	0.08	67,67,67,67	0
55	MG	DA	3054	1/1	0.98	0.10	70,70,70,70	0
55	MG	CA	3040	1/1	0.98	0.07	83,83,83,83	0
55	MG	CA	3018	1/1	0.98	0.18	90,90,90,90	0
55	MG	DA	3090	1/1	0.98	0.14	30,30,30,30	0
55	MG	DA	3015	1/1	0.98	0.11	40,40,40,40	0
55	MG	CA	3042	1/1	0.98	0.10	82,82,82,82	0
55	MG	CA	3101	1/1	0.98	0.09	97,97,97,97	0
55	MG	DA	3063	1/1	0.98	0.07	85,85,85,85	0
55	MG	DA	3087	1/1	0.98	0.14	34,34,34,34	0
57	MPD	DS	203	8/8	0.98	0.20	47,50,57,58	0
55	MG	CA	3086	1/1	0.98	0.08	59,59,59,59	0
55	MG	DA	3082	1/1	0.98	0.12	72,72,72,72	0
55	MG	CA	3050	1/1	0.98	0.09	54,54,54,54	0
55	MG	AA	1633	1/1	0.98	0.23	128,128,128,128	0
55	MG	CA	3081	1/1	0.98	0.06	84,84,84,84	0
55	MG	BA	1621	1/1	0.98	0.22	36,36,36,36	0
55	MG	DA	3230	1/1	0.98	0.07	48,48,48,48	0
55	MG	DA	3100	1/1	0.98	0.15	26,26,26,26	0
55	MG	DA	3081	1/1	0.98	0.09	45,45,45,45	0
55	MG	CA	3020	1/1	0.98	0.13	86,86,86,86	0
55	MG	AA	1653	1/1	0.98	0.07	61,61,61,61	0
55	MG	AA	1669	1/1	0.98	0.14	172,172,172,172	0
55	MG	DA	3070	1/1	0.98	0.07	62,62,62,62	0
55	MG	DA	3053	1/1	0.98	0.11	44,44,44,44	0
55	MG	DA	3031	1/1	0.98	0.17	27,27,27,27	0
55	MG	DA	3157	1/1	0.98	0.14	54,54,54,54	0
55	MG	DA	3118	1/1	0.98	0.08	36,36,36,36	0
55	MG	BA	1620	1/1	0.98	0.09	113,113,113,113	0
55	MG	BA	1601	1/1	0.98	0.25	130,130,130,130	0
55	MG	DA	3079	1/1	0.98	0.16	124,124,124,124	0
55	MG	AA	1648	1/1	0.98	0.08	60,60,60,60	0
55	MG	AA	1638	1/1	0.98	0.07	86,86,86,86	0
55	MG	DA	3085	1/1	0.98	0.12	50,50,50,50	0
55	MG	DA	3016	1/1	0.98	0.09	43,43,43,43	0
55	MG	DA	3113	1/1	0.98	0.09	52,52,52,52	0
55	MG	BA	1615	1/1	0.98	0.06	65,65,65,65	0
55	MG	CA	3015	1/1	0.98	0.18	57,57,57,57	0
55	MG	DA	3089	1/1	0.98	0.18	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1629	1/1	0.98	0.10	71,71,71,71	0
55	MG	DA	3072	1/1	0.98	0.19	55,55,55,55	0
55	MG	DA	3125	1/1	0.98	0.19	58,58,58,58	0
55	MG	DA	3107	1/1	0.98	0.14	35,35,35,35	0
55	MG	AA	1656	1/1	0.98	0.13	140,140,140,140	0
55	MG	DA	3021	1/1	0.98	0.13	27,27,27,27	0
55	MG	BA	1618	1/1	0.98	0.07	69,69,69,69	0
55	MG	DA	3080	1/1	0.98	0.14	149,149,149,149	0
55	MG	AA	1679	1/1	0.98	0.21	62,62,62,62	0
55	MG	DA	3006	1/1	0.98	0.06	75,75,75,75	0
55	MG	AA	1652	1/1	0.98	0.25	21,21,21,21	0
55	MG	DA	3105	1/1	0.98	0.19	31,31,31,31	0
55	MG	DA	3078	1/1	0.98	0.07	52,52,52,52	0
55	MG	AA	1662	1/1	0.98	0.15	73,73,73,73	0
55	MG	DA	3028	1/1	0.98	0.12	56,56,56,56	0
55	MG	DA	3101	1/1	0.98	0.09	45,45,45,45	0
55	MG	DA	3027	1/1	0.98	0.13	33,33,33,33	0
55	MG	DA	3228	1/1	0.99	0.16	36,36,36,36	0
55	MG	DA	3005	1/1	0.99	0.12	60,60,60,60	0
55	MG	DA	3096	1/1	0.99	0.12	36,36,36,36	0
55	MG	AA	1646	1/1	0.99	0.06	49,49,49,49	0
55	MG	DA	3014	1/1	0.99	0.15	14,14,14,14	0
55	MG	DA	3057	1/1	0.99	0.08	13,13,13,13	0
55	MG	DA	3025	1/1	0.99	0.10	31,31,31,31	0
55	MG	DA	3040	1/1	0.99	0.08	36,36,36,36	0
55	MG	DA	3115	1/1	0.99	0.16	37,37,37,37	0
55	MG	DB	205	1/1	0.99	0.13	46,46,46,46	0
55	MG	DA	3071	1/1	0.99	0.10	34,34,34,34	0
55	MG	DA	3034	1/1	0.99	0.13	16,16,16,16	0
55	MG	DA	3050	1/1	0.99	0.13	18,18,18,18	0
55	MG	DA	3035	1/1	0.99	0.20	32,32,32,32	0
55	MG	BA	1613	1/1	0.99	0.16	79,79,79,79	0
55	MG	DA	3029	1/1	0.99	0.18	29,29,29,29	0
55	MG	CA	3041	1/1	0.99	0.05	50,50,50,50	0
55	MG	DA	3088	1/1	0.99	0.10	42,42,42,42	0
55	MG	AA	1643	1/1	0.99	0.12	53,53,53,53	0
55	MG	DA	3024	1/1	0.99	0.18	36,36,36,36	0
55	MG	DA	3114	1/1	0.99	0.12	39,39,39,39	0
55	MG	DA	3004	1/1	0.99	0.09	60,60,60,60	0
55	MG	DM	202	1/1	0.99	0.04	34,34,34,34	0
55	MG	DA	3041	1/1	0.99	0.20	11,11,11,11	0
55	MG	DA	3042	1/1	0.99	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3103	1/1	0.99	0.12	35,35,35,35	0
55	MG	DA	3069	1/1	0.99	0.15	46,46,46,46	0
55	MG	DA	3102	1/1	0.99	0.09	30,30,30,30	0
55	MG	AA	1635	1/1	0.99	0.08	104,104,104,104	0
55	MG	DA	3099	1/1	0.99	0.14	23,23,23,23	0
55	MG	DA	3068	1/1	0.99	0.16	35,35,35,35	0
55	MG	DA	3056	1/1	0.99	0.17	42,42,42,42	0
55	MG	CA	3059	1/1	0.99	0.09	74,74,74,74	0
55	MG	DA	3009	1/1	0.99	0.12	23,23,23,23	0
55	MG	DA	3110	1/1	0.99	0.16	35,35,35,35	0
55	MG	DA	3108	1/1	0.99	0.09	30,30,30,30	0
55	MG	DA	3119	1/1	0.99	0.31	69,69,69,69	0
55	MG	DA	3104	1/1	0.99	0.19	34,34,34,34	0
55	MG	DA	3075	1/1	0.99	0.15	37,37,37,37	0
55	MG	DA	3032	1/1	0.99	0.18	23,23,23,23	0
55	MG	AA	1639	1/1	0.99	0.08	89,89,89,89	0
55	MG	DA	3055	1/1	0.99	0.21	24,24,24,24	0
55	MG	DA	3013	1/1	0.99	0.19	19,19,19,19	0
55	MG	DA	3150	1/1	0.99	0.10	50,50,50,50	0
55	MG	BA	1622	1/1	0.99	0.07	99,99,99,99	0
55	MG	DA	3022	1/1	0.99	0.15	21,21,21,21	0
55	MG	DA	3112	1/1	0.99	0.18	24,24,24,24	0
55	MG	DA	3018	1/1	0.99	0.08	43,43,43,43	0
55	MG	AA	1668	1/1	0.99	0.13	59,59,59,59	0
55	MG	DA	3048	1/1	0.99	0.13	26,26,26,26	0
55	MG	DA	3061	1/1	0.99	0.14	30,30,30,30	0
55	MG	DA	3067	1/1	0.99	0.06	36,36,36,36	0
55	MG	DA	3231	1/1	0.99	0.24	36,36,36,36	0
55	MG	DA	3064	1/1	0.99	0.11	49,49,49,49	0
55	MG	DA	3077	1/1	0.99	0.07	30,30,30,30	0
55	MG	DA	3145	1/1	0.99	0.11	78,78,78,78	0
55	MG	DA	3036	1/1	0.99	0.19	25,25,25,25	0
55	MG	DA	3229	1/1	0.99	0.07	36,36,36,36	0
55	MG	DA	3106	1/1	0.99	0.17	41,41,41,41	0
55	MG	DA	3023	1/1	0.99	0.18	20,20,20,20	0
55	MG	DA	3019	1/1	0.99	0.28	8,8,8,8	0
55	MG	DA	3076	1/1	0.99	0.13	23,23,23,23	0
55	MG	CA	3087	1/1	0.99	0.05	59,59,59,59	0
55	MG	BA	1611	1/1	0.99	0.10	56,56,56,56	0
55	MG	DA	3038	1/1	0.99	0.09	19,19,19,19	0
55	MG	DA	3084	1/1	0.99	0.11	35,35,35,35	0
55	MG	DA	3059	1/1	0.99	0.08	23,23,23,23	0

*Continued on next page...*

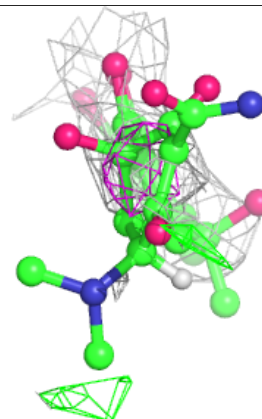
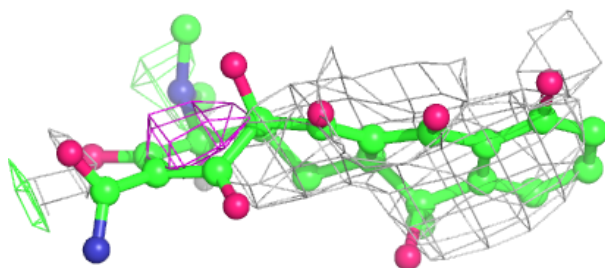
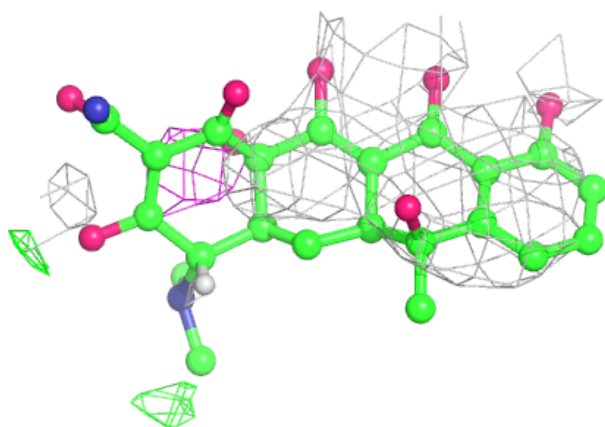
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3066	1/1	0.99	0.17	40,40,40,40	0
55	MG	DA	3091	1/1	0.99	0.16	17,17,17,17	0
55	MG	AA	1637	1/1	0.99	0.07	53,53,53,53	0
55	MG	DA	3045	1/1	0.99	0.05	49,49,49,49	0
55	MG	DA	3051	1/1	0.99	0.09	14,14,14,14	0
55	MG	DA	3093	1/1	0.99	0.18	23,23,23,23	0
55	MG	DA	3058	1/1	1.00	0.09	32,32,32,32	0
55	MG	DA	3086	1/1	1.00	0.11	29,29,29,29	0
55	MG	DA	3020	1/1	1.00	0.05	45,45,45,45	0
60	ZN	D5	101	1/1	1.00	0.12	55,55,55,55	0
55	MG	DA	3109	1/1	1.00	0.16	23,23,23,23	0
55	MG	DA	3060	1/1	1.00	0.14	21,21,21,21	0
55	MG	DA	3046	1/1	1.00	0.13	31,31,31,31	0
55	MG	DA	3017	1/1	1.00	0.14	20,20,20,20	0
55	MG	DA	3073	1/1	1.00	0.13	31,31,31,31	0
55	MG	DB	203	1/1	1.00	0.10	30,30,30,30	0
55	MG	DA	3039	1/1	1.00	0.13	23,23,23,23	0
55	MG	DA	3010	1/1	1.00	0.11	17,17,17,17	0
55	MG	DA	3011	1/1	1.00	0.08	33,33,33,33	0

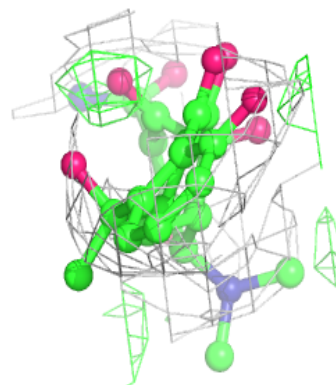
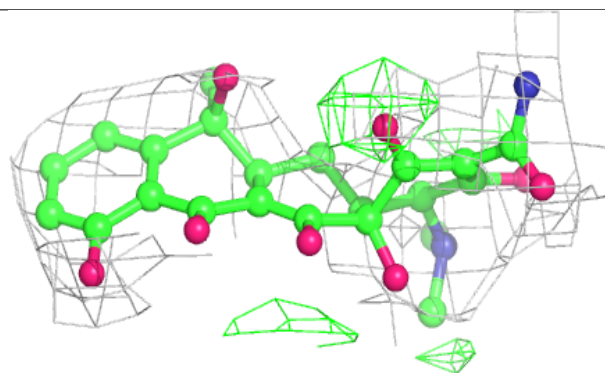
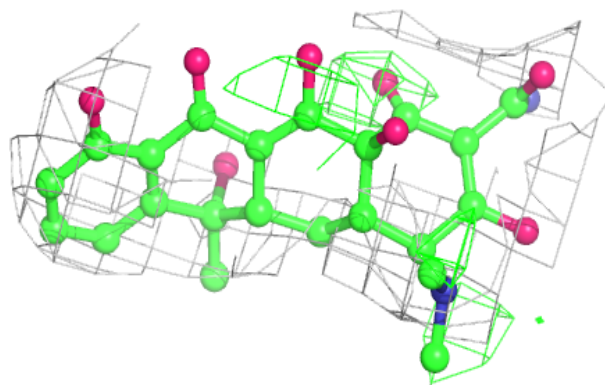
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

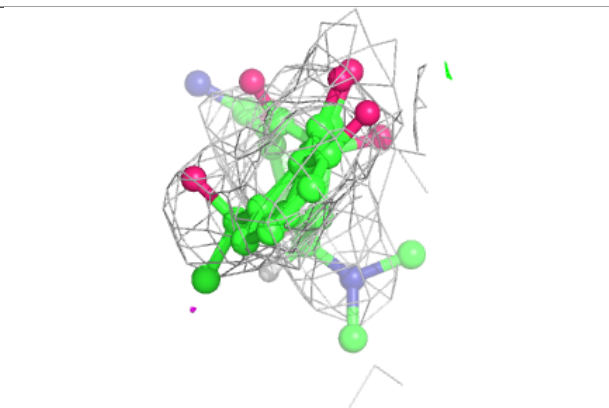
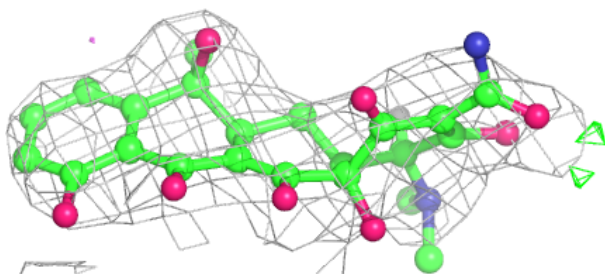
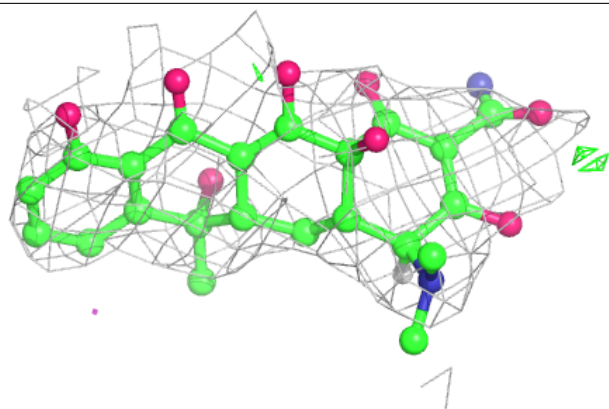
**Electron density around TAC BA 1643:**

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

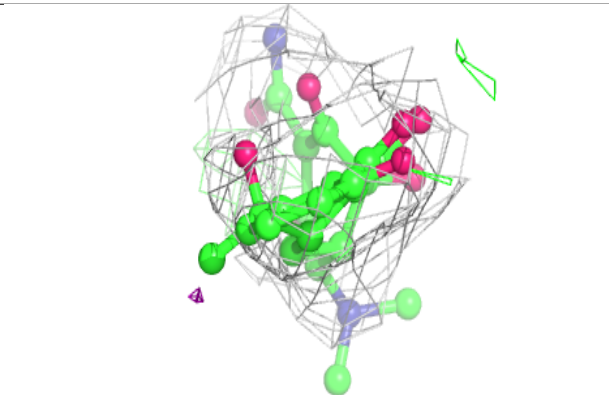
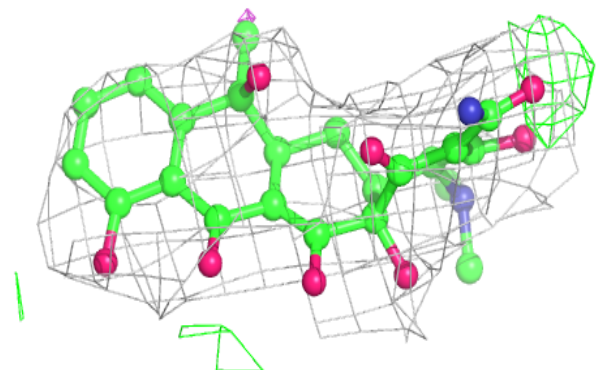
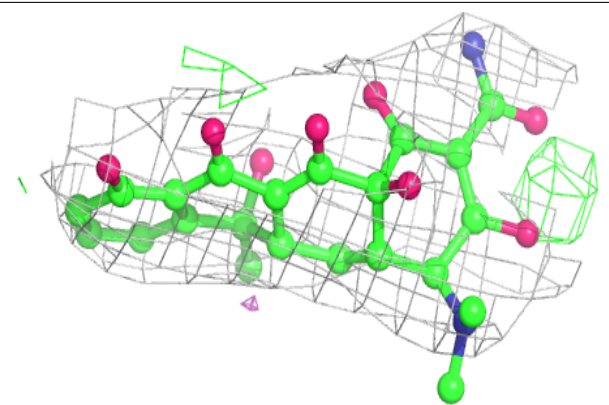


**Electron density around TAC AA 1681:**

$2mF_o-DF_c$  (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.