



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:30 pm BST

PDB ID : 6N1D
Title : X-ray Crystal complex showing Spontaneous Ribosomal Translocation of mRNA and tRNAs into a Chimeric Hybrid State
Authors : Noller, H.F.; Donohue, J.P.; Lancaster, L.; Zhou, J.
Deposited on : 2018-11-08
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

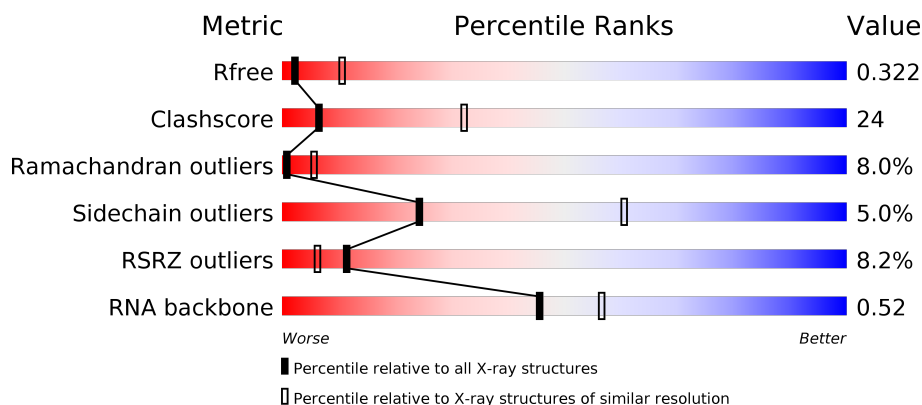
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A16S	1518	<div> <div>3%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
1	B16S	1518	<div> <div>3%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	A23S	2881	<div> <div>%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
2	B23S	2881	<div> <div>%</div> <div>78%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	A5S	119	
3	B5S	119	
4	AL01	228	
4	BL01	228	
5	AL02	276	
5	BL02	276	
6	AL03	206	
6	BL03	206	
7	AL04	205	
7	BL04	205	
8	AL05	181	
8	BL05	181	
9	AL06	180	
9	BL06	180	
10	AL09	148	
10	BL09	148	
11	AL13	140	
11	BL13	140	
12	AL14	122	
12	BL14	122	
13	AL15	150	
13	BL15	150	
14	AL16	141	
14	BL16	141	
15	AL17	118	

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Mol	Chain	Length	Quality of chain
15	BL17	118	
16	AL18	111	
16	BL18	111	
17	AL19	146	
17	BL19	146	
18	AL20	118	
18	BL20	118	
19	AL21	101	
19	BL21	101	
20	AL22	113	
20	BL22	113	
21	AL23	96	
21	BL23	96	
22	AL24	110	
22	BL24	110	
23	AL25	206	
23	BL25	206	
24	AL27	84	
24	BL27	84	
25	AL28	98	
25	BL28	98	
26	AL29	72	
26	BL29	72	
27	AL30	60	
27	BL30	60	

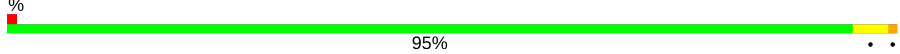


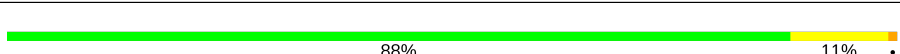
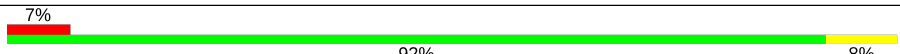
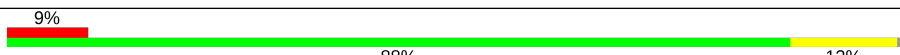
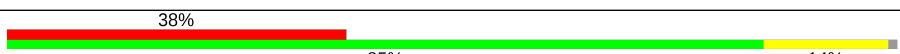
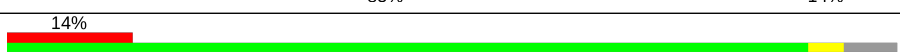
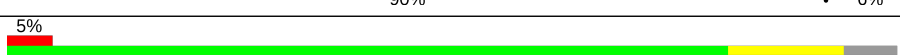
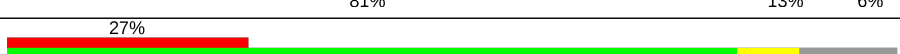

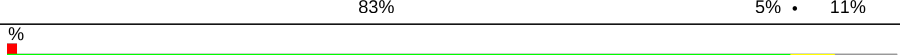
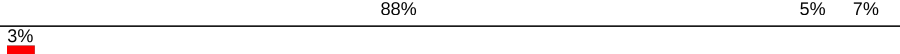
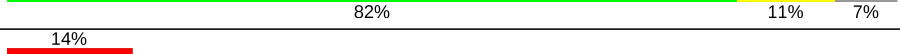





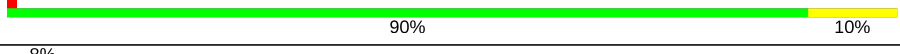

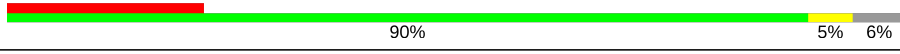
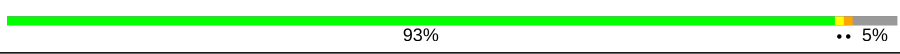


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Mol	Chain	Length	Quality of chain
28	AL31	71	
28	BL31	71	
29	AL32	59	
29	BL32	59	
30	AL33	54	
30	BL33	54	
31	AL34	49	
31	BL34	49	
32	AL35	64	
32	BL35	64	
33	AL36	37	
33	BL36	37	
34	AMRN	17	
34	BMRN	17	
35	APTN	76	
35	BPTN	76	
36	AS02	255	
36	BS02	255	
37	AS03	238	
37	BS03	238	
38	AS04	208	
38	BS04	208	
39	AS05	161	
39	BS05	161	
40	AS06	101	

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Mol	Chain	Length	Quality of chain
40	BS06	101	
41	AS07	155	
41	BS07	155	
42	AS08	138	
42	BS08	138	
43	AS09	128	
43	BS09	128	
44	AS10	104	
44	BS10	104	
45	AS11	128	
45	BS11	128	
46	AS12	131	
46	BS12	131	
47	AS13	125	
47	BS13	125	
48	AS14	60	
48	BS14	60	
49	AS15	88	
49	BS15	88	
50	AS16	88	
50	BS16	88	
51	AS17	104	
51	BS17	104	
52	AS18	87	
52	BS18	87	

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Mol	Chain	Length	Quality of chain
53	AS19	92	
53	BS19	92	
54	AS20	105	
54	BS20	105	
55	ATHX	26	
55	BTHX	26	
56	BATN	85	

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	5MU	BATN	54	-	-	-	X
56	PSU	BATN	55	-	-	-	X
57	MG	A23S	2911	-	-	-	X
57	MG	AL02	302	-	-	-	X
57	MG	AL34	100	-	-	-	X
57	MG	BL23	101	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295025 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	A16S	1517	Total	C	N	O	P	0	0	0
			32600	14510	6031	10542	1517			
1	B16S	1517	Total	C	N	O	P	0	0	0
			32600	14510	6031	10542	1517			

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A23S	2879	Total	C	N	O	P	0	0	0
			61999	27595	11586	19940	2878			
2	B23S	2879	Total	C	N	O	P	0	0	0
			62000	27595	11586	19941	2878			

- Molecule 3 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A5S	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
3	B5S	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 4 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AL01	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
4	BL01	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AL02	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
5	BL02	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AL03	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	BL03	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AL04	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	BL04	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AL05	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
8	BL05	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AL06	167	Total	C	N	O	S	0	0	0
			1282	814	239	228	1			
9	BL06	167	Total	C	N	O	S	0	0	0
			1282	814	239	228	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL09	145	Total	C	N	O	S	0	0	0
			1131	724	199	207	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BL09	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL13	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
11	BL13	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL14	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	BL14	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AL15	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
13	BL15	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL16	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	5			
14	BL16	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	5			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AL17	117	Total	C	N	O	0	0	0
			960	599	202	159			
15	BL17	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AL18	98	Total	C	N	O	0	0	0
			770	486	154	130			
16	BL18	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AL19	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	BL19	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AL20	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	BL20	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AL21	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	BL21	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AL22	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	BL22	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AL23	92	Total	C	N	O	0	0	0
			725	471	131	123			
21	BL23	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AL24	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
22	BL24	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AL25	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	2			
23	BL25	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AL27	82	Total	C	N	O	S	0	0	0
			647	401	136	109	1			
24	BL27	82	Total	C	N	O	S	0	0	0
			647	401	136	109	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	AL28	88	Total	C	N	O	0	0	0
			694	435	141	118			
25	BL28	88	Total	C	N	O	0	0	0
			694	435	141	118			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AL29	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BL29	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AL30	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
27	BL30	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AL31	45	Total	C	N	O	S	0	0	0
			351	224	61	62	4			
28	BL31	45	Total	C	N	O	S	0	0	0
			351	224	61	62	4			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AL32	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
29	BL32	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AL33	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			
30	BL33	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AL34	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	BL34	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AL35	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
32	BL35	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AL36	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	BL36	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AMRN	10	Total	C	N	O	P	0	0	0
			223	99	47	67	10			
34	BMRN	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

- Molecule 35 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
35	APTN	76	Total	C	N	O	P	S	0	0	0
			1631	728	292	534	76	1			
35	BPTN	76	Total	C	N	O	P	S	0	0	0
			1631	728	292	534	76	1			

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AS02	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	BS02	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AS03	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	BS03	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AS04	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
38	BS04	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AS05	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	BS05	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AS06	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	BS06	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AS07	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	BS07	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AS08	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS08	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AS09	127	Total	C	N	O		0	0	0
			1011	639	198	174				
43	BS09	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AS10	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
44	BS10	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AS11	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			
45	BS11	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AS12	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
46	BS12	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	AS13	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	BS13	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	AS14	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	BS14	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	AS15	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	BS15	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	AS16	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	BS16	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	AS17	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	BS17	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	AS18	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	BS18	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	AS19	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
53	BS19	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	AS20	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	BS20	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	ATHX	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	BTHX	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 56 is a RNA chain called A tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BATN	85	Total	C	N	O	P S	0	0	0
			1824	821	323	594	85 1			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL19	2	Total	Mg	0	0
			2	2		
57	BTHX	1	Total	Mg	0	0
			1	1		
57	A16S	33	Total	Mg	0	0
			33	33		
57	AS08	1	Total	Mg	0	0
			1	1		
57	BL31	1	Total	Mg	0	0
			1	1		
57	BL33	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL36	1	Total 1	Mg 1	0	0
57	BL04	1	Total 1	Mg 1	0	0
57	B16S	32	Total 32	Mg 32	0	0
57	BS17	1	Total 1	Mg 1	0	0
57	BL23	1	Total 1	Mg 1	0	0
57	AL17	2	Total 2	Mg 2	0	0
57	BL18	3	Total 3	Mg 3	0	0
57	AL02	2	Total 2	Mg 2	0	0
57	BL28	2	Total 2	Mg 2	0	0
57	AL06	1	Total 1	Mg 1	0	0
57	AL34	1	Total 1	Mg 1	0	0
57	BL01	2	Total 2	Mg 2	0	0
57	BL35	1	Total 1	Mg 1	0	0
57	BATN	1	Total 1	Mg 1	0	0
57	AL21	3	Total 3	Mg 3	0	0
57	AL28	2	Total 2	Mg 2	0	0
57	AS02	1	Total 1	Mg 1	0	0
57	B23S	133	Total 133	Mg 133	0	0
57	BL24	2	Total 2	Mg 2	0	0
57	AL24	1	Total 1	Mg 1	0	0
57	AS06	2	Total 2	Mg 2	0	0

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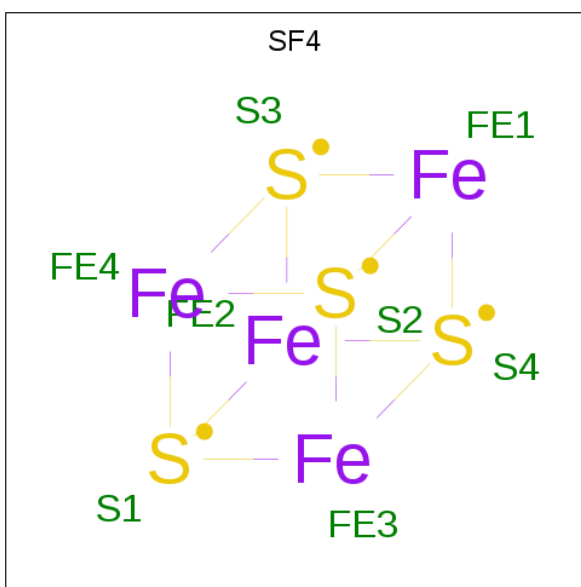
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL32	1	Total 1	Mg 1	0	0
57	BL20	1	Total 1	Mg 1	0	0
57	AL14	1	Total 1	Mg 1	0	0
57	AL20	1	Total 1	Mg 1	0	0
57	BL34	2	Total 2	Mg 2	0	0
57	AL01	2	Total 2	Mg 2	0	0
57	AS03	1	Total 1	Mg 1	0	0
57	BL02	5	Total 5	Mg 5	0	0
57	BL25	1	Total 1	Mg 1	0	0
57	A23S	73	Total 73	Mg 73	0	0
57	AL27	1	Total 1	Mg 1	0	0
57	BL30	1	Total 1	Mg 1	0	0
57	BL15	3	Total 3	Mg 3	0	0
57	AL04	3	Total 3	Mg 3	0	0
57	BL21	1	Total 1	Mg 1	0	0
57	AL15	2	Total 2	Mg 2	0	0
57	AL23	2	Total 2	Mg 2	0	0
57	BL16	3	Total 3	Mg 3	0	0
57	B5S	5	Total 5	Mg 5	0	0
57	BL03	1	Total 1	Mg 1	0	0
57	A5S	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL29	5	Total	Mg	0	0
			5	5		
57	BS16	1	Total	Mg	0	0
			1	1		
57	AL33	3	Total	Mg	0	0
			3	3		
57	BL22	1	Total	Mg	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

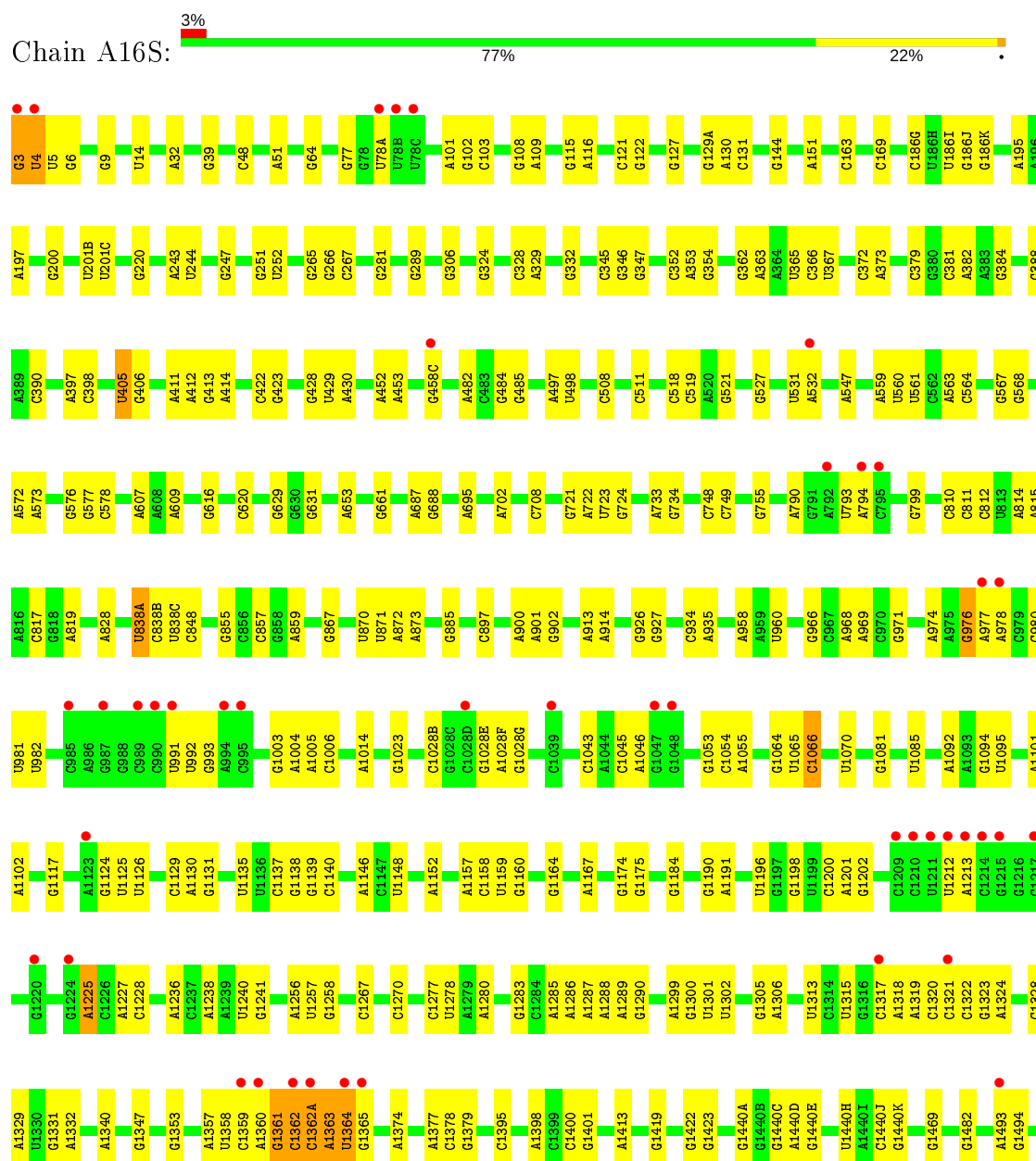


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AS04	1	Total	Fe	S	0	0
			8	4	4		
58	BS04	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

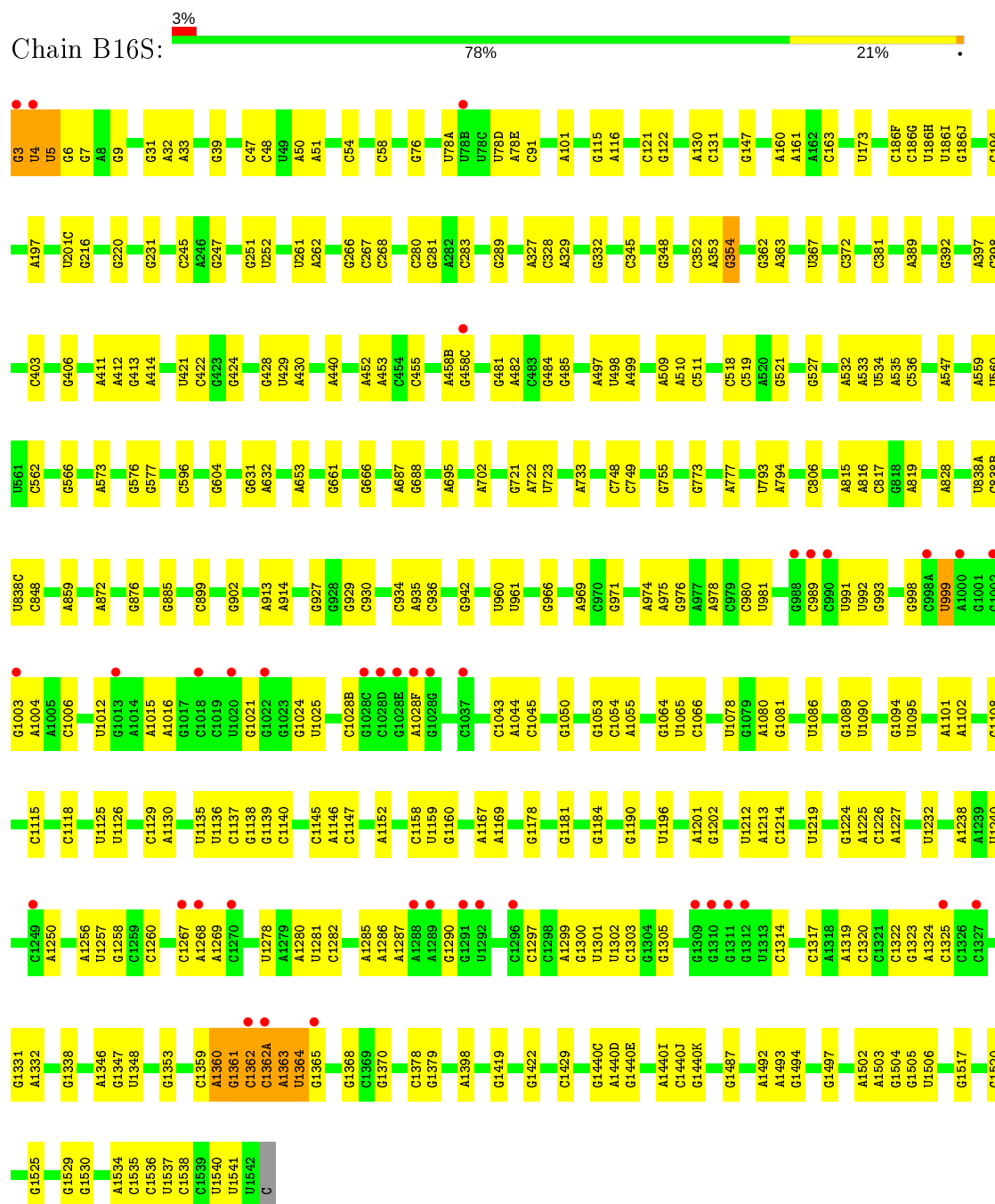
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

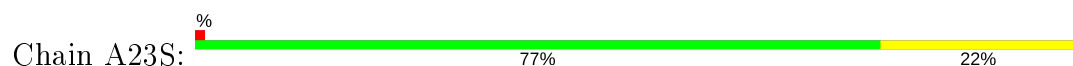




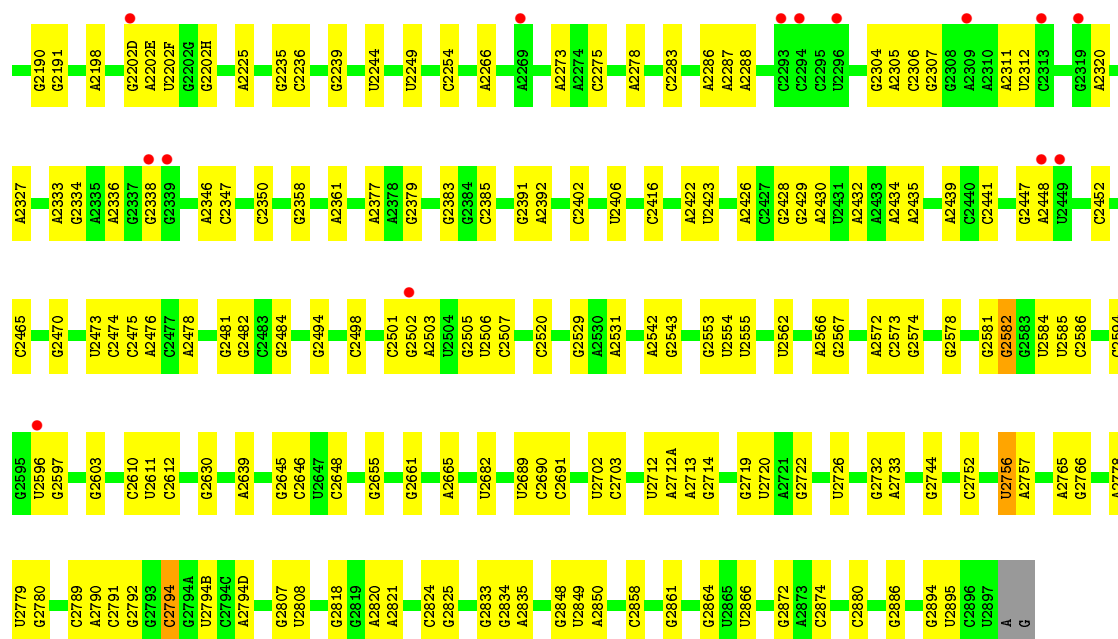
• Molecule 1: 16S rRNA



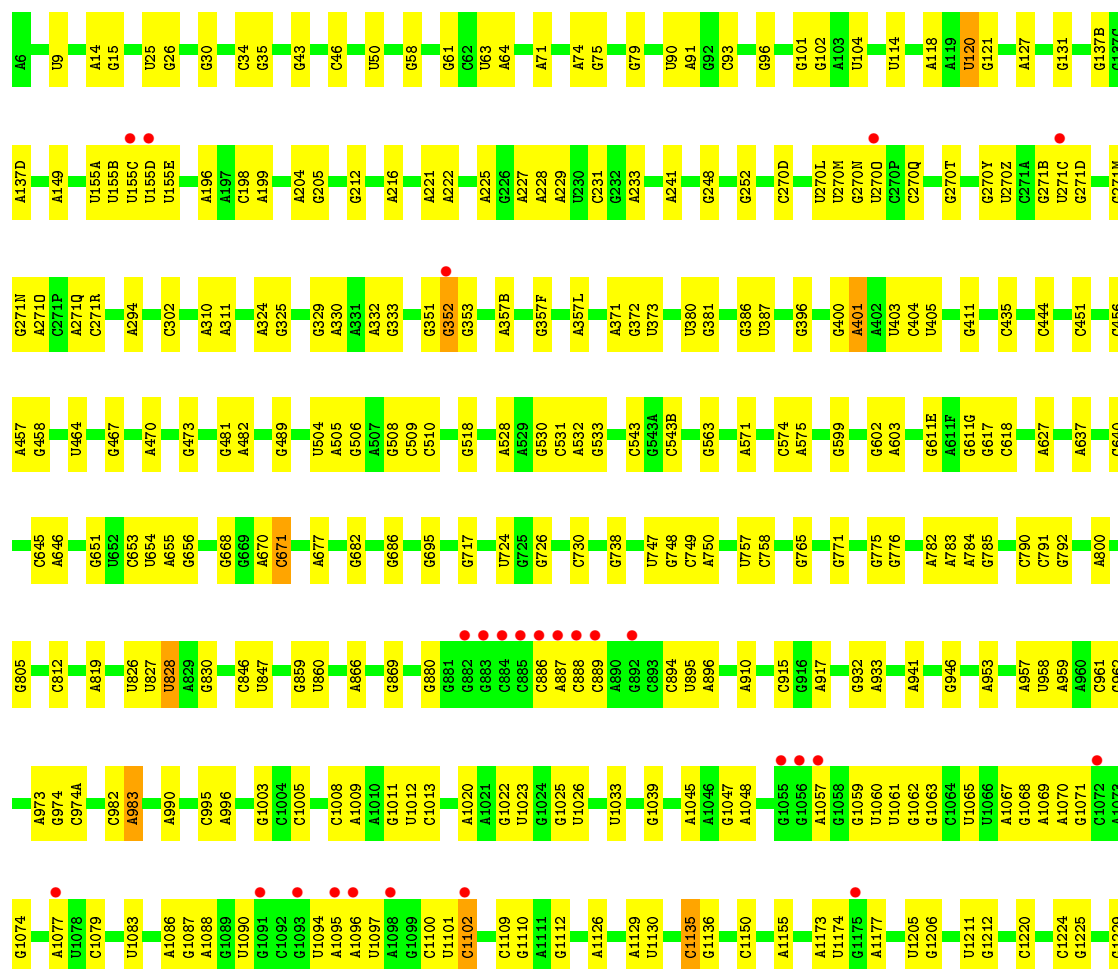
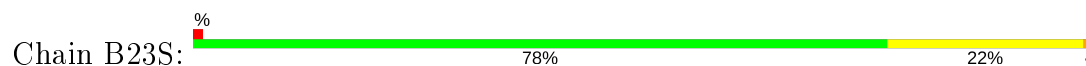
• Molecule 2: 23S rRNA

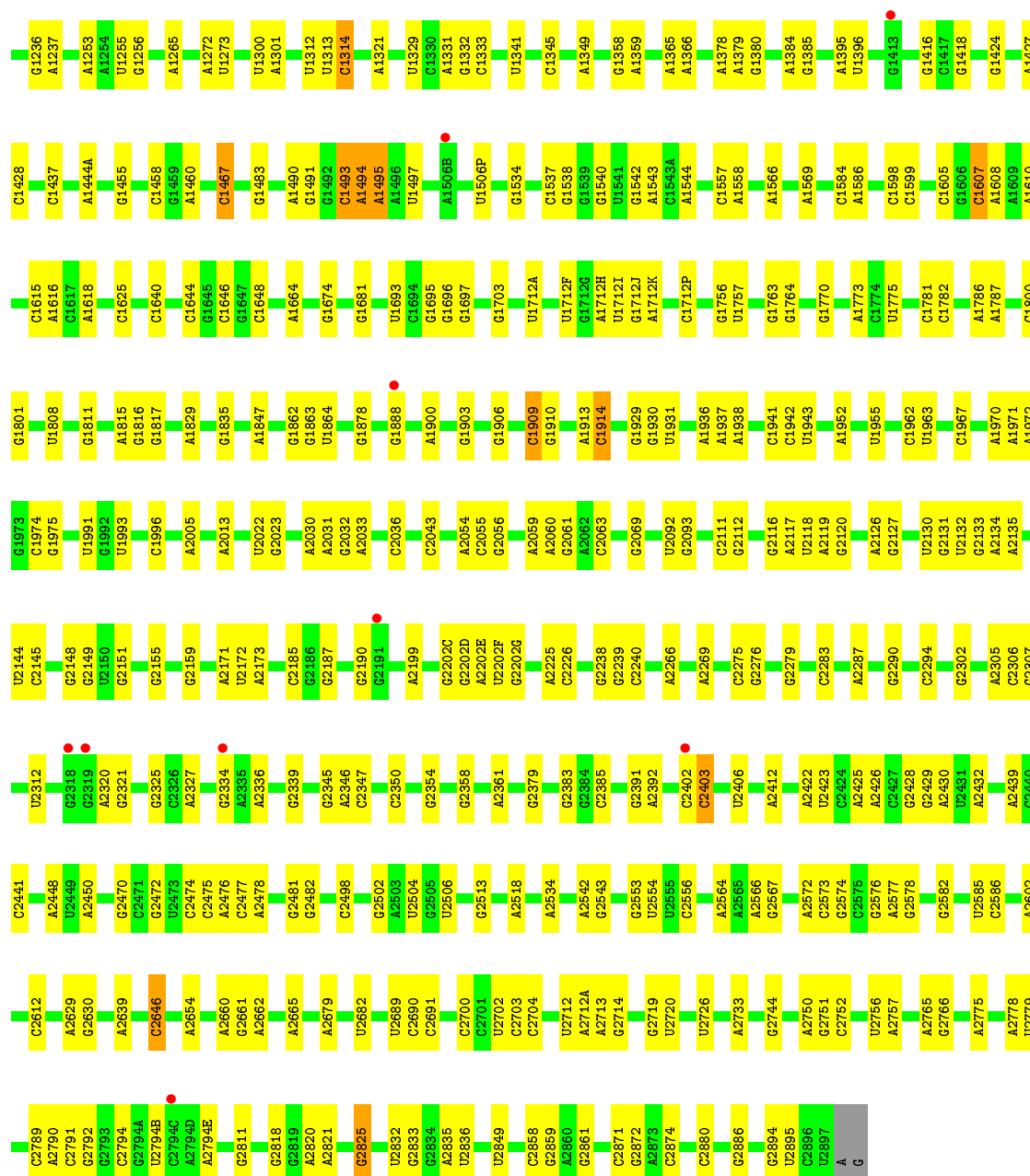


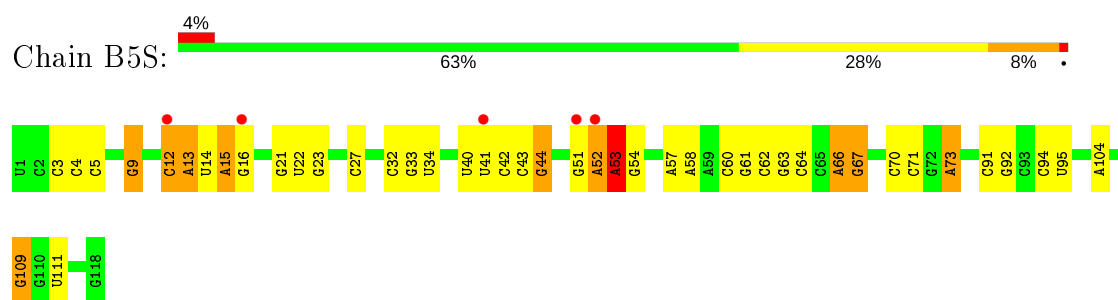




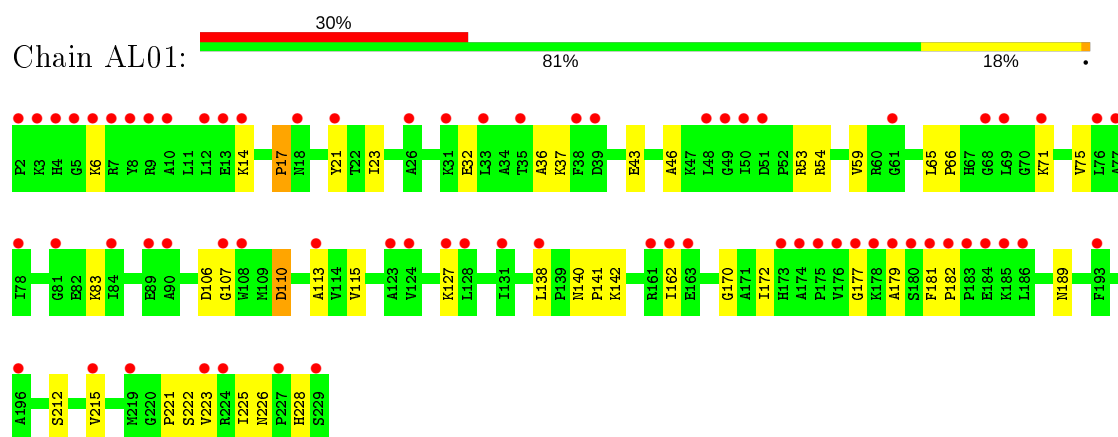
• Molecule 2: 23S rRNA



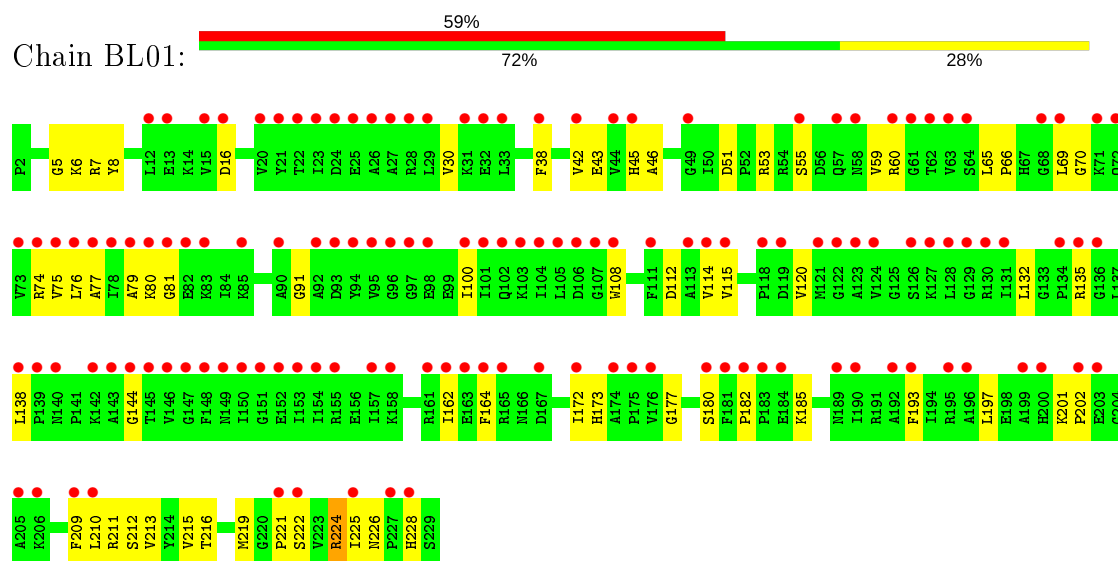




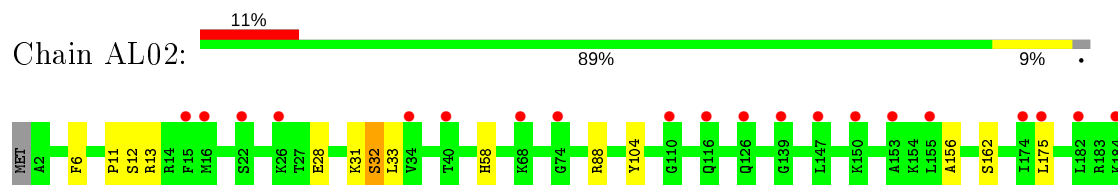
• Molecule 4: 50S ribosomal protein L1

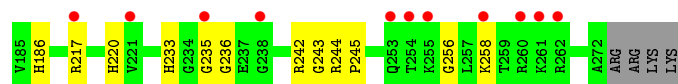


• Molecule 4: 50S ribosomal protein L1

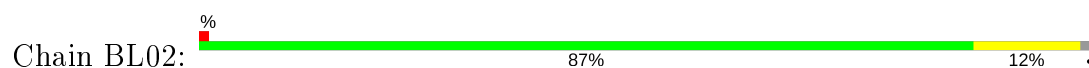


• Molecule 5: 50S ribosomal protein L2

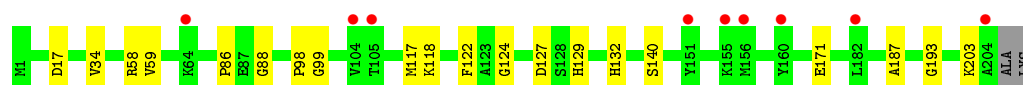




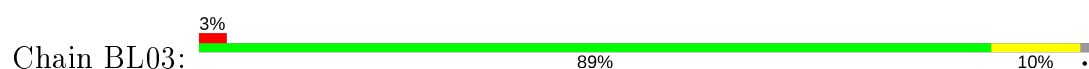
- Molecule 5: 50S ribosomal protein L2



- Molecule 6: 50S ribosomal protein L3

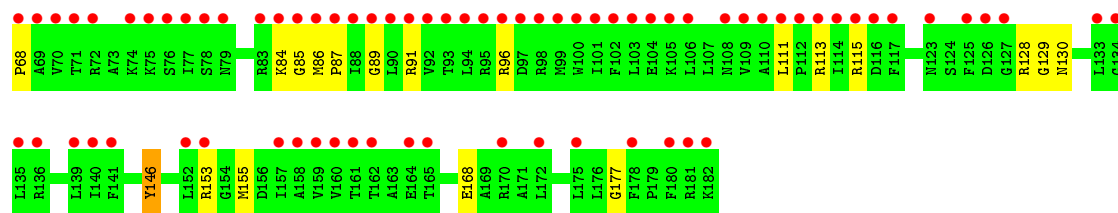


- Molecule 6: 50S ribosomal protein L3

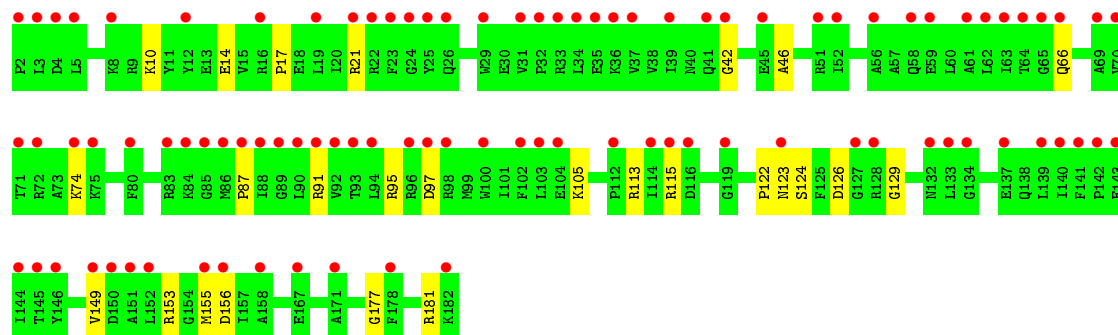
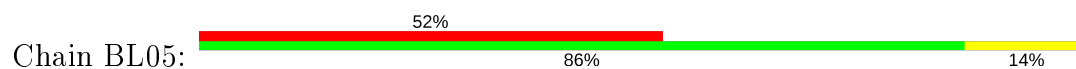


- Molecule 7: 50S ribosomal protein L4

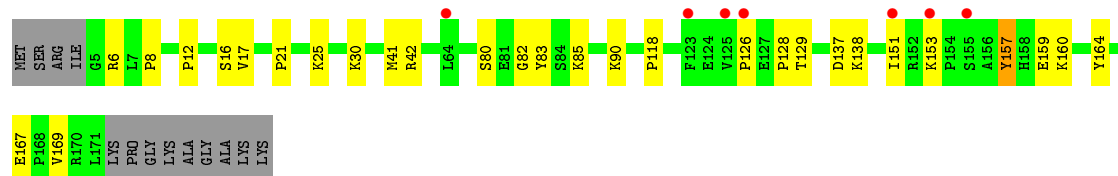
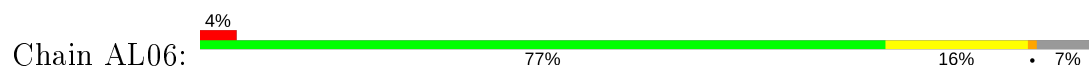




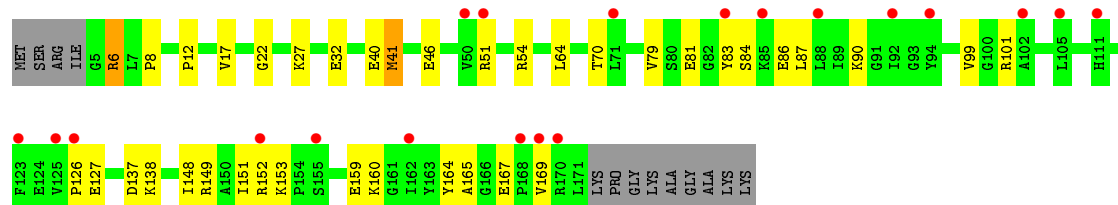
• Molecule 8: 50S ribosomal protein L5



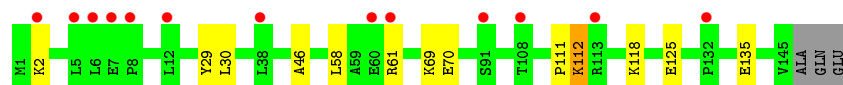
• Molecule 9: 50S ribosomal protein L6



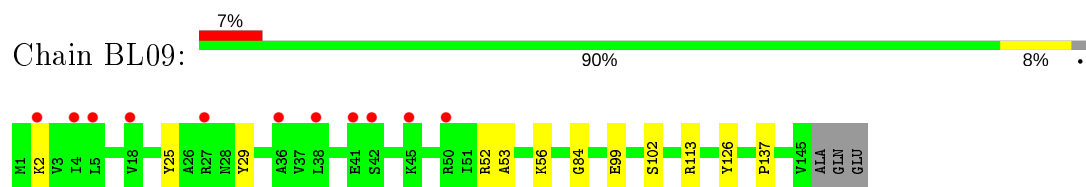
• Molecule 9: 50S ribosomal protein L6



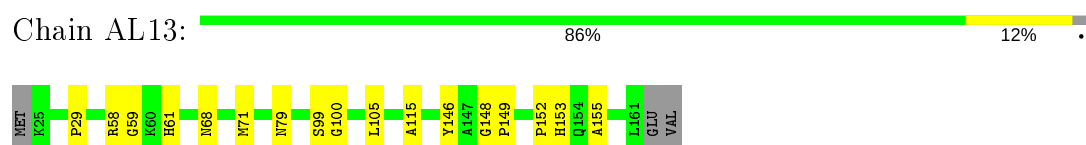
• Molecule 10: 50S ribosomal protein L9



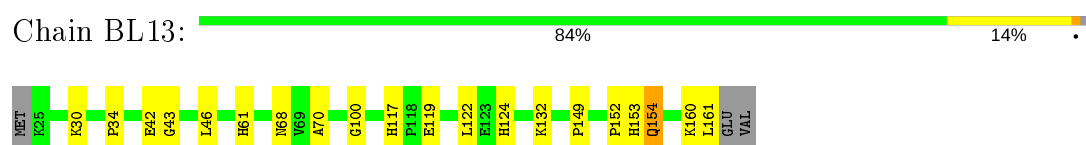
- Molecule 10: 50S ribosomal protein L9



- Molecule 11: 50S ribosomal protein L13



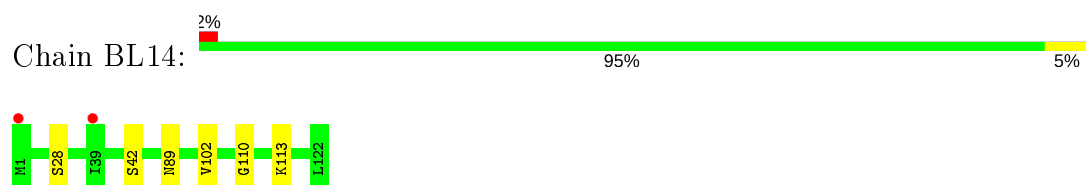
- Molecule 11: 50S ribosomal protein L13



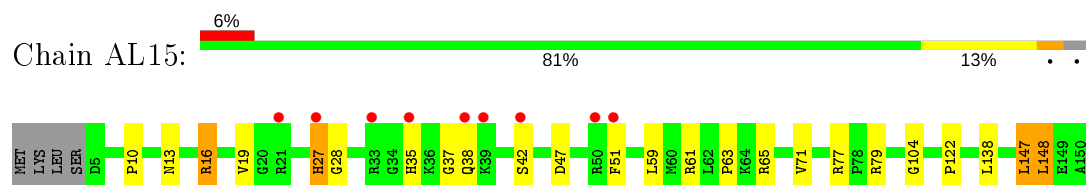
- Molecule 12: 50S ribosomal protein L14



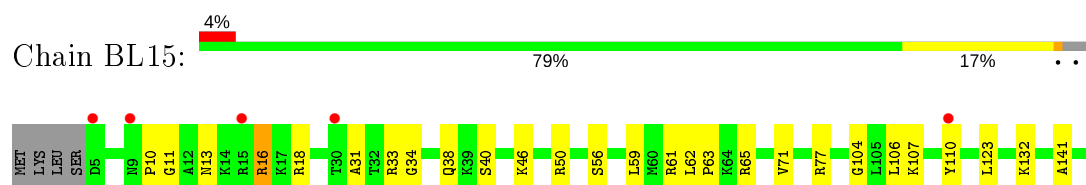
- Molecule 12: 50S ribosomal protein L14



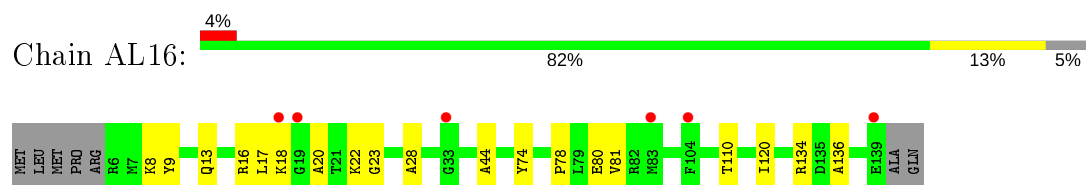
- Molecule 13: 50S ribosomal protein L15



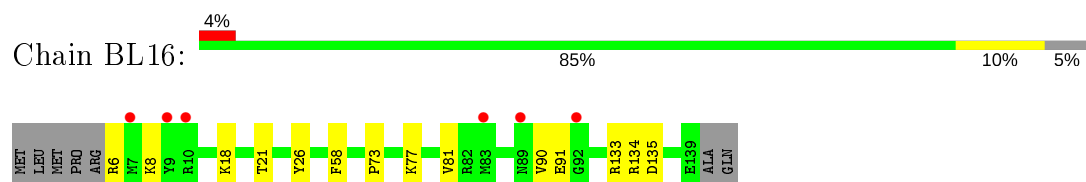
- Molecule 13: 50S ribosomal protein L15



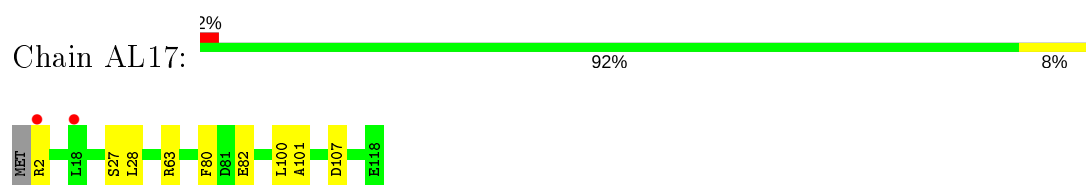
- Molecule 14: 50S ribosomal protein L16



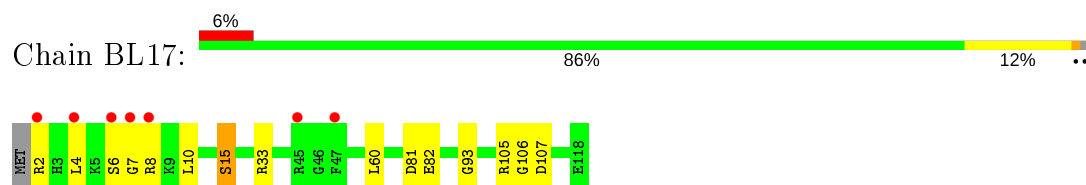
- Molecule 14: 50S ribosomal protein L16



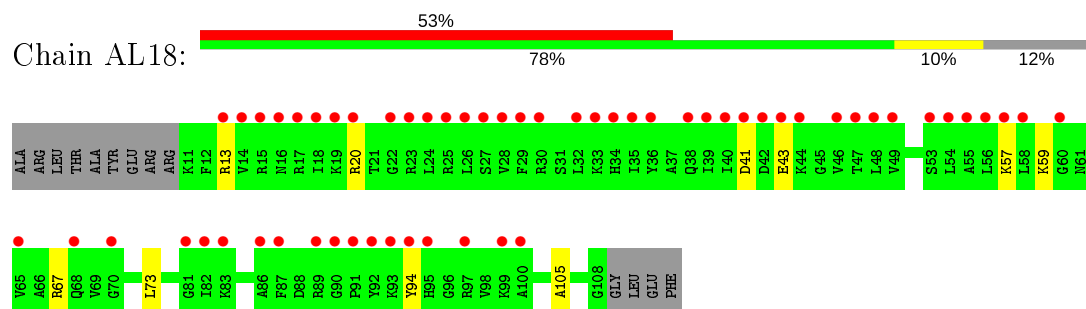
- Molecule 15: 50S ribosomal protein L17



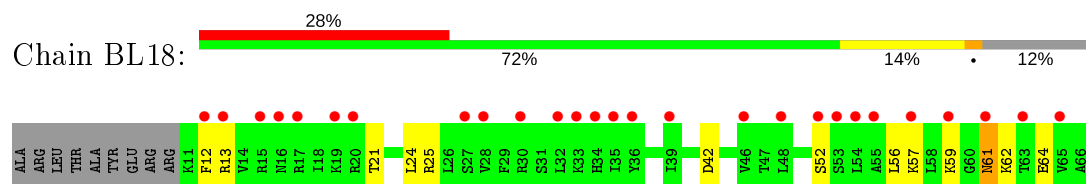
- Molecule 15: 50S ribosomal protein L17

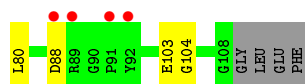


- Molecule 16: 50S ribosomal protein L18

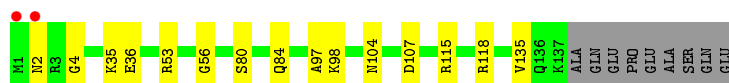
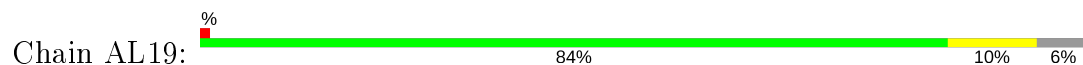


- Molecule 16: 50S ribosomal protein L18





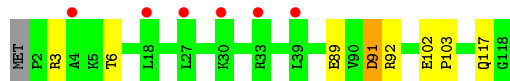
- Molecule 17: 50S ribosomal protein L19



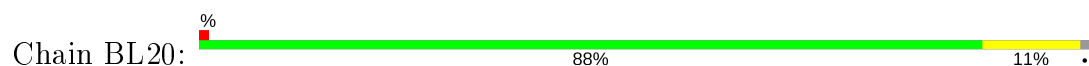
- Molecule 17: 50S ribosomal protein L19



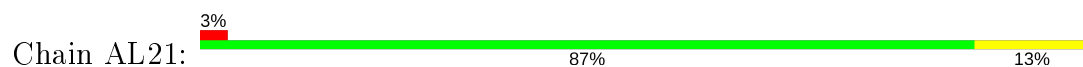
- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20



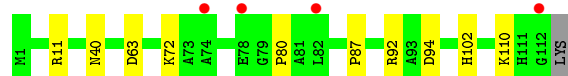
- Molecule 19: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L21



- Molecule 20: 50S ribosomal protein L22



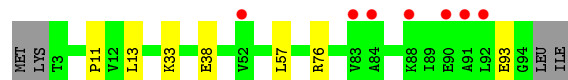
- Molecule 20: 50S ribosomal protein L22



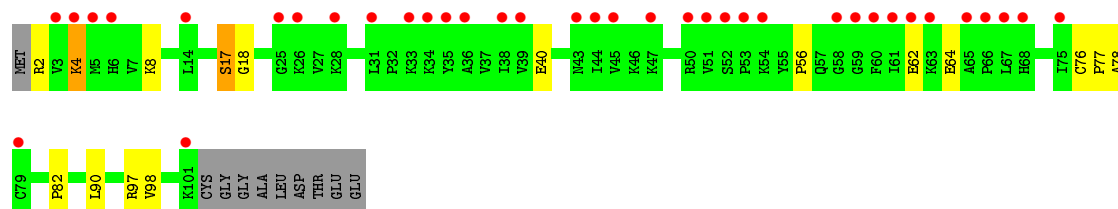
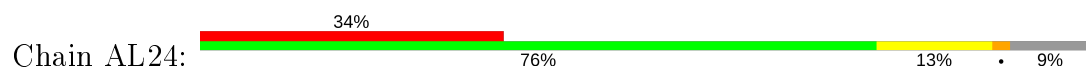
- Molecule 21: 50S ribosomal protein L23



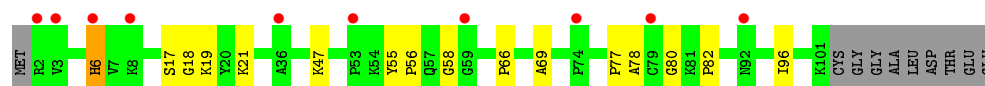
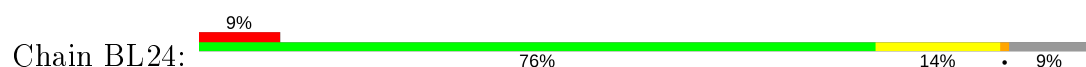
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



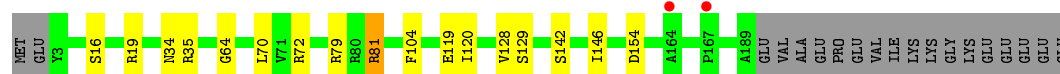
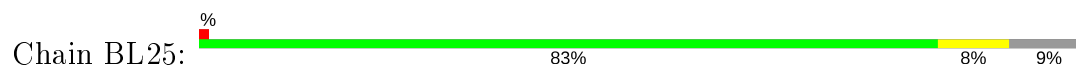
- Molecule 22: 50S ribosomal protein L24



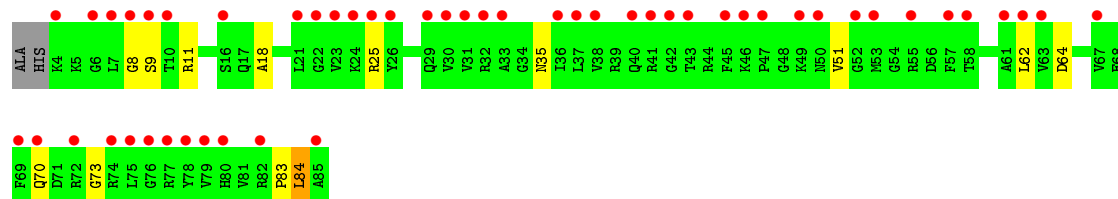
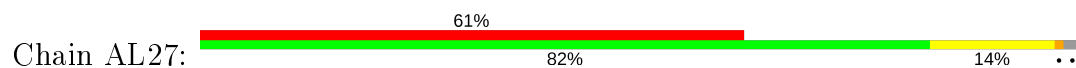
- Molecule 23: 50S ribosomal protein L25



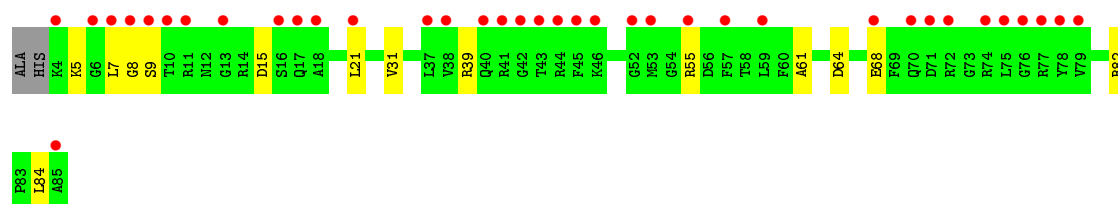
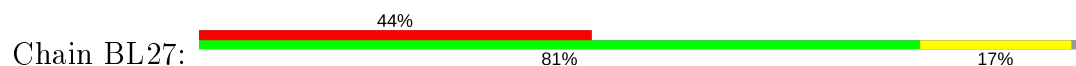
- Molecule 23: 50S ribosomal protein L25



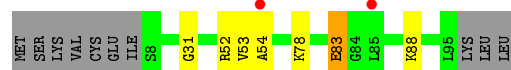
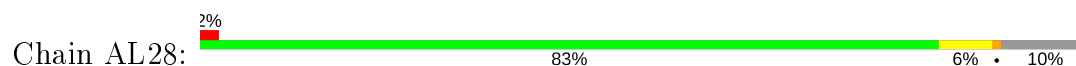
- Molecule 24: 50S ribosomal protein L27



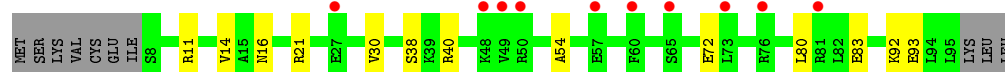
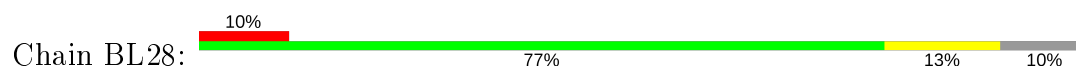
- Molecule 24: 50S ribosomal protein L27



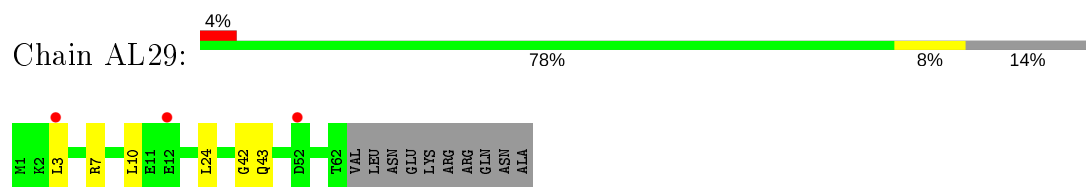
- Molecule 25: 50S ribosomal protein L28



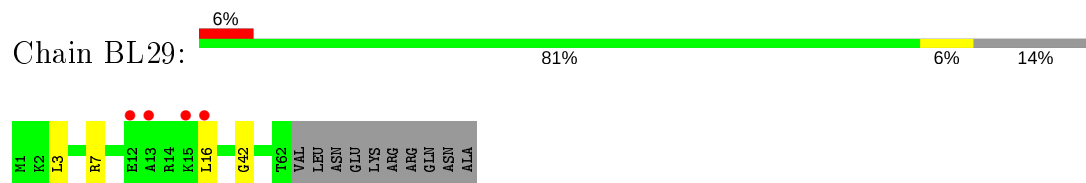
- Molecule 25: 50S ribosomal protein L28



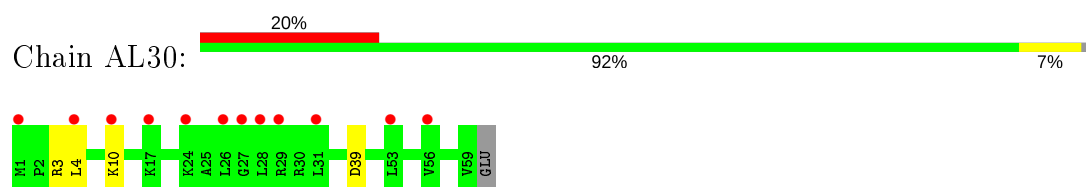
• Molecule 26: 50S ribosomal protein L29



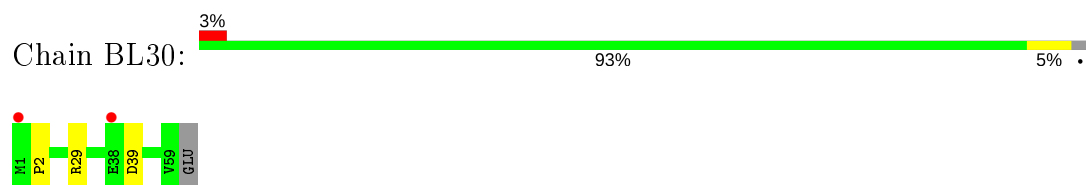
• Molecule 26: 50S ribosomal protein L29



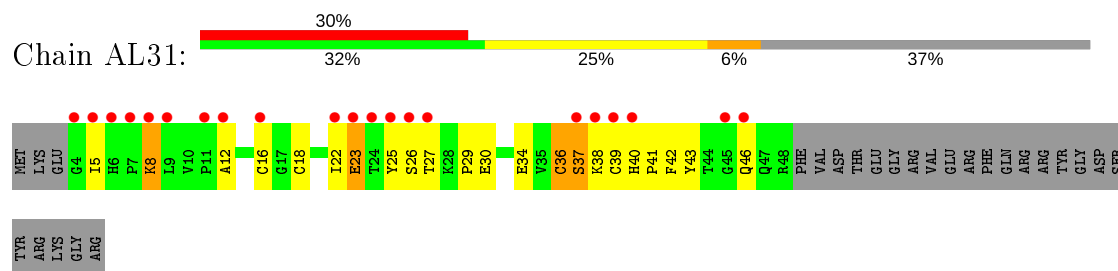
• Molecule 27: 50S ribosomal protein L30



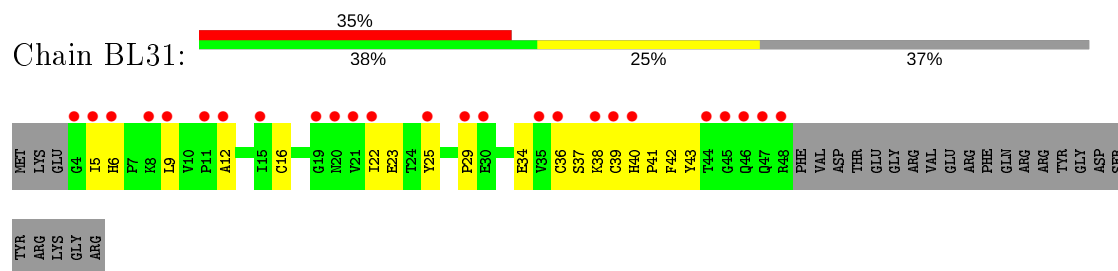
• Molecule 27: 50S ribosomal protein L30



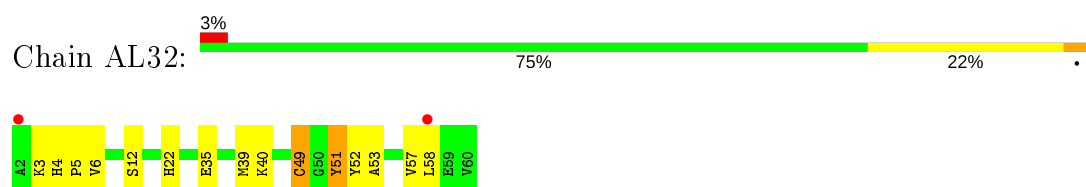
• Molecule 28: 50S ribosomal protein L31



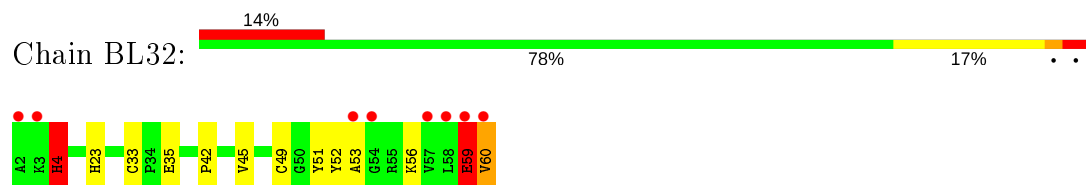
• Molecule 28: 50S ribosomal protein L31



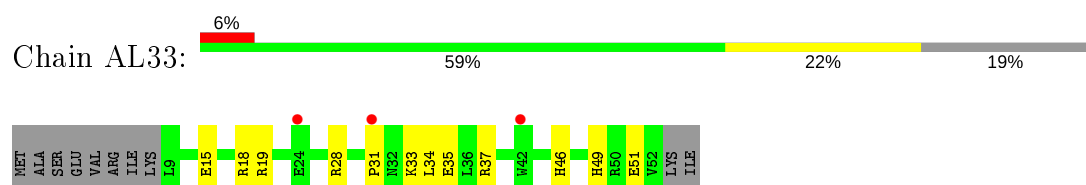
• Molecule 29: 50S ribosomal protein L32



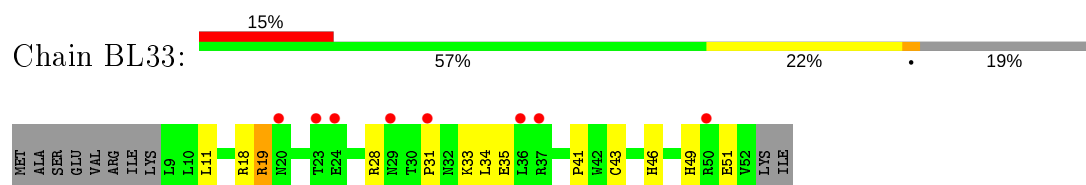
- Molecule 29: 50S ribosomal protein L32



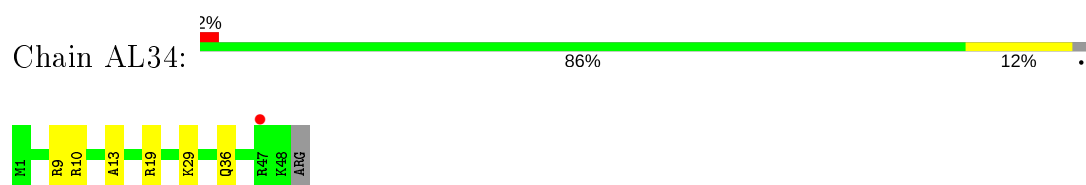
- Molecule 30: 50S ribosomal protein L33



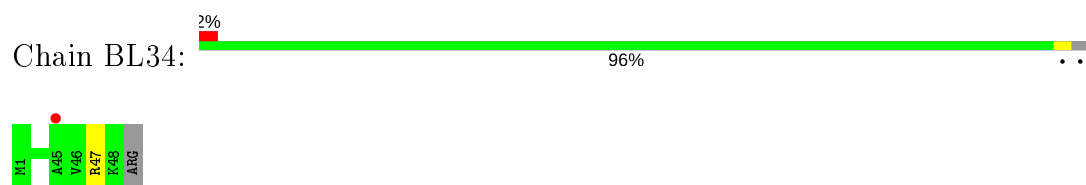
- Molecule 30: 50S ribosomal protein L33



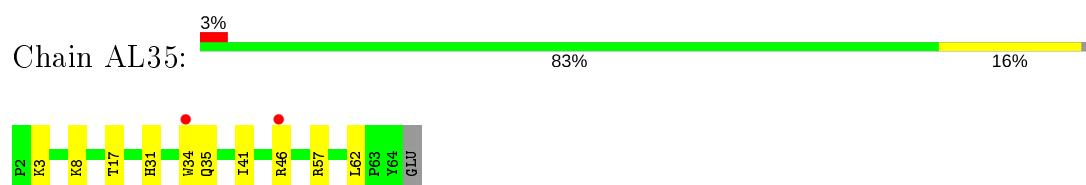
- Molecule 31: 50S ribosomal protein L34



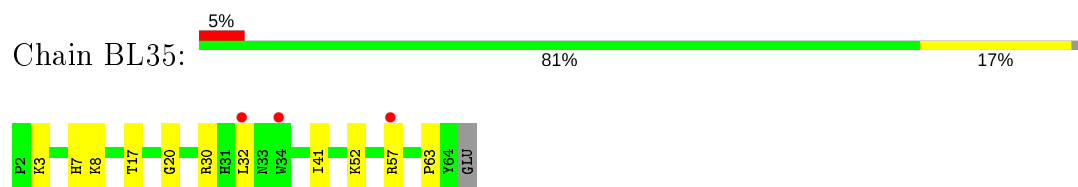
- Molecule 31: 50S ribosomal protein L34



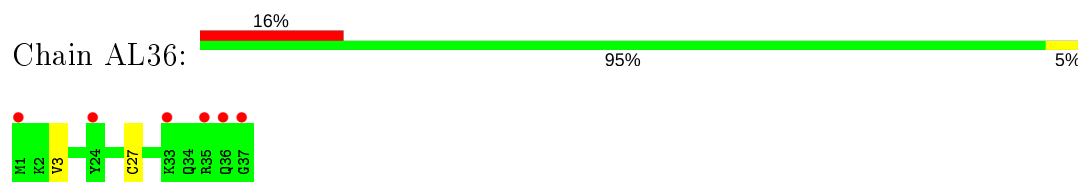
- Molecule 32: 50S ribosomal protein L35



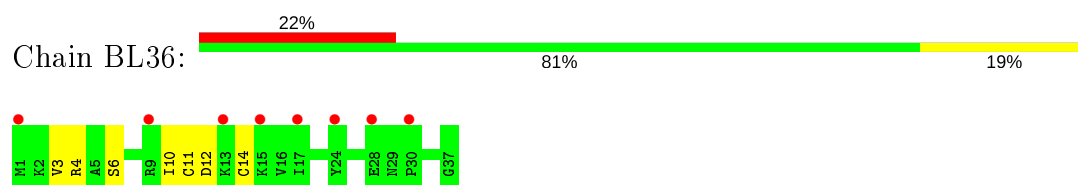
- Molecule 32: 50S ribosomal protein L35



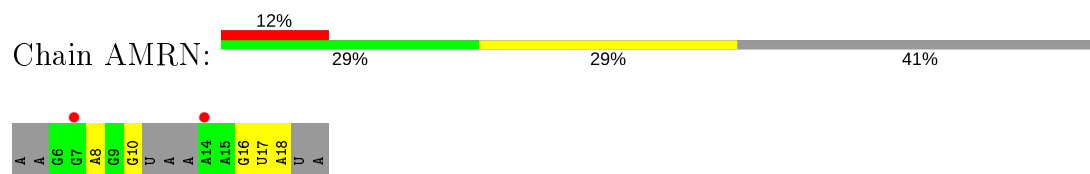
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36



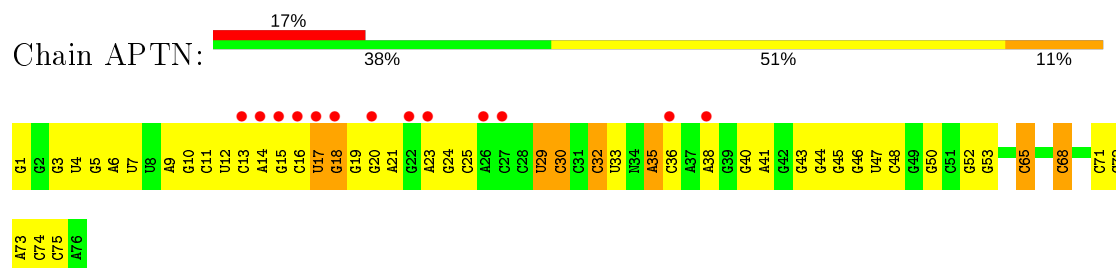
- Molecule 34: mRNA



- Molecule 34: mRNA

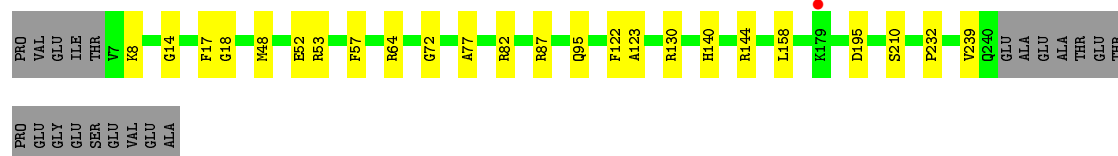


- Molecule 35: P-tRNA



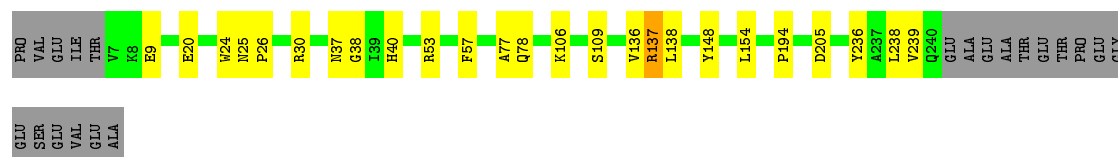
- Molecule 36: 30S ribosomal protein S2

Chain AS02:




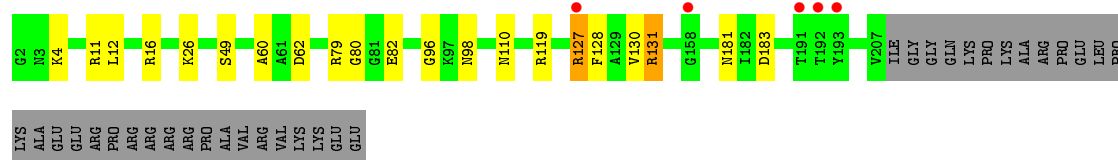
- Molecule 36: 30S ribosomal protein S2

Chain BS02:

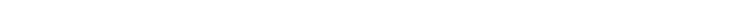


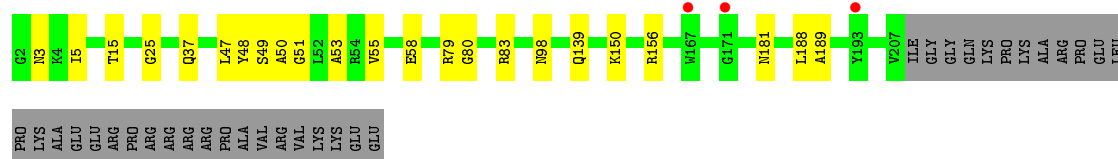
- Molecule 37: 30S ribosomal protein S3

Chain AS03: 



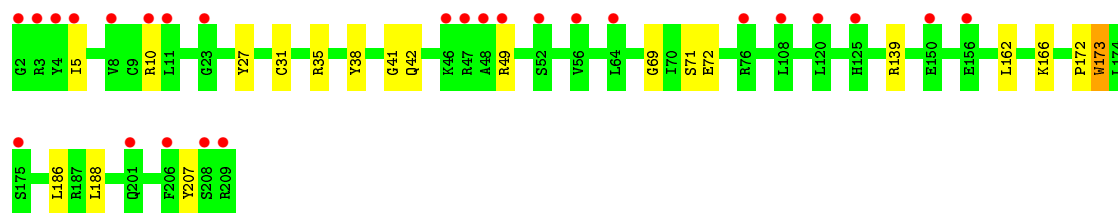
- Molecule 37: 30S ribosomal protein S3

Chain BS03:  %

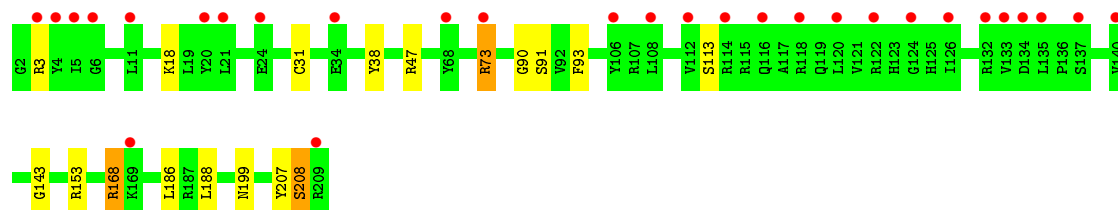


- Molecule 38: 30S ribosomal protein S4

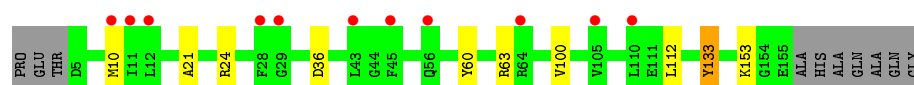
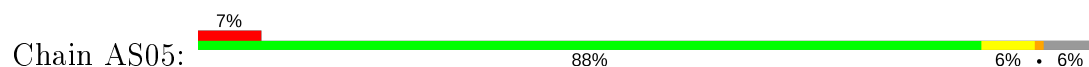
Chain AS04:  13% 90% 9%



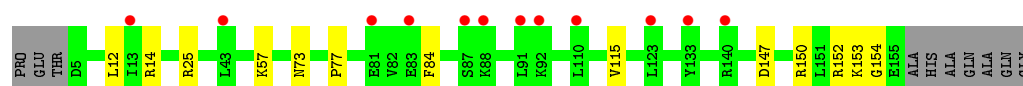
- Molecule 38: 30S ribosomal protein S4



- Molecule 39: 30S ribosomal protein S5



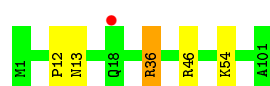
- Molecule 39: 30S ribosomal protein S5



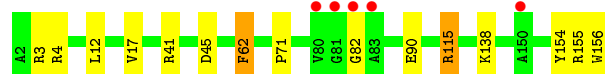
- Molecule 40: 30S ribosomal protein S6



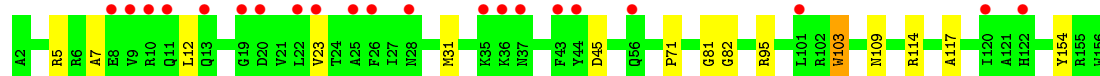
- Molecule 40: 30S ribosomal protein S6



- Molecule 41: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S7



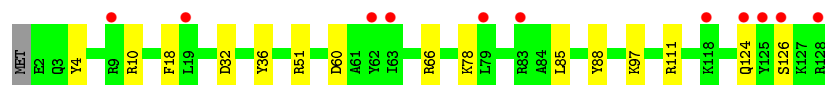
- Molecule 42: 30S ribosomal protein S8



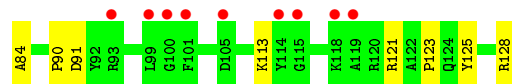
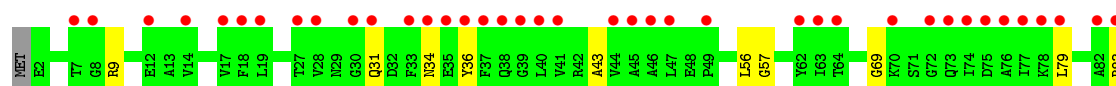
- Molecule 42: 30S ribosomal protein S8



- Molecule 43: 30S ribosomal protein S9

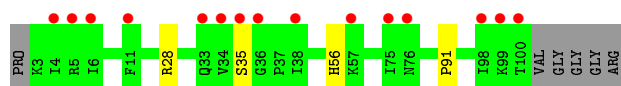


- Molecule 43: 30S ribosomal protein S9

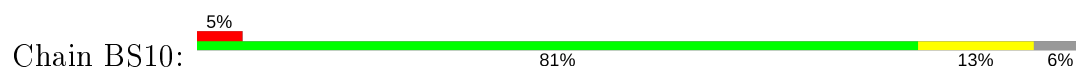


- Molecule 44: 30S ribosomal protein S10

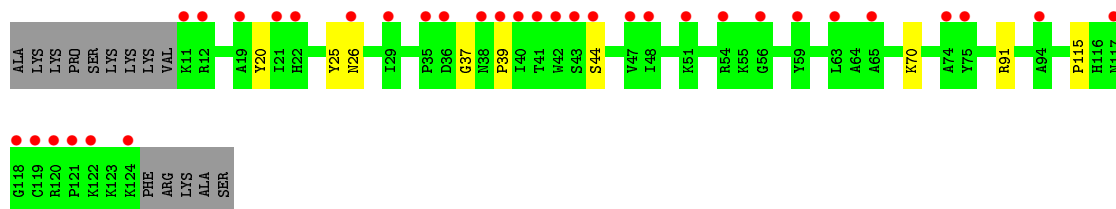
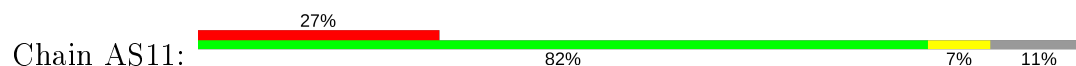




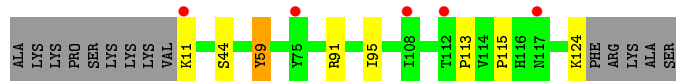
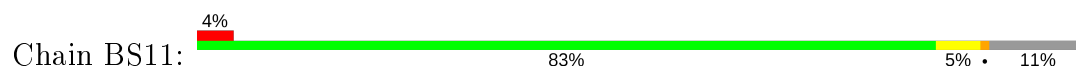
- Molecule 44: 30S ribosomal protein S10



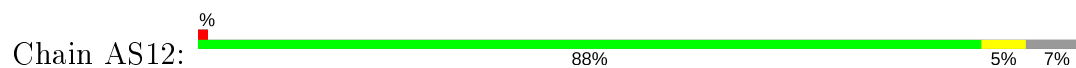
- Molecule 45: 30S ribosomal protein S11



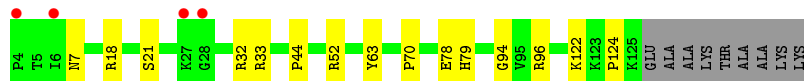
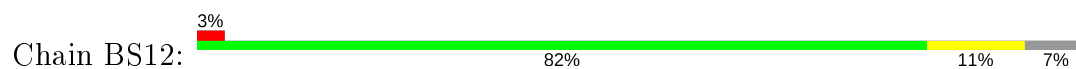
- Molecule 45: 30S ribosomal protein S11



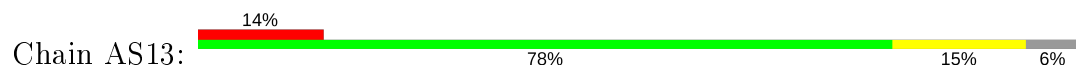
- Molecule 46: 30S ribosomal protein S12

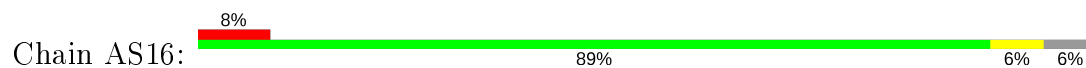


- Molecule 46: 30S ribosomal protein S12



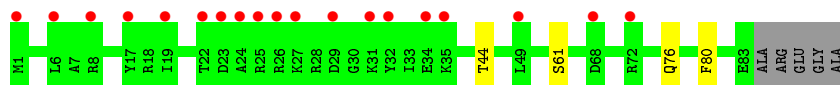
- Molecule 47: 30S ribosomal protein S13



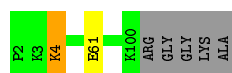




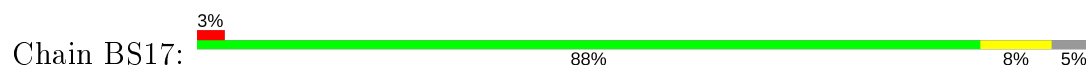
- Molecule 50: 30S ribosomal protein S16



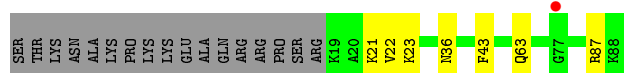
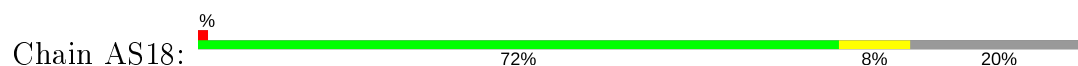
- Molecule 51: 30S ribosomal protein S17



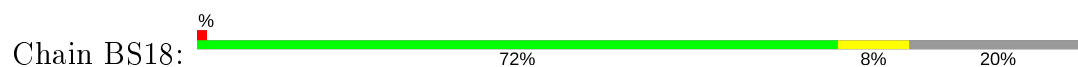
- Molecule 51: 30S ribosomal protein S17



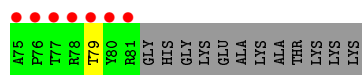
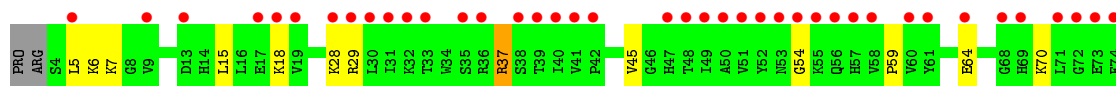
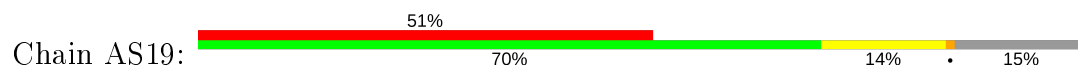
- Molecule 52: 30S ribosomal protein S18




- Molecule 52: 30S ribosomal protein S18



- Molecule 53: 30S ribosomal protein S19



- Chain BS19:
-
- 38% 73% 11% 15%
- PRO ARG S4 L5 K6 K7 G8 V9 F10 V11 L15 L16 A24 E27 K28 R29 L30 I31 M34 S35 S38 T39 I40 V41 P42 G46 H47 T48 I49 A50 L51 V51 Y52 K55 Q56 H57 V58 P59 Y60 Y61 E64 M65 M66 E73 F74 A75 P76 T79 Y80 R81 G82

- Chain AS20: 

- Chain BS20:
-
- | State | Category |
|-------|----------|
| ALA | Grey |
| GLN | Grey |
| LYS | Grey |
| LVS | Grey |
| P80 | Yellow |
| LVS | Yellow |
| R8 | Yellow |
| S11 | Yellow |
| R15 | Yellow |
| K38 | Yellow |
| I63 | Grey |
| G69 | Yellow |
| S70 | Yellow |
| T71 | Yellow |
| L72 | Red |
| I75 | Red |
| R83 | Yellow |
| A37 | Yellow |
| P98 | Yellow |
| L99 | Red |
| I100 | Yellow |
| G101 | Yellow |
| A106 | Green |

- Chain ATHX:
-
- | Category | Percentage |
|----------|------------|
| G2 | 62% |
| K3 | 62% |
| G4 | 62% |
| D5 | 62% |
| R6 | 62% |
| E7 | 62% |
| T8 | 62% |
| R9 | 62% |
| R10 | 62% |
| G11 | 62% |
| K12 | 62% |
| K13 | 62% |
| K14 | 62% |
| R15 | 62% |
| G16 | 62% |
| T17 | 62% |
| Y18 | 62% |
| G19 | 62% |
| K20 | 62% |
| Y21 | 62% |
| R22 | 62% |
| P23 | 62% |
| R24 | 62% |
| K25 | 62% |
| LYS | 23% |
| LYS | 8% |

- Chain BTHX:
-
- | Category | Percentage |
|----------|------------|
| Red | 81% |
| Green | 85% |
| Yellow | 8% |
| Grey | 8% |
- Amino acid sequence: G2, K3, K4, D5, R6, E7, T8, R9, R10, G11, K12, I13, W14, R15, G16, Y17, Y18, G19, K20, Y21, R22, P23, R24, K25, LYS, LYS.

- Chain BATN:
-
- 59%
- 14%
- 35%
- 51%
- 49%
- Legend:
- G1, G2, G3, G4, G5, G6, G7, G8, G9, G10, G11, G12, G13, G14, G15, G16, G18, G19, G20, G21, G22, G23, G24, G25, G26, G27, G28, G29, G30, G31, G32, G33, G34, G35, G36, G37, G38, G39, G40, G41, G42, G43, G44, G45, G46, G47, G48, G49, G50, G51, G52, G53, G54, G55, G56, G57, G58, G59, G60, G61, G62, G63, G64, G65, G66, G67, G68, G69, G70, G71, G72, G73, G74, G75, G76, A1, A2, A3, A4, A5, A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, A20, A21, A22, A23, A24, A25, A26, A27, A28, A29, A30, A31, A32, A33, A34, A35, A36, A37, A38, A39, A40, A41, A42, A43, A44, A45, A46, A47, A48, A49, A50, A51, A52, A53, A54, A55, A56, A57, A58, A59, A60, A61, A62, A63, A64, A65, A66, A67, A68, A69, A70, A71, A72, A73, A74, A75, A76

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.45Å 442.87Å 613.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.20 252.03 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.5 (100.00-3.20) 78.2 (252.03-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.268 , 0.321 0.269 , 0.322	Depositor DCC
R_{free} test set	65984 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	295025	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: 5MU, MG, MIA, SF4, CM0, G7M, 6MZ, 4SU, QUO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A16S	0.71	33/36490 (0.1%)	0.99	80/56951 (0.1%)
1	B16S	0.71	30/36490 (0.1%)	0.99	69/56951 (0.1%)
2	A23S	0.74	3/69437 (0.0%)	0.95	75/108394 (0.1%)
2	B23S	0.83	9/69438 (0.0%)	0.96	76/108396 (0.1%)
3	A5S	0.69	3/2853 (0.1%)	0.98	10/4451 (0.2%)
3	B5S	0.74	2/2853 (0.1%)	1.00	13/4451 (0.3%)
4	AL01	0.28	0/1774	0.52	0/2391
4	BL01	0.28	0/1774	0.51	0/2391
5	AL02	0.48	1/2154 (0.0%)	0.55	0/2905
5	BL02	0.49	0/2154	0.54	0/2905
6	AL03	0.41	0/1596	0.52	0/2153
6	BL03	0.45	0/1596	0.54	0/2153
7	AL04	0.38	0/1621	0.49	0/2194
7	BL04	0.43	0/1621	0.50	0/2194
8	AL05	0.31	0/1500	0.52	0/2017
8	BL05	0.32	0/1500	0.51	0/2017
9	AL06	0.64	0/1307	0.79	0/1769
9	BL06	0.58	0/1307	0.80	0/1769
10	AL09	0.31	0/1146	0.47	0/1551
10	BL09	0.32	0/1147	0.50	0/1552
11	AL13	0.37	0/1123	0.48	0/1515
11	BL13	0.41	0/1123	0.51	0/1515
12	AL14	0.45	0/942	0.51	0/1268
12	BL14	0.46	0/942	0.51	0/1268
13	AL15	0.35	0/1131	0.59	0/1504
13	BL15	0.37	0/1131	0.58	0/1504
14	AL16	0.38	0/1084	0.50	0/1449
14	BL16	0.42	0/1084	0.51	0/1449
15	AL17	0.40	0/974	0.51	0/1302
15	BL17	0.40	0/974	0.53	0/1302
16	AL18	0.36	0/778	0.48	0/1036
16	BL18	0.36	0/778	0.51	0/1036

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AL19	0.39	0/1157	0.52	0/1544
17	BL19	0.42	0/1157	0.48	0/1544
18	AL20	0.36	0/982	0.44	0/1306
18	BL20	0.45	0/982	0.46	0/1306
19	AL21	0.37	0/790	0.55	0/1057
19	BL21	0.41	0/790	0.56	0/1057
20	AL22	0.39	0/901	0.47	0/1209
20	BL22	0.43	0/901	0.51	0/1209
21	AL23	0.40	0/739	0.48	0/993
21	BL23	0.41	0/739	0.53	1/993 (0.1%)
22	AL24	0.34	0/788	0.53	0/1051
22	BL24	0.37	0/788	0.49	0/1051
23	AL25	0.34	0/1514	0.47	0/2056
23	BL25	0.37	0/1514	0.49	0/2056
24	AL27	0.99	0/655	1.13	3/870 (0.3%)
24	BL27	1.03	1/655 (0.2%)	1.31	2/870 (0.2%)
25	AL28	0.37	0/701	0.53	0/932
25	BL28	0.39	0/701	0.55	0/932
26	AL29	0.30	0/522	0.47	0/690
26	BL29	0.33	0/522	0.48	0/690
27	AL30	0.33	0/472	0.48	0/634
27	BL30	0.36	0/472	0.47	0/634
28	AL31	0.85	1/360 (0.3%)	0.96	0/488
28	BL31	0.98	3/360 (0.8%)	1.00	2/488 (0.4%)
29	AL32	1.15	3/473 (0.6%)	1.13	1/639 (0.2%)
29	BL32	1.74	6/473 (1.3%)	1.41	9/639 (1.4%)
30	AL33	0.37	0/387	0.63	0/518
30	BL33	0.38	0/387	0.57	0/518
31	AL34	0.38	0/426	0.51	0/561
31	BL34	0.47	0/426	0.48	0/561
32	AL35	0.38	0/515	0.52	0/679
32	BL35	0.39	0/515	0.59	0/679
33	AL36	0.38	0/310	0.59	1/407 (0.2%)
33	BL36	0.52	0/310	0.63	0/407
34	AMRN	0.47	0/250	0.86	0/387
34	BMRN	1.58	6/420 (1.4%)	3.17	57/654 (8.7%)
35	APTN	0.68	2/1672 (0.1%)	1.30	17/2599 (0.7%)
35	BPTN	1.57	33/1672 (2.0%)	2.69	160/2599 (6.2%)
36	AS02	0.33	0/1935	0.47	0/2609
36	BS02	0.31	0/1935	0.45	0/2609
37	AS03	0.33	0/1636	0.47	0/2205
37	BS03	0.32	0/1636	0.47	0/2205
38	AS04	0.40	0/1695	0.47	0/2274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BS04	0.37	0/1695	0.47	0/2274
39	AS05	0.38	0/1171	0.49	0/1576
39	BS05	0.36	0/1171	0.50	0/1576
40	AS06	0.38	0/856	0.50	0/1154
40	BS06	0.37	0/856	0.47	0/1154
41	AS07	0.30	0/1276	0.43	0/1709
41	BS07	0.29	0/1276	0.43	0/1709
42	AS08	0.40	0/1136	0.47	0/1527
42	BS08	0.39	0/1136	0.49	0/1527
43	AS09	0.31	0/1029	0.51	0/1378
43	BS09	0.31	0/1029	0.48	0/1378
44	AS10	0.29	0/807	0.46	0/1085
44	BS10	0.29	0/807	0.49	0/1085
45	AS11	0.34	0/856	0.48	0/1157
45	BS11	0.32	0/856	0.46	0/1157
46	AS12	0.40	0/972	0.50	0/1301
46	BS12	0.39	0/972	0.52	0/1301
47	AS13	0.29	0/943	0.49	0/1265
47	BS13	0.29	0/943	0.48	0/1265
48	AS14	0.34	0/501	0.51	0/664
48	BS14	0.34	0/501	0.46	0/664
49	AS15	0.35	0/745	0.45	0/992
49	BS15	0.34	0/745	0.46	0/992
50	AS16	0.35	0/716	0.48	0/963
50	BS16	0.38	0/716	0.54	0/963
51	AS17	0.42	0/836	0.48	0/1117
51	BS17	0.41	0/836	0.48	0/1117
52	AS18	0.35	0/579	0.52	0/768
52	BS18	0.32	0/579	0.52	0/768
53	AS19	0.29	0/642	0.49	0/865
53	BS19	0.30	0/642	0.47	0/865
54	AS20	0.29	0/764	0.47	0/1006
54	BS20	0.29	0/764	0.46	0/1006
55	ATHX	0.35	0/212	0.68	1/277 (0.4%)
55	BTHX	0.31	0/212	0.51	0/277
56	BATN	1.35	20/1899 (1.1%)	2.63	197/2952 (6.7%)
All	All	0.69	156/319733 (0.0%)	0.92	774/477946 (0.2%)

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
9	AL06	0	1
15	BL17	0	1
22	BL24	0	1
24	AL27	0	1
24	BL27	0	1
28	AL31	0	2
29	AL32	0	2
29	BL32	0	2
34	BMRN	0	3
43	BS09	0	1
All	All	0	15

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BL32	60	VAL	CB-CG2	-19.93	1.10	1.52
29	BL32	59	GLU	CB-CG	17.61	1.85	1.52
1	B16S	4	U	C2-N3	15.46	1.48	1.37
1	B16S	3	G	C5-C6	14.63	1.56	1.42
1	B16S	3	G	N9-C4	13.83	1.49	1.38

The worst 5 of 774 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BMRN	16	G	N9-C1'-C2'	-31.99	72.41	114.00
35	BPTN	32	C	O4'-C4'-C3'	-29.66	74.34	104.00
35	APTN	35	A	P-O3'-C3'	28.14	153.47	119.70
34	BMRN	12	A	N9-C1'-C2'	-27.96	77.65	114.00
1	A16S	1364	U	C5-C4-O4	-24.36	111.28	125.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AL06	157	TYR	Peptide
24	AL27	8	GLY	Peptide
28	AL31	37	SER	Peptide
28	AL31	42	PHE	Peptide
29	AL32	3	LYS	Peptide

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	A16S	32600	0	0	0	0
1	B16S	32600	0	0	0	1
2	A23S	61999	0	0	0	1
2	B23S	62000	0	0	0	0
3	A5S	2551	0	1295	68	0
3	B5S	2551	0	1295	30	0
4	AL01	1742	0	0	0	0
4	BL01	1742	0	0	0	0
5	AL02	2104	0	0	0	0
5	BL02	2104	0	0	0	0
6	AL03	1563	0	0	0	0
6	BL03	1563	0	0	0	0
7	AL04	1586	0	0	0	0
7	BL04	1586	0	0	0	0
8	AL05	1475	0	0	0	0
8	BL05	1475	0	0	0	0
9	AL06	1282	0	0	0	0
9	BL06	1282	0	0	0	0
10	AL09	1131	0	0	0	0
10	BL09	1132	0	0	0	0
11	AL13	1096	0	0	0	0
11	BL13	1096	0	0	0	0
12	AL14	932	0	0	0	0
12	BL14	932	0	0	0	0
13	AL15	1114	0	0	0	0
13	BL15	1114	0	0	0	0
14	AL16	1064	0	0	0	0
14	BL16	1064	0	0	0	0
15	AL17	960	0	0	0	0
15	BL17	960	0	0	0	0
16	AL18	770	0	0	0	0
16	BL18	770	0	0	0	0
17	AL19	1143	0	0	0	0
17	BL19	1143	0	0	0	0
18	AL20	964	0	0	0	0
18	BL20	964	0	0	0	3
19	AL21	779	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	BL21	779	0	0	0	3
20	AL22	890	0	0	0	0
20	BL22	890	0	0	0	0
21	AL23	725	0	0	0	0
21	BL23	725	0	0	0	0
22	AL24	775	0	0	0	0
22	BL24	775	0	0	0	0
23	AL25	1482	0	0	0	0
23	BL25	1482	0	0	0	0
24	AL27	647	0	0	0	0
24	BL27	647	0	0	0	0
25	AL28	694	0	0	0	0
25	BL28	694	0	0	0	0
26	AL29	520	0	0	0	0
26	BL29	520	0	0	0	0
27	AL30	467	0	0	0	0
27	BL30	467	0	0	0	0
28	AL31	351	0	0	0	0
28	BL31	351	0	0	0	0
29	AL32	459	0	0	0	0
29	BL32	459	0	0	0	6
30	AL33	380	0	0	0	0
30	BL33	380	0	0	0	0
31	AL34	418	0	0	0	0
31	BL34	418	0	0	0	0
32	AL35	507	0	0	0	0
32	BL35	507	0	0	0	0
33	AL36	307	0	0	0	0
33	BL36	307	0	0	0	0
34	AMRN	223	0	0	0	0
34	BMRN	373	0	0	0	0
35	APTN	1631	0	0	0	0
35	BPTN	1631	0	0	0	0
36	AS02	1900	0	0	0	0
36	BS02	1900	0	0	0	0
37	AS03	1612	0	0	0	0
37	BS03	1612	0	0	0	0
38	AS04	1665	0	0	0	0
38	BS04	1665	0	0	0	0
39	AS05	1155	0	0	0	0
39	BS05	1155	0	0	0	0
40	AS06	843	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	BS06	843	0	0	0	0
41	AS07	1257	0	0	0	0
41	BS07	1257	0	0	0	0
42	AS08	1116	0	0	0	0
42	BS08	1116	0	0	0	0
43	AS09	1011	0	0	0	0
43	BS09	1011	0	0	0	0
44	AS10	794	0	0	0	0
44	BS10	794	0	0	0	0
45	AS11	842	0	0	0	0
45	BS11	842	0	0	0	0
46	AS12	956	0	0	0	0
46	BS12	956	0	0	0	0
47	AS13	933	0	0	0	0
47	BS13	933	0	0	0	0
48	AS14	492	0	0	0	0
48	BS14	492	0	0	0	0
49	AS15	734	0	0	0	0
49	BS15	734	0	0	0	0
50	AS16	700	0	0	0	0
50	BS16	700	0	0	0	0
51	AS17	823	0	0	0	0
51	BS17	823	0	0	0	0
52	AS18	574	0	0	0	0
52	BS18	574	0	0	0	0
53	AS19	629	0	0	0	0
53	BS19	629	0	0	0	0
54	AS20	762	0	0	0	0
54	BS20	762	0	0	0	0
55	ATHX	208	0	0	0	0
55	BTHX	208	0	0	0	0
56	BATN	1824	0	0	0	0
57	A16S	33	0	0	0	0
57	A23S	73	0	0	0	0
57	A5S	3	0	0	0	0
57	AL01	2	0	0	0	0
57	AL02	2	0	0	0	0
57	AL04	3	0	0	0	0
57	AL06	1	0	0	0	0
57	AL14	1	0	0	0	0
57	AL15	2	0	0	0	0
57	AL17	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AL20	1	0	0	0	0
57	AL21	3	0	0	0	0
57	AL23	2	0	0	0	0
57	AL24	1	0	0	0	0
57	AL27	1	0	0	0	0
57	AL28	2	0	0	0	0
57	AL33	3	0	0	0	0
57	AL34	1	0	0	0	0
57	AS02	1	0	0	0	0
57	AS03	1	0	0	0	0
57	AS06	2	0	0	0	0
57	AS08	1	0	0	0	0
57	B16S	32	0	0	0	0
57	B23S	133	0	0	0	0
57	B5S	5	0	0	0	0
57	BATN	1	0	0	0	0
57	BL01	2	0	0	0	0
57	BL02	5	0	0	0	0
57	BL03	1	0	0	0	0
57	BL04	1	0	0	0	0
57	BL15	3	0	0	0	0
57	BL16	3	0	0	0	0
57	BL18	3	0	0	0	0
57	BL19	2	0	0	0	0
57	BL20	1	0	0	0	0
57	BL21	1	0	0	0	0
57	BL22	1	0	0	0	0
57	BL23	1	0	0	0	0
57	BL24	2	0	0	0	0
57	BL25	1	0	0	0	0
57	BL28	2	0	0	0	0
57	BL29	5	0	0	0	0
57	BL30	1	0	0	0	0
57	BL31	1	0	0	0	0
57	BL32	1	0	0	0	0
57	BL33	3	0	0	0	0
57	BL34	2	0	0	0	0
57	BL35	1	0	0	0	0
57	BL36	1	0	0	0	0
57	BS16	1	0	0	0	0
57	BS17	1	0	0	0	0
57	BTHX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AS04	8	0	0	0	0
58	BS04	8	0	0	0	0
All	All	295025	0	2590	98	7

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 24.

The worst 5 of 98 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)
3:A5S:78:A:N6	3:A5S:98:G:H21	1.42	1.17
3:A5S:78:A:H62	3:A5S:98:G:N2	1.43	1.16
3:B5S:40:U:N3	3:B5S:44:G:OP2	1.97	0.97
3:B5S:13:A:O2'	3:B5S:15:A:OP2	1.90	0.88
3:B5S:14:U:OP2	3:B5S:70:C:O2'	2.02	0.76

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BL20:89:GLU:N	29:BL32:60:VAL:O[4_455]	1.96	0.24
2:A23S:2154:G:N2	1:B16S:999:U:OP2[4_545]	1.96	0.24
19:BL21:6:LYS:CE	29:BL32:59:GLU:OE2[4_455]	2.02	0.18
19:BL21:6:LYS:NZ	29:BL32:59:GLU:N[4_455]	2.04	0.16
18:BL20:89:GLU:OE2	29:BL32:59:GLU:O[4_455]	2.10	0.10

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
4	AL01	226/228 (99%)	116 (51%)	74 (33%)	36 (16%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BL01	226/228 (99%)	108 (48%)	67 (30%)	51 (23%)	0	0
5	AL02	269/276 (98%)	213 (79%)	39 (14%)	17 (6%)	1	10
5	BL02	269/276 (98%)	198 (74%)	47 (18%)	24 (9%)	1	4
6	AL03	202/206 (98%)	145 (72%)	39 (19%)	18 (9%)	1	4
6	BL03	202/206 (98%)	152 (75%)	36 (18%)	14 (7%)	1	8
7	AL04	200/205 (98%)	162 (81%)	28 (14%)	10 (5%)	2	16
7	BL04	200/205 (98%)	154 (77%)	32 (16%)	14 (7%)	1	8
8	AL05	179/181 (99%)	120 (67%)	40 (22%)	19 (11%)	0	2
8	BL05	179/181 (99%)	120 (67%)	45 (25%)	14 (8%)	1	6
9	AL06	165/180 (92%)	99 (60%)	41 (25%)	25 (15%)	0	1
9	BL06	165/180 (92%)	95 (58%)	37 (22%)	33 (20%)	0	0
10	AL09	143/148 (97%)	116 (81%)	19 (13%)	8 (6%)	2	14
10	BL09	143/148 (97%)	106 (74%)	31 (22%)	6 (4%)	3	20
11	AL13	135/140 (96%)	102 (76%)	19 (14%)	14 (10%)	0	3
11	BL13	135/140 (96%)	106 (78%)	15 (11%)	14 (10%)	0	3
12	AL14	120/122 (98%)	97 (81%)	20 (17%)	3 (2%)	5	32
12	BL14	120/122 (98%)	99 (82%)	16 (13%)	5 (4%)	3	20
13	AL15	144/150 (96%)	90 (62%)	37 (26%)	17 (12%)	0	2
13	BL15	144/150 (96%)	85 (59%)	42 (29%)	17 (12%)	0	2
14	AL16	132/141 (94%)	89 (67%)	28 (21%)	15 (11%)	0	2
14	BL16	132/141 (94%)	103 (78%)	19 (14%)	10 (8%)	1	7
15	AL17	115/118 (98%)	92 (80%)	18 (16%)	5 (4%)	2	20
15	BL17	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	1	8
16	AL18	96/111 (86%)	68 (71%)	21 (22%)	7 (7%)	1	7
16	BL18	96/111 (86%)	67 (70%)	16 (17%)	13 (14%)	0	1
17	AL19	135/146 (92%)	97 (72%)	29 (22%)	9 (7%)	1	9
17	BL19	135/146 (92%)	107 (79%)	23 (17%)	5 (4%)	3	22
18	AL20	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	2	15
18	BL20	115/118 (98%)	82 (71%)	25 (22%)	8 (7%)	1	8
19	AL21	99/101 (98%)	73 (74%)	18 (18%)	8 (8%)	1	5
19	BL21	99/101 (98%)	79 (80%)	16 (16%)	4 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AL22	110/113 (97%)	79 (72%)	25 (23%)	6 (6%)	2	14
20	BL22	110/113 (97%)	81 (74%)	24 (22%)	5 (4%)	2	18
21	AL23	90/96 (94%)	74 (82%)	14 (16%)	2 (2%)	6	35
21	BL23	90/96 (94%)	77 (86%)	10 (11%)	3 (3%)	4	25
22	AL24	98/110 (89%)	54 (55%)	32 (33%)	12 (12%)	0	2
22	BL24	98/110 (89%)	56 (57%)	29 (30%)	13 (13%)	0	1
23	AL25	185/206 (90%)	143 (77%)	32 (17%)	10 (5%)	2	14
23	BL25	185/206 (90%)	144 (78%)	32 (17%)	9 (5%)	2	17
24	AL27	80/84 (95%)	62 (78%)	11 (14%)	7 (9%)	1	4
24	BL27	80/84 (95%)	60 (75%)	11 (14%)	9 (11%)	0	2
25	AL28	86/98 (88%)	59 (69%)	22 (26%)	5 (6%)	1	13
25	BL28	86/98 (88%)	60 (70%)	18 (21%)	8 (9%)	0	3
26	AL29	60/72 (83%)	48 (80%)	8 (13%)	4 (7%)	1	9
26	BL29	60/72 (83%)	45 (75%)	12 (20%)	3 (5%)	2	16
27	AL30	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
27	BL30	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	3	24
28	AL31	43/71 (61%)	16 (37%)	8 (19%)	19 (44%)	0	0
28	BL31	43/71 (61%)	16 (37%)	15 (35%)	12 (28%)	0	0
29	AL32	57/59 (97%)	36 (63%)	12 (21%)	9 (16%)	0	1
29	BL32	57/59 (97%)	43 (75%)	8 (14%)	6 (10%)	0	3
30	AL33	42/54 (78%)	27 (64%)	8 (19%)	7 (17%)	0	0
30	BL33	42/54 (78%)	23 (55%)	11 (26%)	8 (19%)	0	0
31	AL34	46/49 (94%)	39 (85%)	5 (11%)	2 (4%)	2	20
31	BL34	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	35
32	AL35	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	3
32	BL35	61/64 (95%)	40 (66%)	13 (21%)	8 (13%)	0	1
33	AL36	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	4	28
33	BL36	35/37 (95%)	28 (80%)	2 (6%)	5 (14%)	0	1
36	AS02	232/255 (91%)	189 (82%)	27 (12%)	16 (7%)	1	8
36	BS02	232/255 (91%)	174 (75%)	42 (18%)	16 (7%)	1	8
37	AS03	204/238 (86%)	150 (74%)	39 (19%)	15 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BS03	204/238 (86%)	144 (71%)	43 (21%)	17 (8%)	1	5
38	AS04	206/208 (99%)	171 (83%)	24 (12%)	11 (5%)	2	15
38	BS04	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	1	13
39	AS05	149/161 (92%)	122 (82%)	19 (13%)	8 (5%)	2	14
39	BS05	149/161 (92%)	122 (82%)	21 (14%)	6 (4%)	3	21
40	AS06	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	2	15
40	BS06	99/101 (98%)	79 (80%)	17 (17%)	3 (3%)	4	28
41	AS07	153/155 (99%)	119 (78%)	25 (16%)	9 (6%)	1	12
41	BS07	153/155 (99%)	110 (72%)	33 (22%)	10 (6%)	1	10
42	AS08	136/138 (99%)	107 (79%)	22 (16%)	7 (5%)	2	15
42	BS08	136/138 (99%)	115 (85%)	15 (11%)	6 (4%)	2	19
43	AS09	125/128 (98%)	94 (75%)	28 (22%)	3 (2%)	6	34
43	BS09	125/128 (98%)	92 (74%)	21 (17%)	12 (10%)	0	3
44	AS10	96/104 (92%)	83 (86%)	11 (12%)	2 (2%)	7	37
44	BS10	96/104 (92%)	76 (79%)	12 (12%)	8 (8%)	1	5
45	AS11	112/128 (88%)	87 (78%)	21 (19%)	4 (4%)	3	23
45	BS11	112/128 (88%)	89 (80%)	18 (16%)	5 (4%)	2	18
46	AS12	120/131 (92%)	86 (72%)	29 (24%)	5 (4%)	3	20
46	BS12	120/131 (92%)	84 (70%)	28 (23%)	8 (7%)	1	9
47	AS13	115/125 (92%)	72 (63%)	27 (24%)	16 (14%)	0	1
47	BS13	115/125 (92%)	81 (70%)	20 (17%)	14 (12%)	0	2
48	AS14	58/60 (97%)	37 (64%)	12 (21%)	9 (16%)	0	1
48	BS14	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	4
49	AS15	86/88 (98%)	74 (86%)	8 (9%)	4 (5%)	2	17
49	BS15	86/88 (98%)	70 (81%)	9 (10%)	7 (8%)	1	5
50	AS16	81/88 (92%)	63 (78%)	17 (21%)	1 (1%)	13	49
50	BS16	81/88 (92%)	65 (80%)	13 (16%)	3 (4%)	3	22
51	AS17	97/104 (93%)	79 (81%)	16 (16%)	2 (2%)	7	37
51	BS17	97/104 (93%)	75 (77%)	19 (20%)	3 (3%)	4	26
52	AS18	68/87 (78%)	52 (76%)	12 (18%)	4 (6%)	1	12
52	BS18	68/87 (78%)	55 (81%)	10 (15%)	3 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	AS19	76/92 (83%)	46 (60%)	20 (26%)	10 (13%)	0	1
53	BS19	76/92 (83%)	53 (70%)	15 (20%)	8 (10%)	0	3
54	AS20	97/105 (92%)	72 (74%)	20 (21%)	5 (5%)	2	15
54	BS20	97/105 (92%)	75 (77%)	14 (14%)	8 (8%)	1	5
55	ATHX	22/26 (85%)	5 (23%)	13 (59%)	4 (18%)	0	0
55	BTHX	22/26 (85%)	13 (59%)	7 (32%)	2 (9%)	1	3
All	All	11714/12532 (94%)	8611 (74%)	2167 (18%)	936 (8%)	1	6

5 of 936 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AL01	141	PRO
4	AL01	172	ILE
4	AL01	181	PHE
4	AL01	182	PRO
4	AL01	225	ILE

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	
4	AL01	180/180 (100%)	170 (94%)	10 (6%)	21	57
4	BL01	180/180 (100%)	166 (92%)	14 (8%)	12	43
5	AL02	213/218 (98%)	204 (96%)	9 (4%)	30	65
5	BL02	213/218 (98%)	205 (96%)	8 (4%)	33	67
6	AL03	165/166 (99%)	163 (99%)	2 (1%)	71	88
6	BL03	165/166 (99%)	159 (96%)	6 (4%)	35	69
7	AL04	161/162 (99%)	158 (98%)	3 (2%)	57	81
7	BL04	161/162 (99%)	155 (96%)	6 (4%)	34	68
8	AL05	155/155 (100%)	142 (92%)	13 (8%)	11	39
8	BL05	155/155 (100%)	143 (92%)	12 (8%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AL06	139/148 (94%)	135 (97%)	4 (3%)	42	74
9	BL06	139/148 (94%)	132 (95%)	7 (5%)	24	60
10	AL09	121/124 (98%)	115 (95%)	6 (5%)	24	60
10	BL09	122/124 (98%)	116 (95%)	6 (5%)	25	61
11	AL13	116/119 (98%)	113 (97%)	3 (3%)	46	76
11	BL13	116/119 (98%)	109 (94%)	7 (6%)	19	54
12	AL14	100/100 (100%)	100 (100%)	0	100	100
12	BL14	100/100 (100%)	99 (99%)	1 (1%)	76	90
13	AL15	112/116 (97%)	101 (90%)	11 (10%)	8	31
13	BL15	112/116 (97%)	101 (90%)	11 (10%)	8	31
14	AL16	105/111 (95%)	101 (96%)	4 (4%)	33	67
14	BL16	105/111 (95%)	101 (96%)	4 (4%)	33	67
15	AL17	100/101 (99%)	96 (96%)	4 (4%)	31	66
15	BL17	100/101 (99%)	93 (93%)	7 (7%)	15	48
16	AL18	77/87 (88%)	73 (95%)	4 (5%)	23	59
16	BL18	77/87 (88%)	70 (91%)	7 (9%)	9	34
17	AL19	121/128 (94%)	115 (95%)	6 (5%)	24	60
17	BL19	121/128 (94%)	113 (93%)	8 (7%)	16	51
18	AL20	93/94 (99%)	90 (97%)	3 (3%)	39	71
18	BL20	93/94 (99%)	89 (96%)	4 (4%)	29	64
19	AL21	82/82 (100%)	77 (94%)	5 (6%)	18	54
19	BL21	82/82 (100%)	78 (95%)	4 (5%)	25	61
20	AL22	91/92 (99%)	87 (96%)	4 (4%)	28	64
20	BL22	91/92 (99%)	88 (97%)	3 (3%)	38	71
21	AL23	74/78 (95%)	71 (96%)	3 (4%)	30	66
21	BL23	74/78 (95%)	71 (96%)	3 (4%)	30	66
22	AL24	84/91 (92%)	78 (93%)	6 (7%)	14	47
22	BL24	84/91 (92%)	81 (96%)	3 (4%)	35	69
23	AL25	162/179 (90%)	157 (97%)	5 (3%)	40	72
23	BL25	162/179 (90%)	153 (94%)	9 (6%)	21	57
24	AL27	65/66 (98%)	62 (95%)	3 (5%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BL27	65/66 (98%)	64 (98%)	1 (2%)	65	85
25	AL28	73/83 (88%)	70 (96%)	3 (4%)	30	66
25	BL28	73/83 (88%)	68 (93%)	5 (7%)	16	49
26	AL29	58/67 (87%)	56 (97%)	2 (3%)	37	70
26	BL29	58/67 (87%)	57 (98%)	1 (2%)	60	83
27	AL30	51/52 (98%)	48 (94%)	3 (6%)	19	54
27	BL30	51/52 (98%)	50 (98%)	1 (2%)	55	80
28	AL31	40/63 (64%)	36 (90%)	4 (10%)	7	30
28	BL31	40/63 (64%)	39 (98%)	1 (2%)	47	77
29	AL32	51/51 (100%)	48 (94%)	3 (6%)	19	54
29	BL32	51/51 (100%)	48 (94%)	3 (6%)	19	54
30	AL33	43/52 (83%)	38 (88%)	5 (12%)	5	24
30	BL33	43/52 (83%)	37 (86%)	6 (14%)	3	16
31	AL34	41/42 (98%)	37 (90%)	4 (10%)	8	31
31	BL34	41/42 (98%)	41 (100%)	0	100	100
32	AL35	53/54 (98%)	49 (92%)	4 (8%)	13	45
32	BL35	53/54 (98%)	50 (94%)	3 (6%)	20	56
33	AL36	34/34 (100%)	34 (100%)	0	100	100
33	BL36	34/34 (100%)	32 (94%)	2 (6%)	19	54
36	AS02	202/219 (92%)	194 (96%)	8 (4%)	31	66
36	BS02	202/219 (92%)	192 (95%)	10 (5%)	24	60
37	AS03	160/187 (86%)	152 (95%)	8 (5%)	24	60
37	BS03	160/187 (86%)	154 (96%)	6 (4%)	33	67
38	AS04	171/180 (95%)	161 (94%)	10 (6%)	20	55
38	BS04	171/180 (95%)	162 (95%)	9 (5%)	22	58
39	AS05	116/122 (95%)	113 (97%)	3 (3%)	46	76
39	BS05	116/122 (95%)	109 (94%)	7 (6%)	19	54
40	AS06	90/90 (100%)	85 (94%)	5 (6%)	21	57
40	BS06	90/90 (100%)	87 (97%)	3 (3%)	38	71
41	AS07	126/126 (100%)	118 (94%)	8 (6%)	18	52
41	BS07	126/126 (100%)	120 (95%)	6 (5%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	AS08	119/119 (100%)	109 (92%)	10 (8%)	11	39
42	BS08	119/119 (100%)	114 (96%)	5 (4%)	30	65
43	AS09	98/99 (99%)	86 (88%)	12 (12%)	5	22
43	BS09	98/99 (99%)	93 (95%)	5 (5%)	24	60
44	AS10	88/91 (97%)	86 (98%)	2 (2%)	50	78
44	BS10	88/91 (97%)	82 (93%)	6 (7%)	16	49
45	AS11	86/98 (88%)	81 (94%)	5 (6%)	20	55
45	BS11	86/98 (88%)	82 (95%)	4 (5%)	26	62
46	AS12	103/108 (95%)	101 (98%)	2 (2%)	57	81
46	BS12	103/108 (95%)	96 (93%)	7 (7%)	16	49
47	AS13	94/100 (94%)	91 (97%)	3 (3%)	39	71
47	BS13	94/100 (94%)	89 (95%)	5 (5%)	22	58
48	AS14	49/49 (100%)	44 (90%)	5 (10%)	7	29
48	BS14	49/49 (100%)	47 (96%)	2 (4%)	30	66
49	AS15	79/79 (100%)	71 (90%)	8 (10%)	7	29
49	BS15	79/79 (100%)	77 (98%)	2 (2%)	47	77
50	AS16	72/74 (97%)	68 (94%)	4 (6%)	21	57
50	BS16	72/74 (97%)	71 (99%)	1 (1%)	67	86
51	AS17	94/96 (98%)	93 (99%)	1 (1%)	73	88
51	BS17	94/96 (98%)	89 (95%)	5 (5%)	22	58
52	AS18	61/76 (80%)	58 (95%)	3 (5%)	25	61
52	BS18	61/76 (80%)	57 (93%)	4 (7%)	16	51
53	AS19	69/79 (87%)	64 (93%)	5 (7%)	14	47
53	BS19	69/79 (87%)	65 (94%)	4 (6%)	20	55
54	AS20	76/81 (94%)	74 (97%)	2 (3%)	46	76
54	BS20	76/81 (94%)	72 (95%)	4 (5%)	22	58
55	ATHX	19/21 (90%)	14 (74%)	5 (26%)	0	2
55	BTHX	19/21 (90%)	19 (100%)	0	100	100
All	All	9865/10378 (95%)	9372 (95%)	493 (5%)	24	60

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	AS15	79	ARG
7	BL04	68	LYS
45	BS11	11	LYS
51	AS17	4	LYS
4	BL01	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A16S	1517/1518 (99%)	322 (21%)	22 (1%)
1	B16S	1517/1518 (99%)	321 (21%)	26 (1%)
2	A23S	2874/2881 (99%)	618 (21%)	33 (1%)
2	B23S	2875/2881 (99%)	610 (21%)	32 (1%)
3	A5S	118/119 (99%)	23 (19%)	3 (2%)
3	B5S	118/119 (99%)	12 (10%)	1 (0%)
34	AMRN	8/17 (47%)	5 (62%)	0
34	BMRN	17/17 (100%)	16 (94%)	8 (47%)
35	APTIN	72/76 (94%)	38 (52%)	12 (16%)
35	BPTN	72/76 (94%)	54 (75%)	21 (29%)
56	BATN	82/85 (96%)	58 (70%)	10 (12%)
All	All	9270/9307 (99%)	2077 (22%)	168 (1%)

5 of 2077 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A16S	4	U
1	A16S	6	G
1	A16S	9	G
1	A16S	14	U
1	A16S	32	A

5 of 168 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B16S	353	A
1	B16S	1534	A
35	BPTN	17	U
1	B16S	497	A
1	B16S	1145	C

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

17 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
56	PSU	BATN	55	56	17,21,22	1.24	1 (5%)	20,30,33	4.24	7 (35%)
35	PSU	BPTN	55	35	17,21,22	1.03	1 (5%)	20,30,33	2.90	5 (25%)
35	6MZ	BPTN	37	35	18,25,26	1.51	3 (16%)	16,36,39	1.73	4 (25%)
35	G7M	BPTN	46	35	20,26,27	1.98	5 (25%)	20,39,42	3.31	8 (40%)
35	4SU	APTN	8	35	14,21,22	3.36	5 (35%)	15,30,33	1.17	2 (13%)
56	PSU	BATN	39	56	17,21,22	1.79	4 (23%)	20,30,33	3.40	6 (30%)
35	CM0	APTN	34	35	16,26,27	3.20	5 (31%)	18,37,40	2.11	5 (27%)
56	MIA	BATN	37	56	24,31,32	2.20	6 (25%)	26,44,47	4.00	12 (46%)
35	4SU	BPTN	8	35	14,21,22	3.43	7 (50%)	15,30,33	1.30	2 (13%)
56	QUO	BATN	34	56	28,35,36	1.77	4 (14%)	32,52,55	2.99	12 (37%)
35	PSU	APTN	55	35	17,21,22	1.07	2 (11%)	20,30,33	3.18	7 (35%)
35	G7M	APTN	46	35	20,26,27	3.49	7 (35%)	20,39,42	2.26	4 (20%)
35	CM0	BPTN	34	35	16,26,27	1.87	6 (37%)	18,37,40	5.31	13 (72%)
56	5MU	BATN	54	56	15,22,23	2.92	3 (20%)	16,32,35	3.09	2 (12%)
35	5MU	BPTN	54	35	15,22,23	2.86	3 (20%)	16,32,35	2.82	2 (12%)
35	5MU	APTN	54	35	15,22,23	2.89	3 (20%)	16,32,35	2.87	2 (12%)
35	6MZ	APTN	37	35	18,25,26	2.46	3 (16%)	16,36,39	2.47	5 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	BATN	55	56	-	3/7/25/26	0/2/2/2
35	PSU	BPTN	55	35	-	0/7/25/26	0/2/2/2
35	6MZ	BPTN	37	35	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	G7M	BPTN	46	35	-	1/3/25/26	0/3/3/3
35	4SU	APTN	8	35	-	0/5/25/26	0/2/2/2
56	PSU	BATN	39	56	-	0/7/25/26	0/2/2/2
35	CM0	APTN	34	35	-	6/8/30/31	0/2/2/2
56	MIA	BATN	37	56	-	1/11/33/34	0/3/3/3
35	4SU	BPTN	8	35	-	0/5/25/26	0/2/2/2
56	QUO	BATN	34	56	-	1/6/43/44	0/4/4/4
35	PSU	APTN	55	35	-	0/7/25/26	0/2/2/2
35	G7M	APTN	46	35	-	1/3/25/26	0/3/3/3
35	CM0	BPTN	34	35	-	6/8/30/31	0/2/2/2
56	5MU	BATN	54	56	-	2/5/25/26	0/2/2/2
35	5MU	BPTN	54	35	-	0/5/25/26	0/2/2/2
35	5MU	APTN	54	35	-	3/5/25/26	0/2/2/2
35	6MZ	APTN	37	35	-	2/5/27/28	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BATN	54	5MU	C4-C5	9.55	1.61	1.41
35	APTN	37	6MZ	C6-N6	9.53	1.50	1.35
35	APTN	54	5MU	C4-C5	9.32	1.61	1.41
35	BPTN	54	5MU	C4-C5	9.24	1.61	1.41
35	APTN	46	G7M	C4-N3	8.76	1.49	1.35

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BPTN	34	CM0	C4-N3-C2	18.18	130.49	115.14
56	BATN	55	PSU	N1-C2-N3	-13.09	118.02	128.43
56	BATN	34	QUO	C5-C6-N1	-11.68	113.72	124.09
56	BATN	37	MIA	C12-N6-C6	-11.47	105.56	122.55
56	BATN	39	PSU	N1-C2-N3	-10.71	119.92	128.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	BPTN	37	6MZ	N1-C6-N6-C9
35	BPTN	46	G7M	C4'-C5'-O5'-P
35	APTN	34	CM0	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
35	APT	34	CM0	C3'-C4'-C5'-O5'
35	APT	34	CM0	C4-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 361 ligands modelled in this entry, 359 are monoatomic - leaving 2 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	$\# Z > 2$
58	SF4	BS04	501	38	0,12,12	0.00	-	-		
58	SF4	AS04	501	38	0,12,12	0.00	-	-		

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
58	SF4	BS04	501	38	-	-	0/6/5/5
58	SF4	AS04	501	38	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B23S	3
2	A23S	3
35	BPTN	1
35	APTN	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B23S	1141(A):C	O3'	1141:U	P	9.81
1	A23S	1141(A):C	O3'	1141:U	P	9.19
1	B23S	1140:C	O3'	1141(A):C	P	7.44
1	A23S	1140:C	O3'	1141(A):C	P	7.28
1	B23S	1141:U	O3'	1142:A	P	6.83

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A16S	1517/1518 (99%)	-0.01	44 (2%)	51	36	55, 88, 161, 216	0
1	B16S	1517/1518 (99%)	-0.00	39 (2%)	56	40	49, 90, 173, 240	0
2	A23S	2879/2881 (99%)	-0.11	37 (1%)	77	65	36, 76, 173, 238	0
2	B23S	2879/2881 (99%)	0.04	35 (1%)	79	67	28, 63, 165, 232	0
3	A5S	119/119 (100%)	0.49	9 (7%)	13	7	73, 99, 117, 126	0
3	B5S	119/119 (100%)	0.35	5 (4%)	36	23	46, 84, 106, 122	0
4	AL01	228/228 (100%)	1.77	69 (30%)	0	0	131, 167, 179, 191	0
4	BL01	228/228 (100%)	3.10	135 (59%)	0	0	126, 162, 178, 184	0
5	AL02	271/276 (98%)	0.82	31 (11%)	5	3	37, 56, 77, 85	0
5	BL02	271/276 (98%)	-0.05	2 (0%)	87	81	30, 51, 69, 77	0
6	AL03	204/206 (99%)	0.01	9 (4%)	34	21	50, 76, 97, 107	0
6	BL03	204/206 (99%)	0.01	7 (3%)	45	29	39, 66, 92, 107	0
7	AL04	202/205 (98%)	-0.18	3 (1%)	73	61	51, 85, 108, 120	0
7	BL04	202/205 (98%)	0.08	5 (2%)	57	43	34, 67, 91, 103	0
8	AL05	181/181 (100%)	3.17	111 (61%)	0	0	89, 121, 139, 147	0
8	BL05	181/181 (100%)	2.68	94 (51%)	0	0	82, 110, 138, 151	0
9	AL06	167/180 (92%)	0.04	7 (4%)	36	23	114, 151, 173, 182	0
9	BL06	167/180 (92%)	0.88	20 (11%)	4	2	116, 150, 172, 179	0
10	AL09	145/148 (97%)	0.06	13 (8%)	9	5	75, 112, 133, 140	0
10	BL09	145/148 (97%)	0.00	11 (7%)	13	7	78, 101, 118, 127	0
11	AL13	137/140 (97%)	-0.23	0	100	100	66, 87, 116, 122	0
11	BL13	137/140 (97%)	-0.15	0	100	100	48, 66, 91, 105	0
12	AL14	122/122 (100%)	-0.17	0	100	100	51, 63, 77, 85	0
12	BL14	122/122 (100%)	0.05	2 (1%)	72	59	38, 58, 73, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AL15	146/150 (97%)	0.02	9 (6%) 20 11	56, 88, 107, 125	0
13	BL15	146/150 (97%)	0.17	6 (4%) 37 24	45, 77, 98, 123	0
14	AL16	134/141 (95%)	0.19	6 (4%) 33 21	60, 82, 103, 109	0
14	BL16	134/141 (95%)	0.23	6 (4%) 33 21	52, 69, 83, 95	0
15	AL17	117/118 (99%)	0.01	2 (1%) 70 57	50, 69, 83, 92	0
15	BL17	117/118 (99%)	0.18	7 (5%) 21 12	43, 59, 77, 83	0
16	AL18	98/111 (88%)	2.56	59 (60%) 0 0	68, 83, 95, 102	0
16	BL18	98/111 (88%)	1.58	31 (31%) 0 0	47, 69, 94, 101	0
17	AL19	137/146 (93%)	-0.38	2 (1%) 73 61	54, 77, 113, 121	0
17	BL19	137/146 (93%)	-0.31	0 100 100	52, 68, 116, 134	0
18	AL20	117/118 (99%)	0.07	6 (5%) 28 16	50, 84, 101, 108	0
18	BL20	117/118 (99%)	-0.25	1 (0%) 84 75	42, 59, 74, 92	0
19	AL21	101/101 (100%)	-0.22	3 (2%) 50 34	65, 98, 111, 116	0
19	BL21	101/101 (100%)	-0.20	0 100 100	46, 72, 92, 98	0
20	AL22	112/113 (99%)	0.15	4 (3%) 42 27	54, 69, 98, 135	0
20	BL22	112/113 (99%)	-0.39	0 100 100	40, 56, 82, 113	0
21	AL23	92/96 (95%)	0.67	7 (7%) 13 7	48, 71, 96, 108	0
21	BL23	92/96 (95%)	0.19	7 (7%) 13 7	43, 58, 97, 115	0
22	AL24	100/110 (90%)	1.71	37 (37%) 0 0	83, 98, 123, 132	0
22	BL24	100/110 (90%)	0.40	10 (10%) 7 4	60, 80, 116, 141	0
23	AL25	187/206 (90%)	1.20	51 (27%) 0 0	86, 102, 123, 129	0
23	BL25	187/206 (90%)	-0.20	2 (1%) 80 69	65, 91, 108, 121	0
24	AL27	82/84 (97%)	2.84	51 (62%) 0 0	54, 66, 93, 105	0
24	BL27	82/84 (97%)	2.33	37 (45%) 0 0	51, 63, 95, 101	0
25	AL28	88/98 (89%)	0.16	2 (2%) 60 47	52, 78, 107, 121	0
25	BL28	88/98 (89%)	0.64	10 (11%) 5 3	44, 70, 95, 106	0
26	AL29	62/72 (86%)	0.16	3 (4%) 30 18	66, 86, 114, 125	0
26	BL29	62/72 (86%)	0.20	4 (6%) 18 11	40, 74, 102, 114	0
27	AL30	59/60 (98%)	0.79	12 (20%) 1 1	67, 89, 107, 125	0
27	BL30	59/60 (98%)	0.02	2 (3%) 45 29	46, 68, 90, 114	0
28	AL31	45/71 (63%)	2.20	21 (46%) 0 0	124, 142, 151, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BL31	45/71 (63%)	3.38	25 (55%) 0 0	123, 143, 150, 157	0
29	AL32	59/59 (100%)	0.22	2 (3%) 45 29	50, 67, 133, 140	0
29	BL32	59/59 (100%)	0.33	8 (13%) 3 2	42, 63, 126, 135	0
30	AL33	44/54 (81%)	0.08	3 (6%) 17 10	61, 77, 87, 90	0
30	BL33	44/54 (81%)	0.99	8 (18%) 1 1	44, 72, 78, 88	0
31	AL34	48/49 (97%)	-0.06	1 (2%) 63 49	36, 52, 67, 85	0
31	BL34	48/49 (97%)	-0.14	1 (2%) 63 49	29, 39, 62, 69	0
32	AL35	63/64 (98%)	0.36	2 (3%) 47 31	54, 67, 76, 88	0
32	BL35	63/64 (98%)	0.11	3 (4%) 30 18	46, 57, 69, 81	0
33	AL36	37/37 (100%)	0.97	6 (16%) 1 1	70, 80, 95, 115	0
33	BL36	37/37 (100%)	0.96	8 (21%) 0 1	58, 72, 93, 95	0
34	AMRN	10/17 (58%)	1.50	2 (20%) 1 1	108, 136, 165, 166	0
34	BMRN	17/17 (100%)	0.26	0 100 100	109, 144, 173, 178	0
35	APTN	70/76 (92%)	0.99	13 (18%) 1 1	77, 172, 208, 231	0
35	BPTN	70/76 (92%)	0.20	2 (2%) 51 36	70, 140, 172, 182	0
36	AS02	234/255 (91%)	-0.27	1 (0%) 92 89	82, 108, 131, 141	0
36	BS02	234/255 (91%)	-0.39	0 100 100	91, 110, 133, 146	0
37	AS03	206/238 (86%)	-0.19	5 (2%) 59 44	76, 98, 117, 123	0
37	BS03	206/238 (86%)	-0.26	3 (1%) 73 61	83, 106, 123, 132	0
38	AS04	208/208 (100%)	0.85	26 (12%) 3 2	53, 78, 93, 108	0
38	BS04	208/208 (100%)	0.71	29 (13%) 2 1	63, 85, 98, 105	0
39	AS05	151/161 (93%)	0.36	11 (7%) 15 9	59, 76, 96, 102	0
39	BS05	151/161 (93%)	0.44	12 (7%) 12 6	61, 80, 97, 112	0
40	AS06	101/101 (100%)	0.23	6 (5%) 22 13	68, 89, 99, 103	0
40	BS06	101/101 (100%)	-0.21	1 (0%) 82 72	74, 88, 101, 106	0
41	AS07	155/155 (100%)	-0.18	5 (3%) 47 31	101, 122, 141, 158	0
41	BS07	155/155 (100%)	0.41	21 (13%) 3 2	108, 125, 136, 142	0
42	AS08	138/138 (100%)	-0.39	0 100 100	65, 78, 86, 90	0
42	BS08	138/138 (100%)	0.33	10 (7%) 15 9	64, 82, 96, 108	0
43	AS09	127/128 (99%)	0.52	11 (8%) 10 5	97, 133, 144, 150	0
43	BS09	127/128 (99%)	2.06	48 (37%) 0 0	100, 134, 146, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AS10	98/104 (94%)	0.97	15 (15%) 2 1	99, 122, 143, 158	0
44	BS10	98/104 (94%)	-0.02	5 (5%) 28 16	98, 120, 137, 142	0
45	AS11	114/128 (89%)	1.48	34 (29%) 0 0	68, 97, 117, 120	0
45	BS11	114/128 (89%)	-0.01	5 (4%) 34 21	56, 98, 120, 129	0
46	AS12	122/131 (93%)	-0.01	1 (0%) 86 78	56, 74, 88, 98	0
46	BS12	122/131 (93%)	-0.15	4 (3%) 46 30	56, 78, 93, 98	0
47	AS13	117/125 (93%)	0.93	18 (15%) 2 1	115, 132, 144, 166	0
47	BS13	117/125 (93%)	2.31	55 (47%) 0 0	121, 139, 152, 156	0
48	AS14	60/60 (100%)	1.38	17 (28%) 0 0	93, 112, 144, 153	0
48	BS14	60/60 (100%)	0.61	7 (11%) 4 2	95, 112, 148, 156	0
49	AS15	88/88 (100%)	-0.10	3 (3%) 45 29	55, 75, 89, 94	0
49	BS15	88/88 (100%)	-0.01	1 (1%) 80 69	57, 74, 95, 104	0
50	AS16	83/88 (94%)	0.55	7 (8%) 11 6	70, 82, 105, 117	0
50	BS16	83/88 (94%)	1.11	19 (22%) 0 0	66, 78, 99, 124	0
51	AS17	99/104 (95%)	-0.57	0 100 100	56, 70, 83, 91	0
51	BS17	99/104 (95%)	0.29	3 (3%) 50 34	59, 71, 82, 87	0
52	AS18	70/87 (80%)	-0.02	1 (1%) 75 63	68, 82, 100, 108	0
52	BS18	70/87 (80%)	-0.15	1 (1%) 75 63	69, 93, 110, 120	0
53	AS19	78/92 (84%)	2.69	47 (60%) 0 0	124, 135, 144, 152	0
53	BS19	78/92 (84%)	1.95	35 (44%) 0 0	111, 130, 142, 145	0
54	AS20	99/105 (94%)	0.95	18 (18%) 1 1	75, 94, 112, 122	0
54	BS20	99/105 (94%)	0.06	3 (3%) 50 34	64, 84, 105, 112	0
55	ATHX	24/26 (92%)	4.24	16 (66%) 0 0	134, 153, 159, 163	0
55	BTHX	24/26 (92%)	9.19	21 (87%) 0 0	139, 155, 161, 170	0
56	BATN	80/85 (94%)	3.42	50 (62%) 0 0	104, 171, 217, 231	0
All	All	21191/21839 (97%)	0.31	1745 (8%) 11 6	28, 83, 162, 240	0

The worst 5 of 1745 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AL01	3	LYS	27.8
55	BTHX	19	GLY	25.2
4	AL01	5	GLY	24.6

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Mol	Chain	Res	Type	RSRZ
22	AL24	59	GLY	19.6
56	BATN	47(E)	A	19.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	BATN	39	20/21	0.52	0.29	140,150,156,157	0
56	PSU	BATN	55	20/21	0.58	0.41	138,155,160,163	0
56	QUO	BATN	34	32/33	0.60	0.24	125,131,141,145	0
35	G7M	APTN	46	24/25	0.70	0.37	175,184,204,220	0
56	5MU	BATN	54	21/22	0.70	0.61	126,150,160,164	0
35	5MU	BPTN	54	21/22	0.72	0.36	128,135,141,147	0
35	6MZ	BPTN	37	23/24	0.73	0.17	65,76,84,98	0
56	MIA	BATN	37	29/30	0.73	0.22	133,139,142,148	0
35	4SU	APTN	8	20/21	0.73	0.27	179,188,195,198	0
35	4SU	BPTN	8	20/21	0.74	0.16	145,150,159,163	0
35	5MU	APTN	54	21/22	0.75	0.18	155,167,169,170	0
35	6MZ	APTN	37	23/24	0.77	0.30	115,122,128,133	0
35	PSU	BPTN	55	20/21	0.79	0.21	132,146,156,160	0
35	PSU	APTN	55	20/21	0.81	0.16	163,176,182,183	0
35	CM0	APTN	34	25/26	0.83	0.35	119,126,131,132	0
35	G7M	BPTN	46	24/25	0.83	0.16	144,157,172,188	0
35	CM0	BPTN	34	25/26	0.87	0.18	96,104,116,117	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
57	MG	A5S	201	1/1	0.50	0.20	98,98,98,98	0
57	MG	B23S	2924	1/1	0.50	0.18	62,62,62,62	0
57	MG	A23S	2947	1/1	0.51	0.16	47,47,47,47	0
57	MG	B23S	2906	1/1	0.57	0.20	37,37,37,37	0
57	MG	A23S	2910	1/1	0.63	0.22	83,83,83,83	0
57	MG	B23S	2976	1/1	0.64	0.18	46,46,46,46	0
57	MG	AL02	302	1/1	0.65	0.85	50,50,50,50	0
57	MG	BL30	101	1/1	0.66	0.10	72,72,72,72	0
57	MG	A23S	2940	1/1	0.66	0.21	63,63,63,63	0
57	MG	B23S	2949	1/1	0.66	0.20	31,31,31,31	0
57	MG	B23S	3025	1/1	0.67	0.33	45,45,45,45	0
57	MG	B16S	1608	1/1	0.67	0.16	56,56,56,56	0
57	MG	AL14	201	1/1	0.67	0.25	58,58,58,58	0
57	MG	BL01	302	1/1	0.68	0.15	90,90,90,90	0
57	MG	B23S	2959	1/1	0.69	0.13	69,69,69,69	0
57	MG	AL15	202	1/1	0.69	0.17	61,61,61,61	0
57	MG	BATN	101	1/1	0.69	0.22	80,80,80,80	0
57	MG	A16S	1603	1/1	0.69	0.17	57,57,57,57	0
57	MG	B16S	1624	1/1	0.69	0.16	56,56,56,56	0
57	MG	AS06	202	1/1	0.71	0.13	68,68,68,68	0
57	MG	B5S	203	1/1	0.72	0.17	58,58,58,58	0
57	MG	B23S	3011	1/1	0.72	0.14	52,52,52,52	0
57	MG	A23S	2936	1/1	0.72	0.15	40,40,40,40	0
57	MG	B23S	2990	1/1	0.72	0.37	51,51,51,51	0
57	MG	B23S	3015	1/1	0.72	0.10	50,50,50,50	0
57	MG	B16S	1629	1/1	0.73	0.20	82,82,82,82	0
57	MG	BL15	202	1/1	0.73	0.11	64,64,64,64	0
57	MG	B23S	2972	1/1	0.74	0.14	62,62,62,62	0
57	MG	A23S	2927	1/1	0.75	0.15	37,37,37,37	0
57	MG	B23S	2989	1/1	0.75	0.15	56,56,56,56	0
57	MG	BL15	203	1/1	0.75	0.40	48,48,48,48	0
57	MG	B23S	2953	1/1	0.76	0.17	44,44,44,44	0
57	MG	B23S	3000	1/1	0.76	0.15	35,35,35,35	0
57	MG	B23S	2932	1/1	0.76	0.14	43,43,43,43	0
57	MG	B23S	3010	1/1	0.76	0.23	56,56,56,56	0
57	MG	B23S	2974	1/1	0.76	0.17	45,45,45,45	0
57	MG	AL17	202	1/1	0.76	0.10	47,47,47,47	0
57	MG	AL04	301	1/1	0.76	0.10	57,57,57,57	0
57	MG	B16S	1603	1/1	0.77	0.27	57,57,57,57	0
57	MG	BL31	101	1/1	0.77	0.17	78,78,78,78	0
57	MG	A23S	2959	1/1	0.77	0.12	57,57,57,57	0
57	MG	B23S	2936	1/1	0.77	0.10	54,54,54,54	0
57	MG	B23S	3031	1/1	0.78	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	A23S	2911	1/1	0.78	0.65	40,40,40,40	0
57	MG	A23S	2970	1/1	0.78	0.25	73,73,73,73	0
57	MG	BL23	101	1/1	0.78	0.65	46,46,46,46	0
57	MG	BL01	301	1/1	0.78	0.14	105,105,105,105	0
57	MG	A16S	1610	1/1	0.78	0.22	74,74,74,74	0
57	MG	AL34	100	1/1	0.78	0.41	55,55,55,55	0
57	MG	B23S	2963	1/1	0.78	0.18	37,37,37,37	0
57	MG	B5S	204	1/1	0.79	0.10	55,55,55,55	0
57	MG	A23S	2962	1/1	0.79	0.20	50,50,50,50	0
57	MG	B23S	2908	1/1	0.79	0.18	32,32,32,32	0
57	MG	BL33	102	1/1	0.79	0.10	51,51,51,51	0
57	MG	B23S	2960	1/1	0.79	0.25	59,59,59,59	0
57	MG	A16S	1601	1/1	0.80	0.11	47,47,47,47	0
57	MG	A23S	2969	1/1	0.80	0.08	47,47,47,47	0
57	MG	AL23	102	1/1	0.80	0.33	73,73,73,73	0
57	MG	A23S	2953	1/1	0.80	0.09	62,62,62,62	0
57	MG	B16S	1627	1/1	0.80	0.13	85,85,85,85	0
57	MG	BL22	201	1/1	0.80	0.14	34,34,34,34	0
57	MG	AL23	101	1/1	0.80	0.09	57,57,57,57	0
57	MG	B23S	3026	1/1	0.81	0.20	42,42,42,42	0
57	MG	AL06	201	1/1	0.81	0.12	67,67,67,67	0
57	MG	AL01	301	1/1	0.81	0.17	105,105,105,105	0
57	MG	B16S	1630	1/1	0.81	0.11	58,58,58,58	0
57	MG	B23S	2956	1/1	0.81	0.18	42,42,42,42	0
57	MG	B23S	2918	1/1	0.81	0.44	34,34,34,34	0
57	MG	B23S	2986	1/1	0.81	0.09	55,55,55,55	0
57	MG	A16S	1625	1/1	0.81	0.19	62,62,62,62	0
57	MG	A23S	2916	1/1	0.81	0.15	36,36,36,36	0
57	MG	B23S	3009	1/1	0.81	0.36	46,46,46,46	0
57	MG	BL18	201	1/1	0.82	0.30	57,57,57,57	0
57	MG	A16S	1626	1/1	0.82	0.07	58,58,58,58	0
57	MG	B23S	2996	1/1	0.82	0.13	40,40,40,40	0
57	MG	A16S	1619	1/1	0.82	0.14	42,42,42,42	0
57	MG	B23S	2961	1/1	0.82	0.36	42,42,42,42	0
57	MG	BL19	202	1/1	0.82	0.10	63,63,63,63	0
57	MG	B23S	2962	1/1	0.82	0.24	50,50,50,50	0
57	MG	B23S	2934	1/1	0.82	0.17	24,24,24,24	0
57	MG	B23S	2951	1/1	0.82	0.11	50,50,50,50	0
57	MG	B16S	1610	1/1	0.82	0.16	70,70,70,70	0
57	MG	A16S	1613	1/1	0.82	0.18	78,78,78,78	0
57	MG	B16S	1622	1/1	0.83	0.19	44,44,44,44	0
57	MG	B23S	3021	1/1	0.83	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	B23S	2984	1/1	0.83	0.15	41,41,41,41	0
57	MG	BL16	201	1/1	0.83	0.46	52,52,52,52	0
57	MG	BL34	101	1/1	0.83	0.48	41,41,41,41	0
57	MG	B16S	1604	1/1	0.83	0.07	58,58,58,58	0
57	MG	B23S	3002	1/1	0.84	0.22	43,43,43,43	0
57	MG	B23S	3003	1/1	0.84	0.11	46,46,46,46	0
57	MG	B16S	1631	1/1	0.84	0.13	40,40,40,40	0
57	MG	A5S	202	1/1	0.84	0.69	70,70,70,70	0
57	MG	B16S	1626	1/1	0.84	0.14	61,61,61,61	0
57	MG	A23S	2925	1/1	0.84	0.10	44,44,44,44	0
57	MG	B23S	3007	1/1	0.84	0.23	34,34,34,34	0
57	MG	B23S	2910	1/1	0.84	0.36	59,59,59,59	0
57	MG	BL03	301	1/1	0.84	0.43	51,51,51,51	0
57	MG	B23S	2955	1/1	0.84	0.36	45,45,45,45	0
57	MG	B23S	2958	1/1	0.84	0.15	40,40,40,40	0
57	MG	AL01	302	1/1	0.85	0.18	93,93,93,93	0
57	MG	B16S	1628	1/1	0.85	0.15	78,78,78,78	0
57	MG	B23S	3016	1/1	0.85	0.32	47,47,47,47	0
57	MG	AL04	302	1/1	0.85	0.16	73,73,73,73	0
57	MG	AS03	301	1/1	0.85	0.15	67,67,67,67	0
57	MG	A16S	1622	1/1	0.85	0.13	68,68,68,68	0
57	MG	B23S	3032	1/1	0.85	0.19	47,47,47,47	0
57	MG	A16S	1607	1/1	0.85	0.12	51,51,51,51	0
57	MG	B23S	3022	1/1	0.85	0.21	46,46,46,46	0
57	MG	A23S	2941	1/1	0.85	0.13	46,46,46,46	0
57	MG	B23S	2939	1/1	0.85	0.12	57,57,57,57	0
57	MG	BL02	303	1/1	0.85	0.69	60,60,60,60	0
57	MG	B16S	1605	1/1	0.85	0.13	30,30,30,30	0
57	MG	B23S	2994	1/1	0.86	0.11	53,53,53,53	0
57	MG	AL33	103	1/1	0.86	0.18	48,48,48,48	0
57	MG	BL02	301	1/1	0.86	0.13	31,31,31,31	0
57	MG	BL16	202	1/1	0.86	0.08	45,45,45,45	0
57	MG	BL29	104	1/1	0.86	0.22	46,46,46,46	0
57	MG	B23S	2964	1/1	0.86	0.25	62,62,62,62	0
57	MG	B23S	2937	1/1	0.86	0.14	52,52,52,52	0
57	MG	B16S	1613	1/1	0.86	0.14	61,61,61,61	0
57	MG	AL28	101	1/1	0.86	0.26	44,44,44,44	0
57	MG	B23S	2979	1/1	0.86	0.20	51,51,51,51	0
57	MG	B23S	2967	1/1	0.86	0.12	64,64,64,64	0
57	MG	BL29	105	1/1	0.86	0.22	58,58,58,58	0
57	MG	A16S	1611	1/1	0.86	0.10	52,52,52,52	0
57	MG	B23S	2915	1/1	0.86	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	A16S	1614	1/1	0.86	0.16	42,42,42,42	0
57	MG	B23S	3008	1/1	0.86	0.14	53,53,53,53	0
57	MG	B23S	2998	1/1	0.86	0.19	51,51,51,51	0
57	MG	A23S	2943	1/1	0.86	0.11	52,52,52,52	0
57	MG	B23S	2916	1/1	0.87	0.15	43,43,43,43	0
57	MG	B23S	2933	1/1	0.87	0.08	60,60,60,60	0
57	MG	B23S	2926	1/1	0.87	0.22	41,41,41,41	0
57	MG	B23S	3019	1/1	0.87	0.12	51,51,51,51	0
57	MG	B23S	3027	1/1	0.87	0.14	39,39,39,39	0
57	MG	A16S	1624	1/1	0.87	0.10	50,50,50,50	0
57	MG	A23S	2907	1/1	0.87	0.18	51,51,51,51	0
57	MG	B16S	1623	1/1	0.87	0.18	46,46,46,46	0
57	MG	B23S	2954	1/1	0.87	0.14	56,56,56,56	0
57	MG	B5S	205	1/1	0.87	0.13	38,38,38,38	0
57	MG	A16S	1612	1/1	0.87	0.53	54,54,54,54	0
57	MG	A16S	1605	1/1	0.87	0.16	78,78,78,78	0
57	MG	B16S	1618	1/1	0.87	0.28	61,61,61,61	0
57	MG	AL04	303	1/1	0.87	0.11	78,78,78,78	0
57	MG	B23S	3028	1/1	0.87	0.10	69,69,69,69	0
57	MG	A23S	2921	1/1	0.87	0.11	35,35,35,35	0
57	MG	A23S	2964	1/1	0.88	0.10	52,52,52,52	0
57	MG	B23S	2944	1/1	0.88	0.08	41,41,41,41	0
57	MG	B23S	2983	1/1	0.88	0.13	46,46,46,46	0
57	MG	A16S	1608	1/1	0.88	0.17	79,79,79,79	0
57	MG	A23S	2951	1/1	0.88	0.12	50,50,50,50	0
57	MG	B23S	2928	1/1	0.88	0.18	35,35,35,35	0
57	MG	A23S	2971	1/1	0.88	0.09	102,102,102,102	0
57	MG	B23S	2917	1/1	0.88	0.16	50,50,50,50	0
57	MG	A23S	2961	1/1	0.88	0.16	61,61,61,61	0
57	MG	B23S	2948	1/1	0.88	0.12	32,32,32,32	0
57	MG	B23S	2931	1/1	0.88	0.09	33,33,33,33	0
57	MG	B16S	1611	1/1	0.88	0.06	63,63,63,63	0
57	MG	B23S	2985	1/1	0.89	0.08	42,42,42,42	0
57	MG	AL02	301	1/1	0.89	0.37	51,51,51,51	0
57	MG	A23S	2901	1/1	0.89	0.21	33,33,33,33	0
57	MG	A23S	2963	1/1	0.89	0.15	58,58,58,58	0
57	MG	BL19	201	1/1	0.89	0.13	68,68,68,68	0
57	MG	BL28	101	1/1	0.89	0.15	55,55,55,55	0
57	MG	B23S	2938	1/1	0.89	0.10	45,45,45,45	0
57	MG	BTHX	101	1/1	0.89	0.08	117,117,117,117	0
57	MG	A23S	2938	1/1	0.89	0.17	35,35,35,35	0
57	MG	A16S	1620	1/1	0.89	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BL15	201	1/1	0.89	0.17	46,46,46,46	0
57	MG	A23S	2972	1/1	0.89	0.15	50,50,50,50	0
57	MG	A23S	2912	1/1	0.89	0.19	39,39,39,39	0
57	MG	B23S	2977	1/1	0.89	0.11	63,63,63,63	0
57	MG	A16S	1633	1/1	0.89	0.10	48,48,48,48	0
57	MG	A23S	2966	1/1	0.89	0.07	46,46,46,46	0
57	MG	B23S	2999	1/1	0.89	0.10	35,35,35,35	0
57	MG	B23S	3006	1/1	0.89	0.10	70,70,70,70	0
57	MG	A16S	1630	1/1	0.89	0.08	55,55,55,55	0
57	MG	B23S	2942	1/1	0.89	0.09	41,41,41,41	0
57	MG	B16S	1612	1/1	0.90	0.09	61,61,61,61	0
57	MG	B23S	3014	1/1	0.90	0.12	48,48,48,48	0
57	MG	BL21	201	1/1	0.90	0.14	69,69,69,69	0
57	MG	B23S	3017	1/1	0.90	0.07	46,46,46,46	0
57	MG	B16S	1601	1/1	0.90	0.23	58,58,58,58	0
57	MG	B23S	2919	1/1	0.90	0.17	33,33,33,33	0
57	MG	A23S	2919	1/1	0.90	0.58	44,44,44,44	0
57	MG	BL32	101	1/1	0.90	0.21	84,84,84,84	0
57	MG	A16S	1617	1/1	0.90	0.20	61,61,61,61	0
57	MG	B23S	2973	1/1	0.90	0.15	54,54,54,54	0
57	MG	AL21	201	1/1	0.90	0.30	49,49,49,49	0
57	MG	B23S	3013	1/1	0.90	0.15	77,77,77,77	0
57	MG	B16S	1621	1/1	0.90	0.11	38,38,38,38	0
57	MG	B16S	1617	1/1	0.90	0.13	53,53,53,53	0
57	MG	AL24	201	1/1	0.90	0.08	63,63,63,63	0
57	MG	A23S	2935	1/1	0.90	0.18	58,58,58,58	0
57	MG	B23S	3023	1/1	0.90	0.17	54,54,54,54	0
57	MG	BL29	101	1/1	0.90	0.15	46,46,46,46	0
57	MG	B23S	2930	1/1	0.90	0.09	54,54,54,54	0
57	MG	B23S	2905	1/1	0.90	0.14	31,31,31,31	0
57	MG	A16S	1631	1/1	0.90	0.09	46,46,46,46	0
57	MG	A16S	1604	1/1	0.90	0.12	56,56,56,56	0
57	MG	B23S	3018	1/1	0.91	0.06	35,35,35,35	0
57	MG	B23S	2993	1/1	0.91	0.20	43,43,43,43	0
57	MG	B16S	1614	1/1	0.91	0.10	46,46,46,46	0
57	MG	A23S	2973	1/1	0.91	0.08	46,46,46,46	0
57	MG	A16S	1618	1/1	0.91	0.14	65,65,65,65	0
57	MG	B23S	2946	1/1	0.91	0.11	46,46,46,46	0
57	MG	B23S	2987	1/1	0.91	0.11	32,32,32,32	0
57	MG	B23S	2943	1/1	0.91	0.13	50,50,50,50	0
57	MG	A23S	2933	1/1	0.91	0.32	58,58,58,58	0
57	MG	A16S	1606	1/1	0.91	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	A23S	2926	1/1	0.91	0.12	64,64,64,64	0
57	MG	A23S	2967	1/1	0.91	0.08	60,60,60,60	0
57	MG	B23S	3033	1/1	0.91	0.18	67,67,67,67	0
57	MG	AL17	201	1/1	0.91	0.15	51,51,51,51	0
57	MG	B23S	2952	1/1	0.91	0.07	42,42,42,42	0
57	MG	B23S	2995	1/1	0.91	0.20	57,57,57,57	0
57	MG	BL18	202	1/1	0.91	0.39	45,45,45,45	0
57	MG	A16S	1616	1/1	0.91	0.07	62,62,62,62	0
57	MG	BL02	304	1/1	0.92	0.11	45,45,45,45	0
57	MG	A23S	2948	1/1	0.92	0.10	60,60,60,60	0
57	MG	B23S	2941	1/1	0.92	0.14	35,35,35,35	0
57	MG	A23S	2934	1/1	0.92	0.09	39,39,39,39	0
57	MG	B23S	3004	1/1	0.92	0.26	58,58,58,58	0
57	MG	B23S	2997	1/1	0.92	0.23	49,49,49,49	0
57	MG	B23S	2978	1/1	0.92	0.09	39,39,39,39	0
57	MG	A23S	2908	1/1	0.92	0.12	52,52,52,52	0
57	MG	B23S	2971	1/1	0.92	0.13	45,45,45,45	0
57	MG	A23S	2942	1/1	0.92	0.17	38,38,38,38	0
57	MG	A23S	2928	1/1	0.92	0.26	32,32,32,32	0
57	MG	BL29	103	1/1	0.92	0.16	30,30,30,30	0
57	MG	B23S	2911	1/1	0.92	0.18	38,38,38,38	0
57	MG	A16S	1615	1/1	0.92	0.23	51,51,51,51	0
57	MG	A16S	1632	1/1	0.92	0.10	65,65,65,65	0
57	MG	A23S	2965	1/1	0.92	0.11	62,62,62,62	0
57	MG	B16S	1619	1/1	0.92	0.09	50,50,50,50	0
57	MG	B23S	2929	1/1	0.92	0.13	38,38,38,38	0
57	MG	A23S	2960	1/1	0.92	0.08	56,56,56,56	0
57	MG	A16S	1627	1/1	0.92	0.13	47,47,47,47	0
57	MG	A23S	2920	1/1	0.92	0.16	56,56,56,56	0
57	MG	AS08	201	1/1	0.92	0.28	43,43,43,43	0
57	MG	B23S	2968	1/1	0.92	0.13	38,38,38,38	0
57	MG	B23S	3012	1/1	0.92	0.07	54,54,54,54	0
57	MG	B23S	3024	1/1	0.92	0.12	47,47,47,47	0
57	MG	AL27	101	1/1	0.92	0.20	40,40,40,40	0
57	MG	B23S	2923	1/1	0.92	0.13	53,53,53,53	0
57	MG	B16S	1616	1/1	0.92	0.17	44,44,44,44	0
57	MG	A23S	2945	1/1	0.92	0.24	45,45,45,45	0
57	MG	A5S	203	1/1	0.92	0.13	58,58,58,58	0
57	MG	A16S	1623	1/1	0.92	0.17	42,42,42,42	0
57	MG	B23S	2921	1/1	0.92	0.23	56,56,56,56	0
57	MG	BL35	101	1/1	0.92	0.23	58,58,58,58	0
57	MG	B16S	1632	1/1	0.92	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	A23S	2950	1/1	0.92	0.16	34,34,34,34	0
57	MG	A23S	2930	1/1	0.93	0.08	44,44,44,44	0
57	MG	AL28	102	1/1	0.93	0.09	50,50,50,50	0
57	MG	B23S	2935	1/1	0.93	0.10	30,30,30,30	0
57	MG	A23S	2952	1/1	0.93	0.12	43,43,43,43	0
57	MG	B23S	2903	1/1	0.93	0.11	34,34,34,34	0
57	MG	BL25	301	1/1	0.93	0.11	46,46,46,46	0
57	MG	A16S	1629	1/1	0.93	0.41	93,93,93,93	0
57	MG	A23S	2906	1/1	0.93	0.08	41,41,41,41	0
57	MG	A23S	2949	1/1	0.93	0.58	71,71,71,71	0
57	MG	A23S	2929	1/1	0.93	0.11	52,52,52,52	0
57	MG	BL02	305	1/1	0.93	0.09	59,59,59,59	0
57	MG	AS02	301	1/1	0.93	0.12	90,90,90,90	0
57	MG	B23S	2913	1/1	0.93	0.12	28,28,28,28	0
57	MG	A23S	2955	1/1	0.93	0.49	58,58,58,58	0
57	MG	B23S	2966	1/1	0.93	0.14	51,51,51,51	0
57	MG	B23S	2912	1/1	0.93	0.22	27,27,27,27	0
57	MG	A23S	2902	1/1	0.93	0.18	45,45,45,45	0
57	MG	A23S	2932	1/1	0.93	0.13	43,43,43,43	0
57	MG	B23S	2981	1/1	0.93	0.09	31,31,31,31	0
57	MG	B23S	2947	1/1	0.93	0.14	41,41,41,41	0
57	MG	B23S	2940	1/1	0.93	0.31	44,44,44,44	0
57	MG	B23S	2920	1/1	0.94	0.14	31,31,31,31	0
57	MG	BL16	203	1/1	0.94	0.16	69,69,69,69	0
57	MG	B16S	1615	1/1	0.94	0.17	65,65,65,65	0
57	MG	B16S	1602	1/1	0.94	0.15	44,44,44,44	0
57	MG	AL20	201	1/1	0.94	0.12	75,75,75,75	0
57	MG	B23S	3005	1/1	0.94	0.24	50,50,50,50	0
57	MG	B23S	3029	1/1	0.94	0.23	43,43,43,43	0
57	MG	B23S	2957	1/1	0.94	0.22	23,23,23,23	0
57	MG	B23S	2925	1/1	0.94	0.18	46,46,46,46	0
57	MG	BL33	101	1/1	0.94	0.29	57,57,57,57	0
57	MG	A23S	2954	1/1	0.94	0.09	40,40,40,40	0
57	MG	BL04	301	1/1	0.94	0.25	55,55,55,55	0
57	MG	A23S	2958	1/1	0.94	0.11	50,50,50,50	0
57	MG	A23S	2903	1/1	0.94	0.19	41,41,41,41	0
57	MG	B23S	2927	1/1	0.94	0.14	58,58,58,58	0
57	MG	A16S	1602	1/1	0.94	0.08	37,37,37,37	0
57	MG	B23S	2980	1/1	0.94	0.38	47,47,47,47	0
57	MG	B23S	2945	1/1	0.94	0.18	35,35,35,35	0
57	MG	B23S	2988	1/1	0.94	0.11	51,51,51,51	0
57	MG	BL24	201	1/1	0.94	0.21	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	B23S	2991	1/1	0.94	0.04	63,63,63,63	0
57	MG	B23S	2950	1/1	0.94	0.35	33,33,33,33	0
57	MG	B16S	1606	1/1	0.94	0.27	65,65,65,65	0
57	MG	A16S	1609	1/1	0.94	0.15	71,71,71,71	0
57	MG	A23S	2924	1/1	0.94	0.05	46,46,46,46	0
57	MG	A23S	2917	1/1	0.95	0.16	52,52,52,52	0
57	MG	A23S	2914	1/1	0.95	0.12	59,59,59,59	0
57	MG	B5S	201	1/1	0.95	0.28	47,47,47,47	0
57	MG	AS06	201	1/1	0.95	0.12	82,82,82,82	0
57	MG	B23S	2902	1/1	0.95	0.16	24,24,24,24	0
57	MG	A23S	2913	1/1	0.95	0.08	47,47,47,47	0
57	MG	A23S	2956	1/1	0.95	0.22	66,66,66,66	0
57	MG	A23S	2968	1/1	0.95	0.19	51,51,51,51	0
57	MG	A23S	2944	1/1	0.95	0.18	46,46,46,46	0
57	MG	A23S	2957	1/1	0.95	0.12	53,53,53,53	0
57	MG	AL33	102	1/1	0.95	0.07	45,45,45,45	0
57	MG	B23S	2907	1/1	0.95	0.12	31,31,31,31	0
57	MG	BL28	102	1/1	0.95	0.17	41,41,41,41	0
57	MG	B23S	3001	1/1	0.95	0.14	32,32,32,32	0
57	MG	B23S	2914	1/1	0.95	0.24	31,31,31,31	0
57	MG	BL24	202	1/1	0.95	0.09	53,53,53,53	0
57	MG	BS17	201	1/1	0.95	0.09	66,66,66,66	0
57	MG	AL21	203	1/1	0.95	0.09	86,86,86,86	0
57	MG	B23S	2970	1/1	0.95	0.09	57,57,57,57	0
57	MG	BL29	102	1/1	0.96	0.15	23,23,23,23	0
57	MG	BL02	302	1/1	0.96	0.07	65,65,65,65	0
57	MG	A23S	2918	1/1	0.96	0.24	65,65,65,65	0
57	MG	B23S	2901	1/1	0.96	0.22	43,43,43,43	0
57	MG	A23S	2915	1/1	0.96	0.09	40,40,40,40	0
57	MG	B23S	2992	1/1	0.96	0.18	32,32,32,32	0
57	MG	A23S	2905	1/1	0.96	0.08	38,38,38,38	0
57	MG	B23S	2969	1/1	0.96	0.23	67,67,67,67	0
57	MG	B23S	3030	1/1	0.96	0.07	61,61,61,61	0
57	MG	A23S	2922	1/1	0.96	0.13	58,58,58,58	0
57	MG	BL33	103	1/1	0.96	0.18	61,61,61,61	0
57	MG	AL15	201	1/1	0.96	0.12	74,74,74,74	0
57	MG	B16S	1625	1/1	0.96	0.08	52,52,52,52	0
57	MG	A23S	2923	1/1	0.96	0.12	61,61,61,61	0
57	MG	A23S	2909	1/1	0.96	0.13	40,40,40,40	0
57	MG	B23S	2904	1/1	0.96	0.14	40,40,40,40	0
57	MG	BL34	102	1/1	0.97	0.28	38,38,38,38	0
57	MG	B16S	1620	1/1	0.97	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BL36	101	1/1	0.97	0.19	62,62,62,62	0
57	MG	B16S	1607	1/1	0.97	0.15	60,60,60,60	0
57	MG	B23S	2965	1/1	0.97	0.13	43,43,43,43	0
57	MG	A16S	1628	1/1	0.97	0.06	38,38,38,38	0
57	MG	B5S	202	1/1	0.97	0.08	58,58,58,58	0
57	MG	A23S	2931	1/1	0.97	0.10	40,40,40,40	0
57	MG	A23S	2939	1/1	0.97	0.16	55,55,55,55	0
57	MG	BL20	201	1/1	0.97	0.06	44,44,44,44	0
57	MG	A23S	2937	1/1	0.97	0.12	78,78,78,78	0
57	MG	B23S	2922	1/1	0.97	0.13	31,31,31,31	0
57	MG	AL21	202	1/1	0.97	0.06	77,77,77,77	0
57	MG	BS16	101	1/1	0.97	0.19	71,71,71,71	0
57	MG	A23S	2904	1/1	0.98	0.14	48,48,48,48	0
57	MG	B23S	2975	1/1	0.98	0.15	37,37,37,37	0
57	MG	AL33	101	1/1	0.98	0.11	60,60,60,60	0
57	MG	B23S	3020	1/1	0.98	0.09	53,53,53,53	0
58	SF4	BS04	501	8/8	0.98	0.23	76,98,101,103	0
57	MG	BL18	203	1/1	0.99	0.13	80,80,80,80	0
57	MG	B23S	2982	1/1	0.99	0.21	74,74,74,74	0
57	MG	A23S	2946	1/1	0.99	0.03	63,63,63,63	0
57	MG	A16S	1621	1/1	0.99	0.09	63,63,63,63	0
58	SF4	AS04	501	8/8	0.99	0.21	60,86,91,92	0
57	MG	B16S	1609	1/1	0.99	0.18	65,65,65,65	0
57	MG	B23S	2909	1/1	0.99	0.14	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.