



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 07:50 AM EDT

PDB ID : 5J88 / pdb_00005j88
Title : Structure of the E coli 70S ribosome with the U1060A mutation in 16S rRNA
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

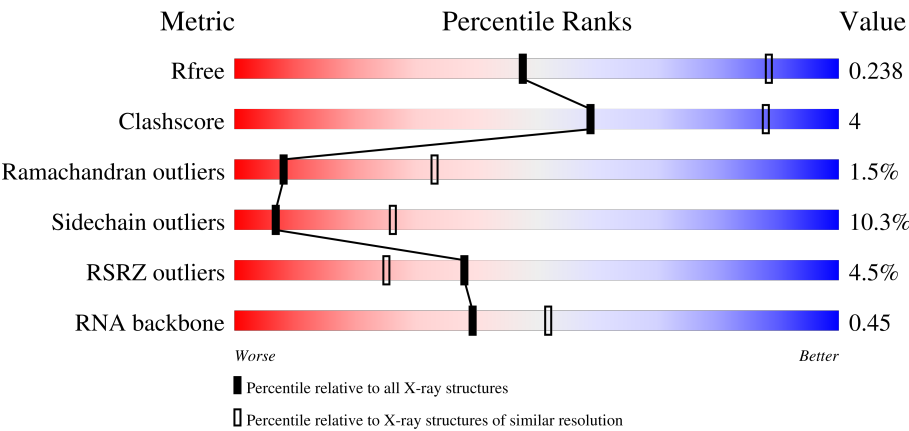
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)
RNA backbone	3983	1067 (3.64-3.00)

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	4% 67% 29%
1	BA	1534	5% 66% 29%
2	AB	224	2% 77% 20%
2	BB	224	% 79% 18%

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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	129	
11	BK	129	
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	84% 13%
16	AP	82	10% 84% 12%
16	BP	82	10% 84% 12%
17	AQ	80	74% 24%
17	BQ	80	5% 75% 20%
18	AR	55	2% 78% 18%
18	BR	55	4% 76% 24%
19	AS	79	10% 66% 29% 5%
19	BS	79	19% 71% 25%
20	AT	86	5% 66% 29% 5%
20	BT	86	12% 70% 24%
21	AU	56	2% 71% 27%
21	BU	56	5% 79% 20%
22	C1	56	21% 68% 29%
22	D1	56	77% 20%
23	C2	51	10% 65% 31%
23	D2	51	2% 71% 29%
24	C3	46	20% 80% 17%
24	D3	46	2% 72% 26%
25	C4	64	42% 84% 16%
25	D4	64	77% 23%
26	C5	38	16% 79% 18%
26	D5	38	82% 16%
27	C0	58	10% 76% 19% 5%
27	D0	58	3% 71% 26%

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	

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Mol	Chain	Length	Quality of chain
42	CO	127	
42	DO	127	
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	100	
48	DU	100	
49	CV	103	
49	DV	103	
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	% 67% 28% 5%

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	CA	3056	-	-	-	X
66	ACY	DA	3196	-	X	-	-
66	ACY	DA	3202	-	-	X	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295119 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
			32932	14695	6044	10659	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32910	14685	6039	10653	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1060	A	U	conflict	GB 675819282
BA	1060	A	U	conflict	GB 675819282

- 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
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	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
			738	466	139	131	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	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
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

- 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 (CCD ID: MG) (formula: Mg).

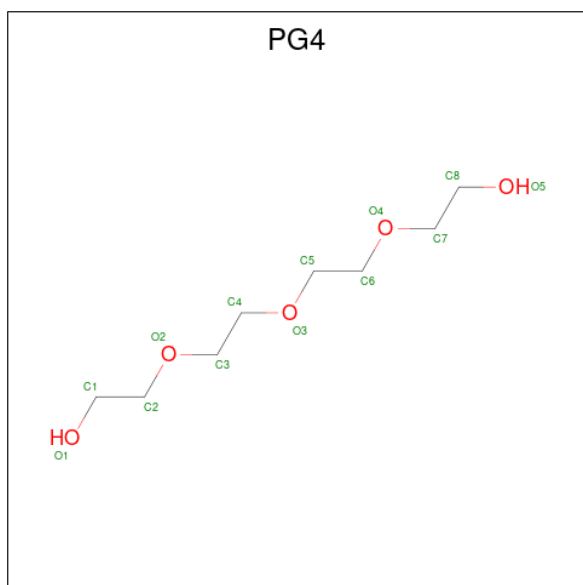
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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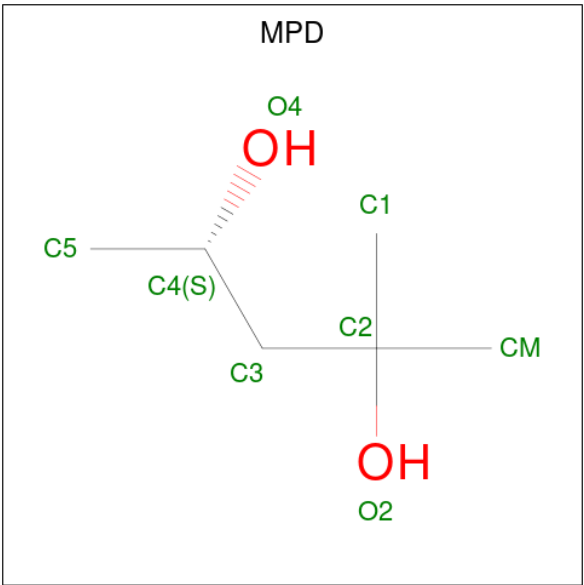
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DA	184	Total	Mg	0	0
			184	184		

- Molecule 57 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



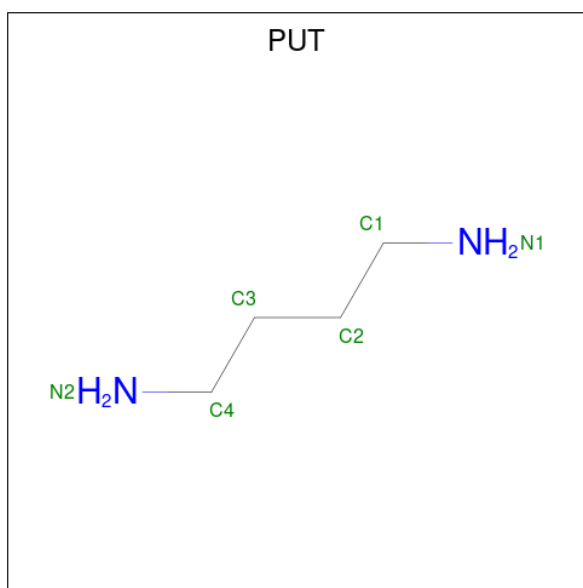
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: 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	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		

- Molecule 59 is 1,4-DIAMINOBUTANE (CCD ID: 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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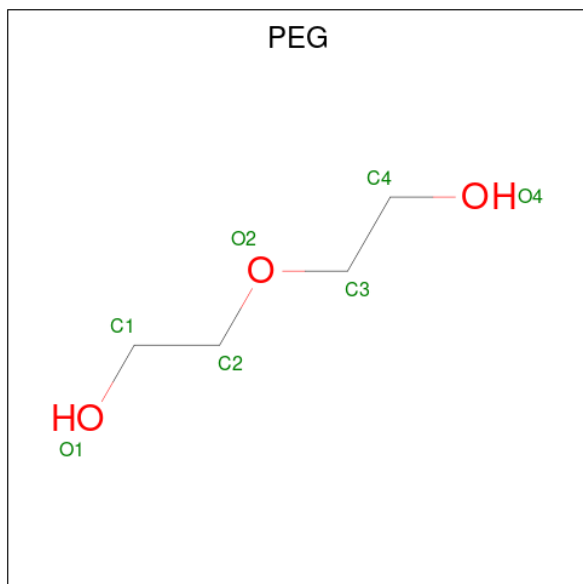
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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

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

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



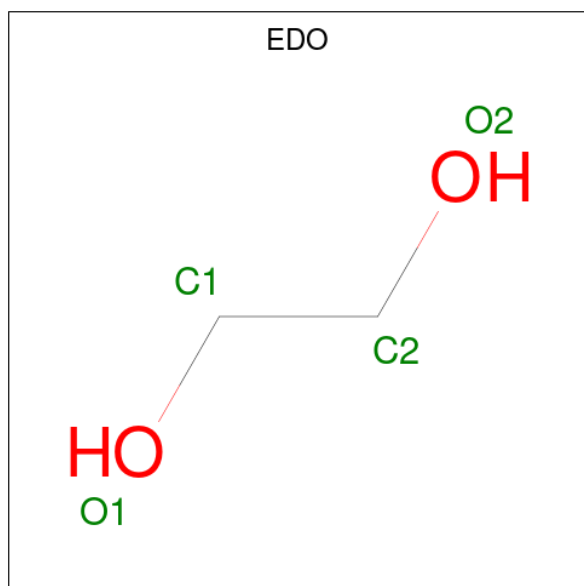
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 62 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



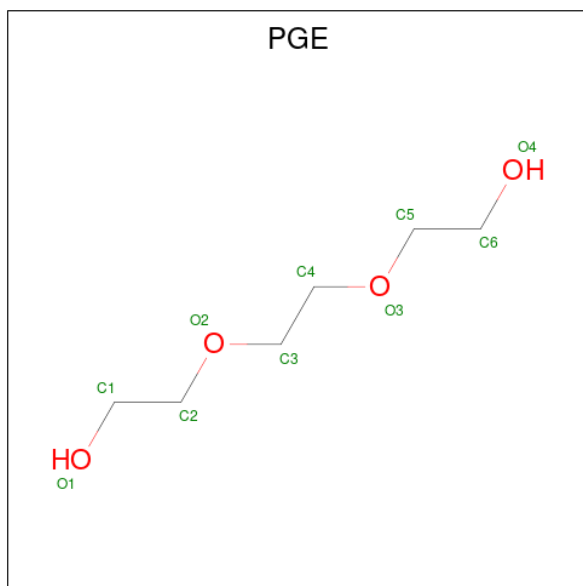
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	D0	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 63 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



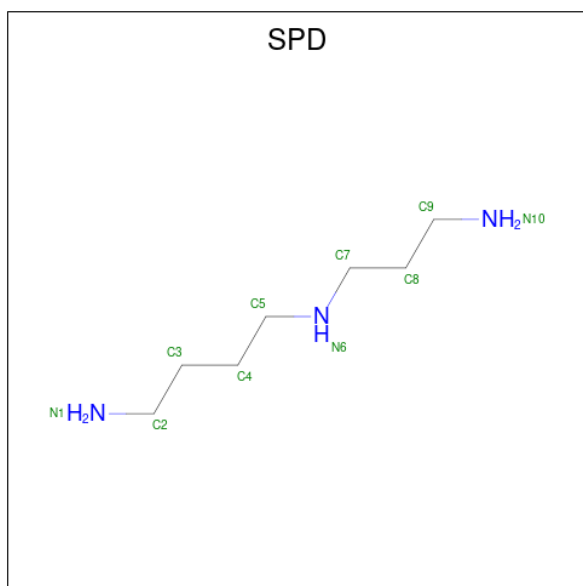
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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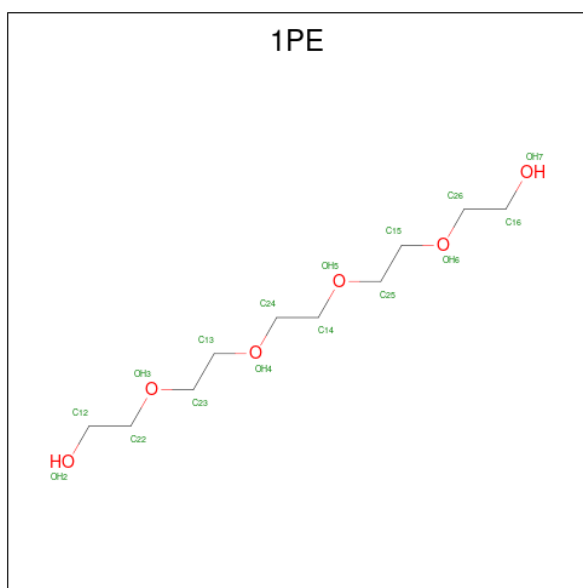
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



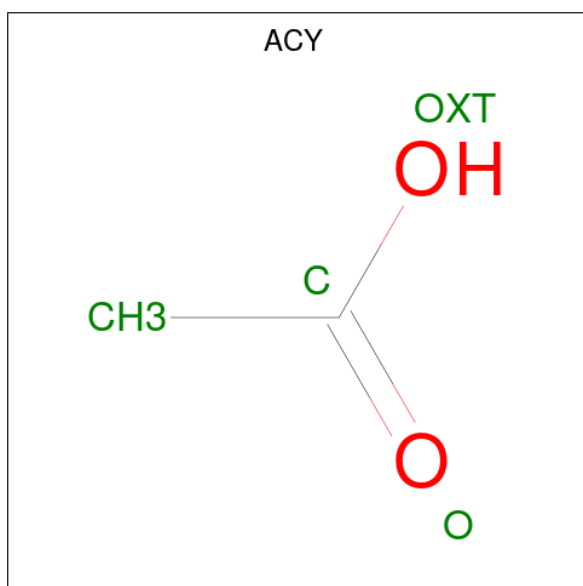
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



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

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



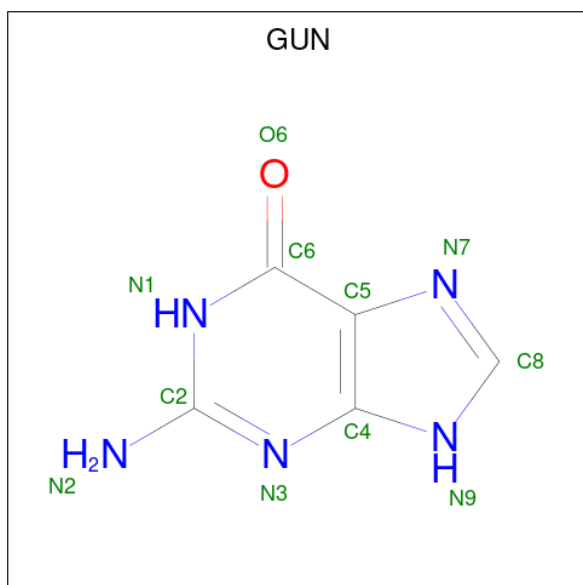
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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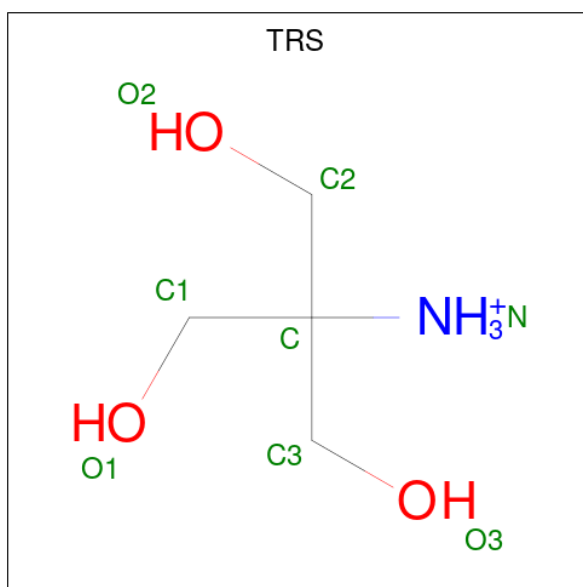
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



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 (CCD ID: 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	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	2	Total	O	0	0
			2	2		
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	5	Total	O	0	0
			5	5		
69	AL	7	Total	O	0	0
			7	7		
69	AM	4	Total	O	0	0
			4	4		
69	AN	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	1	Total 1	O 1	0	0
69	AP	1	Total 1	O 1	0	0
69	AQ	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	4	Total 4	O 4	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	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	3	Total 3	O 3	0	0
69	BN	1	Total 1	O 1	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	4	Total 4	O 4	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	5	Total 5	O 5	0	0
69	D1	37	Total 37	O 37	0	0
69	D2	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	30	Total 30	O 30	0	0
69	D4	40	Total 40	O 40	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	11	Total 11	O 11	0	0
69	CD	4	Total 4	O 4	0	0
69	CA	696	Total 696	O 696	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	97	Total 97	O 97	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	54	Total 54	O 54	0	0
69	DF	13	Total 13	O 13	0	0
69	DG	9	Total 9	O 9	0	0

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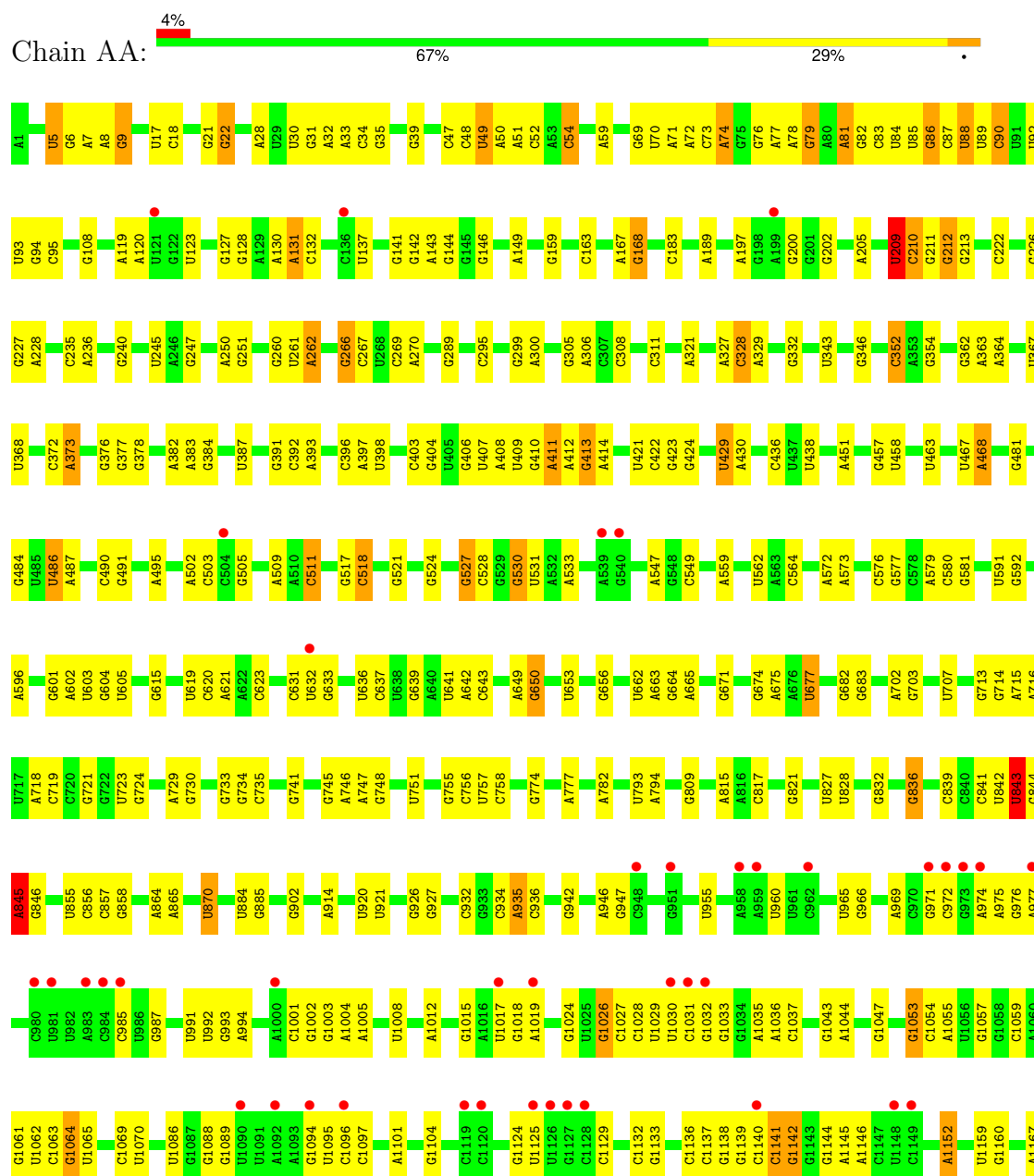
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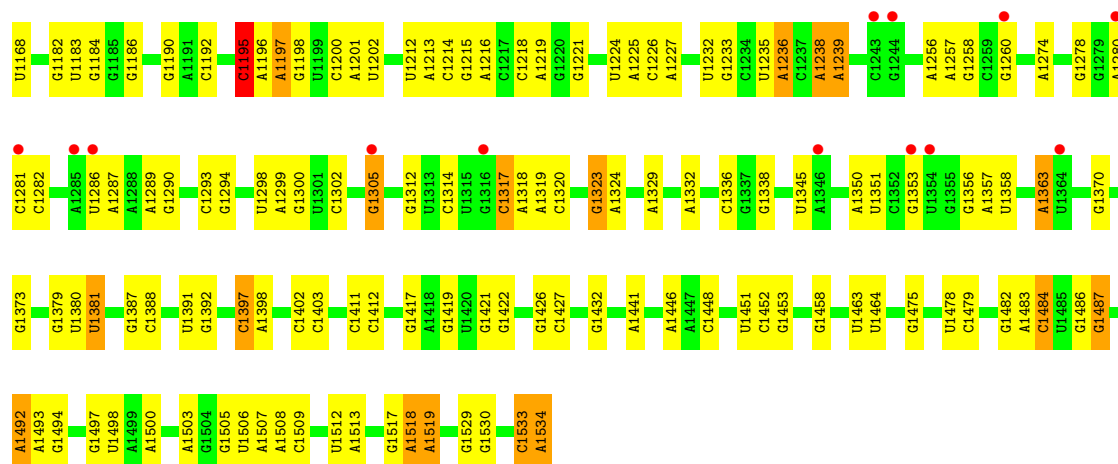
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DH	2	Total 2	O 2	0	0
69	DK	61	Total 61	O 61	0	0
69	DL	50	Total 50	O 50	0	0
69	DM	60	Total 60	O 60	0	0
69	DN	81	Total 81	O 81	0	0
69	DO	42	Total 42	O 42	0	0
69	DP	42	Total 42	O 42	0	0
69	DQ	32	Total 32	O 32	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	52	Total 52	O 52	0	0
69	DT	65	Total 65	O 65	0	0
69	DU	24	Total 24	O 24	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	33	Total 33	O 33	0	0
69	DX	33	Total 33	O 33	0	0
69	DY	11	Total 11	O 11	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	203	Total 203	O 203	0	0
69	DA	4824	Total 4824	O 4824	0	0

3 Residue-property plots

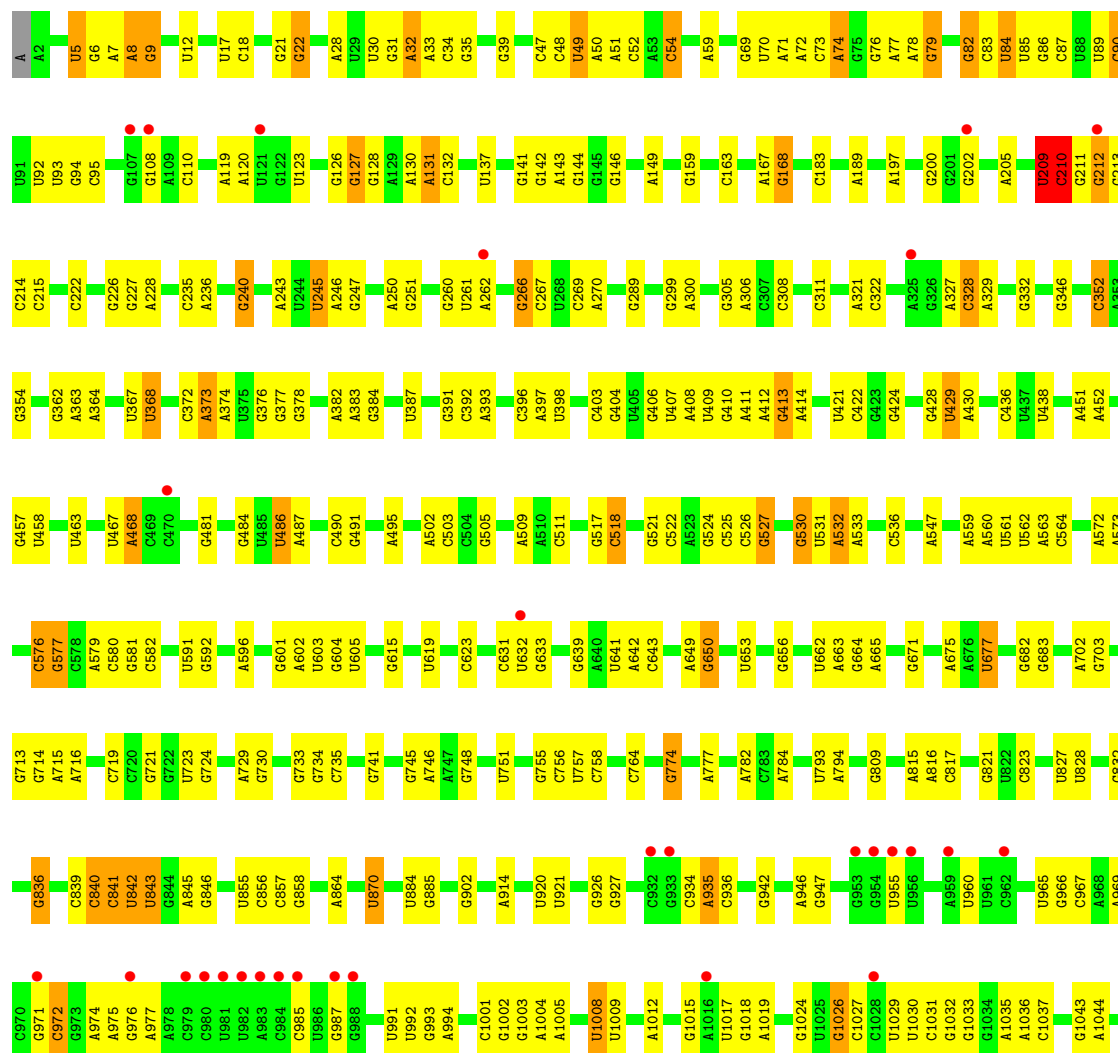
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

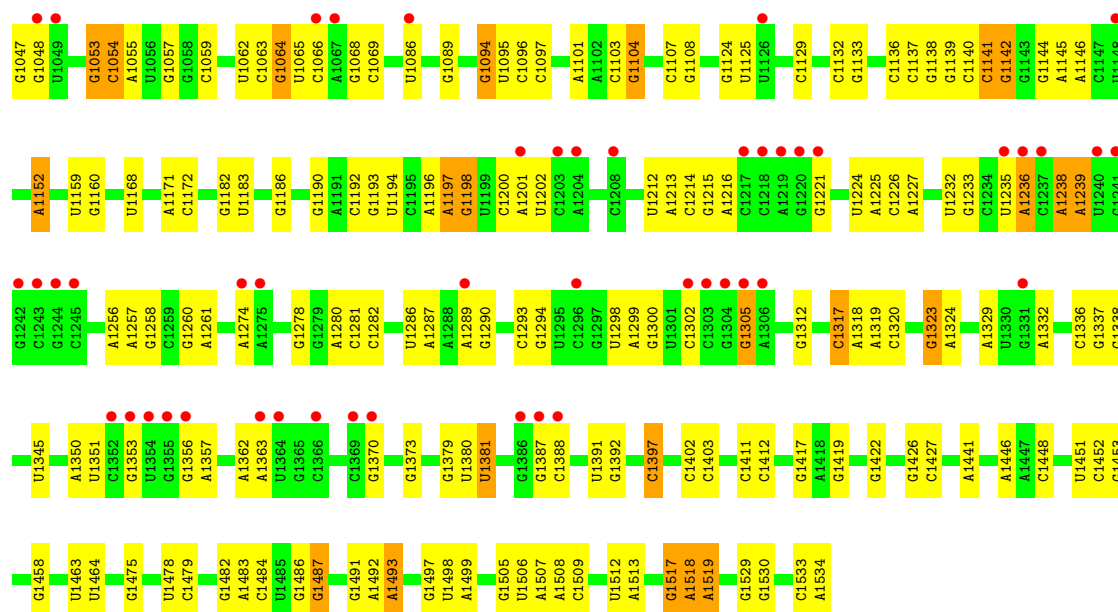
• Molecule 1: 16S rRNA



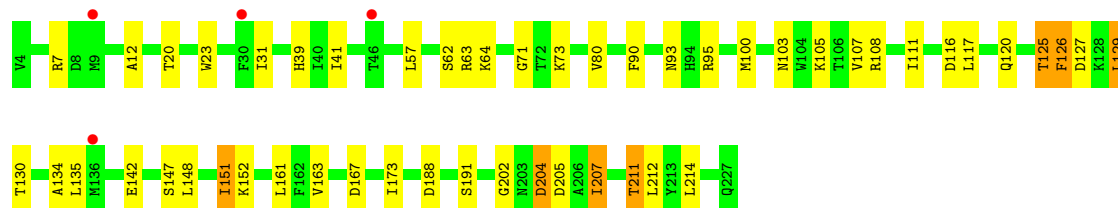
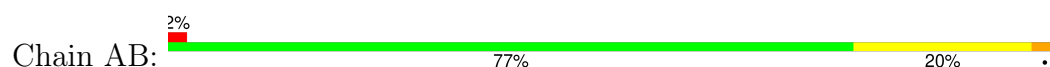


• Molecule 1: 16S rRNA

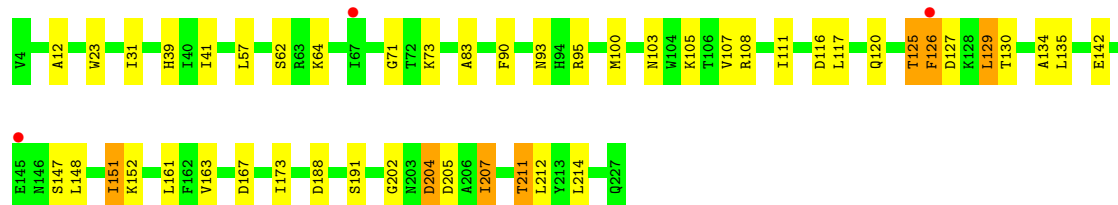
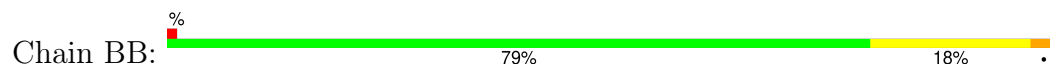




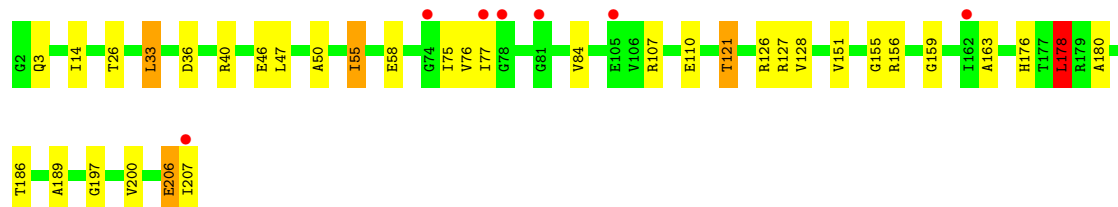
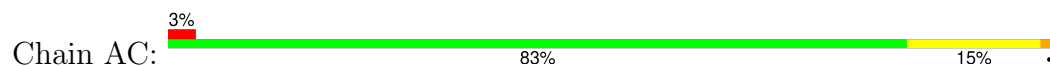
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



- Chain BC:
-
- | Category | Percentage |
|----------|------------|
| Green | 10% |
| Yellow | 82% |
| Red | 14% |
-
-
- | Category | Percentage |
|----------|------------|
| Green | 10% |
| Yellow | 82% |
| Red | 14% |
-

- Chain AD:
-
- | Category | Percentage |
|----------|------------|
| A2 | 80% |
| R3 | 80% |
| Y4 | 80% |
| L9 | 80% |
| K10 | 80% |
| L11 | 80% |
| K22 | 80% |
| S23 | 80% |
| G24 | 80% |
| V25 | 80% |
| R26 | 80% |
| A27 | 80% |
| T30 | 80% |
| R44 | 80% |
| Q64 | 80% |
| K68 | 80% |
| T64 | 80% |
| R73 | 80% |
| E88 | 80% |
| D99 | 80% |
| V102 | 80% |
| M105 | 80% |
| G106 | 80% |
| F107 | 80% |
| Q116 | 80% |
| K121 | 80% |
| V129 | 80% |
| V130 | 80% |
| N131 | 80% |
| I132 | 80% |
| P139 | 80% |
| V142 | 80% |
| V143 | 80% |
| S144 | 80% |
| I145 | 80% |
| R146 | 80% |
| E147 | 80% |
| K150 | 80% |
| R154 | 80% |
| T160 | 80% |

- Chain BD:
-
- | Category | Percentage |
|----------|------------|
| A2 | 79% |
| L9 | |
| K22 | |
| S23 | |
| G24 | |
| V25 | |
| R26 | |
| A27 | |
| T30 | |
| R47 | |
| K58 | |
| N65 | |
| E88 | |
| D99 | |
| V102 | |
| M105 | |
| G106 | |
| F107 | |
| Q116 | |
| V130 | |
| N131 | |
| I132 | |
| P139 | |
| V142 | |
| V143 | |
| S144 | |
| I145 | |
| R146 | |
| E147 | |
| K150 | |
| K151 | |
| R154 | |
| E160 | |
| T169 | |
| W170 | |
| L171 | |
| A175 | |
| P186 | |
| E187 | |
| B189 | |
| S189 | |
| S192 | |
| A193 | |
| D194 | |
| I195 | |
| E197 | |
| I200 | |
| K206 | |

- Chain AE:
-
- 70% 25% 5%
- E10 E13 K14 L15 I16 A17 V18 K26 G27 V38 V39 G40 D41 V46 E55 V56 P57 I60 R69 N70 L76 N77 N78 G79 T80 L81 Q82 V88 H89 T90 G91 S92 R93 V94 Q97 E101 I106 A107 G108 G109 V114 V120 H121 N122 V123 I124
- A125 K126 N132 P133 I134 V137 T140 L144 N148 S149 K159 E162 I163 I164

- Chain BE:
-
- | Node | Color |
|------|--------|
| E10 | Green |
| E13 | Green |
| K14 | Green |
| L15 | Green |
| V18 | Green |
| K23 | Green |
| T24 | Green |
| V25 | Green |
| K26 | Green |
| G27 | Green |
| I30 | Green |
| V39 | Green |
| G40 | Green |
| D41 | Green |
| V46 | Green |
| G47 | Green |
| E55 | Green |
| V56 | Green |
| P57 | Green |
| I60 | Green |
| E65 | Green |
| R69 | Green |
| N70 | Green |
| M71 | Green |
| L76 | Green |
| L81 | Green |
| Q82 | Yellow |
| V83 | Yellow |
| H89 | Yellow |
| T90 | Yellow |
| G91 | Yellow |
| S92 | Yellow |
| R93 | Yellow |
| V94 | Yellow |
| F95 | Yellow |
| H96 | Yellow |
| Q97 | Yellow |
| A99 | Yellow |
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| I105 | Yellow |
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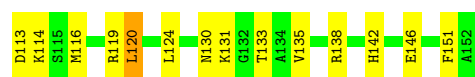
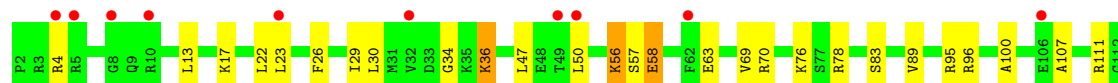
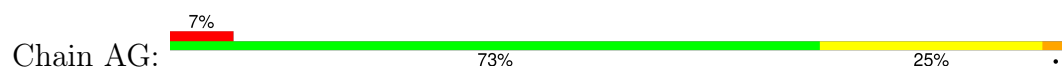
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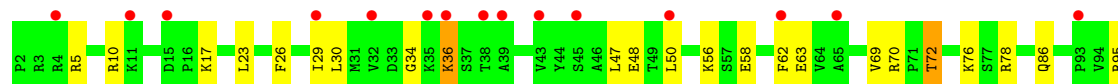
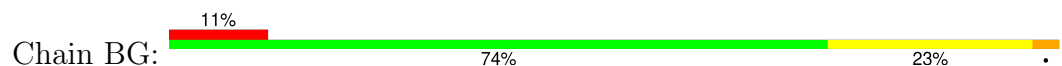
- Molecule 6: 30S ribosomal protein S6



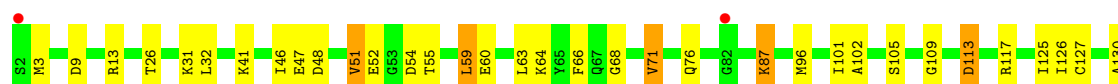
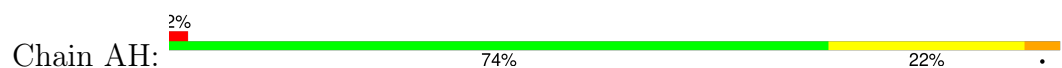
- Molecule 7: 30S ribosomal protein S7



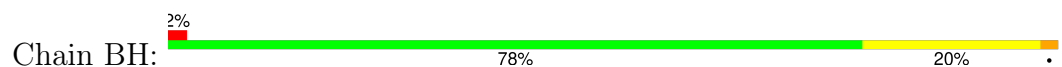
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

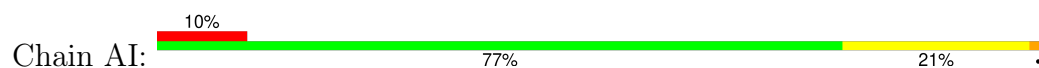


- Molecule 8: 30S ribosomal protein S8

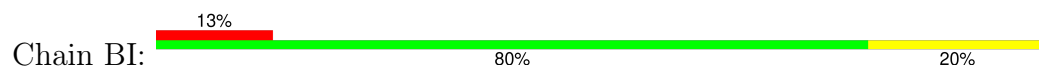




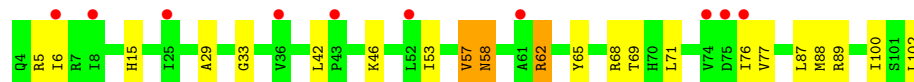
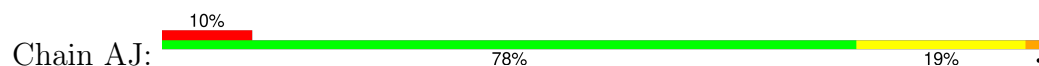
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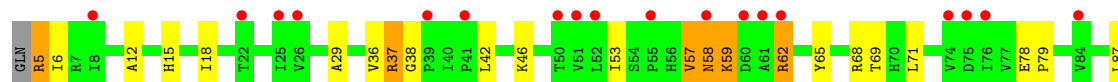
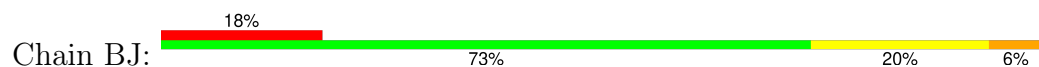
- Molecule 9: 30S ribosomal protein S9



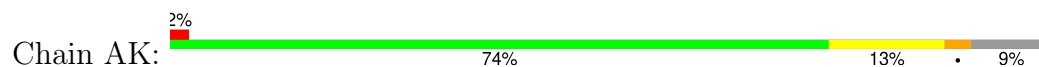
- Molecule 10: 30S ribosomal protein S10



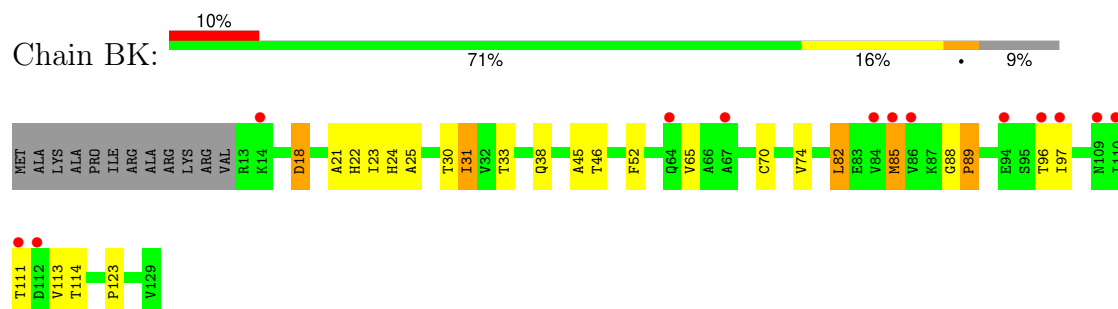
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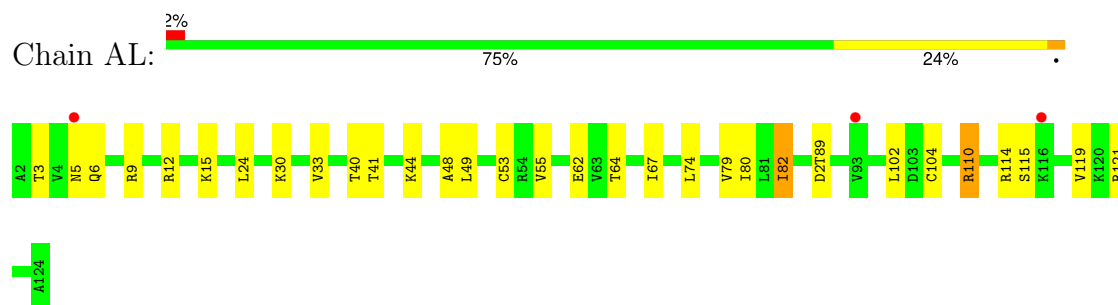
- Molecule 11: 30S ribosomal protein S11



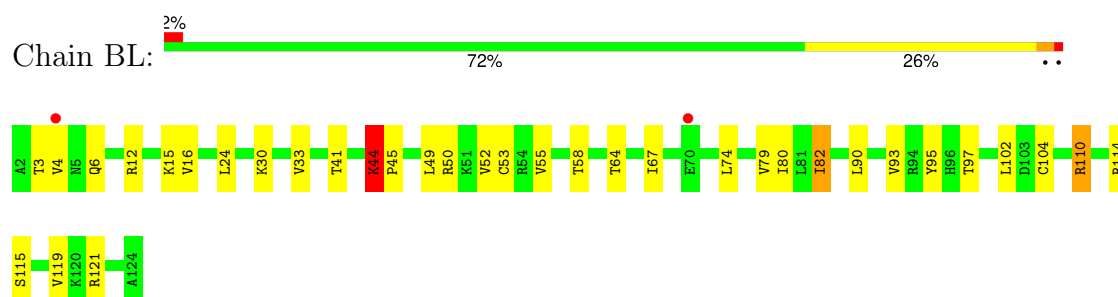
- Molecule 11: 30S ribosomal protein S11



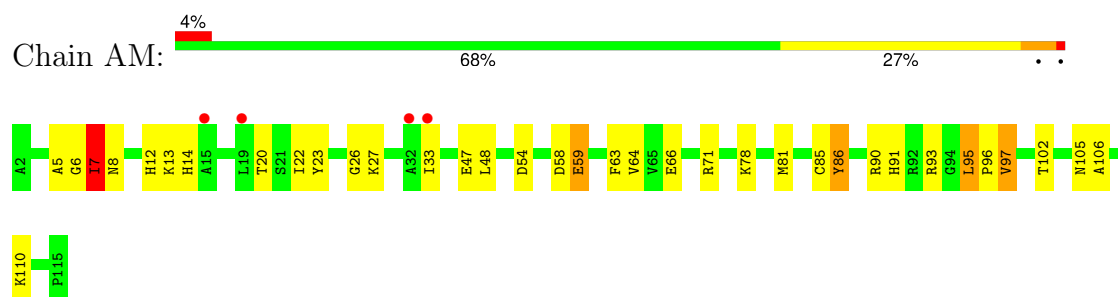
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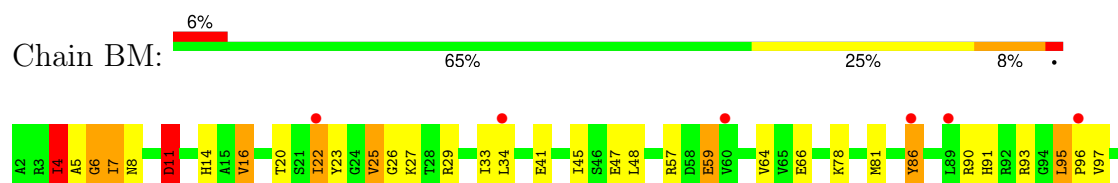
- Molecule 12: 30S ribosomal protein S12

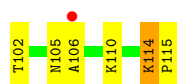


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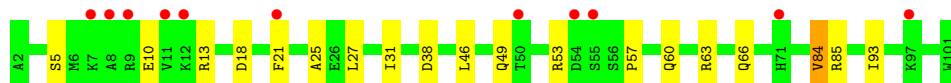
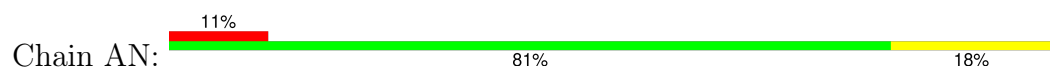


- Molecule 13: 30S ribosomal protein S13

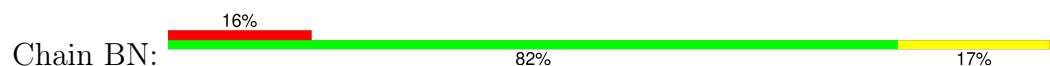




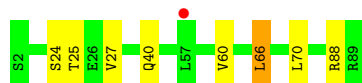
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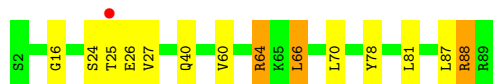
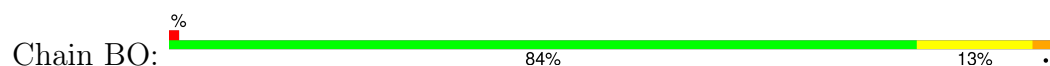
- Molecule 14: 30S ribosomal protein S14



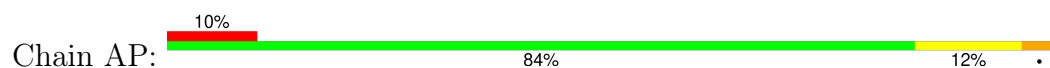
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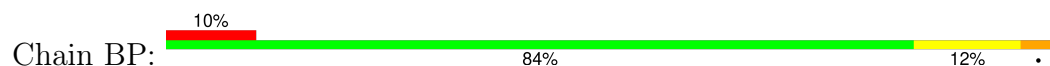
- Molecule 15: 30S ribosomal protein S15



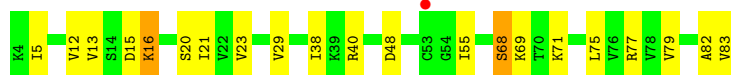
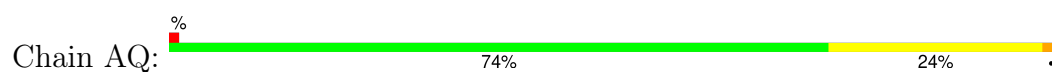
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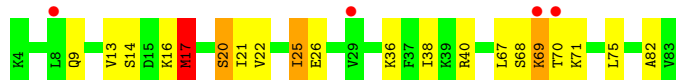
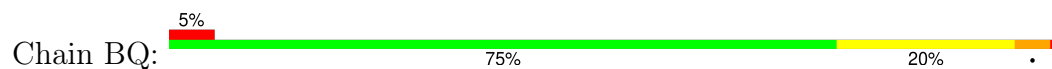
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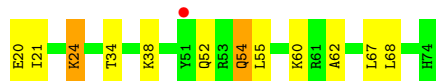
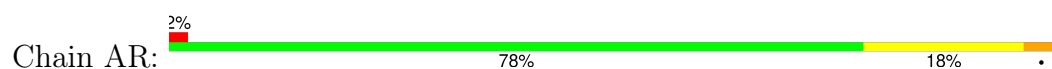
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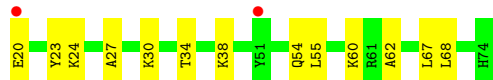
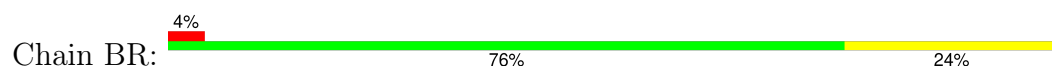
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



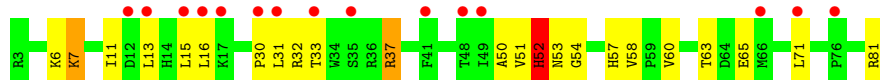
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



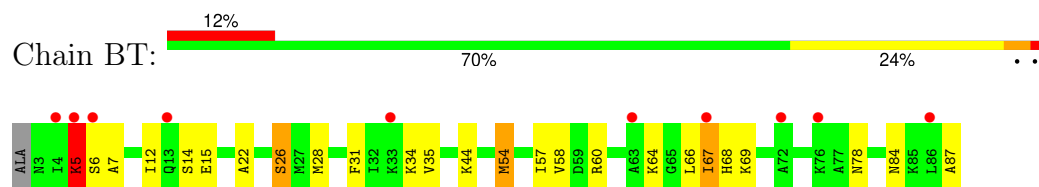
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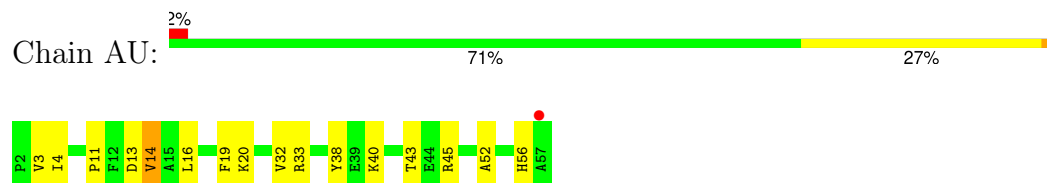
- Molecule 20: 30S ribosomal protein S20



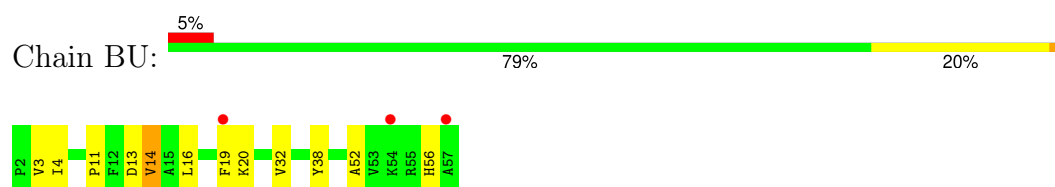
● Molecule 20: 30S ribosomal protein S20



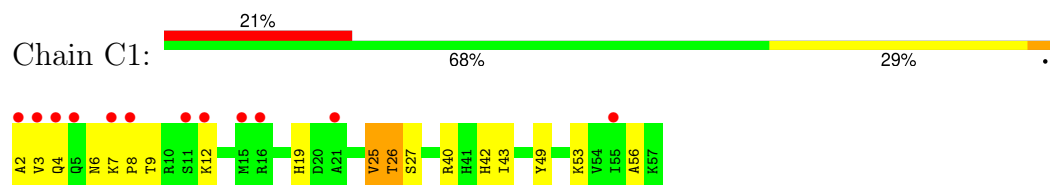
● Molecule 21: 30S ribosomal protein S21



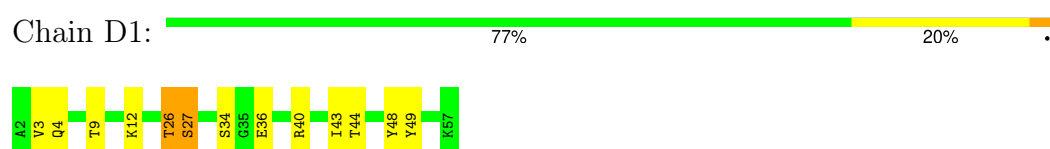
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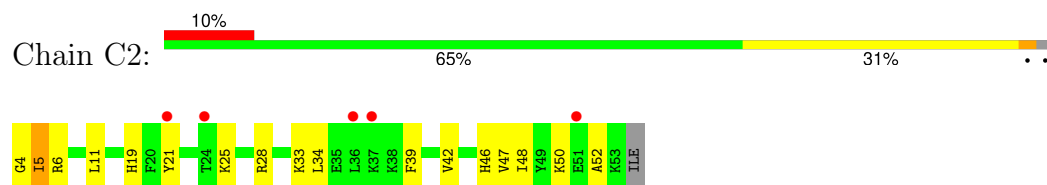
● Molecule 22: 50S ribosomal protein L32



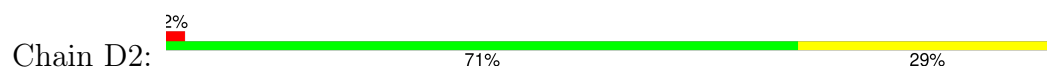
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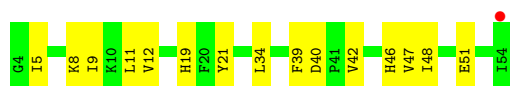


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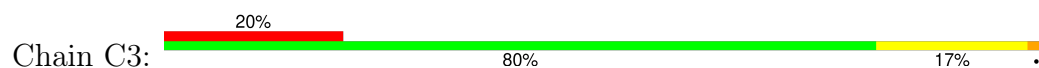


● Molecule 23: 50S ribosomal protein L33

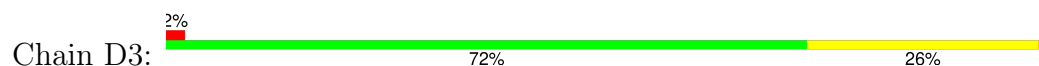




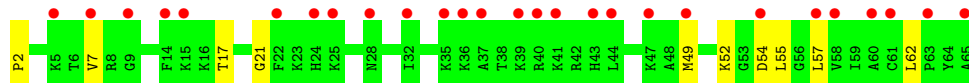
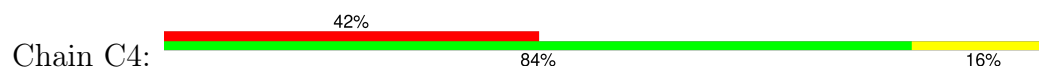
- Molecule 24: 50S ribosomal protein L34



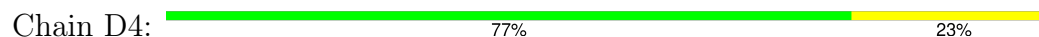
- Molecule 24: 50S ribosomal protein L34



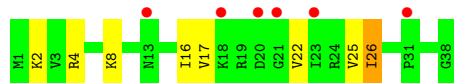
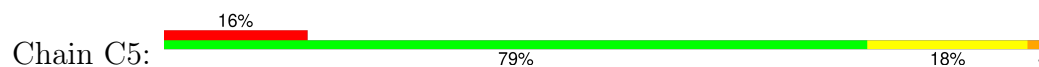
- Molecule 25: 50S ribosomal protein L35



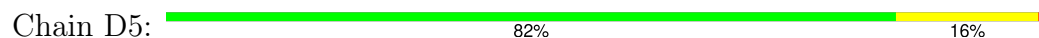
- Molecule 25: 50S ribosomal protein L35



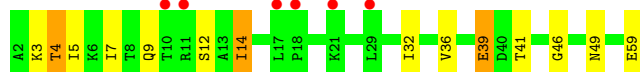
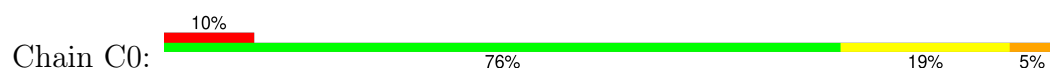
- Molecule 26: 50S ribosomal protein L36



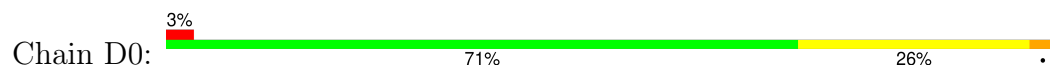
- Molecule 26: 50S ribosomal protein L36



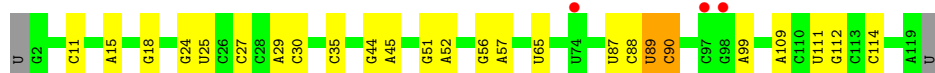
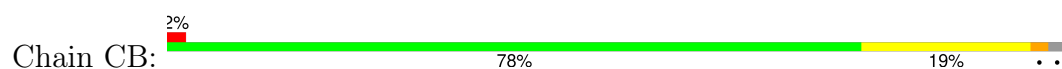
- Molecule 27: 50S ribosomal protein L30



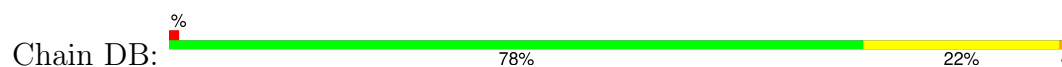
- Molecule 27: 50S ribosomal protein L30



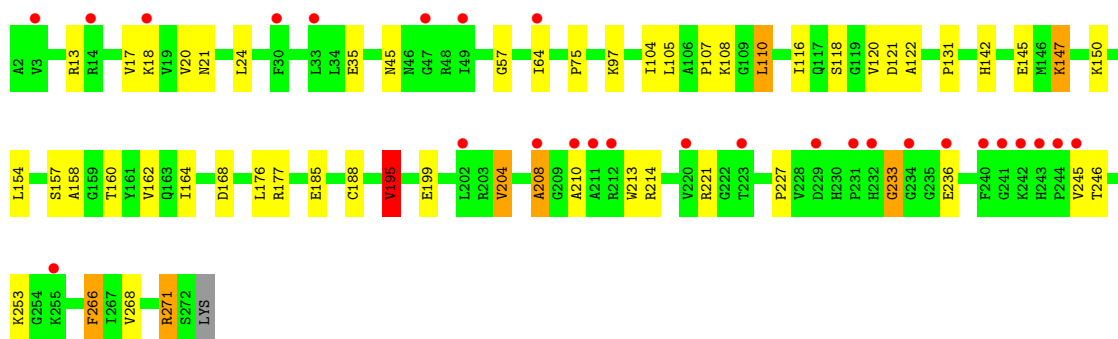
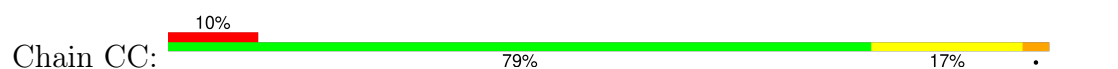
- Molecule 28: 5S rRNA



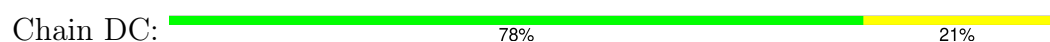
- Molecule 28: 5S rRNA



- Molecule 29: 50S ribosomal protein L2

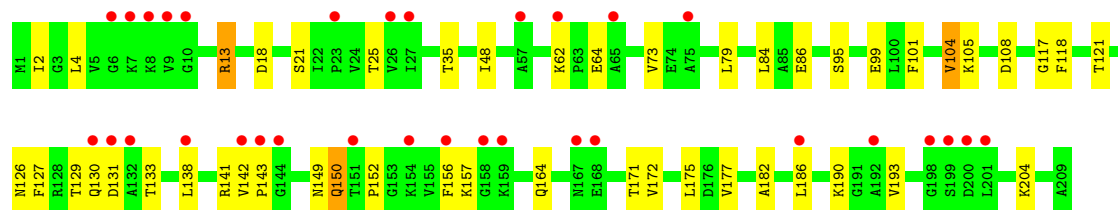
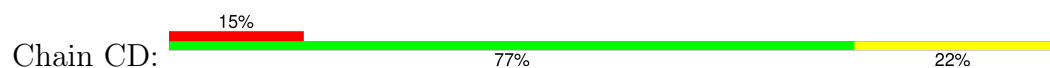


- Molecule 29: 50S ribosomal protein L2

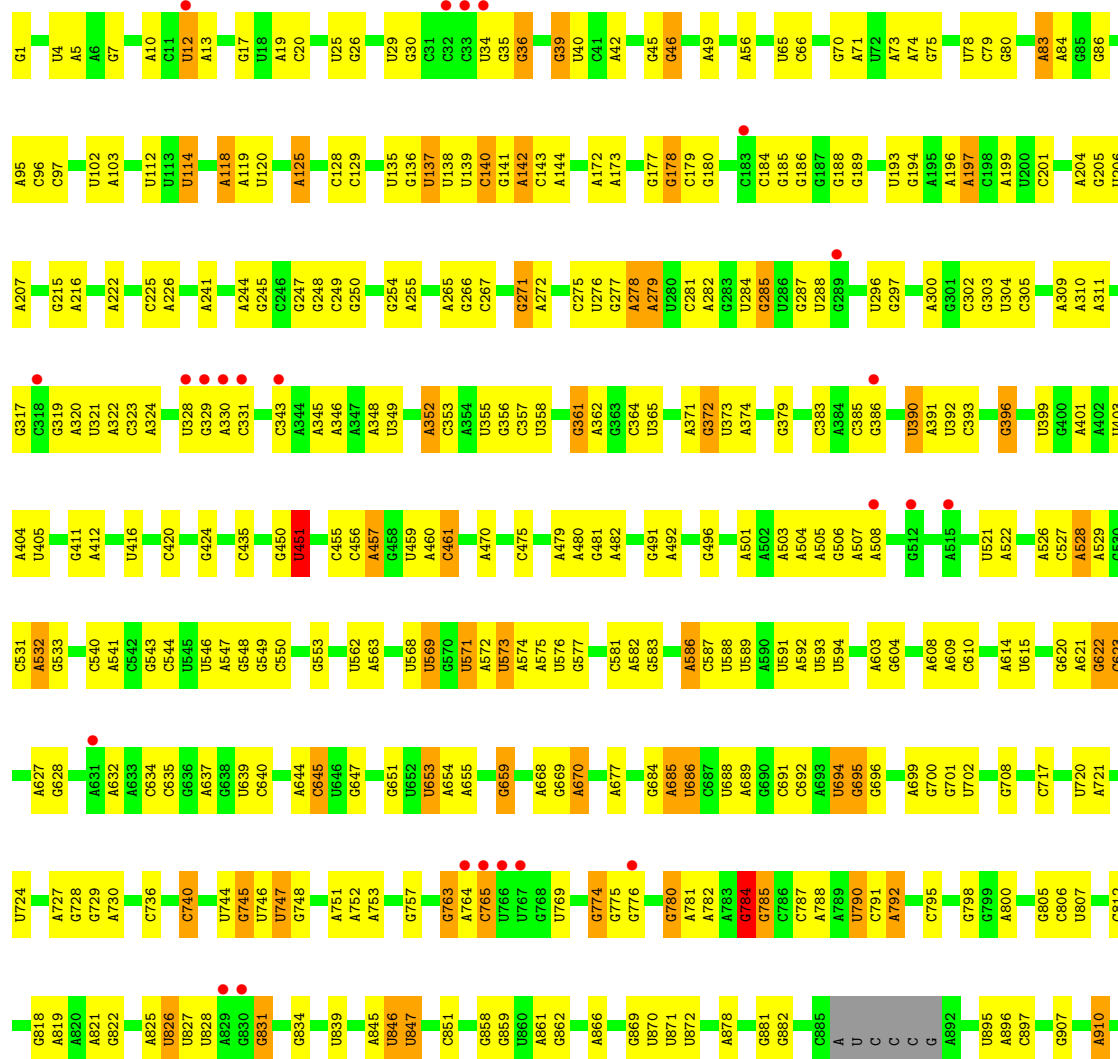




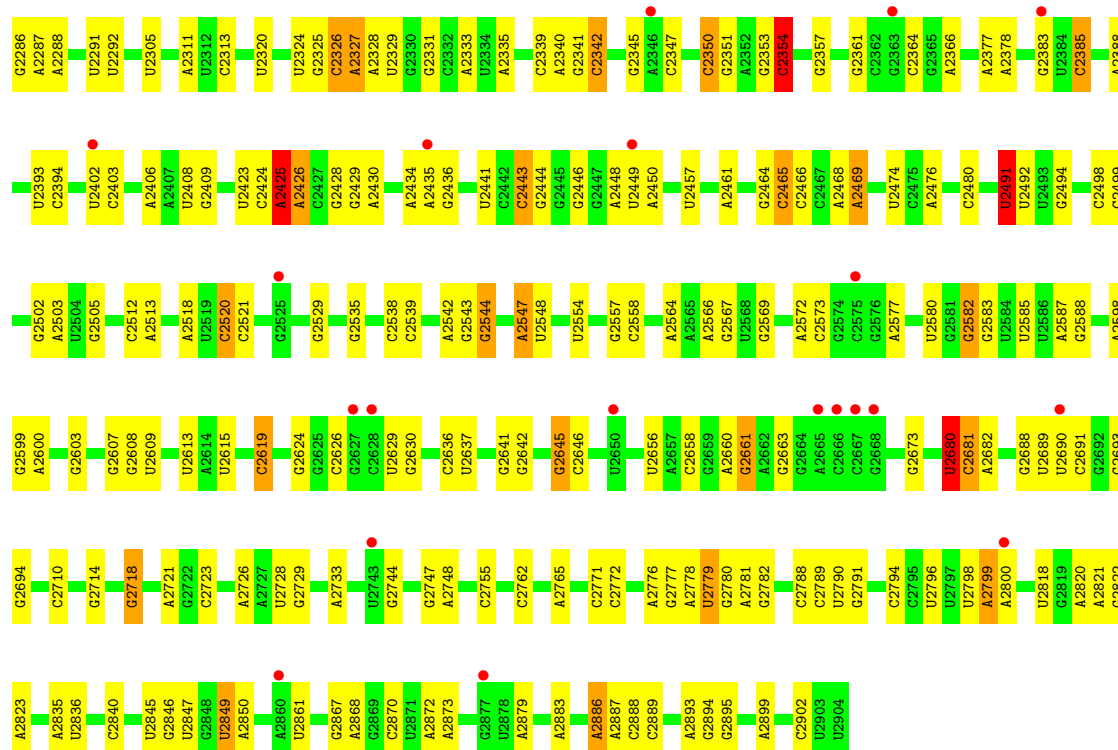
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 23S rRNA



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U2182	G2102	A2015	A1913	A1786	C1675	C1557	U1438	C1330	A1237	C1121	G1024	G914
A2183	C2103	U2016	C1914	C1787	C1676	U1562	G1441	G1332	G1238	G1122	G1025	G930
G2184	C2104	C2020	A1915	C1788	A1677	U1563	U1442	G1331	A1244	G1125	G1026	U931
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G2186	G2106	C2022	A1919	C1790	C1684	C1565	U1444	U1344	G1248	A1129	A1028	C935
G2107	G2107	U2022	A1919	A1791	C1684	A1566	C1447	U1352	G1249	G1132	G1031	A936
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G2109	G2110	G2024	G1929	G1797	G1699	A1569	G1452	A1354	G1251	A1133	U1033	G942
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G2112	G2112	U2028	U1931	A1801	G1703	U1578	U1458	A1359	G1256	G1136	G1045	C944
U2113	U2113	G2029	A1932	A1802	G1703	U1578	G1458	A1359	G1256	G1136	G1045	A945
A2114	G2115	A2030	G1935	A1808	G1707	U1583	U1460	A1365	G1259	U1141	A1046	C946
G2116	G2116	A2031	C1934	A1809	C1708	U1584	U1460	A1365	G1259	U1141	A1046	A946
A2117	A2117	G2032	G1935	A1809	C1708	U1584	U1460	A1365	G1259	U1141	A1046	A946
G2207	G2207	A2033	A1936	A1810	U1709	U1585	G1478	A1377	A1260	A1142	G1047	
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G2119	A2119	G2035	A1938	U1812	G1715	A1591	G1483	U1376	A1262	A1151	G1056	U955
G2120	G2120	C2036	U1939	G1813	G1715	A1603	U1484	C1376	U1263	C1152	U1061	C957
			U1940	A1814	U1720	A1607	U1485	G1377	A1264	A1155	U1062	U958
G2123	G2123	G2040	U1943	C1815	G1721	C1607	U1486	A1378	G1266			
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G2127	G2046	C2046	C1962	A1819	C1728	C1612	G1492	G1382	U1274	G1169	G1068	C964
G2128	U2047	G2047	U1963	U1820	G1729	A1616	A1493	A1384	A1275	C1170	A1069	A973
U2131	G2048	G2048	G1964	A1822	C1730	A1616	A1494	A1385	G1280	G1171	A1070	
G2132	G2049	C2049	C1965	G1823	G1738	C1617	A1495	C1386	G1281	C1172	G1071	G974
G2133	G2050	C2050	A1966	U1824	A1744	A1618	U1497	C1386	U1282			
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G2141	G2055	C2055	U1970	G1826	A1744	A1618	U1497	U1395	G1289	U1176	A1073	
A2142	G2056	G2056	U1971	U1827	G1750	G1627	A1504	U1396	C1290	G1177	U1083	A983
C2145	G1972	G1972	U1972	A1829	U1751	U1629	A1509	U1397	U1294	C1178	A1084	A984
A2146	G1973	G1973	U1973	C1833	A1754	G1633	G1511	C1398	U1297	G1179	A1085	C985
G2147	C1974	G1974	U1974	U1834	U1758	A1634	G1514	G1401	C1297	U1180	A1086	C986
G2148	U2149	G1975	U1975	C1837	A1759	U1636	A1515	U1402	G1298	U1181	G1087	C987
C2150	U1979	U1979	U1979	C1838	C1760	U1637	A1522	A1403	G1299	G1182	A1088	A988
G2157	C2064	C2064	U1979	G1839	C1761	C1638	A1523	U1405	G1300	G1186	A1089	C995
A2158	C2065	C2065	G1984	U1847	C1764	C1639	U1523	U1406	A1301	G1190	A1090	A996
G2159	G2067	U2068	C1985	A1847	C1764	A1640	G1529	U1416	C1306	A1194	G1093	G997
C2160	U2069	G2069	C1986	G1869	G1770	A1641	G1529	C1417	A1307	U1203	U1097	C998
G2161	A2070	A2070	U1991	C1870	A1773	G1642	A1532	C1417	A1308	U1203	A1098	U999
A2162	A2071	A2071	G1992	A1871	C1774	U1647	U1533	A1420	G1309	U1204	G1099	C1006
C2164	C2072	C2072	U1993	A1872	U1775	U1648	U1534	A1420	G1310	A1205	U1101	
C2165	G2078	G2078	C1994	G1873	U1775	U1649	A1535	G1424	G1311	G1212	A1103	A1009
A2171	U2092	U2092	C1997	U1882	G1776	C1656	C1536	A1427	U1312	A1213	A1103	U1012
G2172	G2093	G2093	A1998	U1882	U1777	U1657	G1537	C1428	U1313	A1214	C1104	C1013
A2173	C2093	C2093	C1999	A1900	U1778	C1658	A1544	G1429	C1314	U1105	U1105	U1013
C2174	A2094	A2094	C2000	A1901	U1779	C1658	A1544	G1429	A1321	G1215	G1106	G1017
G2178	C2096	A2096	C2006	C1902	U1781	G1683	C1547	G1430	A1321	G1215	A1111	A1020
C2179	G2100	G2100	U2007	G1903	U1782	A1664	U1554	A1431	G1324	U1231	G1112	A1021
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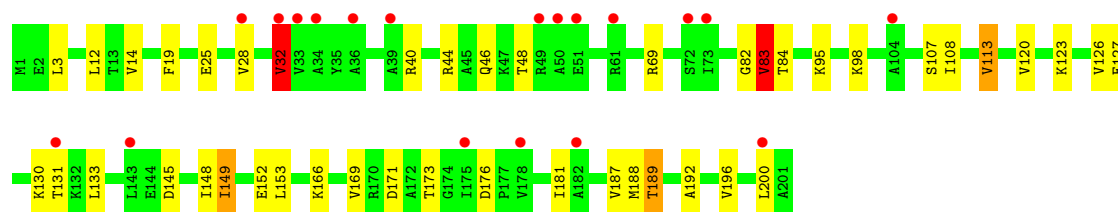
• Molecule 32: 50S ribosomal protein L3

Chain DD: 77% 22% .



• Molecule 33: 50S ribosomal protein L4

Chain CE: 9% 78% 19% ..



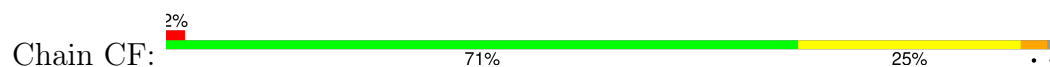
• Molecule 33: 50S ribosomal protein L4

Chain DE: 79% 19% .

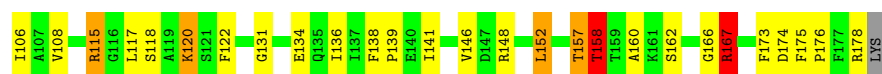




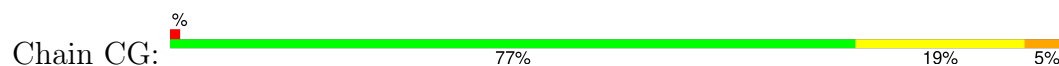
- Molecule 34: 50S ribosomal protein L5



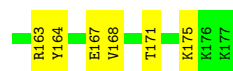
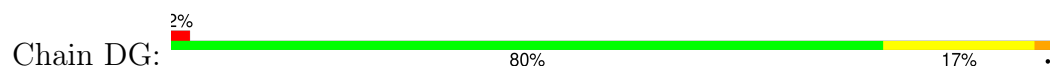
- Molecule 34: 50S ribosomal protein L5



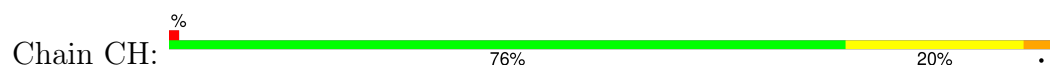
- Molecule 35: 50S ribosomal protein L6

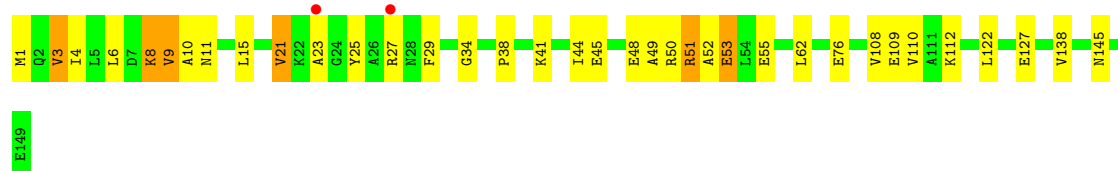


- Molecule 35: 50S ribosomal protein L6

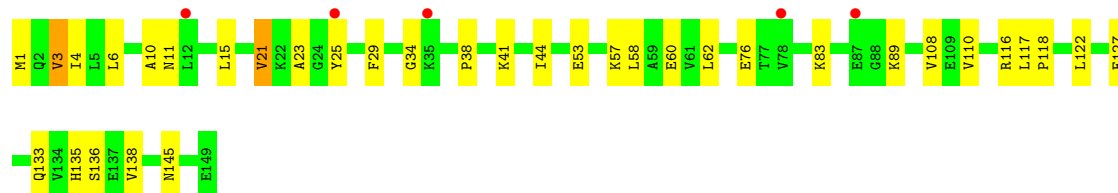


- Molecule 36: 50S ribosomal protein L9

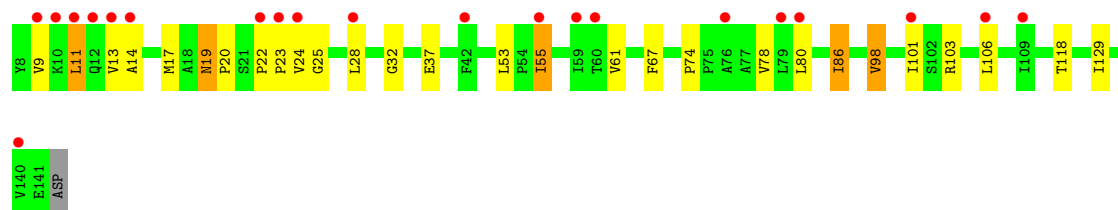
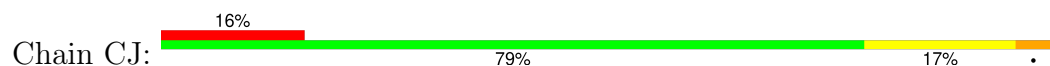




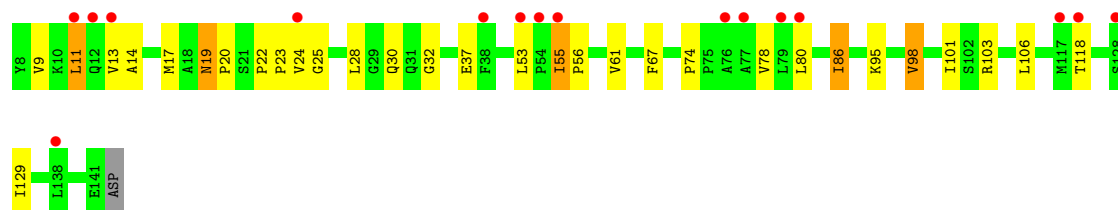
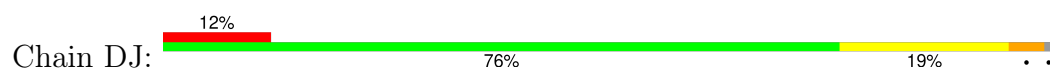
- Molecule 36: 50S ribosomal protein L9



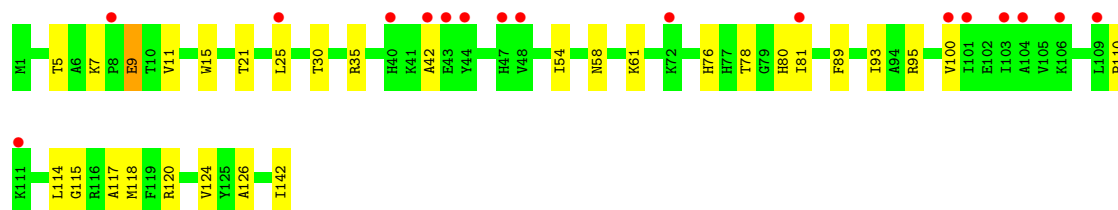
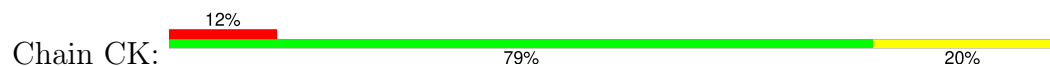
- Molecule 37: 50S ribosomal protein L11



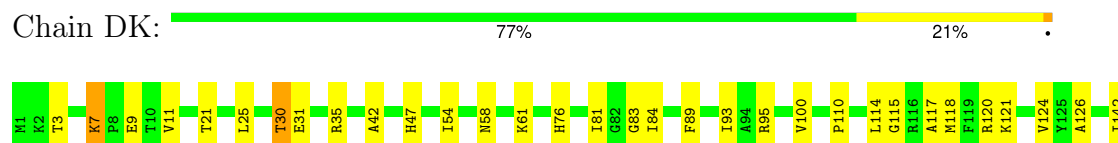
- Molecule 37: 50S ribosomal protein L11



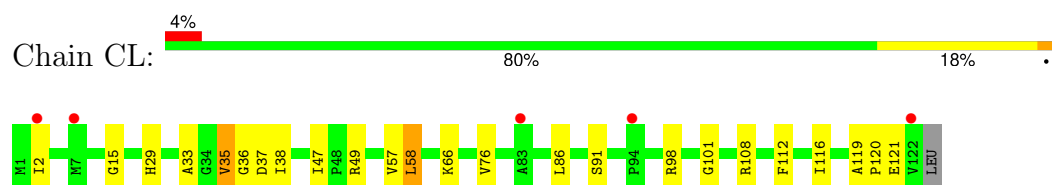
- Molecule 38: 50S ribosomal protein L13



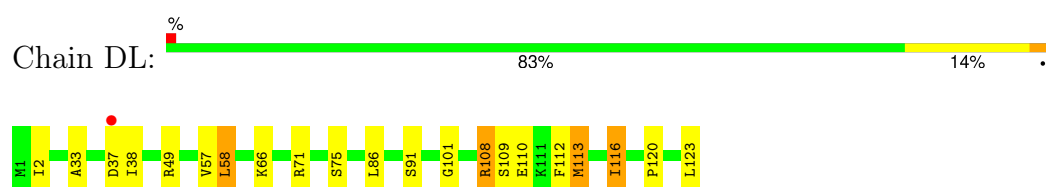
- Molecule 38: 50S ribosomal protein L13



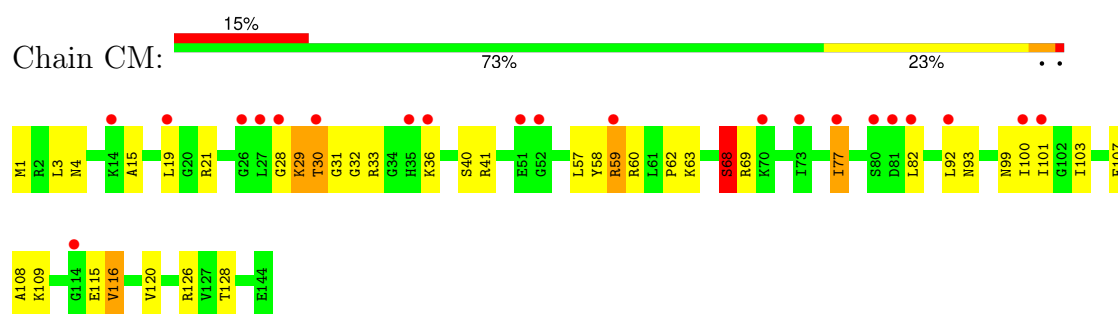
- Molecule 39: 50S ribosomal protein L14



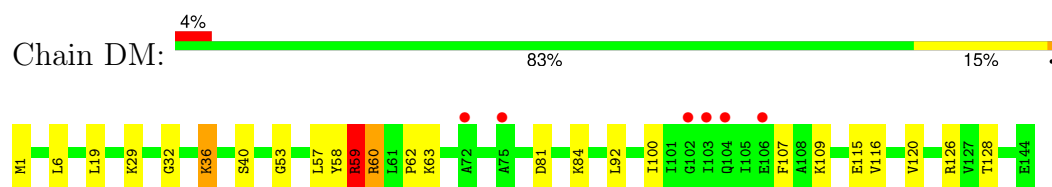
- Molecule 39: 50S ribosomal protein L14



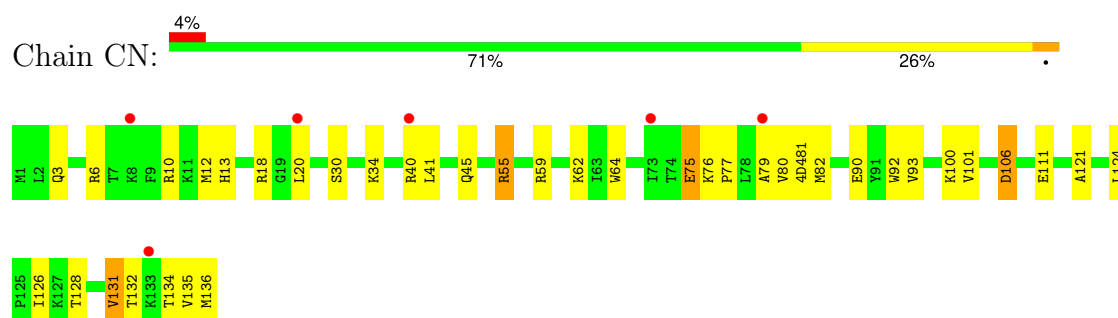
- Molecule 40: 50S ribosomal protein L15



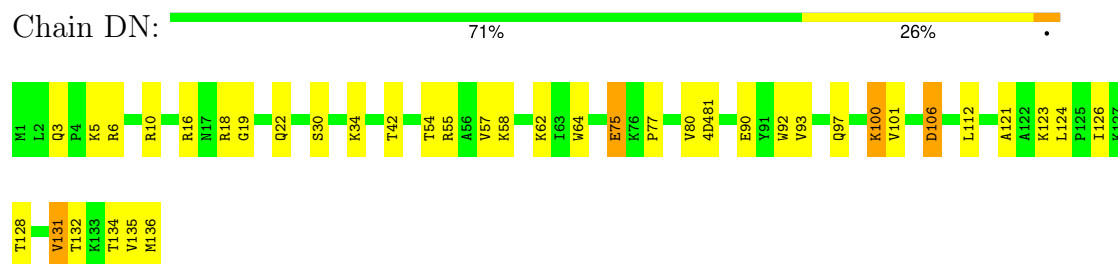
- Molecule 40: 50S ribosomal protein L15



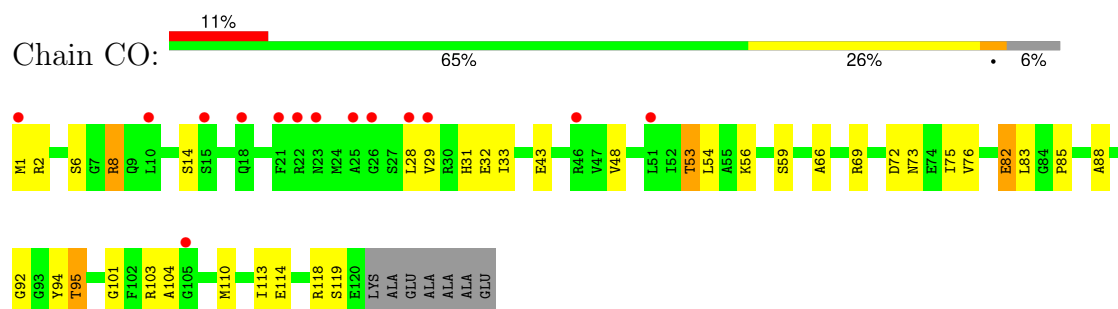
- Molecule 41: 50S ribosomal protein L16



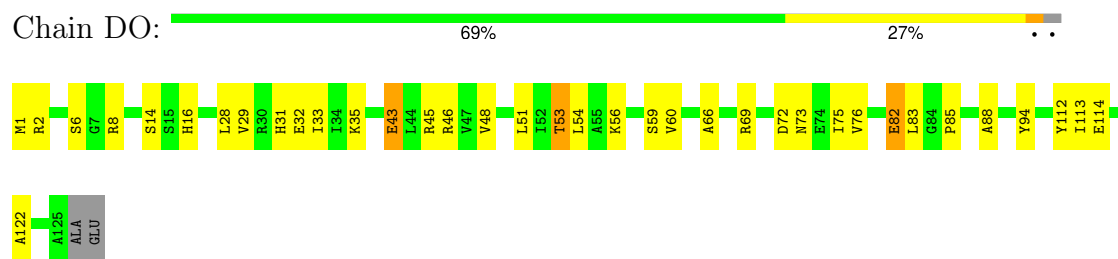
- Molecule 41: 50S ribosomal protein L16



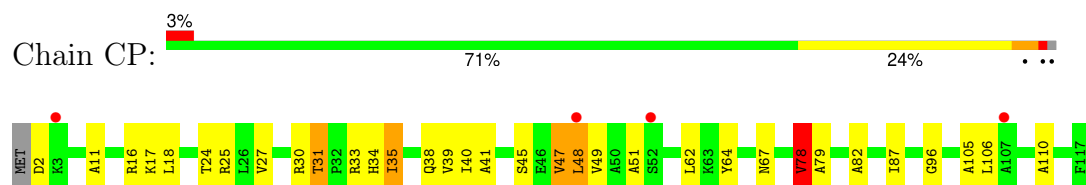
- Molecule 42: 50S ribosomal protein L17



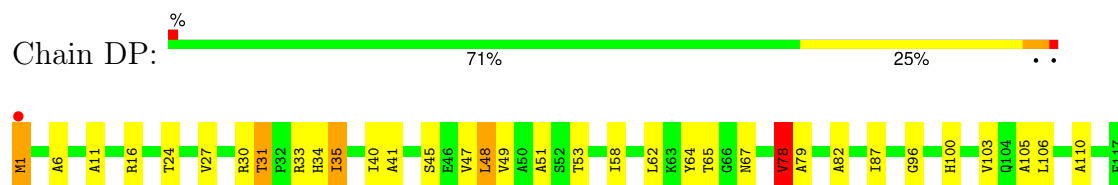
- Molecule 42: 50S ribosomal protein L17



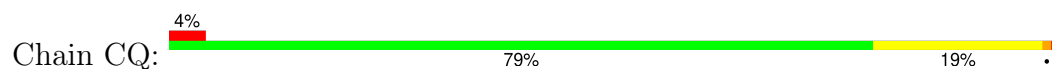
- Molecule 43: 50S ribosomal protein L18



- Molecule 43: 50S ribosomal protein L18

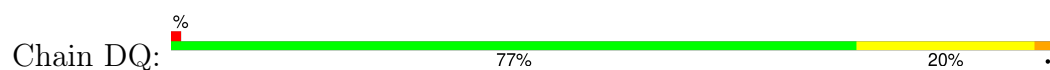


- Molecule 44: 50S ribosomal protein L19

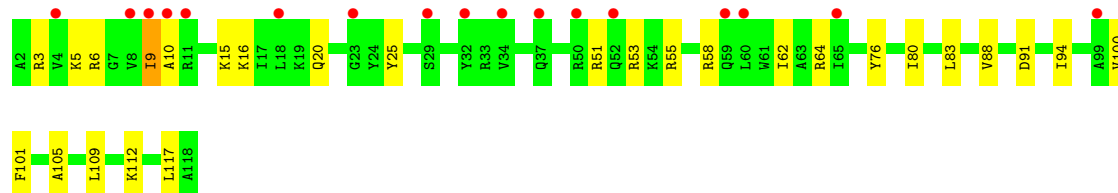
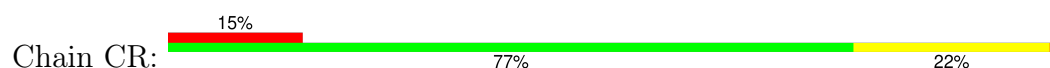




- Molecule 44: 50S ribosomal protein L19



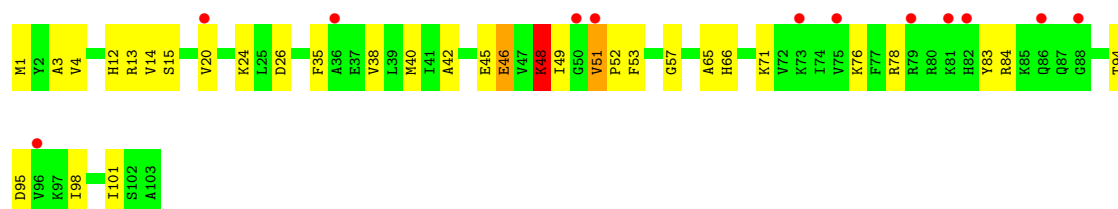
- Molecule 45: 50S ribosomal protein L20



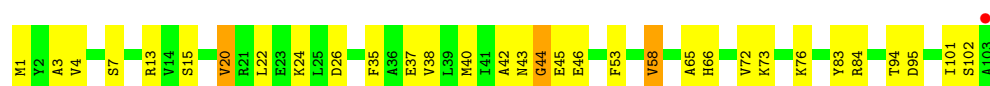
- Molecule 45: 50S ribosomal protein L20



- Molecule 46: 50S ribosomal protein L21

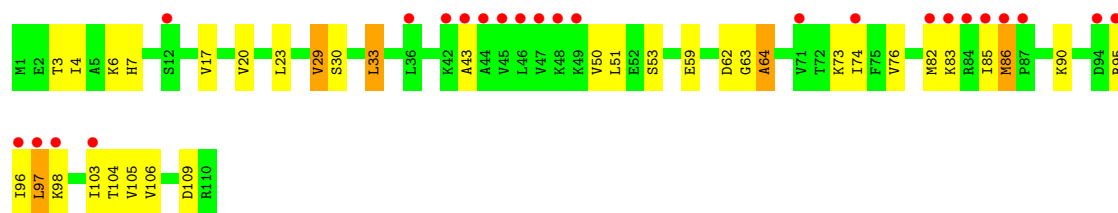


- Molecule 46: 50S ribosomal protein L21

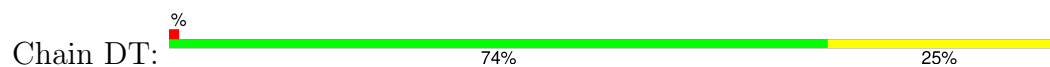


- Molecule 47: 50S ribosomal protein L22

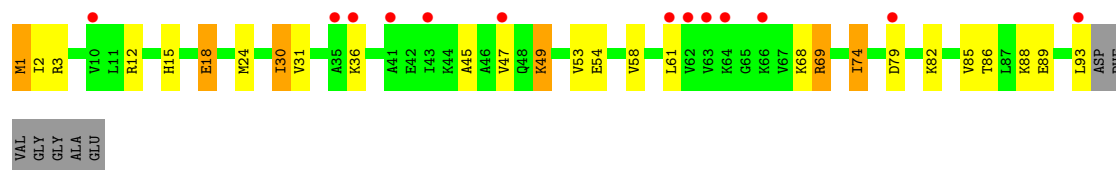




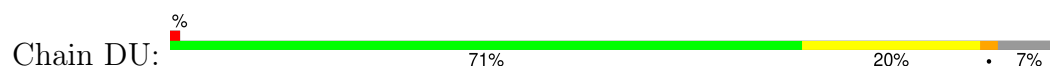
- Molecule 47: 50S ribosomal protein L22



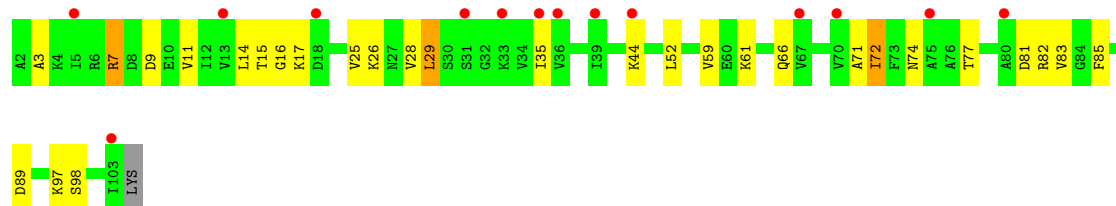
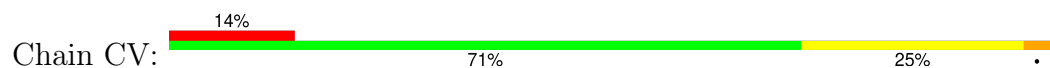
- Molecule 48: 50S ribosomal protein L23



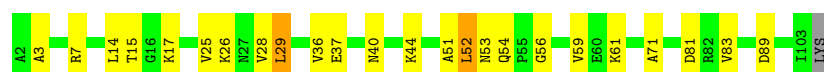
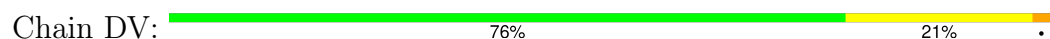
- Molecule 48: 50S ribosomal protein L23



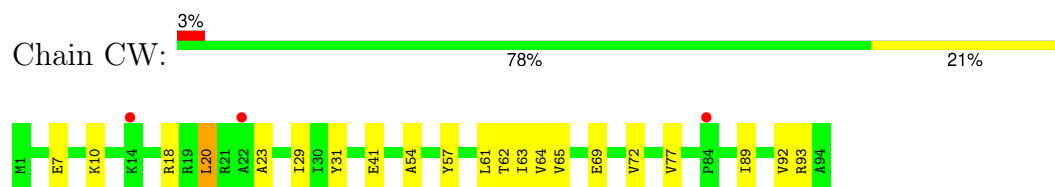
- Molecule 49: 50S ribosomal protein L24



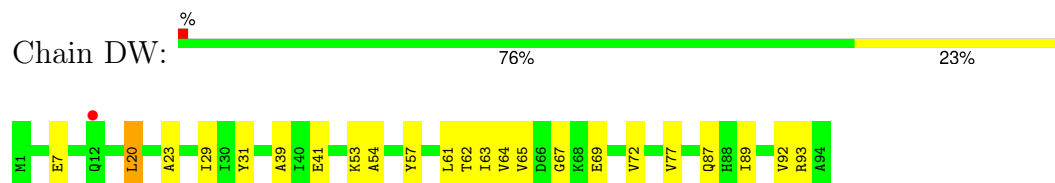
- Molecule 49: 50S ribosomal protein L24



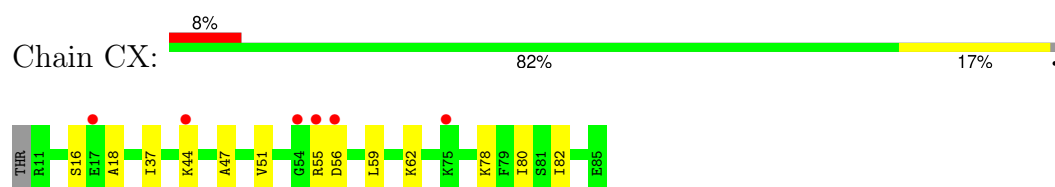
- Molecule 50: 50S ribosomal protein L25



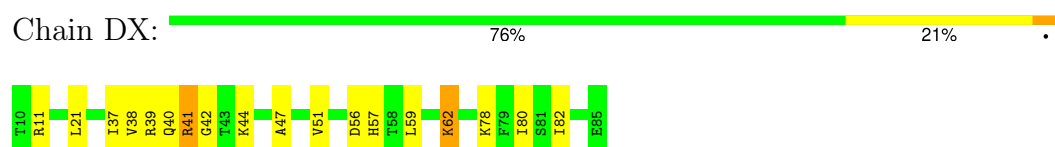
- Molecule 50: 50S ribosomal protein L25



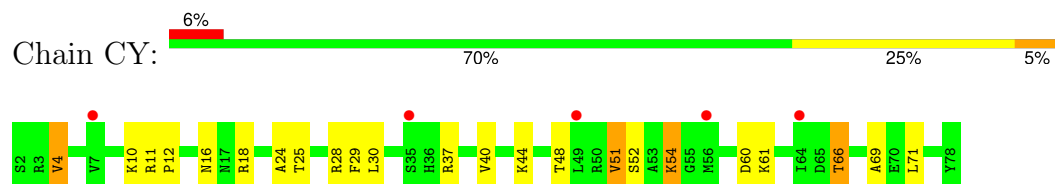
- Molecule 51: 50S ribosomal protein L27



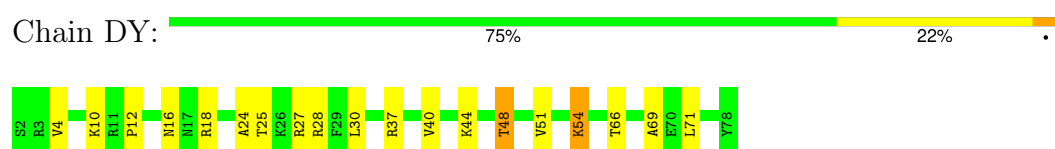
- Molecule 51: 50S ribosomal protein L27



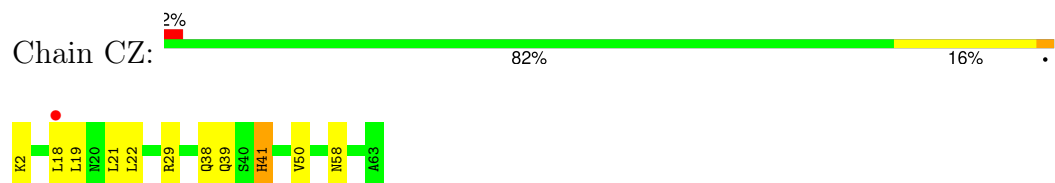
- Molecule 52: 50S ribosomal protein L28



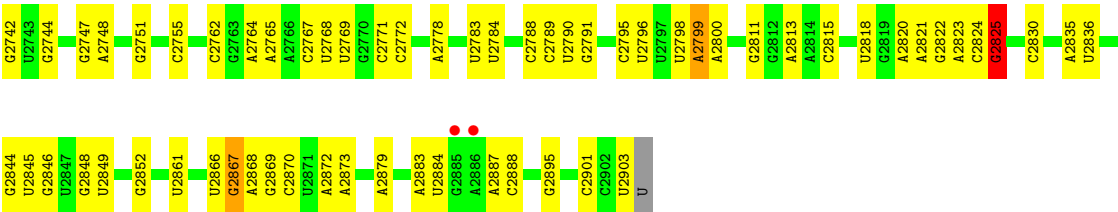
- Molecule 52: 50S ribosomal protein L28



- Molecule 53: 50S ribosomal protein L29



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U2613	U2504	A2287	U2167	A2097	A1885	A1744	A1578	G1451	G1309	U1174	G1068
U2615	G2505	A2288	G2168	U2098	U1886	A1745	A1583	G1452	A1069	A1175	A1068
G2621	U2506	U2292	A2170	G2010	A1900	U1746	G1585	A1453	U1313	G1177	A1070
C2626	C2512	U2305	A2171	A2014	G1906	G1750	A1586	U1460	C1320	G1173	G1072
C2626	A2516	G2308	U2172	A2015	G1907	G1753	G1587	G1478	A1321	U1180	A1073
C2627	C2517	A2311	A2173	G2018	U2106	A1754	G1588	G1482	A1327	U1181	U1083
C2628	U2518	G2312	C2175	A2020	A1913	A1755	U1590	G1483	A1328	G1182	G1087
U2629	G2410	U2313	C2178	C2023	C1914	A1755	A1591	U1484	U1329	U1184	A1088
G2630	A2418	G2320	U2180	G2026	3TD1915	U1758	C1604	U1485	G1332	G1187	A1089
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G2643	U2420	G2325	A2182	G2027	A1927	C1764	A1608	A1490	U1352	A1189	G1093
G2644	U2423	G2326	A2183	A2030	A1928	G1773	C1612	G1491	A1353	G1190	U1094
C2660	C2424	A2327	U2185	A2031	G1929	A1774	G1612	G1492	A1354	G1195	A1095
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A2662	A2426	U2329	G2188	A2033	U1931	U1775	A1614	A1494	G1356	A1097	U1097
G2663	G2427	G2330	A2198	G2034	A1932	U1778	A1618	A1495	A1359	G1212	A1098
C2667	G2428	G2331	G2204	G2035	G1935	U1781	G1622	U1497	A1365	G1226	C1100
C2681	A2434	A2332	G2204	A2037	G1935	U1781	G1622	A1504	A1376	A1244	U1119
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U2695	C2437	A2336	G2220	C2043	U1940	A1784	A1664	G1510	U1396	A1237	G1112
C2703	U2438	G2339	A2225	C2047	C1941	A1786	U1647	G1511	A1383	G1238	G1129
C2704	A2448	A2340	U2233	G2048	A1952	U1796	U1648	A1515	C1386	A1253	G1128
A2706	U2449	G2341	G2234	C2049	U1955	G1797	G1649	A1523	U1397	G1256	A1129
G2714	A2450	G2342	G2234	C2050	C1961	U1798	G1663	U1529	C1398	G1260	U1132
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U2724	C2475	G2365	U2262	G2062	G1972	G1826	G1699	C1547	G1424	G1279	A1142
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G2729	G2382	G2382	A2278	G2069	A1981	A1853	A1722	U1563	U1442	G1300	C1171
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A2740	U2492	U2384	G2280	G2093	U1991	C1870	C1798	A1569	U1443		
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	G2502	A2386	G2282	C2095	U1993	A1872	G1730		C1447		
		G2387	C2283	A2095	C1997						
		A2388									



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.55Å 433.65Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.32 48.13 – 3.32	Depositor EDS
% Data completeness (in resolution range)	83.3 (48.13-3.32) 83.2 (48.13-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	40.28 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.176 , 0.219 0.191 , 0.238	Depositor DCC
R_{free} test set	2784 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 146.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295119	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: MG, PGE, UR3, PUT, H2U, TRS, MPD, 3TD, EDO, MEQ, PSU, OMG, 6MZ, MA6, SPD, GUN, 4OC, 7MG, 2MG, PG4, 5MC, 2MA, OMC, 1MG, ZN, OMU, D2T, 4D4, 1PE, PEG, ACY, 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	0.73	20/36596 (0.1%)	0.68	0/57086
1	BA	0.72	17/36571 (0.0%)	0.68	0/57047
2	AB	0.81	0/1784	1.43	11/2403 (0.5%)
2	BB	0.79	0/1784	1.44	5/2403 (0.2%)
3	AC	0.87	0/1652	1.34	12/2225 (0.5%)
3	BC	0.89	0/1652	1.34	9/2225 (0.4%)
4	AD	0.76	0/1665	1.45	14/2227 (0.6%)
4	BD	0.78	0/1665	1.45	17/2227 (0.8%)
5	AE	0.79	0/1157	1.49	10/1557 (0.6%)
5	BE	0.75	0/1118	1.46	8/1504 (0.5%)
6	AF	0.79	0/881	1.39	7/1189 (0.6%)
6	BF	0.81	0/835	1.46	6/1128 (0.5%)
7	AG	0.89	0/1196	1.37	1/1602 (0.1%)
7	BG	0.88	0/1196	1.37	2/1602 (0.1%)
8	AH	0.74	0/989	1.38	3/1326 (0.2%)
8	BH	0.75	0/989	1.38	3/1326 (0.2%)
9	AI	0.84	0/1034	1.38	6/1375 (0.4%)
9	BI	0.84	0/1034	1.35	1/1375 (0.1%)
10	AJ	0.86	0/806	1.29	2/1089 (0.2%)
10	BJ	0.98	0/797	1.33	2/1077 (0.2%)
11	AK	0.85	1/893 (0.1%)	1.28	0/1205
11	BK	0.82	0/893	1.34	2/1205 (0.2%)
12	AL	0.79	0/960	1.33	1/1286 (0.1%)
12	BL	0.75	0/960	1.29	1/1286 (0.1%)
13	AM	0.94	0/893	1.52	19/1193 (1.6%)
13	BM	0.98	0/893	1.52	18/1193 (1.5%)
14	AN	0.89	0/817	1.35	2/1088 (0.2%)
14	BN	0.87	0/817	1.35	1/1088 (0.1%)
15	AO	0.80	0/722	1.53	3/964 (0.3%)
15	BO	0.76	0/722	1.55	4/964 (0.4%)
16	AP	0.86	0/659	1.38	5/884 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.84	0/659	1.38	0/884
17	AQ	0.81	0/658	1.27	1/881 (0.1%)
17	BQ	0.84	0/658	1.33	2/881 (0.2%)
18	AR	0.86	0/463	1.52	5/621 (0.8%)
18	BR	0.83	0/463	1.50	7/621 (1.1%)
19	AS	0.95	0/653	1.28	2/877 (0.2%)
19	BS	0.96	0/653	1.26	1/877 (0.1%)
20	AT	0.79	0/676	1.58	3/895 (0.3%)
20	BT	0.90	0/671	1.67	2/888 (0.2%)
21	AU	0.74	0/472	1.41	6/627 (1.0%)
21	BU	0.73	0/472	1.43	2/627 (0.3%)
22	C1	0.86	0/450	1.29	0/599
22	D1	0.98	0/450	1.27	1/599 (0.2%)
23	C2	0.85	0/416	1.36	2/554 (0.4%)
23	D2	0.90	0/421	1.33	1/561 (0.2%)
24	C3	0.77	0/380	1.41	0/498
24	D3	0.87	0/380	1.39	0/498
25	C4	0.78	0/513	1.34	2/676 (0.3%)
25	D4	0.88	0/513	1.39	2/676 (0.3%)
26	C5	0.78	0/303	1.21	0/397
26	D5	1.01	1/303 (0.3%)	1.22	0/397
27	C0	0.95	1/453 (0.2%)	1.40	1/605 (0.2%)
27	D0	0.99	0/467	1.40	2/623 (0.3%)
28	CB	0.71	1/2828 (0.0%)	0.70	1/4410 (0.0%)
28	DB	0.79	2/2872 (0.1%)	0.73	0/4478
29	CC	0.77	0/2121	1.34	15/2852 (0.5%)
29	DC	0.82	0/2121	1.31	12/2852 (0.4%)
30	CD	0.79	0/1586	1.23	7/2134 (0.3%)
31	CA	0.76	77/69165 (0.1%)	0.70	8/107896 (0.0%)
32	DD	0.88	0/1576	1.24	4/2119 (0.2%)
33	CE	0.77	0/1571	1.43	9/2113 (0.4%)
33	DE	0.82	1/1571 (0.1%)	1.43	8/2113 (0.4%)
34	CF	0.78	0/1434	1.39	11/1926 (0.6%)
34	DF	0.82	0/1434	1.42	12/1926 (0.6%)
35	CG	0.75	0/1343	1.36	16/1816 (0.9%)
35	DG	0.77	0/1343	1.31	9/1816 (0.5%)
36	CH	0.85	0/1121	1.43	10/1515 (0.7%)
36	DH	0.86	0/1121	1.39	0/1515
37	CJ	1.03	0/993	1.40	4/1341 (0.3%)
37	DJ	1.02	0/993	1.40	5/1341 (0.4%)
38	CK	0.73	0/1152	1.39	4/1551 (0.3%)
38	DK	0.95	0/1152	1.40	3/1551 (0.2%)
39	CL	0.84	0/947	1.29	3/1268 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DL	0.87	0/955	1.32	3/1279 (0.2%)
40	CM	0.80	1/1062 (0.1%)	1.43	9/1413 (0.6%)
40	DM	0.86	0/1062	1.36	7/1413 (0.5%)
41	CN	0.78	0/1081	1.33	5/1443 (0.3%)
41	DN	0.88	0/1092	1.32	5/1457 (0.3%)
42	CO	0.81	0/973	1.35	2/1301 (0.2%)
42	DO	0.97	0/1006	1.41	6/1345 (0.4%)
43	CP	0.80	0/902	1.46	9/1209 (0.7%)
43	DP	0.87	0/910	1.41	5/1219 (0.4%)
44	CQ	0.74	0/929	1.25	6/1242 (0.5%)
44	DQ	0.84	0/929	1.24	5/1242 (0.4%)
45	CR	0.81	0/960	1.55	10/1278 (0.8%)
45	DR	1.00	0/960	1.53	11/1278 (0.9%)
46	CS	0.78	0/829	1.27	2/1107 (0.2%)
46	DS	0.94	0/829	1.31	2/1107 (0.2%)
47	CT	0.77	0/864	1.48	4/1156 (0.3%)
47	DT	0.97	0/864	1.47	1/1156 (0.1%)
48	CU	0.84	0/744	1.29	0/994
48	DU	0.88	0/744	1.30	0/994
49	CV	0.87	0/787	1.42	4/1051 (0.4%)
49	DV	0.84	0/787	1.43	12/1051 (1.1%)
50	CW	0.76	0/766	1.33	2/1025 (0.2%)
50	DW	0.86	1/766 (0.1%)	1.33	4/1025 (0.4%)
51	CX	0.68	0/576	1.24	1/762 (0.1%)
51	DX	0.83	0/598	1.22	2/790 (0.3%)
52	CY	0.67	0/635	1.39	2/848 (0.2%)
52	DY	0.75	0/635	1.37	2/848 (0.2%)
53	CZ	0.77	0/502	1.60	1/667 (0.1%)
53	DZ	0.85	0/502	1.62	1/667 (0.1%)
54	DI	0.94	1/1037 (0.1%)	1.55	9/1402 (0.6%)
55	DA	0.83	54/69364 (0.1%)	0.76	5/108207 (0.0%)
All	All	0.79	178/309271 (0.1%)	0.94	495/462220 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	BJ	0	1
28	DB	0	1
31	CA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DA	0	26
All	All	0	29

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-10.48	1.26	1.42
55	DA	2585	U	C1'-N1	9.24	1.61	1.47
55	DA	2097	A	O5'-C5'	-8.84	1.29	1.42
26	D5	26	ILE	CG1-CD1	8.54	1.85	1.51
31	CA	2225	A	C3'-O3'	8.50	1.55	1.43

The worst 5 of 495 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DI	132	TYR	CA-C-N	9.75	139.24	121.70
54	DI	132	TYR	C-N-CA	9.75	139.24	121.70
4	AD	99	ASP	CA-CB-CG	8.31	120.91	112.60
4	BD	99	ASP	CA-CB-CG	8.08	120.68	112.60
34	DF	10	ASP	CA-CB-CG	7.93	120.53	112.60

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	BJ	37	ARG	Mainchain
31	CA	780	G	Sidechain
55	DA	329	G	Sidechain
55	DA	452	G	Sidechain
28	DB	13	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	32932	0	16593	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	32910	0	16582	179	0
2	AB	1753	0	1780	17	0
2	BB	1753	0	1780	18	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	19	0
4	BD	1643	0	1707	19	0
5	AE	1144	0	1185	17	0
5	BE	1105	0	1148	26	0
6	AF	862	0	864	14	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	17	0
7	BG	1182	0	1238	17	0
8	AH	979	0	1031	10	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	11	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	8	0
10	BJ	787	0	828	11	0
11	AK	877	0	887	12	0
11	BK	877	0	887	14	0
12	AL	957	0	1017	14	0
12	BL	957	0	1017	16	0
13	AM	884	0	941	12	0
13	BM	884	0	941	15	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	3	0
15	BO	714	0	734	7	0
16	AP	649	0	666	6	0
16	BP	649	0	666	8	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	6	0
18	BR	456	0	478	5	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	12	0
20	BT	665	0	714	9	0
21	AU	465	0	491	6	0
21	BU	465	0	491	5	0
22	C1	444	0	458	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	10	0
23	C2	409	0	440	6	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	7	0
25	C4	504	0	572	4	0
25	D4	504	0	572	8	0
26	C5	302	0	340	5	0
26	D5	302	0	340	4	0
27	C0	449	0	488	4	0
27	D0	463	0	504	7	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	10	0
29	CC	2082	0	2154	24	0
29	DC	2082	0	2154	24	0
30	CD	1565	0	1616	22	0
31	CA	62229	0	31319	399	0
32	DD	1576	0	1627	29	0
33	CE	1552	0	1619	22	0
33	DE	1552	0	1619	21	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	26	0
35	CG	1323	0	1371	17	0
35	DG	1323	0	1371	15	0
36	CH	1110	0	1148	10	0
36	DH	1110	0	1148	11	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	10	0
38	CK	1129	0	1162	14	0
38	DK	1129	0	1162	15	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	8	0
40	CM	1053	0	1129	23	0
40	DM	1053	0	1129	18	0
41	CN	1075	0	1154	16	0
41	DN	1092	0	1177	18	0
42	CO	960	0	1000	17	0
42	DO	993	0	1034	17	0
43	CP	892	0	923	14	0
43	DP	900	0	935	17	0
44	CQ	917	0	962	8	0
44	DQ	917	0	962	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CR	947	0	1019	14	0
45	DR	947	0	1019	21	0
46	CS	816	0	839	18	0
46	DS	816	0	839	22	0
47	CT	857	0	922	16	0
47	DT	857	0	922	14	0
48	CU	738	0	807	9	0
48	DU	738	0	807	6	0
49	CV	779	0	831	12	0
49	DV	779	0	831	9	0
50	CW	753	0	780	7	0
50	DW	753	0	780	8	0
51	CX	569	0	581	8	0
51	DX	591	0	606	14	0
52	CY	625	0	652	11	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	5	0
53	DZ	501	0	531	6	0
54	DI	1023	0	1052	26	0
55	DA	62423	0	31411	382	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	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	0	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	1	0
57	DS	13	0	18	0	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	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	16	0	28	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	D3	7	0	10	1	0
61	DA	42	0	60	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	1	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	4	0
62	DB	8	0	12	0	0
63	D1	10	0	14	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	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	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	2	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	3	0
69	AC	4	0	0	0	0
69	AD	2	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	5	0	0	0	0
69	AL	7	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	1	0
69	AO	1	0	0	0	0
69	AP	1	0	0	0	0
69	AQ	1	0	0	0	0
69	AS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AT	2	0	0	0	0
69	AU	4	0	0	0	0
69	BA	287	0	0	2	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	3	0	0	0	0
69	BN	1	0	0	0	0
69	BO	1	0	0	0	0
69	BP	4	0	0	0	0
69	BR	1	0	0	0	0
69	BT	5	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	CA	696	0	0	3	0
69	CB	13	0	0	0	0
69	CC	11	0	0	0	0
69	CD	4	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	2	0
69	D1	37	0	0	0	0
69	D2	5	0	0	0	0
69	D3	30	0	0	0	0
69	D4	40	0	0	1	0
69	D5	13	0	0	1	0
69	DA	4824	0	0	39	0
69	DB	203	0	0	3	0
69	DC	100	0	0	1	0
69	DD	97	0	0	5	0
69	DE	54	0	0	2	0
69	DF	13	0	0	1	0
69	DG	9	0	0	0	0
69	DH	2	0	0	0	0
69	DK	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DL	50	0	0	0	0
69	DM	60	0	0	0	0
69	DN	81	0	0	1	0
69	DO	42	0	0	1	0
69	DP	42	0	0	2	0
69	DQ	32	0	0	1	0
69	DR	68	0	0	3	0
69	DS	52	0	0	5	0
69	DT	65	0	0	1	0
69	DU	24	0	0	0	0
69	DV	19	0	0	1	0
69	DW	33	0	0	1	0
69	DX	33	0	0	2	0
69	DY	11	0	0	1	0
69	DZ	7	0	0	0	0
All	All	295119	0	194415	2104	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 4.

The worst 5 of 2104 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	1.85	1.50
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.16
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.62	0.99
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.44	0.95
31:CA:1311:G:H21	31:CA:1603:A:H62	1.16	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	5	26
2	BB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	5	26
3	AC	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	12	41
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	8	33
4	AD	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	9	35
5	BE	148/155 (96%)	126 (85%)	17 (12%)	5 (3%)	3	19
6	AF	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	12	41
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	3	21
7	AG	149/151 (99%)	137 (92%)	10 (7%)	2 (1%)	9	35
7	BG	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	9	35
8	AH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	32
8	BH	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
9	AI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
9	BI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
10	AJ	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	3	21
10	BJ	96/99 (97%)	78 (81%)	14 (15%)	4 (4%)	2	15
11	AK	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	14	43
11	BK	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	14	43
12	AL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	7	31
12	BL	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	31
13	AM	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	2	18
13	BM	112/114 (98%)	96 (86%)	10 (9%)	6 (5%)	1	10
14	AN	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	12	41
14	BN	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	12	41
15	AO	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	BO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	10	37
16	AP	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	24
16	BP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	2	17
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	2	17
17	BQ	78/80 (98%)	69 (88%)	5 (6%)	4 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	6 (8%)	3 (4%)	2	16
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	4	24
20	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	BT	83/86 (96%)	78 (94%)	4 (5%)	1 (1%)	10	37
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%)	45 (83%)	6 (11%)	3 (6%)	1	10
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	4 (8%)	1 (2%)	5	27
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	26
24	D3	44/46 (96%)	44 (100%)	0	0	100	100
25	C4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	32
25	D4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	32
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%)	51 (91%)	3 (5%)	2 (4%)	2	18
27	D0	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
29	CC	269/272 (99%)	243 (90%)	21 (8%)	5 (2%)	6	29
29	DC	269/272 (99%)	245 (91%)	19 (7%)	5 (2%)	6	29
30	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	9	34
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
33	CE	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	24	56
33	DE	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
34	CF	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
34	DF	175/178 (98%)	163 (93%)	12 (7%)	0	100	100
35	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	5	26
35	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	21	52
36	CH	147/149 (99%)	129 (88%)	12 (8%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DH	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	4	23
37	CJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	3	21
37	DJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	3	21
38	CK	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	5	27
38	DK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	27
39	CL	120/123 (98%)	111 (92%)	7 (6%)	2 (2%)	7	31
39	DL	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	16	45
40	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	2	15
40	DM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	27
41	CN	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	DN	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	CO	118/127 (93%)	98 (83%)	16 (14%)	4 (3%)	3	19
42	DO	123/127 (97%)	106 (86%)	16 (13%)	1 (1%)	16	45
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	CQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	43
44	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	43
45	CR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
45	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
46	CS	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	6	28
46	DS	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12	41
47	CT	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
47	DT	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	43
48	CU	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	11	40
48	DU	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	11	40
49	CV	100/103 (97%)	85 (85%)	12 (12%)	3 (3%)	3	21
49	DV	100/103 (97%)	87 (87%)	11 (11%)	2 (2%)	6	28
50	CW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	11	40
50	DW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	11	40
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	CY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
52	DY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
53	CZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	7	31
53	DZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	7	31
54	DI	133/135 (98%)	112 (84%)	17 (13%)	4 (3%)	3	21
All	All	11407/11679 (98%)	10425 (91%)	815 (7%)	167 (2%)	8	33

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	ARG
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	169 (91%)	17 (9%)	9	32
2	BB	186/186 (100%)	169 (91%)	17 (9%)	9	32
3	AC	170/170 (100%)	157 (92%)	13 (8%)	12	38
3	BC	170/170 (100%)	155 (91%)	15 (9%)	9	33
4	AD	172/172 (100%)	160 (93%)	12 (7%)	14	41
4	BD	172/172 (100%)	159 (92%)	13 (8%)	12	38
5	AE	118/118 (100%)	98 (83%)	20 (17%)	2	10
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	12
6	AF	92/92 (100%)	79 (86%)	13 (14%)	3	15
6	BF	87/92 (95%)	72 (83%)	15 (17%)	2	10
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BG	124/124 (100%)	107 (86%)	17 (14%)	3	16
8	AH	104/104 (100%)	86 (83%)	18 (17%)	2	9
8	BH	104/104 (100%)	88 (85%)	16 (15%)	2	13
9	AI	105/105 (100%)	95 (90%)	10 (10%)	8	30
9	BI	105/105 (100%)	94 (90%)	11 (10%)	6	25
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	8	31
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5	21
11	AK	90/99 (91%)	86 (96%)	4 (4%)	25	54
11	BK	90/99 (91%)	82 (91%)	8 (9%)	9	32
12	AL	102/102 (100%)	93 (91%)	9 (9%)	9	33
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	21
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	20
13	BM	92/92 (100%)	79 (86%)	13 (14%)	3	15
14	AN	83/83 (100%)	80 (96%)	3 (4%)	31	58
14	BN	83/83 (100%)	80 (96%)	3 (4%)	31	58
15	AO	76/76 (100%)	72 (95%)	4 (5%)	20	49
15	BO	76/76 (100%)	70 (92%)	6 (8%)	11	37
16	AP	65/65 (100%)	61 (94%)	4 (6%)	16	45
16	BP	65/65 (100%)	60 (92%)	5 (8%)	12	38
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	20
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	3	14
18	AR	48/48 (100%)	46 (96%)	2 (4%)	26	55
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	66
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	18
19	BS	70/70 (100%)	62 (89%)	8 (11%)	5	22
20	AT	65/65 (100%)	53 (82%)	12 (18%)	1	8
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7	25
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	25
22	C1	47/47 (100%)	46 (98%)	1 (2%)	47	66
22	D1	47/47 (100%)	45 (96%)	2 (4%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	C2	45/46 (98%)	40 (89%)	5 (11%)	6	23
23	D2	45/46 (98%)	40 (89%)	5 (11%)	6	23
24	C3	38/38 (100%)	34 (90%)	4 (10%)	6	25
24	D3	38/38 (100%)	33 (87%)	5 (13%)	4	17
25	C4	51/51 (100%)	48 (94%)	3 (6%)	18	46
25	D4	51/51 (100%)	48 (94%)	3 (6%)	18	46
26	C5	34/34 (100%)	31 (91%)	3 (9%)	9	33
26	D5	34/34 (100%)	32 (94%)	2 (6%)	18	46
27	C0	48/48 (100%)	41 (85%)	7 (15%)	3	14
27	D0	49/48 (102%)	41 (84%)	8 (16%)	2	11
29	CC	216/217 (100%)	198 (92%)	18 (8%)	10	35
29	DC	216/217 (100%)	200 (93%)	16 (7%)	13	39
30	CD	164/164 (100%)	150 (92%)	14 (8%)	10	34
32	DD	163/163 (100%)	150 (92%)	13 (8%)	11	37
33	CE	165/165 (100%)	147 (89%)	18 (11%)	6	24
33	DE	165/165 (100%)	151 (92%)	14 (8%)	10	34
34	CF	148/149 (99%)	126 (85%)	22 (15%)	3	14
34	DF	148/149 (99%)	127 (86%)	21 (14%)	3	15
35	CG	137/137 (100%)	126 (92%)	11 (8%)	11	37
35	DG	137/137 (100%)	125 (91%)	12 (9%)	9	33
36	CH	114/114 (100%)	98 (86%)	16 (14%)	3	15
36	DH	114/114 (100%)	100 (88%)	14 (12%)	4	19
37	CJ	104/105 (99%)	92 (88%)	12 (12%)	5	21
37	DJ	104/105 (99%)	92 (88%)	12 (12%)	5	21
38	CK	116/116 (100%)	111 (96%)	5 (4%)	26	54
38	DK	116/116 (100%)	110 (95%)	6 (5%)	21	49
39	CL	103/104 (99%)	95 (92%)	8 (8%)	11	37
39	DL	104/104 (100%)	94 (90%)	10 (10%)	8	29
40	CM	103/103 (100%)	90 (87%)	13 (13%)	4	19
40	DM	103/103 (100%)	96 (93%)	7 (7%)	14	42
41	CN	108/108 (100%)	94 (87%)	14 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DN	109/108 (101%)	97 (89%)	12 (11%)	6	23
42	CO	100/103 (97%)	91 (91%)	9 (9%)	9	32
42	DO	102/103 (99%)	94 (92%)	8 (8%)	11	37
43	CP	86/87 (99%)	77 (90%)	9 (10%)	6	25
43	DP	87/87 (100%)	77 (88%)	10 (12%)	5	21
44	CQ	99/99 (100%)	89 (90%)	10 (10%)	7	27
44	DQ	99/99 (100%)	89 (90%)	10 (10%)	7	27
45	CR	89/89 (100%)	83 (93%)	6 (7%)	15	43
45	DR	89/89 (100%)	83 (93%)	6 (7%)	15	43
46	CS	84/84 (100%)	73 (87%)	11 (13%)	4	17
46	DS	84/84 (100%)	76 (90%)	8 (10%)	8	30
47	CT	93/93 (100%)	80 (86%)	13 (14%)	3	15
47	DT	93/93 (100%)	80 (86%)	13 (14%)	3	15
48	CU	80/84 (95%)	62 (78%)	18 (22%)	1	5
48	DU	80/84 (95%)	67 (84%)	13 (16%)	2	11
49	CV	83/84 (99%)	72 (87%)	11 (13%)	4	17
49	DV	83/84 (99%)	76 (92%)	7 (8%)	10	35
50	CW	78/78 (100%)	70 (90%)	8 (10%)	7	26
50	DW	78/78 (100%)	71 (91%)	7 (9%)	9	32
51	CX	56/58 (97%)	54 (96%)	2 (4%)	31	58
51	DX	58/58 (100%)	53 (91%)	5 (9%)	10	34
52	CY	67/67 (100%)	59 (88%)	8 (12%)	5	20
52	DY	67/67 (100%)	59 (88%)	8 (12%)	5	20
53	CZ	54/54 (100%)	49 (91%)	5 (9%)	8	31
53	DZ	54/54 (100%)	50 (93%)	4 (7%)	13	39
54	DI	103/103 (100%)	91 (88%)	12 (12%)	5	21
All	All	9461/9514 (99%)	8488 (90%)	973 (10%)	7	26

5 of 973 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	D0	58	GLU
44	DQ	65	SER

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Mol	Chain	Res	Type
35	CG	167	GLU
43	DP	58	ILE
51	DX	41[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
36	CH	66	ASN
36	DH	2	GLN
38	CK	47	HIS
45	CR	56	GLN
38	DK	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	305 (19%)	48 (3%)
1	BA	1532/1534 (99%)	307 (20%)	52 (3%)
28	CB	117/120 (97%)	14 (11%)	2 (1%)
28	DB	119/120 (99%)	14 (11%)	1 (0%)
31	CA	2896/2904 (99%)	593 (20%)	110 (3%)
55	DA	2884/2904 (99%)	504 (17%)	73 (2%)
All	All	9081/9116 (99%)	1737 (19%)	286 (3%)

5 of 1737 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 286 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	DA	603	A
55	DA	984	A
55	DA	1800	C
1	BA	1380	U

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Mol	Chain	Res	Type
1	BA	1345	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	CA	2580	31	18,21,22	0.58	0	21,30,33	0.78	2 (9%)
1	MA6	AA	1518	1	23,26,27	0.50	0	33,38,41	1.21	4 (12%)
55	PSU	DA	955	55	18,21,22	0.69	0	21,30,33	0.50	0
1	2MG	AA	966	1	23,26,27	0.49	0	33,38,41	0.57	0
31	OMC	CA	2498	31,56	19,22,23	0.36	0	25,31,34	0.36	0
1	7MG	BA	527	1	23,26,27	4.22	2 (8%)	27,39,42	2.52	6 (22%)
55	PSU	DA	2457	55	18,21,22	0.56	0	21,30,33	0.52	0
31	OMG	CA	2251	31	23,26,27	0.46	0	32,38,41	0.42	0
41	4D4	DN	81[B]	-	9,11,12	1.82	2 (22%)	7,13,15	2.27	2 (28%)
55	5MU	DA	747	55	19,22,23	0.48	0	27,32,35	0.35	0
31	2MG	CA	1835	31	23,26,27	0.34	0	33,38,41	0.35	0
31	PSU	CA	955	31	18,21,22	0.39	0	21,30,33	0.57	1 (4%)
55	5MU	DA	1939	55	19,22,23	0.65	0	27,32,35	0.40	0
1	5MC	BA	1407	1	19,22,23	0.36	0	26,32,35	0.41	0
31	2MA	CA	2503	31	22,25,26	0.73	0	32,37,40	1.87	6 (18%)
1	PSU	BA	516	1	18,21,22	0.47	0	21,30,33	0.48	0
1	UR3	AA	1498	1	19,22,23	0.60	0	26,32,35	0.60	1 (3%)
31	PSU	CA	2504	31	18,21,22	0.35	0	21,30,33	0.43	0
55	7MG	DA	2069	55	23,26,27	4.22	1 (4%)	27,39,42	2.25	6 (22%)
55	H2U	DA	2449	55	18,21,22	0.84	0	19,30,33	0.41	0
55	6MZ	DA	1618	55	22,25,26	0.66	0	29,36,39	1.32	1 (3%)
31	5MU	CA	747	31	19,22,23	0.26	0	27,32,35	0.28	0
55	OMU	DA	2552	55	19,22,23	0.51	0	25,31,34	0.33	0
55	PSU	DA	746	56,55	18,21,22	1.12	2 (11%)	21,30,33	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	2MA	DA	2503	56,55	22,25,26	0.70	0	32,37,40	1.62	6 (18%)
55	PSU	DA	2604	55	18,21,22	0.79	1 (5%)	21,30,33	0.51	0
1	MA6	BA	1519	1	23,26,27	0.49	0	33,38,41	1.05	3 (9%)
55	OMC	DA	2498	56,55	19,22,23	0.65	1 (5%)	25,31,34	0.46	0
31	7MG	CA	2069	31	23,26,27	4.21	4 (17%)	27,39,42	2.32	6 (22%)
31	PSU	CA	2457	31	18,21,22	0.83	1 (5%)	21,30,33	0.42	0
31	OMU	CA	2552	31	19,22,23	0.27	0	25,31,34	0.37	0
1	2MG	BA	1207	1	23,26,27	0.35	0	33,38,41	0.42	0
1	5MC	AA	1407	1	19,22,23	0.30	0	26,32,35	0.41	0
55	6MZ	DA	2030	55	22,25,26	0.39	0	29,36,39	0.67	1 (3%)
32	MEQ	DD	150[A]	32	8,9,10	0.40	0	5,10,12	0.54	0
1	2MG	AA	1516	1	23,26,27	0.33	0	33,38,41	0.46	0
1	7MG	AA	527	1	23,26,27	4.11	3 (13%)	27,39,42	2.49	6 (22%)
1	2MG	AA	1207	1	23,26,27	0.32	0	33,38,41	0.40	0
31	3TD	CA	1915	31	19,22,23	0.46	0	23,32,35	0.82	1 (4%)
55	5MC	DA	1962	55	19,22,23	0.67	0	26,32,35	0.45	0
55	OMG	DA	2251	55	23,26,27	0.42	0	32,38,41	0.38	0
55	2MG	DA	2445	55	23,26,27	0.47	0	33,38,41	0.44	0
55	PSU	DA	2605	55	18,21,22	0.48	0	21,30,33	0.51	0
1	2MG	BA	1516	1	23,26,27	0.33	0	33,38,41	0.47	0
1	MA6	BA	1518	1	23,26,27	0.49	0	33,38,41	1.27	4 (12%)
55	2MG	DA	1835	55	23,26,27	0.40	0	33,38,41	0.38	0
31	PSU	CA	746	31,56	18,21,22	0.70	1 (5%)	21,30,33	0.43	0
1	2MG	BA	966	1	23,26,27	0.49	0	33,38,41	0.48	0
12	D2T	AL	89	12	8,9,10	0.96	1 (12%)	6,11,13	0.75	0
31	PSU	CA	1911	31	18,21,22	0.37	0	21,30,33	0.42	0
31	6MZ	CA	1618	31	22,25,26	0.61	0	29,36,39	0.78	1 (3%)
31	6MZ	CA	2030	31	22,25,26	0.37	0	29,36,39	0.47	0
31	5MU	CA	1939	31	19,22,23	0.48	0	27,32,35	0.36	0
32	MEQ	DD	150[B]	32	8,9,10	1.47	1 (12%)	5,10,12	1.46	1 (20%)
55	PSU	DA	1917	55	18,21,22	0.50	0	21,30,33	0.42	0
1	5MC	AA	967	1	19,22,23	0.34	0	26,32,35	0.38	0
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.44	0
1	UR3	BA	1498	1	19,22,23	0.56	0	26,32,35	0.73	1 (3%)
12	D2T	BL	89	12	8,9,10	0.91	0	6,11,13	0.67	0
55	PSU	DA	2580	55	18,21,22	0.63	0	21,30,33	0.61	0
31	5MC	CA	1962	31	19,22,23	0.26	0	26,32,35	0.39	0
1	PSU	AA	516	56,1	18,21,22	0.44	0	21,30,33	0.48	0
31	2MG	CA	2445	31	23,26,27	0.36	0	33,38,41	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	1MG	CA	745	31	23,26,27	0.76	1 (4%)	33,39,42	0.70	1 (3%)
1	5MC	BA	967	1	19,22,23	0.34	0	26,32,35	0.37	0
55	3TD	DA	1915	55	19,22,23	0.43	0	23,32,35	0.80	1 (4%)
1	MA6	AA	1519	1	23,26,27	0.54	0	33,38,41	1.03	4 (12%)
31	PSU	CA	2605	31	18,21,22	0.35	0	21,30,33	0.50	0
41	4D4	CN	81	41	9,11,12	2.36	2 (22%)	7,13,15	2.40	2 (28%)
55	PSU	DA	1911	55	18,21,22	0.40	0	21,30,33	0.43	0
55	1MG	DA	745	55	23,26,27	0.95	1 (4%)	33,39,42	0.73	1 (3%)
55	PSU	DA	2504	55	18,21,22	0.45	0	21,30,33	0.39	0
31	PSU	CA	1917	31	18,21,22	0.40	0	21,30,33	0.39	0
41	4D4	DN	81[A]	-	9,11,12	1.67	1 (11%)	7,13,15	3.20	2 (28%)
1	4OC	BA	1402	1	20,23,24	0.40	0	25,32,35	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
31	OMC	CA	2498	31,56	-	2/9/27/28	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	0/9/27/28	0/3/3/3
41	4D4	DN	81[B]	-	-	3/11/12/14	-
55	5MU	DA	747	55	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	0/9/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	2/7/25/26	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
55	7MG	DA	2069	55	-	1/7/37/38	0/3/3/3
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
55	6MZ	DA	1618	55	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/9/27/28	0/2/2/2
55	PSU	DA	746	56,55	-	2/7/25/26	0/2/2/2
55	2MA	DA	2503	56,55	-	2/7/25/26	0/3/3/3
55	PSU	DA	2604	55	-	1/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	3/11/29/30	0/3/3/3
55	OMC	DA	2498	56,55	-	0/9/27/28	0/2/2/2
31	7MG	CA	2069	31	-	0/7/37/38	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
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	6MZ	DA	2030	55	-	1/9/27/28	0/3/3/3
32	MEQ	DD	150[A]	32	-	5/8/9/11	-
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	1/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	0/9/27/28	0/3/3/3
55	2MG	DA	2445	55	-	2/9/27/28	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
55	2MG	DA	1835	55	-	0/9/27/28	0/3/3/3
31	PSU	CA	746	31,56	-	2/7/25/26	0/2/2/2
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
12	D2T	AL	89	12	-	3/7/12/14	-
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	2/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	1/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	3/8/9/11	-
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	6/7/12/14	-
55	PSU	DA	2580	55	-	1/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/9/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/11/29/30	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
41	4D4	CN	81	41	-	1/11/12/14	-
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/7/25/26	0/3/3/3
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
41	4D4	DN	81[A]	-	-	1/11/12/14	-
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2069	7MG	C8-N9	-19.89	1.33	1.45
1	BA	527	7MG	C8-N9	-19.74	1.33	1.45
31	CA	2069	7MG	C8-N9	-19.20	1.33	1.45
1	AA	527	7MG	C8-N9	-19.14	1.33	1.45
41	CN	81	4D4	CZ-NE	6.34	1.45	1.33

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	N6-C6-N1	7.89	127.68	117.03
1	BA	527	7MG	C6-C5-C4	-6.80	110.43	122.40
41	DN	81[A]	4D4	NE-CZ-NH2	6.72	132.21	120.67
1	AA	527	7MG	C6-C5-N7	-6.66	121.61	131.93
55	DA	2503	2MA	N6-C6-N1	6.65	126.00	117.03

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	O-C-CA-CB
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	O-C-CA-CB
12	BL	89	D2T	CA-CB-SB-CB1

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Mol	Chain	Res	Type	Atoms
12	BL	89	D2T	CA-CB-CG-OD1

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
55	DA	747	5MU	1	0
31	CA	747	5MU	1	0
1	BA	1519	MA6	1	0
55	DA	2498	OMC	1	0
55	DA	2030	6MZ	2	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
31	CA	2030	6MZ	5	0
31	CA	1939	5MU	1	0
32	DD	150[B]	MEQ	1	0
1	AA	1402	4OC	1	0
31	CA	745	1MG	1	0
1	BA	967	5MC	2	0
1	AA	1519	MA6	1	0
1	BA	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PUT	AA	1672	-	5,5,5	0.06	0	4,4,4	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PG4	DA	3216	-	12,12,12	0.14	0	11,11,11	0.14	0
58	MPD	AA	1676	-	7,7,7	0.65	0	9,10,10	0.59	0
58	MPD	DA	3192	-	7,7,7	0.74	0	9,10,10	0.69	0
61	PEG	DA	3226	-	6,6,6	0.20	0	5,5,5	0.06	0
66	ACY	DA	3196	-	3,3,3	2.84	1 (33%)	3,3,3	1.89	2 (66%)
58	MPD	DS	203	-	7,7,7	0.36	0	9,10,10	0.37	0
62	EDO	DA	3208	-	3,3,3	0.53	0	2,2,2	0.36	0
62	EDO	D1	101	-	3,3,3	0.62	0	2,2,2	0.26	0
59	PUT	DA	3221	-	5,5,5	0.25	0	4,4,4	0.17	0
59	PUT	DM	201	-	5,5,5	0.21	0	4,4,4	0.28	0
58	MPD	DE	302	-	7,7,7	0.86	0	9,10,10	0.76	0
61	PEG	DA	3200	-	6,6,6	0.24	0	5,5,5	0.09	0
57	PG4	AA	1670	-	12,12,12	0.18	0	11,11,11	0.20	0
62	EDO	DA	3003	-	3,3,3	0.61	0	2,2,2	0.36	0
64	SPD	DA	3187	-	9,9,9	0.12	0	8,8,8	0.22	0
64	SPD	DA	3183	-	9,9,9	0.21	0	8,8,8	0.36	0
58	MPD	AA	1671	-	7,7,7	0.36	0	9,10,10	0.54	0
61	PEG	DA	3227	-	6,6,6	0.25	0	5,5,5	0.15	0
64	SPD	DA	3224	-	9,9,9	0.12	0	8,8,8	0.25	0
59	PUT	DA	3212	-	5,5,5	0.24	0	4,4,4	0.16	0
63	PGE	DA	3217	-	9,9,9	0.22	0	8,8,8	0.19	0
63	PGE	DA	3214	-	9,9,9	0.24	0	8,8,8	0.33	0
58	MPD	DA	3210	-	7,7,7	0.71	0	9,10,10	0.37	0
62	EDO	DA	3002	-	3,3,3	0.56	0	2,2,2	0.21	0
59	PUT	AA	1673	-	5,5,5	0.13	0	4,4,4	0.06	0
63	PGE	DU	201	-	9,9,9	0.32	0	8,8,8	0.29	0
61	PEG	DA	3218	-	6,6,6	0.15	0	5,5,5	0.07	0
59	PUT	DA	3222	-	5,5,5	0.26	0	4,4,4	0.53	0
67	GUN	DA	3211	-	12,12,12	0.26	0	15,17,17	0.76	0
66	ACY	DA	3191	-	3,3,3	0.66	0	3,3,3	1.30	0
62	EDO	DA	3209	-	3,3,3	0.48	0	2,2,2	0.37	0
66	ACY	DA	3202	-	3,3,3	0.66	0	3,3,3	0.86	0
59	PUT	DA	3188	-	5,5,5	0.11	0	4,4,4	0.15	0
59	PUT	DA	3184	-	5,5,5	0.16	0	4,4,4	0.19	0
58	MPD	DK	201	-	7,7,7	0.92	1 (14%)	9,10,10	0.37	0
62	EDO	DA	3215	-	3,3,3	0.65	0	2,2,2	0.27	0
62	EDO	DA	3198	-	3,3,3	0.68	0	2,2,2	0.25	0
62	EDO	DB	210	-	3,3,3	0.62	0	2,2,2	0.20	0
59	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.17	0
61	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.19	0
57	PG4	DA	3193	-	12,12,12	0.28	0	11,11,11	0.26	0
65	1PE	DA	3203	-	15,15,15	0.21	0	14,14,14	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DN	201	-	7,7,7	1.06	1 (14%)	9,10,10	0.54	0
59	PUT	DA	3195	-	5,5,5	0.28	0	4,4,4	0.28	0
59	PUT	DA	3213	-	5,5,5	0.23	0	4,4,4	0.20	0
62	EDO	D0	101	-	3,3,3	0.57	0	2,2,2	0.57	0
62	EDO	DA	3194	-	3,3,3	0.67	0	2,2,2	0.07	0
61	PEG	DQ	201	-	6,6,6	0.22	0	5,5,5	0.12	0
58	MPD	DA	3204	-	7,7,7	0.64	0	9,10,10	0.49	0
63	PGE	D1	102	-	9,9,9	0.11	0	8,8,8	0.13	0
58	MPD	DT	201	-	7,7,7	0.69	0	9,10,10	0.33	0
59	PUT	AA	1674	-	5,5,5	0.13	0	4,4,4	0.10	0
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.08	0
58	MPD	DA	3207	-	7,7,7	0.33	0	9,10,10	0.50	0
59	PUT	AA	1675	-	5,5,5	0.17	0	4,4,4	0.09	0
61	PEG	DA	3201	-	6,6,6	0.14	0	5,5,5	0.14	0
61	PEG	AL	201	-	6,6,6	0.19	0	5,5,5	0.15	0
63	PGE	D3	101	-	9,9,9	0.22	0	8,8,8	0.11	0
61	PEG	DA	3199	-	6,6,6	0.18	0	5,5,5	0.12	0
63	PGE	DA	3225	-	9,9,9	0.26	0	8,8,8	0.31	0
64	SPD	DA	3206	-	9,9,9	0.22	0	8,8,8	0.24	0
63	PGE	DA	3186	-	9,9,9	0.33	0	8,8,8	0.35	0
62	EDO	DB	211	-	3,3,3	0.52	0	2,2,2	0.35	0
58	MPD	DA	3190	-	7,7,7	0.47	0	9,10,10	0.46	0
57	PG4	DQ	202	-	12,12,12	0.13	0	11,11,11	0.15	0
59	PUT	DA	3223	-	5,5,5	0.19	0	4,4,4	0.18	0
68	TRS	DA	3220	-	7,7,7	0.28	0	9,9,9	0.27	0
61	PEG	DP	201	-	6,6,6	0.17	0	5,5,5	0.13	0
63	PGE	DS	201	-	9,9,9	0.22	0	8,8,8	0.18	0
59	PUT	DA	3205	-	5,5,5	0.17	0	4,4,4	0.16	0
57	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.18	0
62	EDO	DA	3197	-	3,3,3	0.60	0	2,2,2	0.19	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.15	0
58	MPD	DT	202	-	7,7,7	0.70	0	9,10,10	0.49	0
57	PG4	DR	201	-	12,12,12	0.22	0	11,11,11	0.25	0
63	PGE	DD	301	-	9,9,9	0.21	0	8,8,8	0.16	0
57	PG4	DS	202	-	12,12,12	0.19	0	11,11,11	0.23	0
59	PUT	DA	3189	-	5,5,5	0.08	0	4,4,4	0.19	0
58	MPD	DE	301	-	7,7,7	0.59	0	9,10,10	0.47	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	AA	1672	-	-	0/3/3/3	-
57	PG4	DA	3216	-	-	5/10/10/10	-
58	MPD	AA	1676	-	-	1/5/5/5	-
58	MPD	DA	3192	-	-	2/5/5/5	-
61	PEG	DA	3226	-	-	0/4/4/4	-
58	MPD	DS	203	-	-	1/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
62	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	DA	3221	-	-	0/3/3/3	-
59	PUT	DM	201	-	-	0/3/3/3	-
58	MPD	DE	302	-	-	3/5/5/5	-
61	PEG	DA	3200	-	-	1/4/4/4	-
57	PG4	AA	1670	-	-	6/10/10/10	-
62	EDO	DA	3003	-	-	1/1/1/1	-
64	SPD	DA	3187	-	-	2/7/7/7	-
64	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	AA	1671	-	-	0/5/5/5	-
61	PEG	DA	3227	-	-	0/4/4/4	-
64	SPD	DA	3224	-	-	3/7/7/7	-
59	PUT	DA	3212	-	-	0/3/3/3	-
63	PGE	DA	3217	-	-	3/7/7/7	-
63	PGE	DA	3214	-	-	4/7/7/7	-
58	MPD	DA	3210	-	-	2/5/5/5	-
62	EDO	DA	3002	-	-	0/1/1/1	-
59	PUT	AA	1673	-	-	0/3/3/3	-
63	PGE	DU	201	-	-	4/7/7/7	-
61	PEG	DA	3218	-	-	1/4/4/4	-
59	PUT	DA	3222	-	-	0/3/3/3	-
67	GUN	DA	3211	-	-	-	0/2/2/2
62	EDO	DA	3209	-	-	0/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
59	PUT	DA	3184	-	-	1/3/3/3	-
58	MPD	DK	201	-	-	4/5/5/5	-
62	EDO	DA	3215	-	-	0/1/1/1	-
62	EDO	DA	3198	-	-	1/1/1/1	-
62	EDO	DB	210	-	-	1/1/1/1	-
59	PUT	DA	3219	-	-	0/3/3/3	-
61	PEG	D3	102	-	-	1/4/4/4	-
57	PG4	DA	3193	-	-	4/10/10/10	-
65	1PE	DA	3203	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	DN	201	-	-	1/5/5/5	-
59	PUT	DA	3195	-	-	0/3/3/3	-
59	PUT	DA	3213	-	-	1/3/3/3	-
62	EDO	D0	101	-	-	0/1/1/1	-
62	EDO	DA	3194	-	-	0/1/1/1	-
61	PEG	DQ	201	-	-	2/4/4/4	-
58	MPD	DA	3204	-	-	3/5/5/5	-
63	PGE	D1	102	-	-	5/7/7/7	-
58	MPD	DT	201	-	-	2/5/5/5	-
59	PUT	AA	1674	-	-	0/3/3/3	-
61	PEG	DL	201	-	-	3/4/4/4	-
58	MPD	DA	3207	-	-	2/5/5/5	-
59	PUT	AA	1675	-	-	1/3/3/3	-
61	PEG	DA	3201	-	-	1/4/4/4	-
61	PEG	AL	201	-	-	2/4/4/4	-
63	PGE	D3	101	-	-	4/7/7/7	-
61	PEG	DA	3199	-	-	2/4/4/4	-
63	PGE	DA	3225	-	-	4/7/7/7	-
64	SPD	DA	3206	-	-	2/7/7/7	-
63	PGE	DA	3186	-	-	2/7/7/7	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	MPD	DA	3190	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
59	PUT	DA	3223	-	-	1/3/3/3	-
68	TRS	DA	3220	-	-	0/9/9/9	-
61	PEG	DP	201	-	-	1/4/4/4	-
63	PGE	DS	201	-	-	4/7/7/7	-
59	PUT	DA	3205	-	-	0/3/3/3	-
57	PG4	BA	1642	-	-	5/10/10/10	-
62	EDO	DA	3197	-	-	0/1/1/1	-
65	1PE	DA	3185	-	-	4/13/13/13	-
58	MPD	DT	202	-	-	3/5/5/5	-
57	PG4	DR	201	-	-	4/10/10/10	-
63	PGE	DD	301	-	-	5/7/7/7	-
57	PG4	DS	202	-	-	4/10/10/10	-
59	PUT	DA	3189	-	-	0/3/3/3	-
58	MPD	DE	301	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.72	1.42	1.22
58	DN	201	MPD	C3-C2	2.36	1.61	1.54
58	DK	201	MPD	C3-C2	2.04	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3196	ACY	OXT-C-CH3	2.45	125.31	115.05
66	DA	3196	ACY	O-C-CH3	-2.15	113.72	122.53

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DE	302	MPD	C1-C2-C3-C4
58	DE	302	MPD	O2-C2-C3-C4
63	DA	3225	PGE	O2-C3-C4-O3
57	BA	1642	PG4	O4-C7-C8-O5
63	DS	201	PGE	O2-C3-C4-O3

There are no ring outliers.

19 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DA	3192	MPD	2	0
58	DS	203	MPD	3	0
59	DA	3212	PUT	1	0
63	DA	3214	PGE	1	0
62	DA	3002	EDO	1	0
63	DU	201	PGE	1	0
66	DA	3202	ACY	2	0
59	DA	3219	PUT	1	0
61	D3	102	PEG	1	0
59	DA	3213	PUT	1	0
62	DA	3194	EDO	3	0
61	DQ	201	PEG	1	0
61	DA	3201	PEG	1	0
63	DA	3225	PGE	4	0
59	DA	3223	PUT	1	0
68	DA	3220	TRS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	1642	PG4	1	0
65	DA	3185	1PE	1	0
57	DR	201	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.04	54 (3%) 47 31	65, 138, 270, 291	0
1	BA	1522/1534 (99%)	0.15	78 (5%) 33 22	86, 162, 293, 294	0
2	AB	224/224 (100%)	0.18	4 (1%) 67 49	108, 156, 231, 272	0
2	BB	224/224 (100%)	0.20	3 (1%) 75 57	138, 181, 229, 262	0
3	AC	206/206 (100%)	0.25	7 (3%) 48 32	138, 174, 208, 228	0
3	BC	206/206 (100%)	0.72	20 (9%) 13 11	223, 253, 269, 279	0
4	AD	205/205 (100%)	0.28	6 (2%) 53 35	100, 145, 174, 190	0
4	BD	205/205 (100%)	-0.27	1 (0%) 87 76	71, 100, 137, 174	0
5	AE	155/155 (100%)	-0.11	1 (0%) 85 73	83, 119, 150, 176	0
5	BE	150/155 (96%)	0.26	6 (4%) 42 28	92, 125, 168, 236	0
6	AF	106/106 (100%)	-0.10	1 (0%) 81 66	89, 126, 149, 187	0
6	BF	100/106 (94%)	0.18	3 (3%) 52 35	135, 162, 188, 196	0
7	AG	151/151 (100%)	0.35	10 (6%) 24 16	159, 186, 216, 229	0
7	BG	151/151 (100%)	0.91	17 (11%) 10 9	198, 247, 263, 268	0
8	AH	129/129 (100%)	0.01	2 (1%) 70 52	89, 122, 148, 158	0
8	BH	129/129 (100%)	0.12	3 (2%) 61 42	119, 151, 179, 192	0
9	AI	127/127 (100%)	0.70	13 (10%) 12 10	168, 196, 251, 270	0
9	BI	127/127 (100%)	0.85	16 (12%) 8 7	198, 234, 277, 283	0
10	AJ	99/99 (100%)	0.80	10 (10%) 12 10	169, 190, 228, 238	0
10	BJ	98/99 (98%)	1.12	18 (18%) 3 3	209, 248, 280, 287	0
11	AK	117/129 (90%)	0.02	3 (2%) 57 38	77, 139, 174, 190	0
11	BK	117/129 (90%)	0.65	13 (11%) 10 9	111, 166, 186, 202	0
12	AL	122/123 (99%)	0.18	3 (2%) 58 39	78, 112, 137, 178	0
12	BL	122/123 (99%)	0.20	2 (1%) 70 52	96, 121, 148, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.46	4 (3%) 47 31	167, 198, 220, 233	0
13	BM	114/114 (100%)	0.83	7 (6%) 27 19	254, 271, 288, 292	0
14	AN	100/100 (100%)	0.95	11 (11%) 10 9	166, 188, 252, 260	0
14	BN	100/100 (100%)	1.08	16 (16%) 5 4	226, 252, 282, 288	0
15	AO	88/88 (100%)	-0.03	1 (1%) 78 61	75, 109, 142, 169	0
15	BO	88/88 (100%)	0.28	1 (1%) 78 61	127, 160, 180, 197	0
16	AP	82/82 (100%)	0.59	8 (9%) 13 11	88, 128, 168, 195	0
16	BP	82/82 (100%)	0.83	8 (9%) 13 11	106, 136, 168, 184	0
17	AQ	80/80 (100%)	0.07	1 (1%) 75 57	86, 115, 149, 157	0
17	BQ	80/80 (100%)	0.37	4 (5%) 34 23	120, 159, 182, 197	0
18	AR	55/55 (100%)	0.11	1 (1%) 67 49	86, 116, 172, 194	0
18	BR	55/55 (100%)	0.21	2 (3%) 46 31	126, 143, 173, 216	0
19	AS	79/79 (100%)	0.71	8 (10%) 12 10	180, 201, 215, 222	0
19	BS	79/79 (100%)	1.14	15 (18%) 3 3	229, 265, 274, 278	0
20	AT	86/86 (100%)	0.46	4 (4%) 36 24	91, 122, 151, 161	0
20	BT	85/86 (98%)	0.87	10 (11%) 9 8	136, 157, 183, 193	0
21	AU	56/56 (100%)	0.19	1 (1%) 67 49	114, 146, 208, 223	0
21	BU	56/56 (100%)	0.41	3 (5%) 31 21	112, 151, 191, 204	0
22	C1	56/56 (100%)	1.12	12 (21%) 2 2	131, 187, 206, 219	0
22	D1	56/56 (100%)	-0.62	0 100 100	31, 57, 81, 120	0
23	C2	50/51 (98%)	0.67	5 (10%) 12 11	179, 197, 215, 237	0
23	D2	51/51 (100%)	0.07	1 (1%) 65 46	81, 98, 130, 145	0
24	C3	46/46 (100%)	1.37	9 (19%) 3 3	129, 153, 170, 177	0
24	D3	46/46 (100%)	-0.50	1 (2%) 62 43	42, 51, 71, 143	0
25	C4	64/64 (100%)	1.99	27 (42%) 0 0	145, 165, 182, 187	0
25	D4	64/64 (100%)	-0.29	0 100 100	51, 64, 78, 105	0
26	C5	38/38 (100%)	1.10	6 (15%) 5 4	126, 153, 166, 174	0
26	D5	38/38 (100%)	-0.23	0 100 100	52, 68, 95, 120	0
27	C0	58/58 (100%)	0.67	6 (10%) 12 10	123, 142, 171, 180	0
27	D0	58/58 (100%)	-0.48	2 (3%) 48 32	30, 47, 85, 112	2 (3%)
28	CB	118/120 (98%)	0.13	3 (2%) 58 39	134, 208, 253, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.67	1 (0%) 82 68	45, 87, 138, 167	0
29	CC	271/272 (99%)	0.58	27 (9%) 12 11	102, 130, 160, 176	0
29	DC	271/272 (99%)	-0.46	1 (0%) 88 79	42, 75, 106, 142	0
30	CD	209/209 (100%)	0.84	32 (15%) 5 5	100, 154, 179, 193	0
31	CA	2876/2904 (99%)	0.30	95 (3%) 49 33	92, 184, 267, 286	0
32	DD	208/209 (99%)	-0.65	1 (0%) 87 76	27, 55, 93, 121	0
33	CE	201/201 (100%)	0.83	19 (9%) 14 11	133, 193, 233, 243	0
33	DE	201/201 (100%)	-0.54	0 100 100	30, 82, 132, 150	0
34	CF	177/178 (99%)	0.30	3 (1%) 69 50	212, 233, 249, 254	0
34	DF	177/178 (99%)	0.00	3 (1%) 69 50	78, 120, 170, 188	0
35	CG	176/176 (100%)	0.27	2 (1%) 78 61	168, 196, 232, 244	0
35	DG	176/176 (100%)	-0.25	3 (1%) 69 50	57, 93, 122, 156	0
36	CH	149/149 (100%)	0.11	2 (1%) 75 57	131, 172, 197, 208	0
36	DH	149/149 (100%)	0.10	5 (3%) 48 32	82, 173, 211, 231	0
37	CJ	134/135 (99%)	0.95	21 (15%) 5 4	259, 279, 289, 291	0
37	DJ	134/135 (99%)	0.76	16 (11%) 9 8	228, 249, 266, 272	0
38	CK	142/142 (100%)	0.73	17 (11%) 9 8	115, 144, 168, 182	0
38	DK	142/142 (100%)	-0.67	0 100 100	28, 49, 82, 106	0
39	CL	122/123 (99%)	0.44	5 (4%) 41 27	105, 133, 168, 181	0
39	DL	123/123 (100%)	-0.54	1 (0%) 82 68	43, 62, 95, 135	0
40	CM	144/144 (100%)	1.05	21 (14%) 6 5	131, 195, 243, 260	0
40	DM	144/144 (100%)	-0.26	6 (4%) 40 26	26, 78, 114, 152	0
41	CN	135/136 (99%)	0.42	6 (4%) 39 25	107, 145, 176, 205	0
41	DN	135/136 (99%)	-0.66	0 100 100	24, 59, 90, 112	1 (0%)
42	CO	120/127 (94%)	0.88	14 (11%) 9 8	127, 158, 186, 233	0
42	DO	125/127 (98%)	-0.61	0 100 100	33, 52, 96, 155	0
43	CP	116/117 (99%)	0.46	4 (3%) 48 32	165, 195, 217, 223	0
43	DP	117/117 (100%)	-0.28	1 (0%) 81 66	56, 84, 121, 136	0
44	CQ	114/114 (100%)	0.52	4 (3%) 47 31	124, 150, 174, 186	0
44	DQ	114/114 (100%)	-0.40	1 (0%) 81 66	47, 72, 105, 135	0
45	CR	117/117 (100%)	1.02	17 (14%) 6 5	117, 144, 166, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.70	0 100 100	24, 41, 63, 114	0
46	CS	103/103 (100%)	0.72	12 (11%) 9 8	117, 159, 195, 202	0
46	DS	103/103 (100%)	-0.56	1 (0%) 79 63	30, 55, 92, 126	0
47	CT	110/110 (100%)	1.27	24 (21%) 2 2	140, 171, 196, 207	0
47	DT	110/110 (100%)	-0.55	1 (0%) 81 66	26, 45, 79, 128	0
48	CU	93/100 (93%)	1.11	13 (13%) 6 6	159, 194, 219, 229	0
48	DU	93/100 (93%)	-0.24	1 (1%) 78 61	51, 73, 136, 154	0
49	CV	102/103 (99%)	1.04	14 (13%) 6 6	157, 198, 231, 242	0
49	DV	102/103 (99%)	-0.28	0 100 100	57, 82, 126, 156	0
50	CW	94/94 (100%)	0.21	3 (3%) 50 33	132, 172, 186, 192	0
50	DW	94/94 (100%)	-0.36	1 (1%) 78 61	43, 73, 110, 119	0
51	CX	75/76 (98%)	0.61	6 (8%) 18 14	129, 161, 175, 206	0
51	DX	76/76 (100%)	-0.30	0 100 100	24, 62, 92, 157	1 (1%)
52	CY	77/77 (100%)	0.65	5 (6%) 25 17	120, 145, 173, 185	0
52	DY	77/77 (100%)	-0.17	0 100 100	56, 76, 111, 130	0
53	CZ	62/62 (100%)	0.64	1 (1%) 70 52	177, 199, 210, 217	0
53	DZ	62/62 (100%)	-0.22	0 100 100	64, 97, 136, 174	0
54	DI	135/135 (100%)	0.74	16 (11%) 9 8	98, 179, 244, 266	1 (0%)
55	DA	2873/2904 (98%)	-0.87	27 (0%) 81 66	29, 65, 231, 294	11 (0%)
All	All	20634/20795 (99%)	0.08	924 (4%) 38 25	24, 144, 266, 294	16 (0%)

The worst 5 of 924 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	121	U	8.8
1	BA	1243	C	8.7
1	BA	1305	G	8.5
55	DA	2120	G	8.1
40	CM	81	ASP	8.0

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	966	24/25	0.33	0.14	258,264,268,268	0
1	2MG	AA	1207	24/25	0.62	0.10	234,239,241,243	0
1	2MG	BA	1207	24/25	0.62	0.13	256,257,258,259	0
1	5MC	BA	967	21/22	0.66	0.14	258,263,266,266	0
1	2MG	AA	966	24/25	0.71	0.12	211,213,215,216	0
31	PSU	CA	1917	20/21	0.76	0.09	132,140,149,149	0
1	PSU	AA	516	20/21	0.81	0.11	135,138,139,141	0
31	3TD	CA	1915	21/22	0.82	0.08	162,165,170,171	0
1	5MC	AA	967	21/22	0.82	0.10	214,216,219,220	0
31	PSU	CA	2580	20/21	0.83	0.11	118,125,130,131	0
31	PSU	CA	955	20/21	0.85	0.11	126,130,135,136	0
31	PSU	CA	2457	20/21	0.88	0.11	118,122,126,127	0
31	PSU	CA	1911	20/21	0.88	0.06	152,158,159,161	0
41	4D4	CN	81	12/13	0.88	0.14	118,121,132,133	0
31	PSU	CA	746	20/21	0.89	0.10	135,137,142,142	0
1	PSU	BA	516	20/21	0.89	0.08	111,121,128,129	0
31	6MZ	CA	1618	23/24	0.89	0.12	160,164,168,172	0
31	PSU	CA	2504	20/21	0.90	0.11	106,114,117,120	0
31	5MC	CA	1962	21/22	0.90	0.12	103,106,110,112	0
31	2MA	CA	2503	23/24	0.90	0.12	117,126,137,138	0
1	UR3	BA	1498	21/22	0.91	0.10	118,122,126,127	0
1	2MG	BA	1516	24/25	0.91	0.09	105,110,116,117	0
31	OMG	CA	2251	24/25	0.92	0.14	111,114,115,116	0
12	D2T	BL	89	10/11	0.92	0.17	106,110,113,114	0
31	1MG	CA	745	24/25	0.92	0.09	123,126,132,134	0
1	5MC	BA	1407	21/22	0.92	0.09	111,121,124,125	0
31	6MZ	CA	2030	23/24	0.92	0.09	117,125,134,134	0
55	PSU	DA	1911	20/21	0.92	0.06	107,118,120,121	0
55	3TD	DA	1915	21/22	0.92	0.07	133,140,146,147	0
55	PSU	DA	1917	20/21	0.92	0.07	109,113,119,119	0
31	7MG	CA	2069	24/25	0.92	0.15	104,111,124,124	0
31	2MG	CA	1835	24/25	0.93	0.10	100,103,106,110	0
31	5MU	CA	1939	21/22	0.93	0.10	95,99,105,107	0
1	7MG	AA	527	24/25	0.94	0.09	102,109,115,118	0
1	7MG	BA	527	24/25	0.94	0.08	100,108,118,120	0
31	2MG	CA	2445	24/25	0.94	0.14	103,109,112,114	0
31	5MU	CA	747	21/22	0.94	0.08	131,134,136,137	0
31	OMC	CA	2498	21/22	0.94	0.12	116,124,130,132	0
12	D2T	AL	89	10/11	0.94	0.10	109,114,125,128	0
31	OMU	CA	2552	21/22	0.95	0.18	106,111,115,116	0
1	MA6	BA	1518	24/25	0.95	0.08	91,97,102,103	0
1	4OC	AA	1402	22/23	0.96	0.09	94,99,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	5MC	DA	1962	21/22	0.96	0.09	46,61,65,66	0
31	PSU	CA	2605	20/21	0.96	0.07	97,101,106,106	0
1	5MC	AA	1407	21/22	0.97	0.06	80,88,90,91	0
1	4OC	BA	1402	22/23	0.97	0.07	111,116,127,128	0
1	UR3	AA	1498	21/22	0.97	0.07	86,92,97,100	0
1	2MG	AA	1516	24/25	0.97	0.06	74,82,84,86	0
1	MA6	AA	1518	24/25	0.97	0.07	67,77,81,85	0
1	MA6	AA	1519	24/25	0.97	0.08	72,76,80,81	0
55	PSU	DA	2604	20/21	0.97	0.06	58,63,70,72	0
55	PSU	DA	2605	20/21	0.97	0.08	51,59,64,65	0
1	MA6	BA	1519	24/25	0.97	0.08	100,102,107,110	0
41	4D4	DN	81[A]	12/13	0.97	0.10	49,59,65,66	9
41	4D4	DN	81[B]	12/13	0.97	0.10	37,45,50,50	9
55	5MU	DA	1939	21/22	0.98	0.06	53,58,65,69	0
55	2MG	DA	1835	24/25	0.98	0.06	59,65,71,72	0
55	H2U	DA	2449	20/21	0.98	0.11	33,39,46,46	0
55	PSU	DA	2504	20/21	0.98	0.07	50,51,54,56	0
55	OMU	DA	2552	21/22	0.98	0.06	45,48,52,57	0
55	7MG	DA	2069	24/25	0.99	0.06	41,48,53,53	0
55	OMG	DA	2251	24/25	0.99	0.05	29,48,54,62	0
55	2MG	DA	2445	24/25	0.99	0.06	39,45,50,62	0
55	6MZ	DA	1618	23/24	0.99	0.06	34,42,47,49	0
55	PSU	DA	2457	20/21	0.99	0.05	44,46,52,53	0
55	OMC	DA	2498	21/22	0.99	0.05	37,39,46,47	0
55	2MA	DA	2503	23/24	0.99	0.05	44,51,58,62	0
32	MEQ	DD	150[A]	10/11	0.99	0.09	31,32,37,37	10
32	MEQ	DD	150[B]	10/11	0.99	0.09	35,38,44,45	10
55	PSU	DA	2580	20/21	0.99	0.06	30,35,41,43	0
55	1MG	DA	745	24/25	0.99	0.04	31,37,42,44	0
55	PSU	DA	746	20/21	0.99	0.04	38,44,46,47	0
55	5MU	DA	747	21/22	0.99	0.05	41,43,52,58	0
55	PSU	DA	955	20/21	0.99	0.06	32,35,39,41	0
55	6MZ	DA	2030	23/24	0.99	0.06	27,33,38,40	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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	3139	1/1	0.35	0.20	140,140,140,140	0
56	MG	AA	1628	1/1	0.37	0.17	137,137,137,137	0
56	MG	BA	1624	1/1	0.40	0.12	293,293,293,293	0
56	MG	AA	1606	1/1	0.46	0.18	124,124,124,124	0
56	MG	CA	3132	1/1	0.48	0.14	157,157,157,157	0
56	MG	CA	3123	1/1	0.49	0.09	142,142,142,142	0
56	MG	BA	1626	1/1	0.50	0.13	255,255,255,255	0
56	MG	CA	3124	1/1	0.53	0.16	159,159,159,159	0
56	MG	BA	1641	1/1	0.56	0.15	140,140,140,140	0
56	MG	BA	1625	1/1	0.58	0.20	288,288,288,288	0
56	MG	CA	3061	1/1	0.58	0.14	270,270,270,270	0
56	MG	CA	3155	1/1	0.60	0.17	181,181,181,181	0
56	MG	AA	1622	1/1	0.63	0.18	106,106,106,106	0
56	MG	AA	1616	1/1	0.64	0.40	105,105,105,105	0
56	MG	CA	3104	1/1	0.65	0.14	249,249,249,249	0
56	MG	DA	3130	1/1	0.66	0.21	109,109,109,109	0
56	MG	AA	1609	1/1	0.67	0.28	107,107,107,107	0
56	MG	CA	3077	1/1	0.68	0.12	244,244,244,244	0
56	MG	AA	1608	1/1	0.68	0.22	128,128,128,128	0
56	MG	AA	1660	1/1	0.69	0.12	283,283,283,283	0
56	MG	CA	3140	1/1	0.69	0.15	108,108,108,108	0
56	MG	CA	3075	1/1	0.70	0.20	231,231,231,231	0
56	MG	CA	3007	1/1	0.70	0.06	257,257,257,257	0
56	MG	CA	3126	1/1	0.71	0.14	115,115,115,115	0
56	MG	DA	3171	1/1	0.71	0.23	111,111,111,111	0
61	PEG	DP	201	7/7	0.71	0.15	149,153,164,165	0
62	EDO	DA	3003	4/4	0.72	0.27	135,137,140,141	0
56	MG	BA	1604	1/1	0.73	0.12	257,257,257,257	0
56	MG	AA	1605	1/1	0.73	0.27	87,87,87,87	0
56	MG	DA	3168	1/1	0.73	0.17	119,119,119,119	0
56	MG	CA	3130	1/1	0.75	0.16	84,84,84,84	0
56	MG	CA	3115	1/1	0.75	0.19	111,111,111,111	0
56	MG	DA	3062	1/1	0.76	0.09	269,269,269,269	0
56	MG	AA	1626	1/1	0.76	0.14	120,120,120,120	0
56	MG	CA	3021	1/1	0.76	0.29	253,253,253,253	0
56	MG	CA	3060	1/1	0.76	0.10	238,238,238,238	0
56	MG	CA	3142	1/1	0.76	0.10	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1658	1/1	0.76	0.13	212,212,212,212	0
56	MG	BA	1607	1/1	0.77	0.14	280,280,280,280	0
56	MG	BA	1619	1/1	0.77	0.19	228,228,228,228	0
56	MG	CA	3056	1/1	0.77	0.61	77,77,77,77	0
56	MG	CA	3014	1/1	0.78	0.11	273,273,273,273	0
56	MG	DA	3152	1/1	0.78	0.29	115,115,115,115	0
56	MG	CA	3148	1/1	0.79	0.28	43,43,43,43	1
56	MG	CA	3112	1/1	0.79	0.12	103,103,103,103	0
56	MG	BA	1629	1/1	0.79	0.30	217,217,217,217	0
59	PUT	DA	3221	6/6	0.80	0.20	112,120,122,122	0
56	MG	CA	3111	1/1	0.80	0.13	103,103,103,103	0
58	MPD	DE	301	8/8	0.80	0.20	172,174,179,179	0
56	MG	CA	3009	1/1	0.81	0.15	259,259,259,259	0
56	MG	DA	3176	1/1	0.81	0.20	81,81,81,81	0
56	MG	AA	1603	1/1	0.81	0.19	111,111,111,111	0
56	MG	CA	3083	1/1	0.81	0.12	254,254,254,254	0
56	MG	CA	3145	1/1	0.81	0.33	78,78,78,78	0
56	MG	CA	3067	1/1	0.81	0.08	274,274,274,274	0
56	MG	CA	3154	1/1	0.82	0.16	110,110,110,110	0
56	MG	BA	1638	1/1	0.82	0.23	65,65,65,65	0
56	MG	AA	1627	1/1	0.82	0.13	115,115,115,115	0
62	EDO	DB	210	4/4	0.82	0.36	125,126,126,127	0
56	MG	BA	1623	1/1	0.82	0.30	277,277,277,277	0
56	MG	CA	3002	1/1	0.83	0.14	224,224,224,224	0
56	MG	CA	3003	1/1	0.83	0.32	272,272,272,272	0
56	MG	CA	3110	1/1	0.83	0.16	129,129,129,129	0
59	PUT	AA	1673	6/6	0.83	0.10	142,145,148,150	0
56	MG	DA	3131	1/1	0.83	0.30	83,83,83,83	0
56	MG	DA	3147	1/1	0.83	0.17	108,108,108,108	0
56	MG	CA	3135	1/1	0.83	0.11	78,78,78,78	0
56	MG	AA	1615	1/1	0.83	0.69	129,129,129,129	0
56	MG	CA	3072	1/1	0.84	0.18	258,258,258,258	0
56	MG	AA	1623	1/1	0.84	0.22	87,87,87,87	0
56	MG	CA	3026	1/1	0.84	0.21	245,245,245,245	0
56	MG	BA	1639	1/1	0.84	0.07	117,117,117,117	0
56	MG	BA	1606	1/1	0.85	0.10	270,270,270,270	0
56	MG	CB	203	1/1	0.85	0.09	237,237,237,237	0
56	MG	CA	3105	1/1	0.85	0.09	252,252,252,252	0
58	MPD	DK	201	8/8	0.85	0.11	125,126,127,127	0
56	MG	CA	3125	1/1	0.85	0.10	136,136,136,136	0
56	MG	DA	3137	1/1	0.85	0.13	61,61,61,61	0
61	PEG	AL	201	7/7	0.85	0.12	132,133,135,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3034	1/1	0.85	0.16	228,228,228,228	0
61	PEG	DQ	201	7/7	0.85	0.28	162,166,170,170	0
56	MG	CA	3001	1/1	0.85	0.15	291,291,291,291	0
56	MG	BA	1635	1/1	0.85	0.12	209,209,209,209	0
56	MG	CA	3048	1/1	0.86	0.11	147,147,147,147	0
56	MG	CA	3137	1/1	0.86	0.16	164,164,164,164	0
56	MG	CA	3028	1/1	0.86	0.11	284,284,284,284	0
56	MG	CA	3129	1/1	0.86	0.13	135,135,135,135	0
56	MG	AA	1659	1/1	0.86	0.07	273,273,273,273	0
56	MG	CA	3087	1/1	0.86	0.13	232,232,232,232	0
56	MG	CA	3146	1/1	0.86	0.08	174,174,174,174	0
56	MG	CA	3038	1/1	0.87	0.09	252,252,252,252	0
56	MG	BA	1627	1/1	0.87	0.28	203,203,203,203	0
56	MG	DA	3170	1/1	0.87	0.21	59,59,59,59	0
56	MG	CA	3152	1/1	0.87	0.07	160,160,160,160	0
56	MG	AA	1618	1/1	0.87	0.44	172,172,172,172	0
57	PG4	AA	1670	13/13	0.87	0.12	111,116,118,119	0
56	MG	AA	1604	1/1	0.87	0.26	79,79,79,79	0
56	MG	CA	3156	1/1	0.87	0.11	263,263,263,263	0
56	MG	CA	3138	1/1	0.87	0.13	98,98,98,98	0
56	MG	BA	1637	1/1	0.87	0.34	121,121,121,121	0
56	MG	AA	1613	1/1	0.87	0.14	80,80,80,80	0
56	MG	CA	3109	1/1	0.87	0.10	67,67,67,67	0
56	MG	DA	3138	1/1	0.87	0.38	29,29,29,29	1
56	MG	DA	3142	1/1	0.87	0.32	80,80,80,80	0
56	MG	AA	1665	1/1	0.87	0.23	274,274,274,274	0
56	MG	CA	3016	1/1	0.88	0.34	218,218,218,218	0
56	MG	AA	1601	1/1	0.88	0.24	62,62,62,62	0
56	MG	CA	3022	1/1	0.88	0.15	259,259,259,259	0
56	MG	DA	3123	1/1	0.88	0.18	84,84,84,84	0
56	MG	DA	3127	1/1	0.88	0.34	69,69,69,69	0
56	MG	CA	3088	1/1	0.88	0.19	86,86,86,86	0
58	MPD	DA	3204	8/8	0.88	0.16	116,119,125,127	0
59	PUT	AA	1672	6/6	0.88	0.23	149,150,150,150	0
56	MG	CA	3141	1/1	0.88	0.23	78,78,78,78	0
59	PUT	AA	1674	6/6	0.88	0.26	109,113,116,117	0
56	MG	AA	1630	1/1	0.88	0.09	205,205,205,205	0
56	MG	CB	201	1/1	0.88	0.06	235,235,235,235	0
56	MG	CA	3107	1/1	0.88	0.20	81,81,81,81	0
56	MG	CA	3071	1/1	0.88	0.09	228,228,228,228	0
56	MG	AA	1642	1/1	0.88	0.13	275,275,275,275	0
56	MG	AA	1624	1/1	0.88	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
68	TRS	DA	3220	8/8	0.88	0.15	184,187,190,191	0
56	MG	CA	3134	1/1	0.89	0.08	167,167,167,167	0
56	MG	CA	3070	1/1	0.89	0.11	234,234,234,234	0
56	MG	DA	3008	1/1	0.89	0.10	280,280,280,280	0
57	PG4	BA	1642	13/13	0.89	0.10	113,117,132,132	0
56	MG	CA	3118	1/1	0.89	0.22	87,87,87,87	0
56	MG	CA	3119	1/1	0.89	0.16	100,100,100,100	0
58	MPD	DA	3190	8/8	0.89	0.12	100,102,103,106	0
56	MG	CA	3122	1/1	0.89	0.16	89,89,89,89	0
56	MG	BA	1633	1/1	0.89	0.13	237,237,237,237	0
56	MG	CA	3023	1/1	0.89	0.20	255,255,255,255	0
56	MG	CA	3004	1/1	0.89	0.09	192,192,192,192	0
59	PUT	AA	1675	6/6	0.89	0.22	172,174,174,175	0
56	MG	AA	1614	1/1	0.89	0.16	83,83,83,83	0
56	MG	CA	3032	1/1	0.89	0.06	197,197,197,197	0
56	MG	CA	3147	1/1	0.89	0.17	36,36,36,36	1
56	MG	CA	3084	1/1	0.89	0.10	172,172,172,172	0
56	MG	DA	3153	1/1	0.89	0.59	102,102,102,102	0
62	EDO	DA	3002	4/4	0.89	0.48	176,176,176,177	0
56	MG	CA	3131	1/1	0.89	0.13	123,123,123,123	0
66	ACY	DA	3196	4/4	0.89	0.14	61,69,69,72	0
56	MG	CA	3008	1/1	0.89	0.12	202,202,202,202	0
56	MG	AA	1656	1/1	0.90	0.09	274,274,274,274	0
56	MG	CA	3010	1/1	0.90	0.12	259,259,259,259	0
56	MG	CA	3121	1/1	0.90	0.13	83,83,83,83	0
56	MG	BA	1636	1/1	0.90	0.16	77,77,77,77	0
56	MG	AA	1664	1/1	0.90	0.14	265,265,265,265	0
56	MG	AA	1612	1/1	0.90	0.14	77,77,77,77	0
56	MG	DA	3120	1/1	0.90	0.26	66,66,66,66	0
56	MG	AA	1669	1/1	0.90	0.14	239,239,239,239	0
56	MG	AA	1621	1/1	0.90	0.38	97,97,97,97	0
56	MG	BA	1634	1/1	0.90	0.11	216,216,216,216	0
57	PG4	DQ	202	13/13	0.90	0.10	84,89,100,101	0
56	MG	CA	3113	1/1	0.90	0.26	76,76,76,76	0
56	MG	CA	3064	1/1	0.90	0.10	271,271,271,271	0
56	MG	CA	3116	1/1	0.90	0.15	92,92,92,92	0
56	MG	CA	3150	1/1	0.91	0.14	79,79,79,79	0
58	MPD	DN	201	8/8	0.91	0.13	109,117,119,121	0
56	MG	BA	1612	1/1	0.91	0.34	262,262,262,262	0
56	MG	CA	3076	1/1	0.91	0.10	218,218,218,218	0
56	MG	AA	1639	1/1	0.91	0.10	225,225,225,225	0
56	MG	CA	3006	1/1	0.91	0.07	221,221,221,221	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3068	1/1	0.91	0.13	174,174,174,174	0
56	MG	DA	3160	1/1	0.91	0.25	64,64,64,64	0
56	MG	CA	3051	1/1	0.91	0.15	248,248,248,248	0
56	MG	AA	1625	1/1	0.91	0.24	83,83,83,83	0
56	MG	CA	3090	1/1	0.91	0.09	187,187,187,187	0
56	MG	DA	3126	1/1	0.91	0.21	77,77,77,77	0
56	MG	CA	3093	1/1	0.91	0.06	143,143,143,143	0
56	MG	DA	3128	1/1	0.91	0.37	57,57,57,57	0
56	MG	CA	3099	1/1	0.91	0.08	174,174,174,174	0
57	PG4	DA	3193	13/13	0.91	0.22	109,113,119,120	0
56	MG	AA	1663	1/1	0.91	0.10	230,230,230,230	0
56	MG	AA	1607	1/1	0.92	0.17	90,90,90,90	0
56	MG	CA	3092	1/1	0.92	0.05	163,163,163,163	0
56	MG	DA	3111	1/1	0.92	0.24	283,283,283,283	0
56	MG	DA	3155	1/1	0.92	0.18	86,86,86,86	0
56	MG	DA	3157	1/1	0.92	0.20	74,74,74,74	0
56	MG	AA	1636	1/1	0.92	0.13	209,209,209,209	0
56	MG	AA	1661	1/1	0.92	0.21	223,223,223,223	0
56	MG	CA	3100	1/1	0.92	0.18	243,243,243,243	0
59	PUT	DA	3195	6/6	0.92	0.27	100,104,108,108	0
59	PUT	DA	3205	6/6	0.92	0.37	106,108,108,109	0
56	MG	BA	1614	1/1	0.92	0.11	217,217,217,217	0
56	MG	DA	3172	1/1	0.92	0.11	85,85,85,85	0
56	MG	CA	3082	1/1	0.92	0.12	168,168,168,168	0
56	MG	CA	3039	1/1	0.92	0.10	190,190,190,190	0
61	PEG	DA	3226	7/7	0.92	0.39	125,126,131,131	0
62	EDO	D1	101	4/4	0.92	0.09	70,71,73,75	0
56	MG	BA	1603	1/1	0.92	0.07	278,278,278,278	0
56	MG	AA	1610	1/1	0.92	0.15	99,99,99,99	0
56	MG	CA	3054	1/1	0.92	0.08	122,122,122,122	0
63	PGE	D1	102	10/10	0.92	0.18	142,145,152,153	0
63	PGE	DA	3214	10/10	0.92	0.18	67,87,91,92	0
64	SPD	DA	3183	10/10	0.92	0.12	80,95,97,98	0
58	MPD	AA	1676	8/8	0.92	0.29	145,146,148,148	0
56	MG	DA	3006	1/1	0.92	0.20	266,266,266,266	0
59	PUT	DA	3184	6/6	0.93	0.22	65,70,74,74	0
56	MG	CA	3149	1/1	0.93	0.21	76,76,76,76	0
57	PG4	DR	201	13/13	0.93	0.26	156,168,173,173	0
59	PUT	DA	3212	6/6	0.93	0.24	114,115,117,117	0
56	MG	DA	3158	1/1	0.93	0.10	107,107,107,107	0
56	MG	CA	3036	1/1	0.93	0.09	227,227,227,227	0
61	PEG	DL	201	7/7	0.93	0.14	102,103,109,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3162	1/1	0.93	0.07	79,79,79,79	0
58	MPD	DE	302	8/8	0.93	0.18	101,102,103,104	0
61	PEG	DA	3199	7/7	0.93	0.18	99,106,112,113	0
61	PEG	DA	3200	7/7	0.93	0.23	124,124,125,125	0
56	MG	DA	3079	1/1	0.93	0.07	179,179,179,179	0
56	MG	CA	3019	1/1	0.93	0.07	87,87,87,87	0
62	EDO	D0	101	4/4	0.93	0.17	79,80,85,89	0
58	MPD	DT	201	8/8	0.93	0.23	110,115,125,126	0
56	MG	AA	1654	1/1	0.93	0.16	178,178,178,178	0
56	MG	CA	3081	1/1	0.93	0.10	254,254,254,254	0
58	MPD	DA	3207	8/8	0.93	0.17	121,125,128,129	0
63	PGE	DD	301	10/10	0.93	0.21	120,122,129,130	0
63	PGE	DS	201	10/10	0.93	0.09	96,99,101,101	0
56	MG	AA	1634	1/1	0.93	0.18	179,179,179,179	0
56	MG	DA	3180	1/1	0.93	0.11	77,77,77,77	0
56	MG	DR	202	1/1	0.93	0.20	269,269,269,269	0
67	GUN	DA	3211	11/11	0.93	0.16	116,122,123,124	0
56	MG	BA	1609	1/1	0.93	0.12	156,156,156,156	0
56	MG	CA	3106	1/1	0.94	0.08	74,74,74,74	0
59	PUT	DA	3219	6/6	0.94	0.19	100,102,103,103	0
56	MG	DA	3001	1/1	0.94	0.16	47,47,47,47	0
59	PUT	DA	3222	6/6	0.94	0.16	77,81,83,83	0
56	MG	DA	3146	1/1	0.94	0.28	76,76,76,76	0
61	PEG	D3	102	7/7	0.94	0.15	136,138,140,140	0
57	PG4	DA	3216	13/13	0.94	0.13	111,122,132,134	0
58	MPD	AA	1671	8/8	0.94	0.20	143,144,147,148	0
56	MG	CA	3047	1/1	0.94	0.10	100,100,100,100	0
56	MG	CA	3018	1/1	0.94	0.08	147,147,147,147	0
56	MG	CA	3031	1/1	0.94	0.05	128,128,128,128	0
61	PEG	DA	3201	7/7	0.94	0.27	146,150,151,152	0
56	MG	AA	1644	1/1	0.94	0.13	180,180,180,180	0
61	PEG	DA	3227	7/7	0.94	0.20	109,114,120,120	0
56	MG	CA	3127	1/1	0.94	0.17	73,73,73,73	0
56	MG	AA	1662	1/1	0.94	0.07	164,164,164,164	0
58	MPD	DT	202	8/8	0.94	0.23	138,139,144,145	0
56	MG	DA	3121	1/1	0.94	0.11	111,111,111,111	0
56	MG	CA	3059	1/1	0.94	0.08	118,118,118,118	0
62	EDO	DA	3209	4/4	0.94	0.32	94,96,98,99	0
56	MG	CA	3005	1/1	0.94	0.08	233,233,233,233	0
63	PGE	D3	101	10/10	0.94	0.15	121,123,125,126	0
56	MG	AA	1602	1/1	0.94	0.12	78,78,78,78	0
56	MG	CA	3117	1/1	0.94	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3129	1/1	0.94	0.18	51,51,51,51	0
63	PGE	DA	3225	10/10	0.94	0.20	100,120,131,131	0
56	MG	CA	3080	1/1	0.94	0.10	108,108,108,108	0
56	MG	CA	3062	1/1	0.94	0.07	168,168,168,168	0
56	MG	DA	3134	1/1	0.94	0.17	98,98,98,98	0
56	MG	AA	1617	1/1	0.94	0.14	88,88,88,88	0
56	MG	DA	3141	1/1	0.95	0.24	80,80,80,80	0
56	MG	CA	3073	1/1	0.95	0.06	139,139,139,139	0
56	MG	DA	3144	1/1	0.95	0.07	79,79,79,79	0
56	MG	AA	1657	1/1	0.95	0.17	134,134,134,134	0
56	MG	CA	3063	1/1	0.95	0.09	155,155,155,155	0
56	MG	DA	3151	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	1618	1/1	0.95	0.06	172,172,172,172	0
56	MG	DA	3080	1/1	0.95	0.13	195,195,195,195	0
61	PEG	DA	3218	7/7	0.95	0.26	179,180,181,181	0
56	MG	CA	3055	1/1	0.95	0.07	193,193,193,193	0
56	MG	CA	3094	1/1	0.95	0.09	132,132,132,132	0
56	MG	CA	3128	1/1	0.95	0.12	116,116,116,116	0
56	MG	CA	3114	1/1	0.95	0.16	67,67,67,67	0
56	MG	BA	1630	1/1	0.95	0.09	197,197,197,197	0
62	EDO	DB	211	4/4	0.95	0.25	131,131,132,133	0
56	MG	DA	3163	1/1	0.95	0.16	87,87,87,87	0
56	MG	DA	3166	1/1	0.95	0.11	74,74,74,74	0
62	EDO	DA	3197	4/4	0.95	0.09	75,76,77,77	0
56	MG	BA	1602	1/1	0.95	0.05	102,102,102,102	0
62	EDO	DA	3215	4/4	0.95	0.10	64,67,70,73	0
56	MG	DA	3169	1/1	0.95	0.09	41,41,41,41	0
56	MG	CA	3101	1/1	0.95	0.05	239,239,239,239	0
56	MG	CA	3133	1/1	0.95	0.08	110,110,110,110	0
56	MG	BA	1620	1/1	0.95	0.08	172,172,172,172	0
56	MG	DA	3175	1/1	0.95	0.26	115,115,115,115	0
56	MG	BA	1640	1/1	0.95	0.07	103,103,103,103	0
56	MG	DA	3178	1/1	0.95	0.17	93,93,93,93	0
56	MG	CA	3120	1/1	0.95	0.10	130,130,130,130	0
56	MG	DB	207	1/1	0.95	0.17	92,92,92,92	0
56	MG	CA	3086	1/1	0.95	0.08	106,106,106,106	0
60	ZN	C5	101	1/1	0.96	0.06	175,175,175,175	0
56	MG	AA	1620	1/1	0.96	0.23	116,116,116,116	0
57	PG4	DS	202	13/13	0.96	0.10	72,73,85,86	0
56	MG	DA	3125	1/1	0.96	0.09	51,51,51,51	0
56	MG	CA	3103	1/1	0.96	0.06	176,176,176,176	0
56	MG	BA	1605	1/1	0.96	0.05	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	205	1/1	0.96	0.40	148,148,148,148	0
56	MG	DA	3159	1/1	0.96	0.12	131,131,131,131	0
56	MG	CA	3050	1/1	0.96	0.07	166,166,166,166	0
56	MG	BA	1622	1/1	0.96	0.07	240,240,240,240	0
56	MG	BA	1628	1/1	0.96	0.05	120,120,120,120	0
56	MG	DA	3164	1/1	0.96	0.18	78,78,78,78	0
56	MG	DA	3132	1/1	0.96	0.12	56,56,56,56	0
56	MG	DA	3167	1/1	0.96	0.14	97,97,97,97	0
58	MPD	DA	3192	8/8	0.96	0.22	84,90,92,94	0
56	MG	CA	3108	1/1	0.96	0.09	89,89,89,89	0
56	MG	DA	3136	1/1	0.96	0.10	72,72,72,72	0
56	MG	CA	3078	1/1	0.96	0.07	198,198,198,198	0
62	EDO	DA	3194	4/4	0.96	0.13	89,90,90,90	0
56	MG	CA	3037	1/1	0.96	0.12	234,234,234,234	0
62	EDO	DA	3198	4/4	0.96	0.25	109,110,112,112	0
56	MG	AA	1655	1/1	0.96	0.04	152,152,152,152	0
56	MG	DA	3098	1/1	0.96	0.16	246,246,246,246	0
59	PUT	DM	201	6/6	0.96	0.16	63,66,74,75	0
56	MG	CA	3151	1/1	0.96	0.12	102,102,102,102	0
59	PUT	DA	3189	6/6	0.96	0.07	49,55,59,62	0
56	MG	DA	3177	1/1	0.96	0.14	52,52,52,52	0
63	PGE	DU	201	10/10	0.96	0.14	135,141,147,147	0
56	MG	DA	3117	1/1	0.96	0.14	70,70,70,70	0
63	PGE	DA	3217	10/10	0.96	0.11	87,89,93,94	0
56	MG	CA	3057	1/1	0.96	0.06	111,111,111,111	0
59	PUT	DA	3213	6/6	0.96	0.22	156,156,157,157	0
64	SPD	DA	3206	10/10	0.96	0.23	142,143,144,144	0
65	1PE	DA	3185	16/16	0.96	0.10	74,89,123,123	0
56	MG	DA	3148	1/1	0.96	0.16	67,67,67,67	0
56	MG	DA	3149	1/1	0.96	0.08	96,96,96,96	0
56	MG	AA	1647	1/1	0.96	0.06	145,145,145,145	0
59	PUT	DA	3223	6/6	0.97	0.13	75,81,84,84	0
56	MG	DA	3182	1/1	0.97	0.07	55,55,55,55	0
56	MG	CA	3030	1/1	0.97	0.05	82,82,82,82	0
56	MG	CA	3017	1/1	0.97	0.10	192,192,192,192	0
56	MG	DA	3054	1/1	0.97	0.09	167,167,167,167	0
56	MG	CA	3053	1/1	0.97	0.06	86,86,86,86	0
56	MG	AA	1645	1/1	0.97	0.05	70,70,70,70	0
56	MG	AA	1632	1/1	0.97	0.07	162,162,162,162	0
56	MG	DA	3095	1/1	0.97	0.10	65,65,65,65	0
56	MG	CA	3074	1/1	0.97	0.06	145,145,145,145	0
56	MG	DA	3154	1/1	0.97	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3143	1/1	0.97	0.04	72,72,72,72	0
56	MG	BA	1608	1/1	0.97	0.08	144,144,144,144	0
56	MG	AA	1650	1/1	0.97	0.11	115,115,115,115	0
56	MG	CA	3058	1/1	0.97	0.08	124,124,124,124	0
58	MPD	DS	203	8/8	0.97	0.16	62,64,65,67	0
56	MG	AA	1611	1/1	0.97	0.07	133,133,133,133	0
56	MG	DA	3161	1/1	0.97	0.13	73,73,73,73	0
56	MG	CA	3079	1/1	0.97	0.07	131,131,131,131	0
56	MG	CA	3025	1/1	0.97	0.06	133,133,133,133	0
56	MG	CA	3040	1/1	0.97	0.04	122,122,122,122	0
56	MG	CA	3042	1/1	0.97	0.06	96,96,96,96	0
58	MPD	DA	3210	8/8	0.97	0.16	110,118,123,125	0
56	MG	CA	3153	1/1	0.97	0.12	77,77,77,77	0
56	MG	CA	3045	1/1	0.97	0.05	167,167,167,167	0
56	MG	AA	1619	1/1	0.97	0.15	122,122,122,122	0
56	MG	CA	3085	1/1	0.97	0.04	116,116,116,116	0
56	MG	CA	3065	1/1	0.97	0.08	115,115,115,115	0
56	MG	DB	201	1/1	0.97	0.06	121,121,121,121	0
59	PUT	DA	3188	6/6	0.97	0.22	89,93,93,94	0
56	MG	DA	3173	1/1	0.97	0.18	100,100,100,100	0
56	MG	CA	3066	1/1	0.97	0.08	91,91,91,91	0
56	MG	BA	1615	1/1	0.97	0.05	103,103,103,103	0
64	SPD	DA	3187	10/10	0.97	0.14	78,82,85,85	0
56	MG	DA	3139	1/1	0.97	0.07	42,42,42,42	0
64	SPD	DA	3224	10/10	0.97	0.11	58,71,88,88	0
56	MG	DB	208	1/1	0.97	0.07	57,57,57,57	0
65	1PE	DA	3203	16/16	0.97	0.13	98,105,109,109	0
56	MG	DA	3179	1/1	0.97	0.07	85,85,85,85	0
56	MG	CA	3136	1/1	0.97	0.14	107,107,107,107	0
56	MG	DA	3181	1/1	0.97	0.15	66,66,66,66	0
56	MG	BA	1617	1/1	0.98	0.05	165,165,165,165	0
56	MG	DA	3085	1/1	0.98	0.07	100,100,100,100	0
56	MG	DA	3165	1/1	0.98	0.23	63,63,63,63	0
56	MG	DA	3088	1/1	0.98	0.06	75,75,75,75	0
56	MG	AA	1635	1/1	0.98	0.06	220,220,220,220	0
56	MG	DA	3097	1/1	0.98	0.04	75,75,75,75	0
56	MG	AA	1646	1/1	0.98	0.06	80,80,80,80	0
56	MG	CA	3020	1/1	0.98	0.06	116,116,116,116	0
56	MG	CA	3144	1/1	0.98	0.06	66,66,66,66	0
60	ZN	AB	301	1/1	0.98	0.03	165,165,165,165	0
56	MG	CA	3044	1/1	0.98	0.05	113,113,113,113	0
56	MG	AA	1641	1/1	0.98	0.05	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3174	1/1	0.98	0.05	87,87,87,87	0
56	MG	CA	3091	1/1	0.98	0.05	81,81,81,81	0
56	MG	DA	3124	1/1	0.98	0.13	90,90,90,90	0
56	MG	CA	3046	1/1	0.98	0.07	99,99,99,99	0
56	MG	CA	3069	1/1	0.98	0.04	107,107,107,107	0
56	MG	AA	1668	1/1	0.98	0.11	110,110,110,110	0
56	MG	CA	3095	1/1	0.98	0.05	174,174,174,174	0
56	MG	CA	3097	1/1	0.98	0.09	112,112,112,112	0
56	MG	CA	3098	1/1	0.98	0.04	98,98,98,98	0
56	MG	DA	3230	1/1	0.98	0.05	76,76,76,76	0
56	MG	AA	1633	1/1	0.98	0.04	116,116,116,116	0
56	MG	CA	3024	1/1	0.98	0.11	85,85,85,85	0
56	MG	DA	3133	1/1	0.98	0.06	52,52,52,52	0
56	MG	BA	1610	1/1	0.98	0.04	107,107,107,107	0
56	MG	DM	202	1/1	0.98	0.07	90,90,90,90	0
56	MG	CA	3102	1/1	0.98	0.03	99,99,99,99	0
56	MG	CA	3052	1/1	0.98	0.06	124,124,124,124	0
56	MG	AA	1651	1/1	0.98	0.07	75,75,75,75	0
56	MG	DB	206	1/1	0.98	0.09	73,73,73,73	0
62	EDO	DA	3208	4/4	0.98	0.22	111,113,113,113	0
56	MG	BA	1613	1/1	0.98	0.14	149,149,149,149	0
56	MG	DA	3143	1/1	0.98	0.10	63,63,63,63	0
56	MG	CA	3029	1/1	0.98	0.05	143,143,143,143	0
56	MG	DB	209	1/1	0.98	0.10	83,83,83,83	0
56	MG	AA	1643	1/1	0.98	0.05	70,70,70,70	0
56	MG	CA	3011	1/1	0.98	0.05	95,95,95,95	0
56	MG	CA	3012	1/1	0.98	0.06	115,115,115,115	0
63	PGE	DA	3186	10/10	0.98	0.07	58,65,71,71	0
56	MG	DA	3012	1/1	0.98	0.07	141,141,141,141	0
56	MG	DA	3026	1/1	0.98	0.09	228,228,228,228	0
56	MG	DA	3037	1/1	0.98	0.09	13,13,13,13	0
56	MG	DA	3042	1/1	0.98	0.06	87,87,87,87	0
56	MG	DA	3044	1/1	0.98	0.09	124,124,124,124	0
56	MG	DA	3156	1/1	0.98	0.12	83,83,83,83	0
56	MG	DA	3052	1/1	0.98	0.08	251,251,251,251	0
56	MG	CA	3013	1/1	0.98	0.04	71,71,71,71	0
56	MG	AA	1638	1/1	0.98	0.04	142,142,142,142	0
66	ACY	DA	3191	4/4	0.98	0.09	79,80,81,81	0
56	MG	DA	3067	1/1	0.98	0.05	75,75,75,75	0
66	ACY	DA	3202	4/4	0.98	0.10	93,96,96,97	0
56	MG	DA	3070	1/1	0.98	0.08	151,151,151,151	0
56	MG	BA	1616	1/1	0.98	0.07	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3030	1/1	0.99	0.04	88,88,88,88	0
56	MG	DA	3031	1/1	0.99	0.03	51,51,51,51	0
56	MG	AA	1631	1/1	0.99	0.03	75,75,75,75	0
56	MG	CA	3043	1/1	0.99	0.03	90,90,90,90	0
56	MG	DA	3135	1/1	0.99	0.07	146,146,146,146	0
56	MG	CA	3096	1/1	0.99	0.03	89,89,89,89	0
56	MG	CA	3027	1/1	0.99	0.06	88,88,88,88	0
56	MG	DA	3231	1/1	0.99	0.07	70,70,70,70	0
56	MG	DA	3053	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3015	1/1	0.99	0.14	84,84,84,84	0
56	MG	DA	3140	1/1	0.99	0.07	51,51,51,51	0
56	MG	DA	3055	1/1	0.99	0.07	52,52,52,52	0
56	MG	AA	1666	1/1	0.99	0.05	100,100,100,100	0
56	MG	DA	3063	1/1	0.99	0.08	111,111,111,111	0
56	MG	BA	1611	1/1	0.99	0.03	84,84,84,84	0
56	MG	DA	3069	1/1	0.99	0.07	64,64,64,64	0
56	MG	AA	1667	1/1	0.99	0.09	76,76,76,76	0
56	MG	DA	3071	1/1	0.99	0.03	56,56,56,56	0
56	MG	DA	3074	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3049	1/1	0.99	0.05	53,53,53,53	0
56	MG	DB	203	1/1	0.99	0.08	88,88,88,88	0
56	MG	DA	3084	1/1	0.99	0.09	55,55,55,55	0
56	MG	DB	204	1/1	0.99	0.03	85,85,85,85	0
56	MG	AA	1648	1/1	0.99	0.03	84,84,84,84	0
56	MG	CA	3033	1/1	0.99	0.11	150,150,150,150	0
56	MG	BA	1631	1/1	0.99	0.07	132,132,132,132	0
56	MG	BA	1632	1/1	0.99	0.06	74,74,74,74	0
56	MG	DA	3099	1/1	0.99	0.07	45,45,45,45	0
56	MG	DA	3103	1/1	0.99	0.02	59,59,59,59	0
56	MG	CB	202	1/1	0.99	0.08	116,116,116,116	0
56	MG	DA	3113	1/1	0.99	0.08	113,113,113,113	0
56	MG	CA	3089	1/1	0.99	0.08	64,64,64,64	0
56	MG	DA	3118	1/1	0.99	0.03	31,31,31,31	0
56	MG	DA	3119	1/1	0.99	0.08	41,41,41,41	0
56	MG	DA	3005	1/1	0.99	0.07	67,67,67,67	0
56	MG	AA	1640	1/1	0.99	0.05	131,131,131,131	0
56	MG	DA	3122	1/1	0.99	0.29	48,48,48,48	0
56	MG	DA	3007	1/1	0.99	0.04	127,127,127,127	0
56	MG	AA	1677	1/1	0.99	0.04	101,101,101,101	0
56	MG	BA	1601	1/1	0.99	0.04	135,135,135,135	0
56	MG	DA	3015	1/1	0.99	0.03	78,78,78,78	0
56	MG	DA	3018	1/1	0.99	0.07	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3041	1/1	0.99	0.09	50,50,50,50	0
56	MG	DA	3027	1/1	0.99	0.02	49,49,49,49	0
56	MG	DA	3028	1/1	0.99	0.04	116,116,116,116	0
56	MG	AA	1629	1/1	1.00	0.06	110,110,110,110	0
56	MG	DA	3096	1/1	1.00	0.03	28,28,28,28	0
56	MG	DA	3228	1/1	1.00	0.01	18,18,18,18	0
56	MG	DA	3229	1/1	1.00	0.05	107,107,107,107	0
56	MG	AA	1652	1/1	1.00	0.12	42,42,42,42	0
56	MG	DA	3004	1/1	1.00	0.03	149,149,149,149	0
56	MG	DA	3029	1/1	1.00	0.08	44,44,44,44	0
56	MG	DA	3100	1/1	1.00	0.03	34,34,34,34	0
56	MG	DA	3101	1/1	1.00	0.03	90,90,90,90	0
56	MG	DA	3102	1/1	1.00	0.01	32,32,32,32	0
56	MG	DB	202	1/1	1.00	0.03	56,56,56,56	0
56	MG	DA	3104	1/1	1.00	0.07	43,43,43,43	0
56	MG	DA	3105	1/1	1.00	0.04	33,33,33,33	0
56	MG	DA	3106	1/1	1.00	0.07	45,45,45,45	0
56	MG	DA	3107	1/1	1.00	0.02	50,50,50,50	0
56	MG	DA	3108	1/1	1.00	0.02	36,36,36,36	0
56	MG	DA	3109	1/1	1.00	0.02	38,38,38,38	0
56	MG	DA	3110	1/1	1.00	0.02	31,31,31,31	0
56	MG	AA	1653	1/1	1.00	0.02	108,108,108,108	0
56	MG	DA	3112	1/1	1.00	0.01	46,46,46,46	0
56	MG	DA	3032	1/1	1.00	0.04	33,33,33,33	0
56	MG	DA	3114	1/1	1.00	0.02	52,52,52,52	0
56	MG	DA	3115	1/1	1.00	0.02	52,52,52,52	0
56	MG	DA	3116	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3033	1/1	1.00	0.02	46,46,46,46	0
56	MG	DA	3034	1/1	1.00	0.03	44,44,44,44	0
56	MG	DA	3035	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3036	1/1	1.00	0.04	32,32,32,32	0
56	MG	CA	3035	1/1	1.00	0.11	100,100,100,100	0
56	MG	DA	3038	1/1	1.00	0.02	35,35,35,35	0
56	MG	DA	3039	1/1	1.00	0.04	34,34,34,34	0
56	MG	DA	3040	1/1	1.00	0.02	55,55,55,55	0
56	MG	DA	3041	1/1	1.00	0.11	22,22,22,22	0
56	MG	AA	1649	1/1	1.00	0.03	111,111,111,111	0
56	MG	DA	3043	1/1	1.00	0.04	40,40,40,40	0
56	MG	DA	3009	1/1	1.00	0.03	39,39,39,39	0
56	MG	DA	3045	1/1	1.00	0.07	73,73,73,73	0
56	MG	DA	3046	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3047	1/1	1.00	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3048	1/1	1.00	0.03	59,59,59,59	0
56	MG	DA	3049	1/1	1.00	0.04	52,52,52,52	0
56	MG	DA	3050	1/1	1.00	0.02	41,41,41,41	0
56	MG	DA	3051	1/1	1.00	0.01	37,37,37,37	0
56	MG	DA	3010	1/1	1.00	0.05	48,48,48,48	0
56	MG	DA	3011	1/1	1.00	0.02	23,23,23,23	0
60	ZN	D5	101	1/1	1.00	0.01	84,84,84,84	0
56	MG	AA	1637	1/1	1.00	0.07	106,106,106,106	0
56	MG	DA	3013	1/1	1.00	0.01	13,13,13,13	0
56	MG	DA	3056	1/1	1.00	0.03	55,55,55,55	0
56	MG	DA	3057	1/1	1.00	0.01	28,28,28,28	0
56	MG	DA	3058	1/1	1.00	0.01	66,66,66,66	0
56	MG	DA	3059	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3060	1/1	1.00	0.01	23,23,23,23	0
56	MG	DA	3145	1/1	1.00	0.03	45,45,45,45	0
56	MG	DA	3061	1/1	1.00	0.01	44,44,44,44	0
56	MG	DA	3014	1/1	1.00	0.02	31,31,31,31	0
56	MG	DD	302	1/1	1.00	0.04	62,62,62,62	0
56	MG	DA	3064	1/1	1.00	0.06	75,75,75,75	0
56	MG	DA	3150	1/1	1.00	0.02	72,72,72,72	0
56	MG	DA	3065	1/1	1.00	0.01	41,41,41,41	0
56	MG	DA	3066	1/1	1.00	0.03	43,43,43,43	0
56	MG	DA	3016	1/1	1.00	0.02	74,74,74,74	0
56	MG	DA	3068	1/1	1.00	0.05	43,43,43,43	0
56	MG	DA	3017	1/1	1.00	0.01	34,34,34,34	0
56	MG	BA	1621	1/1	1.00	0.07	45,45,45,45	0
56	MG	DA	3019	1/1	1.00	0.11	16,16,16,16	0
56	MG	DA	3072	1/1	1.00	0.04	86,86,86,86	0
56	MG	DA	3073	1/1	1.00	0.02	40,40,40,40	0
56	MG	DA	3020	1/1	1.00	0.04	69,69,69,69	0
56	MG	DA	3075	1/1	1.00	0.05	25,25,25,25	0
56	MG	DA	3076	1/1	1.00	0.05	46,46,46,46	0
56	MG	DA	3077	1/1	1.00	0.03	71,71,71,71	0
56	MG	DA	3078	1/1	1.00	0.02	47,47,47,47	0
56	MG	DA	3021	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3022	1/1	1.00	0.04	40,40,40,40	0
56	MG	DA	3081	1/1	1.00	0.02	46,46,46,46	0
56	MG	DA	3082	1/1	1.00	0.03	109,109,109,109	0
56	MG	DA	3083	1/1	1.00	0.02	57,57,57,57	0
56	MG	DA	3023	1/1	1.00	0.06	57,57,57,57	0
56	MG	DA	3024	1/1	1.00	0.04	44,44,44,44	0
56	MG	DA	3086	1/1	1.00	0.03	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3087	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3025	1/1	1.00	0.01	57,57,57,57	0
56	MG	DA	3089	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3090	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3091	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3092	1/1	1.00	0.02	50,50,50,50	0
56	MG	DA	3093	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3094	1/1	1.00	0.09	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.