



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 03:44 AM EST

PDB ID : 5JC9
Title : Structure of the Escherichia coli ribosome with the U1052G mutation in the 16S rRNA
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-14
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

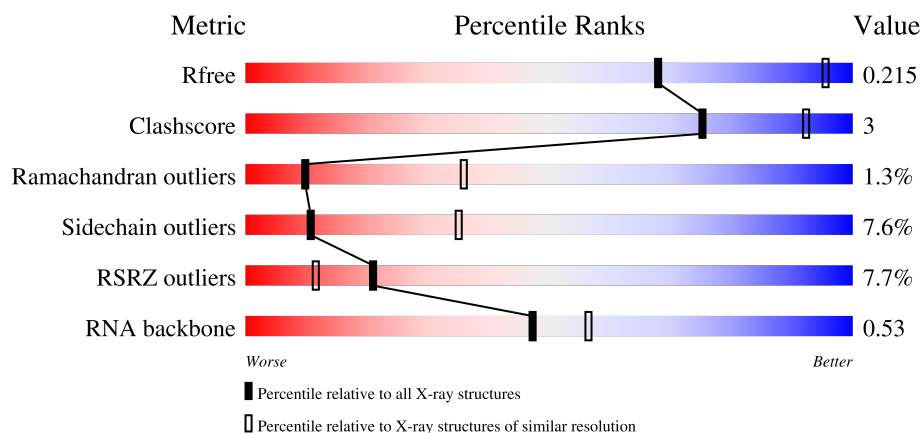
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







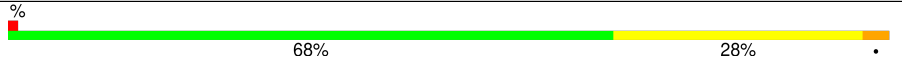
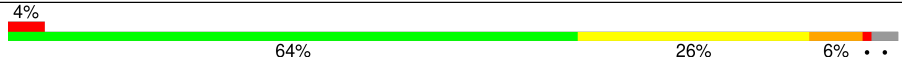
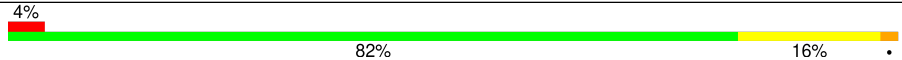
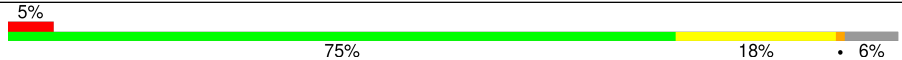
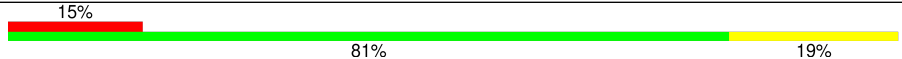
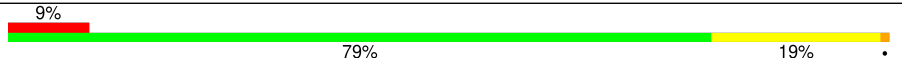
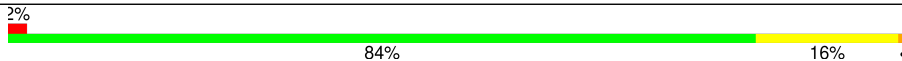



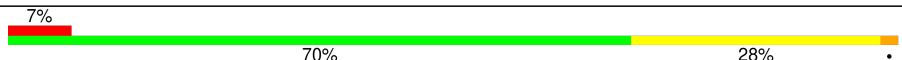
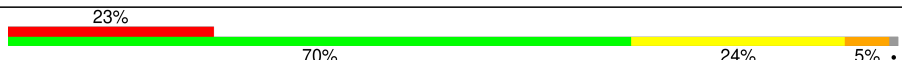
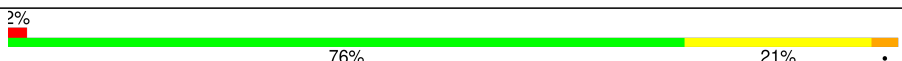
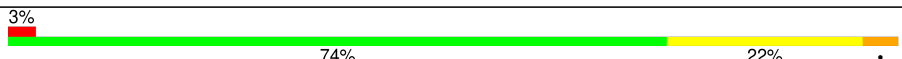
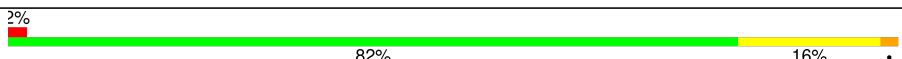

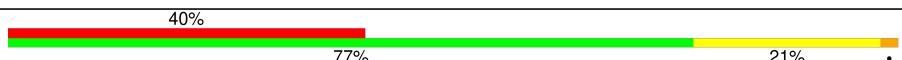
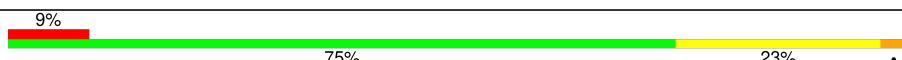
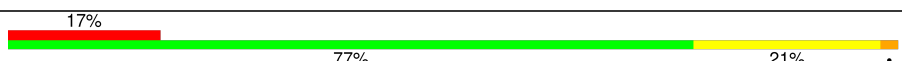
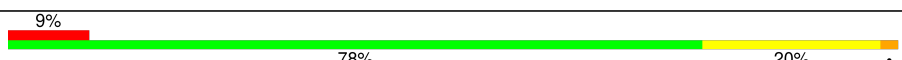
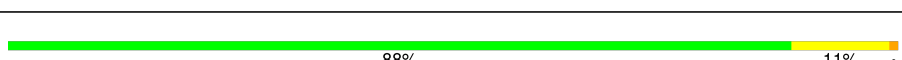
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)
RNA backbone	3690	1071 (3.28-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>5%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	BA	1534	<div> <div>10%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
2	AB	224	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	BB	224	<div> <div>9%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	BO	88	
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	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
28	DB	120	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
29	CC	271	<div> <div>13%</div> <div>82%</div> <div>15%</div> <div>•</div> </div>
29	DC	271	<div> <div>89%</div> <div>10%</div> <div>•</div> </div>
30	CD	209	<div> <div>17%</div> <div>86%</div> <div>13%</div> </div>
31	CA	2904	<div> <div>7%</div> <div>73%</div> <div>23%</div> <div>•</div> </div>
32	DD	209	<div> <div>86%</div> <div>14%</div> </div>
33	CE	201	<div> <div>14%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
33	DE	201	<div> <div>95%</div> <div>5%</div> </div>
34	CF	177	<div> <div>5%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>
34	DF	177	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
35	CG	176	<div> <div>7%</div> <div>82%</div> <div>18%</div> </div>
35	DG	176	<div> <div>%</div> <div>82%</div> <div>18%</div> </div>
36	CH	149	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>•</div> </div>
36	DH	149	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
37	CJ	134	<div> <div>25%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
37	DJ	134	<div> <div>29%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
38	CK	142	<div> <div>5%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
38	DK	142	<div> <div>93%</div> <div>6%</div> <div>•</div> </div>
39	CL	123	<div> <div>9%</div> <div>83%</div> <div>13%</div> <div>• • •</div> </div>
39	DL	123	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
40	CM	144	<div> <div>23%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
40	DM	144	<div> <div>%</div> <div>94%</div> <div>6%</div> </div>
41	CN	136	<div> <div>7%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
41	DN	136	<div> <div>82%</div> <div>17%</div> <div>•</div> </div>


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

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1601	-	-	-	X
56	MG	CA	3021	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3148	-	-	-	X
56	MG	CA	3154	-	-	-	X
66	ACY	DA	3199	-	X	-	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			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 731469900
BA	1052	G	U	engineered mutation	GB 731469900

- 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			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

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

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L10.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 55 is a RNA chain called 23S rRNA.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

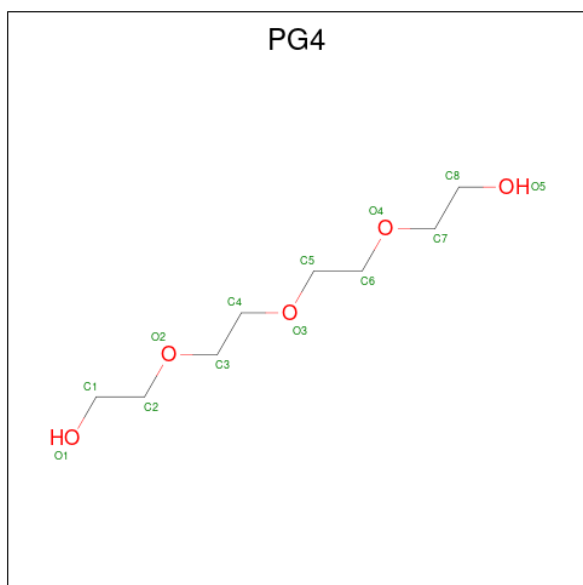
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	71	Total	Mg	0	0
			71	71		
56	BA	43	Total	Mg	0	0
			43	43		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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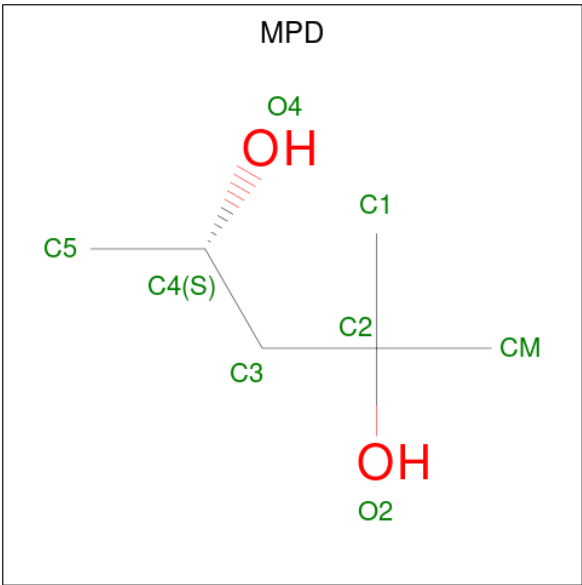
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DA	184	Total	Mg	0	0
			184	184		

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



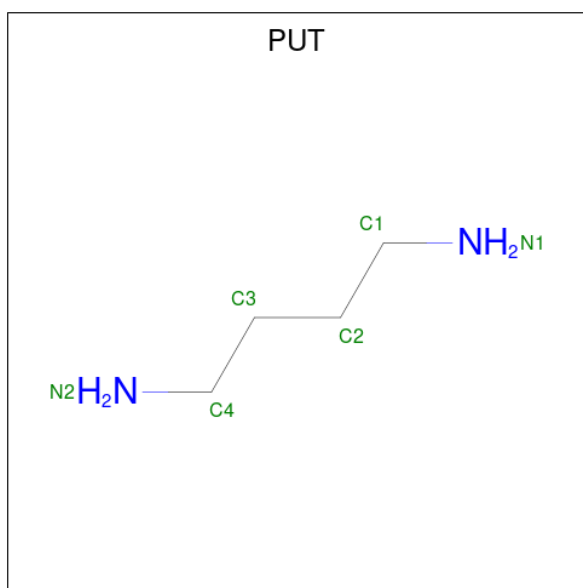
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



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

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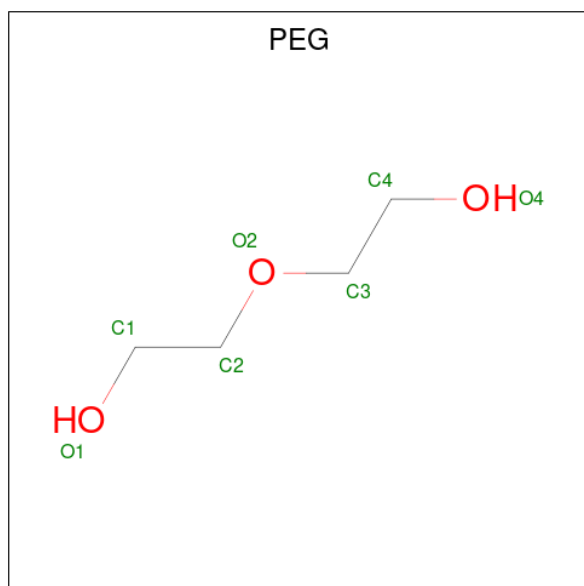
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

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

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



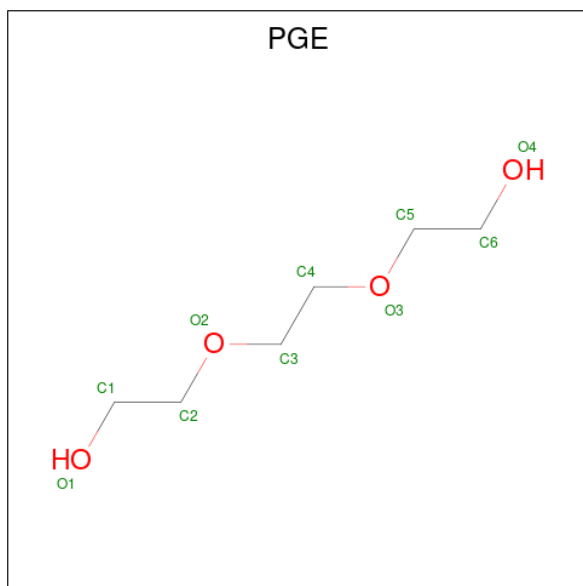
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

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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		
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		

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



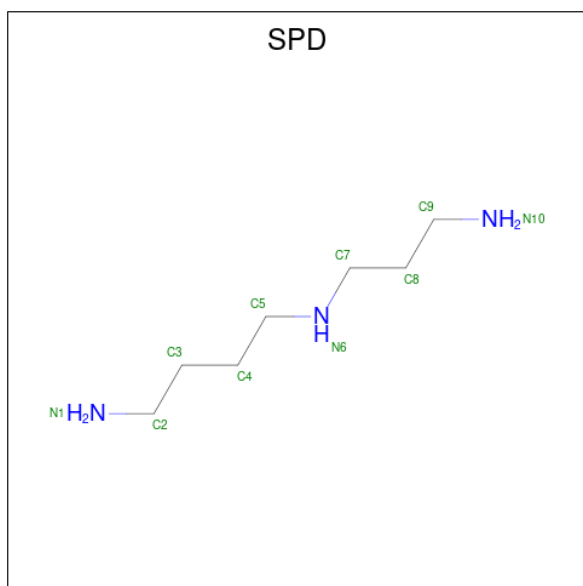
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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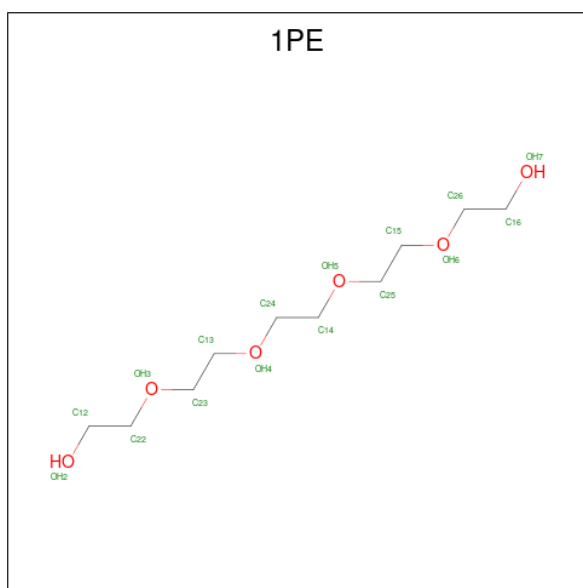
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

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



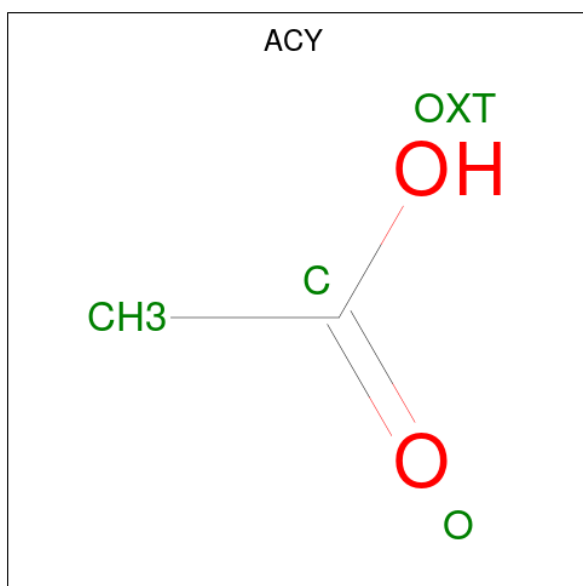
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



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

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



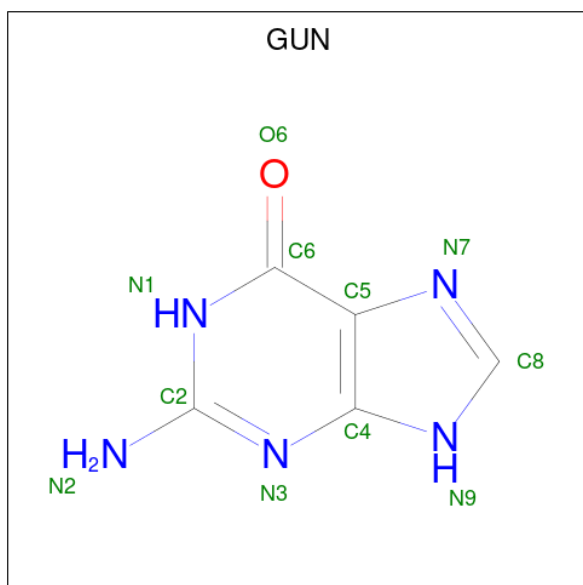
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 67 is GUANINE (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	508	Total	O	0	0
			508	508		
69	AC	5	Total	O	0	0
			5	5		
69	AD	1	Total	O	0	0
			1	1		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	3	Total	O	0	0
			3	3		
69	AK	6	Total	O	0	0
			6	6		
69	AL	10	Total	O	0	0
			10	10		
69	AM	4	Total	O	0	0
			4	4		
69	AN	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AT	4	Total 4	O 4	0	0
69	AU	2	Total 2	O 2	0	0
69	C3	2	Total 2	O 2	0	0
69	C4	1	Total 1	O 1	0	0
69	C5	1	Total 1	O 1	0	0
69	BA	282	Total 282	O 282	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	3	Total 3	O 3	0	0
69	BL	6	Total 6	O 6	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	BR	1	Total 1	O 1	0	0
69	BT	3	Total 3	O 3	0	0
69	BU	3	Total 3	O 3	0	0
69	D1	46	Total 46	O 46	0	0
69	D2	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	28	Total 28	O 28	0	0
69	D4	33	Total 33	O 33	0	0
69	D5	11	Total 11	O 11	0	0
69	D0	26	Total 26	O 26	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	8	Total 8	O 8	0	0
69	CD	7	Total 7	O 7	0	0
69	CA	693	Total 693	O 693	0	0
69	DC	102	Total 102	O 102	0	0
69	DD	95	Total 95	O 95	0	0
69	CE	4	Total 4	O 4	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	4	Total 4	O 4	0	0
69	CO	2	Total 2	O 2	0	0
69	CQ	1	Total 1	O 1	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	63	Total 63	O 63	0	0
69	DF	16	Total 16	O 16	0	0

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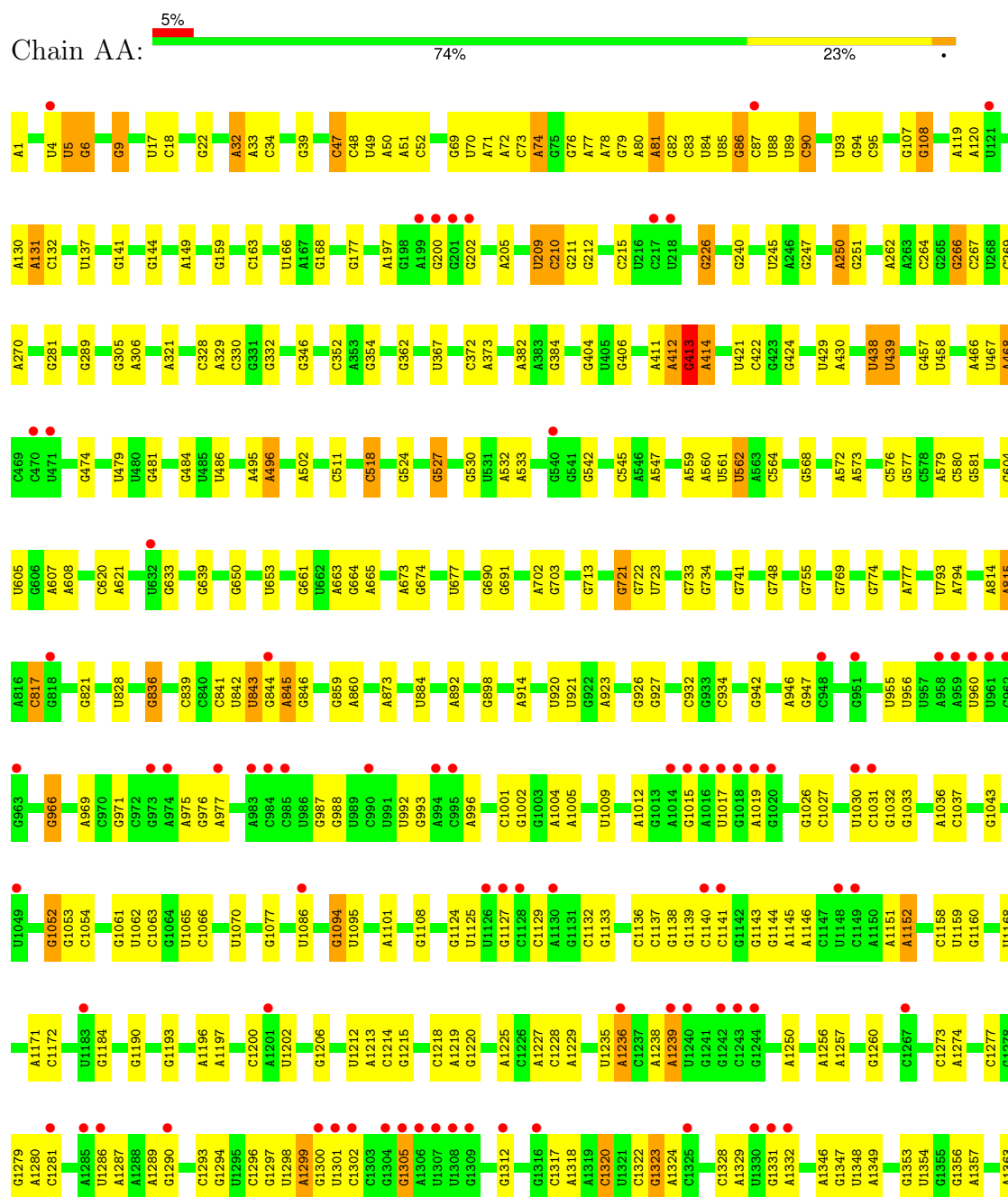
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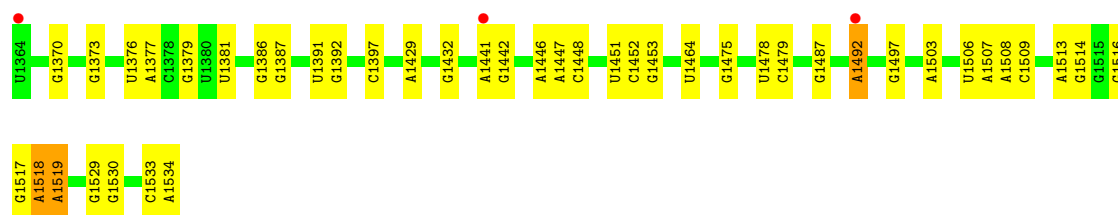
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DG	7	Total	O	0	0
			7	7		
69	DH	2	Total	O	0	0
			2	2		
69	DK	60	Total	O	0	0
			60	60		
69	DL	51	Total	O	0	0
			51	51		
69	DM	68	Total	O	0	0
			68	68		
69	DN	73	Total	O	0	0
			73	73		
69	DO	49	Total	O	0	0
			49	49		
69	DP	38	Total	O	0	0
			38	38		
69	DQ	29	Total	O	0	0
			29	29		
69	DR	61	Total	O	0	0
			61	61		
69	DS	50	Total	O	0	0
			50	50		
69	DT	66	Total	O	0	0
			66	66		
69	DU	19	Total	O	0	0
			19	19		
69	DV	21	Total	O	0	0
			21	21		
69	DW	32	Total	O	0	0
			32	32		
69	DX	25	Total	O	0	0
			25	25		
69	DY	10	Total	O	0	0
			10	10		
69	DZ	6	Total	O	0	0
			6	6		
69	DB	203	Total	O	0	0
			203	203		
69	DA	4830	Total	O	0	0
			4830	4830		

3 Residue-property plots [i](#)

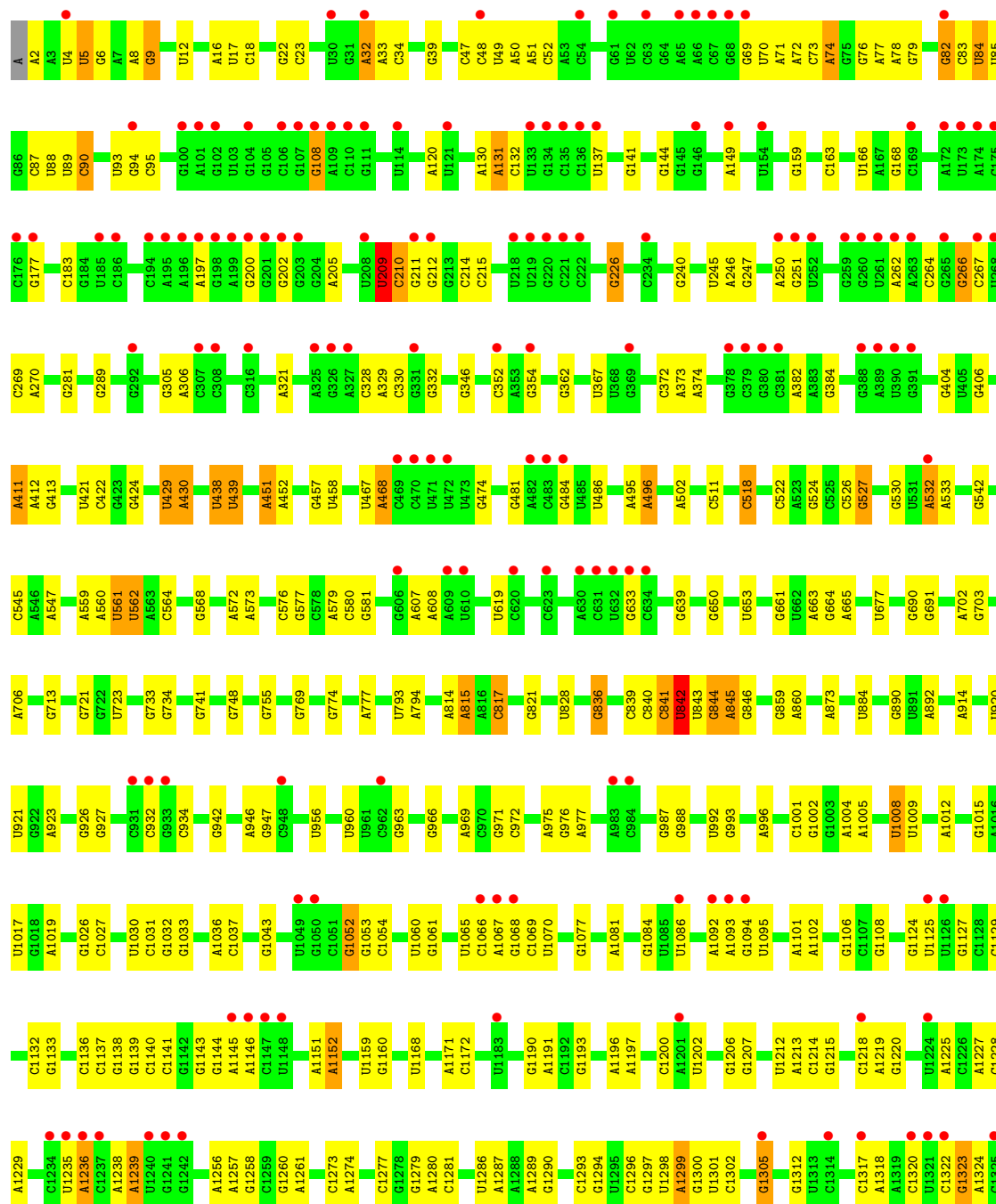
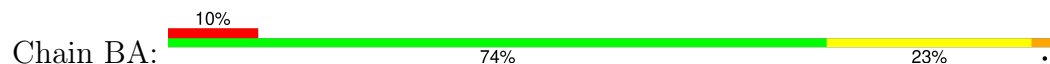
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

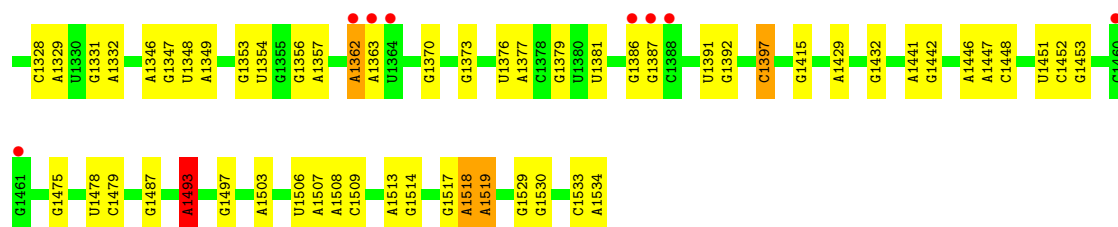
• Molecule 1: 16S rRNA



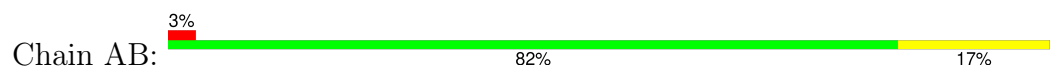


● Molecule 1: 16S rRNA

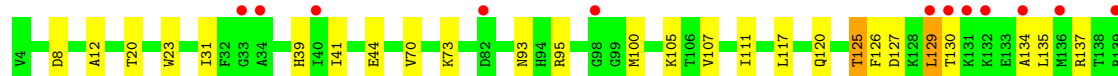
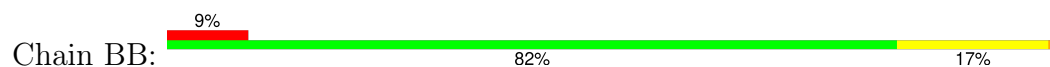




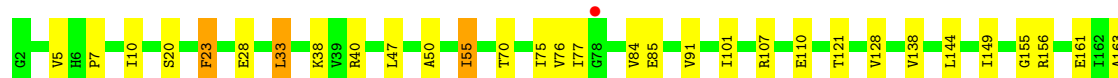
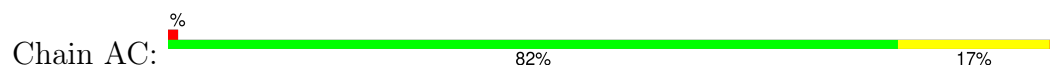
• Molecule 2: 30S ribosomal protein S2



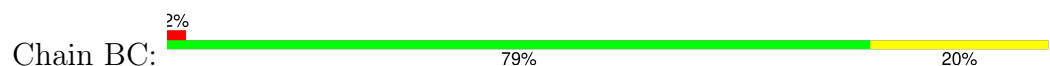
• Molecule 2: 30S ribosomal protein S2



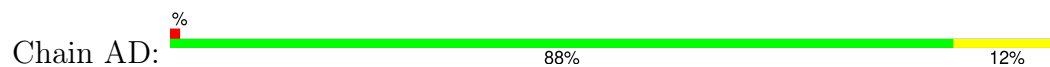
• Molecule 3: 30S ribosomal protein S3



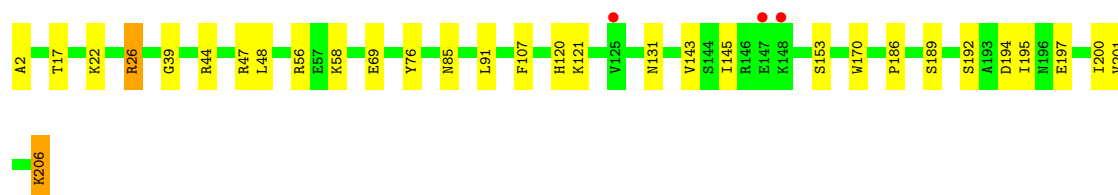
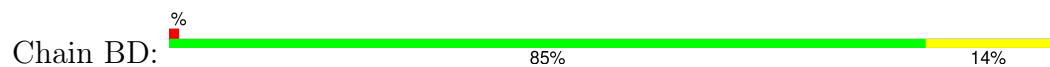
• Molecule 3: 30S ribosomal protein S3



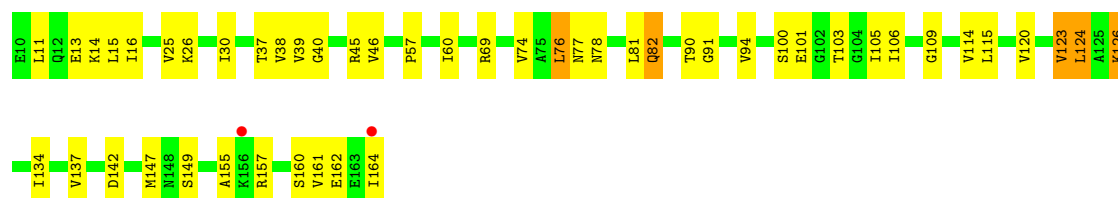
- Molecule 4: 30S ribosomal protein S4



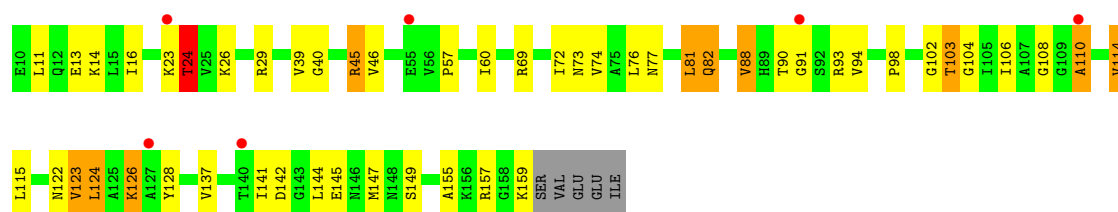
- Molecule 4: 30S ribosomal protein S4



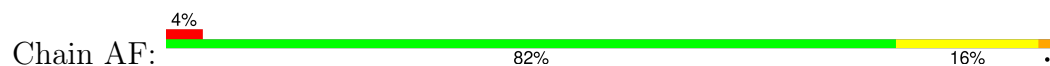
- Molecule 5: 30S ribosomal protein S5



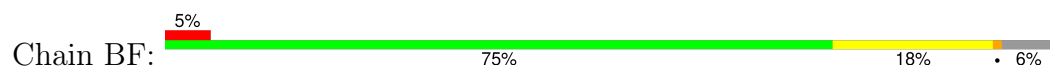
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

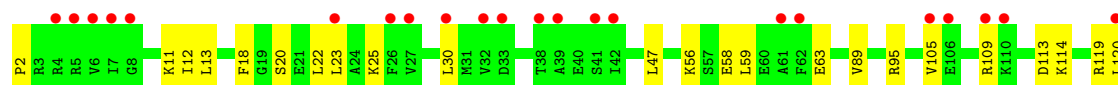
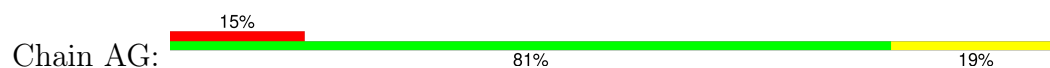


- Molecule 6: 30S ribosomal protein S6

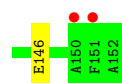
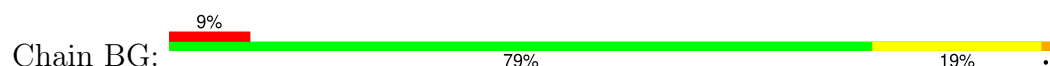




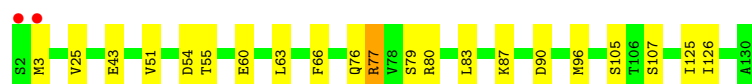
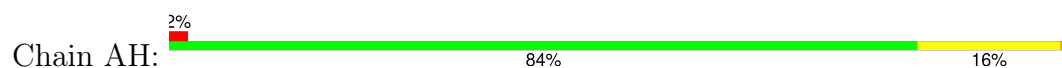
- Molecule 7: 30S ribosomal protein S7



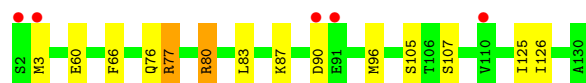
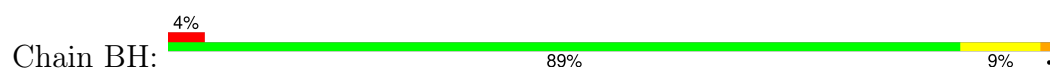
- Molecule 7: 30S ribosomal protein S7



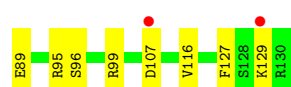
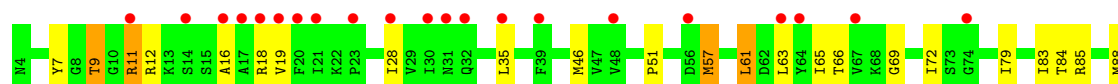
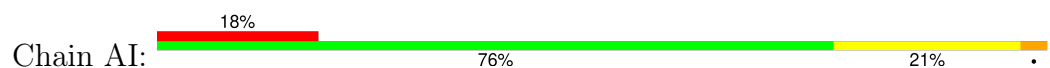
- Molecule 8: 30S ribosomal protein S8



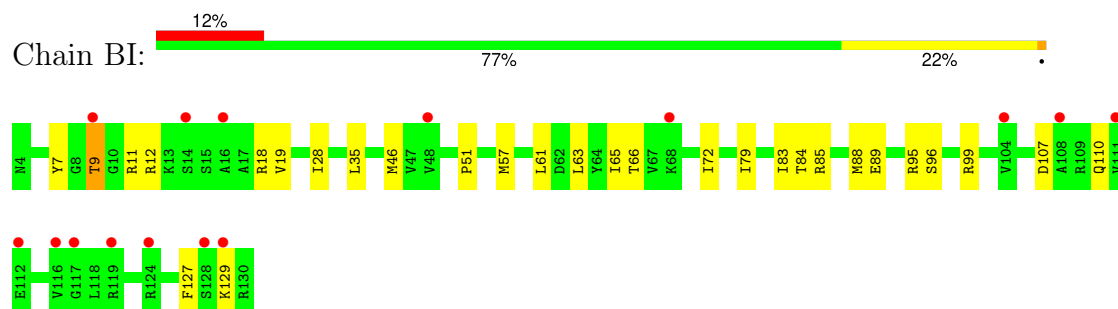
- Molecule 8: 30S ribosomal protein S8



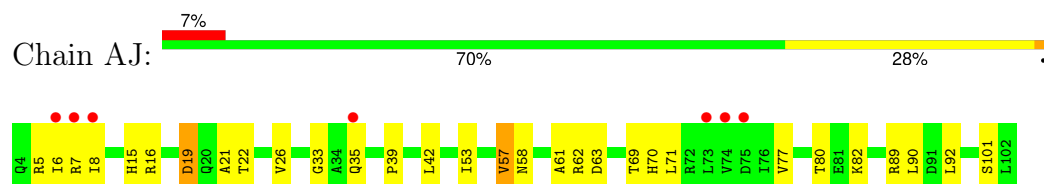
- Molecule 9: 30S ribosomal protein S9



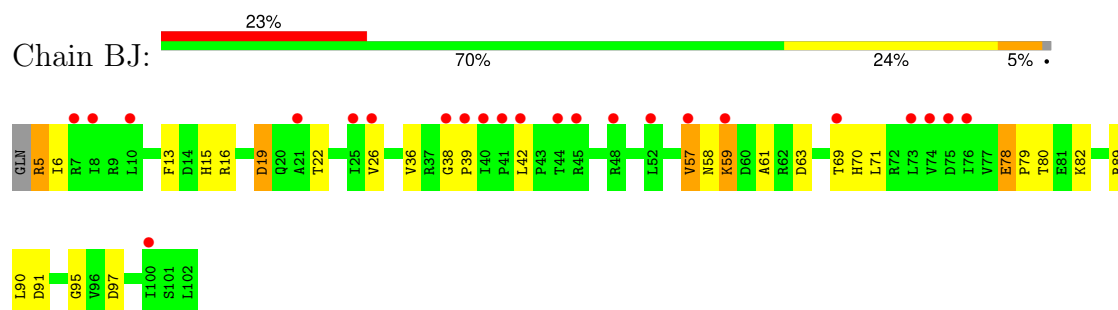
- Molecule 9: 30S ribosomal protein S9



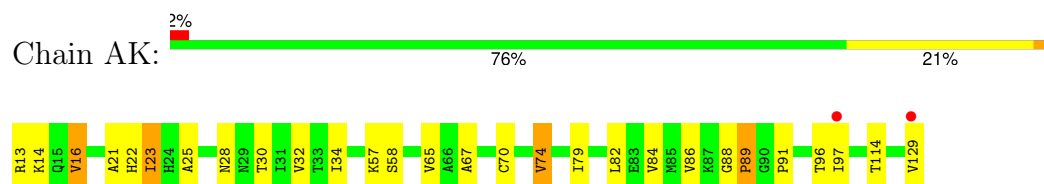
- Molecule 10: 30S ribosomal protein S10



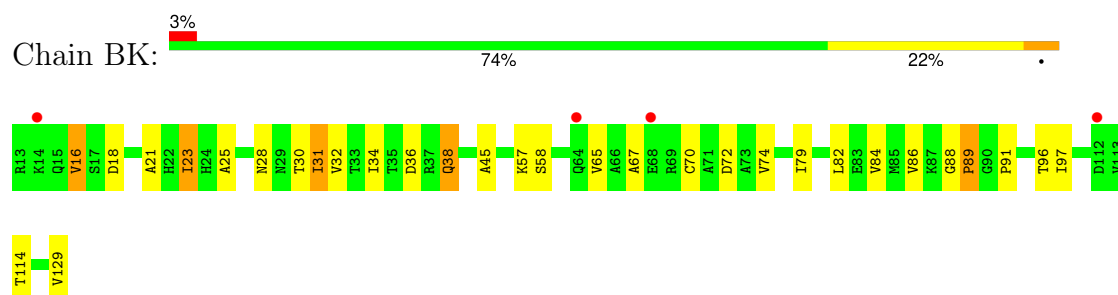
- Molecule 10: 30S ribosomal protein S10



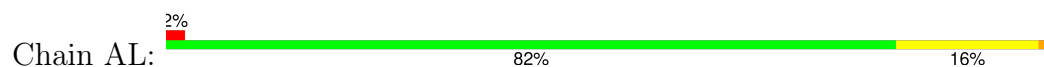
- Molecule 11: 30S ribosomal protein S11




- Molecule 11: 30S ribosomal protein S11




- Molecule 12: 30S ribosomal protein S12

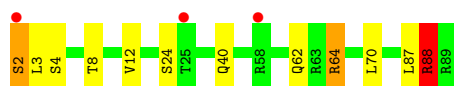


Chain AO:  88% 11%




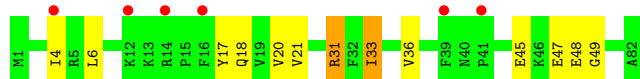
- Molecule 15: 30S ribosomal protein S15

Chain BO:  3% 86% 10%




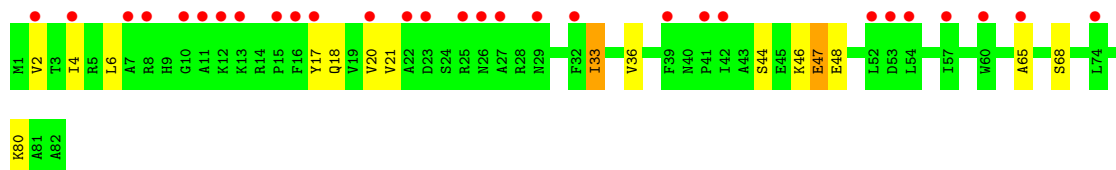
- Molecule 16: 30S ribosomal protein S16

Chain AP:  7% 84% 13%




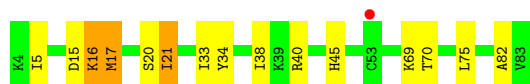
- Molecule 16: 30S ribosomal protein S16

Chain BP:  35% 80% 17%



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  1% 81% 15%




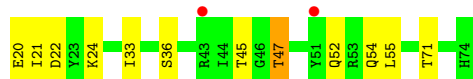
- Molecule 17: 30S ribosomal protein S17

Chain BQ:  10% 68% 25% 6%

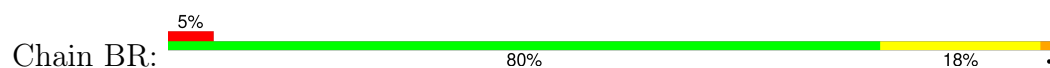


- Molecule 18: 30S ribosomal protein S18

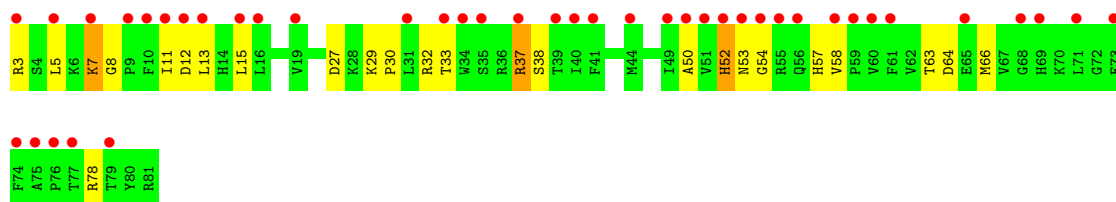
Chain AR:  4% 78% 20%



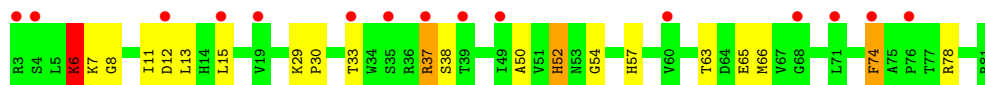
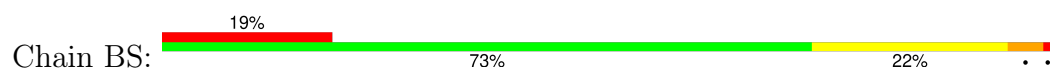
- Molecule 18: 30S ribosomal protein S18



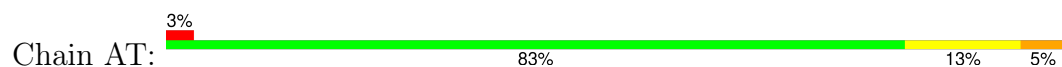
- Molecule 19: 30S ribosomal protein S19



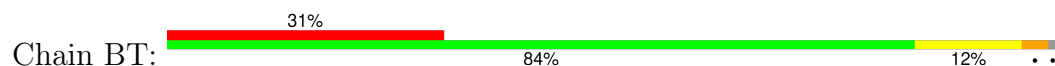
- Molecule 19: 30S ribosomal protein S19



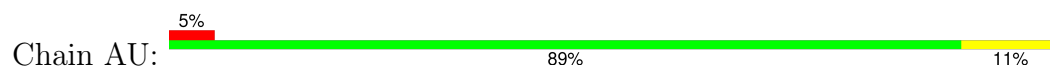
- Molecule 20: 30S ribosomal protein S20

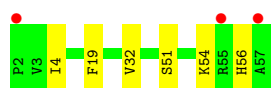


- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

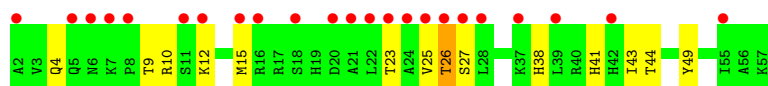
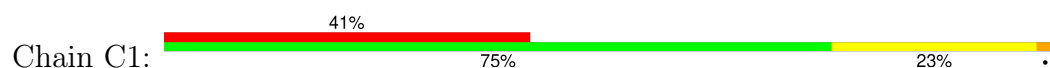




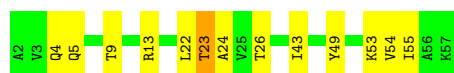
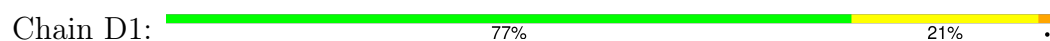
- Molecule 21: 30S ribosomal protein S21



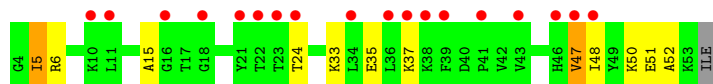
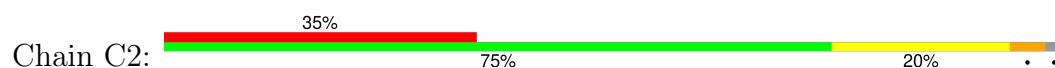
- Molecule 22: 50S ribosomal protein L32



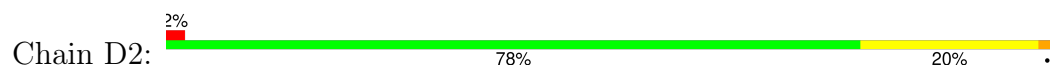
- Molecule 22: 50S ribosomal protein L32



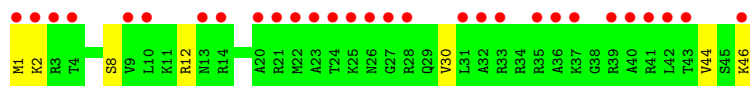
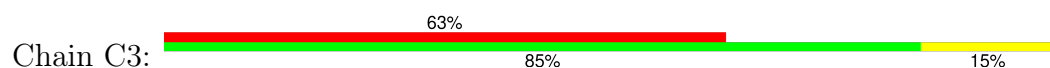
- Molecule 23: 50S ribosomal protein L33



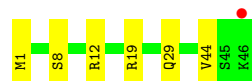
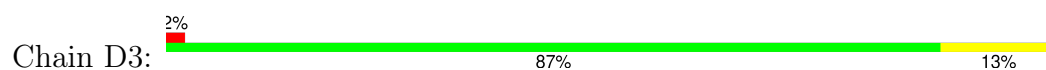
- Molecule 23: 50S ribosomal protein L33



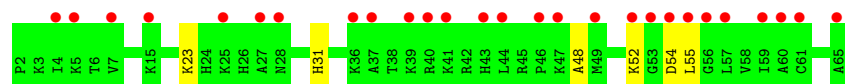
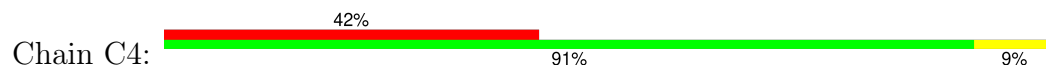
- Molecule 24: 50S ribosomal protein L34



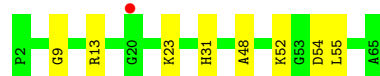
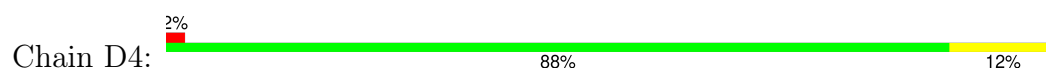
- Molecule 24: 50S ribosomal protein L34



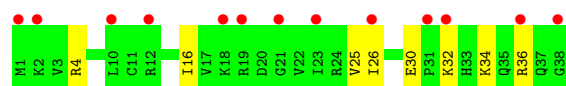
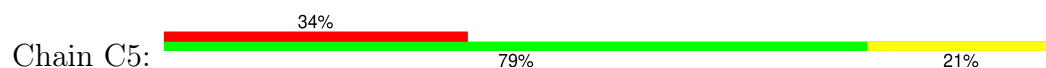
- Molecule 25: 50S ribosomal protein L35



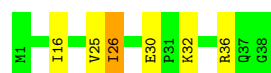
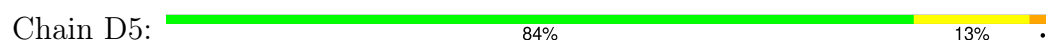
- Molecule 25: 50S ribosomal protein L35



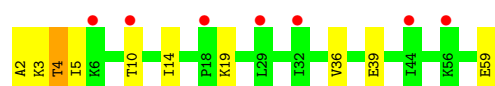
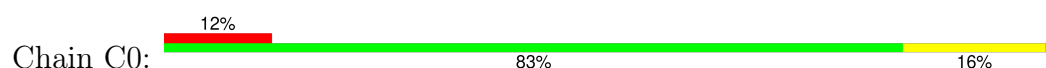
- Molecule 26: 50S ribosomal protein L36



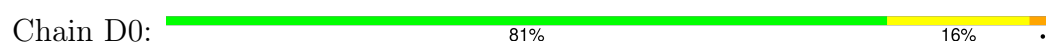
- Molecule 26: 50S ribosomal protein L36



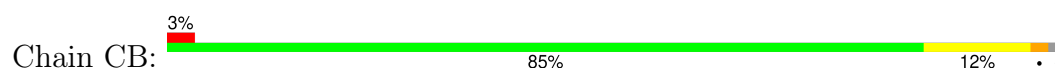
- Molecule 27: 50S ribosomal protein L30



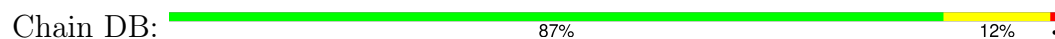
- Molecule 27: 50S ribosomal protein L30



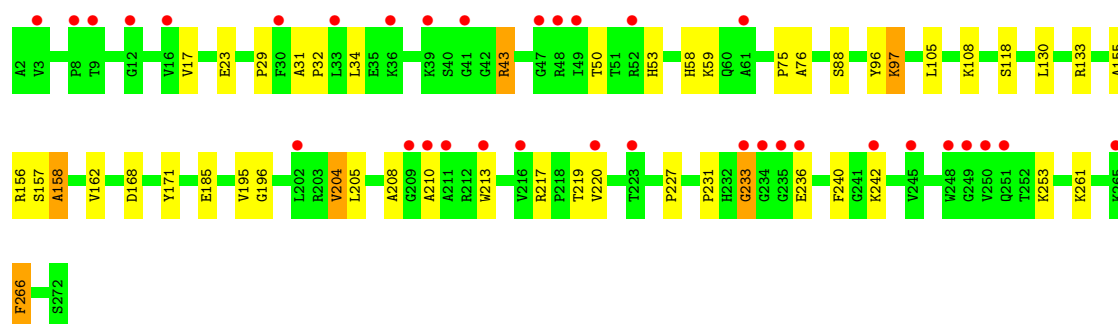
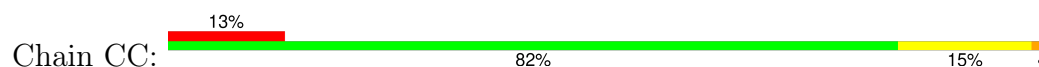
- Molecule 28: 5S rRNA



- Molecule 28: 5S rRNA



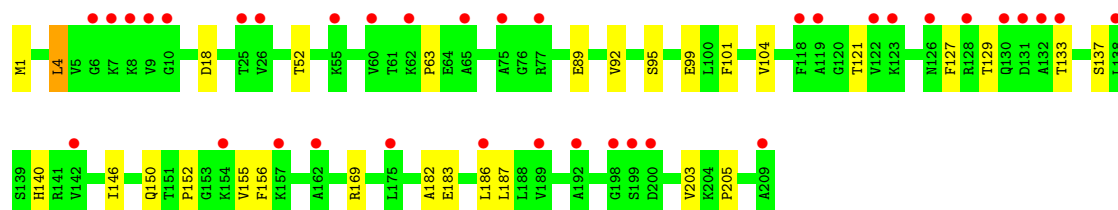
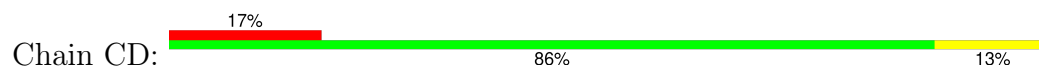
- Molecule 29: 50S ribosomal protein L2



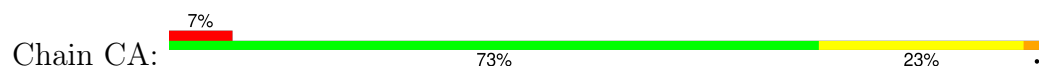
- Molecule 29: 50S ribosomal protein L2

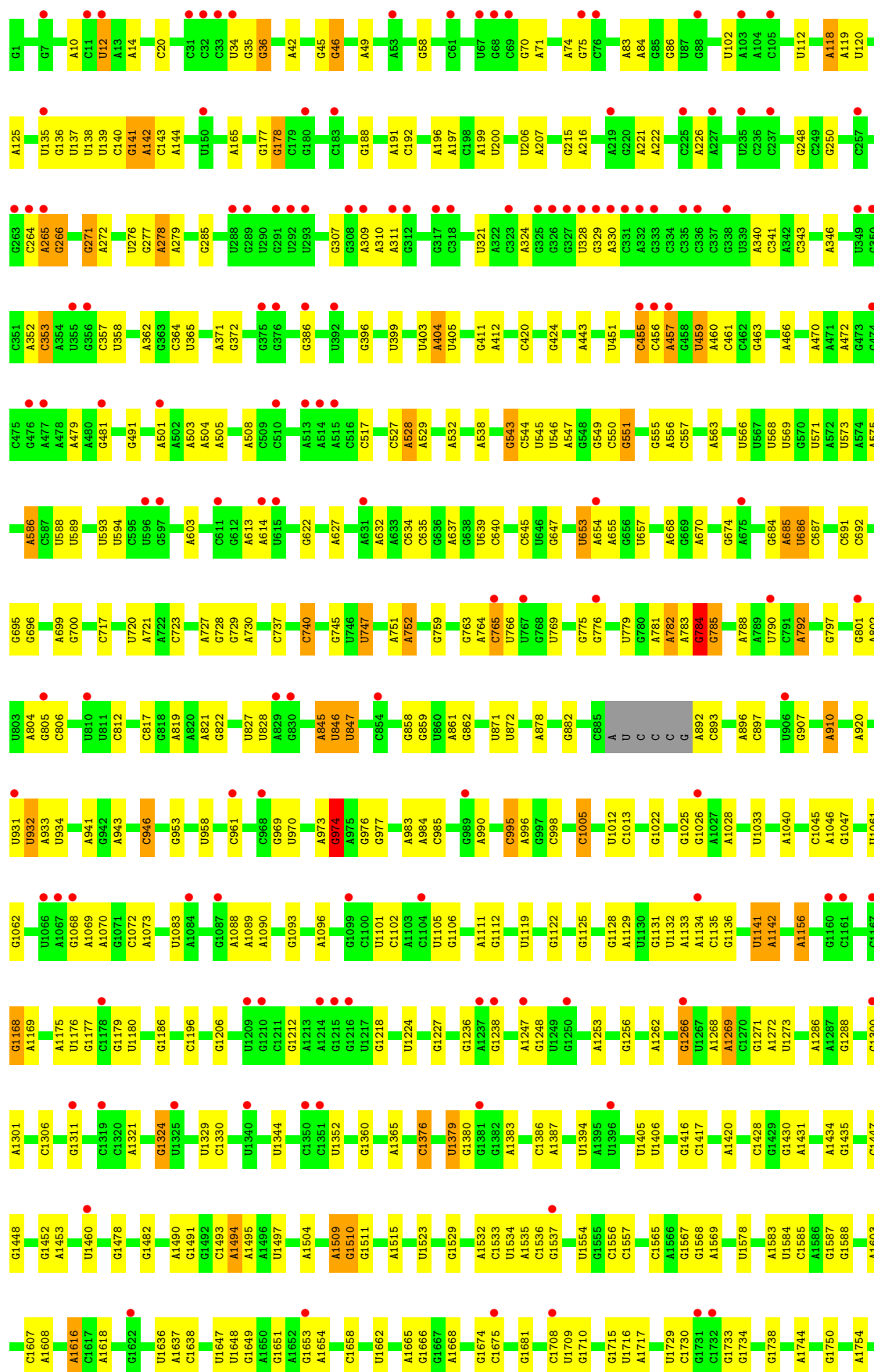


- Molecule 30: 50S ribosomal protein L3



- Molecule 31: 23S rRNA





- Molecule 32: 50S ribosomal protein L3

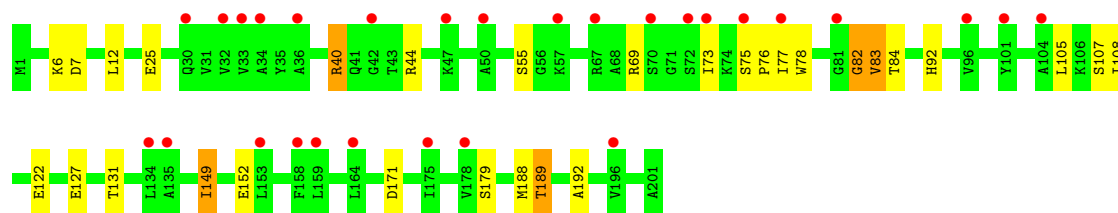
Chain DD:



- Molecule 33: 50S ribosomal protein L4

Chain CE:





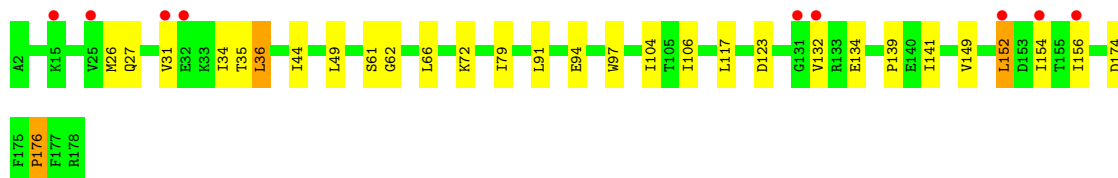
- Molecule 33: 50S ribosomal protein L4

Chain DE: 95% 5%



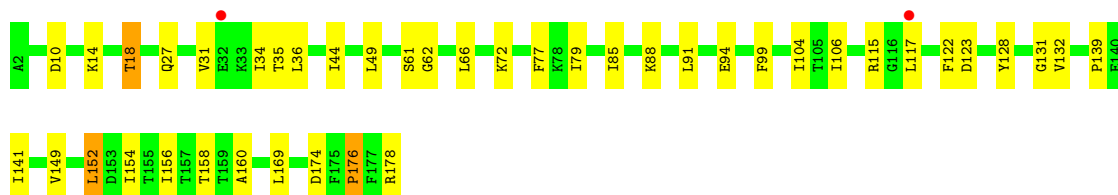
- Molecule 34: 50S ribosomal protein L5

Chain CF: 5% 83% 15%



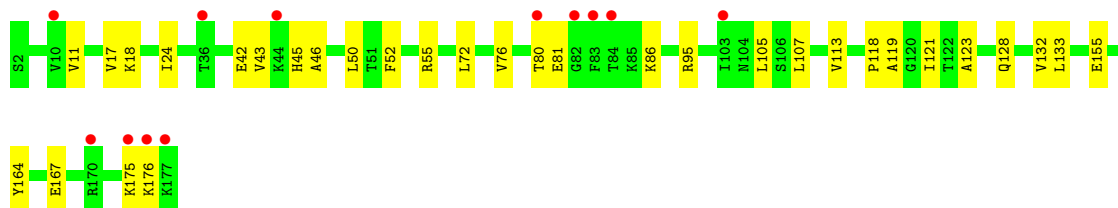
- Molecule 34: 50S ribosomal protein L5

Chain DF: 5% 76% 22%



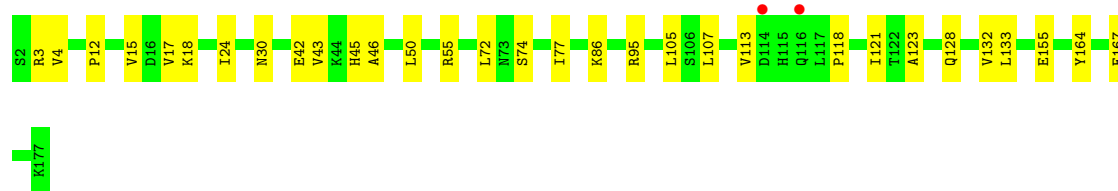
- Molecule 35: 50S ribosomal protein L6

Chain CG: 7% 82% 18%

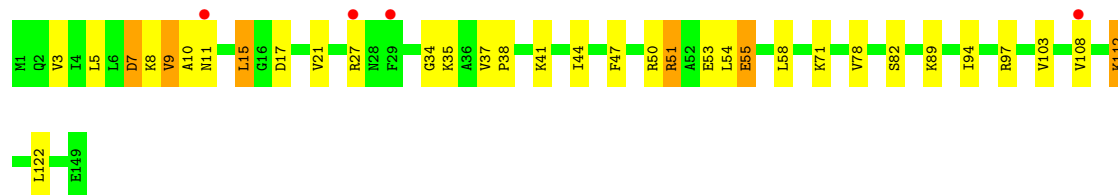
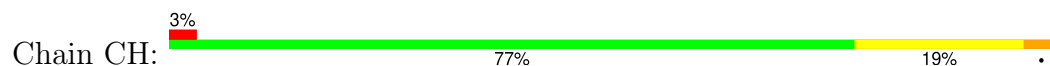


- Molecule 35: 50S ribosomal protein L6

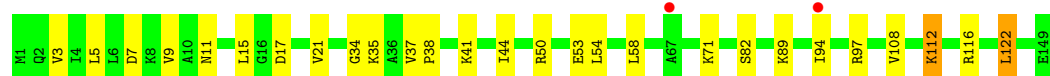
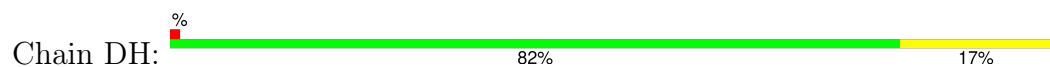
Chain DG: 5% 82% 18%



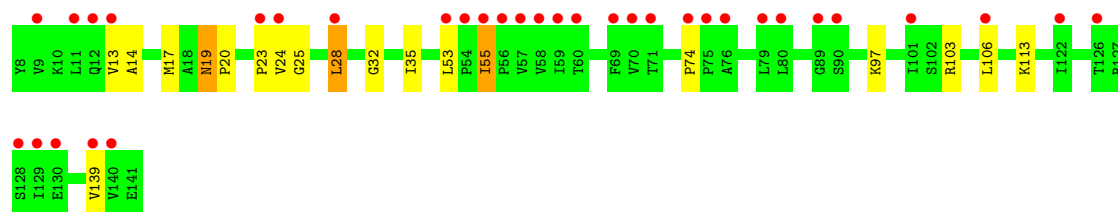
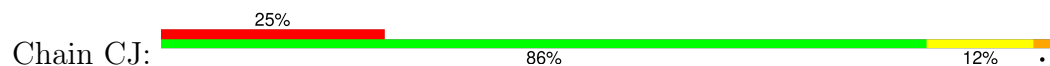
- Molecule 36: 50S ribosomal protein L9



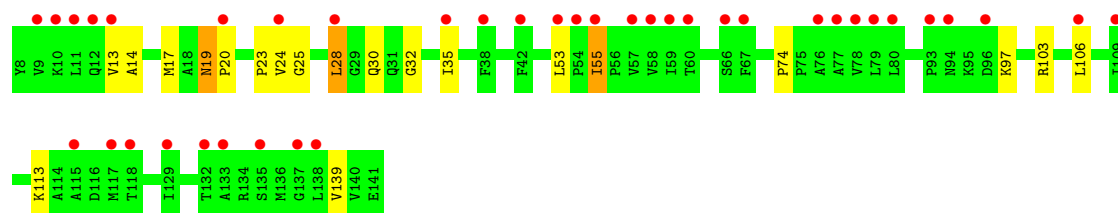
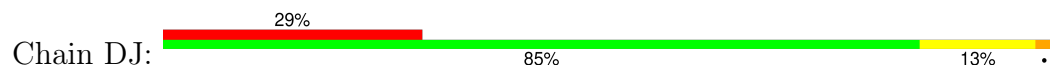
- Molecule 36: 50S ribosomal protein L9



- Molecule 37: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L11



- Molecule 38: 50S ribosomal protein L13





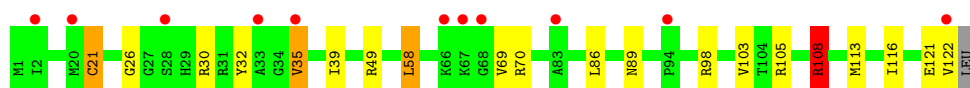
- Molecule 38: 50S ribosomal protein L13

Chain DK: 93% 6% .



- Molecule 39: 50S ribosomal protein L14

Chain CL: 9% 83% 13% ...



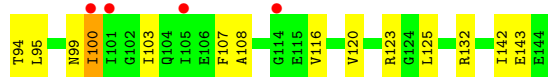
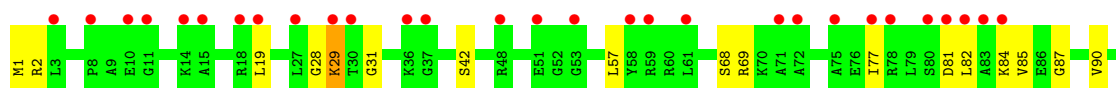
- Molecule 39: 50S ribosomal protein L14

Chain DL: 86% 12% .



- Molecule 40: 50S ribosomal protein L15

Chain CM: 23% 78% 20% .



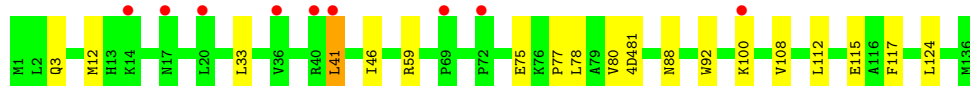
- Molecule 40: 50S ribosomal protein L15

Chain DM: 94% 6%




- Molecule 41: 50S ribosomal protein L16

Chain CN: 7% 86% 13% .




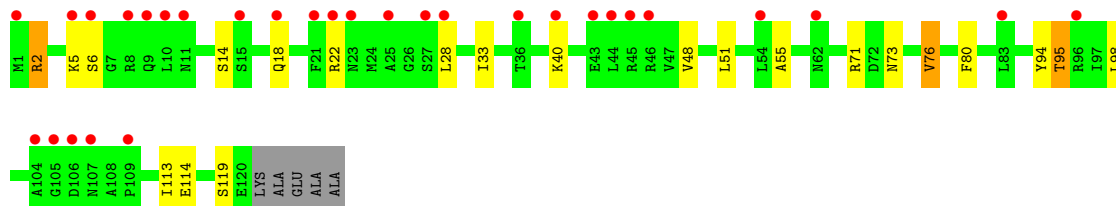
- Molecule 41: 50S ribosomal protein L16

Chain DN:  82% 17%



- Molecule 42: 50S ribosomal protein L17

Chain CO:  24% 78% 15%




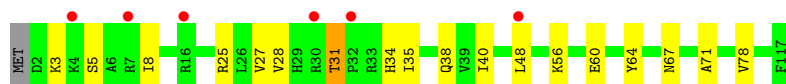
- Molecule 42: 50S ribosomal protein L17

Chain DO:  87% 11%




- Molecule 43: 50S ribosomal protein L18

Chain CP:  5% 84% 15%




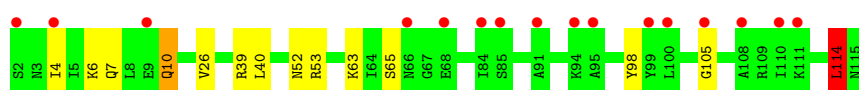
- Molecule 43: 50S ribosomal protein L18

Chain DP:  80% 18%




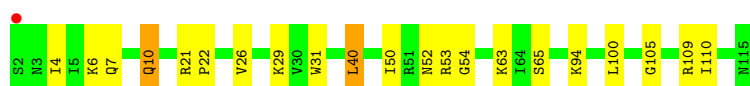
- Molecule 44: 50S ribosomal protein L19

Chain CQ:  14% 88% 11%

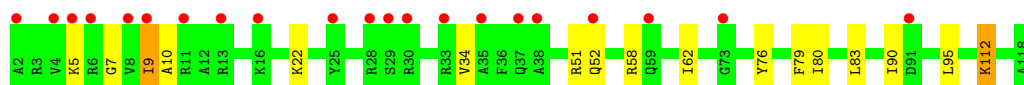
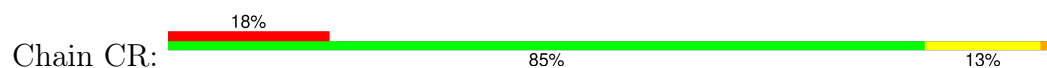


- Molecule 44: 50S ribosomal protein L19

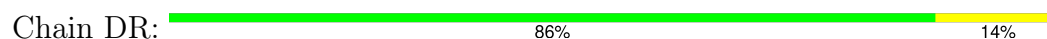
Chain DQ:  82% 17%



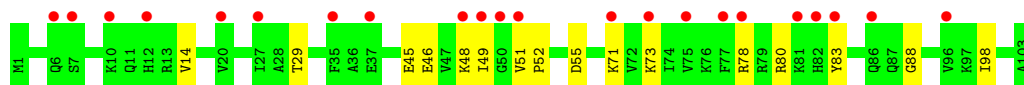
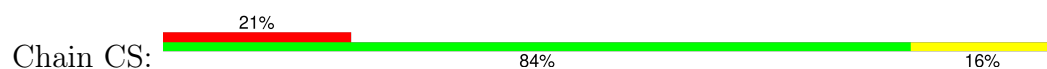
- Molecule 45: 50S ribosomal protein L20



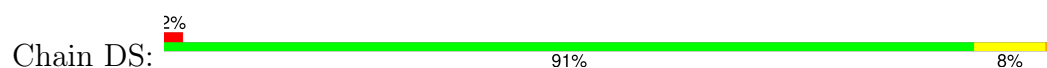
- Molecule 45: 50S ribosomal protein L20



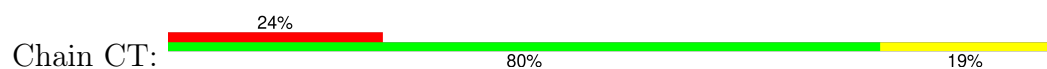
- Molecule 46: 50S ribosomal protein L21



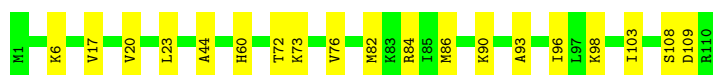
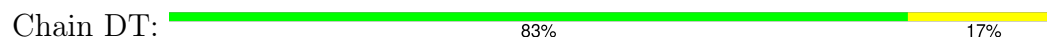
- Molecule 46: 50S ribosomal protein L21



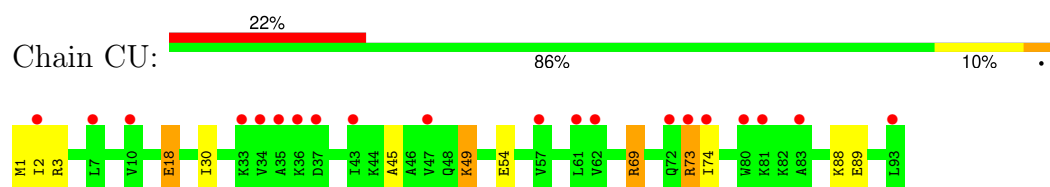
- Molecule 47: 50S ribosomal protein L22



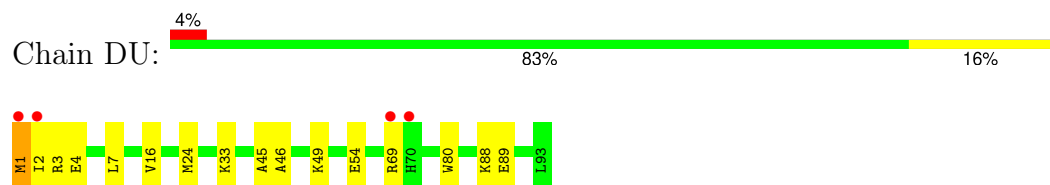
- Molecule 47: 50S ribosomal protein L22



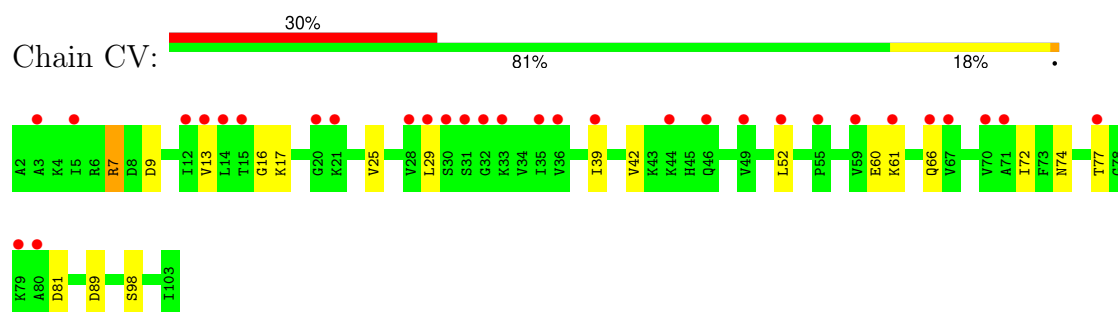
- Molecule 48: 50S ribosomal protein L23



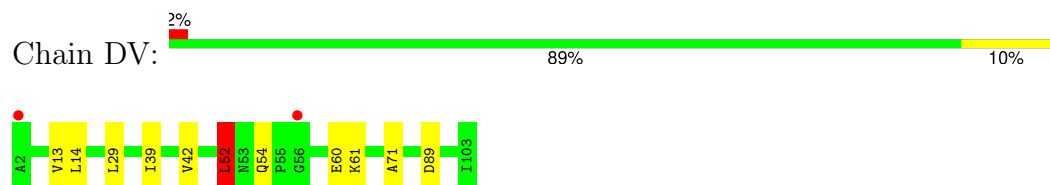
- Molecule 48: 50S ribosomal protein L23



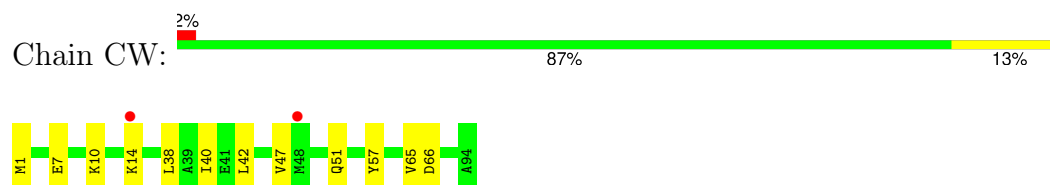
- Molecule 49: 50S ribosomal protein L24



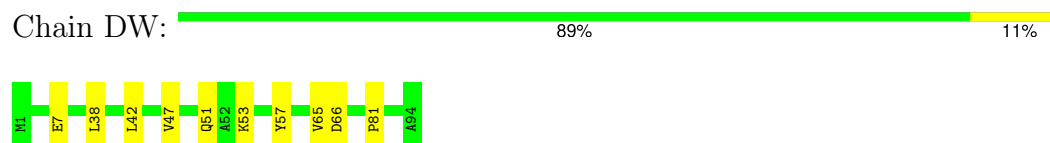
- Molecule 49: 50S ribosomal protein L24



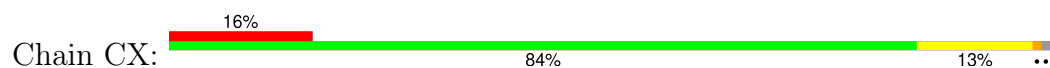
- Molecule 50: 50S ribosomal protein L25

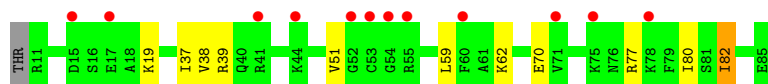


- Molecule 50: 50S ribosomal protein L25

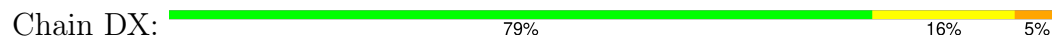


- Molecule 51: 50S ribosomal protein L27

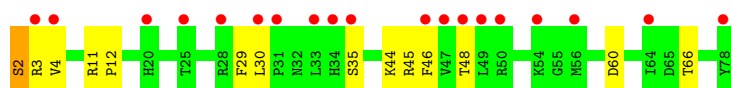
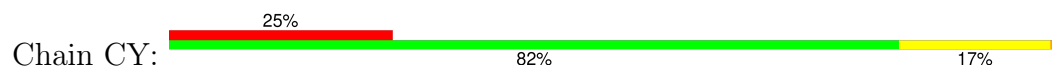




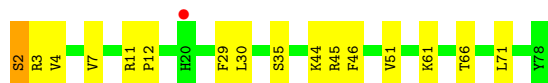
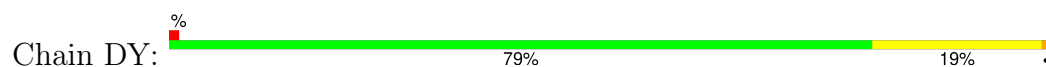
- Molecule 51: 50S ribosomal protein L27



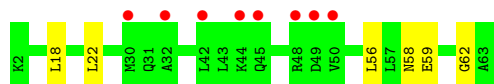
- Molecule 52: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L28



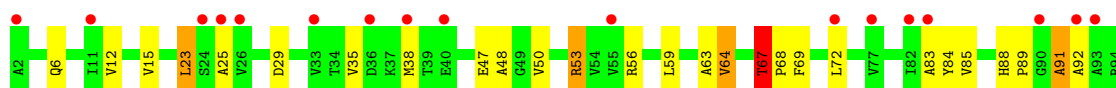
- Molecule 53: 50S ribosomal protein L29



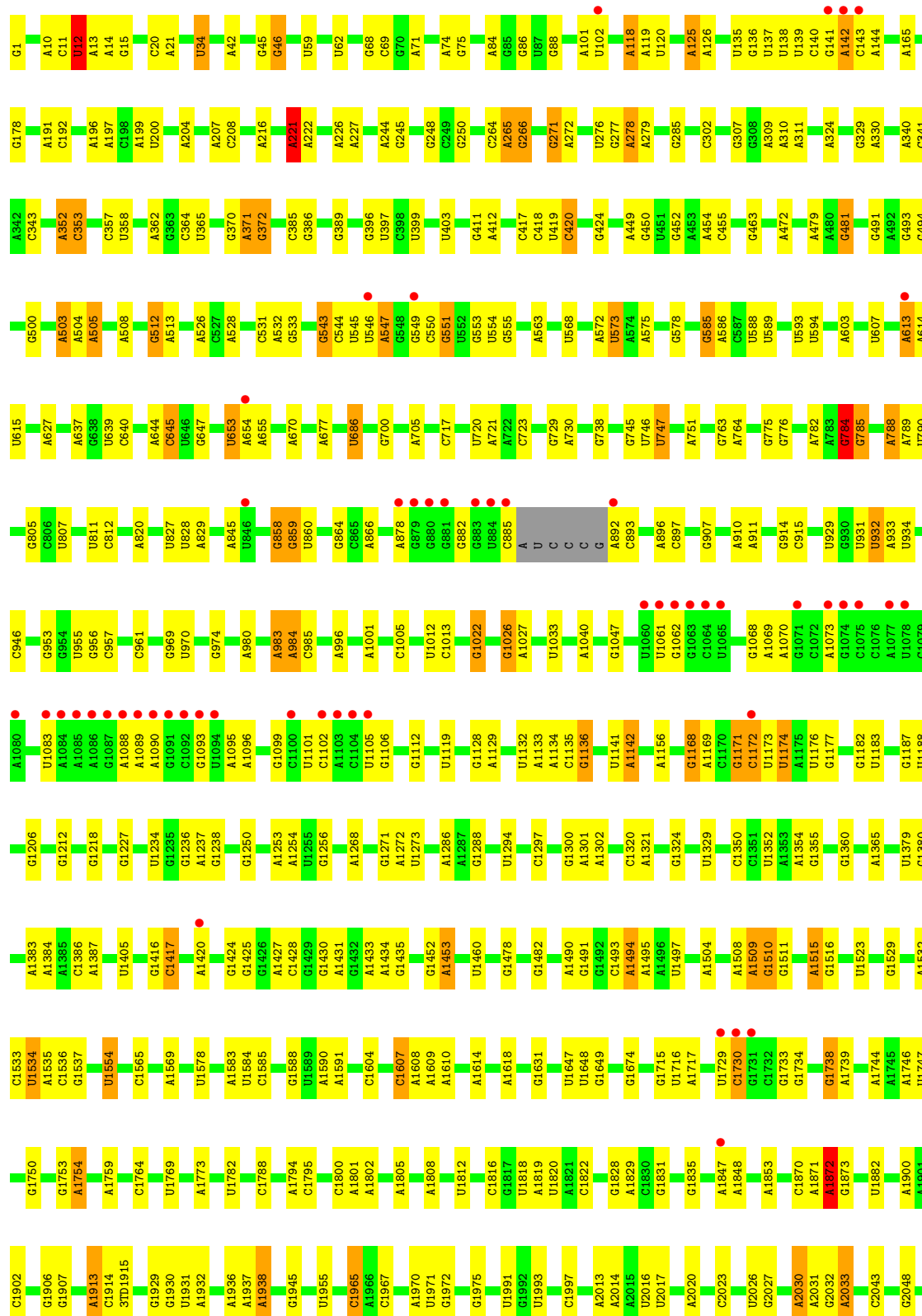
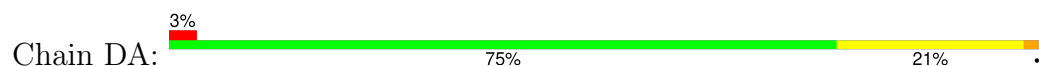
- Molecule 53: 50S ribosomal protein L29

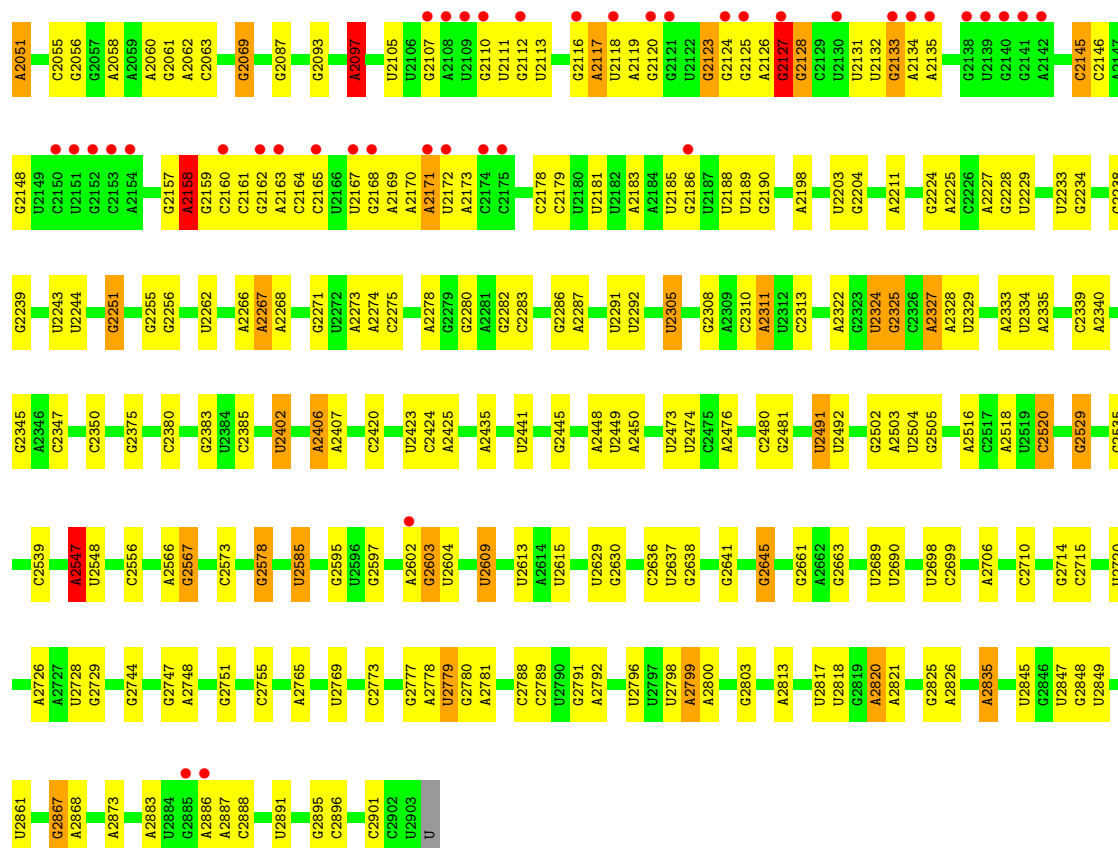


- Molecule 54: 50S ribosomal protein L10



● Molecule 55: 23S rRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.04Å 436.85Å 628.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.03 48.39 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.39-3.03) 96.7 (48.39-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.172 , 0.200 0.186 , 0.215	Depositor DCC
R_{free} test set	4332 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295130	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.98	10/36597 (0.0%)	0.86	2/57088 (0.0%)
1	BA	0.98	10/36572 (0.0%)	0.86	3/57049 (0.0%)
2	AB	0.47	0/1784	0.66	0/2403
2	BB	0.47	0/1784	0.66	0/2403
3	AC	0.44	0/1652	0.67	0/2225
3	BC	0.44	0/1652	0.67	0/2225
4	AD	0.46	0/1665	0.68	0/2227
4	BD	0.44	0/1665	0.69	0/2227
5	AE	0.47	0/1157	0.76	0/1557
5	BE	0.48	0/1118	0.78	0/1504
6	AF	0.46	0/881	0.70	0/1189
6	BF	0.47	0/835	0.80	0/1128
7	AG	0.46	0/1196	0.63	0/1602
7	BG	0.45	0/1196	0.62	0/1602
8	AH	0.44	0/989	0.71	0/1326
8	BH	0.43	0/989	0.69	0/1326
9	AI	0.45	0/1034	0.69	0/1375
9	BI	0.45	0/1034	0.67	0/1375
10	AJ	0.43	0/806	0.67	0/1089
10	BJ	0.47	0/797	0.70	0/1077
11	AK	0.44	0/893	0.65	0/1205
11	BK	0.45	0/893	0.69	0/1205
12	AL	0.45	0/960	0.71	0/1286
12	BL	0.42	0/960	0.72	0/1286
13	AM	0.52	0/893	0.77	0/1193
13	BM	0.51	0/893	0.74	0/1193
14	AN	0.45	0/817	0.65	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.46	0/722	0.63	0/964
15	BO	0.44	0/722	0.62	0/964
16	AP	0.46	0/659	0.70	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.48	0/659	0.74	0/884
17	AQ	0.48	0/658	0.75	0/881
17	BQ	0.50	0/658	0.76	0/881
18	AR	0.51	0/463	0.66	0/621
18	BR	0.49	0/463	0.65	0/621
19	AS	0.47	0/653	0.61	0/877
19	BS	0.47	0/653	0.63	0/877
20	AT	0.49	0/676	0.70	0/895
20	BT	0.52	0/671	0.67	0/888
21	AU	0.40	0/472	0.60	0/627
21	BU	0.39	0/472	0.61	0/627
22	C1	0.48	0/450	0.70	0/599
22	D1	0.59	0/450	0.73	0/599
23	C2	0.48	0/416	0.73	0/554
23	D2	0.49	0/421	0.74	0/561
24	C3	0.45	0/380	0.71	0/498
24	D3	0.58	0/380	0.73	0/498
25	C4	0.44	0/513	0.64	0/676
25	D4	0.51	0/513	0.68	0/676
26	C5	0.44	0/303	0.69	0/397
26	D5	0.59	0/303	0.73	0/397
27	C0	0.51	0/453	0.76	0/605
27	D0	0.66	0/467	0.77	0/623
28	CB	0.94	0/2828	0.89	2/4410 (0.0%)
28	DB	1.08	1/2872 (0.0%)	0.90	0/4478
29	CC	0.46	0/2122	0.75	0/2852
29	DC	0.52	0/2122	0.76	0/2852
30	CD	0.44	0/1586	0.70	0/2134
31	CA	1.02	45/69165 (0.1%)	0.88	19/107896 (0.0%)
32	DD	0.51	0/1576	0.70	0/2119
33	CE	0.43	0/1571	0.72	0/2113
33	DE	0.51	0/1571	0.70	0/2113
34	CF	0.43	0/1435	0.69	0/1926
34	DF	0.52	0/1435	0.73	0/1926
35	CG	0.41	0/1343	0.67	0/1816
35	DG	0.45	0/1343	0.66	0/1816
36	CH	0.47	0/1121	0.68	0/1515
36	DH	0.47	0/1121	0.68	0/1515
37	CJ	0.51	0/993	0.64	0/1341
37	DJ	0.51	0/993	0.64	0/1341
38	CK	0.42	0/1152	0.68	0/1551
38	DK	0.56	0/1152	0.71	0/1551
39	CL	0.44	0/947	0.69	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DL	0.53	0/955	0.70	0/1279
40	CM	0.45	0/1062	0.74	1/1413 (0.1%)
40	DM	0.49	0/1062	0.72	0/1413
41	CN	0.45	0/1081	0.70	0/1443
41	DN	0.57	0/1092	0.76	1/1457 (0.1%)
42	CO	0.45	0/973	0.72	1/1301 (0.1%)
42	DO	0.58	0/1006	0.78	0/1345
43	CP	0.44	0/902	0.72	0/1209
43	DP	0.53	0/910	0.73	0/1219
44	CQ	0.44	0/929	0.73	1/1242 (0.1%)
44	DQ	0.51	0/929	0.72	0/1242
45	CR	0.48	0/960	0.68	0/1278
45	DR	0.58	0/960	0.70	0/1278
46	CS	0.43	0/829	0.74	0/1107
46	DS	0.52	0/829	0.75	0/1107
47	CT	0.41	0/864	0.73	0/1156
47	DT	0.60	0/864	0.72	0/1156
48	CU	0.47	0/745	0.73	0/994
48	DU	0.54	0/745	0.75	0/994
49	CV	0.45	0/788	0.76	0/1051
49	DV	0.51	0/788	0.76	0/1051
50	CW	0.41	0/766	0.66	0/1025
50	DW	0.52	0/766	0.71	0/1025
51	CX	0.40	0/576	0.64	0/762
51	DX	0.54	0/598	0.70	0/790
52	CY	0.45	0/635	0.70	0/848
52	DY	0.51	0/635	0.73	1/848 (0.1%)
53	CZ	0.41	0/502	0.63	0/667
53	DZ	0.48	0/502	0.62	0/667
54	DI	0.54	0/1037	0.78	1/1402 (0.1%)
55	DA	1.19	63/69364 (0.1%)	0.93	15/108207 (0.0%)
All	All	0.93	129/309281 (0.0%)	0.84	47/462224 (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	1
20	AT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	3
55	DA	0	37
All	All	0	45

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.10	1.28	1.42
31	CA	12	U	C1'-N1	8.94	1.62	1.48
55	DA	1237	A	C3'-O3'	-8.70	1.29	1.42
31	CA	1936	A	N9-C4	-8.66	1.32	1.37
31	CA	2225	A	C3'-O3'	8.52	1.54	1.42

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.42	116.54	108.20
31	CA	752	A	O4'-C1'-N9	10.40	116.52	108.20
55	DA	1936	A	O4'-C1'-N9	9.02	115.41	108.20
55	DA	2406	A	C5'-C4'-O4'	-7.61	99.97	109.10
54	DI	132	TYR	C-N-CA	7.10	139.44	121.70

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1077	G	Sidechain
1	AA	1094	G	Sidechain
1	AA	898	G	Sidechain
20	AT	24	ARG	Sidechain
1	BA	1077	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	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	32911	0	16581	118	0
2	AB	1753	0	1780	14	0
2	BB	1753	0	1780	13	0
3	AC	1625	0	1696	17	0
3	BC	1625	0	1696	29	0
4	AD	1643	0	1707	12	0
4	BD	1643	0	1707	18	0
5	AE	1144	0	1185	24	0
5	BE	1105	0	1148	29	0
6	AF	862	0	864	10	0
6	BF	817	0	808	4	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	11	0
8	AH	979	0	1031	6	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	14	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	13	0
10	BJ	787	0	828	13	0
11	AK	877	0	887	15	0
11	BK	877	0	887	19	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	14	0
13	AM	884	0	941	11	0
13	BM	884	0	941	13	0
14	AN	805	0	844	14	0
14	BN	805	0	844	12	0
15	AO	714	0	734	2	0
15	BO	714	0	734	3	0
16	AP	649	0	666	4	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	14	0
18	AR	456	0	478	5	0
18	BR	456	0	478	4	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	6	0
20	BT	665	0	714	3	0
21	AU	465	0	491	3	0
21	BU	465	0	491	2	0
22	C1	444	0	458	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	6	0
25	C4	504	0	572	2	0
25	D4	504	0	572	3	0
26	C5	302	0	340	4	0
26	D5	302	0	340	4	0
27	C0	449	0	488	2	0
27	D0	463	0	504	5	0
28	CB	2529	0	1281	5	0
28	DB	2569	0	1301	7	0
29	CC	2083	0	2154	27	0
29	DC	2083	0	2154	19	0
30	CD	1565	0	1616	18	0
31	CA	62229	0	31318	216	0
32	DD	1576	0	1627	17	0
33	CE	1552	0	1619	13	0
33	DE	1552	0	1619	4	0
34	CF	1411	0	1444	12	0
34	DF	1411	0	1444	18	0
35	CG	1323	0	1371	13	0
35	DG	1323	0	1371	13	0
36	CH	1110	0	1148	17	0
36	DH	1110	0	1148	9	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	8	0
38	CK	1129	0	1162	10	0
38	DK	1129	0	1162	4	0
39	CL	938	0	1012	10	0
39	DL	946	0	1023	6	0
40	CM	1053	0	1129	13	0
40	DM	1053	0	1129	3	0
41	CN	1075	0	1154	7	0
41	DN	1092	0	1177	14	0
42	CO	960	0	1000	9	0
42	DO	993	0	1034	7	0
43	CP	892	0	923	9	0
43	DP	900	0	935	13	0
44	CQ	917	0	962	9	0
44	DQ	917	0	962	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CR	947	0	1019	10	0
45	DR	947	0	1019	12	0
46	CS	816	0	839	11	0
46	DS	816	0	839	7	0
47	CT	857	0	922	10	0
47	DT	857	0	922	11	0
48	CU	739	0	807	5	0
48	DU	739	0	807	7	0
49	CV	780	0	831	6	0
49	DV	780	0	831	4	0
50	CW	753	0	780	4	0
50	DW	753	0	780	4	0
51	CX	569	0	581	4	0
51	DX	591	0	606	10	0
52	CY	625	0	652	8	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	1	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	199	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	1	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	2	0
58	DA	48	0	84	4	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	3	0
58	DT	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	2	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	1	0
62	D1	4	0	6	0	0
62	DA	36	0	54	3	0
62	DB	8	0	12	1	0
63	D1	10	0	14	3	0
63	D3	10	0	14	0	0
63	DA	40	0	56	4	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	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	2	0
69	AA	508	0	0	1	0
69	AC	5	0	0	0	0
69	AD	1	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	1	0
69	AT	4	0	0	0	0
69	AU	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BA	282	0	0	1	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0
69	BL	6	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	1	0
69	BR	1	0	0	0	0
69	BT	3	0	0	0	0
69	BU	3	0	0	0	0
69	C3	2	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	693	0	0	4	0
69	CB	13	0	0	0	0
69	CC	8	0	0	0	0
69	CD	7	0	0	0	0
69	CE	4	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	CQ	1	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	26	0	0	0	0
69	D1	46	0	0	1	0
69	D2	6	0	0	0	0
69	D3	28	0	0	1	0
69	D4	33	0	0	0	0
69	D5	11	0	0	0	0
69	DA	4830	0	0	20	0
69	DB	203	0	0	1	0
69	DC	102	0	0	1	0
69	DD	95	0	0	1	0
69	DE	63	0	0	2	0
69	DF	16	0	0	0	0
69	DG	7	0	0	0	0
69	DH	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DK	60	0	0	1	0
69	DL	51	0	0	0	0
69	DM	68	0	0	1	0
69	DN	73	0	0	1	0
69	DO	49	0	0	0	0
69	DP	38	0	0	0	0
69	DQ	29	0	0	0	0
69	DR	61	0	0	1	0
69	DS	50	0	0	0	0
69	DT	66	0	0	1	0
69	DU	19	0	0	0	0
69	DV	21	0	0	0	0
69	DW	32	0	0	0	0
69	DX	25	0	0	1	0
69	DY	10	0	0	0	0
69	DZ	6	0	0	0	0
All	All	295130	0	194412	1415	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 1415 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D5:26:ILE:CD1	26:D5:26:ILE:CG1	1.82	1.56
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.28	1.11
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.60	1.01
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.39	1.00
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.46	0.96

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%)	204 (92%)	14 (6%)	4 (2%)	7	29
2	BB	222/224 (99%)	202 (91%)	16 (7%)	4 (2%)	7	29
3	AC	204/206 (99%)	195 (96%)	8 (4%)	1 (0%)	25	58
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	13	42
4	AD	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	19	51
5	BE	148/155 (96%)	135 (91%)	10 (7%)	3 (2%)	6	26
6	AF	104/106 (98%)	92 (88%)	12 (12%)	0	100	100
6	BF	98/106 (92%)	82 (84%)	12 (12%)	4 (4%)	2	12
7	AG	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	10	36
7	BG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	19	51
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
9	BI	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
10	AJ	97/99 (98%)	90 (93%)	5 (5%)	2 (2%)	5	25
10	BJ	96/99 (97%)	80 (83%)	11 (12%)	5 (5%)	1	8
11	AK	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	14	45
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	14	45
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	115 (96%)	4 (3%)	1 (1%)	16	47
13	AM	112/114 (98%)	97 (87%)	11 (10%)	4 (4%)	3	14
13	BM	112/114 (98%)	95 (85%)	11 (10%)	6 (5%)	1	8
14	AN	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	3	17
14	BN	98/100 (98%)	93 (95%)	2 (2%)	3 (3%)	3	17
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	11	38
16	AP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	2	13
16	BP	80/82 (98%)	63 (79%)	14 (18%)	3 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	2	13
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	8
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
19	AS	77/79 (98%)	66 (86%)	9 (12%)	2 (3%)	4	20
19	BS	77/79 (98%)	64 (83%)	11 (14%)	2 (3%)	4	20
20	AT	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	5	22
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%)	3 (6%)	4 (7%)	1	4
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2	11
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3	14
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	242 (90%)	21 (8%)	6 (2%)	5	24
29	DC	269/271 (99%)	249 (93%)	18 (7%)	2 (1%)	19	51
30	CD	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
32	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
33	CE	199/201 (99%)	186 (94%)	10 (5%)	3 (2%)	8	33
33	DE	199/201 (99%)	189 (95%)	9 (4%)	1 (0%)	25	58
34	CF	175/177 (99%)	161 (92%)	12 (7%)	2 (1%)	12	40
34	DF	175/177 (99%)	160 (91%)	12 (7%)	3 (2%)	7	30
35	CG	174/176 (99%)	160 (92%)	9 (5%)	5 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DG	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	12	40
36	CH	147/149 (99%)	127 (86%)	15 (10%)	5 (3%)	3	15
36	DH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	26
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	17
37	DJ	132/134 (98%)	126 (96%)	2 (2%)	4 (3%)	3	17
38	CK	140/142 (99%)	133 (95%)	5 (4%)	2 (1%)	9	34
38	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	19	51
39	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7	30
39	DL	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	16	47
40	CM	142/144 (99%)	131 (92%)	8 (6%)	3 (2%)	5	25
40	DM	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
41	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
41	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
42	CO	118/125 (94%)	110 (93%)	7 (6%)	1 (1%)	16	47
42	DO	123/125 (98%)	115 (94%)	8 (6%)	0	100	100
43	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
44	CQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	14	45
44	DQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	14	45
45	CR	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	14	45
45	DR	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
46	CS	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	42
46	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	13	42
47	CT	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	6	27
47	DT	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	14	45
48	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	12	40
48	DU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	12	40
49	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	2	12
49	DV	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	6	26
50	CW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
52	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
52	DY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	30
53	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
54	DI	133/135 (98%)	112 (84%)	15 (11%)	6 (4%)	2	10
All	All	11407/11629 (98%)	10595 (93%)	661 (6%)	151 (1%)	10	36

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
5	AE	109	GLY
7	AG	56	LYS
10	AJ	57	VAL
13	AM	5	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%)	168 (90%)	18 (10%)	6	24
2	BB	186/186 (100%)	168 (90%)	18 (10%)	6	24
3	AC	170/170 (100%)	153 (90%)	17 (10%)	6	23
3	BC	170/170 (100%)	160 (94%)	10 (6%)	16	44
4	AD	172/172 (100%)	166 (96%)	6 (4%)	31	62
4	BD	172/172 (100%)	163 (95%)	9 (5%)	19	49
5	AE	118/118 (100%)	100 (85%)	18 (15%)	2	10
5	BE	113/118 (96%)	93 (82%)	20 (18%)	1	7
6	AF	92/92 (100%)	87 (95%)	5 (5%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BF	87/92 (95%)	78 (90%)	9 (10%)	6	22
7	AG	124/124 (100%)	109 (88%)	15 (12%)	4	16
7	BG	124/124 (100%)	109 (88%)	15 (12%)	4	16
8	AH	104/104 (100%)	92 (88%)	12 (12%)	4	18
8	BH	104/104 (100%)	95 (91%)	9 (9%)	8	29
9	AI	105/105 (100%)	95 (90%)	10 (10%)	7	25
9	BI	105/105 (100%)	94 (90%)	11 (10%)	5	21
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	7	27
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	4	18
11	AK	90/90 (100%)	84 (93%)	6 (7%)	13	40
11	BK	90/90 (100%)	82 (91%)	8 (9%)	8	28
12	AL	102/102 (100%)	94 (92%)	8 (8%)	10	34
12	BL	102/102 (100%)	91 (89%)	11 (11%)	5	20
13	AM	92/92 (100%)	81 (88%)	11 (12%)	4	17
13	BM	92/92 (100%)	84 (91%)	8 (9%)	8	29
14	AN	83/83 (100%)	80 (96%)	3 (4%)	30	61
14	BN	83/83 (100%)	79 (95%)	4 (5%)	21	52
15	AO	76/76 (100%)	68 (90%)	8 (10%)	5	21
15	BO	76/76 (100%)	67 (88%)	9 (12%)	4	17
16	AP	65/65 (100%)	59 (91%)	6 (9%)	7	27
16	BP	65/65 (100%)	58 (89%)	7 (11%)	5	20
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	9	32
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	2	10
18	AR	48/48 (100%)	43 (90%)	5 (10%)	5	21
18	BR	48/48 (100%)	44 (92%)	4 (8%)	9	31
19	AS	70/70 (100%)	62 (89%)	8 (11%)	4	18
19	BS	70/70 (100%)	63 (90%)	7 (10%)	6	23
20	AT	65/65 (100%)	55 (85%)	10 (15%)	2	10
20	BT	65/65 (100%)	56 (86%)	9 (14%)	3	12
21	AU	48/48 (100%)	47 (98%)	1 (2%)	48	74
21	BU	48/48 (100%)	47 (98%)	1 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	C1	47/47 (100%)	44 (94%)	3 (6%)	14	41
22	D1	47/47 (100%)	46 (98%)	1 (2%)	48	74
23	C2	45/46 (98%)	43 (96%)	2 (4%)	24	55
23	D2	45/46 (98%)	42 (93%)	3 (7%)	13	40
24	C3	38/38 (100%)	35 (92%)	3 (8%)	10	33
24	D3	38/38 (100%)	36 (95%)	2 (5%)	19	48
25	C4	51/51 (100%)	48 (94%)	3 (6%)	16	44
25	D4	51/51 (100%)	48 (94%)	3 (6%)	16	44
26	C5	34/34 (100%)	32 (94%)	2 (6%)	16	44
26	D5	34/34 (100%)	33 (97%)	1 (3%)	37	67
27	C0	48/48 (100%)	42 (88%)	6 (12%)	3	15
27	D0	49/48 (102%)	42 (86%)	7 (14%)	2	12
29	CC	216/216 (100%)	201 (93%)	15 (7%)	13	39
29	DC	216/216 (100%)	207 (96%)	9 (4%)	25	56
30	CD	164/164 (100%)	156 (95%)	8 (5%)	21	51
32	DD	163/163 (100%)	156 (96%)	7 (4%)	25	55
33	CE	165/165 (100%)	149 (90%)	16 (10%)	6	24
33	DE	165/165 (100%)	158 (96%)	7 (4%)	25	56
34	CF	148/148 (100%)	134 (90%)	14 (10%)	7	25
34	DF	148/148 (100%)	134 (90%)	14 (10%)	7	25
35	CG	137/137 (100%)	133 (97%)	4 (3%)	37	67
35	DG	137/137 (100%)	132 (96%)	5 (4%)	30	61
36	CH	114/114 (100%)	103 (90%)	11 (10%)	7	25
36	DH	114/114 (100%)	104 (91%)	10 (9%)	8	29
37	CJ	104/104 (100%)	98 (94%)	6 (6%)	17	45
37	DJ	104/104 (100%)	98 (94%)	6 (6%)	17	45
38	CK	116/116 (100%)	113 (97%)	3 (3%)	41	69
38	DK	116/116 (100%)	112 (97%)	4 (3%)	32	63
39	CL	103/104 (99%)	96 (93%)	7 (7%)	13	39
39	DL	104/104 (100%)	96 (92%)	8 (8%)	10	34
40	CM	103/103 (100%)	94 (91%)	9 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DM	103/103 (100%)	97 (94%)	6 (6%)	17	45
41	CN	108/108 (100%)	101 (94%)	7 (6%)	14	41
41	DN	109/108 (101%)	103 (94%)	6 (6%)	18	47
42	CO	100/102 (98%)	91 (91%)	9 (9%)	8	28
42	DO	102/102 (100%)	95 (93%)	7 (7%)	13	39
43	CP	86/87 (99%)	79 (92%)	7 (8%)	9	32
43	DP	87/87 (100%)	79 (91%)	8 (9%)	7	27
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	9	32
44	DQ	99/99 (100%)	93 (94%)	6 (6%)	15	43
45	CR	89/89 (100%)	83 (93%)	6 (7%)	13	40
45	DR	89/89 (100%)	85 (96%)	4 (4%)	23	54
46	CS	84/84 (100%)	81 (96%)	3 (4%)	30	61
46	DS	84/84 (100%)	82 (98%)	2 (2%)	44	71
47	CT	93/93 (100%)	88 (95%)	5 (5%)	18	47
47	DT	93/93 (100%)	91 (98%)	2 (2%)	47	73
48	CU	80/80 (100%)	72 (90%)	8 (10%)	6	23
48	DU	80/80 (100%)	74 (92%)	6 (8%)	11	35
49	CV	83/83 (100%)	77 (93%)	6 (7%)	12	37
49	DV	83/83 (100%)	80 (96%)	3 (4%)	30	61
50	CW	78/78 (100%)	73 (94%)	5 (6%)	14	41
50	DW	78/78 (100%)	75 (96%)	3 (4%)	28	59
51	CX	56/58 (97%)	50 (89%)	6 (11%)	5	20
51	DX	58/58 (100%)	49 (84%)	9 (16%)	2	9
52	CY	67/67 (100%)	62 (92%)	5 (8%)	11	35
52	DY	67/67 (100%)	62 (92%)	5 (8%)	11	35
53	CZ	54/54 (100%)	51 (94%)	3 (6%)	17	46
53	DZ	54/54 (100%)	53 (98%)	1 (2%)	52	76
54	DI	103/103 (100%)	94 (91%)	9 (9%)	8	29
All	All	9461/9478 (100%)	8736 (92%)	725 (8%)	11	34

5 of 725 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	CF	35	THR
49	CV	81	ASP
35	CG	11	VAL
34	CF	27	GLN
41	CN	88	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
20	BT	48	GLN
37	CJ	43	ASN
54	DI	122	GLN
20	BT	52	ASN
34	CF	27	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	256 (16%)	35 (2%)
1	BA	1529/1534 (99%)	259 (16%)	39 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	11 (9%)	0
31	CA	2892/2904 (99%)	488 (16%)	79 (2%)
55	DA	2880/2904 (99%)	423 (14%)	63 (2%)
All	All	9067/9116 (99%)	1449 (15%)	216 (2%)

5 of 1449 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 216 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	1452	G
31	CA	2423	U
55	DA	2157	G

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Mol	Chain	Res	Type
31	CA	1535	A
31	CA	2095	A

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

75 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	2MG	DA	1835	55	18,26,27	0.94	2 (11%)	16,38,41	0.64	0
31	PSU	CA	955	31	18,21,22	0.33	0	21,30,33	0.54	0
1	MA6	AA	1518	1	19,26,27	0.93	0	18,38,41	1.02	1 (5%)
1	2MG	BA	1516	1	18,26,27	0.81	0	16,38,41	0.66	0
55	OMC	DA	2498	56,55	19,22,23	0.46	0	25,31,34	0.60	0
55	OMU	DA	2552	55	19,22,23	0.52	0	25,31,34	0.25	0
55	PSU	DA	2605	55	18,21,22	0.67	0	21,30,33	0.67	0
55	1MG	DA	745	55	19,26,27	1.23	1 (5%)	18,39,42	0.84	1 (5%)
55	6MZ	DA	1618	55	17,25,26	1.14	2 (11%)	15,36,39	1.32	1 (6%)
31	OMG	CA	2251	31	19,26,27	0.86	0	21,38,41	0.60	0
1	5MC	AA	1407	1	19,22,23	0.42	0	26,32,35	0.53	0
55	OMG	DA	2251	55	19,26,27	0.93	3 (15%)	21,38,41	0.52	0
55	PSU	DA	2504	55	18,21,22	0.48	0	21,30,33	0.49	0
31	2MG	CA	1835	31	18,26,27	0.94	1 (5%)	16,38,41	0.51	0
31	PSU	CA	2457	31	18,21,22	0.64	0	21,30,33	0.50	0
31	OMU	CA	2552	31	19,22,23	0.34	0	25,31,34	0.29	0
31	PSU	CA	2605	31	18,21,22	0.43	0	21,30,33	0.59	0
31	OMC	CA	2498	56,31	19,22,23	0.36	0	25,31,34	0.39	0
55	PSU	DA	1911	55	18,21,22	0.29	0	21,30,33	0.43	0
1	PSU	AA	516	1,56	18,21,22	0.41	0	21,30,33	0.49	0
31	PSU	CA	1911	31	18,21,22	0.30	0	21,30,33	0.43	0
1	MA6	AA	1519	1	19,26,27	1.09	0	18,38,41	1.20	2 (11%)
55	2MA	DA	2503	56,55	17,25,26	1.09	2 (11%)	16,37,40	2.13	1 (6%)
1	5MC	AA	967	1	19,22,23	0.30	0	26,32,35	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	CA	2504	31	18,21,22	0.48	0	21,30,33	0.43	0
41	4D4	DN	81[B]	-	9,11,12	1.71	2 (22%)	7,13,15	2.87	2 (28%)
1	4OC	AA	1402	1	20,23,24	0.33	0	25,32,35	0.40	0
1	5MC	BA	967	1	19,22,23	0.26	0	26,32,35	0.38	0
1	UR3	BA	1498	1	19,22,23	0.36	0	26,32,35	0.41	0
55	H2U	DA	2449	55	18,21,22	0.41	0	19,30,33	0.60	1 (5%)
12	D2T	BL	89	12	8,9,10	1.94	2 (25%)	6,11,13	0.81	0
1	MA6	BA	1519	1	19,26,27	1.07	0	18,38,41	1.18	2 (11%)
31	5MU	CA	747	31	19,22,23	0.27	0	27,32,35	0.26	0
55	PSU	DA	955	55	18,21,22	0.70	1 (5%)	21,30,33	0.55	0
31	6MZ	CA	1618	31	17,25,26	0.92	1 (5%)	15,36,39	0.86	1 (6%)
1	4OC	BA	1402	1	20,23,24	0.35	0	25,32,35	0.41	0
31	3TD	CA	1915	31	19,22,23	0.54	0	23,32,35	0.73	1 (4%)
55	G7M	DA	2069	55	20,26,27	0.69	1 (5%)	16,39,42	1.55	1 (6%)
55	PSU	DA	2457	55	18,21,22	0.51	0	21,30,33	0.51	0
41	4D4	CN	81	41	9,11,12	2.14	2 (22%)	7,13,15	2.66	2 (28%)
31	2MA	CA	2503	31	17,25,26	1.03	2 (11%)	16,37,40	2.29	1 (6%)
31	2MG	CA	2445	31	18,26,27	0.97	2 (11%)	16,38,41	0.64	0
32	MEQ	DD	150[B]	32	8,9,10	1.02	1 (12%)	5,10,12	0.89	0
12	D2T	AL	89	12	8,9,10	1.61	2 (25%)	6,11,13	0.97	0
55	5MC	DA	1962	55	19,22,23	0.63	0	26,32,35	0.46	0
1	MA6	BA	1518	1	19,26,27	0.89	0	18,38,41	0.99	1 (5%)
41	4D4	DN	81[A]	-	9,11,12	2.04	2 (22%)	7,13,15	2.48	2 (28%)
1	2MG	BA	1207	1	18,26,27	0.88	1 (5%)	16,38,41	0.59	0
1	2MG	AA	1207	1	18,26,27	0.89	0	16,38,41	0.56	0
31	PSU	CA	1917	31	18,21,22	0.30	0	21,30,33	0.45	0
55	PSU	DA	2580	55	18,21,22	0.73	0	21,30,33	0.71	0
31	1MG	CA	745	31	19,26,27	1.30	2 (10%)	18,39,42	0.76	1 (5%)
55	5MU	DA	747	55	19,22,23	0.30	0	27,32,35	0.36	0
1	2MG	AA	1516	1	18,26,27	0.87	1 (5%)	16,38,41	0.68	0
31	5MC	CA	1962	31	19,22,23	0.34	0	26,32,35	0.38	0
32	MEQ	DD	150[A]	32	8,9,10	0.52	0	5,10,12	0.44	0
31	G7M	CA	2069	31	20,26,27	0.84	1 (5%)	16,39,42	1.30	1 (6%)
31	PSU	CA	2580	31	18,21,22	0.54	0	21,30,33	0.78	2 (9%)
31	PSU	CA	746	56,31	18,21,22	0.55	0	21,30,33	0.36	0
1	G7M	AA	527	1	20,26,27	0.73	1 (5%)	16,39,42	1.53	1 (6%)
55	6MZ	DA	2030	55	17,25,26	1.32	3 (17%)	15,36,39	0.91	1 (6%)
1	2MG	BA	966	1	18,26,27	0.84	0	16,38,41	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	BA	1407	1	19,22,23	0.45	0	26,32,35	0.52	0
1	2MG	AA	966	1	18,26,27	0.86	1 (5%)	16,38,41	0.63	0
1	PSU	BA	516	1	18,21,22	0.42	0	21,30,33	0.46	0
31	5MU	CA	1939	31	19,22,23	0.40	0	27,32,35	0.30	0
31	6MZ	CA	2030	31	17,25,26	0.99	0	15,36,39	1.10	2 (13%)
55	5MU	DA	1939	55	19,22,23	0.57	0	27,32,35	0.39	0
55	PSU	DA	2604	55	18,21,22	0.89	1 (5%)	21,30,33	0.57	0
55	PSU	DA	746	56,55	18,21,22	1.02	1 (5%)	21,30,33	0.36	0
55	PSU	DA	1917	55	18,21,22	0.41	0	21,30,33	0.45	0
1	UR3	AA	1498	1	19,22,23	0.64	0	26,32,35	0.29	0
55	3TD	DA	1915	55	19,22,23	0.52	0	23,32,35	0.74	1 (4%)
1	G7M	BA	527	1	20,26,27	0.80	0	16,39,42	1.67	1 (6%)
55	2MG	DA	2445	55	18,26,27	1.20	3 (16%)	16,38,41	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	2MG	DA	1835	55	-	2/5/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	1/7/29/30	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
55	OMC	DA	2498	56,55	-	0/9/27/28	0/2/2/2
55	OMU	DA	2552	55	-	0/9/27/28	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	1/5/27/28	0/3/3/3
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	56,31	-	0/9/27/28	0/2/2/2
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
55	2MA	DA	2503	56,55	-	2/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	3/11/12/14	-
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
31	5MU	CA	747	31	-	1/7/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
55	G7M	DA	2069	55	-	1/3/25/26	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
41	4D4	CN	81	41	-	2/11/12/14	-
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
31	2MG	CA	2445	31	-	1/5/27/28	0/3/3/3
32	MEQ	DD	150[B]	32	-	6/8/9/11	-
12	D2T	AL	89	12	-	2/7/12/14	-
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	1/7/29/30	0/3/3/3
41	4D4	DN	81[A]	-	-	2/11/12/14	-
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
55	5MU	DA	747	55	-	1/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	3/8/9/11	-
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	746	56,31	-	3/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	6MZ	DA	2030	55	-	1/5/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	746	56,55	-	4/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	CN	81	4D4	CZ-NE	5.78	1.44	1.33
41	DN	81[A]	4D4	CZ-NE	4.91	1.42	1.33
31	CA	745	1MG	C2-N1	4.40	1.45	1.37
41	DN	81[B]	4D4	CZ-NE	4.24	1.41	1.33
12	BL	89	D2T	CB-SB	3.89	1.86	1.82

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	C4-N3-C2	-8.96	116.42	123.30
55	DA	2503	2MA	C4-N3-C2	-8.25	116.96	123.30
1	BA	527	G7M	O4'-C1'-N9	6.44	117.29	108.75
41	DN	81[B]	4D4	NE-CZ-NH2	6.01	130.98	120.67
41	CN	81	4D4	NE-CZ-NH2	5.95	130.89	120.67

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1518	MA6	C5-C6-N6-C9
1	AA	1519	MA6	C5-C6-N6-C9
12	AL	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	2	0
31	CA	2251	OMG	1	0
55	DA	2251	OMG	1	0
31	CA	2498	OMC	1	0
1	AA	1519	MA6	2	0
1	BA	1519	MA6	2	0
31	CA	747	5MU	1	0
31	CA	2503	2MA	1	0
32	DD	150[B]	MEQ	1	0
1	BA	1518	MA6	2	0
55	DA	747	5MU	1	0
32	DD	150[A]	MEQ	2	0
55	DA	2030	6MZ	2	0
31	CA	2030	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 552 ligands modelled in this entry, 472 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PUT	DA	3192	-	5,5,5	0.36	0	4,4,4	0.45	0
63	PGE	DD	301	-	9,9,9	0.18	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PG4	DQ	202	-	12,12,12	0.28	0	11,11,11	0.25	0
59	PUT	AA	1674	-	5,5,5	0.17	0	4,4,4	0.11	0
57	PG4	DS	202	-	12,12,12	0.38	0	11,11,11	0.33	0
61	PEG	DA	3228	-	6,6,6	0.41	0	5,5,5	0.31	0
63	PGE	DA	3219	-	9,9,9	0.22	0	8,8,8	0.27	0
62	EDO	DA	3211	-	3,3,3	0.62	0	2,2,2	0.24	0
59	PUT	DA	3214	-	5,5,5	0.22	0	4,4,4	0.10	0
62	EDO	DA	3003	-	3,3,3	0.57	0	2,2,2	0.32	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.12	0
63	PGE	D1	102	-	9,9,9	0.27	0	8,8,8	0.25	0
66	ACY	DA	3204	-	3,3,3	0.64	0	3,3,3	1.07	0
62	EDO	DA	3005	-	3,3,3	0.52	0	2,2,2	0.34	0
58	MPD	DA	3004	-	7,7,7	0.57	0	9,10,10	0.31	0
62	EDO	DB	210	-	3,3,3	0.62	0	2,2,2	0.06	0
62	EDO	D1	101	-	3,3,3	0.56	0	2,2,2	0.24	0
59	PUT	DA	3221	-	5,5,5	0.14	0	4,4,4	0.08	0
58	MPD	DA	3212	-	7,7,7	0.74	0	9,10,10	0.42	0
59	PUT	DA	3215	-	5,5,5	0.26	0	4,4,4	0.21	0
59	PUT	DA	3198	-	5,5,5	0.23	0	4,4,4	0.23	0
66	ACY	DA	3199	-	3,3,3	2.24	1 (33%)	3,3,3	2.25	2 (66%)
61	PEG	DQ	201	-	6,6,6	0.34	0	5,5,5	0.28	0
64	SPD	DA	3190	-	9,9,9	0.12	0	8,8,8	0.19	0
58	MPD	DA	3195	-	7,7,7	0.58	0	9,10,10	0.67	0
61	PEG	D1	103	-	6,6,6	0.28	0	5,5,5	0.16	0
66	ACY	DA	3194	-	3,3,3	0.61	0	3,3,3	1.03	0
58	MPD	DA	3209	-	7,7,7	0.66	0	9,10,10	0.53	0
65	1PE	DA	3188	-	15,15,15	0.19	0	14,14,14	0.29	0
57	PG4	DR	202	-	12,12,12	0.31	0	11,11,11	0.35	0
62	EDO	DA	3201	-	3,3,3	0.47	0	2,2,2	0.48	0
61	PEG	D3	102	-	6,6,6	0.50	0	5,5,5	0.38	0
63	PGE	DA	3189	-	9,9,9	0.42	0	8,8,8	0.30	0
58	MPD	DA	3193	-	7,7,7	0.30	0	9,10,10	0.48	0
62	EDO	DA	3217	-	3,3,3	0.57	0	2,2,2	0.31	0
63	PGE	DU	101	-	9,9,9	0.29	0	8,8,8	0.21	0
65	1PE	DA	3205	-	15,15,15	0.40	0	14,14,14	0.50	0
63	PGE	DA	3216	-	9,9,9	0.30	0	8,8,8	0.34	0
58	MPD	AA	1676	-	7,7,7	0.61	0	9,10,10	0.35	0
61	PEG	DA	3220	-	6,6,6	0.20	0	5,5,5	0.07	0
59	PUT	AA	1672	-	5,5,5	0.25	0	4,4,4	0.16	0
58	MPD	DE	302	-	7,7,7	0.96	1 (14%)	9,10,10	0.54	0
61	PEG	DL	201	-	6,6,6	0.18	0	5,5,5	0.12	0
62	EDO	DA	3200	-	3,3,3	0.68	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	DS	201	-	9,9,9	0.39	0	8,8,8	0.31	0
58	MPD	AA	1671	-	7,7,7	0.63	0	9,10,10	0.45	0
57	PG4	DA	3218	-	12,12,12	0.19	0	11,11,11	0.25	0
64	SPD	DA	3208	-	9,9,9	0.19	0	8,8,8	0.20	0
64	SPD	DA	3186	-	9,9,9	0.18	0	8,8,8	0.17	0
62	EDO	DA	3210	-	3,3,3	0.59	0	2,2,2	0.30	0
62	EDO	DA	3197	-	3,3,3	0.99	0	2,2,2	0.27	0
58	MPD	DS	203	-	7,7,7	0.44	0	9,10,10	0.45	0
57	PG4	DA	3196	-	12,12,12	0.38	0	11,11,11	0.30	0
61	PEG	DA	3203	-	6,6,6	0.30	0	5,5,5	0.19	0
59	PUT	DA	3207	-	5,5,5	0.20	0	4,4,4	0.17	0
61	PEG	AL	201	-	6,6,6	0.26	0	5,5,5	0.23	0
63	PGE	D3	101	-	9,9,9	0.30	0	8,8,8	0.29	0
57	PG4	AA	1670	-	12,12,12	0.36	0	11,11,11	0.35	0
64	SPD	DA	3226	-	9,9,9	0.34	0	8,8,8	0.47	0
58	MPD	DT	201	-	7,7,7	0.71	0	9,10,10	0.46	0
67	GUN	DA	3213	-	7,12,12	0.43	0	8,17,17	0.71	0
59	PUT	DM	201	-	5,5,5	0.16	0	4,4,4	0.15	0
62	EDO	DB	211	-	3,3,3	0.65	0	2,2,2	0.07	0
58	MPD	DK	201	-	7,7,7	0.60	0	9,10,10	0.36	0
61	PEG	DA	3202	-	6,6,6	0.22	0	5,5,5	0.14	0
59	PUT	DA	3223	-	5,5,5	0.26	0	4,4,4	0.24	0
58	MPD	DE	301	-	7,7,7	0.64	0	9,10,10	0.53	0
61	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.16	0
63	PGE	DA	3227	-	9,9,9	0.18	0	8,8,8	0.23	0
59	PUT	DA	3225	-	5,5,5	0.26	0	4,4,4	0.19	0
61	PEG	DA	3229	-	6,6,6	0.38	0	5,5,5	0.24	0
68	TRS	DA	3222	-	7,7,7	0.35	0	9,9,9	0.38	0
59	PUT	DA	3224	-	5,5,5	0.46	0	4,4,4	0.72	0
59	PUT	AA	1673	-	5,5,5	0.13	0	4,4,4	0.10	0
59	PUT	DA	3187	-	5,5,5	0.46	0	4,4,4	0.30	0
57	PG4	BA	1642	-	12,12,12	0.34	0	11,11,11	0.27	0
58	MPD	DN	201	-	7,7,7	1.05	1 (14%)	9,10,10	0.64	0
59	PUT	DA	3191	-	5,5,5	0.10	0	4,4,4	0.17	0
58	MPD	DA	3206	-	7,7,7	0.88	0	9,10,10	0.73	0
62	EDO	DA	3002	-	3,3,3	0.62	0	2,2,2	0.19	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	PUT	DA	3192	-	-	0/3/3/3	-
63	PGE	DD	301	-	-	4/7/7/7	-
57	PG4	DQ	202	-	-	3/10/10/10	-
59	PUT	AA	1674	-	-	0/3/3/3	-
57	PG4	DS	202	-	-	6/10/10/10	-
61	PEG	DA	3228	-	-	3/4/4/4	-
63	PGE	DA	3219	-	-	3/7/7/7	-
62	EDO	DA	3211	-	-	0/1/1/1	-
59	PUT	DA	3214	-	-	1/3/3/3	-
62	EDO	DA	3003	-	-	0/1/1/1	-
59	PUT	AA	1675	-	-	1/3/3/3	-
63	PGE	D1	102	-	-	3/7/7/7	-
62	EDO	DA	3005	-	-	0/1/1/1	-
58	MPD	DA	3004	-	-	3/5/5/5	-
62	EDO	DB	210	-	-	0/1/1/1	-
62	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	DA	3221	-	-	0/3/3/3	-
58	MPD	DA	3212	-	-	0/5/5/5	-
59	PUT	DA	3215	-	-	0/3/3/3	-
59	PUT	DA	3198	-	-	1/3/3/3	-
61	PEG	DQ	201	-	-	0/4/4/4	-
64	SPD	DA	3190	-	-	2/7/7/7	-
58	MPD	DA	3195	-	-	2/5/5/5	-
61	PEG	D1	103	-	-	0/4/4/4	-
58	MPD	DA	3209	-	-	3/5/5/5	-
65	1PE	DA	3188	-	-	4/13/13/13	-
57	PG4	DR	202	-	-	6/10/10/10	-
62	EDO	DA	3201	-	-	0/1/1/1	-
61	PEG	D3	102	-	-	2/4/4/4	-
63	PGE	DA	3189	-	-	1/7/7/7	-
58	MPD	DA	3193	-	-	1/5/5/5	-
62	EDO	DA	3217	-	-	0/1/1/1	-
63	PGE	DU	101	-	-	2/7/7/7	-
65	1PE	DA	3205	-	-	4/13/13/13	-
63	PGE	DA	3216	-	-	2/7/7/7	-
58	MPD	AA	1676	-	-	0/5/5/5	-
61	PEG	DA	3220	-	-	2/4/4/4	-
59	PUT	AA	1672	-	-	1/3/3/3	-
58	MPD	DE	302	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PEG	DL	201	-	-	2/4/4/4	-
62	EDO	DA	3200	-	-	1/1/1/1	-
63	PGE	DS	201	-	-	2/7/7/7	-
58	MPD	AA	1671	-	-	0/5/5/5	-
57	PG4	DA	3218	-	-	4/10/10/10	-
64	SPD	DA	3208	-	-	2/7/7/7	-
64	SPD	DA	3186	-	-	1/7/7/7	-
62	EDO	DA	3210	-	-	1/1/1/1	-
62	EDO	DA	3197	-	-	0/1/1/1	-
58	MPD	DS	203	-	-	1/5/5/5	-
57	PG4	DA	3196	-	-	5/10/10/10	-
61	PEG	DA	3203	-	-	3/4/4/4	-
59	PUT	DA	3207	-	-	0/3/3/3	-
61	PEG	AL	201	-	-	2/4/4/4	-
63	PGE	D3	101	-	-	3/7/7/7	-
57	PG4	AA	1670	-	-	6/10/10/10	-
64	SPD	DA	3226	-	-	4/7/7/7	-
58	MPD	DT	201	-	-	2/5/5/5	-
67	GUN	DA	3213	-	-	-	0/2/2/2
59	PUT	DM	201	-	-	0/3/3/3	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	MPD	DK	201	-	-	1/5/5/5	-
61	PEG	DA	3202	-	-	2/4/4/4	-
59	PUT	DA	3223	-	-	0/3/3/3	-
58	MPD	DE	301	-	-	2/5/5/5	-
61	PEG	DP	201	-	-	2/4/4/4	-
63	PGE	DA	3227	-	-	4/7/7/7	-
59	PUT	DA	3225	-	-	1/3/3/3	-
61	PEG	DA	3229	-	-	1/4/4/4	-
68	TRS	DA	3222	-	-	1/9/9/9	-
59	PUT	DA	3224	-	-	0/3/3/3	-
59	PUT	AA	1673	-	-	0/3/3/3	-
59	PUT	DA	3187	-	-	0/3/3/3	-
57	PG4	BA	1642	-	-	3/10/10/10	-
58	MPD	DN	201	-	-	2/5/5/5	-
59	PUT	DA	3191	-	-	0/3/3/3	-
58	MPD	DA	3206	-	-	2/5/5/5	-
62	EDO	DA	3002	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3199	ACY	O-C	3.63	1.38	1.22
58	DN	201	MPD	C3-C2	2.23	1.60	1.54
58	DE	302	MPD	C3-C2	2.14	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3199	ACY	OXT-C-CH3	2.96	127.47	115.05
66	DA	3199	ACY	O-C-CH3	-2.48	112.36	122.53

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DA	3209	MPD	C2-C3-C4-O4
57	DR	202	PG4	O2-C3-C4-O3
65	DA	3205	1PE	OH5-C14-C24-OH4
65	DA	3205	1PE	OH4-C13-C23-OH3
61	D3	102	PEG	O1-C1-C2-O2

There are no ring outliers.

30 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DQ	202	PG4	1	0
57	DS	202	PG4	1	0
63	D1	102	PGE	3	0
59	DA	3221	PUT	1	0
61	DQ	201	PEG	1	0
58	DA	3195	MPD	1	0
61	D1	103	PEG	1	0
58	DA	3209	MPD	1	0
65	DA	3188	1PE	1	0
57	DR	202	PG4	3	0
62	DA	3201	EDO	1	0
61	D3	102	PEG	2	0
63	DU	101	PGE	1	0
63	DA	3216	PGE	1	0
58	AA	1671	MPD	2	0
57	DA	3218	PG4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	DA	3208	SPD	1	0
62	DA	3197	EDO	2	0
58	DS	203	MPD	3	0
57	DA	3196	PG4	1	0
57	AA	1670	PG4	1	0
64	DA	3226	SPD	1	0
62	DB	211	EDO	1	0
61	DP	201	PEG	1	0
63	DA	3227	PGE	3	0
68	DA	3222	TRS	2	0
59	DA	3224	PUT	2	0
59	DA	3187	PUT	1	0
57	BA	1642	PG4	1	0
58	DA	3206	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.08	82 (5%) 32 18	37, 95, 237, 293	0
1	BA	1522/1534 (99%)	0.62	158 (10%) 13 7	58, 133, 255, 272	0
2	AB	224/224 (100%)	0.36	7 (3%) 51 31	76, 123, 192, 236	0
2	BB	224/224 (100%)	0.58	20 (8%) 17 9	101, 145, 205, 239	0
3	AC	206/206 (100%)	0.02	2 (0%) 79 61	65, 93, 121, 147	0
3	BC	206/206 (100%)	0.26	5 (2%) 59 38	86, 121, 150, 169	0
4	AD	205/205 (100%)	0.24	3 (1%) 71 51	69, 97, 128, 136	0
4	BD	205/205 (100%)	0.28	3 (1%) 71 51	68, 101, 127, 138	0
5	AE	155/155 (100%)	-0.01	2 (1%) 74 54	60, 84, 120, 175	0
5	BE	150/155 (96%)	0.44	6 (4%) 43 25	72, 106, 138, 202	0
6	AF	106/106 (100%)	0.21	4 (3%) 44 26	69, 103, 126, 144	0
6	BF	100/106 (94%)	0.45	5 (5%) 35 20	82, 115, 140, 149	0
7	AG	151/151 (100%)	1.03	22 (14%) 7 4	106, 150, 177, 189	0
7	BG	151/151 (100%)	0.83	13 (8%) 18 10	137, 190, 215, 221	0
8	AH	129/129 (100%)	0.24	2 (1%) 70 49	68, 91, 119, 130	0
8	BH	129/129 (100%)	0.51	5 (3%) 44 26	98, 126, 151, 161	0
9	AI	127/127 (100%)	1.10	23 (18%) 4 3	75, 144, 180, 187	0
9	BI	127/127 (100%)	1.07	15 (11%) 10 6	111, 162, 195, 202	0
10	AJ	99/99 (100%)	0.74	7 (7%) 23 13	82, 112, 142, 147	0
10	BJ	98/99 (98%)	1.28	23 (23%) 2 2	111, 152, 181, 187	0
11	AK	117/117 (100%)	0.21	2 (1%) 69 47	54, 104, 138, 152	0
11	BK	117/117 (100%)	0.33	4 (3%) 48 29	62, 97, 134, 165	0
12	AL	122/123 (99%)	-0.09	3 (2%) 58 37	48, 65, 106, 141	0
12	BL	122/123 (99%)	0.87	19 (15%) 6 4	82, 102, 129, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.83	46 (40%) 1 1	126, 159, 182, 189	0
13	BM	114/114 (100%)	0.89	10 (8%) 17 9	187, 224, 236, 244	0
14	AN	100/100 (100%)	1.15	17 (17%) 5 3	72, 110, 177, 184	0
14	BN	100/100 (100%)	0.98	9 (9%) 17 9	107, 167, 215, 218	0
15	AO	88/88 (100%)	0.21	0 100 100	63, 91, 115, 142	0
15	BO	88/88 (100%)	0.41	3 (3%) 48 29	84, 114, 143, 156	0
16	AP	82/82 (100%)	0.58	6 (7%) 22 12	68, 85, 126, 145	0
16	BP	82/82 (100%)	1.76	29 (35%) 1 1	100, 125, 161, 175	0
17	AQ	80/80 (100%)	0.14	1 (1%) 74 54	63, 87, 116, 138	0
17	BQ	80/80 (100%)	1.09	8 (10%) 14 8	101, 142, 165, 173	0
18	AR	55/55 (100%)	0.27	2 (3%) 46 28	73, 97, 142, 174	0
18	BR	55/55 (100%)	0.32	3 (5%) 32 18	67, 90, 125, 166	0
19	AS	79/79 (100%)	2.02	42 (53%) 0 0	138, 162, 179, 182	0
19	BS	79/79 (100%)	1.10	15 (18%) 4 3	197, 221, 238, 243	0
20	AT	86/86 (100%)	0.39	3 (3%) 47 28	63, 85, 116, 128	0
20	BT	85/86 (98%)	1.54	27 (31%) 1 1	110, 143, 164, 169	0
21	AU	56/56 (100%)	0.39	3 (5%) 32 18	75, 113, 153, 163	0
21	BU	56/56 (100%)	0.26	2 (3%) 46 28	69, 94, 123, 138	0
22	C1	56/56 (100%)	1.71	23 (41%) 1 1	93, 155, 176, 188	0
22	D1	56/56 (100%)	-0.68	0 100 100	21, 45, 74, 114	0
23	C2	50/51 (98%)	1.99	18 (36%) 1 1	150, 178, 190, 205	0
23	D2	51/51 (100%)	-0.41	1 (1%) 64 43	47, 63, 89, 108	0
24	C3	46/46 (100%)	2.54	29 (63%) 0 0	100, 132, 149, 173	0
24	D3	46/46 (100%)	-0.42	1 (2%) 62 41	25, 35, 54, 118	0
25	C4	64/64 (100%)	2.15	27 (42%) 1 1	95, 116, 139, 151	0
25	D4	64/64 (100%)	-0.53	1 (1%) 70 49	29, 39, 57, 68	0
26	C5	38/38 (100%)	1.75	13 (34%) 1 1	97, 115, 133, 149	0
26	D5	38/38 (100%)	-0.47	0 100 100	32, 45, 71, 83	0
27	C0	58/58 (100%)	0.94	7 (12%) 10 6	99, 121, 149, 157	0
27	D0	58/58 (100%)	-0.74	0 100 100	22, 32, 54, 88	2 (3%)
28	CB	118/120 (98%)	0.65	4 (3%) 48 29	104, 167, 221, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.70	0 100 100	28, 53, 86, 134	0
29	CC	271/271 (100%)	0.84	34 (12%) 9 5	76, 98, 120, 132	0
29	DC	271/271 (100%)	-0.57	1 (0%) 89 77	23, 52, 80, 100	0
30	CD	209/209 (100%)	1.00	36 (17%) 5 3	88, 118, 149, 165	0
31	CA	2876/2904 (99%)	0.77	198 (6%) 24 13	65, 132, 252, 292	0
32	DD	208/209 (99%)	-0.74	0 100 100	18, 38, 71, 100	0
33	CE	201/201 (100%)	1.08	28 (13%) 7 4	88, 159, 186, 195	0
33	DE	201/201 (100%)	-0.59	0 100 100	20, 52, 98, 127	0
34	CF	177/177 (100%)	0.62	9 (5%) 34 19	186, 212, 225, 231	0
34	DF	177/177 (100%)	0.07	2 (1%) 77 58	45, 78, 126, 139	0
35	CG	176/176 (100%)	0.62	12 (6%) 25 14	138, 164, 187, 198	0
35	DG	176/176 (100%)	-0.13	2 (1%) 77 58	45, 74, 105, 131	0
36	CH	149/149 (100%)	0.44	4 (2%) 56 35	81, 148, 176, 186	0
36	DH	149/149 (100%)	0.47	2 (1%) 74 54	60, 158, 195, 208	0
37	CJ	134/134 (100%)	1.34	34 (25%) 2 2	237, 258, 270, 275	0
37	DJ	134/134 (100%)	1.61	39 (29%) 1 1	204, 238, 246, 254	0
38	CK	142/142 (100%)	0.69	7 (4%) 36 20	91, 108, 135, 150	0
38	DK	142/142 (100%)	-0.82	0 100 100	18, 36, 58, 94	0
39	CL	122/123 (99%)	0.90	11 (9%) 17 9	91, 114, 148, 163	0
39	DL	123/123 (100%)	-0.73	0 100 100	29, 43, 72, 106	0
40	CM	144/144 (100%)	1.23	33 (22%) 2 2	87, 146, 186, 214	0
40	DM	144/144 (100%)	-0.50	1 (0%) 84 68	19, 50, 81, 115	0
41	CN	135/136 (99%)	0.50	9 (6%) 25 14	75, 113, 134, 162	0
41	DN	135/136 (99%)	-0.66	0 100 100	16, 39, 68, 99	1 (0%)
42	CO	120/125 (96%)	1.40	30 (25%) 2 2	107, 124, 146, 197	0
42	DO	125/125 (100%)	-0.73	0 100 100	23, 37, 73, 145	0
43	CP	116/117 (99%)	0.57	6 (5%) 34 19	132, 154, 173, 181	0
43	DP	117/117 (100%)	-0.42	0 100 100	36, 54, 81, 96	0
44	CQ	114/114 (100%)	1.11	16 (14%) 7 4	110, 127, 146, 168	0
44	DQ	114/114 (100%)	-0.57	1 (0%) 81 63	28, 50, 84, 119	0
45	CR	117/117 (100%)	1.18	21 (17%) 4 3	76, 107, 129, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.85	0 100 100	15, 30, 49, 85	0
46	CS	103/103 (100%)	1.17	22 (21%) 3 2	94, 127, 152, 164	0
46	DS	103/103 (100%)	-0.75	2 (1%) 66 44	21, 41, 70, 99	0
47	CT	110/110 (100%)	1.45	26 (23%) 2 2	99, 123, 157, 176	0
47	DT	110/110 (100%)	-0.68	0 100 100	17, 32, 61, 114	0
48	CU	93/93 (100%)	1.50	20 (21%) 3 2	129, 147, 176, 181	0
48	DU	93/93 (100%)	-0.10	4 (4%) 40 23	31, 52, 115, 130	0
49	CV	102/102 (100%)	1.62	31 (30%) 1 1	148, 166, 201, 204	0
49	DV	102/102 (100%)	-0.36	2 (1%) 64 43	40, 62, 97, 129	0
50	CW	94/94 (100%)	0.51	2 (2%) 63 42	114, 140, 159, 164	0
50	DW	94/94 (100%)	-0.41	0 100 100	31, 52, 84, 96	0
51	CX	75/76 (98%)	0.91	12 (16%) 6 3	92, 120, 134, 183	0
51	DX	76/76 (100%)	-0.49	0 100 100	17, 39, 67, 116	1 (1%)
52	CY	77/77 (100%)	1.50	19 (24%) 2 2	78, 117, 147, 166	0
52	DY	77/77 (100%)	-0.39	1 (1%) 74 54	32, 53, 93, 111	0
53	CZ	62/62 (100%)	1.13	8 (12%) 9 5	133, 169, 183, 190	0
53	DZ	62/62 (100%)	-0.04	1 (1%) 70 49	42, 70, 110, 138	0
54	DI	135/135 (100%)	1.11	26 (19%) 4 2	78, 152, 215, 229	1 (0%)
55	DA	2873/2904 (98%)	-0.76	93 (3%) 50 30	18, 44, 227, 299	11 (0%)
All	All	20634/20745 (99%)	0.31	1590 (7%) 21 11	15, 106, 233, 299	16 (0%)

The worst 5 of 1590 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	13.9
31	CA	2172	U	9.6
7	BG	4	ARG	8.9
1	AA	121	U	8.5
55	DA	2172	U	8.5

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	3TD	CA	1915	21/22	0.78	0.09	142,145,154,156	0
31	PSU	CA	1917	20/21	0.78	0.10	120,123,132,132	0
31	PSU	CA	1911	20/21	0.82	0.09	104,121,124,125	0
1	2MG	BA	966	24/25	0.86	0.09	119,123,135,135	0
1	5MC	BA	967	21/22	0.87	0.11	115,124,127,128	0
1	2MG	BA	1207	24/25	0.87	0.10	140,147,149,151	0
12	D2T	BL	89	10/11	0.87	0.18	92,99,108,108	0
31	2MA	CA	2503	23/24	0.88	0.16	90,100,103,104	0
55	3TD	DA	1915	21/22	0.88	0.10	91,98,111,112	0
31	6MZ	CA	2030	23/24	0.89	0.12	81,86,89,90	0
31	PSU	CA	2457	20/21	0.90	0.11	87,89,92,92	0
31	PSU	CA	746	20/21	0.90	0.09	86,98,100,101	0
31	PSU	CA	2504	20/21	0.90	0.12	76,87,89,93	0
31	6MZ	CA	1618	23/24	0.90	0.12	109,114,116,117	0
55	PSU	DA	1917	20/21	0.90	0.09	77,81,87,88	0
41	4D4	CN	81	12/13	0.90	0.12	90,96,114,114	0
12	D2T	AL	89	10/11	0.91	0.13	59,64,75,78	0
31	PSU	CA	2580	20/21	0.91	0.10	83,91,93,93	0
31	2MG	CA	1835	24/25	0.91	0.12	76,80,83,83	0
31	1MG	CA	745	24/25	0.91	0.11	90,92,94,96	0
1	2MG	AA	1207	24/25	0.91	0.09	89,100,106,109	0
31	PSU	CA	955	20/21	0.92	0.11	85,87,92,92	0
31	5MC	CA	1962	21/22	0.92	0.13	81,88,89,92	0
31	PSU	CA	2605	20/21	0.93	0.09	82,84,87,88	0
31	5MU	CA	747	21/22	0.93	0.09	97,103,106,106	0
31	G7M	CA	2069	24/25	0.93	0.12	80,84,87,88	0
1	PSU	BA	516	20/21	0.93	0.07	100,101,104,104	0
1	2MG	BA	1516	24/25	0.94	0.10	66,73,79,81	0
31	5MU	CA	1939	21/22	0.94	0.11	74,76,85,88	0
1	PSU	AA	516	20/21	0.94	0.07	75,79,82,82	0
1	2MG	AA	966	24/25	0.94	0.10	76,84,94,94	0
1	5MC	BA	1407	21/22	0.94	0.10	86,95,98,102	0
31	2MG	CA	2445	24/25	0.94	0.15	74,80,84,85	0
1	UR3	BA	1498	21/22	0.94	0.09	80,82,84,88	0
1	MA6	BA	1518	24/25	0.95	0.10	74,80,82,83	0
1	5MC	AA	967	21/22	0.95	0.10	80,86,94,96	0
31	OMC	CA	2498	21/22	0.95	0.11	84,87,93,97	0
1	G7M	BA	527	24/25	0.95	0.09	93,95,98,99	0
31	OMG	CA	2251	24/25	0.95	0.12	82,83,85,86	0
31	OMU	CA	2552	21/22	0.96	0.14	83,84,98,101	0
1	G7M	AA	527	24/25	0.96	0.09	58,70,72,74	0
1	UR3	AA	1498	21/22	0.96	0.08	55,59,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	PSU	DA	1911	20/21	0.96	0.06	66,80,82,83	0
1	2MG	AA	1516	24/25	0.96	0.07	50,54,57,58	0
1	4OC	BA	1402	22/23	0.96	0.08	78,79,81,82	0
1	MA6	BA	1519	24/25	0.96	0.09	76,78,81,82	0
1	4OC	AA	1402	22/23	0.97	0.07	60,61,63,64	0
1	5MC	AA	1407	21/22	0.97	0.08	50,55,58,61	0
55	5MC	DA	1962	21/22	0.97	0.10	33,44,47,50	0
55	PSU	DA	2604	20/21	0.97	0.07	33,39,50,51	0
1	MA6	AA	1518	24/25	0.97	0.09	41,46,49,51	0
41	4D4	DN	81[A]	12/13	0.97	0.08	29,40,50,51	9
41	4D4	DN	81[B]	12/13	0.97	0.08	21,29,35,36	9
55	OMU	DA	2552	21/22	0.98	0.06	30,32,35,44	0
1	MA6	AA	1519	24/25	0.98	0.07	44,48,49,50	0
55	PSU	DA	2605	20/21	0.98	0.06	30,35,41,44	0
55	5MU	DA	1939	21/22	0.98	0.08	31,36,39,44	0
55	2MG	DA	1835	24/25	0.98	0.06	43,49,53,53	0
55	2MA	DA	2503	23/24	0.98	0.07	17,29,37,40	0
55	6MZ	DA	2030	23/24	0.99	0.05	13,20,24,33	0
55	G7M	DA	2069	24/25	0.99	0.05	30,33,35,38	0
55	OMG	DA	2251	24/25	0.99	0.05	22,27,45,51	0
55	2MG	DA	2445	24/25	0.99	0.08	17,23,27,29	0
55	H2U	DA	2449	20/21	0.99	0.07	25,28,29,32	0
55	PSU	DA	2457	20/21	0.99	0.04	23,26,31,32	0
55	OMC	DA	2498	21/22	0.99	0.04	15,24,25,29	0
55	6MZ	DA	1618	23/24	0.99	0.05	24,29,32,37	0
55	PSU	DA	2504	20/21	0.99	0.06	33,36,37,40	0
32	MEQ	DD	150[A]	10/11	0.99	0.06	7,12,22,24	10
55	PSU	DA	2580	20/21	0.99	0.06	20,24,29,32	0
32	MEQ	DD	150[B]	10/11	0.99	0.06	18,24,29,30	10
55	1MG	DA	745	24/25	0.99	0.04	18,25,33,38	0
55	PSU	DA	746	20/21	0.99	0.04	18,24,29,33	0
55	5MU	DA	747	21/22	0.99	0.05	24,31,35,40	0
55	PSU	DA	955	20/21	0.99	0.05	24,25,28,28	0

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	CA	3154	1/1	0.13	0.42	152,152,152,152	0
56	MG	CA	3129	1/1	0.35	0.25	125,125,125,125	0
56	MG	CA	3075	1/1	0.38	0.37	238,238,238,238	0
56	MG	BA	1604	1/1	0.39	0.26	272,272,272,272	0
56	MG	CA	3139	1/1	0.41	0.33	114,114,114,114	0
56	MG	CA	3055	1/1	0.41	0.09	260,260,260,260	0
56	MG	CA	3060	1/1	0.50	0.13	194,194,194,194	0
56	MG	CA	3155	1/1	0.50	0.27	126,126,126,126	0
56	MG	CA	3061	1/1	0.51	0.15	250,250,250,250	0
56	MG	CA	3126	1/1	0.52	0.25	107,107,107,107	0
56	MG	CA	3152	1/1	0.54	0.20	158,158,158,158	0
56	MG	CA	3132	1/1	0.58	0.28	102,102,102,102	0
56	MG	CA	3122	1/1	0.60	0.55	100,100,100,100	0
56	MG	CA	3124	1/1	0.60	0.16	156,156,156,156	0
56	MG	AA	1628	1/1	0.60	0.13	118,118,118,118	0
56	MG	AA	1622	1/1	0.61	0.39	112,112,112,112	0
56	MG	CA	3001	1/1	0.62	0.28	291,291,291,291	0
56	MG	CA	3123	1/1	0.65	0.15	104,104,104,104	0
56	MG	CA	3111	1/1	0.65	0.18	83,83,83,83	0
56	MG	CA	3146	1/1	0.65	0.25	149,149,149,149	0
56	MG	CA	3148	1/1	0.66	0.76	50,50,50,50	1
56	MG	BA	1603	1/1	0.68	0.14	276,276,276,276	0
56	MG	BA	1638	1/1	0.68	0.35	109,109,109,109	0
56	MG	CA	3021	1/1	0.69	0.42	260,260,260,260	0
56	MG	CA	3140	1/1	0.70	0.20	88,88,88,88	0
56	MG	CA	3007	1/1	0.70	0.12	216,216,216,216	0
56	MG	CA	3067	1/1	0.70	0.13	278,278,278,278	0
56	MG	AA	1606	1/1	0.70	0.32	125,125,125,125	0
56	MG	CA	3135	1/1	0.70	0.19	81,81,81,81	0
56	MG	CA	3077	1/1	0.70	0.16	206,206,206,206	0
56	MG	CA	3110	1/1	0.71	0.20	92,92,92,92	0
56	MG	CA	3038	1/1	0.71	0.12	234,234,234,234	0
56	MG	BA	1639	1/1	0.72	0.28	103,103,103,103	0
56	MG	CA	3105	1/1	0.72	0.23	250,250,250,250	0
56	MG	BA	1634	1/1	0.72	0.18	199,199,199,199	0
56	MG	DA	3149	1/1	0.72	0.36	123,123,123,123	0
56	MG	AA	1655	1/1	0.73	0.13	214,214,214,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1643	1/1	0.73	0.25	105,105,105,105	0
56	MG	BA	1609	1/1	0.73	0.11	270,270,270,270	0
56	MG	BA	1640	1/1	0.74	0.32	118,118,118,118	0
56	MG	AA	1601	1/1	0.74	0.61	86,86,86,86	0
56	MG	BA	1606	1/1	0.74	0.19	273,273,273,273	0
61	PEG	DP	201	7/7	0.74	0.17	108,109,109,110	0
56	MG	BA	1641	1/1	0.75	0.28	94,94,94,94	0
56	MG	CA	3116	1/1	0.75	0.33	79,79,79,79	0
56	MG	CA	3104	1/1	0.75	0.15	196,196,196,196	0
56	MG	CA	3014	1/1	0.76	0.12	161,161,161,161	0
56	MG	CA	3026	1/1	0.77	0.14	129,129,129,129	0
56	MG	CA	3134	1/1	0.79	0.14	107,107,107,107	0
56	MG	CA	3002	1/1	0.79	0.15	265,265,265,265	0
56	MG	CA	3005	1/1	0.79	0.18	235,235,235,235	0
56	MG	AA	1624	1/1	0.79	0.33	107,107,107,107	0
56	MG	AA	1614	1/1	0.79	0.13	117,117,117,117	0
56	MG	CA	3147	1/1	0.79	0.27	25,25,25,25	1
62	EDO	DA	3005	4/4	0.79	0.25	104,105,107,110	0
56	MG	BA	1616	1/1	0.80	0.26	185,185,185,185	0
56	MG	DA	3179	1/1	0.80	0.30	102,102,102,102	0
58	MPD	DE	301	8/8	0.80	0.26	153,155,156,156	0
58	MPD	DK	201	8/8	0.80	0.17	104,107,110,111	0
58	MPD	DN	201	8/8	0.80	0.21	91,96,102,102	0
56	MG	AA	1609	1/1	0.80	0.32	84,84,84,84	0
56	MG	CA	3127	1/1	0.80	0.29	87,87,87,87	0
56	MG	CA	3022	1/1	0.81	0.20	170,170,170,170	0
56	MG	CA	3115	1/1	0.81	0.26	77,77,77,77	0
56	MG	CA	3009	1/1	0.81	0.22	222,222,222,222	0
56	MG	BA	1636	1/1	0.81	0.23	97,97,97,97	0
56	MG	AA	1603	1/1	0.81	0.41	108,108,108,108	0
56	MG	DA	3064	1/1	0.81	0.14	243,243,243,243	0
56	MG	DA	3148	1/1	0.81	0.34	84,84,84,84	0
63	PGE	D1	102	10/10	0.81	0.26	113,119,122,122	0
59	PUT	AA	1673	6/6	0.82	0.16	110,110,112,112	0
59	PUT	DA	3224	6/6	0.82	0.22	50,53,55,56	0
56	MG	CA	3113	1/1	0.82	0.47	90,90,90,90	0
56	MG	AA	1617	1/1	0.82	0.49	101,101,101,101	0
56	MG	DA	3183	1/1	0.82	0.20	97,97,97,97	0
68	TRS	DA	3222	8/8	0.82	0.20	107,112,117,117	0
56	MG	DA	3166	1/1	0.83	0.30	81,81,81,81	0
66	ACY	DA	3199	4/4	0.83	0.29	108,109,109,109	0
56	MG	CA	3137	1/1	0.83	0.16	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3106	1/1	0.84	0.15	84,84,84,84	0
56	MG	AA	1677	1/1	0.84	0.14	155,155,155,155	0
56	MG	CA	3130	1/1	0.84	0.16	72,72,72,72	0
56	MG	AA	1633	1/1	0.84	0.10	225,225,225,225	0
56	MG	AA	1660	1/1	0.84	0.18	277,277,277,277	0
56	MG	CA	3003	1/1	0.84	0.25	258,258,258,258	0
67	GUN	DA	3213	11/11	0.84	0.23	119,121,122,122	0
59	PUT	AA	1672	6/6	0.84	0.33	79,82,85,85	0
56	MG	DA	3174	1/1	0.85	0.17	90,90,90,90	0
59	PUT	AA	1675	6/6	0.85	0.20	101,102,103,103	0
56	MG	CA	3156	1/1	0.85	0.12	210,210,210,210	0
56	MG	AA	1664	1/1	0.85	0.13	225,225,225,225	0
56	MG	DA	3139	1/1	0.85	0.36	86,86,86,86	0
56	MG	CA	3142	1/1	0.85	0.12	69,69,69,69	0
56	MG	AA	1654	1/1	0.85	0.36	244,244,244,244	0
58	MPD	DA	3193	8/8	0.85	0.18	89,91,93,93	0
56	MG	CA	3034	1/1	0.85	0.26	235,235,235,235	0
56	MG	DA	3171	1/1	0.86	0.19	111,111,111,111	0
56	MG	AA	1605	1/1	0.86	0.48	91,91,91,91	0
59	PUT	AA	1674	6/6	0.86	0.34	112,117,121,123	0
56	MG	AA	1615	1/1	0.86	0.36	81,81,81,81	0
56	MG	AA	1611	1/1	0.86	0.23	91,91,91,91	0
61	PEG	AL	201	7/7	0.86	0.17	87,91,98,100	0
56	MG	CA	3092	1/1	0.86	0.10	195,195,195,195	0
61	PEG	DQ	201	7/7	0.86	0.38	92,94,96,97	0
58	MPD	DE	302	8/8	0.86	0.28	91,94,97,97	0
56	MG	AA	1619	1/1	0.86	0.27	90,90,90,90	0
63	PGE	DS	201	10/10	0.86	0.17	87,98,101,102	0
56	MG	DA	3154	1/1	0.86	0.26	80,80,80,80	0
56	MG	CA	3133	1/1	0.86	0.21	88,88,88,88	0
58	MPD	DA	3206	8/8	0.86	0.25	85,88,99,101	0
62	EDO	DA	3201	4/4	0.87	0.25	91,92,93,94	0
62	EDO	DA	3217	4/4	0.87	0.23	84,85,86,87	0
56	MG	BA	1630	1/1	0.87	0.16	271,271,271,271	0
56	MG	AA	1608	1/1	0.87	0.35	87,87,87,87	0
56	MG	CA	3047	1/1	0.87	0.31	272,272,272,272	0
66	ACY	DA	3204	4/4	0.87	0.26	75,76,77,77	0
56	MG	BA	1629	1/1	0.87	0.21	144,144,144,144	0
59	PUT	DA	3198	6/6	0.87	0.34	102,102,104,105	0
56	MG	CA	3062	1/1	0.88	0.12	232,232,232,232	0
56	MG	CA	3032	1/1	0.88	0.11	236,236,236,236	0
56	MG	CA	3073	1/1	0.88	0.10	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1642	1/1	0.88	0.13	126,126,126,126	0
62	EDO	DB	211	4/4	0.88	0.26	98,99,99,100	0
56	MG	CA	3010	1/1	0.88	0.21	270,270,270,270	0
56	MG	CA	3117	1/1	0.88	0.31	76,76,76,76	0
56	MG	CA	3084	1/1	0.88	0.10	181,181,181,181	0
56	MG	AA	1661	1/1	0.88	0.10	178,178,178,178	0
56	MG	AA	1607	1/1	0.88	0.28	90,90,90,90	0
56	MG	BA	1607	1/1	0.88	0.19	195,195,195,195	0
56	MG	CA	3145	1/1	0.88	0.18	60,60,60,60	0
56	MG	AA	1626	1/1	0.88	0.17	111,111,111,111	0
56	MG	CA	3128	1/1	0.88	0.19	81,81,81,81	0
56	MG	CA	3112	1/1	0.89	0.09	65,65,65,65	0
56	MG	CA	3136	1/1	0.89	0.15	82,82,82,82	0
56	MG	CA	3153	1/1	0.89	0.14	58,58,58,58	0
59	PUT	DA	3214	6/6	0.89	0.25	71,79,82,85	0
56	MG	BA	1625	1/1	0.89	0.09	235,235,235,235	0
56	MG	DA	3181	1/1	0.89	0.29	85,85,85,85	0
61	PEG	D3	102	7/7	0.89	0.60	88,94,99,99	0
56	MG	CA	3138	1/1	0.89	0.21	74,74,74,74	0
57	PG4	BA	1642	13/13	0.89	0.13	77,87,100,100	0
61	PEG	DA	3228	7/7	0.89	0.23	64,78,90,90	0
58	MPD	AA	1671	8/8	0.89	0.25	109,110,113,114	0
56	MG	CA	3099	1/1	0.89	0.10	129,129,129,129	0
56	MG	CA	3068	1/1	0.89	0.14	185,185,185,185	0
56	MG	AA	1636	1/1	0.89	0.11	110,110,110,110	0
56	MG	DA	3140	1/1	0.89	0.59	43,43,43,43	1
63	PGE	D3	101	10/10	0.89	0.21	105,111,114,114	0
58	MPD	DA	3004	8/8	0.89	0.30	106,109,119,121	0
64	SPD	DA	3186	10/10	0.89	0.19	84,87,91,91	0
56	MG	DA	3146	1/1	0.89	0.17	80,80,80,80	0
56	MG	AA	1625	1/1	0.89	0.16	90,90,90,90	0
56	MG	CA	3031	1/1	0.89	0.06	87,87,87,87	0
56	MG	CA	3064	1/1	0.89	0.14	274,274,274,274	0
57	PG4	DS	202	13/13	0.90	0.16	67,78,83,83	0
57	PG4	DA	3218	13/13	0.90	0.14	90,94,98,99	0
56	MG	AA	1618	1/1	0.90	0.39	83,83,83,83	0
56	MG	CA	3039	1/1	0.90	0.20	252,252,252,252	0
56	MG	AA	1616	1/1	0.90	0.42	75,75,75,75	0
56	MG	CA	3080	1/1	0.90	0.18	143,143,143,143	0
56	MG	BA	1612	1/1	0.90	0.29	201,201,201,201	0
58	MPD	DT	201	8/8	0.90	0.30	111,114,115,115	0
56	MG	CA	3119	1/1	0.90	0.14	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3082	1/1	0.90	0.15	173,173,173,173	0
62	EDO	DA	3211	4/4	0.90	0.30	103,104,104,106	0
58	MPD	DA	3195	8/8	0.90	0.28	92,97,98,98	0
56	MG	DA	3129	1/1	0.90	0.37	64,64,64,64	0
58	MPD	DA	3209	8/8	0.90	0.19	90,94,98,98	0
56	MG	AA	1678	1/1	0.90	0.18	59,59,59,59	0
56	MG	CA	3151	1/1	0.90	0.14	72,72,72,72	0
56	MG	DA	3185	1/1	0.90	0.32	70,70,70,70	0
57	PG4	AA	1670	13/13	0.90	0.13	74,86,104,104	0
56	MG	DA	3144	1/1	0.90	0.28	72,72,72,72	0
59	PUT	DA	3207	6/6	0.90	0.28	95,100,104,105	0
62	EDO	DB	210	4/4	0.91	0.26	95,95,96,97	0
56	MG	AA	1610	1/1	0.91	0.33	85,85,85,85	0
56	MG	AA	1612	1/1	0.91	0.22	78,78,78,78	0
56	MG	CA	3109	1/1	0.91	0.14	63,63,63,63	0
56	MG	CA	3149	1/1	0.91	0.30	76,76,76,76	0
56	MG	BA	1637	1/1	0.91	0.20	87,87,87,87	0
59	PUT	DA	3223	6/6	0.91	0.22	118,122,122,123	0
56	MG	DA	3125	1/1	0.91	0.23	81,81,81,81	0
56	MG	DA	3126	1/1	0.91	0.42	83,83,83,83	0
63	PGE	DU	101	10/10	0.91	0.18	71,82,92,93	0
57	PG4	DA	3196	13/13	0.91	0.21	90,94,96,97	0
65	1PE	DA	3205	16/16	0.91	0.20	77,84,87,88	0
56	MG	DA	3168	1/1	0.91	0.25	65,65,65,65	0
56	MG	AA	1647	1/1	0.91	0.10	157,157,157,157	0
56	MG	AA	1613	1/1	0.91	0.30	64,64,64,64	0
62	EDO	D1	101	4/4	0.91	0.10	61,62,64,66	0
56	MG	DA	3132	1/1	0.92	0.31	78,78,78,78	0
56	MG	CA	3076	1/1	0.92	0.10	163,163,163,163	0
56	MG	CA	3013	1/1	0.92	0.09	123,123,123,123	0
56	MG	CA	3008	1/1	0.92	0.10	131,131,131,131	0
56	MG	CA	3072	1/1	0.92	0.13	274,274,274,274	0
58	MPD	DA	3212	8/8	0.92	0.22	83,85,86,90	0
57	PG4	DQ	202	13/13	0.92	0.09	66,71,76,78	0
57	PG4	DR	202	13/13	0.92	0.24	98,111,116,116	0
56	MG	CA	3090	1/1	0.92	0.08	118,118,118,118	0
56	MG	DA	3100	1/1	0.92	0.20	207,207,207,207	0
56	MG	DA	3123	1/1	0.92	0.24	78,78,78,78	0
56	MG	DA	3155	1/1	0.92	0.30	73,73,73,73	0
56	MG	CA	3120	1/1	0.92	0.12	168,168,168,168	0
59	PUT	DA	3215	6/6	0.92	0.26	83,90,96,98	0
63	PGE	DA	3227	10/10	0.92	0.18	81,90,107,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1627	1/1	0.92	0.25	83,83,83,83	0
56	MG	DA	3127	1/1	0.92	0.25	60,60,60,60	0
56	MG	AA	1623	1/1	0.92	0.12	77,77,77,77	0
61	PEG	D1	103	7/7	0.92	0.28	81,87,93,95	0
56	MG	DA	3131	1/1	0.92	0.43	79,79,79,79	0
61	PEG	DL	201	7/7	0.92	0.14	73,79,80,80	0
61	PEG	DA	3229	7/7	0.93	0.16	79,83,88,88	0
56	MG	BA	1633	1/1	0.93	0.13	163,163,163,163	0
56	MG	CA	3063	1/1	0.93	0.09	103,103,103,103	0
59	PUT	DA	3191	6/6	0.93	0.16	48,54,57,59	0
62	EDO	DA	3003	4/4	0.93	0.26	97,98,98,98	0
59	PUT	DA	3192	6/6	0.93	0.13	44,49,50,50	0
56	MG	DA	3173	1/1	0.93	0.16	69,69,69,69	0
56	MG	CA	3108	1/1	0.93	0.13	65,65,65,65	0
56	MG	DA	3175	1/1	0.93	0.40	97,97,97,97	0
56	MG	CA	3143	1/1	0.93	0.16	104,104,104,104	0
56	MG	DB	206	1/1	0.93	0.25	129,129,129,129	0
56	MG	BA	1614	1/1	0.93	0.09	136,136,136,136	0
56	MG	CA	3121	1/1	0.93	0.15	60,60,60,60	0
63	PGE	DA	3219	10/10	0.93	0.15	85,88,91,91	0
56	MG	CA	3028	1/1	0.93	0.10	277,277,277,277	0
56	MG	CA	3048	1/1	0.93	0.08	97,97,97,97	0
64	SPD	DA	3226	10/10	0.93	0.14	37,46,63,65	0
56	MG	BA	1605	1/1	0.93	0.09	206,206,206,206	0
56	MG	CA	3016	1/1	0.93	0.23	150,150,150,150	0
56	MG	DA	3165	1/1	0.93	0.14	72,72,72,72	0
61	PEG	DA	3202	7/7	0.93	0.22	87,88,91,91	0
56	MG	BA	1624	1/1	0.93	0.08	157,157,157,157	0
56	MG	DA	3156	1/1	0.94	0.47	83,83,83,83	0
56	MG	DA	3159	1/1	0.94	0.25	70,70,70,70	0
56	MG	CA	3093	1/1	0.94	0.07	72,72,72,72	0
56	MG	CA	3057	1/1	0.94	0.11	121,121,121,121	0
56	MG	DA	3130	1/1	0.94	0.57	68,68,68,68	0
56	MG	DA	3170	1/1	0.94	0.36	106,106,106,106	0
56	MG	BA	1623	1/1	0.94	0.14	166,166,166,166	0
56	MG	DA	3172	1/1	0.94	0.18	57,57,57,57	0
59	PUT	DA	3221	6/6	0.94	0.16	65,71,74,75	0
56	MG	CA	3045	1/1	0.94	0.09	110,110,110,110	0
56	MG	DA	3136	1/1	0.94	0.14	87,87,87,87	0
63	PGE	DD	301	10/10	0.94	0.19	86,89,95,96	0
59	PUT	DA	3225	6/6	0.94	0.18	61,62,70,72	0
56	MG	BA	1627	1/1	0.94	0.13	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3107	1/1	0.94	0.21	65,65,65,65	0
56	MG	AA	1602	1/1	0.94	0.24	81,81,81,81	0
56	MG	CA	3049	1/1	0.94	0.07	56,56,56,56	0
64	SPD	DA	3208	10/10	0.94	0.24	112,117,118,119	0
56	MG	DA	3113	1/1	0.94	0.23	280,280,280,280	0
65	1PE	DA	3188	16/16	0.94	0.11	47,60,87,91	0
56	MG	CA	3054	1/1	0.94	0.07	105,105,105,105	0
56	MG	CA	3019	1/1	0.94	0.07	62,62,62,62	0
61	PEG	DA	3203	7/7	0.94	0.31	84,88,95,96	0
61	PEG	DA	3220	7/7	0.94	0.27	136,137,139,139	0
56	MG	CA	3069	1/1	0.94	0.10	135,135,135,135	0
56	MG	CA	3065	1/1	0.95	0.08	107,107,107,107	0
56	MG	DA	3135	1/1	0.95	0.07	56,56,56,56	0
56	MG	CA	3083	1/1	0.95	0.09	136,136,136,136	0
56	MG	DA	3176	1/1	0.95	0.17	92,92,92,92	0
56	MG	CA	3029	1/1	0.95	0.10	166,166,166,166	0
62	EDO	DA	3002	4/4	0.95	0.14	78,79,79,79	0
56	MG	CA	3125	1/1	0.95	0.09	97,97,97,97	0
56	MG	DA	3143	1/1	0.95	0.09	51,51,51,51	0
56	MG	DA	3054	1/1	0.95	0.18	190,190,190,190	0
62	EDO	DA	3210	4/4	0.95	0.20	88,88,89,89	0
56	MG	CA	3056	1/1	0.95	0.31	66,66,66,66	0
56	MG	DA	3147	1/1	0.95	0.12	95,95,95,95	0
56	MG	CA	3043	1/1	0.95	0.06	90,90,90,90	0
56	MG	CA	3071	1/1	0.95	0.06	146,146,146,146	0
56	MG	CA	3114	1/1	0.95	0.08	51,51,51,51	0
56	MG	DA	3121	1/1	0.95	0.17	64,64,64,64	0
56	MG	CA	3094	1/1	0.95	0.08	68,68,68,68	0
63	PGE	DA	3216	10/10	0.95	0.10	68,72,83,84	0
56	MG	AA	1604	1/1	0.95	0.24	66,66,66,66	0
60	ZN	C5	101	1/1	0.95	0.05	155,155,155,155	0
56	MG	DA	3161	1/1	0.95	0.12	119,119,119,119	0
56	MG	DA	3164	1/1	0.95	0.20	62,62,62,62	0
56	MG	CA	3023	1/1	0.95	0.24	245,245,245,245	0
56	MG	CA	3150	1/1	0.95	0.19	89,89,89,89	0
56	MG	DA	3167	1/1	0.95	0.19	63,63,63,63	0
66	ACY	DA	3194	4/4	0.95	0.18	92,93,94,94	0
56	MG	DA	3128	1/1	0.95	0.30	54,54,54,54	0
56	MG	AA	1621	1/1	0.95	0.31	69,69,69,69	0
56	MG	CA	3036	1/1	0.95	0.04	102,102,102,102	0
56	MG	AA	1665	1/1	0.95	0.11	123,123,123,123	0
58	MPD	AA	1676	8/8	0.96	0.12	87,90,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3074	1/1	0.96	0.08	131,131,131,131	0
56	MG	CA	3141	1/1	0.96	0.21	53,53,53,53	0
56	MG	CA	3046	1/1	0.96	0.09	116,116,116,116	0
56	MG	DA	3158	1/1	0.96	0.24	75,75,75,75	0
56	MG	DA	3119	1/1	0.96	0.32	82,82,82,82	0
56	MG	DA	3120	1/1	0.96	0.13	48,48,48,48	0
56	MG	DA	3163	1/1	0.96	0.37	78,78,78,78	0
56	MG	AA	1669	1/1	0.96	0.06	89,89,89,89	0
56	MG	DA	3122	1/1	0.96	0.22	76,76,76,76	0
56	MG	AA	1620	1/1	0.96	0.14	67,67,67,67	0
62	EDO	DA	3197	4/4	0.96	0.16	52,57,59,60	0
56	MG	CA	3078	1/1	0.96	0.08	133,133,133,133	0
56	MG	AA	1634	1/1	0.96	0.09	163,163,163,163	0
56	MG	CA	3066	1/1	0.96	0.06	129,129,129,129	0
56	MG	CA	3006	1/1	0.96	0.07	144,144,144,144	0
56	MG	BA	1608	1/1	0.96	0.07	114,114,114,114	0
56	MG	CA	3131	1/1	0.96	0.05	56,56,56,56	0
56	MG	AA	1644	1/1	0.96	0.18	115,115,115,115	0
56	MG	CA	3070	1/1	0.96	0.05	79,79,79,79	0
56	MG	DA	3133	1/1	0.96	0.30	68,68,68,68	0
63	PGE	DA	3189	10/10	0.96	0.10	42,45,49,49	0
56	MG	DA	3178	1/1	0.96	0.17	89,89,89,89	0
56	MG	DA	3134	1/1	0.96	0.17	68,68,68,68	0
56	MG	BA	1644	1/1	0.96	0.10	64,64,64,64	0
56	MG	CA	3097	1/1	0.96	0.10	109,109,109,109	0
56	MG	CA	3118	1/1	0.96	0.13	47,47,47,47	0
56	MG	AA	1658	1/1	0.96	0.07	65,65,65,65	0
56	MG	DB	207	1/1	0.96	0.10	84,84,84,84	0
56	MG	DB	208	1/1	0.96	0.07	56,56,56,56	0
56	MG	DB	209	1/1	0.96	0.22	71,71,71,71	0
56	MG	DA	3014	1/1	0.96	0.07	122,122,122,122	0
56	MG	CA	3102	1/1	0.96	0.07	107,107,107,107	0
56	MG	CA	3012	1/1	0.96	0.06	89,89,89,89	0
56	MG	DA	3150	1/1	0.96	0.35	63,63,63,63	0
58	MPD	DS	203	8/8	0.97	0.13	55,56,58,61	0
56	MG	BA	1613	1/1	0.97	0.12	112,112,112,112	0
56	MG	CA	3024	1/1	0.97	0.10	75,75,75,75	0
56	MG	DA	3039	1/1	0.97	0.14	21,21,21,21	0
56	MG	AA	1663	1/1	0.97	0.08	99,99,99,99	0
56	MG	AA	1657	1/1	0.97	0.11	116,116,116,116	0
56	MG	BA	1617	1/1	0.97	0.05	130,130,130,130	0
56	MG	DA	3142	1/1	0.97	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3087	1/1	0.97	0.05	49,49,49,49	0
56	MG	CB	201	1/1	0.97	0.07	157,157,157,157	0
62	EDO	DA	3200	4/4	0.97	0.09	53,54,54,55	0
56	MG	DA	3145	1/1	0.97	0.10	63,63,63,63	0
56	MG	CB	203	1/1	0.97	0.06	125,125,125,125	0
59	PUT	DM	201	6/6	0.97	0.13	49,50,53,56	0
59	PUT	DA	3187	6/6	0.97	0.12	49,51,53,54	0
56	MG	DA	3180	1/1	0.97	0.12	54,54,54,54	0
56	MG	BA	1618	1/1	0.97	0.06	106,106,106,106	0
56	MG	DA	3182	1/1	0.97	0.13	109,109,109,109	0
56	MG	CA	3035	1/1	0.97	0.17	83,83,83,83	0
56	MG	DA	3184	1/1	0.97	0.12	74,74,74,74	0
56	MG	CA	3079	1/1	0.97	0.04	110,110,110,110	0
56	MG	AA	1630	1/1	0.97	0.07	102,102,102,102	0
56	MG	DA	3151	1/1	0.97	0.04	41,41,41,41	0
56	MG	CA	3018	1/1	0.97	0.10	125,125,125,125	0
56	MG	DA	3124	1/1	0.97	0.36	49,49,49,49	0
56	MG	BA	1610	1/1	0.97	0.06	130,130,130,130	0
56	MG	DA	3157	1/1	0.97	0.21	69,69,69,69	0
56	MG	CA	3087	1/1	0.97	0.06	65,65,65,65	0
56	MG	CA	3042	1/1	0.97	0.07	87,87,87,87	0
56	MG	CA	3020	1/1	0.97	0.07	60,60,60,60	0
56	MG	DB	205	1/1	0.97	0.16	73,73,73,73	0
56	MG	CA	3044	1/1	0.97	0.08	49,49,49,49	0
56	MG	BA	1601	1/1	0.97	0.10	158,158,158,158	0
56	MG	BA	1626	1/1	0.97	0.04	92,92,92,92	0
56	MG	BA	1620	1/1	0.98	0.04	115,115,115,115	0
56	MG	CA	3144	1/1	0.98	0.03	60,60,60,60	0
56	MG	CA	3051	1/1	0.98	0.05	52,52,52,52	0
56	MG	CA	3053	1/1	0.98	0.07	58,58,58,58	0
56	MG	AA	1641	1/1	0.98	0.04	65,65,65,65	0
60	ZN	AB	301	1/1	0.98	0.06	141,141,141,141	0
56	MG	AA	1632	1/1	0.98	0.06	94,94,94,94	0
56	MG	DA	3177	1/1	0.98	0.08	80,80,80,80	0
56	MG	CA	3011	1/1	0.98	0.06	72,72,72,72	0
56	MG	CA	3081	1/1	0.98	0.07	82,82,82,82	0
56	MG	AA	1662	1/1	0.98	0.09	89,89,89,89	0
56	MG	CA	3058	1/1	0.98	0.10	87,87,87,87	0
56	MG	CA	3086	1/1	0.98	0.04	74,74,74,74	0
56	MG	CA	3059	1/1	0.98	0.05	70,70,70,70	0
56	MG	CA	3088	1/1	0.98	0.03	78,78,78,78	0
56	MG	DA	3137	1/1	0.98	0.04	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3231	1/1	0.98	0.13	46,46,46,46	0
56	MG	DA	3138	1/1	0.98	0.15	72,72,72,72	0
56	MG	CA	3089	1/1	0.98	0.10	54,54,54,54	0
56	MG	DR	201	1/1	0.98	0.04	30,30,30,30	0
56	MG	DA	3141	1/1	0.98	0.06	57,57,57,57	0
56	MG	CA	3033	1/1	0.98	0.07	79,79,79,79	0
56	MG	CA	3091	1/1	0.98	0.05	71,71,71,71	0
56	MG	BA	1611	1/1	0.98	0.04	80,80,80,80	0
56	MG	BA	1602	1/1	0.98	0.05	90,90,90,90	0
56	MG	AA	1656	1/1	0.98	0.04	95,95,95,95	0
56	MG	DA	3007	1/1	0.98	0.09	77,77,77,77	0
56	MG	CA	3095	1/1	0.98	0.06	68,68,68,68	0
56	MG	DA	3017	1/1	0.98	0.06	60,60,60,60	0
56	MG	CA	3037	1/1	0.98	0.08	107,107,107,107	0
56	MG	DA	3045	1/1	0.98	0.09	41,41,41,41	0
56	MG	DA	3153	1/1	0.98	0.12	33,33,33,33	0
56	MG	CA	3098	1/1	0.98	0.05	91,91,91,91	0
56	MG	DA	3056	1/1	0.98	0.09	151,151,151,151	0
56	MG	CA	3017	1/1	0.98	0.10	97,97,97,97	0
56	MG	DA	3081	1/1	0.98	0.04	130,130,130,130	0
56	MG	AA	1638	1/1	0.98	0.04	100,100,100,100	0
56	MG	CA	3040	1/1	0.98	0.07	85,85,85,85	0
56	MG	DA	3160	1/1	0.98	0.20	57,57,57,57	0
56	MG	DA	3097	1/1	0.98	0.09	106,106,106,106	0
64	SPD	DA	3190	10/10	0.98	0.09	38,46,49,53	0
56	MG	DA	3162	1/1	0.98	0.09	67,67,67,67	0
56	MG	BA	1631	1/1	0.98	0.06	63,63,63,63	0
56	MG	BA	1632	1/1	0.98	0.10	85,85,85,85	0
56	MG	AA	1639	1/1	0.98	0.05	122,122,122,122	0
56	MG	AA	1666	1/1	0.98	0.07	97,97,97,97	0
56	MG	AA	1659	1/1	0.98	0.04	61,61,61,61	0
56	MG	BA	1619	1/1	0.98	0.05	70,70,70,70	0
56	MG	DA	3169	1/1	0.98	0.12	95,95,95,95	0
56	MG	CA	3025	1/1	0.98	0.06	88,88,88,88	0
56	MG	CA	3101	1/1	0.99	0.03	71,71,71,71	0
56	MG	AA	1653	1/1	0.99	0.06	67,67,67,67	0
56	MG	DD	302	1/1	0.99	0.05	41,41,41,41	0
56	MG	CA	3103	1/1	0.99	0.04	82,82,82,82	0
56	MG	DB	201	1/1	0.99	0.07	56,56,56,56	0
56	MG	DB	203	1/1	0.99	0.07	34,34,34,34	0
60	ZN	D5	101	1/1	0.99	0.04	56,56,56,56	0
56	MG	DB	204	1/1	0.99	0.03	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3015	1/1	0.99	0.09	48,48,48,48	0
56	MG	CB	202	1/1	0.99	0.05	100,100,100,100	0
56	MG	AA	1629	1/1	0.99	0.06	99,99,99,99	0
56	MG	AA	1643	1/1	0.99	0.06	69,69,69,69	0
56	MG	AA	1640	1/1	0.99	0.04	60,60,60,60	0
56	MG	DA	3006	1/1	0.99	0.04	75,75,75,75	0
56	MG	CA	3082	1/1	0.99	0.07	90,90,90,90	0
56	MG	DA	3008	1/1	0.99	0.05	77,77,77,77	0
56	MG	DA	3232	1/1	0.99	0.07	30,30,30,30	0
56	MG	DA	3009	1/1	0.99	0.06	82,82,82,82	0
56	MG	AA	1667	1/1	0.99	0.05	42,42,42,42	0
56	MG	CA	3004	1/1	0.99	0.05	83,83,83,83	0
56	MG	DA	3028	1/1	0.99	0.06	83,83,83,83	0
56	MG	DA	3032	1/1	0.99	0.05	47,47,47,47	0
56	MG	DA	3037	1/1	0.99	0.06	29,29,29,29	0
56	MG	CA	3085	1/1	0.99	0.04	56,56,56,56	0
56	MG	BA	1635	1/1	0.99	0.06	106,106,106,106	0
56	MG	DA	3046	1/1	0.99	0.04	61,61,61,61	0
56	MG	DA	3049	1/1	0.99	0.05	48,48,48,48	0
56	MG	BA	1621	1/1	0.99	0.10	29,29,29,29	0
56	MG	BA	1622	1/1	0.99	0.05	104,104,104,104	0
56	MG	AA	1645	1/1	0.99	0.04	61,61,61,61	0
56	MG	DA	3152	1/1	0.99	0.07	53,53,53,53	0
56	MG	DA	3065	1/1	0.99	0.06	120,120,120,120	0
56	MG	DA	3072	1/1	0.99	0.06	86,86,86,86	0
56	MG	DA	3074	1/1	0.99	0.06	53,53,53,53	0
56	MG	DA	3076	1/1	0.99	0.08	39,39,39,39	0
56	MG	AA	1635	1/1	0.99	0.05	119,119,119,119	0
56	MG	CA	3027	1/1	0.99	0.04	61,61,61,61	0
56	MG	DA	3084	1/1	0.99	0.02	75,75,75,75	0
56	MG	AA	1649	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3094	1/1	0.99	0.04	36,36,36,36	0
56	MG	DA	3096	1/1	0.99	0.04	19,19,19,19	0
56	MG	AA	1650	1/1	0.99	0.04	87,87,87,87	0
56	MG	DA	3099	1/1	0.99	0.03	31,31,31,31	0
56	MG	CA	3050	1/1	0.99	0.03	51,51,51,51	0
56	MG	CA	3030	1/1	0.99	0.04	84,84,84,84	0
56	MG	CA	3096	1/1	0.99	0.04	97,97,97,97	0
56	MG	CA	3052	1/1	0.99	0.08	60,60,60,60	0
56	MG	AA	1651	1/1	0.99	0.04	68,68,68,68	0
56	MG	AA	1652	1/1	0.99	0.14	30,30,30,30	0
56	MG	CA	3100	1/1	0.99	0.09	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3083	1/1	1.00	0.04	46,46,46,46	0
56	MG	AA	1668	1/1	1.00	0.06	58,58,58,58	0
56	MG	DA	3085	1/1	1.00	0.05	52,52,52,52	0
56	MG	DA	3086	1/1	1.00	0.03	30,30,30,30	0
56	MG	DA	3018	1/1	1.00	0.05	69,69,69,69	0
56	MG	DA	3088	1/1	1.00	0.01	36,36,36,36	0
56	MG	DA	3089	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3090	1/1	1.00	0.02	52,52,52,52	0
56	MG	DA	3091	1/1	1.00	0.05	30,30,30,30	0
56	MG	DA	3230	1/1	1.00	0.02	53,53,53,53	0
56	MG	DA	3092	1/1	1.00	0.02	23,23,23,23	0
56	MG	DA	3093	1/1	1.00	0.02	23,23,23,23	0
56	MG	DA	3019	1/1	1.00	0.02	17,17,17,17	0
56	MG	DA	3095	1/1	1.00	0.06	26,26,26,26	0
56	MG	DA	3020	1/1	1.00	0.04	42,42,42,42	0
56	MG	DA	3021	1/1	1.00	0.11	9,9,9,9	0
56	MG	DA	3098	1/1	1.00	0.05	32,32,32,32	0
56	MG	DA	3022	1/1	1.00	0.05	43,43,43,43	0
56	MG	DA	3023	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3101	1/1	1.00	0.04	22,22,22,22	0
56	MG	DA	3102	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3103	1/1	1.00	0.05	50,50,50,50	0
56	MG	DA	3104	1/1	1.00	0.02	37,37,37,37	0
56	MG	DA	3105	1/1	1.00	0.01	38,38,38,38	0
56	MG	DA	3106	1/1	1.00	0.05	25,25,25,25	0
56	MG	DA	3107	1/1	1.00	0.05	25,25,25,25	0
56	MG	DA	3108	1/1	1.00	0.09	37,37,37,37	0
56	MG	DA	3109	1/1	1.00	0.04	34,34,34,34	0
56	MG	DA	3110	1/1	1.00	0.04	32,32,32,32	0
56	MG	DA	3111	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3112	1/1	1.00	0.03	35,35,35,35	0
56	MG	DA	3024	1/1	1.00	0.05	28,28,28,28	0
56	MG	DA	3114	1/1	1.00	0.01	27,27,27,27	0
56	MG	DA	3115	1/1	1.00	0.03	81,81,81,81	0
56	MG	DA	3116	1/1	1.00	0.02	40,40,40,40	0
56	MG	DA	3117	1/1	1.00	0.01	36,36,36,36	0
56	MG	DA	3118	1/1	1.00	0.01	45,45,45,45	0
56	MG	DA	3025	1/1	1.00	0.05	26,26,26,26	0
56	MG	DA	3026	1/1	1.00	0.07	33,33,33,33	0
56	MG	DA	3027	1/1	1.00	0.03	43,43,43,43	0
56	MG	AA	1648	1/1	1.00	0.03	77,77,77,77	0
56	MG	DA	3029	1/1	1.00	0.03	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3030	1/1	1.00	0.06	55,55,55,55	0
56	MG	DA	3031	1/1	1.00	0.06	23,23,23,23	0
56	MG	AA	1637	1/1	1.00	0.03	43,43,43,43	0
56	MG	DA	3033	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3034	1/1	1.00	0.04	22,22,22,22	0
56	MG	DA	3035	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3036	1/1	1.00	0.01	28,28,28,28	0
56	MG	BA	1615	1/1	1.00	0.07	65,65,65,65	0
56	MG	DA	3038	1/1	1.00	0.05	20,20,20,20	0
56	MG	DM	202	1/1	1.00	0.03	43,43,43,43	0
56	MG	DA	3040	1/1	1.00	0.02	20,20,20,20	0
56	MG	DA	3041	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3042	1/1	1.00	0.04	56,56,56,56	0
56	MG	DA	3043	1/1	1.00	0.08	13,13,13,13	0
56	MG	DA	3044	1/1	1.00	0.05	29,29,29,29	0
56	MG	DA	3001	1/1	1.00	0.02	25,25,25,25	0
56	MG	BA	1628	1/1	1.00	0.02	70,70,70,70	0
56	MG	DA	3047	1/1	1.00	0.03	61,61,61,61	0
56	MG	DA	3048	1/1	1.00	0.02	36,36,36,36	0
56	MG	AA	1646	1/1	1.00	0.02	57,57,57,57	0
56	MG	DA	3050	1/1	1.00	0.02	25,25,25,25	0
56	MG	DA	3051	1/1	1.00	0.02	46,46,46,46	0
56	MG	DA	3052	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3053	1/1	1.00	0.02	22,22,22,22	0
56	MG	DB	202	1/1	1.00	0.02	30,30,30,30	0
56	MG	DA	3055	1/1	1.00	0.03	40,40,40,40	0
56	MG	AA	1631	1/1	1.00	0.03	43,43,43,43	0
56	MG	DA	3057	1/1	1.00	0.06	30,30,30,30	0
56	MG	DA	3058	1/1	1.00	0.02	38,38,38,38	0
56	MG	DA	3059	1/1	1.00	0.01	27,27,27,27	0
56	MG	DA	3060	1/1	1.00	0.02	31,31,31,31	0
56	MG	DA	3061	1/1	1.00	0.01	33,33,33,33	0
56	MG	DA	3062	1/1	1.00	0.04	28,28,28,28	0
56	MG	DA	3063	1/1	1.00	0.04	36,36,36,36	0
56	MG	DA	3010	1/1	1.00	0.08	74,74,74,74	0
56	MG	DA	3011	1/1	1.00	0.04	20,20,20,20	0
56	MG	DA	3066	1/1	1.00	0.08	44,44,44,44	0
56	MG	DA	3067	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3068	1/1	1.00	0.05	37,37,37,37	0
56	MG	DA	3069	1/1	1.00	0.03	42,42,42,42	0
56	MG	DA	3070	1/1	1.00	0.04	37,37,37,37	0
56	MG	DA	3071	1/1	1.00	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3012	1/1	1.00	0.07	31,31,31,31	0
56	MG	DA	3073	1/1	1.00	0.04	49,49,49,49	0
56	MG	DA	3013	1/1	1.00	0.02	33,33,33,33	0
56	MG	DA	3075	1/1	1.00	0.03	23,23,23,23	0
56	MG	CA	3041	1/1	1.00	0.04	62,62,62,62	0
56	MG	DA	3077	1/1	1.00	0.03	42,42,42,42	0
56	MG	DA	3078	1/1	1.00	0.01	32,32,32,32	0
56	MG	DA	3079	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3080	1/1	1.00	0.03	50,50,50,50	0
56	MG	DA	3015	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3016	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.