



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 10:18 AM EDT

PDB ID : 6N1D / pdb_00006n1d
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

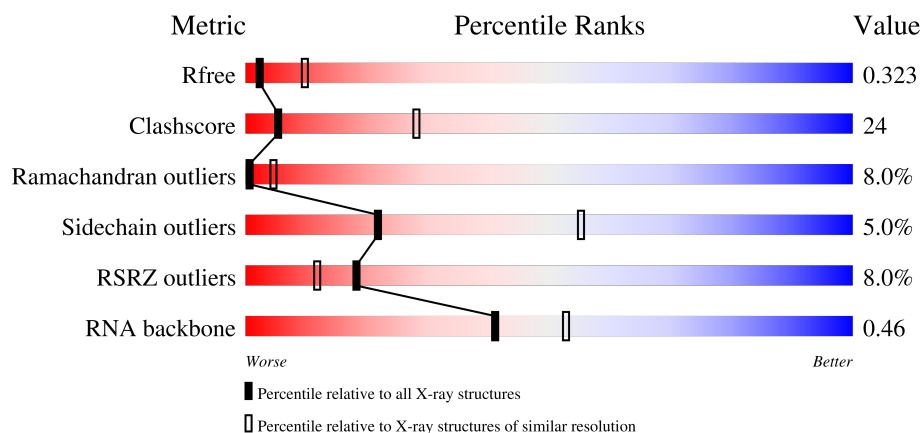
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A16S	1518	5% 78% 22%
1	B16S	1518	5% 78% 22%
2	A23S	2881	3% 78% 22%
2	B23S	2881	2% 78% 21%

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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	

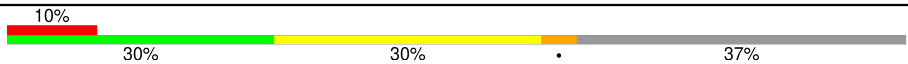
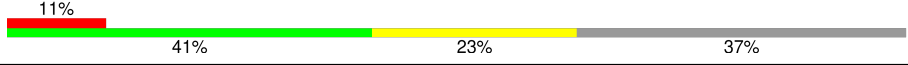
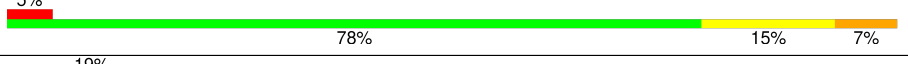
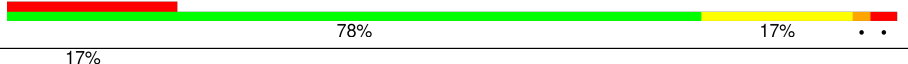
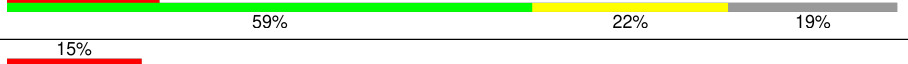
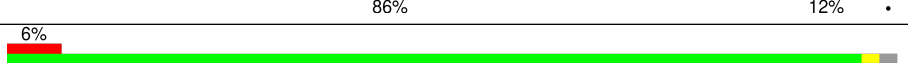
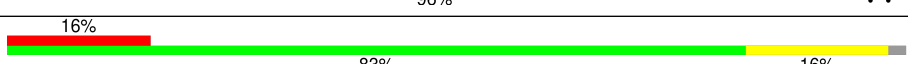
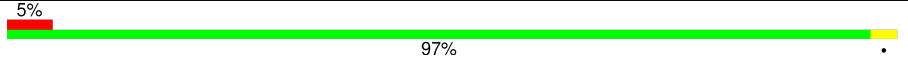
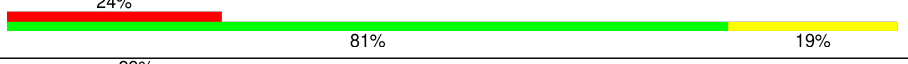
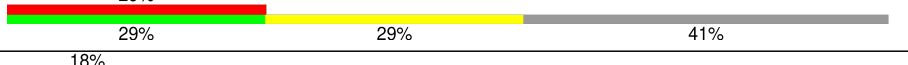
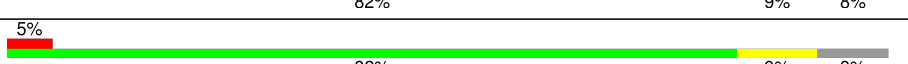
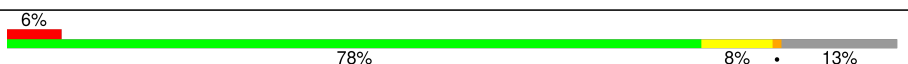
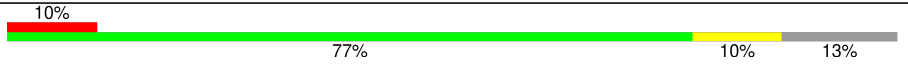
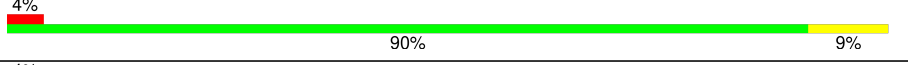
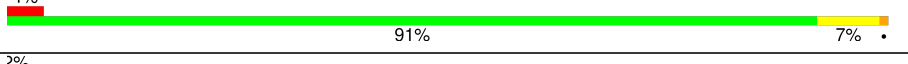
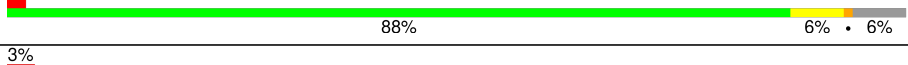
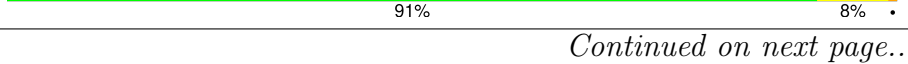
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Mol	Chain	Length	Quality of chain
15	BL17	118	
16	AL18	111	
16	BL18	111	
17	AL19	146	
17	BL19	146	
18	AL20	118	
18	BL20	118	
19	AL21	101	
19	BL21	101	
20	AL22	113	
20	BL22	113	
21	AL23	96	
21	BL23	96	
22	AL24	110	
22	BL24	110	
23	AL25	206	
23	BL25	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	

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	A16S	33	Total	Mg	0	0
			33	33		
57	A23S	73	Total	Mg	0	0
			73	73		
57	A5S	3	Total	Mg	0	0
			3	3		
57	AL01	2	Total	Mg	0	0
			2	2		
57	AL02	2	Total	Mg	0	0
			2	2		
57	AL04	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AL06	1	Total 1	Mg 1	0	0
57	AL14	1	Total 1	Mg 1	0	0
57	AL15	2	Total 2	Mg 2	0	0
57	AL17	2	Total 2	Mg 2	0	0
57	AL20	1	Total 1	Mg 1	0	0
57	AL21	3	Total 3	Mg 3	0	0
57	AL23	2	Total 2	Mg 2	0	0
57	AL24	1	Total 1	Mg 1	0	0
57	AL27	1	Total 1	Mg 1	0	0
57	AL28	2	Total 2	Mg 2	0	0
57	AL33	3	Total 3	Mg 3	0	0
57	AL34	1	Total 1	Mg 1	0	0
57	AS02	1	Total 1	Mg 1	0	0
57	AS03	1	Total 1	Mg 1	0	0
57	AS06	2	Total 2	Mg 2	0	0
57	AS08	1	Total 1	Mg 1	0	0
57	B16S	32	Total 32	Mg 32	0	0
57	B23S	133	Total 133	Mg 133	0	0
57	B5S	5	Total 5	Mg 5	0	0
57	BATN	1	Total 1	Mg 1	0	0
57	BL01	2	Total 2	Mg 2	0	0

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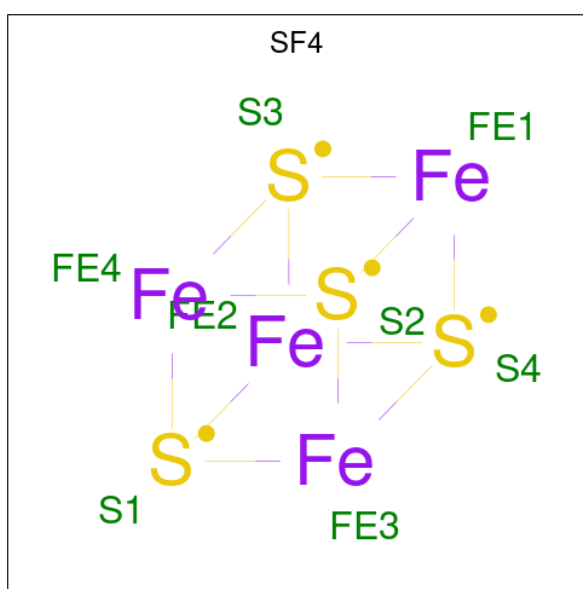
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL02	5	Total 5	Mg 5	0	0
57	BL03	1	Total 1	Mg 1	0	0
57	BL04	1	Total 1	Mg 1	0	0
57	BL15	3	Total 3	Mg 3	0	0
57	BL16	3	Total 3	Mg 3	0	0
57	BL18	3	Total 3	Mg 3	0	0
57	BL19	2	Total 2	Mg 2	0	0
57	BL20	1	Total 1	Mg 1	0	0
57	BL21	1	Total 1	Mg 1	0	0
57	BL22	1	Total 1	Mg 1	0	0
57	BL23	1	Total 1	Mg 1	0	0
57	BL24	2	Total 2	Mg 2	0	0
57	BL25	1	Total 1	Mg 1	0	0
57	BL28	2	Total 2	Mg 2	0	0
57	BL29	5	Total 5	Mg 5	0	0
57	BL30	1	Total 1	Mg 1	0	0
57	BL31	1	Total 1	Mg 1	0	0
57	BL32	1	Total 1	Mg 1	0	0
57	BL33	3	Total 3	Mg 3	0	0
57	BL34	2	Total 2	Mg 2	0	0
57	BL35	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BL36	1	Total	Mg	0	0
			1	1		
57	BS16	1	Total	Mg	0	0
			1	1		
57	BS17	1	Total	Mg	0	0
			1	1		
57	BTHX	1	Total	Mg	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

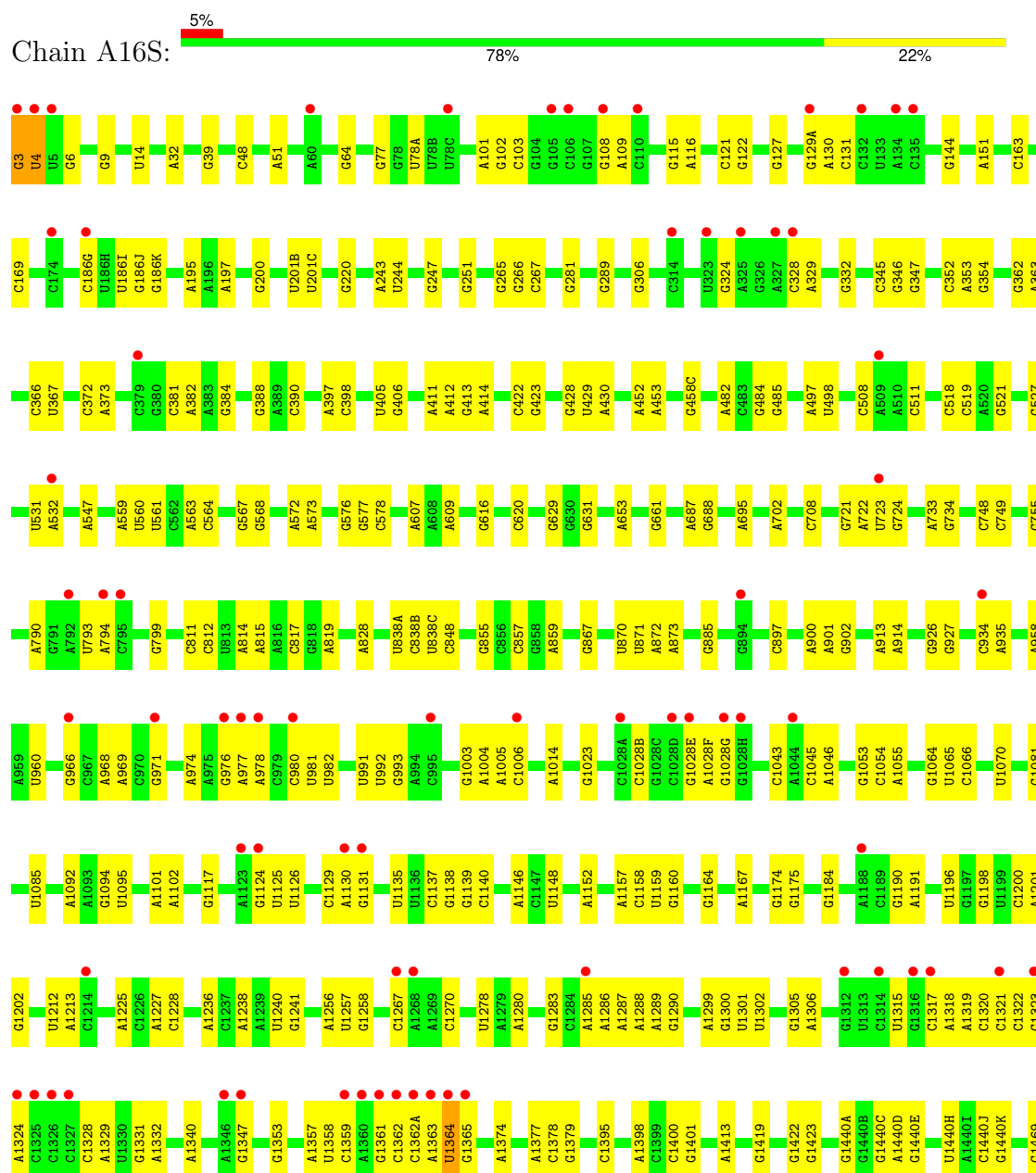


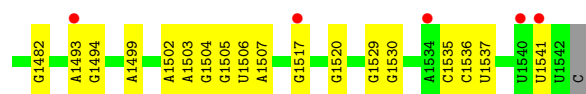
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AS04	1	Total	Fe	S	0	0
			8	4	4		
58	BS04	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots [i](#)

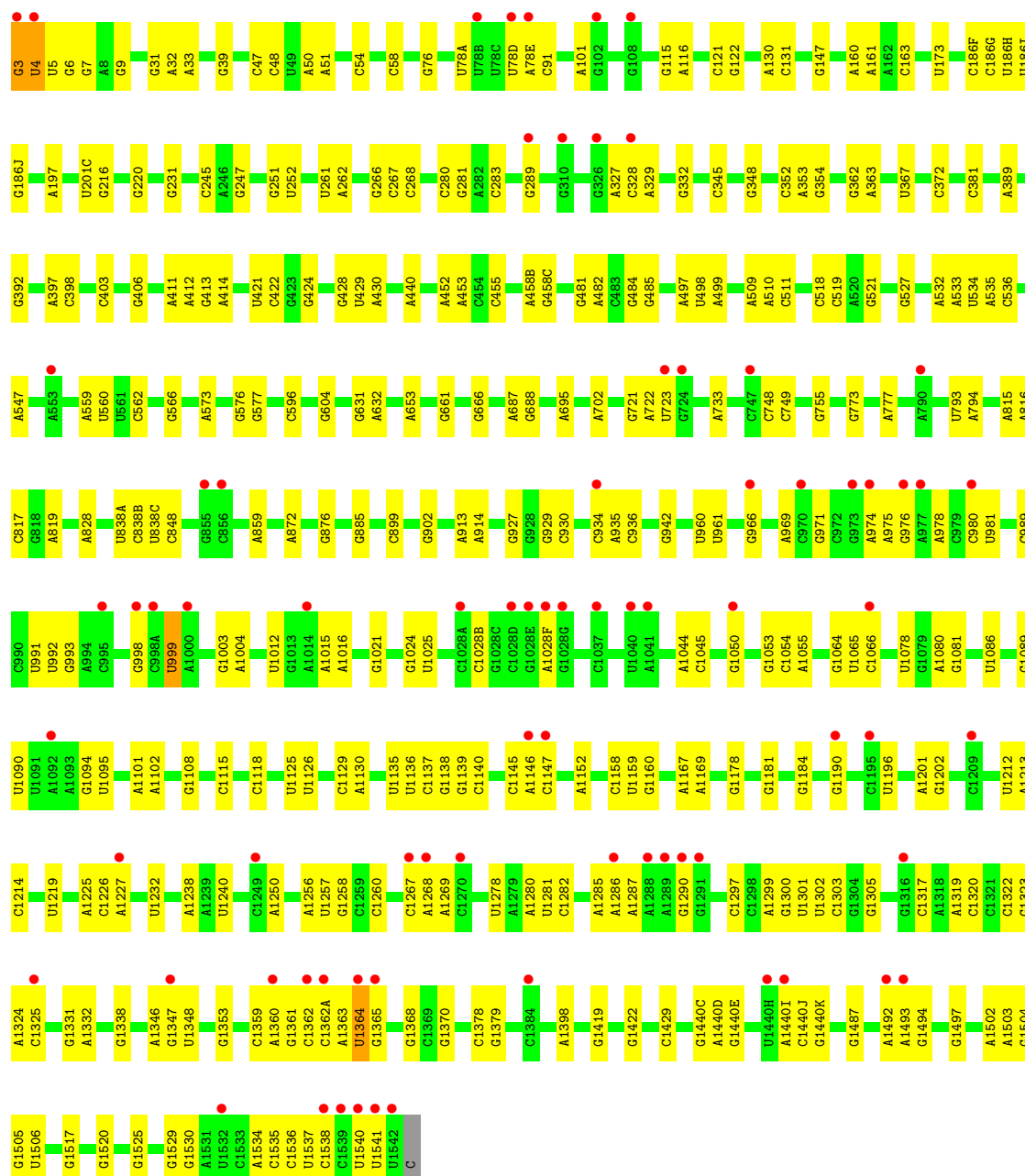
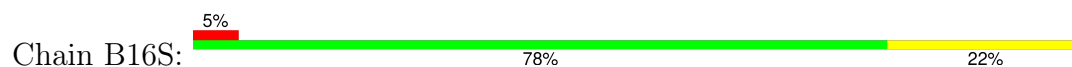
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

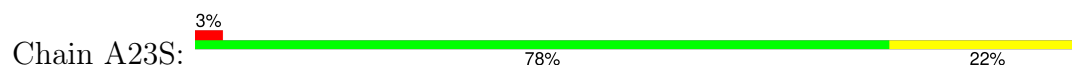


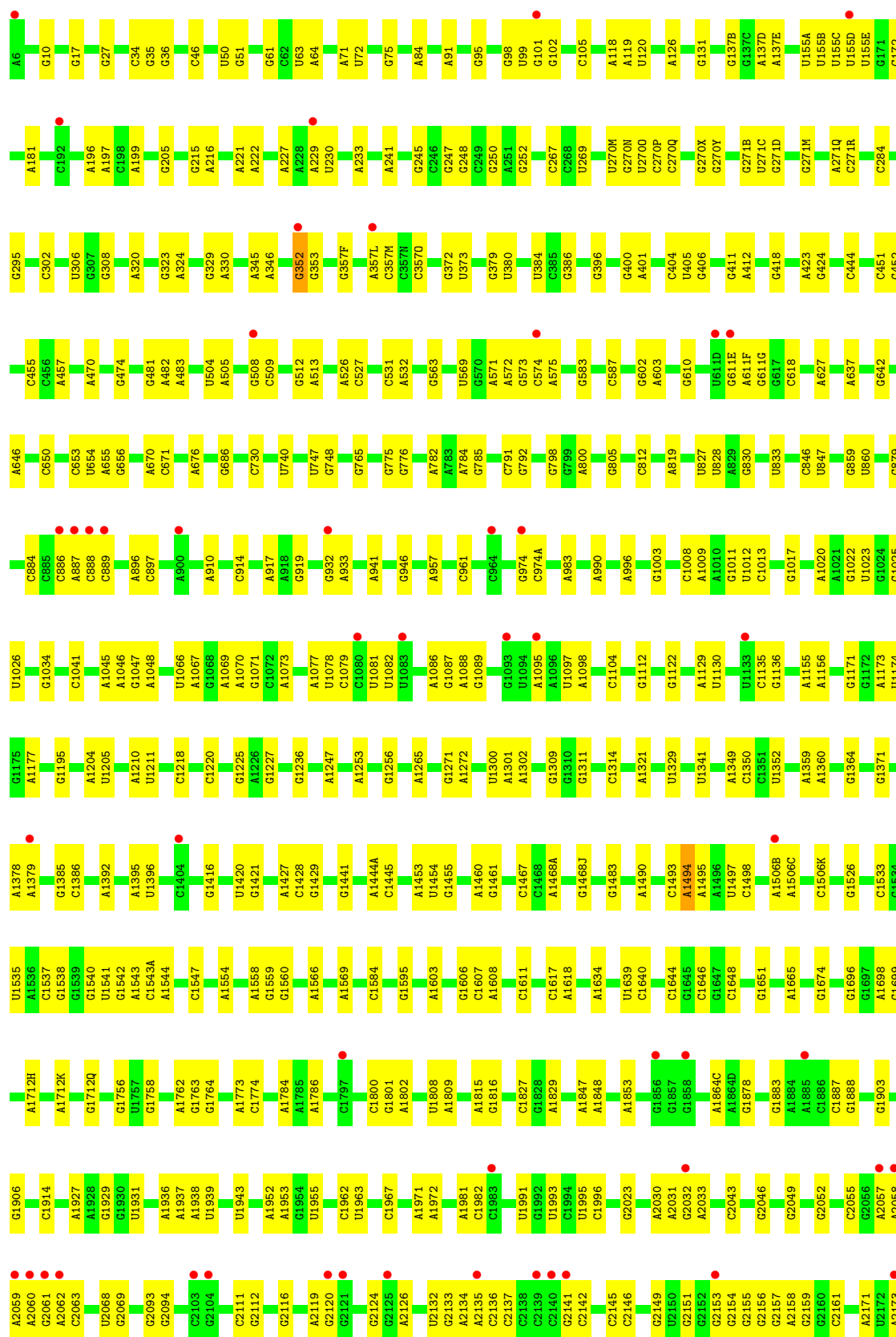


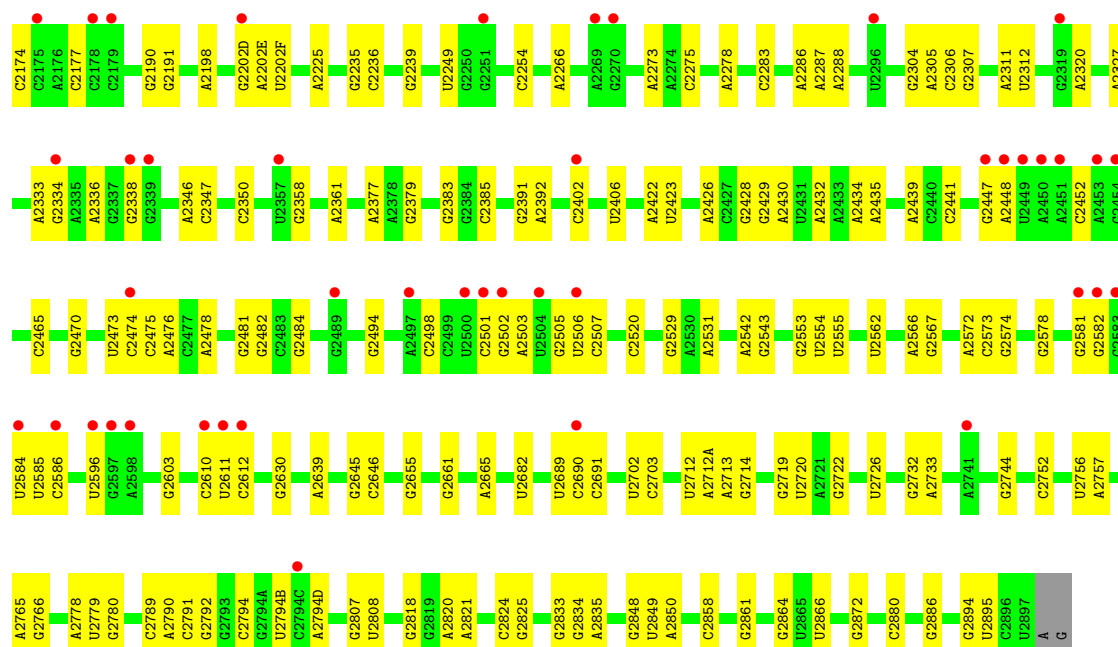
• Molecule 1: 16S rRNA



• Molecule 2: 23S rRNA

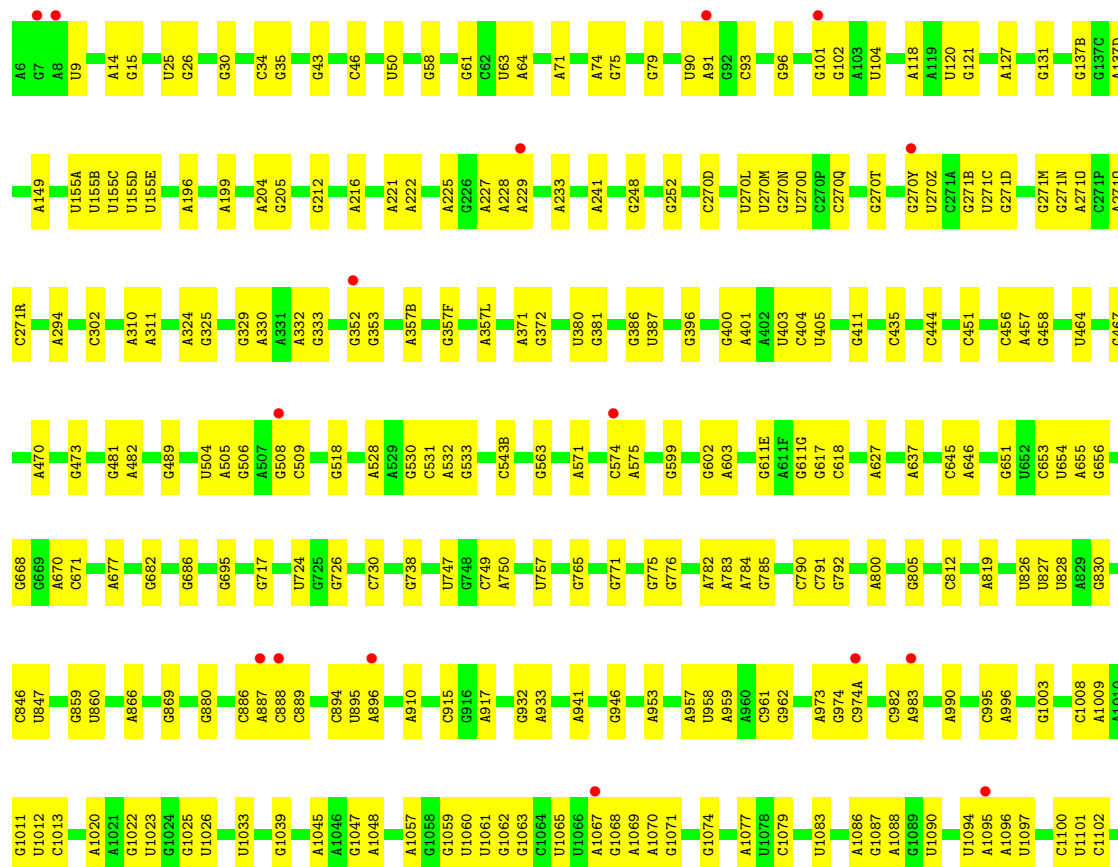


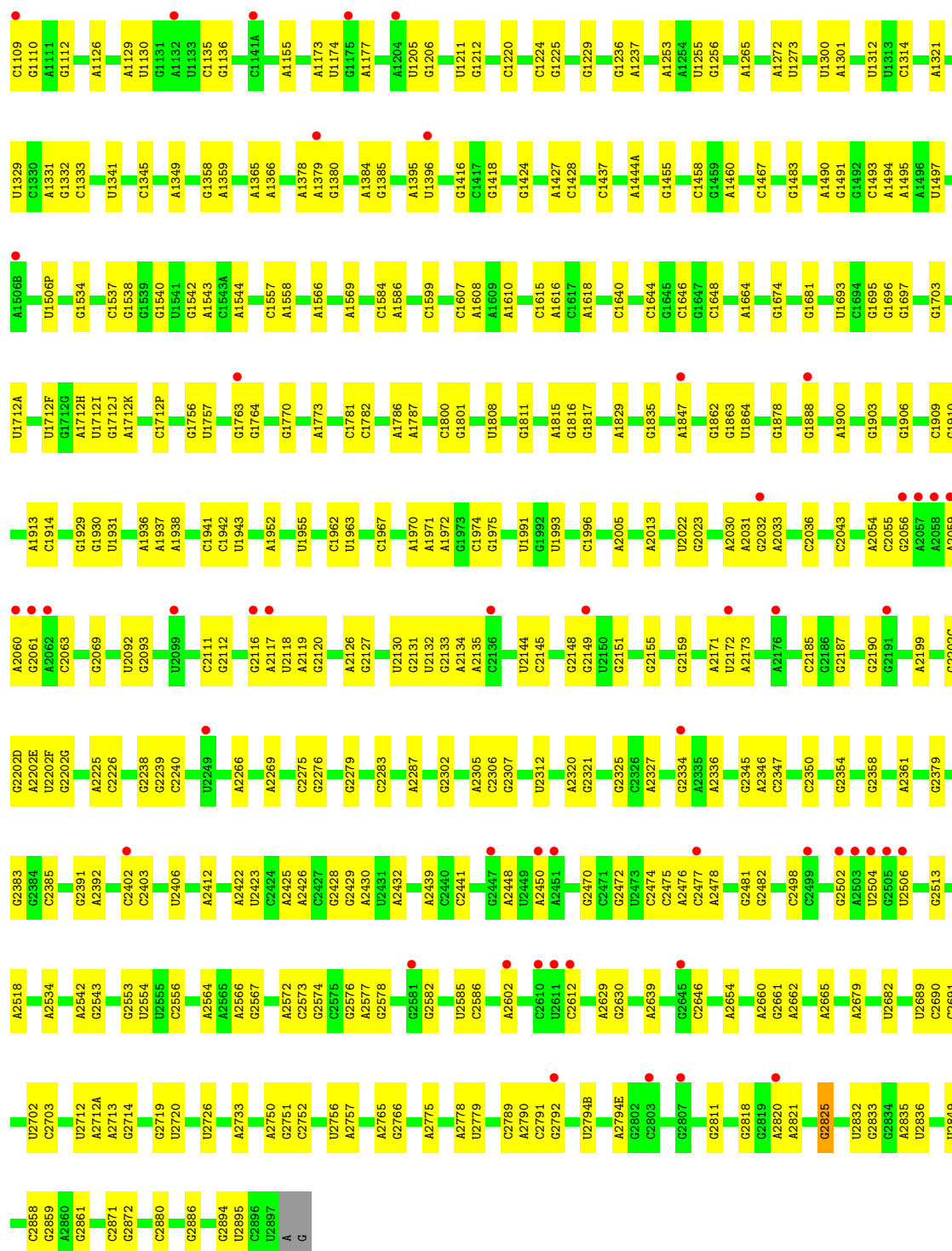


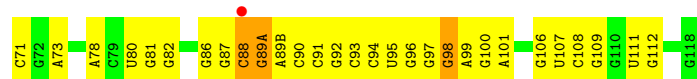


- Molecule 2: 23S rRNA

Chain B23S: 



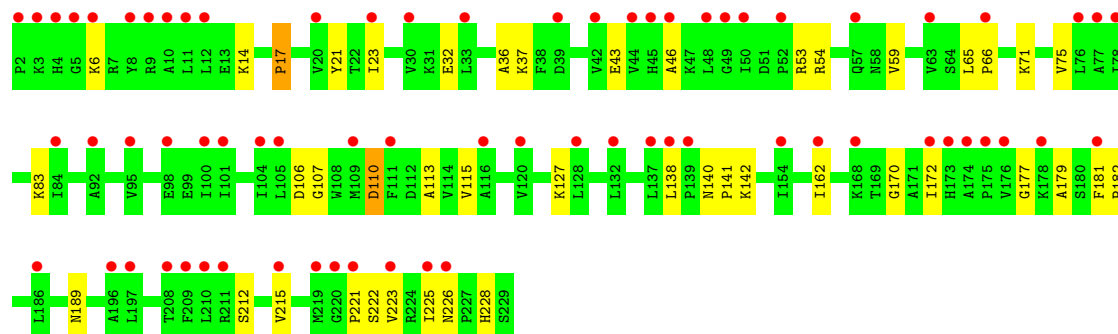
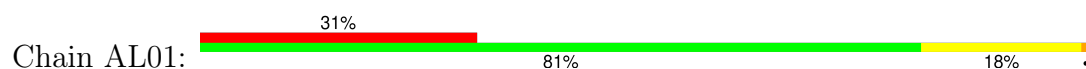




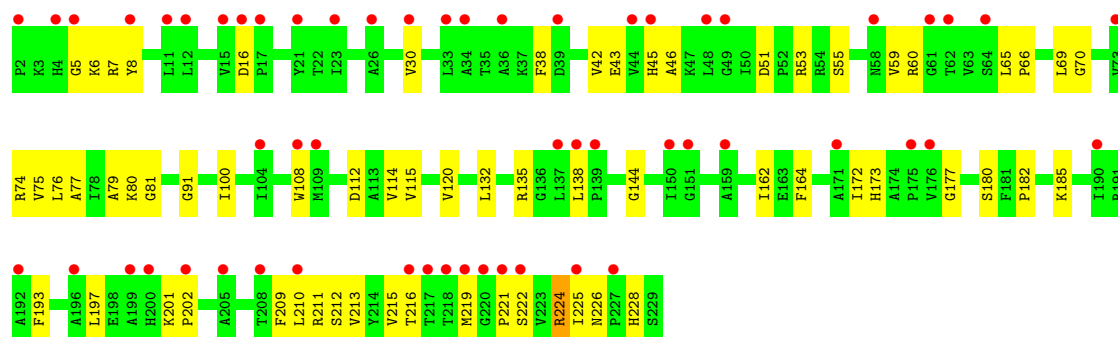
• Molecule 3: 5s rRNA



• Molecule 4: 50S ribosomal protein L1

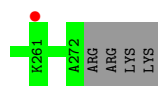


• Molecule 4: 50S ribosomal protein L1

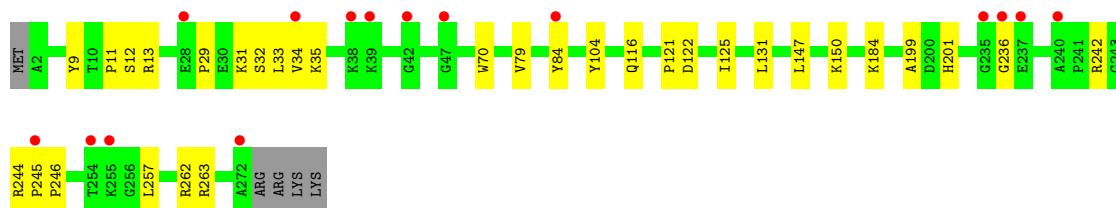
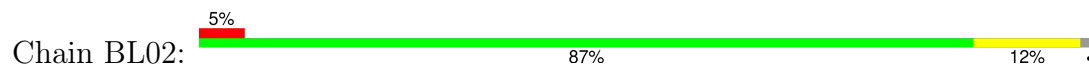


• Molecule 5: 50S ribosomal protein L2

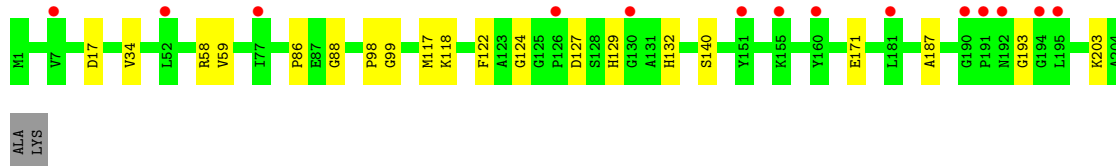




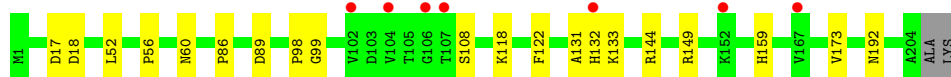
- Molecule 5: 50S ribosomal protein L2



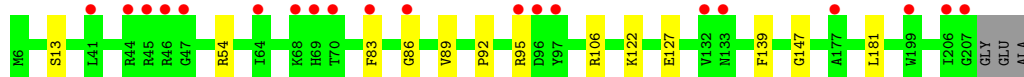
- Molecule 6: 50S ribosomal protein L3



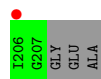
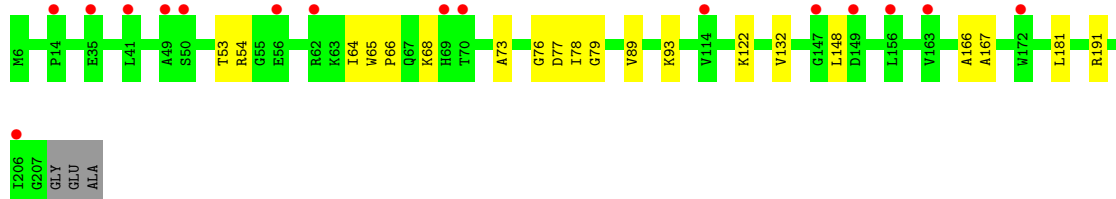
- Molecule 6: 50S ribosomal protein L3



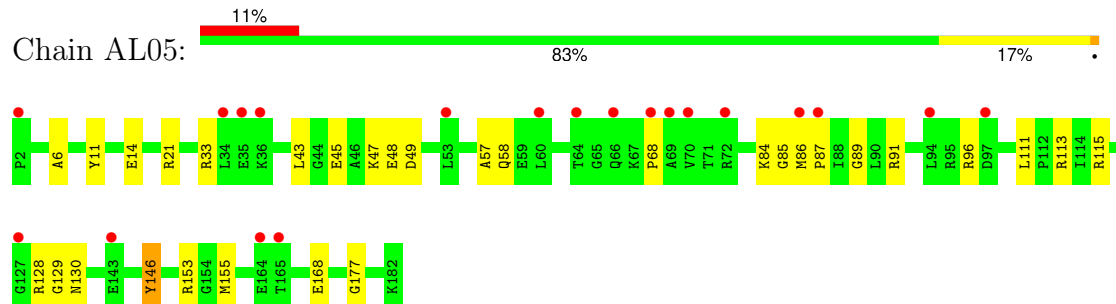
- Molecule 7: 50S ribosomal protein L4



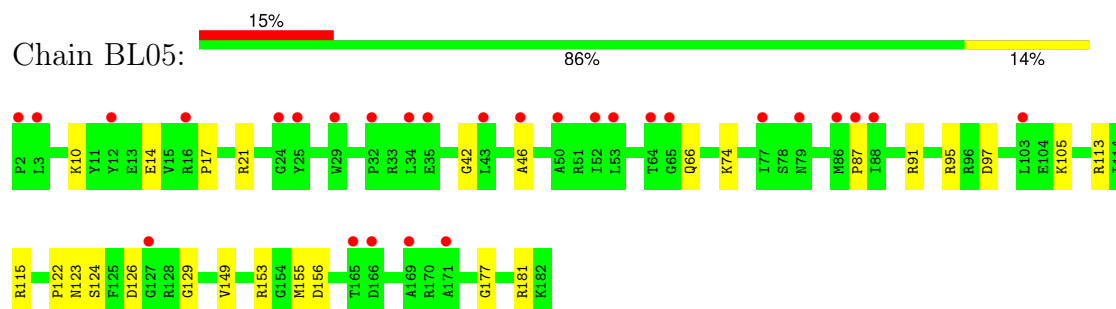
- Molecule 7: 50S ribosomal protein L4



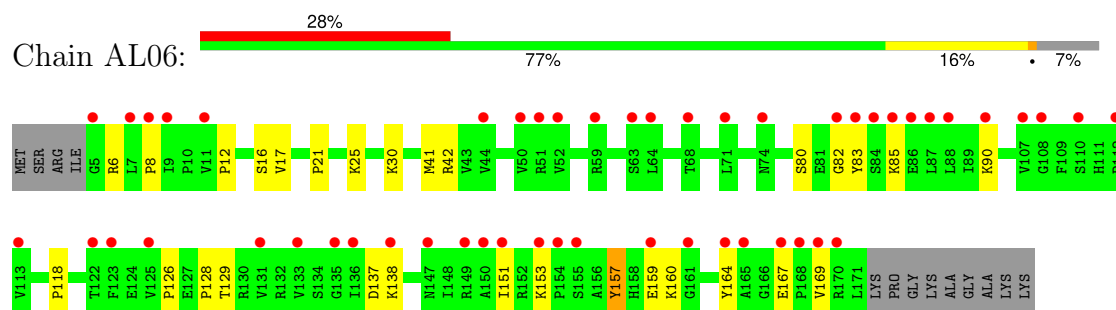
- Molecule 8: 50S ribosomal protein L5



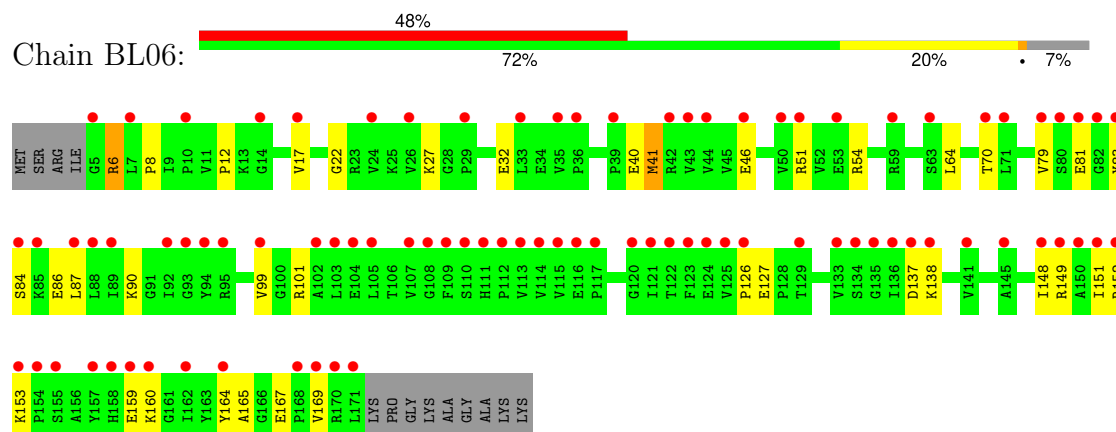
- Molecule 8: 50S ribosomal protein L5



- Molecule 9: 50S ribosomal protein L6



- Molecule 9: 50S ribosomal protein L6

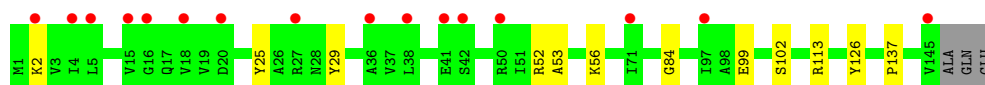


- Molecule 10: 50S ribosomal protein L9

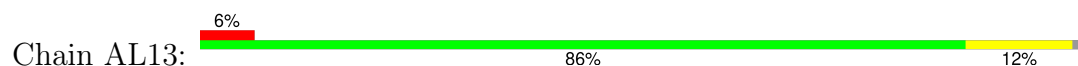




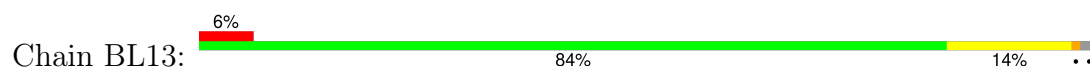
- Molecule 10: 50S ribosomal protein L9



- Molecule 11: 50S ribosomal protein L13



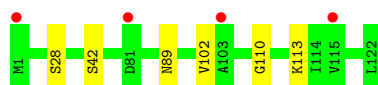
- Molecule 11: 50S ribosomal protein L13



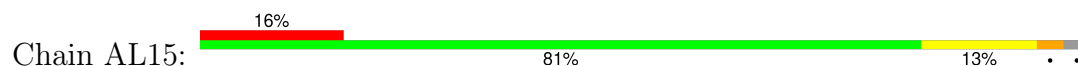
- Molecule 12: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L14

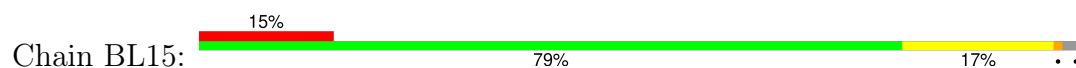


- Molecule 13: 50S ribosomal protein L15

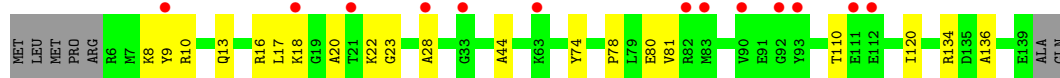
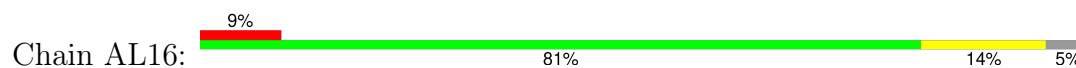




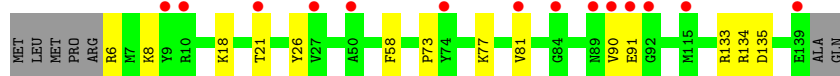
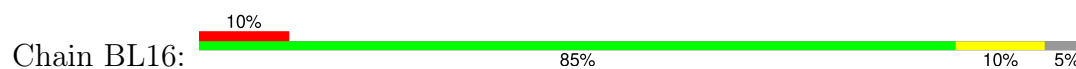
- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16



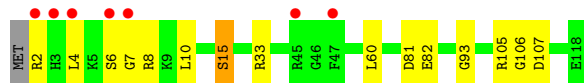
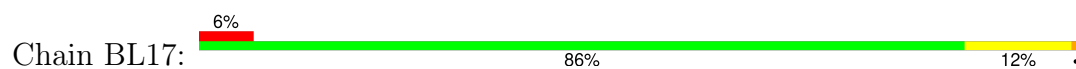
- Molecule 14: 50S ribosomal protein L16



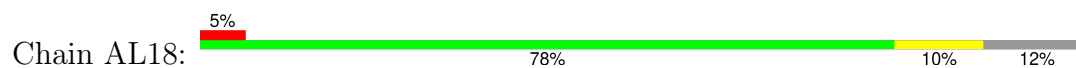
- Molecule 15: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L17

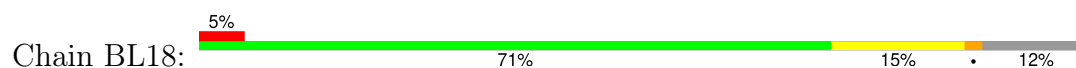


- Molecule 16: 50S ribosomal protein L18

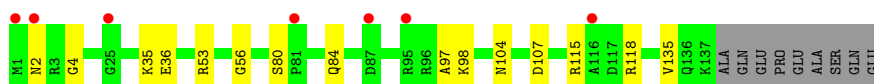
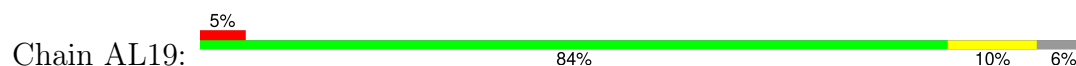




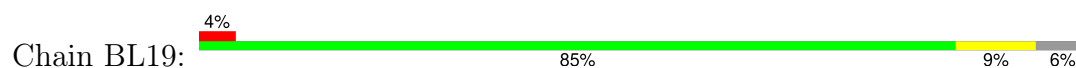
- Molecule 16: 50S ribosomal protein L18



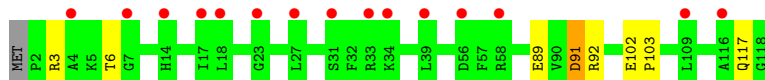
- Molecule 17: 50S ribosomal protein L19



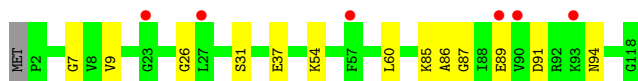
- Molecule 17: 50S ribosomal protein L19



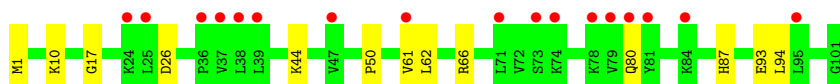
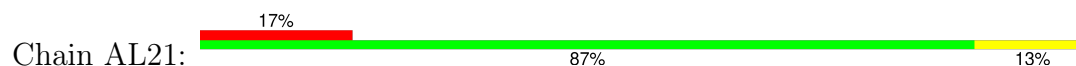
- Molecule 18: 50S ribosomal protein L20



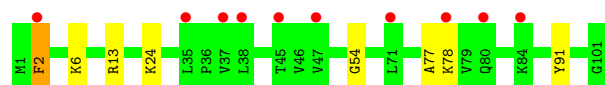
- Molecule 18: 50S ribosomal protein L20



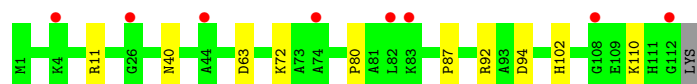
- Molecule 19: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L21



- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22



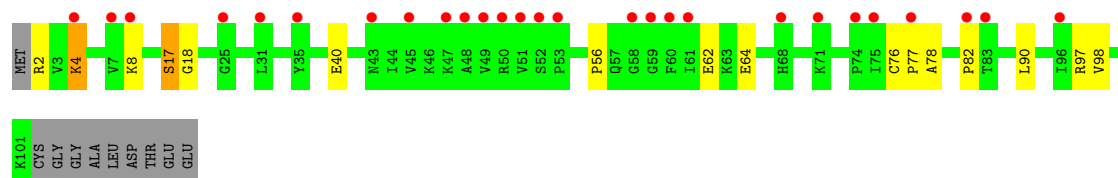
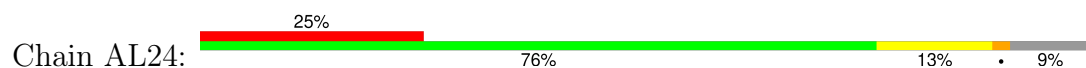
- Molecule 21: 50S ribosomal protein L23



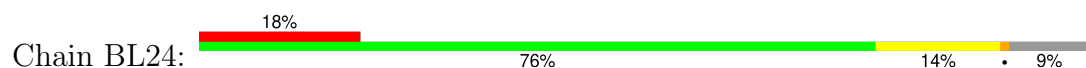
- Molecule 21: 50S ribosomal protein L23

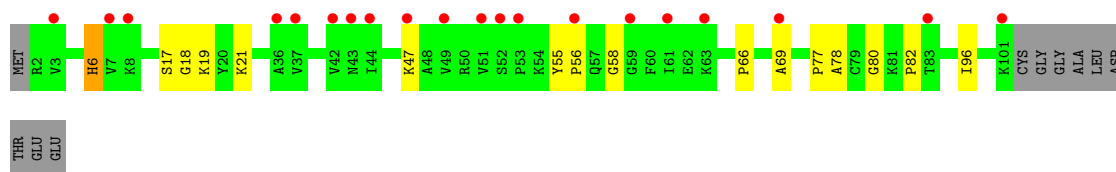


- Molecule 22: 50S ribosomal protein L24

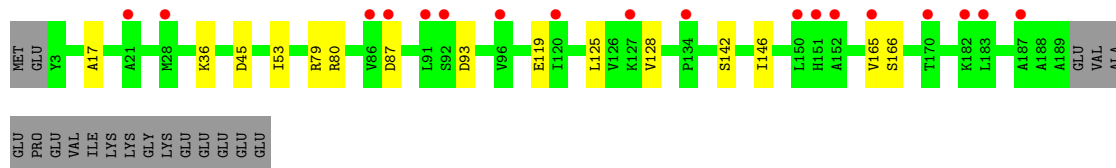
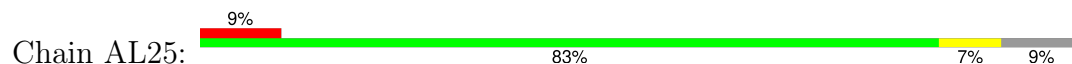


- Molecule 22: 50S ribosomal protein L24

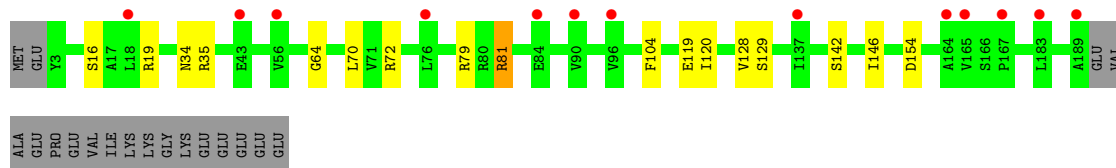




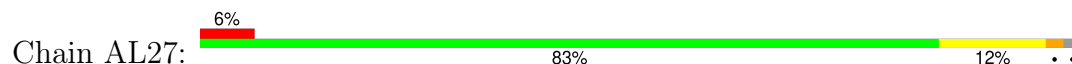
- Molecule 23: 50S ribosomal protein L25



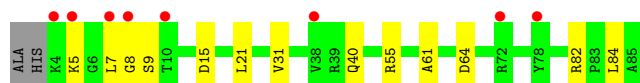
- Molecule 23: 50S ribosomal protein L25



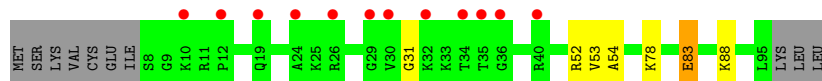
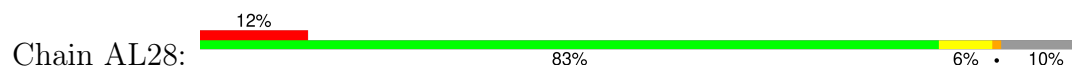
- Molecule 24: 50S ribosomal protein L27



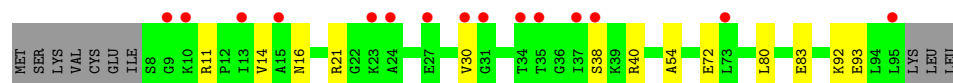
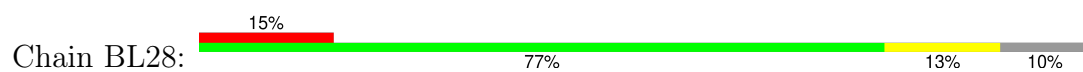
- Molecule 24: 50S ribosomal protein L27



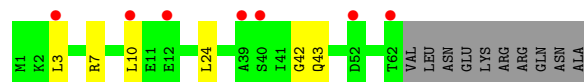
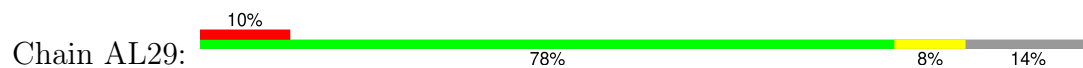
- Molecule 25: 50S ribosomal protein L28



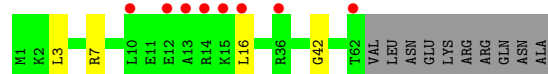
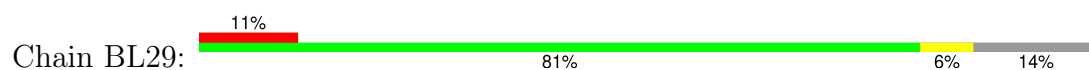
- Molecule 25: 50S ribosomal protein L28



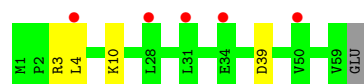
- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29



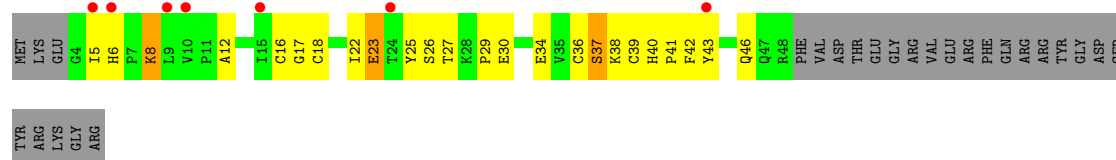
- Molecule 27: 50S ribosomal protein L30



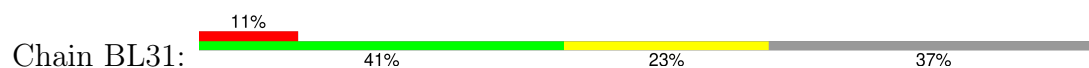
- Molecule 27: 50S ribosomal protein L30

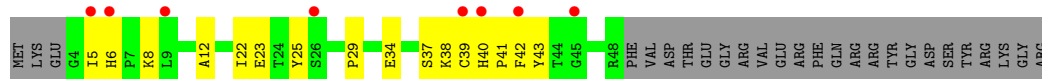


- Molecule 28: 50S ribosomal protein L31

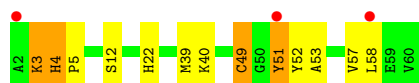
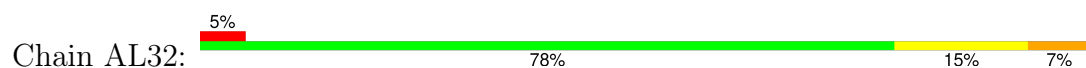


- Molecule 28: 50S ribosomal protein L31

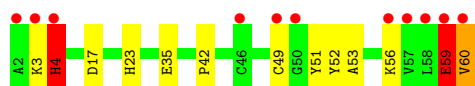
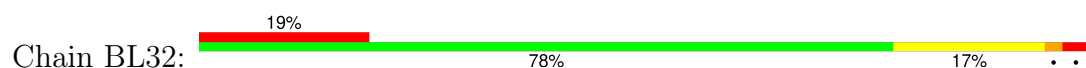




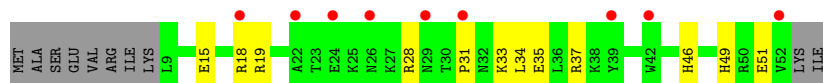
- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



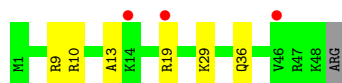
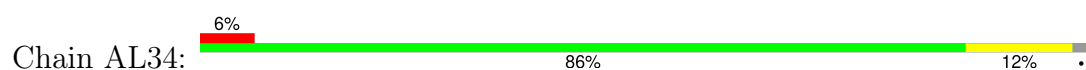
- Molecule 30: 50S ribosomal protein L33



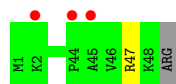
- Molecule 30: 50S ribosomal protein L33



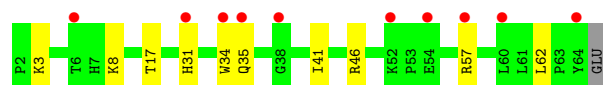
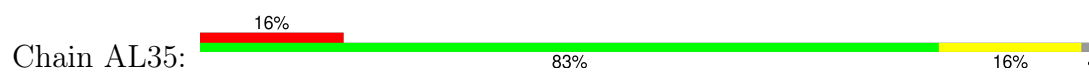
- Molecule 31: 50S ribosomal protein L34



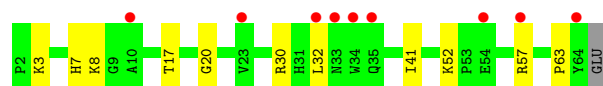
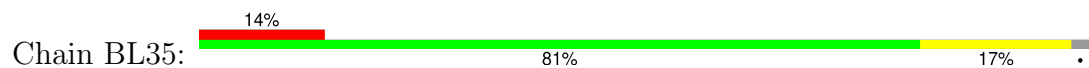
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



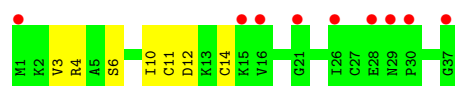
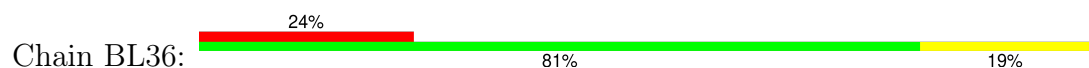
- Molecule 32: 50S ribosomal protein L35



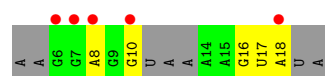
- Molecule 33: 50S ribosomal protein L36



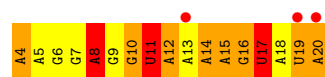
- Molecule 33: 50S ribosomal protein L36



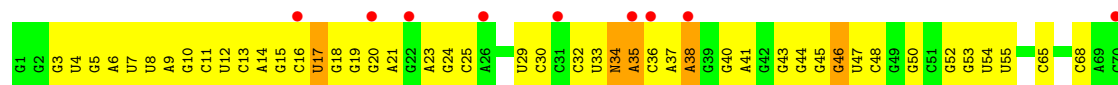
- Molecule 34: mRNA

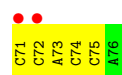


- Molecule 34: mRNA

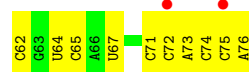
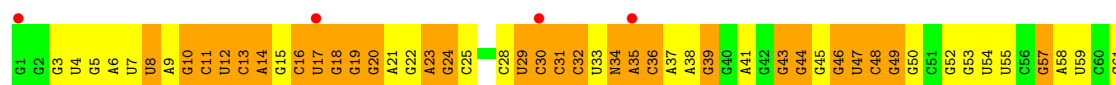
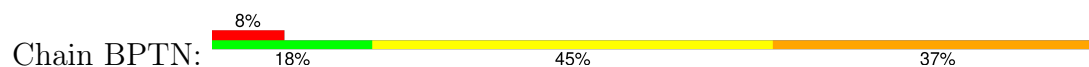


- Molecule 35: P-tRNA

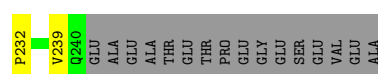
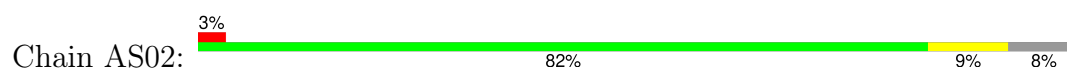




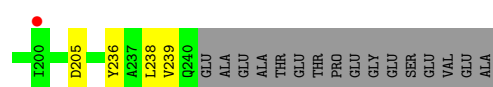
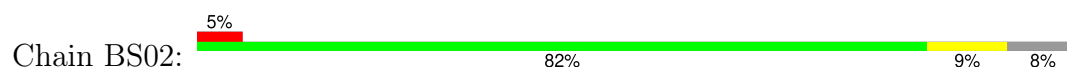
• Molecule 35: P-tRNA



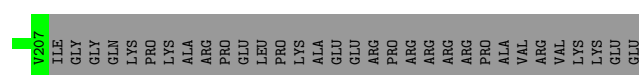
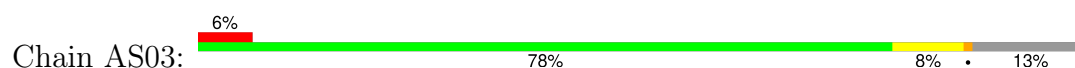
• Molecule 36: 30S ribosomal protein S2



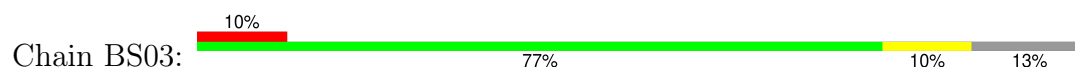
• Molecule 36: 30S ribosomal protein S2

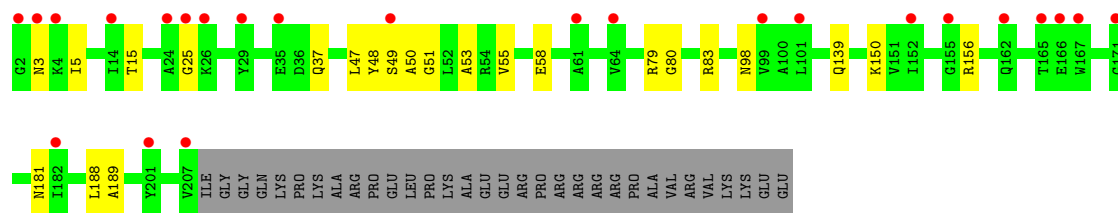


• Molecule 37: 30S ribosomal protein S3

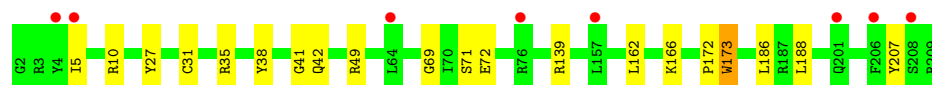


• Molecule 37: 30S ribosomal protein S3

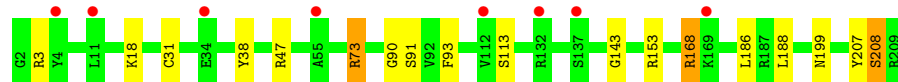




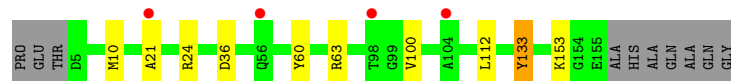
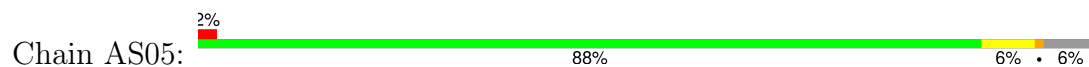
- Molecule 38: 30S ribosomal protein S4



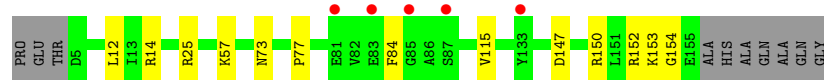
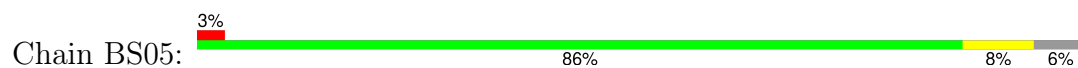
- Molecule 38: 30S ribosomal protein S4



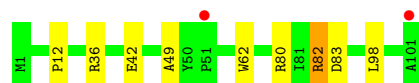
- Molecule 39: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S5



- Molecule 40: 30S ribosomal protein S6

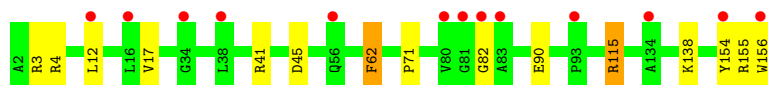


- Molecule 40: 30S ribosomal protein S6

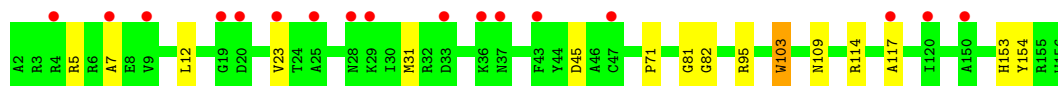




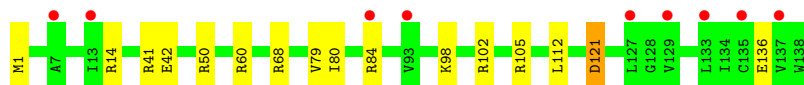
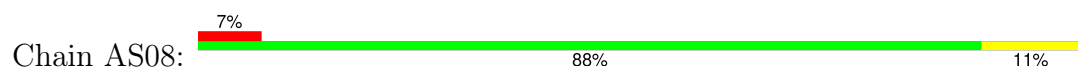
- Molecule 41: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S7



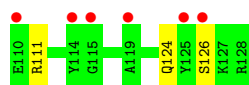
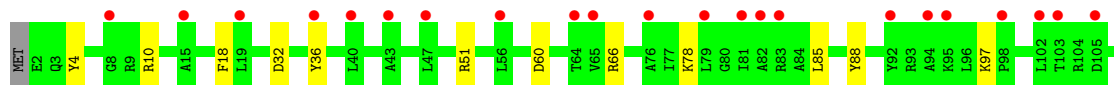
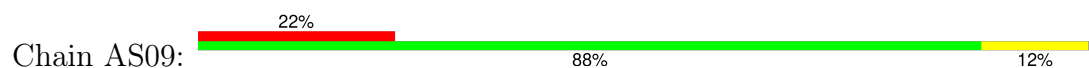
- Molecule 42: 30S ribosomal protein S8



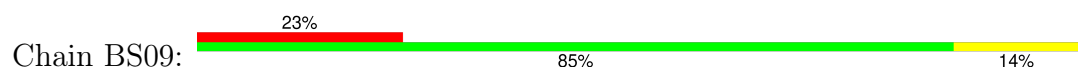
- Molecule 42: 30S ribosomal protein S8

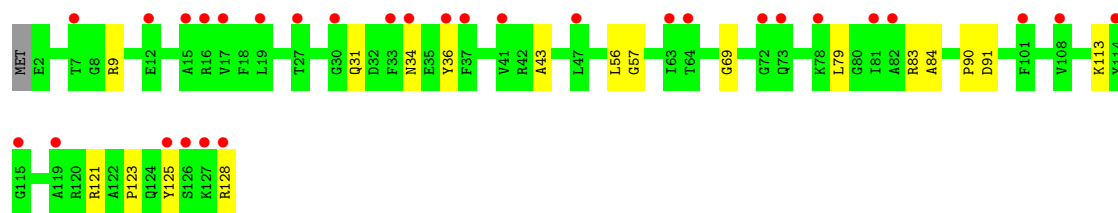


- Molecule 43: 30S ribosomal protein S9

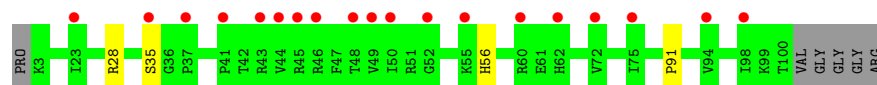


- Molecule 43: 30S ribosomal protein S9

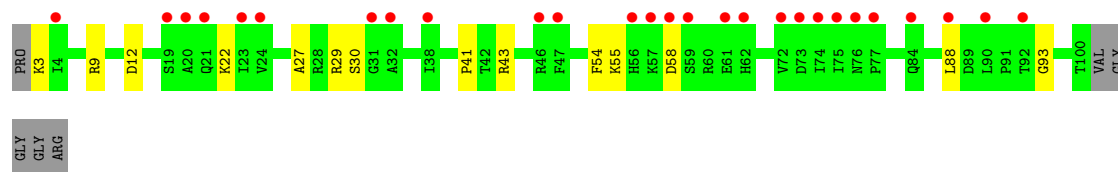
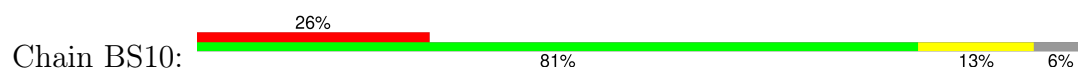




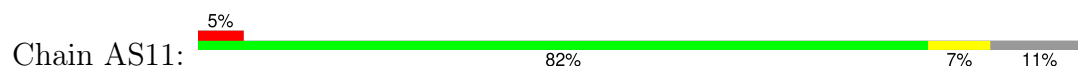
- Molecule 44: 30S ribosomal protein S10



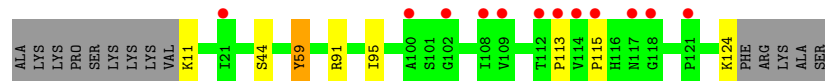
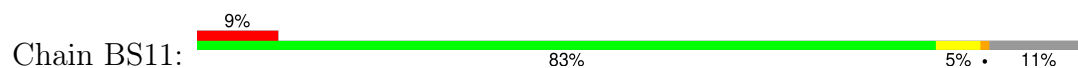
- Molecule 44: 30S ribosomal protein S10



- Molecule 45: 30S ribosomal protein S11



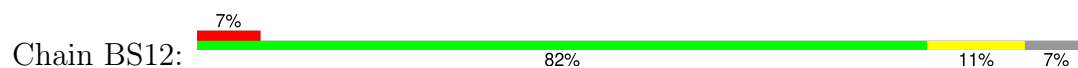
- Molecule 45: 30S ribosomal protein S11



- Molecule 46: 30S ribosomal protein S12

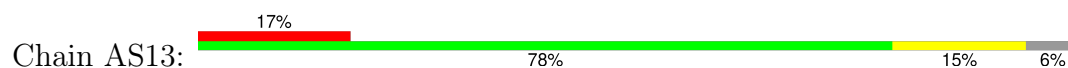


- Molecule 46: 30S ribosomal protein S12

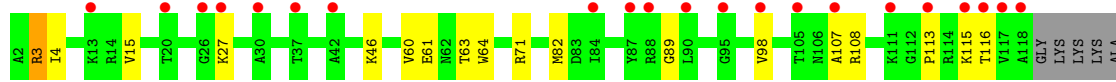
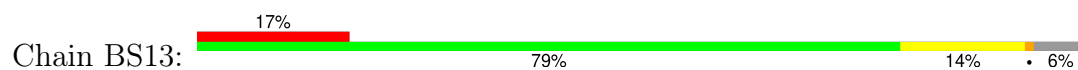




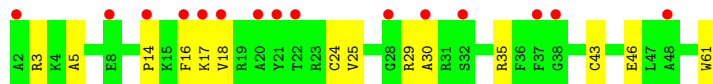
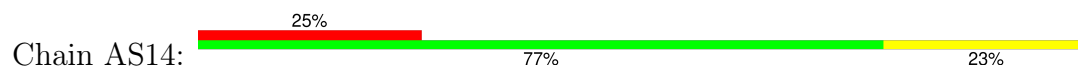
- Molecule 47: 30S ribosomal protein S13



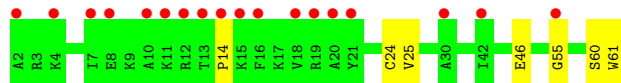
- Molecule 47: 30S ribosomal protein S13



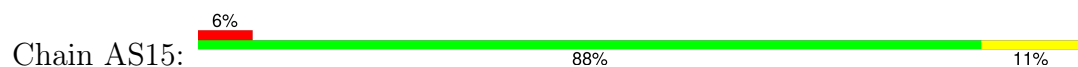
- Molecule 48: 30S ribosomal protein S14 type Z



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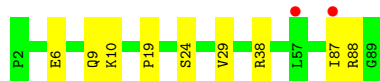


- Molecule 49: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S15

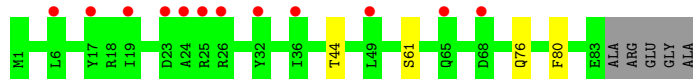




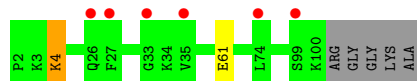
- Molecule 50: 30S ribosomal protein S16



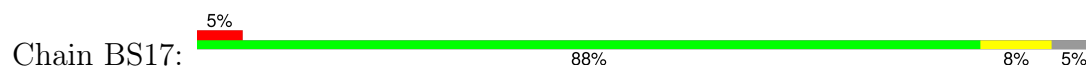
- Molecule 50: 30S ribosomal protein S16



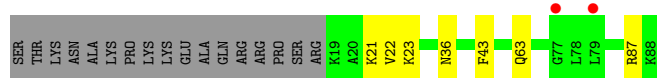
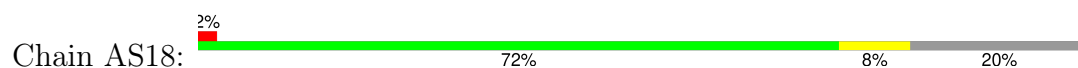
- Molecule 51: 30S ribosomal protein S17



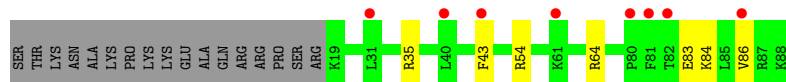
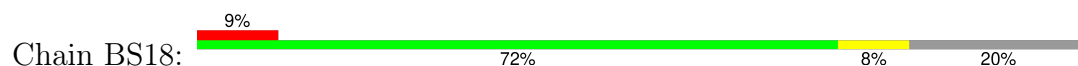
- Molecule 51: 30S ribosomal protein S17



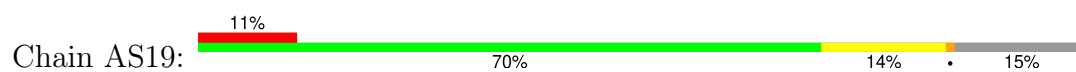
- Molecule 52: 30S ribosomal protein S18



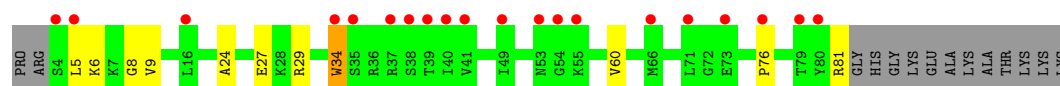
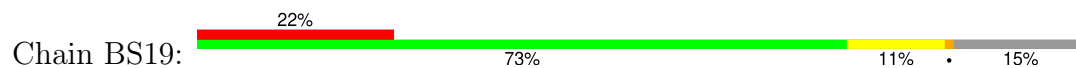
- Molecule 52: 30S ribosomal protein S18



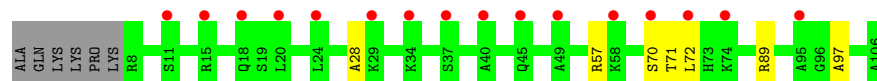
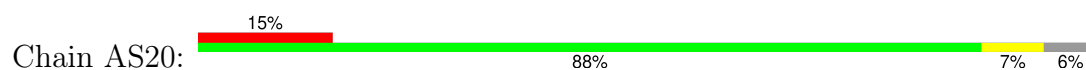
- Molecule 53: 30S ribosomal protein S19



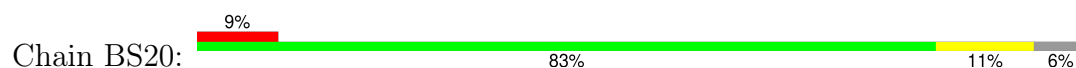
• Molecule 53: 30S ribosomal protein S19



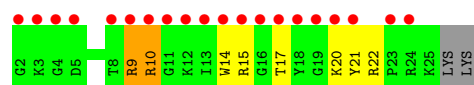
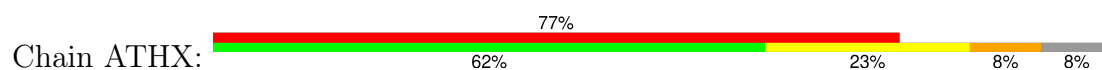
• Molecule 54: 30S ribosomal protein S20



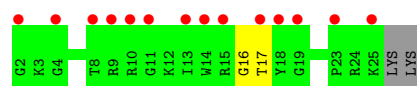
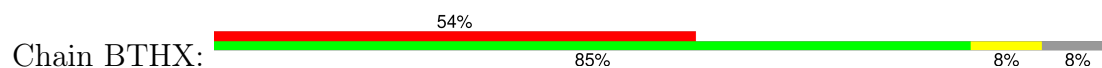
• Molecule 54: 30S ribosomal protein S20



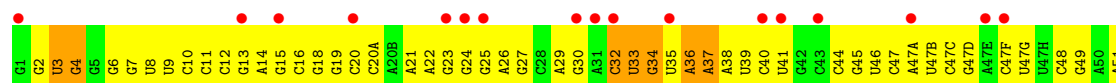
• Molecule 55: 30S ribosomal protein Thx



• Molecule 55: 30S ribosomal protein Thx



• Molecule 56: A tRNA





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 – 3.20 100.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (100.00-3.20) 95.2 (100.00-3.20)	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 0.270 , 0.323	Depositor DCC
R_{free} test set	65984 reflections (3.92%)	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)	0.31 , 92.2	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: 4SU, MG, G7M, MIA, CM0, 6MZ, SF4, 5MU, PSU, QUO

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	0.36	5/36490 (0.0%)	0.40	7/56951 (0.0%)
1	B16S	0.36	4/36490 (0.0%)	0.40	2/56951 (0.0%)
2	A23S	0.37	1/69437 (0.0%)	0.39	2/108394 (0.0%)
2	B23S	0.42	1/69438 (0.0%)	0.40	0/108396
3	A5S	0.34	0/2853	0.40	0/4451
3	B5S	0.37	0/2853	0.39	0/4451
4	AL01	0.21	0/1774	0.59	0/2391
4	BL01	0.21	0/1774	0.57	0/2391
5	AL02	0.42	0/2154	0.56	0/2905
5	BL02	0.43	0/2154	0.52	0/2905
6	AL03	0.35	0/1596	0.50	0/2153
6	BL03	0.39	0/1596	0.48	0/2153
7	AL04	0.33	0/1621	0.47	0/2194
7	BL04	0.37	0/1621	0.48	0/2194
8	AL05	0.24	0/1500	0.49	0/2017
8	BL05	0.26	0/1500	0.49	0/2017
9	AL06	0.60	0/1307	0.90	0/1769
9	BL06	0.56	0/1307	0.90	0/1769
10	AL09	0.23	0/1146	0.46	1/1551 (0.1%)
10	BL09	0.26	0/1147	0.47	0/1552
11	AL13	0.31	0/1123	0.47	0/1515
11	BL13	0.36	0/1123	0.50	0/1515
12	AL14	0.39	0/942	0.42	0/1268
12	BL14	0.40	0/942	0.46	0/1268
13	AL15	0.30	0/1131	0.63	0/1504
13	BL15	0.33	0/1131	0.64	0/1504
14	AL16	0.32	0/1084	0.54	1/1449 (0.1%)
14	BL16	0.38	0/1084	0.52	0/1449
15	AL17	0.34	0/974	0.49	0/1302
15	BL17	0.40	0/974	0.54	0/1302
16	AL18	0.31	0/778	0.48	0/1036
16	BL18	0.31	0/778	0.53	1/1036 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AL19	0.34	0/1157	0.52	0/1544
17	BL19	0.36	0/1157	0.51	0/1544
18	AL20	0.32	0/982	0.47	0/1306
18	BL20	0.41	0/982	0.48	0/1306
19	AL21	0.29	0/790	0.48	0/1057
19	BL21	0.33	0/790	0.52	0/1057
20	AL22	0.34	0/901	0.45	0/1209
20	BL22	0.39	0/901	0.46	0/1209
21	AL23	0.34	0/739	0.47	0/993
21	BL23	0.35	0/739	0.50	0/993
22	AL24	0.26	0/788	0.55	0/1051
22	BL24	0.28	0/788	0.50	0/1051
23	AL25	0.26	0/1514	0.45	0/2056
23	BL25	0.28	0/1514	0.44	0/2056
24	AL27	1.05	0/655	1.22	4/870 (0.5%)
24	BL27	1.03	0/655	1.33	2/870 (0.2%)
25	AL28	0.32	0/701	0.55	0/932
25	BL28	0.36	0/701	0.57	0/932
26	AL29	0.27	0/522	0.53	0/690
26	BL29	0.32	0/522	0.52	0/690
27	AL30	0.27	0/472	0.47	0/634
27	BL30	0.33	0/472	0.45	0/634
28	AL31	0.90	1/360 (0.3%)	1.24	1/488 (0.2%)
28	BL31	1.03	1/360 (0.3%)	1.27	4/488 (0.8%)
29	AL32	1.12	0/473	1.25	3/639 (0.5%)
29	BL32	1.41	6/473 (1.3%)	1.60	10/639 (1.6%)
30	AL33	0.30	0/387	0.60	0/518
30	BL33	0.32	0/387	0.61	0/518
31	AL34	0.38	0/426	0.56	0/561
31	BL34	0.45	0/426	0.49	0/561
32	AL35	0.34	0/515	0.55	0/679
32	BL35	0.36	0/515	0.57	0/679
33	AL36	0.33	0/310	0.54	0/407
33	BL36	0.35	0/310	0.60	0/407
34	AMRN	0.22	0/250	0.32	0/387
34	BMRN	1.19	1/420 (0.2%)	2.66	32/654 (4.9%)
35	APTN	0.42	2/1672 (0.1%)	0.82	8/2599 (0.3%)
35	BPTN	1.07	15/1672 (0.9%)	2.03	73/2599 (2.8%)
36	AS02	0.26	0/1935	0.44	0/2609
36	BS02	0.25	0/1935	0.46	0/2609
37	AS03	0.26	0/1636	0.46	0/2205
37	BS03	0.24	0/1636	0.44	0/2205
38	AS04	0.33	0/1695	0.47	0/2274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BS04	0.32	0/1695	0.49	0/2274
39	AS05	0.33	0/1171	0.45	0/1576
39	BS05	0.31	0/1171	0.47	0/1576
40	AS06	0.29	0/856	0.45	0/1154
40	BS06	0.29	0/856	0.44	0/1154
41	AS07	0.22	0/1276	0.43	0/1709
41	BS07	0.24	0/1276	0.48	1/1709 (0.1%)
42	AS08	0.32	0/1136	0.47	0/1527
42	BS08	0.32	0/1136	0.49	0/1527
43	AS09	0.24	0/1029	0.49	0/1378
43	BS09	0.24	0/1029	0.49	0/1378
44	AS10	0.22	0/807	0.40	0/1085
44	BS10	0.24	0/807	0.44	0/1085
45	AS11	0.26	0/856	0.41	0/1157
45	BS11	0.26	0/856	0.40	0/1157
46	AS12	0.33	0/972	0.49	0/1301
46	BS12	0.33	0/972	0.53	0/1301
47	AS13	0.23	0/943	0.52	0/1265
47	BS13	0.22	0/943	0.50	0/1265
48	AS14	0.27	0/501	0.51	0/664
48	BS14	0.27	0/501	0.54	0/664
49	AS15	0.32	0/745	0.42	0/992
49	BS15	0.32	0/745	0.43	0/992
50	AS16	0.30	0/716	0.49	0/963
50	BS16	0.34	0/716	0.52	0/963
51	AS17	0.33	0/836	0.45	0/1117
51	BS17	0.33	0/836	0.48	0/1117
52	AS18	0.31	0/579	0.50	0/768
52	BS18	0.27	0/579	0.45	0/768
53	AS19	0.20	0/642	0.51	0/865
53	BS19	0.22	0/642	0.43	0/865
54	AS20	0.27	0/764	0.47	0/1006
54	BS20	0.28	0/764	0.45	0/1006
55	ATHX	0.33	0/212	0.93	2/277 (0.7%)
55	BTHX	0.27	0/212	0.61	0/277
56	BATN	0.76	2/1899 (0.1%)	1.20	12/2952 (0.4%)
All	All	0.39	39/319733 (0.0%)	0.49	166/477946 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BL32	60	VAL	CB-CG2	-12.59	1.10	1.52
29	BL32	59	GLU	CB-CG	11.05	1.85	1.52
35	BPTN	12	U	C3'-O3'	9.28	1.56	1.42
35	APTN	38	A	O3'-P	-8.93	1.47	1.61
35	BPTN	24	G	O3'-P	-8.03	1.49	1.61
35	BPTN	24	G	C3'-O3'	-7.54	1.30	1.42
2	B23S	2825	G	C1'-N9	-7.33	1.36	1.48
1	B16S	3	G	C5-C6	7.32	1.56	1.42
35	BPTN	18	G	O3'-P	-7.21	1.50	1.61
35	BPTN	31	C	C3'-O3'	7.17	1.52	1.42
35	BPTN	36	C	O5'-C5'	6.67	1.52	1.42
2	A23S	2825	G	C1'-N9	-6.61	1.38	1.48
35	BPTN	48	C	O3'-P	-6.57	1.51	1.61
35	BPTN	31	C	O3'-P	-6.47	1.51	1.61
29	BL32	59	GLU	CG-CD	6.25	1.67	1.52
35	BPTN	32	C	C4'-C3'	-6.14	1.43	1.52
29	BL32	60	VAL	CB-CG1	6.12	1.72	1.52
1	A16S	4	U	P-O5'	6.05	1.68	1.59
56	BATN	67	C	N1-C2	-6.04	1.28	1.40
35	BPTN	18	G	C3'-O3'	-6.03	1.34	1.43
29	BL32	59	GLU	CA-CB	5.96	1.63	1.53
1	A16S	3	G	O3'-P	5.75	1.69	1.61
35	BPTN	32	C	O3'-P	-5.71	1.52	1.61
56	BATN	33	U	C3'-O3'	-5.68	1.33	1.42
35	BPTN	24	G	C4'-C3'	-5.63	1.44	1.52
35	BPTN	57	G	O3'-P	-5.58	1.52	1.61
1	B16S	3	G	N9-C4	5.53	1.49	1.38
35	BPTN	16	C	O3'-P	-5.47	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B16S	4	U	C2-N3	5.41	1.48	1.37
28	AL31	6	HIS	C-N	5.38	1.40	1.33
28	BL31	6	HIS	C-N	5.33	1.46	1.33
35	BPTN	12	U	O3'-P	5.33	1.69	1.61
1	A16S	1364	U	C3'-O3'	-5.30	1.35	1.43
35	APTN	8	4SU	O3'-P	5.25	1.61	1.56
1	A16S	3	G	C3'-O3'	5.22	1.50	1.42
29	BL32	3	LYS	C-N	5.20	1.44	1.33
34	BMRN	4	A	O3'-P	-5.16	1.53	1.61
1	A16S	4	U	O5'-C5'	5.11	1.50	1.42
1	B16S	3	G	C6-O6	5.04	1.34	1.24

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BPTN	32	C	O4'-C4'-C3'	-29.66	74.34	104.00
34	BMRN	16	G	N9-C1'-C2'	-26.39	72.41	112.00
34	BMRN	12	A	N9-C1'-C2'	-22.90	77.65	112.00
35	APTN	35	A	P-O3'-C3'	22.18	153.47	120.20
35	BPTN	11	C	O4'-C4'-C3'	-18.38	85.62	104.00
34	BMRN	17	U	N1-C1'-C2'	-17.62	85.56	112.00
35	BPTN	14	A	C3'-C2'-C1'	-16.67	84.63	101.30
35	BPTN	32	C	C3'-C2'-C1'	-16.11	85.19	101.30
35	BPTN	14	A	O4'-C4'-C3'	-16.08	87.92	104.00
35	BPTN	16	C	P-O3'-C3'	15.62	143.63	120.20
35	BPTN	35	A	C2'-C3'-O3'	-15.06	91.11	113.70
56	BATN	32	C	O4'-C4'-C3'	-14.72	89.28	104.00
35	BPTN	16	C	O3'-P-O5'	-14.35	82.48	104.00
35	BPTN	28	C	P-O3'-C3'	-13.89	99.36	120.20
35	BPTN	35	A	O3'-P-O5'	13.26	123.89	104.00
35	BPTN	18	G	P-O3'-C3'	-13.09	100.56	120.20
29	BL32	59	GLU	CB-CG-CD	13.06	134.81	112.60
35	BPTN	17	U	C2'-C3'-O3'	12.77	132.85	113.70
35	BPTN	32	C	P-O3'-C3'	-11.97	102.24	120.20
35	BPTN	17	U	O4'-C4'-C3'	-11.07	92.93	104.00
34	BMRN	4	A	C4'-C3'-C2'	10.90	113.50	102.60
35	BPTN	18	G	O4'-C4'-C3'	-10.68	95.42	106.10
35	APTN	35	A	C4'-C3'-O3'	10.64	128.97	113.00
35	BPTN	17	U	P-O5'-C5'	-10.45	105.23	120.90
35	BPTN	48	C	P-O3'-C3'	10.37	135.76	120.20
35	BPTN	11	C	C3'-C2'-C1'	-10.33	90.97	101.30
34	BMRN	4	A	C2'-C3'-O3'	-10.31	98.23	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BATN	33	U	C4'-C3'-C2'	10.30	112.90	102.60
24	BL27	7	LEU	CA-CB-CG	10.14	151.80	116.30
34	BMRN	11	U	P-O3'-C3'	-9.86	105.41	120.20
35	BPTN	32	C	O4'-C1'-N1	9.84	123.26	108.50
34	BMRN	4	A	C4'-C3'-O3'	-9.68	98.47	113.00
35	BPTN	24	G	O4'-C4'-C3'	-9.48	94.52	104.00
35	APTN	35	A	C2'-C3'-O3'	-9.21	99.88	113.70
35	BPTN	17	U	C3'-C2'-C1'	-9.18	92.12	101.30
35	BPTN	11	C	P-O3'-C3'	-9.03	106.66	120.20
56	BATN	4	G	O3'-P-O5'	-9.02	90.47	104.00
1	A16S	1364	U	O3'-P-O5'	9.01	117.52	104.00
35	BPTN	14	A	N9-C1'-C2'	-8.96	98.55	112.00
35	BPTN	24	G	C4'-C3'-C2'	8.80	111.40	102.60
29	BL32	60	VAL	CA-CB-CG2	-8.47	96.00	110.40
35	APTN	17	U	OP1-P-O3'	-8.46	82.63	108.00
34	BMRN	4	A	P-O5'-C5'	-8.34	108.38	120.90
56	BATN	4	G	N9-C1'-C2'	8.30	124.45	112.00
35	BPTN	29	U	O4'-C4'-C3'	-8.30	95.70	104.00
34	BMRN	10	G	O4'-C4'-C3'	-8.28	95.72	104.00
56	BATN	4	G	C2'-C3'-O3'	8.27	126.11	113.70
35	BPTN	18	G	C3'-C2'-C1'	-8.24	93.26	101.50
35	APTN	17	U	OP2-P-O3'	-8.21	83.36	108.00
35	BPTN	36	C	C4'-C3'-O3'	8.10	125.15	113.00
35	BPTN	12	U	C4'-C3'-C2'	-8.08	94.52	102.60
34	BMRN	15	A	P-O3'-C3'	-7.87	108.40	120.20
34	BMRN	8	A	N9-C1'-C2'	-7.81	100.28	112.00
35	BPTN	17	U	N1-C1'-C2'	7.81	123.71	112.00
35	BPTN	24	G	P-O5'-C5'	-7.77	109.24	120.90
34	BMRN	12	A	C4'-C3'-C2'	7.66	110.26	102.60
35	BPTN	24	G	C2'-C3'-O3'	-7.55	102.38	113.70
35	BPTN	36	C	P-O5'-C5'	-7.48	109.68	120.90
35	APTN	35	A	OP2-P-O3'	-7.46	85.64	108.00
56	BATN	3	U	C4'-C3'-O3'	7.43	120.54	109.40
35	BPTN	24	G	C3'-C2'-C1'	-7.37	93.93	101.30
29	BL32	59	GLU	CA-CB-CG	7.30	128.70	114.10
29	BL32	60	VAL	N-CA-C	7.30	131.44	111.00
35	BPTN	17	U	C5'-C4'-O4'	7.29	120.73	109.80
35	BPTN	49	G	O5'-C5'-C4'	-7.23	100.66	111.50
28	AL31	17	GLY	N-CA-C	7.21	121.21	112.49
35	BPTN	17	U	C4'-C3'-C2'	-7.19	95.41	102.60
34	BMRN	11	U	C3'-C2'-C1'	-7.14	94.16	101.30
35	BPTN	13	C	P-O3'-C3'	-7.10	109.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	ATHX	21	TYR	CA-C-N	7.09	139.09	121.80
55	ATHX	21	TYR	C-N-CA	7.09	139.09	121.80
35	BPTN	24	G	C4'-C3'-O3'	-7.07	102.40	113.00
35	BPTN	35	A	C3'-C2'-O2'	7.01	121.21	110.70
35	BPTN	24	G	P-O3'-C3'	-7.00	109.69	120.20
34	BMRN	20	A	C2'-C3'-O3'	7.00	120.00	109.50
35	BPTN	32	C	O3'-P-O5'	-6.96	93.56	104.00
35	BPTN	30	C	P-O5'-C5'	-6.95	110.47	120.90
35	BPTN	29	U	C3'-C2'-C1'	-6.93	94.37	101.30
56	BATN	32	C	P-O3'-C3'	-6.92	109.82	120.20
35	BPTN	19	G	C4'-C3'-O3'	-6.92	102.62	113.00
34	BMRN	17	U	O4'-C4'-C3'	6.90	110.90	104.00
35	BPTN	48	C	C4'-C3'-O3'	-6.88	102.68	113.00
35	BPTN	35	A	P-O3'-C3'	6.84	130.47	120.20
1	A16S	1364	U	N1-C1'-C2'	-6.76	103.86	114.00
35	BPTN	32	C	C4'-C3'-O3'	-6.73	102.91	113.00
35	APTN	35	A	O3'-P-O5'	6.72	114.08	104.00
35	BPTN	29	U	C2'-C3'-O3'	6.68	123.72	113.70
34	BMRN	20	A	P-O5'-C5'	-6.67	110.90	120.90
1	A16S	1364	U	C6-N1-C1'	-6.66	101.22	121.20
35	BPTN	17	U	O3'-P-O5'	6.63	113.95	104.00
35	BPTN	43	G	O3'-P-O5'	6.62	113.93	104.00
1	B16S	1364	U	O3'-P-O5'	6.52	113.78	104.00
34	BMRN	11	U	O4'-C4'-C3'	-6.51	97.49	104.00
34	BMRN	19	U	N1-C1'-C2'	6.50	123.75	114.00
35	BPTN	58	A	P-O5'-C5'	-6.41	111.29	120.90
34	BMRN	12	A	C3'-C2'-C1'	-6.40	94.90	101.30
35	BPTN	17	U	C5'-C4'-C3'	-6.38	106.43	116.00
1	A16S	4	U	C4'-C3'-O3'	6.37	122.56	113.00
35	BPTN	32	C	C5'-C4'-C3'	-6.36	106.46	116.00
34	BMRN	10	G	C4'-C3'-O3'	6.32	122.49	113.00
34	BMRN	4	A	N9-C1'-C2'	-6.28	102.58	112.00
35	BPTN	18	G	C4'-C3'-C2'	6.24	108.84	102.60
34	BMRN	17	U	O4'-C1'-C2'	6.22	113.82	107.60
29	AL32	40	LYS	CD-CE-NZ	6.20	131.73	111.90
24	AL27	84	LEU	CA-CB-CG	6.19	137.96	116.30
56	BATN	32	C	P-O5'-C5'	-6.18	111.63	120.90
2	A23S	352	G	C2'-C3'-O3'	6.13	118.69	109.50
29	BL32	60	VAL	CA-CB-CG1	6.08	120.73	110.40
1	A16S	1364	U	C4'-C3'-O3'	-6.06	100.31	109.40
10	AL09	11	ASN	N-CA-C	-6.04	107.73	114.62
35	BPTN	10	G	C4'-C3'-C2'	5.96	108.56	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BMRN	10	G	P-O3'-C3'	5.91	129.06	120.20
34	BMRN	12	A	O4'-C1'-C2'	5.89	113.49	107.60
29	BL32	4	HIS	CB-CA-C	5.87	121.73	110.17
35	BPTN	12	U	O4'-C4'-C3'	5.84	109.84	104.00
16	BL18	65	VAL	N-CA-C	-5.82	107.19	111.90
34	BMRN	16	G	P-O3'-C3'	-5.81	111.48	120.20
35	BPTN	44	G	O3'-P-O5'	-5.73	95.41	104.00
34	BMRN	16	G	O4'-C1'-C2'	5.73	113.33	107.60
29	AL32	3	LYS	CG-CD-CE	5.71	124.44	111.30
29	BL32	35	GLU	CA-C-N	-5.70	110.74	122.82
29	BL32	35	GLU	C-N-CA	-5.70	110.74	122.82
34	BMRN	14	A	P-O3'-C3'	5.69	128.73	120.20
35	BPTN	12	U	P-O3'-C3'	5.63	128.65	120.20
35	BPTN	20	G	N9-C1'-C2'	-5.60	105.61	114.00
35	BPTN	35	A	C1'-C2'-O2'	5.58	116.77	108.40
29	AL32	4	HIS	N-CA-C	5.57	122.12	109.81
35	BPTN	11	C	N1-C1'-C2'	-5.56	103.66	112.00
1	B16S	3	G	C4'-C3'-O3'	5.49	121.24	113.00
28	BL31	5	ILE	CA-C-N	5.49	135.20	121.80
28	BL31	5	ILE	C-N-CA	5.49	135.20	121.80
1	A16S	4	U	P-O5'-C5'	5.49	129.13	120.90
56	BATN	3	U	O3'-P-O5'	5.48	112.23	104.00
1	A16S	1364	U	C2-N1-C1'	5.47	134.12	117.70
35	BPTN	16	C	C5'-C4'-C3'	-5.46	107.01	115.20
56	BATN	2	G	C3'-C2'-C1'	-5.43	95.87	101.30
35	BPTN	23	A	C4'-C3'-O3'	5.43	121.14	113.00
34	BMRN	14	A	N9-C1'-C2'	5.38	120.06	112.00
35	BPTN	47	U	N1-C1'-C2'	-5.36	105.96	114.00
56	BATN	33	U	O4'-C4'-C3'	-5.36	98.64	104.00
34	BMRN	4	A	O4'-C1'-C2'	5.33	112.94	107.60
35	BPTN	17	U	O5'-C5'-C4'	5.33	119.49	111.50
35	APTN	38	A	O3'-P-O5'	-5.32	96.02	104.00
35	BPTN	11	C	C1'-C2'-O2'	5.30	116.36	108.40
2	A23S	1494	A	N9-C1'-C2'	5.30	121.95	114.00
35	BPTN	29	U	P-O3'-C3'	5.29	128.14	120.20
41	BS07	153	HIS	N-CA-C	-5.28	108.60	114.62
34	BMRN	20	A	O4'-C4'-C3'	5.26	111.36	106.10
35	BPTN	35	A	N9-C1'-C2'	-5.24	104.15	112.00
29	BL32	17	ASP	CA-C-N	5.23	129.58	120.68
29	BL32	17	ASP	C-N-CA	5.23	129.58	120.68
24	AL27	35	ASN	N-CA-CB	5.22	117.39	110.29
14	AL16	10	ARG	CB-CA-C	-5.21	110.14	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BPTN	12	U	C2'-C3'-O3'	5.20	121.50	113.70
34	BMRN	10	G	O3'-P-O5'	5.18	111.77	104.00
56	BATN	36	A	C4'-C3'-O3'	5.17	120.75	113.00
24	AL27	64	ASP	CA-C-N	-5.14	111.33	121.41
24	AL27	64	ASP	C-N-CA	-5.14	111.33	121.41
28	BL31	8	LYS	CA-C-N	5.13	128.15	120.87
28	BL31	8	LYS	C-N-CA	5.13	128.15	120.87
35	BPTN	47	U	O4'-C1'-C2'	5.13	110.93	105.80
35	BPTN	47	U	C4'-C3'-O3'	5.10	117.06	109.40
34	BMRN	12	A	C4'-C3'-O3'	-5.04	105.43	113.00
35	BPTN	17	U	P-O3'-C3'	5.04	127.75	120.20
24	BL27	40	GLN	N-CA-C	5.03	116.49	108.79
35	BPTN	39	G	P-O3'-C3'	-5.03	112.65	120.20

There are no chirality outliers.

All (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
29	AL32	39	MET	Peptide
15	BL17	10	LEU	Peptide
22	BL24	6	HIS	Peptide
24	BL27	8	GLY	Peptide
29	BL32	59	GLU	Mainchain,Peptide
34	BMRN	11	U	Sidechain
34	BMRN	17	U	Sidechain
34	BMRN	8	A	Sidechain
43	BS09	128	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
3:A5S:87:G:N1	3:A5S:89(A):G:OP2	2.21	0.72
3:B5S:5:C:OP1	3:B5S:61:G:O2'	2.06	0.71
3:A5S:81:G:N1	3:A5S:95:U:N3	2.37	0.71
3:B5S:12:C:O2'	3:B5S:13:A:OP2	2.10	0.69
3:A5S:80:U:O2	3:A5S:96:G:O6	2.11	0.68
3:A5S:13:A:N1	3:A5S:69:G:O2'	2.22	0.66
3:A5S:57:A:OP2	3:A5S:58:A:OP2	2.14	0.66
3:A5S:81:G:O6	3:A5S:95:U:O2	2.14	0.65
3:A5S:14:U:H4'	3:A5S:15:A:OP2	1.97	0.65
3:B5S:57:A:OP2	3:B5S:58:A:OP2	2.16	0.64
3:A5S:14:U:H3'	3:A5S:15:A:H2	1.63	0.63
3:B5S:3:C:H2'	3:B5S:4:C:C6	2.35	0.61
3:A5S:111:U:H2'	3:A5S:112:G:H8	1.65	0.61
3:A5S:14:U:OP2	3:A5S:70:C:O2'	2.17	0.61
3:B5S:32:C:H2'	3:B5S:33:G:H8	1.66	0.60
3:A5S:9:G:H1	3:A5S:111:U:H3	1.50	0.60
3:A5S:91:C:H2'	3:A5S:92:G:H8	1.68	0.59
3:A5S:78:A:H62	3:A5S:98:G:H21	0.68	0.58
3:A5S:33:G:N2	3:A5S:35:U:O4	2.34	0.57
3:B5S:5:C:O2'	3:B5S:27:C:O2	2.23	0.56
3:B5S:9:G:H1	3:B5S:111:U:H3	1.53	0.55
3:A5S:51:G:N3	3:A5S:52:A:N7	2.55	0.55
3:A5S:66:A:O2'	3:A5S:67:G:O5'	2.24	0.55
3:B5S:66:A:O2'	3:B5S:67:G:O5'	2.20	0.55
3:A5S:81:G:O6	3:A5S:95:U:C2	2.60	0.54
3:A5S:22:U:H3	3:A5S:61:G:H1	1.56	0.54
3:A5S:97:G:H5'	3:A5S:98:G:OP2	2.08	0.54
3:A5S:45:A:C4	3:A5S:46:A:C8	2.96	0.53
3:A5S:88:C:HO2'	3:A5S:89(A):G:P	2.31	0.52
3:B5S:32:C:H2'	3:B5S:33:G:C8	2.45	0.52
3:A5S:14:U:H3'	3:A5S:15:A:C2	2.44	0.52
3:A5S:14:U:O3'	3:A5S:107:U:O2'	2.28	0.52
3:A5S:86:G:H2'	3:A5S:87:G:H8	1.76	0.51
3:A5S:87:G:C6	3:A5S:89(A):G:OP2	2.64	0.51
3:B5S:21:G:H2'	3:B5S:22:U:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B5S:66:A:HO2'	3:B5S:67:G:P	2.33	0.50
3:A5S:51:G:C4	3:A5S:52:A:N7	2.79	0.50
3:A5S:62:C:H2'	3:A5S:63:G:H8	1.77	0.50
3:A5S:9:G:H2'	3:A5S:10:C:H6	1.77	0.50
3:A5S:3:C:H2'	3:A5S:4:C:H6	1.77	0.50
3:A5S:106:G:H2'	3:A5S:107:U:O4'	2.12	0.50
3:A5S:28:C:H2'	3:A5S:29:A:C8	2.46	0.49
3:A5S:32:C:H2'	3:A5S:33:G:H8	1.76	0.49
3:B5S:32:C:C2	3:B5S:33:G:C8	3.00	0.49
3:A5S:28:C:H2'	3:A5S:29:A:H8	1.78	0.49
3:A5S:87:G:O6	3:A5S:90:C:N4	2.46	0.49
3:A5S:80:U:C2	3:A5S:96:G:O6	2.66	0.49
3:A5S:66:A:O2'	3:A5S:67:G:C8	2.62	0.49
3:B5S:3:C:H2'	3:B5S:4:C:H6	1.78	0.48
3:A5S:35:U:H2'	3:A5S:36:C:C6	2.49	0.48
3:B5S:3:C:H2'	3:B5S:4:C:C5	2.49	0.48
3:A5S:88:C:O2'	3:A5S:89(A):G:OP1	2.23	0.48
3:A5S:39:A:C2	3:A5S:44:G:C2	3.02	0.47
3:A5S:31:C:C2	3:A5S:32:C:C5	3.03	0.47
3:A5S:13:A:O2'	3:A5S:15:A:OP2	2.33	0.47
3:A5S:62:C:H2'	3:A5S:63:G:C8	2.50	0.46
3:A5S:14:U:O2	3:A5S:106:G:O2'	2.32	0.46
3:A5S:51:G:H2'	3:A5S:52:A:N7	2.31	0.46
3:B5S:60:C:C2	3:B5S:61:G:C8	3.04	0.45
3:B5S:34:U:O4	3:B5S:44:G:O2'	2.22	0.45
3:A5S:44:G:C2	3:A5S:48:A:C2	3.05	0.45
3:B5S:14:U:OP2	3:B5S:71:C:H5'	2.16	0.45
3:A5S:14:U:OP2	3:A5S:71:C:H5'	2.18	0.44
3:A5S:93:C:H2'	3:A5S:94:C:H6	1.83	0.44
3:A5S:99:A:C4	3:A5S:100:G:C8	3.06	0.44
3:B5S:94:C:H2'	3:B5S:95:U:C6	2.53	0.44
3:A5S:91:C:H2'	3:A5S:92:G:C8	2.52	0.44
3:A5S:63:G:H2'	3:A5S:64:C:C6	2.53	0.43
3:A5S:81:G:N2	3:A5S:95:U:O4	2.48	0.43
3:A5S:92:G:C2	3:A5S:93:C:C5	3.06	0.43
3:B5S:15:A:H1'	3:B5S:109:G:N7	2.34	0.43
3:A5S:9:G:N2	3:A5S:111:U:O2	2.46	0.43
3:B5S:91:C:H2'	3:B5S:92:G:C8	2.55	0.42
3:A5S:61:G:C6	3:A5S:62:C:C4	3.08	0.42
3:A5S:81:G:C6	3:A5S:95:U:N3	2.87	0.42
3:A5S:19:G:H2'	3:A5S:20:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5S:15:A:O2'	3:A5S:16:G:OP1	2.35	0.42
3:B5S:73:A:C5	3:B5S:104:A:C2	3.08	0.42
3:A5S:15:A:OP1	3:A5S:107:U:O2'	2.38	0.41
3:B5S:52:A:O2'	3:B5S:53:A:OP2	2.38	0.41
3:B5S:53:A:H2'	3:B5S:54:G:H8	1.84	0.41
3:A5S:66:A:N3	3:A5S:108:C:N4	2.68	0.41
3:B5S:22:U:H2'	3:B5S:23:G:H8	1.85	0.41
3:A5S:3:C:C2	3:A5S:4:C:C5	3.08	0.41
3:A5S:35:U:OP2	3:A5S:36:C:OP2	2.39	0.41
3:A5S:100:G:H3'	3:A5S:101:A:H8	1.85	0.41
3:B5S:62:C:H2'	3:B5S:63:G:H8	1.86	0.41
3:B5S:63:G:H2'	3:B5S:64:C:C6	2.56	0.40
3:A5S:30:C:C4	3:A5S:31:C:C6	3.09	0.40
3:A5S:56:G:H4'	3:A5S:57:A:C8	2.57	0.40
3:A5S:24:G:C2	3:A5S:56:G:C2	3.09	0.40
3:A5S:87:G:C2	3:A5S:89(A):G:OP2	2.75	0.40
3:B5S:40:U:C2	3:B5S:43:C:OP2	2.75	0.40

All (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)
2:A23S:2154:G:N2	1:B16S:999:U:OP2[4_545]	1.96	0.24
18:BL20:89:GLU:N	29:BL32:60:VAL:O[4_455]	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
19:BL21:6:LYS:NZ	29:BL32:59:GLU:CB[4_455]	2.14	0.06
18:BL20:89:GLU:O	29:BL32:60:VAL:CA[4_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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	8
5	BL02	269/276 (98%)	198 (74%)	47 (18%)	24 (9%)	0	3
6	AL03	202/206 (98%)	145 (72%)	39 (19%)	18 (9%)	0	3
6	BL03	202/206 (98%)	152 (75%)	36 (18%)	14 (7%)	1	7
7	AL04	200/205 (98%)	162 (81%)	28 (14%)	10 (5%)	1	13
7	BL04	200/205 (98%)	154 (77%)	32 (16%)	14 (7%)	1	6
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	5
9	AL06	165/180 (92%)	99 (60%)	41 (25%)	25 (15%)	0	0
9	BL06	165/180 (92%)	95 (58%)	37 (22%)	33 (20%)	0	0
10	AL09	143/148 (97%)	116 (81%)	19 (13%)	8 (6%)	1	11
10	BL09	143/148 (97%)	106 (74%)	31 (22%)	6 (4%)	2	16
11	AL13	135/140 (96%)	102 (76%)	19 (14%)	14 (10%)	0	2
11	BL13	135/140 (96%)	106 (78%)	15 (11%)	14 (10%)	0	2
12	AL14	120/122 (98%)	97 (81%)	20 (17%)	3 (2%)	4	27
12	BL14	120/122 (98%)	99 (82%)	16 (13%)	5 (4%)	2	16
13	AL15	144/150 (96%)	90 (62%)	37 (26%)	17 (12%)	0	1
13	BL15	144/150 (96%)	85 (59%)	42 (29%)	17 (12%)	0	1
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	5
15	AL17	115/118 (98%)	92 (80%)	18 (16%)	5 (4%)	2	16
15	BL17	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	1	6
16	AL18	96/111 (86%)	68 (71%)	21 (22%)	7 (7%)	1	6
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	7
17	BL19	135/146 (92%)	107 (79%)	23 (17%)	5 (4%)	2	18
18	AL20	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	1	12
18	BL20	115/118 (98%)	82 (71%)	25 (22%)	8 (7%)	1	6
19	AL21	99/101 (98%)	73 (74%)	18 (18%)	8 (8%)	1	4
19	BL21	99/101 (98%)	79 (80%)	16 (16%)	4 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AL22	110/113 (97%)	79 (72%)	25 (23%)	6 (6%)	1	11
20	BL22	110/113 (97%)	81 (74%)	24 (22%)	5 (4%)	2	15
21	AL23	90/96 (94%)	74 (82%)	14 (16%)	2 (2%)	5	29
21	BL23	90/96 (94%)	77 (86%)	10 (11%)	3 (3%)	3	21
22	AL24	98/110 (89%)	54 (55%)	32 (33%)	12 (12%)	0	1
22	BL24	98/110 (89%)	56 (57%)	29 (30%)	13 (13%)	0	1
23	AL25	185/206 (90%)	143 (77%)	32 (17%)	10 (5%)	1	12
23	BL25	185/206 (90%)	144 (78%)	32 (17%)	9 (5%)	1	13
24	AL27	80/84 (95%)	62 (78%)	11 (14%)	7 (9%)	0	3
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	10
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	7
26	BL29	60/72 (83%)	45 (75%)	12 (20%)	3 (5%)	1	13
27	AL30	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	6	34
27	BL30	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	3	20
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	0
29	BL32	57/59 (97%)	43 (75%)	8 (14%)	6 (10%)	0	2
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	16
31	BL34	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	29
32	AL35	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	2
32	BL35	61/64 (95%)	40 (66%)	13 (21%)	8 (13%)	0	1
33	AL36	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	24
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	7
36	BS02	232/255 (91%)	174 (75%)	42 (18%)	16 (7%)	1	7
37	AS03	204/238 (86%)	150 (74%)	39 (19%)	15 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BS03	204/238 (86%)	144 (71%)	43 (21%)	17 (8%)	0	4
38	AS04	206/208 (99%)	171 (83%)	24 (12%)	11 (5%)	1	12
38	BS04	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	1	10
39	AS05	149/161 (92%)	122 (82%)	19 (13%)	8 (5%)	1	12
39	BS05	149/161 (92%)	122 (82%)	21 (14%)	6 (4%)	2	17
40	AS06	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	1	13
40	BS06	99/101 (98%)	79 (80%)	17 (17%)	3 (3%)	3	23
41	AS07	153/155 (99%)	119 (78%)	25 (16%)	9 (6%)	1	10
41	BS07	153/155 (99%)	110 (72%)	33 (22%)	10 (6%)	1	8
42	AS08	136/138 (99%)	107 (79%)	22 (16%)	7 (5%)	1	13
42	BS08	136/138 (99%)	115 (85%)	15 (11%)	6 (4%)	2	15
43	AS09	125/128 (98%)	94 (75%)	28 (22%)	3 (2%)	4	28
43	BS09	125/128 (98%)	92 (74%)	21 (17%)	12 (10%)	0	3
44	AS10	96/104 (92%)	83 (86%)	11 (12%)	2 (2%)	5	31
44	BS10	96/104 (92%)	76 (79%)	12 (12%)	8 (8%)	0	4
45	AS11	112/128 (88%)	87 (78%)	21 (19%)	4 (4%)	2	19
45	BS11	112/128 (88%)	89 (80%)	18 (16%)	5 (4%)	2	15
46	AS12	120/131 (92%)	86 (72%)	29 (24%)	5 (4%)	2	16
46	BS12	120/131 (92%)	84 (70%)	28 (23%)	8 (7%)	1	7
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	1
48	AS14	58/60 (97%)	37 (64%)	12 (21%)	9 (16%)	0	0
48	BS14	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	0	3
49	AS15	86/88 (98%)	74 (86%)	8 (9%)	4 (5%)	2	14
49	BS15	86/88 (98%)	70 (81%)	9 (10%)	7 (8%)	1	4
50	AS16	81/88 (92%)	63 (78%)	17 (21%)	1 (1%)	10	42
50	BS16	81/88 (92%)	65 (80%)	13 (16%)	3 (4%)	2	18
51	AS17	97/104 (93%)	79 (81%)	16 (16%)	2 (2%)	5	31
51	BS17	97/104 (93%)	75 (77%)	19 (20%)	3 (3%)	3	22
52	AS18	68/87 (78%)	52 (76%)	12 (18%)	4 (6%)	1	10
52	BS18	68/87 (78%)	55 (81%)	10 (15%)	3 (4%)	2	15

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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	2
54	AS20	97/105 (92%)	72 (74%)	20 (21%)	5 (5%)	1	12
54	BS20	97/105 (92%)	75 (77%)	14 (14%)	8 (8%)	0	4
55	ATHX	22/26 (85%)	5 (23%)	13 (59%)	4 (18%)	0	0
55	BTHX	22/26 (85%)	13 (59%)	7 (32%)	2 (9%)	0	3
All	All	11714/12532 (94%)	8611 (74%)	2167 (18%)	936 (8%)	1	4

All (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	AL02	28	GLU
5	AL02	235	GLY
5	AL02	242	ARG
5	AL02	244	ARG
5	AL02	258	LYS
6	AL03	17	ASP
7	AL04	83	PHE
8	AL05	84	LYS
8	AL05	129	GLY
9	AL06	25	LYS
9	AL06	83	TYR
9	AL06	90	LYS
9	AL06	137	ASP
9	AL06	138	LYS
9	AL06	153	LYS
9	AL06	169	VAL
10	AL09	111	PRO
11	AL13	58	ARG
11	AL13	59	GLY
11	AL13	153	HIS
11	AL13	155	ALA
12	AL14	28	SER
13	AL15	10	PRO
13	AL15	65	ARG

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Mol	Chain	Res	Type
13	AL15	147	LEU
13	AL15	148	LEU
14	AL16	18	LYS
14	AL16	20	ALA
14	AL16	110	THR
16	AL18	13	ARG
16	AL18	43	GLU
16	AL18	94	TYR
18	AL20	91	ASP
20	AL22	63	ASP
22	AL24	17	SER
22	AL24	40	GLU
22	AL24	56	PRO
22	AL24	62	GLU
23	AL25	17	ALA
23	AL25	165	VAL
24	AL27	18	ALA
24	AL27	83	PRO
25	AL28	54	ALA
25	AL28	83	GLU
27	AL30	39	ASP
28	AL31	5	ILE
28	AL31	12	ALA
28	AL31	18	CYS
28	AL31	30	GLU
28	AL31	39	CYS
28	AL31	40	HIS
28	AL31	41	PRO
29	AL32	4	HIS
29	AL32	49	CYS
29	AL32	52	TYR
29	AL32	57	VAL
32	AL35	17	THR
32	AL35	62	LEU
36	AS02	8	LYS
36	AS02	82	ARG
38	AS04	166	LYS
39	AS05	21	ALA
40	AS06	42	GLU
42	AS08	121	ASP
43	AS09	85	LEU
44	AS10	56	HIS

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Mol	Chain	Res	Type
44	AS10	91	PRO
47	AS13	6	GLY
47	AS13	7	VAL
47	AS13	23	TYR
47	AS13	38	GLY
47	AS13	77	ASN
48	AS14	14	PRO
48	AS14	17	LYS
52	AS18	87	ARG
55	ATHX	10	ARG
4	BL01	6	LYS
4	BL01	69	LEU
4	BL01	74	ARG
4	BL01	81	GLY
4	BL01	115	VAL
4	BL01	180	SER
4	BL01	182	PRO
4	BL01	185	LYS
4	BL01	193	PHE
4	BL01	215	VAL
4	BL01	222	SER
5	BL02	32	SER
5	BL02	242	ARG
5	BL02	244	ARG
6	BL03	17	ASP
6	BL03	60	ASN
7	BL04	64	ILE
8	BL05	66	GLN
8	BL05	123	ASN
9	BL06	6	ARG
9	BL06	81	GLU
9	BL06	83	TYR
9	BL06	84	SER
9	BL06	87	LEU
9	BL06	126	PRO
9	BL06	152	ARG
9	BL06	153	LYS
9	BL06	159	GLU
9	BL06	160	LYS
9	BL06	164	TYR
9	BL06	165	ALA
10	BL09	53	ALA

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Mol	Chain	Res	Type
11	BL13	100	GLY
11	BL13	149	PRO
12	BL14	28	SER
13	BL15	65	ARG
14	BL16	133	ARG
16	BL18	21	THR
17	BL19	107	ASP
18	BL20	26	GLY
18	BL20	60	LEU
18	BL20	91	ASP
19	BL21	77	ALA
19	BL21	78	LYS
20	BL22	63	ASP
21	BL23	11	PRO
22	BL24	77	PRO
22	BL24	82	PRO
23	BL25	81	ARG
23	BL25	128	VAL
24	BL27	9	SER
24	BL27	55	ARG
24	BL27	61	ALA
24	BL27	82	ARG
25	BL28	16	ASN
28	BL31	34	GLU
28	BL31	38	LYS
28	BL31	39	CYS
28	BL31	40	HIS
29	BL32	49	CYS
29	BL32	56	LYS
30	BL33	31	PRO
32	BL35	7	HIS
33	BL36	11	CYS
36	BS02	9	GLU
36	BS02	37	ASN
36	BS02	78	GLN
36	BS02	136	VAL
36	BS02	137	ARG
37	BS03	3	ASN
37	BS03	15	THR
37	BS03	49	SER
37	BS03	189	ALA
38	BS04	168	ARG

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Mol	Chain	Res	Type
41	BS07	31	MET
42	BS08	46	LYS
43	BS09	43	ALA
43	BS09	125	TYR
44	BS10	30	SER
46	BS12	124	PRO
47	BS13	98	VAL
47	BS13	108	ARG
48	BS14	14	PRO
50	BS16	76	GLN
53	BS19	27	GLU
4	AL01	17	PRO
4	AL01	21	TYR
4	AL01	23	ILE
4	AL01	36	ALA
4	AL01	37	LYS
4	AL01	66	PRO
4	AL01	71	LYS
4	AL01	115	VAL
4	AL01	170	GLY
4	AL01	223	VAL
4	AL01	226	ASN
5	AL02	12	SER
5	AL02	32	SER
5	AL02	33	LEU
5	AL02	243	GLY
6	AL03	58	ARG
6	AL03	59	VAL
6	AL03	88	GLY
6	AL03	118	LYS
6	AL03	140	SER
6	AL03	187	ALA
6	AL03	203	LYS
7	AL04	54	ARG
7	AL04	86	GLY
7	AL04	89	VAL
8	AL05	48	GLU
8	AL05	49	ASP
8	AL05	146	TYR
8	AL05	168	GLU
9	AL06	12	PRO
9	AL06	16	SER

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Mol	Chain	Res	Type
9	AL06	80	SER
9	AL06	129	THR
9	AL06	151	ILE
9	AL06	157	TYR
9	AL06	160	LYS
9	AL06	164	TYR
11	AL13	99	SER
13	AL15	13	ASN
13	AL15	28	GLY
13	AL15	38	GLN
14	AL16	8	LYS
14	AL16	17	LEU
14	AL16	23	GLY
14	AL16	78	PRO
14	AL16	136	ALA
15	AL17	80	PHE
15	AL17	101	ALA
16	AL18	59	LYS
16	AL18	105	ALA
17	AL19	84	GLN
17	AL19	97	ALA
18	AL20	6	THR
18	AL20	117	GLN
19	AL21	26	ASP
19	AL21	50	PRO
19	AL21	93	GLU
20	AL22	40	ASN
22	AL24	64	GLU
22	AL24	78	ALA
23	AL25	119	GLU
23	AL25	146	ILE
24	AL27	9	SER
24	AL27	73	GLY
25	AL28	78	LYS
28	AL31	8	LYS
28	AL31	22	ILE
28	AL31	29	PRO
28	AL31	46	GLN
29	AL32	51	TYR
29	AL32	53	ALA
30	AL33	28	ARG
30	AL33	34	LEU

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Mol	Chain	Res	Type
30	AL33	35	GLU
30	AL33	46	HIS
36	AS02	14	GLY
36	AS02	52	GLU
36	AS02	53	ARG
36	AS02	95	GLN
36	AS02	123	ALA
36	AS02	232	PRO
36	AS02	239	VAL
37	AS03	11	ARG
37	AS03	49	SER
37	AS03	96	GLY
37	AS03	127	ARG
37	AS03	130	VAL
38	AS04	5	ILE
38	AS04	42	GLN
38	AS04	71	SER
38	AS04	139	ARG
38	AS04	186	LEU
41	AS07	4	ARG
41	AS07	154	TYR
42	AS08	42	GLU
42	AS08	79	VAL
45	AS11	70	LYS
45	AS11	91	ARG
46	AS12	72	GLU
46	AS12	124	PRO
47	AS13	4	ILE
47	AS13	10	PRO
47	AS13	100	GLY
48	AS14	16	PHE
48	AS14	30	ALA
49	AS15	16	ALA
49	AS15	78	TYR
52	AS18	23	LYS
53	AS19	5	LEU
53	AS19	7	LYS
53	AS19	64	GLU
54	AS20	71	THR
55	ATHX	17	THR
4	BL01	66	PRO
4	BL01	76	LEU

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Mol	Chain	Res	Type
4	BL01	79	ALA
4	BL01	100	ILE
4	BL01	112	ASP
4	BL01	135	ARG
4	BL01	162	ILE
4	BL01	172	ILE
4	BL01	212	SER
4	BL01	213	VAL
4	BL01	225	ILE
5	BL02	31	LYS
5	BL02	33	LEU
5	BL02	79	VAL
5	BL02	121	PRO
5	BL02	122	ASP
5	BL02	199	ALA
6	BL03	144	ARG
6	BL03	173	VAL
6	BL03	192	ASN
7	BL04	89	VAL
7	BL04	148	LEU
8	BL05	10	LYS
8	BL05	122	PRO
8	BL05	177	GLY
9	BL06	46	GLU
9	BL06	64	LEU
9	BL06	86	GLU
9	BL06	90	LYS
9	BL06	137	ASP
9	BL06	138	LYS
9	BL06	148	ILE
10	BL09	2	LYS
11	BL13	46	LEU
11	BL13	154	GLN
13	BL15	18	ARG
13	BL15	34	GLY
13	BL15	46	LYS
13	BL15	59	LEU
14	BL16	8	LYS
14	BL16	18	LYS
14	BL16	21	THR
16	BL18	13	ARG
16	BL18	52	SER

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Mol	Chain	Res	Type
16	BL18	57	LYS
16	BL18	61	ASN
16	BL18	88	ASP
16	BL18	104	GLY
17	BL19	79	HIS
17	BL19	86	ILE
18	BL20	7	GLY
18	BL20	86	ALA
18	BL20	87	GLY
19	BL21	2	PHE
20	BL22	80	PRO
20	BL22	88	ARG
22	BL24	56	PRO
23	BL25	34	ASN
23	BL25	119	GLU
23	BL25	120	ILE
23	BL25	142	SER
25	BL28	30	VAL
25	BL28	54	ALA
25	BL28	83	GLU
27	BL30	2	PRO
29	BL32	4	HIS
30	BL33	41	PRO
31	BL34	47	ARG
32	BL35	8	LYS
32	BL35	41	ILE
32	BL35	63	PRO
36	BS02	38	GLY
36	BS02	236	TYR
37	BS03	47	LEU
37	BS03	53	ALA
37	BS03	55	VAL
37	BS03	83	ARG
38	BS04	3	ARG
38	BS04	18	LYS
38	BS04	90	GLY
38	BS04	91	SER
38	BS04	186	LEU
38	BS04	199	ASN
38	BS04	207	TYR
38	BS04	208	SER
39	BS05	77	PRO

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Mol	Chain	Res	Type
39	BS05	115	VAL
40	BS06	13	ASN
41	BS07	81	GLY
41	BS07	117	ALA
42	BS08	2	LEU
42	BS08	60	ARG
42	BS08	74	PRO
43	BS09	83	ARG
43	BS09	91	ASP
44	BS10	55	LYS
44	BS10	88	LEU
45	BS11	91	ARG
45	BS11	95	ILE
46	BS12	33	ARG
47	BS13	61	GLU
47	BS13	82	MET
47	BS13	113	PRO
49	BS15	9	GLN
49	BS15	88	ARG
50	BS16	44	THR
52	BS18	84	LYS
53	BS19	34	TRP
54	BS20	11	SER
54	BS20	71	THR
54	BS20	101	GLY
55	BTHX	16	GLY
4	AL01	43	GLU
4	AL01	54	ARG
4	AL01	110	ASP
4	AL01	138	LEU
4	AL01	142	LYS
4	AL01	179	ALA
4	AL01	228	HIS
5	AL02	233	HIS
5	AL02	236	GLY
5	AL02	256	GLY
6	AL03	117	MET
7	AL04	139	PHE
7	AL04	181	LEU
8	AL05	6	ALA
8	AL05	14	GLU
8	AL05	45	GLU

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Mol	Chain	Res	Type
8	AL05	87	PRO
8	AL05	96	ARG
8	AL05	111	LEU
9	AL06	82	GLY
10	AL09	29	TYR
10	AL09	30	LEU
10	AL09	112	LYS
10	AL09	125	GLU
11	AL13	68	ASN
11	AL13	79	ASN
11	AL13	105	LEU
11	AL13	149	PRO
12	AL14	70	LYS
13	AL15	16	ARG
13	AL15	27	HIS
13	AL15	35	HIS
13	AL15	42	SER
14	AL16	134	ARG
15	AL17	107	ASP
17	AL19	2	ASN
17	AL19	4	GLY
18	AL20	89	GLU
18	AL20	102	GLU
19	AL21	61	VAL
19	AL21	80	GLN
21	AL23	15	GLU
22	AL24	4	LYS
23	AL25	79	ARG
26	AL29	43	GLN
28	AL31	37	SER
30	AL33	18	ARG
30	AL33	31	PRO
30	AL33	51	GLU
31	AL34	13	ALA
36	AS02	18	GLY
36	AS02	77	ALA
36	AS02	122	PHE
37	AS03	60	ALA
37	AS03	98	ASN
38	AS04	41	GLY
38	AS04	173	TRP
39	AS05	60	TYR

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Mol	Chain	Res	Type
39	AS05	133	TYR
40	AS06	12	PRO
40	AS06	80	ARG
41	AS07	90	GLU
42	AS08	68	ARG
42	AS08	80	ILE
45	AS11	37	GLY
46	AS12	27	LYS
46	AS12	70	PRO
46	AS12	115	SER
47	AS13	15	VAL
47	AS13	26	GLY
47	AS13	57	ARG
47	AS13	70	LEU
48	AS14	5	ALA
51	AS17	4	LYS
53	AS19	6	LYS
53	AS19	37	ARG
55	ATHX	9	ARG
4	BL01	43	GLU
4	BL01	46	ALA
4	BL01	60	ARG
4	BL01	108	TRP
4	BL01	216	THR
4	BL01	221	PRO
5	BL02	12	SER
6	BL03	56	PRO
6	BL03	89	ASP
6	BL03	99	GLY
6	BL03	122	PHE
7	BL04	78	ILE
7	BL04	166	ALA
7	BL04	167	ALA
7	BL04	181	LEU
8	BL05	42	GLY
8	BL05	74	LYS
8	BL05	87	PRO
9	BL06	27	LYS
9	BL06	41	MET
9	BL06	169	VAL
11	BL13	30	LYS
11	BL13	43	GLY

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Mol	Chain	Res	Type
11	BL13	68	ASN
11	BL13	119	GLU
11	BL13	124	HIS
13	BL15	10	PRO
13	BL15	31	ALA
13	BL15	33	ARG
14	BL16	134	ARG
15	BL17	4	LEU
15	BL17	15	SER
15	BL17	82	GLU
16	BL18	56	LEU
18	BL20	9	VAL
22	BL24	17	SER
23	BL25	79	ARG
24	BL27	5	LYS
24	BL27	15	ASP
24	BL27	21	LEU
24	BL27	84	LEU
25	BL28	92	LYS
26	BL29	3	LEU
28	BL31	22	ILE
28	BL31	23	GLU
28	BL31	29	PRO
30	BL33	19	ARG
30	BL33	35	GLU
30	BL33	51	GLU
33	BL36	12	ASP
36	BS02	77	ALA
36	BS02	138	LEU
37	BS03	25	GLY
37	BS03	50	ALA
37	BS03	80	GLY
37	BS03	156	ARG
38	BS04	153	ARG
39	BS05	152	ARG
39	BS05	153	LYS
43	BS09	79	LEU
43	BS09	84	ALA
43	BS09	123	PRO
44	BS10	27	ALA
44	BS10	93	GLY
46	BS12	18	ARG

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Mol	Chain	Res	Type
46	BS12	78	GLU
47	BS13	3	ARG
47	BS13	63	THR
47	BS13	107	ALA
48	BS14	55	GLY
49	BS15	10	LYS
51	BS17	67	LYS
52	BS18	86	VAL
54	BS20	99	LEU
55	BTHX	17	THR
4	AL01	46	ALA
4	AL01	59	VAL
4	AL01	65	LEU
4	AL01	107	GLY
4	AL01	222	SER
5	AL02	156	ALA
6	AL03	122	PHE
6	AL03	132	HIS
7	AL04	122	LYS
8	AL05	43	LEU
8	AL05	57	ALA
9	AL06	8	PRO
9	AL06	118	PRO
9	AL06	159	GLU
10	AL09	46	ALA
10	AL09	70	GLU
11	AL13	115	ALA
13	AL15	71	VAL
13	AL15	122	PRO
14	AL16	28	ALA
15	AL17	82	GLU
16	AL18	62	LYS
17	AL19	35	LYS
19	AL21	17	GLY
19	AL21	44	LYS
19	AL21	62	LEU
20	AL22	80	PRO
20	AL22	110	LYS
21	AL23	6	ASP
22	AL24	18	GLY
22	AL24	77	PRO
22	AL24	90	LEU

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Mol	Chain	Res	Type
23	AL25	80	ARG
23	AL25	93	ASP
23	AL25	142	SER
24	AL27	11	ARG
24	AL27	84	LEU
26	AL29	3	LEU
26	AL29	10	LEU
28	AL31	23	GLU
28	AL31	25	TYR
28	AL31	26	SER
28	AL31	38	LYS
28	AL31	43	TYR
29	AL32	5	PRO
29	AL32	22	HIS
29	AL32	58	LEU
31	AL34	36	GLN
32	AL35	35	GLN
36	AS02	64	ARG
36	AS02	72	GLY
37	AS03	62	ASP
37	AS03	181	ASN
38	AS04	69	GLY
39	AS05	100	VAL
39	AS05	153	LYS
40	AS06	49	ALA
41	AS07	71	PRO
41	AS07	115	ARG
41	AS07	155	ARG
42	AS08	98	LYS
43	AS09	78	LYS
47	AS13	94	ARG
47	AS13	116	THR
48	AS14	3	ARG
48	AS14	46	GLU
52	AS18	36	ASN
54	AS20	28	ALA
4	BL01	45	HIS
4	BL01	77	ALA
4	BL01	210	LEU
4	BL01	224	ARG
5	BL02	13	ARG
5	BL02	116	GLN

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Mol	Chain	Res	Type
5	BL02	147	LEU
5	BL02	236	GLY
5	BL02	245	PRO
5	BL02	246	PRO
6	BL03	52	LEU
6	BL03	131	ALA
7	BL04	77	ASP
9	BL06	22	GLY
9	BL06	40	GLU
9	BL06	149	ARG
10	BL09	99	GLU
11	BL13	42	GLU
11	BL13	160	LYS
12	BL14	89	ASN
12	BL14	113	LYS
13	BL15	16	ARG
13	BL15	38	GLN
13	BL15	56	SER
13	BL15	71	VAL
13	BL15	104	GLY
13	BL15	141	ALA
14	BL16	81	VAL
15	BL17	93	GLY
15	BL17	107	ASP
16	BL18	24	LEU
16	BL18	64	GLU
16	BL18	67	ARG
16	BL18	103	GLU
17	BL19	84	GLN
18	BL20	37	GLU
20	BL22	90	ARG
22	BL24	19	LYS
22	BL24	58	GLY
22	BL24	69	ALA
25	BL28	11	ARG
28	BL31	12	ALA
28	BL31	25	TYR
28	BL31	37	SER
29	BL32	42	PRO
29	BL32	51	TYR
29	BL32	53	ALA
30	BL33	28	ARG

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Mol	Chain	Res	Type
32	BL35	17	THR
33	BL36	14	CYS
36	BS02	20	GLU
36	BS02	109	SER
37	BS03	150	LYS
37	BS03	188	LEU
38	BS04	73	ARG
39	BS05	73	ASN
39	BS05	154	GLY
40	BS06	36	ARG
41	BS07	5	ARG
41	BS07	7	ALA
41	BS07	103	TRP
42	BS08	20	TYR
43	BS09	90	PRO
45	BS11	115	PRO
46	BS12	94	GLY
47	BS13	27	LYS
47	BS13	116	THR
48	BS14	46	GLU
48	BS14	60	SER
50	BS16	80	PHE
51	BS17	4	LYS
51	BS17	11	VAL
52	BS18	54	ARG
54	BS20	83	ARG
4	AL01	113	ALA
4	AL01	140	ASN
4	AL01	162	ILE
4	AL01	212	SER
4	AL01	215	VAL
4	AL01	221	PRO
5	AL02	13	ARG
5	AL02	31	LYS
6	AL03	86	PRO
6	AL03	129	HIS
7	AL04	127	GLU
8	AL05	11	TYR
9	AL06	41	MET
9	AL06	128	PRO
10	AL09	58	LEU
13	AL15	19	VAL

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Mol	Chain	Res	Type
14	AL16	13	GLN
14	AL16	80	GLU
14	AL16	120	ILE
15	AL17	100	LEU
16	AL18	57	LYS
17	AL19	107	ASP
22	AL24	82	PRO
22	AL24	98	VAL
23	AL25	128	VAL
26	AL29	42	GLY
28	AL31	27	THR
28	AL31	34	GLU
36	AS02	158	LEU
36	AS02	210	SER
37	AS03	12	LEU
37	AS03	80	GLY
37	AS03	82	GLU
37	AS03	131	ARG
38	AS04	207	TYR
39	AS05	36	ASP
39	AS05	112	LEU
40	AS06	82	ARG
41	AS07	62	PHE
42	AS08	105	ARG
47	AS13	117	VAL
49	AS15	88	ARG
52	AS18	22	VAL
53	AS19	28	LYS
53	AS19	79	THR
54	AS20	72	LEU
54	AS20	89	ARG
55	ATHX	14	TRP
4	BL01	51	ASP
4	BL01	59	VAL
4	BL01	114	VAL
4	BL01	228	HIS
5	BL02	35	LYS
5	BL02	70	TRP
5	BL02	262	ARG
6	BL03	86	PRO
7	BL04	53	THR
7	BL04	73	ALA

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Mol	Chain	Res	Type
8	BL05	14	GLU
8	BL05	17	PRO
8	BL05	124	SER
8	BL05	129	GLY
9	BL06	17	VAL
9	BL06	79	VAL
10	BL09	29	TYR
10	BL09	137	PRO
11	BL13	70	ALA
14	BL16	90	VAL
14	BL16	91	GLU
15	BL17	8	ARG
15	BL17	106	GLY
16	BL18	62	LYS
20	BL22	87	PRO
21	BL23	93	GLU
22	BL24	18	GLY
22	BL24	78	ALA
25	BL28	93	GLU
28	BL31	42	PHE
30	BL33	33	LYS
30	BL33	46	HIS
32	BL35	3	LYS
33	BL36	10	ILE
36	BS02	106	LYS
42	BS08	79	VAL
43	BS09	34	ASN
44	BS10	29	ARG
44	BS10	41	PRO
44	BS10	54	PHE
46	BS12	122	LYS
47	BS13	4	ILE
49	BS15	6	GLU
49	BS15	87	ILE
53	BS19	5	LEU
53	BS19	24	ALA
53	BS19	60	VAL
5	AL02	11	PRO
6	AL03	98	PRO
8	AL05	68	PRO
9	AL06	17	VAL
9	AL06	167	GLU

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Mol	Chain	Res	Type
11	AL13	152	PRO
13	AL15	37	GLY
14	AL16	44	ALA
14	AL16	81	VAL
17	AL19	115	ARG
20	AL22	11	ARG
20	AL22	87	PRO
25	AL28	31	GLY
32	AL35	3	LYS
32	AL35	31	HIS
33	AL36	3	VAL
37	AS03	26	LYS
37	AS03	110	ASN
39	AS05	63	ARG
41	AS07	17	VAL
43	AS09	32	ASP
51	AS17	61	GLU
4	BL01	5	GLY
4	BL01	42	VAL
4	BL01	55	SER
4	BL01	164	PHE
4	BL01	177	GLY
5	BL02	29	PRO
5	BL02	150	LYS
6	BL03	18	ASP
8	BL05	46	ALA
9	BL06	70	THR
9	BL06	151	ILE
9	BL06	167	GLU
12	BL14	110	GLY
13	BL15	106	LEU
14	BL16	135	ASP
17	BL19	78	LEU
21	BL23	38	GLU
22	BL24	55	TYR
22	BL24	80	GLY
22	BL24	96	ILE
23	BL25	64	GLY
26	BL29	16	LEU
27	BL30	39	ASP
32	BL35	52	LYS
33	BL36	3	VAL

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Mol	Chain	Res	Type
36	BS02	238	LEU
37	BS03	181	ASN
41	BS07	23	VAL
41	BS07	71	PRO
41	BS07	114	ARG
43	BS09	56	LEU
43	BS09	69	GLY
45	BS11	59	TYR
45	BS11	113	PRO
48	BS14	25	VAL
54	BS20	63	ILE
54	BS20	69	GLY
6	AL03	99	GLY
6	AL03	193	GLY
18	AL20	103	PRO
23	AL25	53	ILE
24	AL27	51	VAL
38	AS04	172	PRO
41	AS07	82	GLY
49	AS15	86	GLY
50	AS16	66	PRO
53	AS19	59	PRO
4	BL01	16	ASP
5	BL02	34	VAL
24	BL27	31	VAL
28	BL31	41	PRO
36	BS02	26	PRO
36	BS02	239	VAL
37	BS03	5	ILE
46	BS12	44	PRO
54	BS20	97	ALA
7	AL04	92	PRO
11	AL13	148	GLY
13	AL15	63	PRO
32	AL35	41	ILE
48	AS14	18	VAL
53	AS19	54	GLY
4	BL01	65	LEU
4	BL01	91	GLY
4	BL01	144	GLY
4	BL01	202	PRO
7	BL04	76	GLY

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Mol	Chain	Res	Type
9	BL06	8	PRO
13	BL15	11	GLY
13	BL15	63	PRO
14	BL16	73	PRO
15	BL17	7	GLY
32	BL35	20	GLY
37	BS03	51	GLY
40	BS06	12	PRO
41	BS07	82	GLY
47	BS13	15	VAL
53	BS19	9	VAL
53	BS19	76	PRO
4	AL01	75	VAL
11	AL13	100	GLY
25	AL28	53	VAL
47	AS13	113	PRO
53	AS19	45	VAL
4	BL01	70	GLY
7	BL04	132	VAL
9	BL06	12	PRO
9	BL06	99	VAL
11	BL13	152	PRO
23	BL25	146	ILE
25	BL28	14	VAL
43	BS09	57	GLY
46	BS12	70	PRO
53	BS19	8	GLY
6	AL03	34	VAL
6	AL03	124	GLY
8	AL05	85	GLY
8	AL05	177	GLY
9	AL06	21	PRO
11	AL13	29	PRO
12	AL14	43	VAL
17	AL19	56	GLY
17	AL19	135	VAL
45	AS11	115	PRO
48	AS14	25	VAL
54	AS20	97	ALA
4	BL01	30	VAL
4	BL01	75	VAL
4	BL01	120	VAL

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Mol	Chain	Res	Type
4	BL01	138	LEU
5	BL02	11	PRO
7	BL04	79	GLY
8	BL05	149	VAL
10	BL09	84	GLY
12	BL14	102	VAL
22	BL24	66	PRO
26	BL29	42	GLY
36	BS02	194	PRO
38	BS04	143	GLY
47	BS13	60	VAL
47	BS13	89	GLY
49	BS15	19	PRO
4	AL01	177	GLY
7	AL04	147	GLY
8	AL05	89	GLY
13	AL15	104	GLY
5	BL02	125	ILE
6	BL03	98	PRO
7	BL04	66	PRO
11	BL13	34	PRO
19	BL21	54	GLY
49	BS15	29	VAL
5	AL02	245	PRO
9	AL06	126	PRO

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%)	19	52
4	BL01	180/180 (100%)	166 (92%)	14 (8%)	11	41
5	AL02	213/218 (98%)	204 (96%)	9 (4%)	26	60
5	BL02	213/218 (98%)	205 (96%)	8 (4%)	29	62
6	AL03	165/166 (99%)	163 (99%)	2 (1%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BL03	165/166 (99%)	159 (96%)	6 (4%)	31	63
7	AL04	161/162 (99%)	158 (98%)	3 (2%)	50	73
7	BL04	161/162 (99%)	155 (96%)	6 (4%)	30	63
8	AL05	155/155 (100%)	142 (92%)	13 (8%)	10	38
8	BL05	155/155 (100%)	143 (92%)	12 (8%)	12	41
9	AL06	139/148 (94%)	135 (97%)	4 (3%)	37	67
9	BL06	139/148 (94%)	132 (95%)	7 (5%)	22	55
10	AL09	121/124 (98%)	115 (95%)	6 (5%)	22	55
10	BL09	122/124 (98%)	116 (95%)	6 (5%)	22	55
11	AL13	116/119 (98%)	113 (97%)	3 (3%)	40	69
11	BL13	116/119 (98%)	109 (94%)	7 (6%)	17	50
12	AL14	100/100 (100%)	100 (100%)	0	100	100
12	BL14	100/100 (100%)	99 (99%)	1 (1%)	68	80
13	AL15	112/116 (97%)	101 (90%)	11 (10%)	7	31
13	BL15	112/116 (97%)	101 (90%)	11 (10%)	7	31
14	AL16	105/111 (95%)	101 (96%)	4 (4%)	29	62
14	BL16	105/111 (95%)	101 (96%)	4 (4%)	29	62
15	AL17	100/101 (99%)	96 (96%)	4 (4%)	28	61
15	BL17	100/101 (99%)	93 (93%)	7 (7%)	14	45
16	AL18	77/87 (88%)	73 (95%)	4 (5%)	21	54
16	BL18	77/87 (88%)	70 (91%)	7 (9%)	9	34
17	AL19	121/128 (94%)	115 (95%)	6 (5%)	22	55
17	BL19	121/128 (94%)	113 (93%)	8 (7%)	15	47
18	AL20	93/94 (99%)	90 (97%)	3 (3%)	34	65
18	BL20	93/94 (99%)	89 (96%)	4 (4%)	26	59
19	AL21	82/82 (100%)	77 (94%)	5 (6%)	17	49
19	BL21	82/82 (100%)	78 (95%)	4 (5%)	22	55
20	AL22	91/92 (99%)	87 (96%)	4 (4%)	25	59
20	BL22	91/92 (99%)	88 (97%)	3 (3%)	33	65
21	AL23	74/78 (95%)	71 (96%)	3 (4%)	27	60
21	BL23	74/78 (95%)	71 (96%)	3 (4%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	AL24	84/91 (92%)	78 (93%)	6 (7%)	13	44
22	BL24	84/91 (92%)	81 (96%)	3 (4%)	31	63
23	AL25	162/179 (90%)	157 (97%)	5 (3%)	35	66
23	BL25	162/179 (90%)	153 (94%)	9 (6%)	19	52
24	AL27	65/66 (98%)	62 (95%)	3 (5%)	24	58
24	BL27	65/66 (98%)	64 (98%)	1 (2%)	57	76
25	AL28	73/83 (88%)	70 (96%)	3 (4%)	27	60
25	BL28	73/83 (88%)	68 (93%)	5 (7%)	14	46
26	AL29	58/67 (87%)	56 (97%)	2 (3%)	32	64
26	BL29	58/67 (87%)	57 (98%)	1 (2%)	53	75
27	AL30	51/52 (98%)	48 (94%)	3 (6%)	18	50
27	BL30	51/52 (98%)	50 (98%)	1 (2%)	48	72
28	AL31	40/63 (64%)	36 (90%)	4 (10%)	7	30
28	BL31	40/63 (64%)	39 (98%)	1 (2%)	42	69
29	AL32	51/51 (100%)	48 (94%)	3 (6%)	18	50
29	BL32	51/51 (100%)	48 (94%)	3 (6%)	18	50
30	AL33	43/52 (83%)	38 (88%)	5 (12%)	5	24
30	BL33	43/52 (83%)	37 (86%)	6 (14%)	3	17
31	AL34	41/42 (98%)	37 (90%)	4 (10%)	7	31
31	BL34	41/42 (98%)	41 (100%)	0	100	100
32	AL35	53/54 (98%)	49 (92%)	4 (8%)	12	42
32	BL35	53/54 (98%)	50 (94%)	3 (6%)	18	51
33	AL36	34/34 (100%)	34 (100%)	0	100	100
33	BL36	34/34 (100%)	32 (94%)	2 (6%)	18	50
36	AS02	202/219 (92%)	194 (96%)	8 (4%)	28	61
36	BS02	202/219 (92%)	192 (95%)	10 (5%)	22	55
37	AS03	160/187 (86%)	152 (95%)	8 (5%)	22	55
37	BS03	160/187 (86%)	154 (96%)	6 (4%)	29	62
38	AS04	171/180 (95%)	161 (94%)	10 (6%)	18	51
38	BS04	171/180 (95%)	162 (95%)	9 (5%)	20	53
39	AS05	116/122 (95%)	113 (97%)	3 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BS05	116/122 (95%)	109 (94%)	7 (6%)	17	50
40	AS06	90/90 (100%)	85 (94%)	5 (6%)	19	52
40	BS06	90/90 (100%)	87 (97%)	3 (3%)	33	65
41	AS07	126/126 (100%)	118 (94%)	8 (6%)	16	48
41	BS07	126/126 (100%)	120 (95%)	6 (5%)	23	56
42	AS08	119/119 (100%)	109 (92%)	10 (8%)	10	38
42	BS08	119/119 (100%)	114 (96%)	5 (4%)	26	60
43	AS09	98/99 (99%)	86 (88%)	12 (12%)	5	22
43	BS09	98/99 (99%)	93 (95%)	5 (5%)	21	54
44	AS10	88/91 (97%)	86 (98%)	2 (2%)	44	70
44	BS10	88/91 (97%)	82 (93%)	6 (7%)	14	46
45	AS11	86/98 (88%)	81 (94%)	5 (6%)	18	51
45	BS11	86/98 (88%)	82 (95%)	4 (5%)	23	57
46	AS12	103/108 (95%)	101 (98%)	2 (2%)	50	73
46	BS12	103/108 (95%)	96 (93%)	7 (7%)	14	46
47	AS13	94/100 (94%)	91 (97%)	3 (3%)	34	65
47	BS13	94/100 (94%)	89 (95%)	5 (5%)	20	53
48	AS14	49/49 (100%)	44 (90%)	5 (10%)	7	29
48	BS14	49/49 (100%)	47 (96%)	2 (4%)	27	60
49	AS15	79/79 (100%)	71 (90%)	8 (10%)	7	30
49	BS15	79/79 (100%)	77 (98%)	2 (2%)	42	69
50	AS16	72/74 (97%)	68 (94%)	4 (6%)	19	52
50	BS16	72/74 (97%)	71 (99%)	1 (1%)	59	77
51	AS17	94/96 (98%)	93 (99%)	1 (1%)	65	79
51	BS17	94/96 (98%)	89 (95%)	5 (5%)	20	53
52	AS18	61/76 (80%)	58 (95%)	3 (5%)	22	55
52	BS18	61/76 (80%)	57 (93%)	4 (7%)	15	47
53	AS19	69/79 (87%)	64 (93%)	5 (7%)	13	44
53	BS19	69/79 (87%)	65 (94%)	4 (6%)	18	51
54	AS20	76/81 (94%)	74 (97%)	2 (3%)	40	69
54	BS20	76/81 (94%)	72 (95%)	4 (5%)	20	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	ATHX	19/21 (90%)	14 (74%)	5 (26%)	0	3
55	BTHX	19/21 (90%)	19 (100%)	0	100	100
All	All	9865/10378 (95%)	9372 (95%)	493 (5%)	22	55

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AL01	6	LYS
4	AL01	14	LYS
4	AL01	17	PRO
4	AL01	32	GLU
4	AL01	53	ARG
4	AL01	83	LYS
4	AL01	106	ASP
4	AL01	110	ASP
4	AL01	127	LYS
4	AL01	189	ASN
5	AL02	32	SER
5	AL02	58	HIS
5	AL02	88	ARG
5	AL02	104	TYR
5	AL02	162	SER
5	AL02	175	LEU
5	AL02	186	HIS
5	AL02	217	ARG
5	AL02	220	HIS
6	AL03	127	ASP
6	AL03	171	GLU
7	AL04	13	SER
7	AL04	95	ARG
7	AL04	106	ARG
8	AL05	21	ARG
8	AL05	33	ARG
8	AL05	47	LYS
8	AL05	58	GLN
8	AL05	86	MET
8	AL05	91	ARG
8	AL05	113	ARG
8	AL05	115	ARG
8	AL05	128	ARG
8	AL05	130	ASN

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Mol	Chain	Res	Type
8	AL05	146	TYR
8	AL05	153	ARG
8	AL05	155	MET
9	AL06	6	ARG
9	AL06	30	LYS
9	AL06	42	ARG
9	AL06	85	LYS
10	AL09	2	LYS
10	AL09	61	ARG
10	AL09	69	LYS
10	AL09	112	LYS
10	AL09	118	LYS
10	AL09	135	GLU
11	AL13	61	HIS
11	AL13	71	MET
11	AL13	146	TYR
13	AL15	16	ARG
13	AL15	27	HIS
13	AL15	47	ASP
13	AL15	51	PHE
13	AL15	59	LEU
13	AL15	61	ARG
13	AL15	77	ARG
13	AL15	79	ARG
13	AL15	138	LEU
13	AL15	147	LEU
13	AL15	148	LEU
14	AL16	9	TYR
14	AL16	16	ARG
14	AL16	22	LYS
14	AL16	74	TYR
15	AL17	2	ARG
15	AL17	27	SER
15	AL17	28	LEU
15	AL17	63	ARG
16	AL18	20	ARG
16	AL18	41	ASP
16	AL18	67	ARG
16	AL18	73	LEU
17	AL19	36	GLU
17	AL19	53	ARG
17	AL19	80	SER

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Mol	Chain	Res	Type
17	AL19	98	LYS
17	AL19	104	ASN
17	AL19	118	ARG
18	AL20	3	ARG
18	AL20	91	ASP
18	AL20	92	ARG
19	AL21	1	MET
19	AL21	10	LYS
19	AL21	66	ARG
19	AL21	87	HIS
19	AL21	94	LEU
20	AL22	72	LYS
20	AL22	92	ARG
20	AL22	94	ASP
20	AL22	102	HIS
21	AL23	40	LYS
21	AL23	65	ARG
21	AL23	75	ASP
22	AL24	2	ARG
22	AL24	4	LYS
22	AL24	8	LYS
22	AL24	17	SER
22	AL24	76	CYS
22	AL24	97	ARG
23	AL25	36	LYS
23	AL25	45	ASP
23	AL25	87	ASP
23	AL25	125	LEU
23	AL25	166	SER
24	AL27	25	ARG
24	AL27	35	ASN
24	AL27	70	GLN
25	AL28	52	ARG
25	AL28	83	GLU
25	AL28	88	LYS
26	AL29	7	ARG
26	AL29	24	LEU
27	AL30	3	ARG
27	AL30	4	LEU
27	AL30	10	LYS
28	AL31	8	LYS
28	AL31	16	CYS

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Mol	Chain	Res	Type
28	AL31	23	GLU
28	AL31	36	CYS
29	AL32	12	SER
29	AL32	49	CYS
29	AL32	51	TYR
30	AL33	15	GLU
30	AL33	19	ARG
30	AL33	33	LYS
30	AL33	37	ARG
30	AL33	49	HIS
31	AL34	9	ARG
31	AL34	10	ARG
31	AL34	19	ARG
31	AL34	29	LYS
32	AL35	8	LYS
32	AL35	34	TRP
32	AL35	46	ARG
32	AL35	57	ARG
36	AS02	17	PHE
36	AS02	48	MET
36	AS02	57	PHE
36	AS02	87	ARG
36	AS02	130	ARG
36	AS02	140	HIS
36	AS02	144	ARG
36	AS02	195	ASP
37	AS03	4	LYS
37	AS03	16	ARG
37	AS03	79	ARG
37	AS03	119	ARG
37	AS03	127	ARG
37	AS03	128	PHE
37	AS03	131	ARG
37	AS03	183	ASP
38	AS04	10	ARG
38	AS04	27	TYR
38	AS04	31	CYS
38	AS04	35	ARG
38	AS04	38	TYR
38	AS04	49	ARG
38	AS04	72	GLU
38	AS04	162	LEU

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Mol	Chain	Res	Type
38	AS04	173	TRP
38	AS04	188	LEU
39	AS05	10	MET
39	AS05	24	ARG
39	AS05	133	TYR
40	AS06	36	ARG
40	AS06	62	TRP
40	AS06	82	ARG
40	AS06	83	ASP
40	AS06	98	LEU
41	AS07	3	ARG
41	AS07	12	LEU
41	AS07	41	ARG
41	AS07	45	ASP
41	AS07	62	PHE
41	AS07	115	ARG
41	AS07	138	LYS
41	AS07	156	TRP
42	AS08	1	MET
42	AS08	14	ARG
42	AS08	41	ARG
42	AS08	50	ARG
42	AS08	60	ARG
42	AS08	84	ARG
42	AS08	102	ARG
42	AS08	112	LEU
42	AS08	121	ASP
42	AS08	136	GLU
43	AS09	4	TYR
43	AS09	10	ARG
43	AS09	18	PHE
43	AS09	36	TYR
43	AS09	51	ARG
43	AS09	60	ASP
43	AS09	66	ARG
43	AS09	88	TYR
43	AS09	97	LYS
43	AS09	111	ARG
43	AS09	124	GLN
43	AS09	126	SER
44	AS10	28	ARG
44	AS10	35	SER

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Mol	Chain	Res	Type
45	AS11	20	TYR
45	AS11	25	TYR
45	AS11	26	ASN
45	AS11	39	PRO
45	AS11	44	SER
46	AS12	19	LYS
46	AS12	26	LEU
47	AS13	32	GLU
47	AS13	92	HIS
47	AS13	93	ARG
48	AS14	24	CYS
48	AS14	29	ARG
48	AS14	35	ARG
48	AS14	43	CYS
48	AS14	61	TRP
49	AS15	5	LYS
49	AS15	26	GLU
49	AS15	57	LEU
49	AS15	65	ARG
49	AS15	68	ARG
49	AS15	74	ASP
49	AS15	79	ARG
49	AS15	88	ARG
50	AS16	1	MET
50	AS16	43	LYS
50	AS16	50	LYS
50	AS16	72	ARG
51	AS17	4	LYS
52	AS18	21	LYS
52	AS18	43	PHE
52	AS18	63	GLN
53	AS19	15	LEU
53	AS19	18	LYS
53	AS19	29	ARG
53	AS19	37	ARG
53	AS19	70	LYS
54	AS20	57	ARG
54	AS20	70	SER
55	ATHX	9	ARG
55	ATHX	10	ARG
55	ATHX	15	ARG
55	ATHX	20	LYS

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Mol	Chain	Res	Type
55	ATHX	22	ARG
4	BL01	7	ARG
4	BL01	8	TYR
4	BL01	38	PHE
4	BL01	53	ARG
4	BL01	80	LYS
4	BL01	132	LEU
4	BL01	173	HIS
4	BL01	197	LEU
4	BL01	201	LYS
4	BL01	209	PHE
4	BL01	211	ARG
4	BL01	219	MET
4	BL01	224	ARG
4	BL01	226	ASN
5	BL02	9	TYR
5	BL02	84	TYR
5	BL02	104	TYR
5	BL02	131	LEU
5	BL02	184	LYS
5	BL02	201	HIS
5	BL02	257	LEU
5	BL02	263	ARG
6	BL03	108	SER
6	BL03	118	LYS
6	BL03	132	HIS
6	BL03	133	LYS
6	BL03	149	ARG
6	BL03	159	HIS
7	BL04	54	ARG
7	BL04	65	TRP
7	BL04	68	LYS
7	BL04	93	LYS
7	BL04	122	LYS
7	BL04	191	ARG
8	BL05	21	ARG
8	BL05	91	ARG
8	BL05	95	ARG
8	BL05	97	ASP
8	BL05	105	LYS
8	BL05	113	ARG
8	BL05	115	ARG

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Mol	Chain	Res	Type
8	BL05	126	ASP
8	BL05	153	ARG
8	BL05	155	MET
8	BL05	156	ASP
8	BL05	181	ARG
9	BL06	6	ARG
9	BL06	32	GLU
9	BL06	41	MET
9	BL06	51	ARG
9	BL06	54	ARG
9	BL06	101	ARG
9	BL06	127	GLU
10	BL09	25	TYR
10	BL09	52	ARG
10	BL09	56	LYS
10	BL09	102	SER
10	BL09	113	ARG
10	BL09	126	TYR
11	BL13	61	HIS
11	BL13	117	HIS
11	BL13	122	LEU
11	BL13	132	LYS
11	BL13	153	HIS
11	BL13	154	GLN
11	BL13	161	LEU
12	BL14	42	SER
13	BL15	13	ASN
13	BL15	16	ARG
13	BL15	40	SER
13	BL15	50	ARG
13	BL15	61	ARG
13	BL15	62	LEU
13	BL15	77	ARG
13	BL15	107	LYS
13	BL15	110	TYR
13	BL15	123	LEU
13	BL15	132	LYS
14	BL16	6	ARG
14	BL16	26	TYR
14	BL16	58	PHE
14	BL16	77	LYS
15	BL17	2	ARG

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Mol	Chain	Res	Type
15	BL17	6	SER
15	BL17	15	SER
15	BL17	33	ARG
15	BL17	60	LEU
15	BL17	81	ASP
15	BL17	105	ARG
16	BL18	12	PHE
16	BL18	25	ARG
16	BL18	42	ASP
16	BL18	59	LYS
16	BL18	61	ASN
16	BL18	67	ARG
16	BL18	80	LEU
17	BL19	23	ARG
17	BL19	29	ARG
17	BL19	39	ARG
17	BL19	53	ARG
17	BL19	65	LYS
17	BL19	80	SER
17	BL19	122	ASP
17	BL19	128	GLU
18	BL20	31	SER
18	BL20	54	LYS
18	BL20	85	LYS
18	BL20	94	ASN
19	BL21	2	PHE
19	BL21	13	ARG
19	BL21	24	LYS
19	BL21	91	TYR
20	BL22	63	ASP
20	BL22	67	ASP
20	BL22	77	ASP
21	BL23	33	LYS
21	BL23	57	LEU
21	BL23	76	ARG
22	BL24	6	HIS
22	BL24	21	LYS
22	BL24	47	LYS
23	BL25	16	SER
23	BL25	19	ARG
23	BL25	35	ARG
23	BL25	70	LEU

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Mol	Chain	Res	Type
23	BL25	72	ARG
23	BL25	81	ARG
23	BL25	104	PHE
23	BL25	129	SER
23	BL25	154	ASP
24	BL27	64	ASP
25	BL28	21	ARG
25	BL28	38	SER
25	BL28	40	ARG
25	BL28	72	GLU
25	BL28	80	LEU
26	BL29	7	ARG
27	BL30	29	ARG
28	BL31	43	TYR
29	BL32	4	HIS
29	BL32	23	HIS
29	BL32	52	TYR
30	BL33	11	LEU
30	BL33	18	ARG
30	BL33	19	ARG
30	BL33	34	LEU
30	BL33	43	CYS
30	BL33	49	HIS
32	BL35	30	ARG
32	BL35	32	LEU
32	BL35	57	ARG
33	BL36	4	ARG
33	BL36	6	SER
36	BS02	24	TRP
36	BS02	25	ASN
36	BS02	30	ARG
36	BS02	40	HIS
36	BS02	53	ARG
36	BS02	57	PHE
36	BS02	137	ARG
36	BS02	148	TYR
36	BS02	154	LEU
36	BS02	205	ASP
37	BS03	37	GLN
37	BS03	48	TYR
37	BS03	58	GLU
37	BS03	79	ARG

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Mol	Chain	Res	Type
37	BS03	98	ASN
37	BS03	139	GLN
38	BS04	31	CYS
38	BS04	38	TYR
38	BS04	47	ARG
38	BS04	73	ARG
38	BS04	93	PHE
38	BS04	113	SER
38	BS04	168	ARG
38	BS04	188	LEU
38	BS04	208	SER
39	BS05	12	LEU
39	BS05	14	ARG
39	BS05	25	ARG
39	BS05	57	LYS
39	BS05	84	PHE
39	BS05	147	ASP
39	BS05	150	ARG
40	BS06	36	ARG
40	BS06	46	ARG
40	BS06	54	LYS
41	BS07	12	LEU
41	BS07	45	ASP
41	BS07	95	ARG
41	BS07	103	TRP
41	BS07	109	ASN
41	BS07	154	TYR
42	BS08	1	MET
42	BS08	50	ARG
42	BS08	85	ARG
42	BS08	102	ARG
42	BS08	112	LEU
43	BS09	9	ARG
43	BS09	31	GLN
43	BS09	36	TYR
43	BS09	113	LYS
43	BS09	121	ARG
44	BS10	3	LYS
44	BS10	9	ARG
44	BS10	12	ASP
44	BS10	22	LYS
44	BS10	43	ARG

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Mol	Chain	Res	Type
44	BS10	58	ASP
45	BS11	11	LYS
45	BS11	44	SER
45	BS11	59	TYR
45	BS11	124	LYS
46	BS12	7	ASN
46	BS12	21	SER
46	BS12	32	ARG
46	BS12	52	ARG
46	BS12	63	TYR
46	BS12	79	HIS
46	BS12	96	ARG
47	BS13	3	ARG
47	BS13	46	LYS
47	BS13	64	TRP
47	BS13	71	ARG
47	BS13	115	LYS
48	BS14	24	CYS
48	BS14	61	TRP
49	BS15	24	SER
49	BS15	38	ARG
50	BS16	61	SER
51	BS17	12	SER
51	BS17	26	GLN
51	BS17	43	LEU
51	BS17	52	LYS
51	BS17	68	ARG
52	BS18	35	ARG
52	BS18	43	PHE
52	BS18	64	ARG
52	BS18	83	GLU
53	BS19	6	LYS
53	BS19	29	ARG
53	BS19	34	TRP
53	BS19	81	ARG
54	BS20	8	ARG
54	BS20	15	ARG
54	BS20	38	LYS
54	BS20	70	SER

Sometimes 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%)	323 (21%)	22 (1%)
1	B16S	1517/1518 (99%)	321 (21%)	26 (1%)
2	A23S	2873/2881 (99%)	617 (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	APTn	75/76 (98%)	40 (53%)	12 (16%)
35	BPTn	75/76 (98%)	56 (74%)	21 (28%)
56	BATn	84/85 (98%)	60 (71%)	10 (11%)
All	All	9277/9307 (99%)	2083 (22%)	168 (1%)

All (2083) 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
1	A16S	39	G
1	A16S	48	C
1	A16S	51	A
1	A16S	64	G
1	A16S	77	G
1	A16S	78(A)	U
1	A16S	101	A
1	A16S	103	C
1	A16S	108	G
1	A16S	109	A
1	A16S	116	A
1	A16S	121	C
1	A16S	122	G
1	A16S	127	G
1	A16S	129(A)	G
1	A16S	130	A
1	A16S	131	C
1	A16S	144	G
1	A16S	151	A
1	A16S	163	C

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Mol	Chain	Res	Type
1	A16S	169	C
1	A16S	186(G)	C
1	A16S	186(I)	U
1	A16S	186(J)	G
1	A16S	186(K)	G
1	A16S	195	A
1	A16S	197	A
1	A16S	200	G
1	A16S	201(B)	U
1	A16S	201(C)	U
1	A16S	220	G
1	A16S	244	U
1	A16S	247	G
1	A16S	251	G
1	A16S	265	G
1	A16S	267	C
1	A16S	281	G
1	A16S	289	G
1	A16S	306	G
1	A16S	324	G
1	A16S	328	C
1	A16S	329	A
1	A16S	332	G
1	A16S	345	C
1	A16S	346	G
1	A16S	347	G
1	A16S	352	C
1	A16S	353	A
1	A16S	354	G
1	A16S	362	G
1	A16S	363	A
1	A16S	366	C
1	A16S	367	U
1	A16S	372	C
1	A16S	373	A
1	A16S	381	C
1	A16S	382	A
1	A16S	384	G
1	A16S	388	G
1	A16S	390	C
1	A16S	397	A
1	A16S	398	C

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Mol	Chain	Res	Type
1	A16S	405	U
1	A16S	406	G
1	A16S	411	A
1	A16S	412	A
1	A16S	413	G
1	A16S	414	A
1	A16S	422	C
1	A16S	423	G
1	A16S	428	G
1	A16S	429	U
1	A16S	430	A
1	A16S	452	A
1	A16S	453	A
1	A16S	458(C)	G
1	A16S	482	A
1	A16S	484	G
1	A16S	485	G
1	A16S	497	A
1	A16S	498	U
1	A16S	508	C
1	A16S	511	C
1	A16S	518	C
1	A16S	519	C
1	A16S	521	G
1	A16S	527	G
1	A16S	531	U
1	A16S	532	A
1	A16S	547	A
1	A16S	559	A
1	A16S	560	U
1	A16S	561	U
1	A16S	563	A
1	A16S	564	C
1	A16S	568	G
1	A16S	572	A
1	A16S	573	A
1	A16S	576	G
1	A16S	577	G
1	A16S	578	C
1	A16S	607	A
1	A16S	609	A
1	A16S	616	G

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Mol	Chain	Res	Type
1	A16S	620	C
1	A16S	629	G
1	A16S	631	G
1	A16S	653	A
1	A16S	661	G
1	A16S	687	A
1	A16S	688	G
1	A16S	695	A
1	A16S	702	A
1	A16S	708	C
1	A16S	721	G
1	A16S	722	A
1	A16S	723	U
1	A16S	724	G
1	A16S	733	A
1	A16S	734	G
1	A16S	748	C
1	A16S	749	C
1	A16S	755	G
1	A16S	790	A
1	A16S	793	U
1	A16S	794	A
1	A16S	799	G
1	A16S	811	C
1	A16S	812	C
1	A16S	814	A
1	A16S	815	A
1	A16S	817	C
1	A16S	819	A
1	A16S	828	A
1	A16S	838(A)	U
1	A16S	838(B)	C
1	A16S	838(C)	U
1	A16S	848	C
1	A16S	855	G
1	A16S	857	C
1	A16S	859	A
1	A16S	867	G
1	A16S	870	U
1	A16S	871	U
1	A16S	872	A
1	A16S	873	A

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Mol	Chain	Res	Type
1	A16S	885	G
1	A16S	897	C
1	A16S	900	A
1	A16S	901	A
1	A16S	902	G
1	A16S	914	A
1	A16S	926	G
1	A16S	927	G
1	A16S	934	C
1	A16S	935	A
1	A16S	958	A
1	A16S	960	U
1	A16S	966	G
1	A16S	968	A
1	A16S	969	A
1	A16S	971	G
1	A16S	974	A
1	A16S	976	G
1	A16S	977	A
1	A16S	978	A
1	A16S	981	U
1	A16S	982	U
1	A16S	991	U
1	A16S	992	U
1	A16S	993	G
1	A16S	1003	G
1	A16S	1004	A
1	A16S	1005	A
1	A16S	1006	C
1	A16S	1014	A
1	A16S	1023	G
1	A16S	1028(B)	C
1	A16S	1028(E)	G
1	A16S	1028(F)	A
1	A16S	1028(G)	G
1	A16S	1043	C
1	A16S	1045	C
1	A16S	1046	A
1	A16S	1053	G
1	A16S	1054	C
1	A16S	1055	A
1	A16S	1064	G

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Mol	Chain	Res	Type
1	A16S	1065	U
1	A16S	1066	C
1	A16S	1070	U
1	A16S	1081	G
1	A16S	1085	U
1	A16S	1092	A
1	A16S	1094	G
1	A16S	1095	U
1	A16S	1101	A
1	A16S	1102	A
1	A16S	1117	G
1	A16S	1124	G
1	A16S	1125	U
1	A16S	1126	U
1	A16S	1129	C
1	A16S	1130	A
1	A16S	1131	G
1	A16S	1135	U
1	A16S	1137	C
1	A16S	1138	G
1	A16S	1139	G
1	A16S	1140	C
1	A16S	1146	A
1	A16S	1148	U
1	A16S	1152	A
1	A16S	1157	A
1	A16S	1158	C
1	A16S	1159	U
1	A16S	1160	G
1	A16S	1164	G
1	A16S	1167	A
1	A16S	1174	G
1	A16S	1175	G
1	A16S	1184	G
1	A16S	1190	G
1	A16S	1191	A
1	A16S	1196	U
1	A16S	1198	G
1	A16S	1200	C
1	A16S	1202	G
1	A16S	1212	U
1	A16S	1213	A

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Mol	Chain	Res	Type
1	A16S	1225	A
1	A16S	1227	A
1	A16S	1228	C
1	A16S	1236	A
1	A16S	1238	A
1	A16S	1240	U
1	A16S	1241	G
1	A16S	1256	A
1	A16S	1257	U
1	A16S	1258	G
1	A16S	1267	C
1	A16S	1270	C
1	A16S	1278	U
1	A16S	1280	A
1	A16S	1283	G
1	A16S	1286	A
1	A16S	1287	A
1	A16S	1288	A
1	A16S	1290	G
1	A16S	1299	A
1	A16S	1300	G
1	A16S	1301	U
1	A16S	1302	U
1	A16S	1305	G
1	A16S	1306	A
1	A16S	1315	U
1	A16S	1317	C
1	A16S	1318	A
1	A16S	1319	A
1	A16S	1320	C
1	A16S	1321	C
1	A16S	1322	C
1	A16S	1323	G
1	A16S	1324	A
1	A16S	1328	C
1	A16S	1329	A
1	A16S	1331	G
1	A16S	1332	A
1	A16S	1340	A
1	A16S	1347	G
1	A16S	1353	G
1	A16S	1357	A

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Mol	Chain	Res	Type
1	A16S	1358	U
1	A16S	1359	C
1	A16S	1361	G
1	A16S	1362	C
1	A16S	1362(A)	C
1	A16S	1363	A
1	A16S	1364	U
1	A16S	1365	G
1	A16S	1374	A
1	A16S	1377	A
1	A16S	1378	C
1	A16S	1379	G
1	A16S	1395	C
1	A16S	1398	A
1	A16S	1400	C
1	A16S	1401	G
1	A16S	1413	A
1	A16S	1419	G
1	A16S	1422	G
1	A16S	1423	G
1	A16S	1440(A)	G
1	A16S	1440(C)	G
1	A16S	1440(D)	A
1	A16S	1440(E)	G
1	A16S	1440(H)	U
1	A16S	1440(J)	C
1	A16S	1440(K)	G
1	A16S	1469	G
1	A16S	1482	G
1	A16S	1493	A
1	A16S	1494	G
1	A16S	1499	A
1	A16S	1502	A
1	A16S	1503	A
1	A16S	1504	G
1	A16S	1505	G
1	A16S	1506	U
1	A16S	1507	A
1	A16S	1517	G
1	A16S	1520	G
1	A16S	1529	G
1	A16S	1530	G

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Mol	Chain	Res	Type
1	A16S	1535	C
1	A16S	1536	C
1	A16S	1537	U
1	A16S	1541	U
2	A23S	10	G
2	A23S	17	G
2	A23S	27	G
2	A23S	34	C
2	A23S	35	G
2	A23S	36	G
2	A23S	46	C
2	A23S	50	U
2	A23S	51	G
2	A23S	61	G
2	A23S	63	U
2	A23S	64	A
2	A23S	71	A
2	A23S	72	U
2	A23S	75	G
2	A23S	84	A
2	A23S	91	A
2	A23S	95	G
2	A23S	98	G
2	A23S	99	U
2	A23S	101	G
2	A23S	102	G
2	A23S	105	C
2	A23S	118	A
2	A23S	119	A
2	A23S	120	U
2	A23S	126	A
2	A23S	131	G
2	A23S	137(B)	G
2	A23S	137(D)	A
2	A23S	137(E)	A
2	A23S	155(A)	U
2	A23S	155(B)	U
2	A23S	155(C)	U
2	A23S	155(D)	U
2	A23S	155(E)	U
2	A23S	172	C
2	A23S	181	A

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Mol	Chain	Res	Type
2	A23S	196	A
2	A23S	197	A
2	A23S	199	A
2	A23S	205	G
2	A23S	215	G
2	A23S	216	A
2	A23S	221	A
2	A23S	222	A
2	A23S	227	A
2	A23S	229	A
2	A23S	230	U
2	A23S	233	A
2	A23S	241	A
2	A23S	245	G
2	A23S	247	G
2	A23S	248	G
2	A23S	250	G
2	A23S	252	G
2	A23S	267	C
2	A23S	269	U
2	A23S	270(M)	U
2	A23S	270(N)	G
2	A23S	270(O)	U
2	A23S	270(P)	C
2	A23S	270(Q)	C
2	A23S	270(Y)	G
2	A23S	271(B)	G
2	A23S	271(C)	U
2	A23S	271(D)	G
2	A23S	271(M)	G
2	A23S	271(Q)	A
2	A23S	271(R)	C
2	A23S	284	C
2	A23S	295	G
2	A23S	302	C
2	A23S	306	U
2	A23S	308	G
2	A23S	320	A
2	A23S	323	G
2	A23S	324	A
2	A23S	329	G
2	A23S	330	A

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Mol	Chain	Res	Type
2	A23S	345	A
2	A23S	346	A
2	A23S	352	G
2	A23S	353	G
2	A23S	357(F)	G
2	A23S	357(L)	A
2	A23S	357(M)	C
2	A23S	357(O)	C
2	A23S	372	G
2	A23S	373	U
2	A23S	379	G
2	A23S	380	U
2	A23S	384	U
2	A23S	386	G
2	A23S	396	G
2	A23S	401	A
2	A23S	404	C
2	A23S	405	U
2	A23S	406	G
2	A23S	411	G
2	A23S	412	A
2	A23S	418	G
2	A23S	423	A
2	A23S	424	G
2	A23S	444	C
2	A23S	451	C
2	A23S	452	G
2	A23S	455	C
2	A23S	457	A
2	A23S	470	A
2	A23S	474	G
2	A23S	481	G
2	A23S	482	A
2	A23S	483	A
2	A23S	504	U
2	A23S	505	A
2	A23S	508	G
2	A23S	509	C
2	A23S	512	G
2	A23S	513	A
2	A23S	526	A
2	A23S	527	C

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Mol	Chain	Res	Type
2	A23S	531	C
2	A23S	532	A
2	A23S	563	G
2	A23S	569	U
2	A23S	571	A
2	A23S	572	A
2	A23S	573	G
2	A23S	574	C
2	A23S	575	A
2	A23S	583	G
2	A23S	587	C
2	A23S	602	G
2	A23S	603	A
2	A23S	610	G
2	A23S	611(E)	G
2	A23S	611(F)	A
2	A23S	611(G)	G
2	A23S	618	C
2	A23S	627	A
2	A23S	637	A
2	A23S	642	G
2	A23S	646	A
2	A23S	650	C
2	A23S	653	C
2	A23S	654	U
2	A23S	655	A
2	A23S	656	G
2	A23S	670	A
2	A23S	671	C
2	A23S	676	A
2	A23S	686	G
2	A23S	730	C
2	A23S	740	U
2	A23S	747	U
2	A23S	748	G
2	A23S	765	G
2	A23S	775	G
2	A23S	776	G
2	A23S	782	A
2	A23S	784	A
2	A23S	785	G
2	A23S	791	C

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Mol	Chain	Res	Type
2	A23S	792	G
2	A23S	798	G
2	A23S	800	A
2	A23S	805	G
2	A23S	812	C
2	A23S	819	A
2	A23S	827	U
2	A23S	828	U
2	A23S	830	G
2	A23S	833	U
2	A23S	846	C
2	A23S	847	U
2	A23S	859	G
2	A23S	860	U
2	A23S	879	G
2	A23S	884	C
2	A23S	886	C
2	A23S	887	A
2	A23S	888	C
2	A23S	889	C
2	A23S	896	A
2	A23S	897	C
2	A23S	910	A
2	A23S	914	C
2	A23S	917	A
2	A23S	919	G
2	A23S	932	G
2	A23S	933	A
2	A23S	941	A
2	A23S	946	G
2	A23S	957	A
2	A23S	961	C
2	A23S	974	G
2	A23S	974(A)	C
2	A23S	983	A
2	A23S	990	A
2	A23S	996	A
2	A23S	1003	G
2	A23S	1008	C
2	A23S	1009	A
2	A23S	1011	G
2	A23S	1012	U

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Mol	Chain	Res	Type
2	A23S	1013	C
2	A23S	1017	G
2	A23S	1020	A
2	A23S	1022	G
2	A23S	1023	U
2	A23S	1025	G
2	A23S	1026	U
2	A23S	1034	G
2	A23S	1041	C
2	A23S	1045	A
2	A23S	1046	A
2	A23S	1047	G
2	A23S	1048	A
2	A23S	1066	U
2	A23S	1067	A
2	A23S	1069	A
2	A23S	1070	A
2	A23S	1071	G
2	A23S	1073	A
2	A23S	1077	A
2	A23S	1078	U
2	A23S	1079	C
2	A23S	1081	U
2	A23S	1082	U
2	A23S	1086	A
2	A23S	1087	G
2	A23S	1088	A
2	A23S	1089	G
2	A23S	1095	A
2	A23S	1097	U
2	A23S	1098	A
2	A23S	1104	C
2	A23S	1112	G
2	A23S	1122	G
2	A23S	1129	A
2	A23S	1130	U
2	A23S	1135	C
2	A23S	1136	G
2	A23S	1155	A
2	A23S	1156	A
2	A23S	1171	G
2	A23S	1173	A

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Mol	Chain	Res	Type
2	A23S	1174	U
2	A23S	1177	A
2	A23S	1195	G
2	A23S	1204	A
2	A23S	1205	U
2	A23S	1210	A
2	A23S	1211	U
2	A23S	1218	C
2	A23S	1220	C
2	A23S	1225	G
2	A23S	1227	G
2	A23S	1236	G
2	A23S	1247	A
2	A23S	1253	A
2	A23S	1256	G
2	A23S	1265	A
2	A23S	1271	G
2	A23S	1272	A
2	A23S	1300	U
2	A23S	1301	A
2	A23S	1302	A
2	A23S	1309	G
2	A23S	1311	G
2	A23S	1314	C
2	A23S	1321	A
2	A23S	1329	U
2	A23S	1341	U
2	A23S	1349	A
2	A23S	1350	C
2	A23S	1352	U
2	A23S	1359	A
2	A23S	1360	A
2	A23S	1364	G
2	A23S	1371	G
2	A23S	1378	A
2	A23S	1379	A
2	A23S	1385	G
2	A23S	1386	C
2	A23S	1392	A
2	A23S	1395	A
2	A23S	1396	U
2	A23S	1416	G

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Mol	Chain	Res	Type
2	A23S	1420	U
2	A23S	1421	G
2	A23S	1427	A
2	A23S	1428	C
2	A23S	1429	G
2	A23S	1441	G
2	A23S	1444(A)	A
2	A23S	1445	C
2	A23S	1453	A
2	A23S	1454	U
2	A23S	1455	G
2	A23S	1460	A
2	A23S	1461	G
2	A23S	1467	C
2	A23S	1468(A)	A
2	A23S	1468(J)	G
2	A23S	1483	G
2	A23S	1490	A
2	A23S	1494	A
2	A23S	1495	A
2	A23S	1497	U
2	A23S	1498	C
2	A23S	1506(B)	A
2	A23S	1506(C)	A
2	A23S	1506(K)	C
2	A23S	1526	G
2	A23S	1533	C
2	A23S	1535	U
2	A23S	1537	C
2	A23S	1538	G
2	A23S	1540	G
2	A23S	1541	U
2	A23S	1542	G
2	A23S	1543	A
2	A23S	1543(A)	C
2	A23S	1544	A
2	A23S	1547	C
2	A23S	1554	A
2	A23S	1558	A
2	A23S	1559	G
2	A23S	1560	G
2	A23S	1566	A

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Mol	Chain	Res	Type
2	A23S	1569	A
2	A23S	1584	C
2	A23S	1595	G
2	A23S	1603	A
2	A23S	1606	G
2	A23S	1607	C
2	A23S	1608	A
2	A23S	1611	C
2	A23S	1617	C
2	A23S	1618	A
2	A23S	1634	A
2	A23S	1639	U
2	A23S	1640	C
2	A23S	1644	C
2	A23S	1646	C
2	A23S	1648	C
2	A23S	1651	G
2	A23S	1665	A
2	A23S	1674	G
2	A23S	1696	G
2	A23S	1698	A
2	A23S	1699	G
2	A23S	1712(H)	A
2	A23S	1712(K)	A
2	A23S	1712(Q)	G
2	A23S	1756	G
2	A23S	1758	G
2	A23S	1762	A
2	A23S	1763	G
2	A23S	1764	G
2	A23S	1773	A
2	A23S	1774	C
2	A23S	1784	A
2	A23S	1786	A
2	A23S	1800	C
2	A23S	1801	G
2	A23S	1802	A
2	A23S	1808	U
2	A23S	1809	A
2	A23S	1815	A
2	A23S	1816	G
2	A23S	1827	C

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Mol	Chain	Res	Type
2	A23S	1829	A
2	A23S	1847	A
2	A23S	1848	A
2	A23S	1853	A
2	A23S	1864(C)	A
2	A23S	1878	G
2	A23S	1883	G
2	A23S	1887	C
2	A23S	1888	G
2	A23S	1903	G
2	A23S	1906	G
2	A23S	1914	C
2	A23S	1927	A
2	A23S	1929	G
2	A23S	1931	U
2	A23S	1936	A
2	A23S	1937	A
2	A23S	1938	A
2	A23S	1939	U
2	A23S	1943	U
2	A23S	1952	A
2	A23S	1953	A
2	A23S	1955	U
2	A23S	1962	C
2	A23S	1963	U
2	A23S	1967	C
2	A23S	1971	A
2	A23S	1972	A
2	A23S	1981	A
2	A23S	1982	C
2	A23S	1991	U
2	A23S	1993	U
2	A23S	1995	U
2	A23S	1996	C
2	A23S	2023	G
2	A23S	2030	A
2	A23S	2031	A
2	A23S	2032	G
2	A23S	2033	A
2	A23S	2043	C
2	A23S	2046	G
2	A23S	2049	G

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Mol	Chain	Res	Type
2	A23S	2052	G
2	A23S	2055	C
2	A23S	2057	A
2	A23S	2058	A
2	A23S	2059	A
2	A23S	2060	A
2	A23S	2061	G
2	A23S	2062	A
2	A23S	2063	C
2	A23S	2068	U
2	A23S	2069	G
2	A23S	2093	G
2	A23S	2094	G
2	A23S	2111	C
2	A23S	2112	G
2	A23S	2116	G
2	A23S	2119	A
2	A23S	2120	G
2	A23S	2124	G
2	A23S	2126	A
2	A23S	2132	U
2	A23S	2133	G
2	A23S	2134	A
2	A23S	2135	A
2	A23S	2136	C
2	A23S	2137	C
2	A23S	2141	G
2	A23S	2142	C
2	A23S	2145	C
2	A23S	2146	C
2	A23S	2149	G
2	A23S	2151	G
2	A23S	2153	G
2	A23S	2155	G
2	A23S	2156	G
2	A23S	2157	G
2	A23S	2158	A
2	A23S	2159	G
2	A23S	2161	C
2	A23S	2171	A
2	A23S	2173	A
2	A23S	2174	C

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Mol	Chain	Res	Type
2	A23S	2177	C
2	A23S	2190	G
2	A23S	2191	G
2	A23S	2198	A
2	A23S	2202(D)	G
2	A23S	2202(E)	A
2	A23S	2202(F)	U
2	A23S	2225	A
2	A23S	2235	G
2	A23S	2236	C
2	A23S	2239	G
2	A23S	2249	U
2	A23S	2254	C
2	A23S	2266	A
2	A23S	2273	A
2	A23S	2275	C
2	A23S	2278	A
2	A23S	2283	C
2	A23S	2286	A
2	A23S	2287	A
2	A23S	2288	A
2	A23S	2304	G
2	A23S	2305	A
2	A23S	2306	C
2	A23S	2307	G
2	A23S	2311	A
2	A23S	2312	U
2	A23S	2320	A
2	A23S	2327	A
2	A23S	2333	A
2	A23S	2334	G
2	A23S	2336	A
2	A23S	2338	G
2	A23S	2346	A
2	A23S	2347	C
2	A23S	2350	C
2	A23S	2358	G
2	A23S	2361	A
2	A23S	2377	A
2	A23S	2379	G
2	A23S	2383	G
2	A23S	2385	C

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Mol	Chain	Res	Type
2	A23S	2391	G
2	A23S	2392	A
2	A23S	2402	C
2	A23S	2406	U
2	A23S	2422	A
2	A23S	2423	U
2	A23S	2426	A
2	A23S	2428	G
2	A23S	2429	G
2	A23S	2430	A
2	A23S	2432	A
2	A23S	2434	A
2	A23S	2435	A
2	A23S	2439	A
2	A23S	2441	C
2	A23S	2447	G
2	A23S	2448	A
2	A23S	2452	C
2	A23S	2465	C
2	A23S	2470	G
2	A23S	2473	U
2	A23S	2475	C
2	A23S	2476	A
2	A23S	2478	A
2	A23S	2482	G
2	A23S	2484	G
2	A23S	2494	G
2	A23S	2498	C
2	A23S	2501	C
2	A23S	2502	G
2	A23S	2503	A
2	A23S	2505	G
2	A23S	2506	U
2	A23S	2507	C
2	A23S	2520	C
2	A23S	2529	G
2	A23S	2531	A
2	A23S	2542	A
2	A23S	2543	G
2	A23S	2553	G
2	A23S	2554	U
2	A23S	2555	U

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Mol	Chain	Res	Type
2	A23S	2562	U
2	A23S	2566	A
2	A23S	2567	G
2	A23S	2572	A
2	A23S	2573	C
2	A23S	2574	G
2	A23S	2578	G
2	A23S	2581	G
2	A23S	2582	G
2	A23S	2584	U
2	A23S	2585	U
2	A23S	2586	C
2	A23S	2596	U
2	A23S	2603	G
2	A23S	2610	C
2	A23S	2611	U
2	A23S	2612	C
2	A23S	2630	G
2	A23S	2639	A
2	A23S	2645	G
2	A23S	2646	C
2	A23S	2655	G
2	A23S	2661	G
2	A23S	2665	A
2	A23S	2682	U
2	A23S	2689	U
2	A23S	2690	C
2	A23S	2691	C
2	A23S	2702	U
2	A23S	2703	C
2	A23S	2712	U
2	A23S	2712(A)	A
2	A23S	2713	A
2	A23S	2714	G
2	A23S	2720	U
2	A23S	2722	G
2	A23S	2726	U
2	A23S	2732	G
2	A23S	2733	A
2	A23S	2744	G
2	A23S	2752	C
2	A23S	2757	A

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Mol	Chain	Res	Type
2	A23S	2765	A
2	A23S	2766	G
2	A23S	2778	A
2	A23S	2779	U
2	A23S	2780	G
2	A23S	2789	C
2	A23S	2790	A
2	A23S	2791	C
2	A23S	2792	G
2	A23S	2794	C
2	A23S	2794(B)	U
2	A23S	2794(D)	A
2	A23S	2807	G
2	A23S	2808	U
2	A23S	2818	G
2	A23S	2820	A
2	A23S	2821	A
2	A23S	2824	C
2	A23S	2833	G
2	A23S	2834	G
2	A23S	2835	A
2	A23S	2848	G
2	A23S	2849	U
2	A23S	2850	A
2	A23S	2858	C
2	A23S	2861	G
2	A23S	2864	G
2	A23S	2866	U
2	A23S	2872	G
2	A23S	2880	C
2	A23S	2886	G
2	A23S	2894	G
2	A23S	2895	U
3	A5S	12	C
3	A5S	13	A
3	A5S	14	U
3	A5S	15	A
3	A5S	16	G
3	A5S	24	G
3	A5S	34	U
3	A5S	35	U
3	A5S	41	U

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Mol	Chain	Res	Type
3	A5S	42	C
3	A5S	44	G
3	A5S	52	A
3	A5S	53	A
3	A5S	63	G
3	A5S	66	A
3	A5S	67	G
3	A5S	73	A
3	A5S	82	G
3	A5S	88	C
3	A5S	89(A)	G
3	A5S	89(B)	A
3	A5S	98	G
3	A5S	109	G
34	AMRN	8	A
34	AMRN	10	G
34	AMRN	16	G
34	AMRN	17	U
34	AMRN	18	A
35	APTN	3	G
35	APTN	4	U
35	APTN	5	G
35	APTN	6	A
35	APTN	7	U
35	APTN	9	A
35	APTN	10	G
35	APTN	12	U
35	APTN	13	C
35	APTN	15	G
35	APTN	16	C
35	APTN	17	U
35	APTN	18	G
35	APTN	19	G
35	APTN	20	G
35	APTN	21	A
35	APTN	23	A
35	APTN	24	G
35	APTN	25	C
35	APTN	29	U
35	APTN	30	C
35	APTN	32	C
35	APTN	33	U

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Mol	Chain	Res	Type
35	APTN	34	CM0
35	APTN	36	C
35	APTN	38	A
35	APTN	41	A
35	APTN	44	G
35	APTN	45	G
35	APTN	46	G7M
35	APTN	47	U
35	APTN	48	C
35	APTN	50	G
35	APTN	53	G
35	APTN	65	C
35	APTN	68	C
35	APTN	72	C
35	APTN	73	A
35	APTN	74	C
35	APTN	75	C
1	B16S	4	U
1	B16S	5	U
1	B16S	6	G
1	B16S	7	G
1	B16S	9	G
1	B16S	31	G
1	B16S	32	A
1	B16S	33	A
1	B16S	39	G
1	B16S	47	C
1	B16S	48	C
1	B16S	50	A
1	B16S	51	A
1	B16S	54	C
1	B16S	58	C
1	B16S	76	G
1	B16S	78(A)	U
1	B16S	78(E)	A
1	B16S	91	C
1	B16S	101	A
1	B16S	116	A
1	B16S	121	C
1	B16S	122	G
1	B16S	130	A
1	B16S	131	C

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Mol	Chain	Res	Type
1	B16S	147	G
1	B16S	160	A
1	B16S	161	A
1	B16S	163	C
1	B16S	173	U
1	B16S	186(F)	C
1	B16S	186(G)	C
1	B16S	186(H)	U
1	B16S	186(I)	U
1	B16S	186(J)	G
1	B16S	197	A
1	B16S	201(C)	U
1	B16S	216	G
1	B16S	220	G
1	B16S	231	G
1	B16S	245	C
1	B16S	247	G
1	B16S	251	G
1	B16S	252	U
1	B16S	261	U
1	B16S	262	A
1	B16S	266	G
1	B16S	267	C
1	B16S	268	C
1	B16S	280	C
1	B16S	281	G
1	B16S	283	C
1	B16S	289	G
1	B16S	327	A
1	B16S	328	C
1	B16S	329	A
1	B16S	332	G
1	B16S	345	C
1	B16S	348	G
1	B16S	352	C
1	B16S	353	A
1	B16S	354	G
1	B16S	362	G
1	B16S	363	A
1	B16S	367	U
1	B16S	372	C
1	B16S	381	C

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Mol	Chain	Res	Type
1	B16S	389	A
1	B16S	392	G
1	B16S	397	A
1	B16S	398	C
1	B16S	403	C
1	B16S	406	G
1	B16S	411	A
1	B16S	412	A
1	B16S	413	G
1	B16S	414	A
1	B16S	421	U
1	B16S	422	C
1	B16S	424	G
1	B16S	429	U
1	B16S	430	A
1	B16S	440	A
1	B16S	452	A
1	B16S	453	A
1	B16S	455	C
1	B16S	458(B)	A
1	B16S	458(C)	G
1	B16S	481	G
1	B16S	482	A
1	B16S	484	G
1	B16S	485	G
1	B16S	497	A
1	B16S	498	U
1	B16S	499	A
1	B16S	509	A
1	B16S	510	A
1	B16S	511	C
1	B16S	518	C
1	B16S	519	C
1	B16S	521	G
1	B16S	527	G
1	B16S	532	A
1	B16S	533	A
1	B16S	534	U
1	B16S	535	A
1	B16S	536	C
1	B16S	547	A
1	B16S	559	A

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Mol	Chain	Res	Type
1	B16S	560	U
1	B16S	562	C
1	B16S	566	G
1	B16S	573	A
1	B16S	576	G
1	B16S	577	G
1	B16S	596	C
1	B16S	604	G
1	B16S	631	G
1	B16S	632	A
1	B16S	653	A
1	B16S	661	G
1	B16S	666	G
1	B16S	687	A
1	B16S	688	G
1	B16S	695	A
1	B16S	702	A
1	B16S	721	G
1	B16S	722	A
1	B16S	723	U
1	B16S	733	A
1	B16S	748	C
1	B16S	749	C
1	B16S	755	G
1	B16S	773	G
1	B16S	777	A
1	B16S	793	U
1	B16S	794	A
1	B16S	815	A
1	B16S	816	A
1	B16S	817	C
1	B16S	819	A
1	B16S	828	A
1	B16S	838(A)	U
1	B16S	838(B)	C
1	B16S	838(C)	U
1	B16S	848	C
1	B16S	859	A
1	B16S	872	A
1	B16S	876	G
1	B16S	885	G
1	B16S	899	C

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Mol	Chain	Res	Type
1	B16S	902	G
1	B16S	914	A
1	B16S	927	G
1	B16S	930	C
1	B16S	934	C
1	B16S	935	A
1	B16S	936	C
1	B16S	942	G
1	B16S	960	U
1	B16S	961	U
1	B16S	966	G
1	B16S	969	A
1	B16S	971	G
1	B16S	974	A
1	B16S	975	A
1	B16S	976	G
1	B16S	978	A
1	B16S	980	C
1	B16S	981	U
1	B16S	989	C
1	B16S	991	U
1	B16S	992	U
1	B16S	993	G
1	B16S	998	G
1	B16S	999	U
1	B16S	1003	G
1	B16S	1004	A
1	B16S	1012	U
1	B16S	1015	A
1	B16S	1016	A
1	B16S	1021	G
1	B16S	1024	G
1	B16S	1025	U
1	B16S	1028(B)	C
1	B16S	1028(F)	A
1	B16S	1044	A
1	B16S	1045	C
1	B16S	1050	G
1	B16S	1053	G
1	B16S	1054	C
1	B16S	1055	A
1	B16S	1064	G

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Mol	Chain	Res	Type
1	B16S	1065	U
1	B16S	1066	C
1	B16S	1078	U
1	B16S	1080	A
1	B16S	1081	G
1	B16S	1086	U
1	B16S	1089	G
1	B16S	1090	U
1	B16S	1094	G
1	B16S	1095	U
1	B16S	1101	A
1	B16S	1102	A
1	B16S	1108	G
1	B16S	1115	C
1	B16S	1118	C
1	B16S	1125	U
1	B16S	1126	U
1	B16S	1129	C
1	B16S	1130	A
1	B16S	1135	U
1	B16S	1136	U
1	B16S	1137	C
1	B16S	1138	G
1	B16S	1139	G
1	B16S	1140	C
1	B16S	1146	A
1	B16S	1147	C
1	B16S	1152	A
1	B16S	1158	C
1	B16S	1159	U
1	B16S	1160	G
1	B16S	1167	A
1	B16S	1169	A
1	B16S	1178	G
1	B16S	1181	G
1	B16S	1184	G
1	B16S	1190	G
1	B16S	1196	U
1	B16S	1202	G
1	B16S	1212	U
1	B16S	1213	A
1	B16S	1214	C

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Mol	Chain	Res	Type
1	B16S	1219	U
1	B16S	1225	A
1	B16S	1226	C
1	B16S	1227	A
1	B16S	1232	U
1	B16S	1238	A
1	B16S	1240	U
1	B16S	1250	A
1	B16S	1256	A
1	B16S	1257	U
1	B16S	1258	G
1	B16S	1260	C
1	B16S	1267	C
1	B16S	1268	A
1	B16S	1269	A
1	B16S	1278	U
1	B16S	1280	A
1	B16S	1281	U
1	B16S	1282	C
1	B16S	1286	A
1	B16S	1287	A
1	B16S	1290	G
1	B16S	1297	C
1	B16S	1299	A
1	B16S	1300	G
1	B16S	1301	U
1	B16S	1302	U
1	B16S	1303	C
1	B16S	1305	G
1	B16S	1317	C
1	B16S	1319	A
1	B16S	1320	C
1	B16S	1322	C
1	B16S	1323	G
1	B16S	1324	A
1	B16S	1325	C
1	B16S	1331	G
1	B16S	1332	A
1	B16S	1338	G
1	B16S	1346	A
1	B16S	1347	G
1	B16S	1348	U

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Mol	Chain	Res	Type
1	B16S	1353	G
1	B16S	1359	C
1	B16S	1360	A
1	B16S	1361	G
1	B16S	1362(A)	C
1	B16S	1363	A
1	B16S	1364	U
1	B16S	1365	G
1	B16S	1368	G
1	B16S	1370	G
1	B16S	1378	C
1	B16S	1379	G
1	B16S	1398	A
1	B16S	1419	G
1	B16S	1422	G
1	B16S	1429	C
1	B16S	1440(C)	G
1	B16S	1440(D)	A
1	B16S	1440(E)	G
1	B16S	1440(I)	A
1	B16S	1440(J)	C
1	B16S	1440(K)	G
1	B16S	1487	G
1	B16S	1492	A
1	B16S	1493	A
1	B16S	1494	G
1	B16S	1497	G
1	B16S	1502	A
1	B16S	1503	A
1	B16S	1504	G
1	B16S	1505	G
1	B16S	1506	U
1	B16S	1517	G
1	B16S	1520	G
1	B16S	1525	G
1	B16S	1529	G
1	B16S	1530	G
1	B16S	1534	A
1	B16S	1535	C
1	B16S	1536	C
1	B16S	1537	U
1	B16S	1538	C

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Mol	Chain	Res	Type
1	B16S	1540	U
1	B16S	1541	U
2	B23S	9	U
2	B23S	14	A
2	B23S	15	G
2	B23S	25	U
2	B23S	26	G
2	B23S	30	G
2	B23S	34	C
2	B23S	35	G
2	B23S	43	G
2	B23S	46	C
2	B23S	50	U
2	B23S	58	G
2	B23S	61	G
2	B23S	63	U
2	B23S	64	A
2	B23S	71	A
2	B23S	74	A
2	B23S	75	G
2	B23S	79	G
2	B23S	90	U
2	B23S	91	A
2	B23S	93	C
2	B23S	96	G
2	B23S	101	G
2	B23S	102	G
2	B23S	104	U
2	B23S	118	A
2	B23S	120	U
2	B23S	121	G
2	B23S	127	A
2	B23S	131	G
2	B23S	137(B)	G
2	B23S	137(D)	A
2	B23S	149	A
2	B23S	155(A)	U
2	B23S	155(B)	U
2	B23S	155(C)	U
2	B23S	155(D)	U
2	B23S	155(E)	U
2	B23S	196	A

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Mol	Chain	Res	Type
2	B23S	199	A
2	B23S	204	A
2	B23S	205	G
2	B23S	212	G
2	B23S	216	A
2	B23S	221	A
2	B23S	222	A
2	B23S	225	A
2	B23S	227	A
2	B23S	228	A
2	B23S	229	A
2	B23S	233	A
2	B23S	241	A
2	B23S	248	G
2	B23S	252	G
2	B23S	270(D)	C
2	B23S	270(L)	U
2	B23S	270(M)	U
2	B23S	270(N)	G
2	B23S	270(O)	U
2	B23S	270(Q)	C
2	B23S	270(T)	G
2	B23S	270(Y)	G
2	B23S	270(Z)	U
2	B23S	271(C)	U
2	B23S	271(D)	G
2	B23S	271(M)	G
2	B23S	271(N)	G
2	B23S	271(O)	A
2	B23S	271(Q)	A
2	B23S	271(R)	C
2	B23S	294	A
2	B23S	302	C
2	B23S	310	A
2	B23S	311	A
2	B23S	324	A
2	B23S	325	G
2	B23S	329	G
2	B23S	330	A
2	B23S	332	A
2	B23S	333	G
2	B23S	352	G

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Mol	Chain	Res	Type
2	B23S	353	G
2	B23S	357(B)	A
2	B23S	357(F)	G
2	B23S	357(L)	A
2	B23S	371	A
2	B23S	372	G
2	B23S	380	U
2	B23S	381	G
2	B23S	386	G
2	B23S	387	U
2	B23S	396	G
2	B23S	400	G
2	B23S	401	A
2	B23S	403	U
2	B23S	404	C
2	B23S	405	U
2	B23S	411	G
2	B23S	435	C
2	B23S	444	C
2	B23S	451	C
2	B23S	456	C
2	B23S	457	A
2	B23S	458	G
2	B23S	464	U
2	B23S	467	G
2	B23S	470	A
2	B23S	473	G
2	B23S	481	G
2	B23S	482	A
2	B23S	489	G
2	B23S	504	U
2	B23S	505	A
2	B23S	506	G
2	B23S	508	G
2	B23S	509	C
2	B23S	518	G
2	B23S	528	A
2	B23S	530	G
2	B23S	531	C
2	B23S	532	A
2	B23S	533	G
2	B23S	543(B)	C

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Mol	Chain	Res	Type
2	B23S	563	G
2	B23S	571	A
2	B23S	574	C
2	B23S	575	A
2	B23S	599	G
2	B23S	602	G
2	B23S	603	A
2	B23S	611(E)	G
2	B23S	611(G)	G
2	B23S	617	G
2	B23S	618	C
2	B23S	627	A
2	B23S	637	A
2	B23S	645	C
2	B23S	646	A
2	B23S	651	G
2	B23S	653	C
2	B23S	654	U
2	B23S	655	A
2	B23S	656	G
2	B23S	668	G
2	B23S	670	A
2	B23S	671	C
2	B23S	677	A
2	B23S	682	G
2	B23S	686	G
2	B23S	695	G
2	B23S	717	G
2	B23S	724	U
2	B23S	726	G
2	B23S	730	C
2	B23S	738	G
2	B23S	747	U
2	B23S	749	C
2	B23S	750	A
2	B23S	757	U
2	B23S	765	G
2	B23S	771	G
2	B23S	776	G
2	B23S	782	A
2	B23S	783	A
2	B23S	784	A

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Mol	Chain	Res	Type
2	B23S	785	G
2	B23S	790	C
2	B23S	791	C
2	B23S	792	G
2	B23S	800	A
2	B23S	805	G
2	B23S	812	C
2	B23S	819	A
2	B23S	826	U
2	B23S	827	U
2	B23S	828	U
2	B23S	830	G
2	B23S	846	C
2	B23S	847	U
2	B23S	859	G
2	B23S	860	U
2	B23S	866	A
2	B23S	869	G
2	B23S	880	G
2	B23S	886	C
2	B23S	887	A
2	B23S	888	C
2	B23S	889	C
2	B23S	894	C
2	B23S	895	U
2	B23S	896	A
2	B23S	910	A
2	B23S	915	C
2	B23S	917	A
2	B23S	932	G
2	B23S	933	A
2	B23S	941	A
2	B23S	946	G
2	B23S	953	A
2	B23S	957	A
2	B23S	958	U
2	B23S	959	A
2	B23S	961	C
2	B23S	962	G
2	B23S	973	A
2	B23S	974	G
2	B23S	974(A)	C

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Mol	Chain	Res	Type
2	B23S	982	C
2	B23S	983	A
2	B23S	990	A
2	B23S	995	C
2	B23S	996	A
2	B23S	1003	G
2	B23S	1008	C
2	B23S	1009	A
2	B23S	1011	G
2	B23S	1012	U
2	B23S	1013	C
2	B23S	1020	A
2	B23S	1022	G
2	B23S	1023	U
2	B23S	1025	G
2	B23S	1026	U
2	B23S	1033	U
2	B23S	1039	G
2	B23S	1045	A
2	B23S	1047	G
2	B23S	1048	A
2	B23S	1057	A
2	B23S	1059	G
2	B23S	1060	U
2	B23S	1061	U
2	B23S	1062	G
2	B23S	1063	G
2	B23S	1065	U
2	B23S	1067	A
2	B23S	1068	G
2	B23S	1069	A
2	B23S	1070	A
2	B23S	1071	G
2	B23S	1074	G
2	B23S	1077	A
2	B23S	1079	C
2	B23S	1083	U
2	B23S	1086	A
2	B23S	1087	G
2	B23S	1088	A
2	B23S	1090	U
2	B23S	1094	U

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Mol	Chain	Res	Type
2	B23S	1095	A
2	B23S	1096	A
2	B23S	1097	U
2	B23S	1100	C
2	B23S	1101	U
2	B23S	1102	C
2	B23S	1109	C
2	B23S	1110	G
2	B23S	1112	G
2	B23S	1126	A
2	B23S	1129	A
2	B23S	1130	U
2	B23S	1135	C
2	B23S	1136	G
2	B23S	1155	A
2	B23S	1173	A
2	B23S	1174	U
2	B23S	1177	A
2	B23S	1205	U
2	B23S	1206	G
2	B23S	1211	U
2	B23S	1212	G
2	B23S	1220	C
2	B23S	1224	C
2	B23S	1225	G
2	B23S	1229	G
2	B23S	1236	G
2	B23S	1237	A
2	B23S	1253	A
2	B23S	1255	U
2	B23S	1256	G
2	B23S	1265	A
2	B23S	1272	A
2	B23S	1273	U
2	B23S	1300	U
2	B23S	1301	A
2	B23S	1312	U
2	B23S	1314	C
2	B23S	1321	A
2	B23S	1329	U
2	B23S	1331	A
2	B23S	1332	G

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Mol	Chain	Res	Type
2	B23S	1333	C
2	B23S	1341	U
2	B23S	1345	C
2	B23S	1349	A
2	B23S	1358	G
2	B23S	1359	A
2	B23S	1365	A
2	B23S	1366	A
2	B23S	1378	A
2	B23S	1379	A
2	B23S	1380	G
2	B23S	1384	A
2	B23S	1385	G
2	B23S	1395	A
2	B23S	1396	U
2	B23S	1416	G
2	B23S	1418	G
2	B23S	1424	G
2	B23S	1427	A
2	B23S	1428	C
2	B23S	1437	C
2	B23S	1444(A)	A
2	B23S	1455	G
2	B23S	1458	C
2	B23S	1460	A
2	B23S	1467	C
2	B23S	1483	G
2	B23S	1490	A
2	B23S	1491	G
2	B23S	1493	C
2	B23S	1494	A
2	B23S	1495	A
2	B23S	1497	U
2	B23S	1506(P)	U
2	B23S	1534	G
2	B23S	1537	C
2	B23S	1538	G
2	B23S	1540	G
2	B23S	1542	G
2	B23S	1543	A
2	B23S	1544	A
2	B23S	1557	C

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Mol	Chain	Res	Type
2	B23S	1558	A
2	B23S	1566	A
2	B23S	1569	A
2	B23S	1584	C
2	B23S	1586	A
2	B23S	1599	C
2	B23S	1607	C
2	B23S	1608	A
2	B23S	1610	A
2	B23S	1615	C
2	B23S	1616	A
2	B23S	1618	A
2	B23S	1640	C
2	B23S	1644	C
2	B23S	1646	C
2	B23S	1648	C
2	B23S	1664	A
2	B23S	1674	G
2	B23S	1681	G
2	B23S	1693	U
2	B23S	1695	G
2	B23S	1696	G
2	B23S	1697	G
2	B23S	1703	G
2	B23S	1712(A)	U
2	B23S	1712(F)	U
2	B23S	1712(H)	A
2	B23S	1712(I)	U
2	B23S	1712(J)	G
2	B23S	1712(K)	A
2	B23S	1712(P)	C
2	B23S	1756	G
2	B23S	1757	U
2	B23S	1763	G
2	B23S	1764	G
2	B23S	1770	G
2	B23S	1773	A
2	B23S	1781	C
2	B23S	1782	C
2	B23S	1786	A
2	B23S	1787	A
2	B23S	1800	C

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Mol	Chain	Res	Type
2	B23S	1801	G
2	B23S	1808	U
2	B23S	1811	G
2	B23S	1815	A
2	B23S	1816	G
2	B23S	1817	G
2	B23S	1829	A
2	B23S	1835	G
2	B23S	1847	A
2	B23S	1862	G
2	B23S	1863	G
2	B23S	1864	U
2	B23S	1878	G
2	B23S	1888	G
2	B23S	1900	A
2	B23S	1903	G
2	B23S	1906	G
2	B23S	1909	C
2	B23S	1910	G
2	B23S	1913	A
2	B23S	1914	C
2	B23S	1929	G
2	B23S	1930	G
2	B23S	1931	U
2	B23S	1936	A
2	B23S	1937	A
2	B23S	1938	A
2	B23S	1941	C
2	B23S	1942	C
2	B23S	1943	U
2	B23S	1952	A
2	B23S	1955	U
2	B23S	1962	C
2	B23S	1963	U
2	B23S	1967	C
2	B23S	1970	A
2	B23S	1971	A
2	B23S	1972	A
2	B23S	1975	G
2	B23S	1991	U
2	B23S	1993	U
2	B23S	1996	C

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Mol	Chain	Res	Type
2	B23S	2005	A
2	B23S	2013	A
2	B23S	2022	U
2	B23S	2023	G
2	B23S	2030	A
2	B23S	2031	A
2	B23S	2033	A
2	B23S	2036	C
2	B23S	2043	C
2	B23S	2054	A
2	B23S	2055	C
2	B23S	2056	G
2	B23S	2059	A
2	B23S	2060	A
2	B23S	2061	G
2	B23S	2063	C
2	B23S	2069	G
2	B23S	2092	U
2	B23S	2093	G
2	B23S	2111	C
2	B23S	2112	G
2	B23S	2116	G
2	B23S	2117	A
2	B23S	2118	U
2	B23S	2119	A
2	B23S	2120	G
2	B23S	2126	A
2	B23S	2127	G
2	B23S	2130	U
2	B23S	2131	G
2	B23S	2132	U
2	B23S	2133	G
2	B23S	2134	A
2	B23S	2135	A
2	B23S	2144	U
2	B23S	2145	C
2	B23S	2148	G
2	B23S	2149	G
2	B23S	2151	G
2	B23S	2155	G
2	B23S	2159	G
2	B23S	2172	U

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Mol	Chain	Res	Type
2	B23S	2173	A
2	B23S	2185	C
2	B23S	2187	G
2	B23S	2190	G
2	B23S	2199	A
2	B23S	2202(C)	G
2	B23S	2202(D)	G
2	B23S	2202(E)	A
2	B23S	2202(F)	U
2	B23S	2202(G)	G
2	B23S	2226	C
2	B23S	2238	G
2	B23S	2239	G
2	B23S	2240	C
2	B23S	2266	A
2	B23S	2269	A
2	B23S	2275	C
2	B23S	2276	G
2	B23S	2279	G
2	B23S	2283	C
2	B23S	2287	A
2	B23S	2302	G
2	B23S	2305	A
2	B23S	2306	C
2	B23S	2307	G
2	B23S	2312	U
2	B23S	2320	A
2	B23S	2321	G
2	B23S	2325	G
2	B23S	2327	A
2	B23S	2334	G
2	B23S	2336	A
2	B23S	2345	G
2	B23S	2346	A
2	B23S	2347	C
2	B23S	2350	C
2	B23S	2354	G
2	B23S	2358	G
2	B23S	2361	A
2	B23S	2379	G
2	B23S	2383	G
2	B23S	2385	C

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Mol	Chain	Res	Type
2	B23S	2391	G
2	B23S	2392	A
2	B23S	2402	C
2	B23S	2403	C
2	B23S	2406	U
2	B23S	2412	A
2	B23S	2422	A
2	B23S	2423	U
2	B23S	2425	A
2	B23S	2426	A
2	B23S	2428	G
2	B23S	2429	G
2	B23S	2430	A
2	B23S	2432	A
2	B23S	2439	A
2	B23S	2441	C
2	B23S	2448	A
2	B23S	2450	A
2	B23S	2470	G
2	B23S	2472	G
2	B23S	2475	C
2	B23S	2476	A
2	B23S	2477	C
2	B23S	2478	A
2	B23S	2482	G
2	B23S	2498	C
2	B23S	2502	G
2	B23S	2504	U
2	B23S	2506	U
2	B23S	2513	G
2	B23S	2518	A
2	B23S	2534	A
2	B23S	2542	A
2	B23S	2543	G
2	B23S	2553	G
2	B23S	2554	U
2	B23S	2556	C
2	B23S	2564	A
2	B23S	2566	A
2	B23S	2567	G
2	B23S	2572	A
2	B23S	2573	C

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Mol	Chain	Res	Type
2	B23S	2574	G
2	B23S	2576	G
2	B23S	2577	A
2	B23S	2578	G
2	B23S	2582	G
2	B23S	2585	U
2	B23S	2586	C
2	B23S	2602	A
2	B23S	2612	C
2	B23S	2629	A
2	B23S	2630	G
2	B23S	2639	A
2	B23S	2646	C
2	B23S	2654	A
2	B23S	2660	A
2	B23S	2661	G
2	B23S	2662	A
2	B23S	2665	A
2	B23S	2679	A
2	B23S	2682	U
2	B23S	2689	U
2	B23S	2690	C
2	B23S	2691	C
2	B23S	2702	U
2	B23S	2703	C
2	B23S	2712	U
2	B23S	2712(A)	A
2	B23S	2713	A
2	B23S	2714	G
2	B23S	2720	U
2	B23S	2726	U
2	B23S	2733	A
2	B23S	2750	A
2	B23S	2751	G
2	B23S	2752	C
2	B23S	2757	A
2	B23S	2765	A
2	B23S	2766	G
2	B23S	2775	A
2	B23S	2778	A
2	B23S	2779	U
2	B23S	2789	C

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Mol	Chain	Res	Type
2	B23S	2790	A
2	B23S	2791	C
2	B23S	2792	G
2	B23S	2794(B)	U
2	B23S	2794(E)	A
2	B23S	2811	G
2	B23S	2818	G
2	B23S	2820	A
2	B23S	2821	A
2	B23S	2825	G
2	B23S	2832	U
2	B23S	2833	G
2	B23S	2835	A
2	B23S	2836	U
2	B23S	2849	U
2	B23S	2858	C
2	B23S	2859	G
2	B23S	2861	G
2	B23S	2871	C
2	B23S	2872	G
2	B23S	2880	C
2	B23S	2886	G
2	B23S	2894	G
2	B23S	2895	U
3	B5S	9	G
3	B5S	12	C
3	B5S	13	A
3	B5S	15	A
3	B5S	16	G
3	B5S	41	U
3	B5S	42	C
3	B5S	44	G
3	B5S	53	A
3	B5S	67	G
3	B5S	73	A
3	B5S	109	G
56	BATN	3	U
56	BATN	4	G
56	BATN	6	G
56	BATN	7	G
56	BATN	8	U
56	BATN	9	U

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Mol	Chain	Res	Type
56	BATN	10	C
56	BATN	11	C
56	BATN	12	C
56	BATN	13	G
56	BATN	14	A
56	BATN	15	G
56	BATN	16	C
56	BATN	18	G
56	BATN	19	G
56	BATN	20	C
56	BATN	20(A)	C
56	BATN	21	A
56	BATN	22	A
56	BATN	23	G
56	BATN	24	G
56	BATN	25	G
56	BATN	26	A
56	BATN	27	G
56	BATN	29	A
56	BATN	30	G
56	BATN	32	C
56	BATN	33	U
56	BATN	34	QUO
56	BATN	35	U
56	BATN	36	A
56	BATN	37	MIA
56	BATN	38	A
56	BATN	40	C
56	BATN	41	U
56	BATN	44	C
56	BATN	45	G
56	BATN	46	U
56	BATN	47	C
56	BATN	47(A)	A
56	BATN	47(B)	U
56	BATN	47(C)	C
56	BATN	47(D)	G
56	BATN	47(F)	C
56	BATN	47(G)	U
56	BATN	49	G
56	BATN	51	A
56	BATN	53	G

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Mol	Chain	Res	Type
56	BATN	55	PSU
56	BATN	59	A
56	BATN	60	U
56	BATN	61	C
56	BATN	63	U
56	BATN	64	U
56	BATN	66	C
56	BATN	69	C
56	BATN	70	A
56	BATN	71	C
56	BATN	73	A
56	BATN	74	C
34	BMRN	5	A
34	BMRN	6	G
34	BMRN	7	G
34	BMRN	8	A
34	BMRN	9	G
34	BMRN	10	G
34	BMRN	11	U
34	BMRN	12	A
34	BMRN	13	A
34	BMRN	14	A
34	BMRN	15	A
34	BMRN	16	G
34	BMRN	17	U
34	BMRN	18	A
34	BMRN	19	U
34	BMRN	20	A
35	BPTN	4	U
35	BPTN	5	G
35	BPTN	6	A
35	BPTN	7	U
35	BPTN	8	4SU
35	BPTN	9	A
35	BPTN	10	G
35	BPTN	11	C
35	BPTN	12	U
35	BPTN	13	C
35	BPTN	14	A
35	BPTN	15	G
35	BPTN	16	C
35	BPTN	17	U

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Mol	Chain	Res	Type
35	BPTN	18	G
35	BPTN	19	G
35	BPTN	20	G
35	BPTN	21	A
35	BPTN	22	G
35	BPTN	23	A
35	BPTN	24	G
35	BPTN	25	C
35	BPTN	29	U
35	BPTN	30	C
35	BPTN	31	C
35	BPTN	32	C
35	BPTN	33	U
35	BPTN	34	CM0
35	BPTN	35	A
35	BPTN	36	C
35	BPTN	38	A
35	BPTN	39	G
35	BPTN	41	A
35	BPTN	43	G
35	BPTN	44	G
35	BPTN	45	G
35	BPTN	46	G7M
35	BPTN	47	U
35	BPTN	48	C
35	BPTN	49	G
35	BPTN	50	G
35	BPTN	52	G
35	BPTN	53	G
35	BPTN	57	G
35	BPTN	59	U
35	BPTN	61	C
35	BPTN	62	C
35	BPTN	64	U
35	BPTN	65	C
35	BPTN	67	U
35	BPTN	71	C
35	BPTN	72	C
35	BPTN	73	A
35	BPTN	74	C
35	BPTN	75	C
35	BPTN	76	A

All (168) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A16S	3	G
1	A16S	102	G
1	A16S	115	G
1	A16S	243	A
1	A16S	266	G
1	A16S	328	C
1	A16S	428	G
1	A16S	429	U
1	A16S	567	G
1	A16S	687	A
1	A16S	722	A
1	A16S	748	C
1	A16S	913	A
1	A16S	980	C
1	A16S	1101	A
1	A16S	1201	A
1	A16S	1285	A
1	A16S	1289	A
1	A16S	1300	G
1	A16S	1358	U
1	A16S	1362	C
1	A16S	1504	G
2	A23S	155(B)	U
2	A23S	155(C)	U
2	A23S	270(X)	G
2	A23S	271(B)	G
2	A23S	271(Q)	A
2	A23S	352	G
2	A23S	357(L)	A
2	A23S	400	G
2	A23S	481	G
2	A23S	512	G
2	A23S	784	A
2	A23S	1210	A
2	A23S	1225	G
2	A23S	1300	U
2	A23S	1427	A
2	A23S	1493	C
2	A23S	1494	A
2	A23S	1558	A
2	A23S	1808	U
2	A23S	1971	A

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Mol	Chain	Res	Type
2	A23S	2119	A
2	A23S	2133	G
2	A23S	2136	C
2	A23S	2202(E)	A
2	A23S	2311	A
2	A23S	2333	A
2	A23S	2474	C
2	A23S	2475	C
2	A23S	2481	G
2	A23S	2689	U
2	A23S	2719	G
2	A23S	2756	U
2	A23S	2789	C
3	A5S	52	A
3	A5S	66	A
3	A5S	88	C
35	APTN	3	G
35	APTN	11	C
35	APTN	14	A
35	APTN	16	C
35	APTN	29	U
35	APTN	35	A
35	APTN	40	G
35	APTN	43	G
35	APTN	52	G
35	APTN	71	C
35	APTN	72	C
35	APTN	73	A
1	B16S	3	G
1	B16S	78(D)	U
1	B16S	115	G
1	B16S	328	C
1	B16S	352	C
1	B16S	353	A
1	B16S	428	G
1	B16S	429	U
1	B16S	497	A
1	B16S	687	A
1	B16S	748	C
1	B16S	913	A
1	B16S	929	G
1	B16S	1064	G

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Mol	Chain	Res	Type
1	B16S	1101	A
1	B16S	1145	C
1	B16S	1201	A
1	B16S	1257	U
1	B16S	1285	A
1	B16S	1300	G
1	B16S	1362	C
1	B16S	1362(A)	C
1	B16S	1363	A
1	B16S	1504	G
1	B16S	1534	A
1	B16S	1535	C
2	B23S	25	U
2	B23S	155(B)	U
2	B23S	155(C)	U
2	B23S	271(B)	G
2	B23S	271(N)	G
2	B23S	271(Q)	A
2	B23S	352	G
2	B23S	481	G
2	B23S	775	G
2	B23S	784	A
2	B23S	790	C
2	B23S	1022	G
2	B23S	1060	U
2	B23S	1379	A
2	B23S	1427	A
2	B23S	1493	C
2	B23S	1494	A
2	B23S	1974	C
2	B23S	2032	G
2	B23S	2119	A
2	B23S	2126	A
2	B23S	2130	U
2	B23S	2133	G
2	B23S	2171	A
2	B23S	2225	A
2	B23S	2239	G
2	B23S	2474	C
2	B23S	2481	G
2	B23S	2660	A
2	B23S	2689	U

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Mol	Chain	Res	Type
2	B23S	2719	G
2	B23S	2756	U
3	B5S	66	A
56	BATN	3	U
56	BATN	6	G
56	BATN	19	G
56	BATN	20	C
56	BATN	27	G
56	BATN	32	C
56	BATN	45	G
56	BATN	48	C
56	BATN	60	U
56	BATN	69	C
34	BMRN	4	A
34	BMRN	7	G
34	BMRN	10	G
34	BMRN	12	A
34	BMRN	13	A
34	BMRN	14	A
34	BMRN	16	G
34	BMRN	19	U
35	BPTN	3	G
35	BPTN	6	A
35	BPTN	10	G
35	BPTN	11	C
35	BPTN	12	U
35	BPTN	14	A
35	BPTN	15	G
35	BPTN	16	C
35	BPTN	17	U
35	BPTN	18	G
35	BPTN	20	G
35	BPTN	23	A
35	BPTN	29	U
35	BPTN	32	C
35	BPTN	43	G
35	BPTN	47	U
35	BPTN	48	C
35	BPTN	52	G
35	BPTN	64	U
35	BPTN	71	C
35	BPTN	73	A

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
35	G7M	BPTN	46	35	23,26,27	1.05	1 (4%)	34,39,42	1.73	8 (23%)
35	5MU	APTN	54	35	19,22,23	4.94	7 (36%)	27,32,35	3.59	10 (37%)
35	CM0	APTN	34	35	21,26,27	2.88	6 (28%)	26,37,40	1.92	5 (19%)
56	5MU	BATN	54	56	19,22,23	5.03	7 (36%)	27,32,35	3.33	10 (37%)
35	5MU	BPTN	54	35	19,22,23	4.94	7 (36%)	27,32,35	3.53	11 (40%)
56	PSU	BATN	55	56	18,21,22	1.37	1 (5%)	21,30,33	1.89	7 (33%)
35	4SU	BPTN	8	35	18,21,22	3.90	9 (50%)	25,30,33	2.90	7 (28%)
35	6MZ	BPTN	37	35	22,25,26	1.83	4 (18%)	29,36,39	1.69	6 (20%)
35	G7M	APTN	46	35	23,26,27	2.66	8 (34%)	34,39,42	2.34	10 (29%)
35	6MZ	APTN	37	35	22,25,26	3.23	4 (18%)	29,36,39	2.93	13 (44%)
56	PSU	BATN	39	56	18,21,22	1.75	3 (16%)	21,30,33	1.97	4 (19%)
35	4SU	APTN	8	35	18,21,22	3.72	7 (38%)	25,30,33	2.46	5 (20%)
56	MIA	BATN	37	56	28,31,32	1.82	6 (21%)	38,44,47	3.77	20 (52%)
35	PSU	BPTN	55	35	18,21,22	1.23	1 (5%)	21,30,33	2.01	4 (19%)
56	QUO	BATN	34	56	32,35,36	0.95	1 (3%)	36,52,55	2.20	7 (19%)
35	PSU	APTN	55	35	18,21,22	1.04	1 (5%)	21,30,33	2.04	4 (19%)
35	CM0	BPTN	34	35	21,26,27	1.80	6 (28%)	26,37,40	2.48	11 (42%)

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
35	G7M	BPTN	46	35	-	1/7/25/26	0/3/3/3
35	5MU	APTN	54	35	-	3/7/25/26	0/2/2/2
35	CM0	APTN	34	35	-	8/12/30/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	BATN	54	56	-	2/7/25/26	0/2/2/2
35	5MU	BPTN	54	35	-	0/7/25/26	0/2/2/2
56	PSU	BATN	55	56	-	3/7/25/26	0/2/2/2
35	4SU	BPTN	8	35	-	0/7/25/26	0/2/2/2
35	6MZ	BPTN	37	35	-	2/9/27/28	0/3/3/3
35	G7M	APTN	46	35	-	1/7/25/26	0/3/3/3
35	6MZ	APTN	37	35	-	4/9/27/28	0/3/3/3
56	PSU	BATN	39	56	-	0/7/25/26	0/2/2/2
35	4SU	APTN	8	35	-	0/7/25/26	0/2/2/2
56	MIA	BATN	37	56	-	1/15/33/34	0/3/3/3
35	PSU	BPTN	55	35	-	0/7/25/26	0/2/2/2
56	QUO	BATN	34	56	-	1/12/43/44	0/4/4/4
35	PSU	APTN	55	35	-	0/7/25/26	0/2/2/2
35	CM0	BPTN	34	35	-	6/12/30/31	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	APTN	37	6MZ	C6-N6	14.37	1.50	1.34
35	APTN	54	5MU	C2-N1	11.75	1.56	1.38
56	BATN	54	5MU	C6-N1	11.71	1.57	1.38
35	BPTN	54	5MU	C2-N1	11.60	1.56	1.38
56	BATN	54	5MU	C2-N1	11.07	1.55	1.38
35	BPTN	54	5MU	C6-N1	10.56	1.56	1.38
56	BATN	54	5MU	C4-C5	10.48	1.61	1.44
35	APTN	54	5MU	C6-N1	10.41	1.55	1.38
35	APTN	54	5MU	C4-C5	10.18	1.61	1.44
35	BPTN	54	5MU	C4-C5	10.08	1.61	1.44
35	BPTN	8	4SU	C2-N1	8.96	1.52	1.38
35	APTN	8	4SU	C4-N3	8.37	1.46	1.37
35	APTN	54	5MU	C4-N3	-7.95	1.24	1.38
35	BPTN	8	4SU	C4-N3	7.83	1.45	1.37
35	BPTN	54	5MU	C4-N3	-7.82	1.24	1.38
35	APTN	8	4SU	C2-N1	7.31	1.49	1.38
56	BATN	54	5MU	C4-N3	-7.29	1.25	1.38
35	APTN	34	CM0	C2-N3	7.09	1.50	1.38
56	BATN	37	MIA	C13-C14	7.01	1.53	1.32
35	APTN	34	CM0	C2-N1	6.93	1.49	1.38
35	APTN	46	G7M	C4-N3	6.62	1.49	1.34
35	BPTN	37	6MZ	C6-N6	6.57	1.41	1.34
56	BATN	54	5MU	C6-C5	6.44	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	APT	34	CM0	C6-N1	6.28	1.48	1.38
35	BPT	54	5MU	C6-C5	6.26	1.44	1.34
35	BPT	8	4SU	C2-N3	5.95	1.48	1.38
35	APT	54	5MU	C6-C5	5.93	1.44	1.34
35	APT	46	G7M	C2-N3	5.93	1.47	1.33
35	BPT	8	4SU	C6-C5	5.86	1.48	1.35
35	APT	8	4SU	C2-N3	5.83	1.48	1.38
35	APT	8	4SU	C6-C5	5.81	1.48	1.35
35	APT	8	4SU	C4-S4	-5.80	1.58	1.68
35	BPT	8	4SU	C4-S4	-5.49	1.59	1.68
56	BAT	55	PSU	C6-C5	4.81	1.40	1.35
35	APT	46	G7M	C5-N7	-4.79	1.33	1.39
56	BAT	39	PSU	C6-C5	4.71	1.40	1.35
35	APT	46	G7M	C2-N2	4.44	1.44	1.34
35	BPT	55	PSU	C6-C5	4.37	1.40	1.35
35	BPT	34	CM0	C6-N1	4.32	1.45	1.38
35	APT	34	CM0	C4-N3	4.15	1.46	1.38
35	APT	46	G7M	C5-C6	3.98	1.54	1.43
56	BAT	39	PSU	C2'-C1'	3.98	1.59	1.53
35	APT	8	4SU	C5-C4	3.59	1.46	1.42
35	BPT	8	4SU	O2-C2	-3.38	1.17	1.23
35	BPT	34	CM0	C1'-N1	3.34	1.57	1.47
35	APT	55	PSU	C6-C5	3.23	1.38	1.35
56	BAT	39	PSU	O4'-C1'	-3.15	1.39	1.43
56	BAT	37	MIA	C2-S10	2.99	1.78	1.75
35	BPT	46	G7M	C8-N9	2.77	1.43	1.35
35	BPT	34	CM0	O5-C5	2.74	1.42	1.36
35	APT	54	5MU	O4-C4	-2.68	1.18	1.23
35	APT	46	G7M	C2-N1	2.68	1.44	1.37
35	BPT	34	CM0	O3'-C3'	2.65	1.49	1.43
35	APT	8	4SU	O2-C2	-2.61	1.18	1.23
56	BAT	37	MIA	C4-N3	-2.60	1.30	1.34
35	BPT	54	5MU	O2-C2	-2.57	1.18	1.23
35	BPT	8	4SU	C5-C4	2.57	1.45	1.42
35	APT	46	G7M	O6-C6	-2.55	1.18	1.23
56	BAT	54	5MU	O4-C4	-2.53	1.18	1.23
56	BAT	34	QUO	O2'-C2'	-2.52	1.36	1.43
35	BPT	37	6MZ	C2-N1	2.51	1.38	1.33
35	BPT	54	5MU	O4-C4	-2.43	1.19	1.23
35	APT	46	G7M	C6-N1	2.39	1.43	1.38
35	APT	54	5MU	O2-C2	-2.35	1.18	1.23
35	APT	37	6MZ	C8-N7	2.32	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BPTN	8	4SU	C3'-C2'	-2.30	1.47	1.53
56	BATN	54	5MU	O2-C2	-2.29	1.19	1.23
35	APTN	34	CM0	O5-C5	2.28	1.41	1.36
35	BPTN	34	CM0	O5-C7	-2.26	1.39	1.44
35	APTN	34	CM0	O5-C7	-2.25	1.39	1.44
35	APTN	37	6MZ	C9-N6	-2.23	1.41	1.45
35	BPTN	8	4SU	C6-N1	2.21	1.43	1.38
56	BATN	37	MIA	O4'-C1'	2.20	1.47	1.42
35	APTN	37	6MZ	C8-N9	-2.16	1.33	1.37
56	BATN	37	MIA	C5-N7	-2.13	1.35	1.39
35	BPTN	34	CM0	C2'-C3'	2.05	1.58	1.53
56	BATN	37	MIA	C3'-C4'	2.05	1.58	1.53
35	BPTN	37	6MZ	C5-N7	-2.04	1.35	1.39
35	BPTN	37	6MZ	C2-N3	2.00	1.37	1.33

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BATN	54	5MU	C5-C4-N3	11.67	125.47	115.32
35	APTN	54	5MU	C5-C4-N3	11.57	125.38	115.32
56	BATN	37	MIA	C12-C13-C14	-11.28	106.76	127.01
35	BPTN	54	5MU	C5-C4-N3	10.63	124.56	115.32
56	BATN	37	MIA	C2'-C1'-N9	-9.58	89.50	113.30
35	APTN	54	5MU	C5-C6-N1	-9.42	113.08	123.31
35	BPTN	54	5MU	C5-C6-N1	-9.40	113.10	123.31
56	BATN	34	QUO	C2'-C1'-N9	-9.09	87.94	113.25
35	BPTN	8	4SU	C4-N3-C2	-8.93	118.75	127.31
35	APTN	8	4SU	C4-N3-C2	-8.40	119.27	127.31
56	BATN	37	MIA	C5-C4-N3	-7.51	119.27	127.18
56	BATN	54	5MU	C5-C6-N1	-7.08	115.62	123.31
35	BPTN	8	4SU	C5-C4-N3	6.12	120.45	114.75
35	BPTN	8	4SU	C5-C4-S4	-5.98	117.47	124.31
35	APTN	46	G7M	CN7-N7-C5	5.86	134.10	126.80
35	BPTN	34	CM0	C6-N1-C2	-5.80	115.52	121.30
35	APTN	37	6MZ	O4'-C1'-N9	5.70	119.03	108.09
35	APTN	37	6MZ	C5-C4-N3	-5.63	118.97	126.72
35	APTN	8	4SU	C5-C4-N3	5.59	119.95	114.75
56	BATN	37	MIA	C6-C5-N7	5.51	138.43	132.43
56	BATN	54	5MU	C5M-C5-C4	5.49	124.65	118.78
35	APTN	55	PSU	C4-N3-C2	-5.29	119.08	126.37
35	BPTN	55	PSU	N1-C2-N3	5.27	120.73	115.17
35	BPTN	54	5MU	N3-C2-N1	5.25	121.73	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BATN	54	5MU	O4-C4-C5	-5.11	119.07	124.92
35	APTN	34	CM0	C4-N3-C2	-5.05	120.72	127.34
35	BPTN	55	PSU	C4-N3-C2	-5.04	119.44	126.37
56	BATN	37	MIA	C15-C14-C13	-4.92	107.90	122.66
35	APTN	37	6MZ	N9-C8-N7	-4.91	106.97	113.94
35	APTN	55	PSU	N1-C2-N3	4.90	120.34	115.17
35	APTN	37	6MZ	N3-C4-N9	4.90	135.50	127.17
56	BATN	39	PSU	C6-C5-C4	-4.89	114.88	118.17
35	BPTN	34	CM0	C7-O5-C5	-4.81	111.35	117.48
35	BPTN	54	5MU	O4-C4-C5	-4.72	119.52	124.92
35	APTN	46	G7M	CN7-N7-C8	-4.70	117.67	124.79
35	APTN	34	CM0	N3-C2-N1	4.69	121.00	114.89
35	APTN	46	G7M	C2-N3-C4	4.69	120.37	112.30
35	APTN	37	6MZ	C4-N9-C1'	-4.67	115.71	126.63
35	APTN	54	5MU	O4-C4-C5	-4.66	119.58	124.92
35	BPTN	8	4SU	N3-C2-N1	4.66	120.96	114.89
35	BPTN	54	5MU	C4-N3-C2	-4.65	121.25	127.34
35	APTN	37	6MZ	C4-N9-C8	4.62	110.58	105.74
56	BATN	37	MIA	C5-N7-C8	4.59	110.67	103.45
35	APTN	46	G7M	C5-C4-N3	-4.58	119.49	128.15
56	BATN	37	MIA	C4-C5-N7	-4.55	105.38	110.58
56	BATN	37	MIA	N3-C4-N9	4.52	132.73	126.99
56	BATN	39	PSU	N1-C2-N3	4.50	119.92	115.17
35	APTN	54	5MU	C4-N3-C2	-4.50	121.44	127.34
56	BATN	37	MIA	C16-C14-C13	-4.47	109.23	122.66
35	APTN	8	4SU	C5-C4-S4	-4.47	119.20	124.31
35	BPTN	37	6MZ	C4-N9-C8	4.40	110.36	105.74
35	BPTN	34	CM0	C2'-C1'-N1	4.39	125.46	113.25
35	APTN	54	5MU	N3-C2-N1	4.38	120.59	114.89
35	APTN	37	6MZ	C4-C5-C6	4.36	120.41	116.78
56	BATN	37	MIA	C2-N3-C4	4.31	123.59	112.29
35	BPTN	54	5MU	C5M-C5-C6	-4.21	117.15	122.85
35	APTN	46	G7M	C5-C6-N1	4.21	120.53	111.84
35	APTN	37	6MZ	N1-C2-N3	-4.19	122.24	128.58
35	APTN	54	5MU	C5M-C5-C6	-4.17	117.21	122.85
56	BATN	37	MIA	O4'-C1'-N9	4.09	115.94	108.09
35	APTN	54	5MU	C5M-C5-C4	4.04	123.09	118.78
35	APTN	8	4SU	N3-C2-N1	3.98	120.07	114.89
35	BPTN	37	6MZ	N9-C8-N7	-3.91	108.39	113.94
56	BATN	34	QUO	C3'-C2'-C1'	-3.91	94.07	101.46
35	APTN	37	6MZ	C5-N7-C8	3.88	109.55	103.45
56	BATN	37	MIA	N9-C8-N7	-3.85	108.47	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	APTN	34	CM0	C6-N1-C2	-3.78	117.54	121.30
35	BPTN	34	CM0	O4'-C4'-C3'	3.74	112.58	105.15
56	BATN	34	QUO	C7-C8-N9	-3.71	107.61	111.08
35	BPTN	46	G7M	C1'-N9-C4	-3.71	115.53	126.49
56	BATN	34	QUO	C7-C5-C4	-3.64	108.51	112.68
35	BPTN	34	CM0	O3'-C3'-C2'	3.60	123.35	111.82
56	BATN	55	PSU	C6-N1-C2	-3.57	119.38	122.69
35	BPTN	46	G7M	C4-C5-N7	3.57	113.50	107.67
35	APTN	46	G7M	C1'-N9-C4	-3.55	116.01	126.49
35	APTN	46	G7M	N9-C4-N3	3.50	132.95	125.95
35	APTN	46	G7M	O6-C6-C5	-3.47	120.27	128.01
56	BATN	39	PSU	C4-N3-C2	-3.46	121.61	126.37
35	APTN	46	G7M	C2-N1-C6	-3.42	118.91	125.11
56	BATN	55	PSU	O2-C2-N1	-3.41	119.27	122.79
35	BPTN	46	G7M	CN7-N7-C8	3.35	129.87	124.79
35	BPTN	54	5MU	C5M-C5-C4	3.35	122.36	118.78
56	BATN	54	5MU	N3-C2-N1	3.33	119.22	114.89
35	BPTN	46	G7M	C8-N7-C5	-3.25	103.72	107.78
56	BATN	37	MIA	O3'-C3'-C4'	3.25	120.41	111.08
56	BATN	54	5MU	C5M-C5-C6	-3.24	118.46	122.85
56	BATN	39	PSU	O2-C2-N1	-3.23	119.46	122.79
35	APTN	37	6MZ	C2-N3-C4	3.22	119.69	111.83
56	BATN	37	MIA	N3-C2-N1	-3.13	121.29	127.00
35	BPTN	34	CM0	O4'-C1'-C2'	-3.12	99.94	106.62
56	BATN	37	MIA	C3'-C2'-C1'	3.09	107.31	101.46
35	BPTN	46	G7M	C6-C5-C4	-3.01	113.80	119.01
35	BPTN	54	5MU	C6-C5-C4	3.00	120.49	118.02
35	APTN	34	CM0	C7-O5-C5	-2.99	113.67	117.48
35	BPTN	34	CM0	C1'-N1-C6	2.96	126.02	121.15
35	APTN	37	6MZ	C1'-N9-C8	2.95	133.64	127.09
56	BATN	55	PSU	C4-N3-C2	-2.91	122.36	126.37
56	BATN	55	PSU	C6-C5-C4	-2.91	116.21	118.17
35	BPTN	46	G7M	C5-C4-N3	2.90	133.62	128.15
56	BATN	34	QUO	C15-C16-C12	2.90	108.59	103.91
56	BATN	34	QUO	C10-N11-C12	2.87	120.70	114.83
35	APTN	55	PSU	O2-C2-N1	-2.85	119.85	122.79
56	BATN	54	5MU	C4-N3-C2	-2.84	123.61	127.34
35	APTN	37	6MZ	C4-C5-N7	-2.81	107.37	110.58
35	BPTN	54	5MU	O2-C2-N1	-2.77	119.19	122.80
35	BPTN	37	6MZ	C5-N7-C8	2.75	107.78	103.45
35	BPTN	55	PSU	O2-C2-N1	-2.73	119.97	122.79
35	BPTN	8	4SU	C1'-N1-C2	2.72	122.47	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BATN	37	MIA	C4-N9-C1'	-2.71	120.29	126.63
56	BATN	55	PSU	N1-C2-N3	2.71	118.02	115.17
56	BATN	37	MIA	O2'-C2'-C1'	2.70	119.41	110.10
35	APTN	54	5MU	O4-C4-N3	-2.70	115.04	120.11
35	BPTN	55	PSU	C6-N1-C2	-2.67	120.22	122.69
35	APTN	46	G7M	C1'-N9-C8	2.66	135.73	126.74
35	APTN	54	5MU	C1'-N1-C2	2.60	122.27	117.59
35	BPTN	34	CM0	C2'-C3'-C4'	-2.56	97.66	102.61
35	APTN	55	PSU	C6-C5-C4	2.54	119.89	118.17
35	BPTN	46	G7M	C1'-N9-C8	2.49	135.15	126.74
56	BATN	54	5MU	O4-C4-N3	-2.47	115.47	120.11
35	APTN	8	4SU	O2-C2-N1	-2.46	119.59	122.80
35	BPTN	54	5MU	C6-N1-C2	-2.45	118.86	121.30
35	BPTN	37	6MZ	C9-N6-C6	2.43	125.11	122.85
35	BPTN	34	CM0	C4-N3-C2	2.40	130.49	127.34
35	APTN	34	CM0	C1'-N1-C2	2.39	121.88	117.59
35	BPTN	8	4SU	C6-N1-C2	-2.38	118.10	121.00
35	BPTN	8	4SU	O2-C2-N1	-2.38	119.70	122.80
35	BPTN	37	6MZ	C3'-C2'-C1'	2.32	105.86	101.46
56	BATN	37	MIA	C1'-N9-C8	2.30	132.20	127.09
56	BATN	55	PSU	O3'-C3'-C4'	2.26	117.57	111.08
56	BATN	55	PSU	O4-C4-C5	-2.23	118.46	124.01
35	BPTN	54	5MU	O4-C4-N3	-2.23	115.92	120.11
35	BPTN	34	CM0	C3'-C2'-C1'	2.21	105.65	101.46
35	BPTN	34	CM0	C5'-C4'-C3'	-2.20	107.28	115.21
35	BPTN	37	6MZ	C4-N9-C1'	-2.18	121.54	126.63
56	BATN	37	MIA	O4'-C4'-C3'	2.13	109.39	105.15
56	BATN	34	QUO	C5-C4-N3	2.12	129.97	127.53
56	BATN	54	5MU	C6-N1-C2	-2.12	119.19	121.30
35	APTN	37	6MZ	C5'-C4'-C3'	-2.12	107.58	115.21
35	BPTN	46	G7M	O6-C6-N1	-2.12	116.13	120.11
56	BATN	54	5MU	O2-C2-N1	-2.07	120.10	122.80
35	APTN	54	5MU	C6-C5-C4	2.03	119.70	118.02
56	BATN	37	MIA	C5-C4-N9	2.00	108.00	105.81

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BATN	37	MIA	C12-C13-C14-C16
35	BPTN	34	CM0	O4'-C1'-N1-C2
35	BPTN	34	CM0	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
35	BPTN	34	CM0	C3'-C4'-C5'-O5'
35	APTN	37	6MZ	C5-C6-N6-C9
35	APTN	37	6MZ	N1-C6-N6-C9
35	BPTN	37	6MZ	C5-C6-N6-C9
35	BPTN	37	6MZ	N1-C6-N6-C9
35	APTN	46	G7M	C4'-C5'-O5'-P
35	BPTN	46	G7M	C4'-C5'-O5'-P
35	APTN	34	CM0	C3'-C4'-C5'-O5'
35	APTN	34	CM0	O4'-C4'-C5'-O5'
35	BPTN	34	CM0	O4'-C4'-C5'-O5'
35	APTN	54	5MU	O4'-C4'-C5'-O5'
35	APTN	34	CM0	O5-C7-C8-O9
56	BATN	55	PSU	C3'-C4'-C5'-O5'
35	APTN	34	CM0	O5-C7-C8-O8
56	BATN	55	PSU	O4'-C4'-C5'-O5'
35	APTN	34	CM0	C6-C5-O5-C7
35	APTN	34	CM0	C4-C5-O5-C7
35	APTN	34	CM0	C8-C7-O5-C5
35	BPTN	34	CM0	C8-C7-O5-C5
35	APTN	54	5MU	C3'-C4'-C5'-O5'
56	BATN	54	5MU	C3'-C4'-C5'-O5'
56	BATN	54	5MU	O4'-C4'-C5'-O5'
56	BATN	34	QUO	C4'-C5'-O5'-P
56	BATN	55	PSU	O4'-C1'-C5-C4
35	BPTN	34	CM0	C4-C5-O5-C7
35	APTN	54	5MU	C2'-C1'-N1-C6
35	APTN	37	6MZ	C2'-C1'-N9-C8
35	APTN	34	CM0	C2'-C1'-N1-C6
35	APTN	37	6MZ	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	AS04	501	38	0,12,12	-	-	-		
58	SF4	BS04	501	38	0,12,12	-	-	-		

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

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Mol	Chain	Number of breaks
35	APTN	1

All 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
1	A23S	1141:U	O3'	1142:A	P	5.75
1	BPTN	37:6MZ	O3'	38:A	P	2.91
1	APTN	37:6MZ	O3'	38:A	P	2.33

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A16S	1517/1518 (99%)	0.48	77 (5%)	33	21	55, 88, 161, 216	0
1	B16S	1517/1518 (99%)	0.53	76 (5%)	34	22	49, 90, 173, 240	0
2	A23S	2879/2881 (99%)	0.39	93 (3%)	50	31	36, 76, 173, 238	0
2	B23S	2879/2881 (99%)	0.26	66 (2%)	61	41	28, 63, 165, 232	0
3	A5S	119/119 (100%)	0.26	3 (2%)	58	39	73, 99, 117, 126	0
3	B5S	119/119 (100%)	0.31	1 (0%)	82	67	46, 84, 106, 122	0
4	AL01	228/228 (100%)	1.63	70 (30%)	1	1	131, 167, 179, 191	0
4	BL01	228/228 (100%)	1.44	56 (24%)	2	2	126, 162, 178, 184	0
5	AL02	271/276 (98%)	0.47	14 (5%)	33	21	37, 56, 77, 85	0
5	BL02	271/276 (98%)	0.45	15 (5%)	30	19	30, 51, 69, 77	0
6	AL03	204/206 (99%)	0.78	14 (6%)	23	14	50, 76, 97, 107	0
6	BL03	204/206 (99%)	0.38	7 (3%)	48	30	39, 66, 92, 107	0
7	AL04	202/205 (98%)	0.94	20 (9%)	13	8	51, 85, 108, 120	0
7	BL04	202/205 (98%)	0.63	16 (7%)	18	12	34, 67, 91, 103	0
8	AL05	181/181 (100%)	1.03	20 (11%)	10	7	89, 121, 139, 147	0
8	BL05	181/181 (100%)	1.08	28 (15%)	5	4	82, 110, 138, 151	0
9	AL06	167/180 (92%)	1.68	51 (30%)	1	1	114, 151, 173, 182	0
9	BL06	167/180 (92%)	2.15	87 (52%)	0	1	116, 150, 172, 179	0
10	AL09	145/148 (97%)	0.88	17 (11%)	9	6	75, 112, 133, 140	0
10	BL09	145/148 (97%)	0.88	16 (11%)	10	7	78, 101, 118, 127	0
11	AL13	137/140 (97%)	0.89	9 (6%)	24	15	66, 87, 116, 122	0
11	BL13	137/140 (97%)	0.57	8 (5%)	29	18	48, 66, 91, 105	0
12	AL14	122/122 (100%)	0.34	1 (0%)	82	67	51, 63, 77, 85	0
12	BL14	122/122 (100%)	0.26	4 (3%)	49	30	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%)	1.17	24 (16%) 4 3	56, 88, 107, 125	0
13	BL15	146/150 (97%)	1.17	22 (15%) 5 4	45, 77, 98, 123	0
14	AL16	134/141 (95%)	0.98	13 (9%) 13 9	60, 82, 103, 109	0
14	BL16	134/141 (95%)	0.87	14 (10%) 11 8	52, 69, 83, 95	0
15	AL17	117/118 (99%)	0.57	6 (5%) 33 21	50, 69, 83, 92	0
15	BL17	117/118 (99%)	0.51	7 (5%) 27 17	43, 59, 76, 83	0
16	AL18	98/111 (88%)	0.71	5 (5%) 33 21	68, 83, 95, 102	0
16	BL18	98/111 (88%)	0.61	5 (5%) 33 21	47, 69, 94, 101	0
17	AL19	137/146 (93%)	0.58	7 (5%) 33 21	54, 77, 113, 121	0
17	BL19	137/146 (93%)	0.59	6 (4%) 39 24	52, 68, 116, 134	0
18	AL20	117/118 (99%)	0.96	15 (12%) 7 6	50, 84, 101, 108	0
18	BL20	117/118 (99%)	0.57	6 (5%) 33 21	42, 59, 74, 92	0
19	AL21	101/101 (100%)	1.06	17 (16%) 4 3	65, 98, 111, 116	0
19	BL21	101/101 (100%)	0.74	10 (9%) 13 8	46, 72, 92, 98	0
20	AL22	112/113 (99%)	0.69	8 (7%) 22 14	54, 69, 98, 135	0
20	BL22	112/113 (99%)	0.33	4 (3%) 46 28	40, 56, 82, 113	0
21	AL23	92/96 (95%)	0.68	6 (6%) 25 16	48, 71, 96, 108	0
21	BL23	92/96 (95%)	0.40	1 (1%) 78 61	43, 58, 97, 115	0
22	AL24	100/110 (90%)	1.52	27 (27%) 1 1	83, 98, 123, 132	0
22	BL24	100/110 (90%)	1.12	20 (20%) 3 2	60, 80, 116, 141	0
23	AL25	187/206 (90%)	0.92	18 (9%) 13 9	86, 102, 123, 129	0
23	BL25	187/206 (90%)	0.74	13 (6%) 22 14	65, 91, 108, 121	0
24	AL27	82/84 (97%)	0.41	5 (6%) 27 17	54, 66, 93, 105	0
24	BL27	82/84 (97%)	0.58	8 (9%) 13 9	51, 63, 95, 101	0
25	AL28	88/98 (89%)	1.10	12 (13%) 7 5	52, 78, 107, 121	0
25	BL28	88/98 (89%)	0.96	15 (17%) 4 3	44, 70, 95, 106	0
26	AL29	62/72 (86%)	1.03	7 (11%) 10 7	66, 86, 114, 125	0
26	BL29	62/72 (86%)	0.94	8 (12%) 7 6	40, 74, 102, 114	0
27	AL30	59/60 (98%)	0.94	5 (8%) 16 11	67, 89, 107, 124	0
27	BL30	59/60 (98%)	0.59	4 (6%) 23 15	46, 68, 90, 114	0
28	AL31	45/71 (63%)	0.99	7 (15%) 5 4	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%)	1.06	8 (17%) 4 3	123, 143, 150, 157	0
29	AL32	59/59 (100%)	0.67	3 (5%) 33 21	50, 67, 133, 140	0
29	BL32	59/59 (100%)	0.74	11 (18%) 3 3	42, 63, 126, 135	0
30	AL33	44/54 (81%)	1.18	9 (20%) 2 2	61, 77, 87, 90	0
30	BL33	44/54 (81%)	1.07	8 (18%) 3 3	44, 72, 78, 88	0
31	AL34	48/49 (97%)	0.63	3 (6%) 26 17	36, 52, 67, 85	0
31	BL34	48/49 (97%)	0.79	3 (6%) 26 17	29, 39, 62, 69	0
32	AL35	63/64 (98%)	1.16	10 (15%) 5 3	54, 67, 76, 88	0
32	BL35	63/64 (98%)	0.85	9 (14%) 6 5	46, 57, 69, 81	0
33	AL36	37/37 (100%)	0.60	2 (5%) 31 20	70, 80, 95, 115	0
33	BL36	37/37 (100%)	1.50	9 (24%) 2 2	58, 72, 93, 95	0
34	AMRN	10/17 (58%)	2.03	5 (50%) 0 1	108, 136, 165, 166	0
34	BMRN	17/17 (100%)	1.33	3 (17%) 4 3	109, 144, 173, 178	0
35	APTN	70/76 (92%)	1.29	11 (15%) 5 4	77, 172, 208, 231	0
35	BPTN	70/76 (92%)	1.08	6 (8%) 16 11	70, 140, 172, 182	0
36	AS02	234/255 (91%)	0.63	7 (2%) 52 33	82, 108, 131, 141	0
36	BS02	234/255 (91%)	0.80	13 (5%) 30 19	91, 110, 133, 146	0
37	AS03	206/238 (86%)	0.79	15 (7%) 21 13	76, 98, 117, 123	0
37	BS03	206/238 (86%)	0.90	24 (11%) 9 6	83, 106, 123, 132	0
38	AS04	208/208 (100%)	0.49	8 (3%) 44 27	53, 78, 93, 108	0
38	BS04	208/208 (100%)	0.67	8 (3%) 44 27	63, 85, 98, 105	0
39	AS05	151/161 (93%)	0.42	4 (2%) 57 37	59, 76, 96, 102	0
39	BS05	151/161 (93%)	0.62	5 (3%) 49 30	61, 80, 97, 112	0
40	AS06	101/101 (100%)	0.40	2 (1%) 65 45	68, 88, 99, 103	0
40	BS06	101/101 (100%)	0.47	3 (2%) 52 33	74, 88, 101, 106	0
41	AS07	155/155 (100%)	0.77	13 (8%) 17 11	101, 122, 141, 158	0
41	BS07	155/155 (100%)	0.90	17 (10%) 10 7	108, 125, 136, 142	0
42	AS08	138/138 (100%)	0.60	9 (6%) 25 16	65, 78, 86, 90	0
42	BS08	138/138 (100%)	0.47	5 (3%) 46 28	64, 82, 96, 108	0
43	AS09	127/128 (99%)	1.33	28 (22%) 2 2	97, 133, 144, 150	0
43	BS09	127/128 (99%)	1.41	30 (23%) 2 2	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%)	1.28	19 (19%) 3 2	99, 122, 143, 158	0
44	BS10	98/104 (94%)	1.68	27 (27%) 1 1	98, 120, 137, 142	0
45	AS11	114/128 (89%)	0.62	7 (6%) 27 17	68, 97, 117, 120	0
45	BS11	114/128 (89%)	0.86	12 (10%) 11 8	56, 98, 120, 129	0
46	AS12	122/131 (93%)	0.68	8 (6%) 24 15	56, 74, 88, 98	0
46	BS12	122/131 (93%)	0.89	9 (7%) 20 13	56, 78, 93, 98	0
47	AS13	117/125 (93%)	1.30	21 (17%) 3 3	115, 132, 144, 166	0
47	BS13	117/125 (93%)	1.23	21 (17%) 3 3	121, 139, 152, 156	0
48	AS14	60/60 (100%)	1.60	15 (25%) 2 2	93, 112, 144, 153	0
48	BS14	60/60 (100%)	1.72	18 (30%) 1 1	95, 112, 148, 156	0
49	AS15	88/88 (100%)	0.42	5 (5%) 29 19	55, 75, 89, 94	0
49	BS15	88/88 (100%)	0.52	2 (2%) 61 41	57, 74, 95, 104	0
50	AS16	83/88 (94%)	0.80	3 (3%) 46 28	70, 82, 105, 117	0
50	BS16	83/88 (94%)	0.90	12 (14%) 6 5	66, 78, 99, 124	0
51	AS17	99/104 (95%)	0.49	6 (6%) 27 17	56, 70, 83, 91	0
51	BS17	99/104 (95%)	0.65	5 (5%) 33 21	59, 71, 82, 87	0
52	AS18	70/87 (80%)	0.44	2 (2%) 53 35	68, 82, 100, 108	0
52	BS18	70/87 (80%)	0.83	8 (11%) 10 7	69, 93, 110, 120	0
53	AS19	78/92 (84%)	1.22	10 (12%) 7 6	124, 135, 144, 152	0
53	BS19	78/92 (84%)	1.43	20 (25%) 1 2	111, 130, 142, 145	0
54	AS20	99/105 (94%)	1.11	16 (16%) 4 3	75, 94, 112, 122	0
54	BS20	99/105 (94%)	0.88	9 (9%) 15 9	64, 84, 105, 112	0
55	ATHX	24/26 (92%)	3.32	20 (83%) 0 0	134, 153, 159, 163	0
55	BTHX	24/26 (92%)	2.51	14 (58%) 0 0	139, 155, 161, 170	0
56	BATN	80/85 (94%)	1.52	22 (27%) 1 1	104, 171, 217, 231	0
All	All	21191/21839 (97%)	0.66	1696 (8%) 18 12	28, 83, 162, 240	0

All (1696) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	BS10	58	ASP	9.7
4	AL01	5	GLY	9.2
4	AL01	4	HIS	8.9

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Mol	Chain	Res	Type	RSRZ
13	BL15	30	THR	8.7
4	AL01	3	LYS	8.2
44	BS10	59	SER	7.4
13	AL15	51	PHE	7.2
9	BL06	169	VAL	7.0
9	AL06	64	LEU	7.0
47	BS13	118	ALA	6.9
22	AL24	59	GLY	6.9
1	A16S	1362(A)	C	6.8
55	ATHX	16	GLY	6.7
13	AL15	33	ARG	6.7
9	BL06	111	HIS	6.6
1	A16S	1360	A	6.5
24	BL27	4	LYS	6.5
30	BL33	31	PRO	6.5
48	BS14	2	ALA	6.3
26	BL29	13	ALA	6.3
48	BS14	16	PHE	6.2
9	BL06	125	VAL	6.1
1	A16S	3	G	5.9
4	BL01	221	PRO	5.9
2	A23S	2060	A	5.8
9	AL06	5	GLY	5.7
44	BS10	62	HIS	5.7
9	BL06	170	ARG	5.7
4	AL01	104	ILE	5.6
37	BS03	167	TRP	5.5
55	ATHX	23	PRO	5.5
53	BS19	55	LYS	5.5
37	BS03	171	GLY	5.4
1	B16S	3	G	5.3
9	BL06	155	SER	5.3
55	BTHX	4	GLY	5.3
8	AL05	127	GLY	5.3
1	B16S	1362(A)	C	5.3
32	BL35	57	ARG	5.3
48	AS14	16	PHE	5.2
55	BTHX	13	ILE	5.3
55	ATHX	19	GLY	5.2
1	A16S	1362	C	5.2
9	AL06	155	SER	5.2
26	BL29	12	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
9	BL06	108	GLY	5.2
4	AL01	101	ILE	5.1
9	AL06	153	LYS	5.1
43	BS09	34	ASN	5.1
2	B23S	8	A	5.1
25	AL28	19	GLN	5.1
4	AL01	2	PRO	5.1
53	BS19	79	THR	5.0
29	BL32	58	LEU	5.0
22	BL24	59	GLY	5.0
48	AS14	18	VAL	4.9
4	BL01	220	GLY	4.9
48	AS14	2	ALA	4.9
9	AL06	159	GLU	4.9
23	BL25	84	GLU	4.9
46	BS12	28	GLY	4.9
45	BS11	117	ASN	4.9
55	ATHX	8	THR	4.8
2	B23S	983	A	4.8
29	BL32	59	GLU	4.8
29	AL32	2	ALA	4.8
47	AS13	35	GLU	4.8
13	AL15	21	ARG	4.8
43	AS09	83	ARG	4.8
44	AS10	48	THR	4.8
54	AS20	70	SER	4.8
43	BS09	33	PHE	4.8
4	BL01	222	SER	4.8
16	AL18	11	LYS	4.8
13	BL15	110	TYR	4.7
19	AL21	81	TYR	4.7
19	AL21	73	SER	4.7
5	BL02	34	VAL	4.7
34	AMRN	7	G	4.7
41	BS07	37	ASN	4.7
1	A16S	1359	C	4.7
2	B23S	2612	C	4.7
48	BS14	4	LYS	4.6
7	AL04	47	GLY	4.6
9	BL06	152	ARG	4.6
18	AL20	18	LEU	4.6
40	BS06	18	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
7	AL04	96	ASP	4.6
29	BL32	60	VAL	4.6
44	BS10	88	LEU	4.6
51	AS17	26	GLN	4.6
44	AS10	62	HIS	4.6
9	BL06	171	LEU	4.5
4	AL01	215	VAL	4.5
55	ATHX	9	ARG	4.5
9	AL06	167	GLU	4.5
9	BL06	99	VAL	4.5
2	B23S	2117	A	4.5
6	AL03	77	ILE	4.5
53	AS19	5	LEU	4.5
11	BL13	142	ARG	4.5
36	BS02	193	ASP	4.4
4	AL01	132	LEU	4.4
43	BS09	63	ILE	4.4
55	ATHX	17	THR	4.4
9	BL06	5	GLY	4.4
4	BL01	12	LEU	4.4
26	AL29	3	LEU	4.4
43	BS09	64	THR	4.4
53	AS19	35	SER	4.4
15	AL17	2	ARG	4.4
37	BS03	165	THR	4.4
43	AS09	125	TYR	4.4
29	BL32	2	ALA	4.3
4	AL01	175	PRO	4.3
9	AL06	154	PRO	4.3
4	BL01	225	ILE	4.3
2	B23S	2061	G	4.3
37	AS03	35	GLU	4.3
2	A23S	1379	A	4.3
43	BS09	108	VAL	4.3
8	AL05	165	THR	4.3
48	BS14	10	ALA	4.3
18	AL20	58	ARG	4.2
53	AS19	4	SER	4.2
43	AS09	79	LEU	4.2
1	A16S	1365	G	4.2
43	BS09	126	SER	4.2
53	AS19	41	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
31	BL34	45	ALA	4.2
55	BTHX	8	THR	4.2
54	AS20	72	LEU	4.2
18	BL20	89	GLU	4.1
10	BL09	20	ASP	4.1
1	A16S	1363	A	4.1
50	BS16	25	ARG	4.1
22	AL24	75	ILE	4.1
17	BL19	94	ALA	4.1
54	BS20	69	GLY	4.1
4	AL01	20	VAL	4.1
2	B23S	974(A)	C	4.1
9	BL06	93	GLY	4.1
54	BS20	72	LEU	4.1
55	ATHX	18	TYR	4.1
39	BS05	81	GLU	4.1
9	AL06	151	ILE	4.1
55	ATHX	2	GLY	4.1
1	B16S	1362	C	4.1
44	BS10	32	ALA	4.1
15	BL17	2	ARG	4.1
51	BS17	30	PRO	4.1
4	BL01	219	MET	4.0
1	A16S	328	C	4.0
1	A16S	1326	C	4.0
1	B16S	1325	C	4.0
2	B23S	2610	C	4.0
4	AL01	78	ILE	4.0
37	BS03	99	VAL	4.0
25	AL28	35	THR	4.0
10	BL09	16	GLY	4.0
55	BTHX	25	LYS	4.0
48	BS14	21	TYR	4.0
2	A23S	2141	G	4.0
37	BS03	162	GLN	4.0
5	AL02	34	VAL	4.0
45	BS11	114	VAL	4.0
1	B16S	1365	G	4.0
43	BS09	119	ALA	4.0
1	B16S	4	U	3.9
22	AL24	48	ALA	3.9
4	AL01	8	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
9	BL06	71	LEU	3.9
1	A16S	1267	C	3.9
32	AL35	38	GLY	3.9
56	BATN	32	C	3.9
9	BL06	153	LYS	3.9
30	BL33	24	GLU	3.9
9	BL06	110	SER	3.9
29	AL32	58	LEU	3.9
47	AS13	107	ALA	3.9
1	B16S	723	U	3.9
35	BPTN	17	U	3.9
10	BL09	27	ARG	3.9
42	BS08	1	MET	3.9
10	AL09	47	LEU	3.9
23	BL25	164	ALA	3.9
2	A23S	2103	C	3.9
48	BS14	8	GLU	3.9
6	BL03	106	GLY	3.9
41	AS07	93	PRO	3.9
8	BL05	77	ILE	3.9
46	AS12	27	LYS	3.9
4	AL01	12	LEU	3.9
4	AL01	210	LEU	3.9
22	AL24	82	PRO	3.8
17	BL19	104	ASN	3.8
2	A23S	2178	C	3.8
18	AL20	33	ARG	3.8
6	AL03	151	TYR	3.8
4	AL01	181	PHE	3.8
7	BL04	41	LEU	3.8
13	AL15	7	ARG	3.8
2	B23S	352	G	3.8
9	BL06	109	PHE	3.8
8	BL05	3	LEU	3.8
23	AL25	91	LEU	3.8
49	BS15	57	LEU	3.8
8	BL05	79	ASN	3.8
23	BL25	96	VAL	3.8
4	AL01	162	ILE	3.8
47	AS13	38	GLY	3.8
38	AS04	64	LEU	3.8
50	BS16	68	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
50	BS16	32	TYR	3.8
9	AL06	88	LEU	3.8
13	BL15	51	PHE	3.8
1	A16S	4	U	3.8
2	A23S	2501	C	3.7
22	BL24	49	VAL	3.7
55	ATHX	20	LYS	3.7
2	B23S	2505	G	3.7
10	BL09	97	ILE	3.7
23	AL25	183	LEU	3.7
39	BS05	85	GLY	3.7
9	BL06	46	GLU	3.7
4	BL01	217	THR	3.7
1	A16S	1364	U	3.7
29	BL32	57	VAL	3.7
35	APTN	31	C	3.7
22	AL24	25	GLY	3.7
48	BS14	30	ALA	3.7
33	BL36	26	ILE	3.7
36	BS02	200	ILE	3.7
2	B23S	887	A	3.7
43	AS09	126	SER	3.7
47	AS13	42	ALA	3.7
7	AL04	44	ARG	3.7
2	B23S	2581	G	3.7
46	AS12	12	LYS	3.7
1	B16S	78(B)	U	3.7
9	BL06	168	PRO	3.7
13	AL15	52	GLU	3.7
55	ATHX	5	ASP	3.7
4	BL01	36	ALA	3.7
10	BL09	18	VAL	3.7
4	AL01	221	PRO	3.6
10	BL09	42	SER	3.6
9	AL06	50	VAL	3.6
26	BL29	14	ARG	3.6
2	A23S	2062	A	3.6
4	AL01	50	ILE	3.6
9	AL06	138	LYS	3.6
5	BL02	237	GLU	3.6
4	AL01	76	LEU	3.6
2	A23S	2032	G	3.6

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Mol	Chain	Res	Type	RSRZ
1	A16S	978	A	3.6
4	AL01	223	VAL	3.6
48	AS14	21	TYR	3.6
9	BL06	92	ILE	3.6
55	ATHX	3	LYS	3.6
43	BS09	37	PHE	3.6
1	A16S	108	G	3.6
1	B16S	102	G	3.6
4	AL01	219	MET	3.6
9	AL06	164	TYR	3.6
9	BL06	103	LEU	3.6
46	BS12	27	LYS	3.6
39	BS05	87	SER	3.6
55	ATHX	15	ARG	3.6
9	AL06	131	VAL	3.6
9	BL06	102	ALA	3.6
25	BL28	30	VAL	3.6
53	AS19	76	PRO	3.6
9	AL06	87	LEU	3.6
10	BL09	41	GLU	3.6
55	ATHX	21	TYR	3.6
55	BTHX	19	GLY	3.5
47	AS13	10	PRO	3.5
25	BL28	27	GLU	3.5
24	AL27	78	TYR	3.5
9	AL06	51	ARG	3.5
53	BS19	35	SER	3.5
38	BS04	112	VAL	3.5
47	BS13	117	VAL	3.5
2	A23S	2448	A	3.5
2	B23S	2060	A	3.5
37	AS03	193	TYR	3.5
11	AL13	137	ARG	3.5
25	BL28	34	THR	3.5
4	AL01	39	ASP	3.5
22	AL24	47	LYS	3.5
8	AL05	69	ALA	3.5
4	BL01	2	PRO	3.5
10	BL09	38	LEU	3.5
2	B23S	2477	C	3.5
13	BL15	22	GLY	3.5
29	BL32	50	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
4	BL01	26	ALA	3.5
25	AL28	12	PRO	3.5
46	BS12	4	PRO	3.5
9	BL06	50	VAL	3.5
7	AL04	41	LEU	3.5
1	A16S	135	C	3.5
2	B23S	2402	C	3.5
9	AL06	168	PRO	3.5
4	BL01	150	ILE	3.5
44	AS10	75	ILE	3.5
30	AL33	24	GLU	3.4
14	AL16	90	VAL	3.4
13	AL15	30	THR	3.4
14	BL16	10	ARG	3.4
1	A16S	1493	A	3.4
4	AL01	6	LYS	3.4
5	AL02	139	GLY	3.4
45	BS11	118	GLY	3.4
48	AS14	20	ALA	3.4
27	BL30	1	MET	3.4
9	AL06	112	PRO	3.4
1	B16S	1440(I)	A	3.4
4	BL01	30	VAL	3.4
19	AL21	61	VAL	3.4
30	AL33	52	VAL	3.4
44	BS10	24	VAL	3.4
36	BS02	196	LEU	3.4
14	BL16	84	GLY	3.4
37	BS03	25	GLY	3.4
7	AL04	206	ILE	3.4
51	BS17	29	HIS	3.4
9	BL06	126	PRO	3.4
1	B16S	1028(E)	G	3.4
41	AS07	82	GLY	3.4
8	BL05	165	THR	3.4
13	BL15	9	ASN	3.4
32	AL35	31	HIS	3.4
40	AS06	51	PRO	3.4
53	BS19	4	SER	3.4
4	AL01	128	LEU	3.4
6	AL03	181	LEU	3.4
13	BL15	77	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
55	BTHX	9	ARG	3.4
2	A23S	2581	G	3.4
2	B23S	7	G	3.4
9	BL06	94	TYR	3.4
9	BL06	151	ILE	3.4
44	BS10	4	ILE	3.4
4	AL01	111	PHE	3.3
55	BTHX	14	TRP	3.3
1	A16S	1317	C	3.3
9	BL06	26	VAL	3.3
44	BS10	19	SER	3.3
33	BL36	1	MET	3.3
47	AS13	26	GLY	3.3
18	AL20	14	HIS	3.3
38	AS04	201	GLN	3.3
2	A23S	2334	G	3.3
2	A23S	2583	G	3.3
2	B23S	2807	G	3.3
55	BTHX	10	ARG	3.3
24	AL27	7	LEU	3.3
8	BL05	35	GLU	3.3
45	AS11	12	ARG	3.3
9	AL06	123	PHE	3.3
22	AL24	31	LEU	3.3
18	BL20	90	VAL	3.3
4	AL01	84	ILE	3.3
21	AL23	67	GLY	3.3
8	BL05	2	PRO	3.3
8	AL05	64	THR	3.3
25	BL28	73	LEU	3.3
9	AL06	169	VAL	3.3
5	AL02	235	GLY	3.3
22	BL24	52	SER	3.3
7	BL04	149	ASP	3.3
4	AL01	139	PRO	3.3
8	AL05	2	PRO	3.3
9	BL06	154	PRO	3.3
19	AL21	38	LEU	3.3
51	AS17	27	PHE	3.3
1	B16S	1440(H)	U	3.3
35	APTN	38	A	3.3
14	BL16	89	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
9	AL06	150	ALA	3.3
51	AS17	33	GLY	3.3
14	BL16	9	TYR	3.2
24	BL27	7	LEU	3.2
26	BL29	16	LEU	3.2
8	AL05	36	LYS	3.2
9	BL06	107	VAL	3.2
54	BS20	9	ASN	3.2
2	A23S	2120	G	3.2
56	BATN	13	G	3.2
13	BL15	65	ARG	3.2
1	B16S	1028(D)	C	3.2
21	AL23	66	LEU	3.2
35	APTN	36	C	3.2
44	BS10	90	LEU	3.2
54	BS20	99	LEU	3.2
55	BTHX	23	PRO	3.2
23	BL25	165	VAL	3.2
41	AS07	56	GLN	3.2
50	BS16	65	GLN	3.2
32	BL35	34	TRP	3.2
40	BS06	101	ALA	3.2
27	AL30	31	LEU	3.2
9	BL06	117	PRO	3.2
2	A23S	2447	G	3.2
19	BL21	37	VAL	3.2
35	APTN	20	G	3.2
2	A23S	2175	C	3.2
9	AL06	59	ARG	3.2
18	AL20	4	ALA	3.2
50	BS16	24	ALA	3.2
7	BL04	56	GLU	3.2
7	AL04	133	ASN	3.2
8	AL05	60	LEU	3.2
6	AL03	160	TYR	3.2
48	AS14	14	PRO	3.2
14	BL16	81	VAL	3.2
22	AL24	45	VAL	3.2
7	AL04	69	HIS	3.2
2	A23S	357(L)	A	3.2
2	B23S	2334	G	3.2
5	BL02	47	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
30	AL33	42	TRP	3.2
25	BL28	95	LEU	3.2
14	BL16	90	VAL	3.2
30	AL33	31	PRO	3.2
13	AL15	35	HIS	3.2
47	BS13	37	THR	3.2
1	A16S	60	A	3.1
37	BS03	201	TYR	3.1
1	A16S	1327	C	3.1
1	A16S	1517	G	3.1
8	BL05	52	ILE	3.1
13	AL15	27	HIS	3.1
14	AL16	83	MET	3.1
15	BL17	7	GLY	3.1
19	AL21	71	LEU	3.1
45	AS11	118	GLY	3.1
9	BL06	81	GLU	3.1
9	BL06	114	VAL	3.1
12	BL14	115	VAL	3.1
43	BS09	41	VAL	3.1
9	BL06	36	PRO	3.1
43	AS09	114	TYR	3.1
2	A23S	2450	A	3.1
7	AL04	64	ILE	3.1
4	BL01	192	ALA	3.1
13	AL15	38	GLN	3.1
18	AL20	27	LEU	3.1
26	AL29	62	THR	3.1
56	BATN	40	C	3.1
2	A23S	2153	G	3.1
2	A23S	2502	G	3.1
23	BL25	43	GLU	3.1
4	AL01	44	VAL	3.1
19	AL21	37	VAL	3.1
9	BL06	42	ARG	3.1
22	AL24	60	PHE	3.1
4	BL01	190	ILE	3.1
6	AL03	155	LYS	3.1
37	AS03	152	ILE	3.1
41	BS07	28	ASN	3.1
44	BS10	74	ILE	3.1
5	BL02	272	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
13	BL15	150	ALA	3.1
4	BL01	11	LEU	3.1
34	AMRN	8	A	3.1
55	ATHX	4	GLY	3.1
56	BATN	31	A	3.1
7	AL04	95	ARG	3.1
9	BL06	123	PHE	3.1
19	AL21	79	VAL	3.1
4	BL01	175	PRO	3.1
11	BL13	127	LYS	3.1
2	B23S	101	G	3.1
9	AL06	136	ILE	3.1
44	AS10	50	ILE	3.1
4	BL01	45	HIS	3.1
23	AL25	187	ALA	3.1
1	A16S	1541	U	3.1
45	AS11	63	LEU	3.1
8	AL05	70	VAL	3.1
1	A16S	1285	A	3.1
41	BS07	36	LYS	3.1
13	BL15	47	ASP	3.1
37	AS03	183	ASP	3.1
22	BL24	53	PRO	3.1
4	BL01	34	ALA	3.0
4	BL01	137	LEU	3.0
18	AL20	39	LEU	3.0
54	BS20	12	ALA	3.0
2	B23S	2032	G	3.0
9	BL06	82	GLY	3.0
33	BL36	21	GLY	3.0
5	AL02	255	LYS	3.0
53	BS19	40	ILE	3.0
22	AL24	35	TYR	3.0
2	A23S	2453	A	3.0
1	B16S	1538	C	3.0
4	BL01	49	GLY	3.0
9	BL06	120	GLY	3.0
56	BATN	69	C	3.0
42	AS08	93	VAL	3.0
5	BL02	28	GLU	3.0
9	BL06	89	ILE	3.0
2	A23S	2357	U	3.0

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Mol	Chain	Res	Type	RSRZ
9	BL06	7	LEU	3.0
32	BL35	32	LEU	3.0
43	BS09	47	LEU	3.0
9	BL06	83	TYR	3.0
54	AS20	18	GLN	3.0
22	BL24	3	VAL	3.0
32	AL35	34	TRP	3.0
55	ATHX	13	ILE	3.0
26	BL29	10	LEU	3.0
25	AL28	24	ALA	3.0
39	AS05	21	ALA	3.0
2	B23S	2504	U	3.0
2	B23S	2611	U	3.0
4	AL01	220	GLY	3.0
22	BL24	61	ILE	3.0
2	A23S	887	A	3.0
13	AL15	62	LEU	3.0
23	AL25	150	LEU	3.0
16	AL18	27	SER	3.0
51	AS17	99	SER	3.0
1	B16S	1532	U	3.0
2	A23S	2584	U	3.0
19	BL21	80	GLN	3.0
2	A23S	508	G	2.9
2	A23S	1093	G	2.9
11	AL13	152	PRO	2.9
56	BATN	23	G	2.9
4	AL01	77	ALA	2.9
9	AL06	90	LYS	2.9
2	B23S	2602	A	2.9
41	AS07	81	GLY	2.9
49	AS15	20	GLY	2.9
44	BS10	21	GLN	2.9
3	A5S	88	C	2.9
22	BL24	44	ILE	2.9
37	BS03	152	ILE	2.9
2	A23S	2596	U	2.9
4	AL01	9	ARG	2.9
7	AL04	70	THR	2.9
24	BL27	72	ARG	2.9
19	BL21	84	LYS	2.9
30	BL33	42	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
43	AS09	98	PRO	2.9
54	AS20	29	LYS	2.9
4	BL01	171	ALA	2.9
38	AS04	4	TYR	2.9
9	AL06	52	VAL	2.9
42	AS08	129	VAL	2.9
14	AL16	92	GLY	2.9
2	A23S	611(E)	G	2.9
4	AL01	154	ILE	2.9
1	B16S	1092	A	2.9
17	BL19	99	LEU	2.9
53	BS19	5	LEU	2.9
54	AS20	58	LYS	2.9
1	B16S	970	C	2.9
1	B16S	980	C	2.9
1	B16S	1270	C	2.9
4	BL01	205	ALA	2.9
32	BL35	10	ALA	2.9
9	AL06	83	TYR	2.9
9	BL06	35	VAL	2.9
9	BL06	113	VAL	2.9
19	AL21	47	VAL	2.9
22	AL24	49	VAL	2.9
43	BS09	114	TYR	2.9
7	BL04	50	SER	2.9
37	AS03	158	GLY	2.9
4	AL01	109	MET	2.9
23	AL25	28	MET	2.9
32	BL35	35	GLN	2.9
20	AL22	4	LYS	2.9
1	A16S	1361	G	2.9
1	B16S	855	G	2.9
22	BL24	69	ALA	2.9
43	AS09	82	ALA	2.9
56	BATN	76	A	2.9
4	BL01	73	VAL	2.9
9	BL06	141	VAL	2.9
17	BL19	34	VAL	2.9
23	AL25	96	VAL	2.9
37	AS03	99	VAL	2.9
14	AL16	33	GLY	2.9
25	AL28	36	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
25	BL28	31	GLY	2.9
35	APTN	70	C	2.9
44	AS10	46	ARG	2.9
13	AL15	75	ILE	2.9
20	AL22	82	LEU	2.9
22	AL24	4	LYS	2.9
36	BS02	149	LEU	2.9
44	BS10	38	ILE	2.9
13	BL15	76	LYS	2.9
18	AL20	56	ASP	2.9
4	BL01	227	PRO	2.9
13	AL15	74	GLU	2.9
17	AL19	2	ASN	2.9
43	AS09	65	VAL	2.9
4	AL01	49	GLY	2.9
1	B16S	1268	A	2.9
10	AL09	130	TYR	2.9
13	BL15	15	ARG	2.9
53	BS19	80	TYR	2.9
55	BTHX	18	TYR	2.9
10	BL09	4	ILE	2.9
42	BS08	2	LEU	2.9
48	BS14	15	LYS	2.9
22	AL24	68	HIS	2.8
1	B16S	1028(A)	C	2.8
1	B16S	1384	C	2.8
2	B23S	2172	U	2.8
13	BL15	70	GLN	2.8
10	AL09	111	PRO	2.8
20	AL22	44	ALA	2.8
9	AL06	86	GLU	2.8
41	BS07	9	VAL	2.8
44	BS10	76	ASN	2.8
47	AS13	7	VAL	2.8
53	BS19	34	TRP	2.8
50	BS16	26	ARG	2.8
5	BL02	235	GLY	2.8
10	BL09	2	LYS	2.8
4	AL01	225	ILE	2.8
10	AL09	12	LEU	2.8
43	AS09	19	LEU	2.8
46	AS12	26	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
47	BS13	26	GLY	2.8
53	BS19	54	GLY	2.8
28	BL31	5	ILE	2.8
44	BS10	56	HIS	2.8
1	A16S	325	A	2.8
2	A23S	2059	A	2.8
2	B23S	1379	A	2.8
5	BL02	240	ALA	2.8
30	BL33	22	ALA	2.8
1	A16S	976	G	2.8
10	AL09	8	PRO	2.8
32	AL35	57	ARG	2.8
29	BL32	3	LYS	2.8
55	ATHX	12	LYS	2.8
15	BL17	4	LEU	2.8
55	BTHX	2	GLY	2.8
29	BL32	4	HIS	2.8
7	BL04	14	PRO	2.8
19	AL21	74	LYS	2.8
1	A16S	1130	A	2.8
1	B16S	78(E)	A	2.8
56	BATN	47(E)	A	2.8
9	AL06	71	LEU	2.8
43	AS09	40	LEU	2.8
4	AL01	23	ILE	2.8
9	AL06	9	ILE	2.8
9	BL06	162	ILE	2.8
20	AL22	112	GLY	2.8
22	AL24	58	GLY	2.8
2	A23S	888	C	2.8
43	AS09	15	ALA	2.8
11	AL13	121	VAL	2.8
22	BL24	8	LYS	2.8
45	AS11	124	LYS	2.8
9	BL06	148	ILE	2.8
28	BL31	42	PHE	2.8
53	BS19	49	ILE	2.8
13	BL15	109	GLY	2.8
20	BL22	60	ASN	2.8
24	BL27	78	TYR	2.8
7	BL04	69	HIS	2.8
56	BATN	43	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	A16S	1028(E)	G	2.8
2	B23S	2447	G	2.8
34	AMRN	10	G	2.8
44	AS10	44	VAL	2.8
4	BL01	33	LEU	2.8
4	BL01	210	LEU	2.8
6	AL03	195	LEU	2.8
9	BL06	80	SER	2.8
23	AL25	92	SER	2.8
28	BL31	9	LEU	2.8
4	BL01	61	GLY	2.7
5	AL02	110	GLY	2.7
9	BL06	149	ARG	2.7
25	AL28	26	ARG	2.7
30	AL33	18	ARG	2.7
4	AL01	178	LYS	2.7
10	AL09	2	LYS	2.7
25	BL28	15	ALA	2.7
9	AL06	113	VAL	2.7
47	BS13	113	PRO	2.7
54	AS20	20	LEU	2.7
1	A16S	1325	C	2.7
17	AL19	1	MET	2.7
44	BS10	47	PHE	2.7
24	AL27	10	THR	2.7
14	BL16	92	GLY	2.7
2	A23S	2251	G	2.7
2	B23S	508	G	2.7
13	BL15	33	ARG	2.7
38	AS04	76	ARG	2.7
51	BS17	75	ARG	2.7
37	BS03	3	ASN	2.7
37	BS03	26	LYS	2.7
4	BL01	199	ALA	2.7
14	AL16	28	ALA	2.7
47	AS13	30	ALA	2.7
12	AL14	5	GLN	2.7
23	AL25	86	VAL	2.7
25	AL28	30	VAL	2.7
48	BS14	7	ILE	2.7
2	B23S	2062	A	2.7
4	BL01	208	THR	2.7

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Mol	Chain	Res	Type	RSRZ
15	BL17	6	SER	2.7
37	AS03	165	THR	2.7
44	AS10	43	ARG	2.7
5	BL02	39	LYS	2.7
43	AS09	105	ASP	2.7
11	AL13	101	TYR	2.7
11	BL13	124	HIS	2.7
40	AS06	101	ALA	2.7
16	BL18	85	VAL	2.7
10	AL09	38	LEU	2.7
1	A16S	894	G	2.7
1	A16S	1131	G	2.7
9	BL06	136	ILE	2.7
15	BL17	47	PHE	2.7
25	BL28	13	ILE	2.7
5	AL02	42	GLY	2.7
9	AL06	82	GLY	2.7
9	BL06	124	GLU	2.7
9	BL06	51	ARG	2.7
13	AL15	104	GLY	2.7
9	BL06	129	THR	2.7
14	BL16	21	THR	2.7
1	A16S	5	U	2.7
1	B16S	1040	U	2.7
1	B16S	1288	A	2.7
2	A23S	2451	A	2.7
56	BATN	47(A)	A	2.7
9	BL06	157	TYR	2.7
21	AL23	4	ALA	2.7
37	BS03	24	ALA	2.7
4	AL01	176	VAL	2.7
7	AL04	132	VAL	2.7
13	BL15	27	HIS	2.7
36	BS02	15	VAL	2.7
37	BS03	207	VAL	2.7
43	BS09	17	VAL	2.7
44	AS10	49	VAL	2.7
47	BS13	90	LEU	2.7
2	B23S	888	C	2.7
4	AL01	57	GLN	2.7
13	AL15	50	ARG	2.7
6	AL03	194	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
7	AL04	207	GLY	2.7
9	AL06	135	GLY	2.7
13	BL15	52	GLU	2.7
25	AL28	10	LYS	2.7
37	BS03	166	GLU	2.7
54	AS20	34	LYS	2.7
52	BS18	82	THR	2.7
1	A16S	1323	G	2.7
9	BL06	63	SER	2.7
4	BL01	15	VAL	2.7
10	AL09	110	ASP	2.7
50	BS16	23	ASP	2.7
2	A23S	2135	A	2.6
19	AL21	80	GLN	2.6
42	AS08	13	ILE	2.6
48	BS14	19	ARG	2.6
19	AL21	24	LYS	2.6
42	AS08	135	CYS	2.6
4	AL01	105	LEU	2.6
9	BL06	84	SER	2.6
16	BL18	54	LEU	2.6
43	AS09	92	TYR	2.6
1	A16S	1312	G	2.6
2	B23S	2116	G	2.6
2	B23S	2149	G	2.6
22	AL24	61	ILE	2.6
44	BS10	23	ILE	2.6
46	BS12	111	ASP	2.6
18	AL20	34	LYS	2.6
37	AS03	150	LYS	2.6
38	AS04	206	PHE	2.6
48	BS14	14	PRO	2.6
2	A23S	2296	U	2.6
4	AL01	30	VAL	2.6
8	BL05	46	ALA	2.6
9	AL06	125	VAL	2.6
43	AS09	76	ALA	2.6
43	BS09	19	LEU	2.6
46	BS12	29	ALA	2.6
47	BS13	30	ALA	2.6
48	BS14	20	ALA	2.6
50	BS16	49	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
53	BS19	41	VAL	2.6
1	A16S	106	C	2.6
1	A16S	995	C	2.6
2	A23S	2612	C	2.6
2	A23S	2690	C	2.6
53	BS19	38	SER	2.6
11	BL13	141	LYS	2.6
22	AL24	96	ILE	2.6
36	AS02	200	ILE	2.6
47	BS13	84	ILE	2.6
53	BS19	37	ARG	2.6
55	BTHX	15	ARG	2.6
5	BL02	245	PRO	2.6
8	AL05	68	PRO	2.6
45	BS11	121	PRO	2.6
26	AL29	52	ASP	2.6
33	BL36	29	ASN	2.6
2	B23S	2249	U	2.6
2	A23S	2454	G	2.6
25	AL28	34	THR	2.6
27	BL30	58	VAL	2.6
48	BS14	13	THR	2.6
1	B16S	1000	A	2.6
2	A23S	1095	A	2.6
14	AL16	63	LYS	2.6
52	BS18	61	LYS	2.6
4	BL01	4	HIS	2.6
22	AL24	74	PRO	2.6
1	A16S	1314	C	2.6
1	B16S	1539	C	2.6
2	B23S	2499	C	2.6
22	AL24	43	ASN	2.6
43	AS09	115	GLY	2.6
5	AL02	33	LEU	2.6
46	BS12	15	GLU	2.6
9	BL06	115	VAL	2.6
41	BS07	7	ALA	2.6
44	BS10	72	VAL	2.6
47	BS13	42	ALA	2.6
2	A23S	611(D)	U	2.6
2	A23S	1083	U	2.6
2	A23S	2506	U	2.6

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Mol	Chain	Res	Type	RSRZ
47	BS13	105	THR	2.6
20	AL22	83	LYS	2.6
54	BS20	29	LYS	2.6
10	AL09	138	ILE	2.6
37	BS03	14	ILE	2.6
2	A23S	974	G	2.6
4	AL01	173	HIS	2.6
30	BL33	39	TYR	2.6
18	AL20	31	SER	2.6
23	AL25	134	PRO	2.6
2	B23S	1506(B)	A	2.6
18	BL20	23	GLY	2.6
36	AS02	98	LEU	2.6
37	BS03	101	LEU	2.6
54	BS20	24	LEU	2.6
2	A23S	574	C	2.6
26	AL29	12	GLU	2.6
53	BS19	73	GLU	2.6
41	BS07	150	ALA	2.6
4	BL01	218	THR	2.6
18	AL20	17	ILE	2.5
28	AL31	5	ILE	2.5
38	BS04	4	TYR	2.5
31	BL34	44	PRO	2.5
16	BL18	53	SER	2.5
8	BL05	24	GLY	2.5
15	AL17	7	GLY	2.5
33	BL36	37	GLY	2.5
41	AS07	16	LEU	2.5
53	BS19	71	LEU	2.5
2	A23S	2597	G	2.5
4	AL01	168	LYS	2.5
4	BL01	176	VAL	2.5
9	BL06	160	LYS	2.5
13	BL15	5	ASP	2.5
16	AL18	19	LYS	2.5
54	AS20	15	ARG	2.5
30	BL33	12	GLU	2.5
56	BATN	24	G	2.5
2	A23S	2269	A	2.5
2	A23S	2741	A	2.5
14	BL16	50	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
56	BATN	70	A	2.5
43	BS09	81	ILE	2.5
45	AS11	108	ILE	2.5
50	BS16	19	ILE	2.5
1	A16S	174	C	2.5
1	B16S	1195	C	2.5
2	A23S	1404	C	2.5
9	BL06	39	PRO	2.5
44	AS10	37	PRO	2.5
29	BL32	49	CYS	2.5
1	B16S	78(D)	U	2.5
2	A23S	155(D)	U	2.5
9	AL06	7	LEU	2.5
26	AL29	10	LEU	2.5
36	BS02	51	LEU	2.5
13	AL15	107	LYS	2.5
24	AL27	5	LYS	2.5
22	AL24	7	VAL	2.5
47	AS13	53	VAL	2.5
5	AL02	30	GLU	2.5
7	BL04	49	ALA	2.5
27	BL30	48	GLU	2.5
43	BS09	15	ALA	2.5
7	BL04	206	ILE	2.5
14	BL16	115	MET	2.5
55	ATHX	14	TRP	2.5
7	AL04	83	PHE	2.5
1	B16S	1146	A	2.5
1	B16S	1360	A	2.5
2	B23S	896	A	2.5
2	B23S	2058	A	2.5
2	B23S	2450	A	2.5
35	APTN	35	A	2.5
2	A23S	101	G	2.5
34	AMRN	6	G	2.5
9	BL06	29	PRO	2.5
31	AL34	19	ARG	2.5
53	AS19	71	LEU	2.5
1	B16S	747	C	2.5
2	A23S	1983	C	2.5
35	APTN	16	C	2.5
35	BPTN	75	C	2.5

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Mol	Chain	Res	Type	RSRZ
56	BATN	20	C	2.5
44	BS10	84	GLN	2.5
9	BL06	17	VAL	2.5
8	BL05	169	ALA	2.5
1	A16S	78(C)	U	2.5
27	AL30	34	GLU	2.5
38	BS04	34	GLU	2.5
43	BS09	12	GLU	2.5
30	AL33	29	ASN	2.5
46	BS12	6	ILE	2.5
19	BL21	38	LEU	2.5
19	BL21	71	LEU	2.5
23	BL25	18	LEU	2.5
32	AL35	64	TYR	2.5
33	BL36	30	PRO	2.5
53	BS19	76	PRO	2.5
9	BL06	138	LYS	2.5
47	AS13	102	ARG	2.5
54	AS20	24	LEU	2.5
1	B16S	1028(F)	A	2.5
2	B23S	2059	A	2.5
7	BL04	147	GLY	2.5
27	AL30	50	VAL	2.5
2	A23S	2319	G	2.5
2	B23S	1175	G	2.5
2	B23S	1888	G	2.5
35	APTN	22	G	2.5
37	AS03	166	GLU	2.5
43	AS09	110	GLU	2.5
12	BL14	81	ASP	2.5
1	A16S	723	U	2.5
4	AL01	137	LEU	2.5
6	AL03	126	PRO	2.5
8	BL05	34	LEU	2.5
11	AL13	161	LEU	2.5
19	BL21	35	LEU	2.5
21	AL23	60	ARG	2.5
41	BS07	4	ARG	2.5
49	AS15	54	ARG	2.5
28	BL31	40	HIS	2.5
5	BL02	42	GLY	2.5
8	BL05	127	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
31	AL34	46	VAL	2.5
54	AS20	45	GLN	2.5
30	AL33	22	ALA	2.4
47	BS13	107	ALA	2.4
28	BL31	26	SER	2.4
30	BL33	43	CYS	2.4
45	BS11	21	ILE	2.4
4	AL01	98	GLU	2.4
35	APTN	26	A	2.4
52	BS18	43	PHE	2.4
9	BL06	85	LYS	2.4
9	BL06	95	ARG	2.4
19	AL21	84	LYS	2.4
33	AL36	2	LYS	2.4
36	BS02	133	LYS	2.4
37	AS03	192	THR	2.4
41	AS07	156	TRP	2.4
1	A16S	1316	G	2.4
1	B16S	1050	G	2.4
1	B16S	1291	G	2.4
2	B23S	574	C	2.4
4	AL01	48	LEU	2.4
7	BL04	156	LEU	2.4
8	BL05	53	LEU	2.4
9	BL06	105	LEU	2.4
45	BS11	113	PRO	2.4
4	BL01	21	TYR	2.4
4	BL01	200	HIS	2.4
5	BL02	84	TYR	2.4
4	AL01	42	VAL	2.4
4	AL01	95	VAL	2.4
9	AL06	11	VAL	2.4
47	BS13	95	GLY	2.4
43	BS09	82	ALA	2.4
8	AL05	72	ARG	2.4
15	AL17	68	ARG	2.4
33	BL36	15	LYS	2.4
4	BL01	48	LEU	2.4
42	AS08	127	LEU	2.4
1	A16S	794	A	2.4
2	A23S	229	A	2.4
2	B23S	1204	A	2.4

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Mol	Chain	Res	Type	RSRZ
5	AL02	25	THR	2.4
9	AL06	74	ASN	2.4
9	AL06	147	ASN	2.4
13	AL15	5	ASP	2.4
14	AL16	21	THR	2.4
44	BS10	73	ASP	2.4
14	AL16	9	TYR	2.4
14	AL16	93	TYR	2.4
50	BS16	17	TYR	2.4
1	B16S	995	C	2.4
2	A23S	2586	C	2.4
35	APTN	71	C	2.4
47	AS13	33	ALA	2.4
1	B16S	1290	G	2.4
2	A23S	2500	U	2.4
2	B23S	1763	G	2.4
7	AL04	68	LYS	2.4
32	AL35	52	LYS	2.4
10	AL09	7	GLU	2.4
32	AL35	54	GLU	2.4
33	BL36	28	GLU	2.4
22	AL24	52	SER	2.4
8	AL05	53	LEU	2.4
9	BL06	33	LEU	2.4
9	BL06	88	LEU	2.4
15	AL17	4	LEU	2.4
51	AS17	74	LEU	2.4
4	BL01	139	PRO	2.4
7	BL04	70	THR	2.4
28	AL31	24	THR	2.4
36	AS02	159	PRO	2.4
9	BL06	44	VAL	2.4
19	BL21	47	VAL	2.4
23	AL25	151	HIS	2.4
30	AL33	39	TYR	2.4
43	BS09	30	GLY	2.4
1	A16S	1044	A	2.4
1	B16S	1014	A	2.4
17	AL19	95	ARG	2.4
25	AL28	32	LYS	2.4
52	BS18	81	PHE	2.4
1	A16S	314	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	A16S	1321	C	2.4
6	AL03	52	LEU	2.4
8	AL05	35	GLU	2.4
8	AL05	94	LEU	2.4
8	AL05	143	GLU	2.4
41	AS07	12	LEU	2.4
54	AS20	11	SER	2.4
2	A23S	2338	G	2.4
2	B23S	2191	G	2.4
41	BS07	47	CYS	2.4
9	BL06	10	PRO	2.4
30	BL33	41	PRO	2.4
36	BS02	107	THR	2.4
37	BS03	64	VAL	2.4
53	AS19	33	THR	2.4
4	AL01	226	ASN	2.4
4	BL01	5	GLY	2.4
17	AL19	25	GLY	2.4
37	BS03	2	GLY	2.4
4	BL01	159	ALA	2.4
8	BL05	50	ALA	2.4
9	BL06	145	ALA	2.4
43	AS09	43	ALA	2.4
43	BS09	36	TYR	2.4
54	BS20	21	LYS	2.4
11	AL13	56	LEU	2.4
18	BL20	27	LEU	2.4
1	A16S	1268	A	2.4
2	A23S	2598	A	2.4
2	B23S	2451	A	2.4
9	AL06	84	SER	2.4
2	A23S	1133	U	2.4
2	A23S	2611	U	2.4
2	B23S	2099	U	2.4
22	AL24	51	VAL	2.4
52	BS18	86	VAL	2.4
2	A23S	889	C	2.3
28	BL31	39	CYS	2.4
42	BS08	17	THR	2.3
43	BS09	27	THR	2.3
44	AS10	52	GLY	2.3
7	AL04	177	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
8	BL05	88	ILE	2.3
14	AL16	18	LYS	2.3
18	AL20	116	ALA	2.3
23	AL25	182	LYS	2.3
36	AS02	161	ALA	2.3
38	BS04	55	ALA	2.3
41	BS07	25	ALA	2.3
1	B16S	310	G	2.3
2	A23S	932	G	2.3
2	A23S	2339	G	2.3
28	AL31	9	LEU	2.3
32	AL35	35	GLN	2.3
46	AS12	9	LEU	2.3
37	BS03	35	GLU	2.3
48	AS14	8	GLU	2.3
4	BL01	202	PRO	2.3
1	B16S	1227	A	2.3
1	B16S	1286	A	2.3
1	B16S	1492	A	2.3
1	B16S	1493	A	2.3
10	AL09	91	SER	2.3
5	AL02	31	LYS	2.3
37	AS03	167	TRP	2.3
21	BL23	61	GLY	2.3
41	BS07	29	LYS	2.3
44	BS10	57	LYS	2.3
4	AL01	116	ALA	2.3
9	BL06	121	ILE	2.3
10	BL09	50	ARG	2.3
47	AS13	99	ARG	2.3
47	AS13	109	THR	2.3
48	AS14	22	THR	2.3
55	ATHX	11	GLY	2.3
55	BTHX	11	GLY	2.3
8	BL05	171	ALA	2.3
23	AL25	120	ILE	2.3
29	BL32	46	CYS	2.3
1	A16S	323	U	2.3
4	BL01	109	MET	2.3
12	BL14	1	MET	2.3
49	AS15	59	MET	2.3
53	BS19	53	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B16S	1066	C	2.3
4	AL01	197	LEU	2.3
27	AL30	28	LEU	2.3
38	BS04	11	LEU	2.3
47	AS13	81	LEU	2.3
8	AL05	66	GLN	2.3
1	A16S	105	G	2.3
1	A16S	1028(G)	G	2.3
2	A23S	2121	G	2.3
2	B23S	2056	G	2.3
10	AL09	145	VAL	2.3
56	BATN	1	G	2.3
6	BL03	152	LYS	2.3
43	AS09	95	LYS	2.3
4	AL01	52	PRO	2.3
7	AL04	46	ARG	2.3
8	BL05	16	ARG	2.3
22	BL24	56	PRO	2.3
37	AS03	127	ARG	2.3
52	BS18	80	PRO	2.3
4	BL01	64	SER	2.3
20	AL22	26	GLY	2.3
22	BL24	83	THR	2.3
37	BS03	61	ALA	2.3
43	AS09	94	ALA	2.3
43	AS09	103	THR	2.3
44	BS10	20	ALA	2.3
6	BL03	132	HIS	2.3
23	BL25	76	LEU	2.3
41	AS07	38	LEU	2.3
1	A16S	1123	A	2.3
2	A23S	1885	A	2.3
4	AL01	209	PHE	2.3
4	BL01	39	ASP	2.3
2	A23S	2449	U	2.3
1	A16S	1214	C	2.3
2	A23S	2140	C	2.3
3	B5S	12	C	2.3
16	BL18	69	VAL	2.3
29	BL32	56	LYS	2.3
35	BPTN	30	C	2.3
44	AS10	94	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
15	BL17	45	ARG	2.3
8	AL05	87	PRO	2.3
7	AL04	199	TRP	2.3
9	BL06	150	ALA	2.3
37	AS03	92	ALA	2.3
19	BL21	45	THR	2.3
39	AS05	98	THR	2.3
55	BTHX	17	THR	2.3
15	BL17	3	HIS	2.3
19	AL21	25	LEU	2.3
28	BL31	6	HIS	2.3
38	AS04	157	LEU	2.3
1	B16S	976	G	2.3
1	B16S	1028(G)	G	2.3
1	B16S	1190	G	2.3
2	A23S	2061	G	2.3
7	AL04	97	TYR	2.3
43	BS09	125	TYR	2.3
47	BS13	87	TYR	2.3
8	AL05	97	ASP	2.3
51	BS17	26	GLN	2.3
5	BL02	38	LYS	2.3
22	BL24	47	LYS	2.3
47	BS13	13	LYS	2.3
2	B23S	1847	A	2.3
4	BL01	44	VAL	2.3
9	BL06	133	VAL	2.3
22	AL24	50	ARG	2.3
47	BS13	98	VAL	2.3
51	AS17	35	VAL	2.3
2	B23S	2506	U	2.3
8	BL05	32	PRO	2.3
38	AS04	5	ILE	2.3
43	AS09	81	ILE	2.3
44	AS10	23	ILE	2.3
45	BS11	115	PRO	2.3
23	BL25	189	ALA	2.3
28	BL31	45	GLY	2.3
37	BS03	155	GLY	2.3
1	A16S	980	C	2.3
1	B16S	1267	C	2.3
8	BL05	86	MET	2.3

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Mol	Chain	Res	Type	RSRZ
39	AS05	104	ALA	2.3
41	BS07	117	ALA	2.3
54	AS20	95	ALA	2.3
35	APTN	72	C	2.3
8	AL05	34	LEU	2.3
25	BL28	35	THR	2.3
52	BS18	31	LEU	2.3
9	BL06	134	SER	2.3
17	BL19	106	SER	2.3
22	AL24	8	LYS	2.3
55	ATHX	10	ARG	2.3
6	BL03	104	VAL	2.3
10	BL09	145	VAL	2.3
9	BL06	159	GLU	2.2
1	A16S	1347	G	2.2
2	B23S	2502	G	2.2
56	BATN	15	G	2.2
48	BS14	42	ILE	2.2
9	AL06	161	GLY	2.2
22	AL24	77	PRO	2.2
23	AL25	21	ALA	2.2
41	AS07	83	ALA	2.2
1	A16S	532	A	2.2
1	A16S	792	A	2.2
1	A16S	1346	A	2.2
1	B16S	1041	A	2.2
1	B16S	1542	U	2.2
2	B23S	91	A	2.2
2	B23S	229	A	2.2
2	B23S	1067	A	2.2
2	B23S	1396	U	2.2
2	B23S	2503	A	2.2
2	B23S	2820	A	2.2
8	BL05	43	LEU	2.2
10	AL09	6	LEU	2.2
34	AMRN	18	A	2.2
9	BL06	122	THR	2.2
19	BL21	2	PHE	2.2
36	BS02	47	THR	2.2
4	BL01	8	TYR	2.2
9	AL06	110	SER	2.2
25	BL28	10	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
51	BS17	99	SER	2.2
1	A16S	379	C	2.2
1	B16S	998(A)	C	2.2
1	B16S	1037	C	2.2
2	A23S	2610	C	2.2
9	AL06	149	ARG	2.2
43	BS09	16	ARG	2.2
6	BL03	167	VAL	2.2
32	BL35	54	GLU	2.2
39	BS05	83	GLU	2.2
8	BL05	87	PRO	2.2
8	BL05	103	LEU	2.2
18	AL20	23	GLY	2.2
37	AS03	197	GLY	2.2
48	BS14	55	GLY	2.2
2	A23S	2270	G	2.2
2	B23S	2792	G	2.2
22	AL24	83	THR	2.2
53	BS19	39	THR	2.2
1	B16S	1364	U	2.2
7	AL04	45	ARG	2.2
26	BL29	36	ARG	2.2
43	BS09	128	ARG	2.2
50	AS16	32	TYR	2.2
2	A23S	1506(B)	A	2.2
2	A23S	2057	A	2.2
2	A23S	2497	A	2.2
11	AL13	99	SER	2.2
13	AL15	133	SER	2.2
6	AL03	7	VAL	2.2
24	BL27	38	VAL	2.2
32	BL35	23	VAL	2.2
48	BS14	18	VAL	2.2
50	AS16	79	VAL	2.2
8	AL05	164	GLU	2.2
44	BS10	61	GLU	2.2
1	A16S	795	C	2.2
1	B16S	328	C	2.2
1	B16S	856	C	2.2
1	B16S	1209	C	2.2
2	A23S	2474	C	2.2
4	AL01	11	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	BL01	196	ALA	2.2
6	AL03	130	GLY	2.2
13	AL15	100	LEU	2.2
48	AS14	30	ALA	2.2
19	BL21	78	LYS	2.2
7	BL04	62	ARG	2.2
42	AS08	84	ARG	2.2
47	BS13	88	ARG	2.2
5	AL02	27	THR	2.2
8	BL05	64	THR	2.2
9	BL06	70	THR	2.2
11	BL13	96	THR	2.2
21	AL23	5	TYR	2.2
6	BL03	102	VAL	2.2
10	AL09	37	VAL	2.2
23	BL25	56	VAL	2.2
26	AL29	40	SER	2.2
1	A16S	1540	U	2.2
2	A23S	2504	U	2.2
6	AL03	192	ASN	2.2
1	A16S	327	A	2.2
1	A16S	1188	A	2.2
2	A23S	352	G	2.2
2	B23S	1095	A	2.2
2	B23S	2057	A	2.2
2	B23S	2645	G	2.2
14	AL16	112	GLU	2.2
22	BL24	43	ASN	2.2
32	BL35	33	ASN	2.2
40	BS06	98	LEU	2.2
47	AS13	56	LEU	2.2
7	AL04	86	GLY	2.2
9	BL06	14	GLY	2.2
9	BL06	112	PRO	2.2
12	BL14	103	ALA	2.2
25	AL28	29	GLY	2.2
41	AS07	34	GLY	2.2
41	AS07	134	ALA	2.2
45	AS11	35	PRO	2.2
18	BL20	93	LYS	2.2
22	BL24	101	LYS	2.2
47	BS13	27	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
48	BS14	11	LYS	2.2
4	AL01	211	ARG	2.2
13	BL15	91	PHE	2.2
41	BS07	43	PHE	2.2
44	AS10	45	ARG	2.2
2	A23S	886	C	2.2
8	BL05	29	TRP	2.2
35	BPTN	72	C	2.2
9	AL06	68	THR	2.2
9	BL06	158	HIS	2.2
47	AS13	92	HIS	2.2
22	BL24	37	VAL	2.2
29	AL32	51	TYR	2.2
39	BS05	133	TYR	2.2
10	BL09	71	ILE	2.2
25	BL28	37	ILE	2.2
44	AS10	98	ILE	2.2
48	AS14	32	SER	2.2
4	BL01	138	LEU	2.2
9	BL06	87	LEU	2.2
32	AL35	60	LEU	2.2
9	BL06	116	GLU	2.2
11	AL13	68	ASN	2.2
13	AL15	120	ALA	2.2
4	BL01	151	GLY	2.2
22	AL24	71	LYS	2.2
22	BL24	63	LYS	2.2
25	BL28	23	LYS	2.2
44	BS10	31	GLY	2.2
44	BS10	77	PRO	2.2
48	AS14	17	LYS	2.2
8	BL05	166	ASP	2.2
9	BL06	137	ASP	2.2
17	AL19	87	ASP	2.2
1	A16S	134	A	2.2
1	B16S	553	A	2.2
34	BMRN	20	A	2.2
35	BPTN	35	A	2.2
1	B16S	326	G	2.2
1	B16S	966	G	2.2
2	A23S	1858	G	2.2
2	A23S	2125	G	2.2

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Mol	Chain	Res	Type	RSRZ
2	A23S	2202(D)	G	2.2
2	A23S	2582	G	2.2
2	B23S	270(Y)	G	2.2
35	BPTN	1	G	2.2
56	BATN	25	G	2.2
6	BL03	107	THR	2.1
10	AL09	76	THR	2.1
27	BL30	36	VAL	2.1
28	AL31	10	VAL	2.1
32	AL35	6	THR	2.1
41	AS07	80	VAL	2.1
8	BL05	12	TYR	2.1
11	BL13	101	TYR	2.1
14	BL16	74	TYR	2.1
1	B16S	934	C	2.1
2	A23S	1080	C	2.1
4	BL01	23	ILE	2.1
16	AL18	35	ILE	2.1
11	AL13	122	LEU	2.1
37	AS03	91	LEU	2.1
39	AS05	56	GLN	2.1
43	AS09	102	LEU	2.1
53	BS19	16	LEU	2.1
4	AL01	196	ALA	2.1
11	BL13	99	SER	2.1
13	AL15	39	LYS	2.1
19	AL21	78	LYS	2.1
22	BL24	36	ALA	2.1
37	BS03	49	SER	2.1
38	BS04	169	LYS	2.1
46	BS12	115	SER	2.1
9	BL06	53	GLU	2.1
46	BS12	72	GLU	2.1
17	BL19	81	PRO	2.1
24	BL27	8	GLY	2.1
30	AL33	26	ASN	2.1
33	AL36	30	PRO	2.1
43	BS09	115	GLY	2.1
44	BS10	46	ARG	2.1
48	BS14	12	ARG	2.1
53	AS19	42	PRO	2.1
22	BL24	51	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
28	AL31	6	HIS	2.1
42	BS08	79	VAL	2.1
45	BS11	109	VAL	2.1
4	BL01	216	THR	2.1
43	AS09	64	THR	2.1
43	BS09	7	THR	2.1
2	A23S	6	A	2.1
2	A23S	2058	A	2.1
4	AL01	138	LEU	2.1
19	AL21	39	LEU	2.1
26	BL29	15	LYS	2.1
37	BS03	4	LYS	2.1
43	BS09	127	LYS	2.1
1	A16S	966	G	2.1
1	A16S	1124	G	2.1
1	B16S	998	G	2.1
2	A23S	2489	G	2.1
8	AL05	86	MET	2.1
49	AS15	58	MET	2.1
53	BS19	66	MET	2.1
9	BL06	59	ARG	2.1
20	AL22	74	ALA	2.1
6	AL03	190	GLY	2.1
13	AL15	20	GLY	2.1
16	BL18	52	SER	2.1
17	AL19	81	PRO	2.1
43	AS09	8	GLY	2.1
43	BS09	72	GLY	2.1
46	AS12	15	GLU	2.1
52	AS18	77	GLY	2.1
1	A16S	1006	C	2.1
1	A16S	1028(A)	C	2.1
1	A16S	1028(D)	C	2.1
2	B23S	2136	C	2.1
9	AL06	44	VAL	2.1
9	BL06	79	VAL	2.1
33	BL36	16	VAL	2.1
36	BS02	7	VAL	2.1
3	A5S	1	U	2.1
4	AL01	33	LEU	2.1
5	AL02	261	LYS	2.1
10	BL09	5	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
19	AL21	95	LEU	2.1
23	AL25	127	LYS	2.1
24	BL27	5	LYS	2.1
36	BS02	42	ILE	2.1
42	AS08	133	LEU	2.1
43	AS09	36	TYR	2.1
43	AS09	56	LEU	2.1
44	BS10	75	ILE	2.1
47	AS13	63	THR	2.1
47	AS13	87	TYR	2.1
14	AL16	82	ARG	2.1
23	AL25	152	ALA	2.1
1	A16S	977	A	2.1
1	A16S	1324	A	2.1
1	B16S	974	A	2.1
1	B16S	977	A	2.1
2	B23S	2176	A	2.1
4	AL01	66	PRO	2.1
4	BL01	17	PRO	2.1
9	AL06	108	GLY	2.1
9	BL06	135	GLY	2.1
10	AL09	32	PRO	2.1
13	BL15	28	GLY	2.1
14	BL16	139	GLU	2.1
23	BL25	167	PRO	2.1
25	BL28	9	GLY	2.1
9	AL06	63	SER	2.1
54	AS20	37	SER	2.1
4	BL01	58	ASN	2.1
2	A23S	2104	G	2.1
4	AL01	63	VAL	2.1
4	AL01	120	VAL	2.1
7	BL04	114	VAL	2.1
36	AS02	93	VAL	2.1
1	A16S	132	C	2.1
1	B16S	1249	C	2.1
2	A23S	964	C	2.1
2	A23S	2179	C	2.1
2	A23S	2402	C	2.1
2	B23S	1109	C	2.1
15	AL17	99	LYS	2.1
31	AL34	14	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
47	BS13	111	LYS	2.1
4	AL01	172	ILE	2.1
23	BL25	183	LEU	2.1
50	BS16	6	LEU	2.1
9	AL06	170	ARG	2.1
20	BL22	90	ARG	2.1
8	BL05	25	TYR	2.1
28	AL31	43	TYR	2.1
32	BL35	64	TYR	2.1
41	AS07	154	TYR	2.1
47	BS13	116	THR	2.1
4	AL01	46	ALA	2.1
4	AL01	92	ALA	2.1
26	AL29	39	ALA	2.1
48	AS14	48	ALA	2.1
54	AS20	49	ALA	2.1
34	BMRN	19	U	2.1
56	BATN	35	U	2.1
41	BS07	19	GLY	2.1
14	AL16	111	GLU	2.1
18	BL20	57	PHE	2.1
19	AL21	36	PRO	2.1
22	AL24	53	PRO	2.1
25	BL28	38	SER	2.1
9	AL06	107	VAL	2.1
23	AL25	165	VAL	2.1
23	BL25	90	VAL	2.1
41	BS07	23	VAL	2.1
2	B23S	1132	A	2.1
46	AS12	90	LYS	2.1
54	AS20	74	LYS	2.1
4	AL01	186	LEU	2.1
7	BL04	172	TRP	2.1
11	BL13	130	LEU	2.1
23	BL25	137	ILE	2.1
38	BS04	132	ARG	2.1
42	BS08	138	TRP	2.1
45	BS11	108	ILE	2.1
52	AS18	79	LEU	2.1
53	AS19	69	HIS	2.1
41	BS07	20	ASP	2.1
41	BS07	33	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	BL02	254	THR	2.1
9	AL06	122	THR	2.1
23	AL25	170	THR	2.1
26	BL29	62	THR	2.1
44	BS10	92	THR	2.1
49	AS15	25	THR	2.1
1	A16S	186(G)	C	2.1
2	A23S	2139	C	2.1
1	A16S	129(A)	G	2.1
1	A16S	1028(H)	G	2.1
4	AL01	10	ALA	2.1
42	AS08	7	ALA	2.1
46	AS12	25	ALA	2.1
56	BATN	30	G	2.1
56	BATN	53	G	2.1
5	BL02	236	GLY	2.1
8	BL05	65	GLY	2.1
24	AL27	76	GLY	2.1
36	BS02	14	GLY	2.1
36	BS02	18	GLY	2.1
43	BS09	73	GLN	2.1
48	AS14	38	GLY	2.1
6	AL03	191	PRO	2.1
14	BL16	91	GLU	2.1
48	AS14	37	PHE	2.1
16	AL18	85	VAL	2.0
42	AS08	137	VAL	2.0
43	BS09	78	LYS	2.0
44	AS10	55	LYS	2.0
45	AS11	105	VAL	2.0
38	AS04	208	SER	2.0
44	AS10	35	SER	2.0
13	AL15	9	ASN	2.0
18	AL20	109	LEU	2.0
20	BL22	34	ASN	2.0
20	BL22	69	LEU	2.0
21	AL23	89	ILE	2.0
25	AL28	40	ARG	2.0
27	AL30	4	LEU	2.0
28	AL31	15	ILE	2.0
41	BS07	120	ILE	2.0
43	AS09	47	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
52	BS18	40	LEU	2.0
4	AL01	45	HIS	2.0
1	B16S	790	A	2.0
2	A23S	900	A	2.0
2	A23S	2173	A	2.0
4	AL01	174	ALA	2.0
4	AL01	208	THR	2.0
4	BL01	16	ASP	2.0
9	AL06	165	ALA	2.0
13	BL15	120	ALA	2.0
34	BMRN	13	A	2.0
36	AS02	62	ALA	2.0
37	BS03	29	TYR	2.0
43	AS09	119	ALA	2.0
45	BS11	100	ALA	2.0
47	AS13	118	ALA	2.0
47	BS13	20	THR	2.0
10	AL09	90	GLY	2.0
13	AL15	43	GLY	2.0
20	AL22	108	GLY	2.0
36	AS02	146	GLN	2.0
43	BS09	101	PHE	2.0
50	AS16	37	GLY	2.0
9	AL06	8	PRO	2.0
44	AS10	41	PRO	2.0
53	AS19	74	PHE	2.0
7	BL04	35	GLU	2.0
9	BL06	104	GLU	2.0
1	A16S	110	C	2.0
1	A16S	934	C	2.0
1	B16S	1147	C	2.0
3	A5S	12	C	2.0
31	BL34	2	LYS	2.0
9	AL06	133	VAL	2.0
14	BL16	27	VAL	2.0
22	BL24	7	VAL	2.0
44	AS10	72	VAL	2.0
54	BS20	88	VAL	2.0
1	A16S	971	G	2.0
1	B16S	108	G	2.0
1	B16S	289	G	2.0
1	B16S	724	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	B16S	973	G	2.0
1	B16S	1316	G	2.0
1	B16S	1347	G	2.0
2	A23S	1856	G	2.0
5	AL02	48	ARG	2.0
13	BL15	105	LEU	2.0
37	BS03	182	ILE	2.0
38	BS04	137	SER	2.0
49	BS15	87	ILE	2.0
50	BS16	36	ILE	2.0
1	B16S	1540	U	2.0
1	B16S	1541	U	2.0
56	BATN	41	U	2.0
4	BL01	108	TRP	2.0
4	BL01	62	THR	2.0
5	AL02	40	THR	2.0
10	BL09	36	ALA	2.0
17	AL19	116	ALA	2.0
24	BL27	10	THR	2.0
25	BL28	24	ALA	2.0
45	BS11	112	THR	2.0
47	AS13	20	THR	2.0
54	AS20	40	ALA	2.0
9	BL06	164	TYR	2.0
15	AL17	59	ASP	2.0
23	AL25	87	ASP	2.0
18	AL20	7	GLY	2.0
45	BS11	102	GLY	2.0
46	AS12	28	GLY	2.0
48	AS14	28	GLY	2.0
5	BL02	255	LYS	2.0
9	AL06	85	LYS	2.0
47	BS13	115	LYS	2.0
1	A16S	509	A	2.0
1	A16S	1534	A	2.0
1	B16S	1289	A	2.0
7	BL04	163	VAL	2.0
9	BL06	24	VAL	2.0
9	BL06	43	VAL	2.0
10	BL09	15	VAL	2.0
13	AL15	61	ARG	2.0
22	BL24	42	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
44	AS10	60	ARG	2.0
55	ATHX	24	ARG	2.0
13	BL15	62	LEU	2.0
4	AL01	100	ILE	2.0
4	BL01	104	ILE	2.0
47	AS13	4	ILE	2.0
2	A23S	192	C	2.0
2	A23S	1797	C	2.0
2	A23S	2794(C)	C	2.0
2	B23S	1141(A)	C	2.0
2	B23S	2803	C	2.0
56	BATN	47(F)	C	2.0
56	BATN	71	C	2.0

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

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	55	20/21	0.45	0.13	138,155,160,163	0
35	G7M	BPTN	46	24/25	0.45	0.14	144,157,172,188	0
35	G7M	APTN	46	24/25	0.48	0.13	175,184,204,220	0
56	PSU	BATN	39	20/21	0.48	0.22	140,150,156,157	0
56	QUO	BATN	34	32/33	0.58	0.18	125,131,141,145	0
56	MIA	BATN	37	29/30	0.62	0.19	133,139,142,148	0
35	5MU	APTN	54	21/22	0.66	0.12	155,167,169,170	0
56	5MU	BATN	54	21/22	0.68	0.12	126,150,160,164	0
35	6MZ	BPTN	37	23/24	0.71	0.19	65,76,84,98	0
35	4SU	BPTN	8	20/21	0.78	0.10	145,150,159,163	0
35	5MU	BPTN	54	21/22	0.78	0.14	128,135,141,147	0
35	PSU	APTN	55	20/21	0.78	0.10	163,176,182,183	0
35	4SU	APTN	8	20/21	0.79	0.10	179,188,195,198	0
35	CM0	APTN	34	25/26	0.79	0.19	119,126,131,132	0
35	6MZ	APTN	37	23/24	0.79	0.15	115,122,128,133	0
35	PSU	BPTN	55	20/21	0.81	0.11	132,146,156,160	0
35	CM0	BPTN	34	25/26	0.84	0.16	96,104,116,117	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	A5S	201	1/1	0.43	0.16	98,98,98,98	0
57	MG	B16S	1618	1/1	0.62	0.21	61,61,61,61	0
57	MG	A16S	1608	1/1	0.64	0.23	79,79,79,79	0
57	MG	B16S	1601	1/1	0.67	0.21	58,58,58,58	0
57	MG	AL06	201	1/1	0.68	0.15	67,67,67,67	0
57	MG	BL30	101	1/1	0.69	0.11	72,72,72,72	0
57	MG	B16S	1603	1/1	0.71	0.33	57,57,57,57	0
57	MG	AS06	202	1/1	0.71	0.19	68,68,68,68	0
57	MG	B16S	1630	1/1	0.71	0.14	58,58,58,58	0
57	MG	B5S	203	1/1	0.71	0.18	58,58,58,58	0
57	MG	BL02	301	1/1	0.71	0.21	31,31,31,31	0
57	MG	A23S	2967	1/1	0.71	0.23	60,60,60,60	0
57	MG	A16S	1604	1/1	0.72	0.12	56,56,56,56	0
57	MG	A23S	2953	1/1	0.72	0.26	62,62,62,62	0
57	MG	A23S	2963	1/1	0.72	0.18	58,58,58,58	0
57	MG	AL15	202	1/1	0.72	0.22	61,61,61,61	0
57	MG	BATN	101	1/1	0.73	0.24	80,80,80,80	0
57	MG	B23S	3015	1/1	0.73	0.23	50,50,50,50	0
57	MG	AL23	102	1/1	0.73	0.12	73,73,73,73	0
57	MG	B23S	2989	1/1	0.74	0.20	56,56,56,56	0
57	MG	A23S	2956	1/1	0.74	0.23	66,66,66,66	0
57	MG	BL25	301	1/1	0.74	0.12	46,46,46,46	0
57	MG	A23S	2916	1/1	0.74	0.23	36,36,36,36	0
57	MG	BL32	101	1/1	0.74	0.16	84,84,84,84	0
57	MG	AL14	201	1/1	0.75	0.26	58,58,58,58	0
57	MG	B23S	2930	1/1	0.75	0.15	54,54,54,54	0
57	MG	A23S	2917	1/1	0.76	0.15	52,52,52,52	0
57	MG	B16S	1624	1/1	0.76	0.14	56,56,56,56	0
57	MG	B23S	3011	1/1	0.76	0.15	52,52,52,52	0
57	MG	A23S	2918	1/1	0.76	0.22	65,65,65,65	0
57	MG	B23S	2924	1/1	0.76	0.14	62,62,62,62	0
57	MG	A23S	2973	1/1	0.77	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A23S	2910	1/1	0.77	0.23	83,83,83,83	0
57	MG	AL02	302	1/1	0.77	0.16	50,50,50,50	0
57	MG	A23S	2948	1/1	0.77	0.18	60,60,60,60	0
57	MG	B23S	2901	1/1	0.78	0.23	43,43,43,43	0
57	MG	A16S	1626	1/1	0.78	0.21	58,58,58,58	0
57	MG	AL01	301	1/1	0.78	0.20	105,105,105,105	0
57	MG	A23S	2920	1/1	0.78	0.26	56,56,56,56	0
57	MG	AL28	101	1/1	0.78	0.30	44,44,44,44	0
57	MG	A23S	2923	1/1	0.78	0.12	61,61,61,61	0
57	MG	A23S	2925	1/1	0.79	0.18	44,44,44,44	0
57	MG	BL01	301	1/1	0.79	0.15	105,105,105,105	0
57	MG	AL04	301	1/1	0.79	0.25	57,57,57,57	0
57	MG	A16S	1607	1/1	0.80	0.24	51,51,51,51	0
57	MG	B16S	1612	1/1	0.80	0.16	61,61,61,61	0
57	MG	A23S	2949	1/1	0.80	0.13	71,71,71,71	0
57	MG	A16S	1602	1/1	0.80	0.21	37,37,37,37	0
57	MG	B23S	2935	1/1	0.80	0.18	30,30,30,30	0
57	MG	B23S	2939	1/1	0.80	0.17	57,57,57,57	0
57	MG	BL15	202	1/1	0.80	0.17	64,64,64,64	0
57	MG	B23S	2943	1/1	0.80	0.20	50,50,50,50	0
57	MG	B23S	2959	1/1	0.80	0.14	69,69,69,69	0
57	MG	B16S	1627	1/1	0.80	0.14	85,85,85,85	0
57	MG	A23S	2909	1/1	0.81	0.21	40,40,40,40	0
57	MG	AL01	302	1/1	0.81	0.17	93,93,93,93	0
57	MG	B16S	1622	1/1	0.81	0.19	44,44,44,44	0
57	MG	A23S	2905	1/1	0.81	0.16	38,38,38,38	0
57	MG	B16S	1606	1/1	0.82	0.28	65,65,65,65	0
57	MG	B23S	3016	1/1	0.82	0.10	47,47,47,47	0
57	MG	B16S	1610	1/1	0.82	0.16	70,70,70,70	0
57	MG	AL17	201	1/1	0.82	0.24	51,51,51,51	0
57	MG	B23S	2950	1/1	0.82	0.08	33,33,33,33	0
57	MG	A16S	1616	1/1	0.82	0.11	62,62,62,62	0
57	MG	A16S	1633	1/1	0.82	0.10	48,48,48,48	0
57	MG	B23S	2992	1/1	0.82	0.15	32,32,32,32	0
57	MG	B23S	3006	1/1	0.82	0.13	70,70,70,70	0
57	MG	BL31	101	1/1	0.82	0.19	78,78,78,78	0
57	MG	B16S	1623	1/1	0.82	0.20	46,46,46,46	0
57	MG	B5S	201	1/1	0.83	0.28	47,47,47,47	0
57	MG	A23S	2970	1/1	0.83	0.11	73,73,73,73	0
57	MG	AS08	201	1/1	0.83	0.21	43,43,43,43	0
57	MG	AL04	302	1/1	0.83	0.14	73,73,73,73	0
57	MG	BL01	302	1/1	0.83	0.14	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A16S	1610	1/1	0.83	0.14	74,74,74,74	0
57	MG	A23S	2935	1/1	0.83	0.11	58,58,58,58	0
57	MG	B16S	1626	1/1	0.83	0.22	61,61,61,61	0
57	MG	AS02	301	1/1	0.83	0.12	90,90,90,90	0
57	MG	B23S	2946	1/1	0.83	0.09	46,46,46,46	0
57	MG	B23S	3031	1/1	0.83	0.18	53,53,53,53	0
57	MG	A23S	2930	1/1	0.84	0.24	44,44,44,44	0
57	MG	B23S	2949	1/1	0.84	0.12	31,31,31,31	0
57	MG	B16S	1608	1/1	0.84	0.18	56,56,56,56	0
57	MG	A5S	203	1/1	0.84	0.20	58,58,58,58	0
57	MG	BL18	201	1/1	0.84	0.08	57,57,57,57	0
57	MG	B23S	2982	1/1	0.84	0.14	74,74,74,74	0
57	MG	B23S	2987	1/1	0.84	0.15	32,32,32,32	0
57	MG	A16S	1601	1/1	0.84	0.20	47,47,47,47	0
57	MG	B23S	2921	1/1	0.84	0.14	56,56,56,56	0
57	MG	B23S	3029	1/1	0.85	0.17	43,43,43,43	0
57	MG	B23S	2956	1/1	0.85	0.17	42,42,42,42	0
57	MG	A23S	2946	1/1	0.85	0.17	63,63,63,63	0
57	MG	A16S	1613	1/1	0.85	0.08	78,78,78,78	0
57	MG	A23S	2957	1/1	0.85	0.25	53,53,53,53	0
57	MG	A16S	1614	1/1	0.85	0.11	42,42,42,42	0
57	MG	B23S	2990	1/1	0.85	0.16	51,51,51,51	0
57	MG	B16S	1632	1/1	0.85	0.15	50,50,50,50	0
57	MG	BL02	303	1/1	0.85	0.09	60,60,60,60	0
57	MG	A23S	2964	1/1	0.85	0.27	52,52,52,52	0
57	MG	B23S	3010	1/1	0.85	0.17	56,56,56,56	0
57	MG	B23S	2902	1/1	0.85	0.24	24,24,24,24	0
57	MG	B23S	3014	1/1	0.85	0.12	48,48,48,48	0
57	MG	AL04	303	1/1	0.85	0.07	78,78,78,78	0
57	MG	B23S	2955	1/1	0.85	0.12	45,45,45,45	0
57	MG	B16S	1604	1/1	0.86	0.22	58,58,58,58	0
57	MG	B23S	2941	1/1	0.86	0.22	35,35,35,35	0
57	MG	B16S	1613	1/1	0.86	0.15	61,61,61,61	0
57	MG	B23S	2911	1/1	0.86	0.35	38,38,38,38	0
57	MG	B23S	3000	1/1	0.86	0.17	35,35,35,35	0
57	MG	B23S	3003	1/1	0.86	0.21	46,46,46,46	0
57	MG	B23S	2917	1/1	0.86	0.19	50,50,50,50	0
57	MG	B23S	3009	1/1	0.86	0.17	46,46,46,46	0
57	MG	A23S	2903	1/1	0.86	0.27	41,41,41,41	0
57	MG	B16S	1629	1/1	0.86	0.11	82,82,82,82	0
57	MG	B23S	2925	1/1	0.86	0.18	46,46,46,46	0
57	MG	A16S	1603	1/1	0.86	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B23S	2961	1/1	0.86	0.18	42,42,42,42	0
57	MG	A16S	1618	1/1	0.86	0.18	65,65,65,65	0
57	MG	A16S	1619	1/1	0.87	0.10	42,42,42,42	0
57	MG	AS03	301	1/1	0.87	0.10	67,67,67,67	0
57	MG	B23S	2910	1/1	0.87	0.33	59,59,59,59	0
57	MG	A23S	2972	1/1	0.87	0.15	50,50,50,50	0
57	MG	B23S	2915	1/1	0.87	0.14	34,34,34,34	0
57	MG	A23S	2933	1/1	0.87	0.12	58,58,58,58	0
57	MG	A23S	2902	1/1	0.87	0.19	45,45,45,45	0
57	MG	B23S	2922	1/1	0.87	0.23	31,31,31,31	0
57	MG	AL17	202	1/1	0.87	0.20	47,47,47,47	0
57	MG	A5S	202	1/1	0.87	0.17	70,70,70,70	0
57	MG	A23S	2926	1/1	0.87	0.15	64,64,64,64	0
57	MG	B23S	2932	1/1	0.87	0.20	43,43,43,43	0
57	MG	B23S	2996	1/1	0.87	0.17	40,40,40,40	0
57	MG	B23S	2997	1/1	0.87	0.14	49,49,49,49	0
57	MG	B16S	1628	1/1	0.87	0.08	78,78,78,78	0
57	MG	BL16	201	1/1	0.87	0.14	52,52,52,52	0
57	MG	B23S	3002	1/1	0.87	0.12	43,43,43,43	0
57	MG	BL19	202	1/1	0.87	0.10	63,63,63,63	0
57	MG	AL28	102	1/1	0.87	0.22	50,50,50,50	0
57	MG	B23S	3005	1/1	0.87	0.07	50,50,50,50	0
57	MG	AL33	103	1/1	0.87	0.23	48,48,48,48	0
57	MG	B16S	1611	1/1	0.87	0.09	63,63,63,63	0
57	MG	B23S	2963	1/1	0.88	0.07	37,37,37,37	0
57	MG	B23S	2968	1/1	0.88	0.15	38,38,38,38	0
57	MG	AL34	100	1/1	0.88	0.10	55,55,55,55	0
57	MG	A23S	2913	1/1	0.88	0.22	47,47,47,47	0
57	MG	AL21	201	1/1	0.88	0.22	49,49,49,49	0
57	MG	A23S	2906	1/1	0.88	0.18	41,41,41,41	0
57	MG	BL15	203	1/1	0.88	0.14	48,48,48,48	0
57	MG	A23S	2951	1/1	0.88	0.12	50,50,50,50	0
57	MG	B23S	2951	1/1	0.88	0.18	50,50,50,50	0
57	MG	A16S	1617	1/1	0.88	0.13	61,61,61,61	0
57	MG	BL23	101	1/1	0.88	0.22	46,46,46,46	0
57	MG	B23S	2933	1/1	0.88	0.10	60,60,60,60	0
57	MG	B23S	3032	1/1	0.88	0.23	47,47,47,47	0
57	MG	A16S	1611	1/1	0.88	0.11	52,52,52,52	0
57	MG	B16S	1615	1/1	0.88	0.17	65,65,65,65	0
57	MG	A23S	2959	1/1	0.89	0.27	57,57,57,57	0
57	MG	A16S	1625	1/1	0.89	0.19	62,62,62,62	0
57	MG	B16S	1631	1/1	0.89	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B23S	3012	1/1	0.89	0.16	54,54,54,54	0
57	MG	A23S	2938	1/1	0.89	0.23	35,35,35,35	0
57	MG	B23S	2958	1/1	0.89	0.21	40,40,40,40	0
57	MG	A23S	2942	1/1	0.89	0.11	38,38,38,38	0
57	MG	B23S	3024	1/1	0.89	0.07	47,47,47,47	0
57	MG	A23S	2901	1/1	0.89	0.25	33,33,33,33	0
57	MG	B23S	2903	1/1	0.89	0.25	34,34,34,34	0
57	MG	BL24	201	1/1	0.89	0.17	89,89,89,89	0
57	MG	A16S	1620	1/1	0.89	0.17	48,48,48,48	0
57	MG	BL29	101	1/1	0.89	0.17	46,46,46,46	0
57	MG	B23S	2971	1/1	0.89	0.20	45,45,45,45	0
57	MG	B23S	2976	1/1	0.89	0.15	46,46,46,46	0
57	MG	B23S	2980	1/1	0.89	0.11	47,47,47,47	0
57	MG	BL35	101	1/1	0.89	0.10	58,58,58,58	0
57	MG	A16S	1623	1/1	0.90	0.15	42,42,42,42	0
57	MG	A23S	2961	1/1	0.90	0.10	61,61,61,61	0
57	MG	BL15	201	1/1	0.90	0.11	46,46,46,46	0
57	MG	B23S	2953	1/1	0.90	0.19	44,44,44,44	0
57	MG	B16S	1625	1/1	0.90	0.27	52,52,52,52	0
57	MG	B23S	2918	1/1	0.90	0.18	34,34,34,34	0
57	MG	B23S	2936	1/1	0.90	0.15	54,54,54,54	0
57	MG	BL19	201	1/1	0.90	0.11	68,68,68,68	0
57	MG	A23S	2944	1/1	0.90	0.26	46,46,46,46	0
57	MG	B23S	2960	1/1	0.90	0.11	59,59,59,59	0
57	MG	B16S	1617	1/1	0.90	0.18	53,53,53,53	0
57	MG	B23S	2962	1/1	0.90	0.32	50,50,50,50	0
57	MG	BL28	101	1/1	0.90	0.14	55,55,55,55	0
57	MG	B23S	2923	1/1	0.90	0.12	53,53,53,53	0
57	MG	BL29	105	1/1	0.90	0.10	58,58,58,58	0
57	MG	B23S	2964	1/1	0.90	0.12	62,62,62,62	0
57	MG	A23S	2927	1/1	0.90	0.24	37,37,37,37	0
57	MG	B23S	2969	1/1	0.90	0.12	67,67,67,67	0
57	MG	AL24	201	1/1	0.90	0.19	63,63,63,63	0
57	MG	B23S	2908	1/1	0.91	0.20	32,32,32,32	0
57	MG	A16S	1624	1/1	0.91	0.10	50,50,50,50	0
57	MG	A23S	2937	1/1	0.91	0.09	78,78,78,78	0
57	MG	B23S	3004	1/1	0.91	0.30	58,58,58,58	0
57	MG	B23S	2914	1/1	0.91	0.31	31,31,31,31	0
57	MG	A16S	1627	1/1	0.91	0.18	47,47,47,47	0
57	MG	A23S	2940	1/1	0.91	0.08	63,63,63,63	0
57	MG	B16S	1602	1/1	0.91	0.27	44,44,44,44	0
57	MG	B23S	2919	1/1	0.91	0.27	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A23S	2907	1/1	0.91	0.22	51,51,51,51	0
57	MG	A23S	2921	1/1	0.91	0.15	35,35,35,35	0
57	MG	BL20	201	1/1	0.91	0.09	44,44,44,44	0
57	MG	BL22	201	1/1	0.91	0.16	34,34,34,34	0
57	MG	A23S	2945	1/1	0.91	0.26	45,45,45,45	0
57	MG	A23S	2908	1/1	0.91	0.13	52,52,52,52	0
57	MG	B23S	2988	1/1	0.91	0.11	51,51,51,51	0
57	MG	A23S	2947	1/1	0.91	0.22	47,47,47,47	0
57	MG	B23S	2927	1/1	0.91	0.11	58,58,58,58	0
57	MG	BL29	103	1/1	0.91	0.12	30,30,30,30	0
57	MG	B23S	2957	1/1	0.91	0.07	23,23,23,23	0
57	MG	B23S	3033	1/1	0.91	0.08	67,67,67,67	0
57	MG	B23S	2994	1/1	0.91	0.09	53,53,53,53	0
57	MG	B23S	2928	1/1	0.91	0.25	35,35,35,35	0
57	MG	BL33	102	1/1	0.91	0.22	51,51,51,51	0
57	MG	B23S	2907	1/1	0.91	0.15	31,31,31,31	0
57	MG	A23S	2914	1/1	0.92	0.07	59,59,59,59	0
57	MG	B23S	2991	1/1	0.92	0.09	63,63,63,63	0
57	MG	A16S	1605	1/1	0.92	0.15	78,78,78,78	0
57	MG	B23S	3018	1/1	0.92	0.14	35,35,35,35	0
57	MG	B23S	3023	1/1	0.92	0.13	54,54,54,54	0
57	MG	A16S	1631	1/1	0.92	0.20	46,46,46,46	0
57	MG	B23S	3028	1/1	0.92	0.09	69,69,69,69	0
57	MG	B23S	2966	1/1	0.92	0.10	51,51,51,51	0
57	MG	A23S	2904	1/1	0.92	0.20	48,48,48,48	0
57	MG	A23S	2919	1/1	0.92	0.12	44,44,44,44	0
57	MG	B16S	1607	1/1	0.92	0.19	60,60,60,60	0
57	MG	A16S	1622	1/1	0.92	0.10	68,68,68,68	0
57	MG	A23S	2912	1/1	0.92	0.39	39,39,39,39	0
57	MG	B23S	2981	1/1	0.92	0.11	31,31,31,31	0
57	MG	B23S	2938	1/1	0.92	0.29	45,45,45,45	0
57	MG	B23S	2986	1/1	0.92	0.05	55,55,55,55	0
57	MG	B23S	2904	1/1	0.92	0.23	40,40,40,40	0
57	MG	A16S	1612	1/1	0.92	0.12	54,54,54,54	0
57	MG	BL04	301	1/1	0.92	0.13	55,55,55,55	0
57	MG	A23S	2939	1/1	0.92	0.11	55,55,55,55	0
57	MG	BL02	304	1/1	0.93	0.13	45,45,45,45	0
57	MG	BL03	301	1/1	0.93	0.19	51,51,51,51	0
57	MG	A23S	2962	1/1	0.93	0.12	50,50,50,50	0
57	MG	B23S	2937	1/1	0.93	0.07	52,52,52,52	0
57	MG	B16S	1605	1/1	0.93	0.15	30,30,30,30	0
57	MG	A23S	2936	1/1	0.93	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B23S	3022	1/1	0.93	0.21	46,46,46,46	0
57	MG	BL16	202	1/1	0.93	0.16	45,45,45,45	0
57	MG	B23S	2940	1/1	0.93	0.27	44,44,44,44	0
57	MG	A23S	2932	1/1	0.93	0.26	43,43,43,43	0
57	MG	B23S	3026	1/1	0.93	0.11	42,42,42,42	0
57	MG	AS06	201	1/1	0.93	0.08	82,82,82,82	0
57	MG	A23S	2943	1/1	0.93	0.15	52,52,52,52	0
57	MG	B23S	2948	1/1	0.93	0.28	32,32,32,32	0
57	MG	A23S	2969	1/1	0.93	0.12	47,47,47,47	0
57	MG	A16S	1609	1/1	0.93	0.08	71,71,71,71	0
57	MG	AL33	102	1/1	0.93	0.05	45,45,45,45	0
57	MG	B23S	2952	1/1	0.93	0.10	42,42,42,42	0
57	MG	B5S	205	1/1	0.93	0.10	38,38,38,38	0
57	MG	B16S	1614	1/1	0.93	0.14	46,46,46,46	0
57	MG	A16S	1630	1/1	0.93	0.29	55,55,55,55	0
57	MG	B23S	2983	1/1	0.93	0.07	46,46,46,46	0
57	MG	B23S	2916	1/1	0.93	0.12	43,43,43,43	0
57	MG	BL02	302	1/1	0.93	0.08	65,65,65,65	0
57	MG	B16S	1616	1/1	0.93	0.09	44,44,44,44	0
57	MG	BTHX	101	1/1	0.93	0.06	117,117,117,117	0
57	MG	BL18	202	1/1	0.94	0.06	45,45,45,45	0
57	MG	B23S	2912	1/1	0.94	0.28	27,27,27,27	0
57	MG	B23S	2913	1/1	0.94	0.14	28,28,28,28	0
57	MG	B23S	2954	1/1	0.94	0.06	56,56,56,56	0
57	MG	BL21	201	1/1	0.94	0.06	69,69,69,69	0
57	MG	A23S	2911	1/1	0.94	0.07	40,40,40,40	0
57	MG	B23S	3021	1/1	0.94	0.08	63,63,63,63	0
57	MG	B23S	2926	1/1	0.94	0.26	41,41,41,41	0
57	MG	BL24	202	1/1	0.94	0.05	53,53,53,53	0
57	MG	A16S	1632	1/1	0.94	0.09	65,65,65,65	0
57	MG	A16S	1629	1/1	0.94	0.06	93,93,93,93	0
57	MG	B23S	3025	1/1	0.94	0.14	45,45,45,45	0
57	MG	BL29	102	1/1	0.94	0.15	23,23,23,23	0
57	MG	B23S	2944	1/1	0.94	0.12	41,41,41,41	0
57	MG	BL29	104	1/1	0.94	0.12	46,46,46,46	0
57	MG	B23S	3027	1/1	0.94	0.10	39,39,39,39	0
57	MG	B23S	2945	1/1	0.94	0.27	35,35,35,35	0
57	MG	A16S	1606	1/1	0.94	0.11	29,29,29,29	0
57	MG	B16S	1619	1/1	0.94	0.10	50,50,50,50	0
57	MG	A23S	2928	1/1	0.94	0.10	32,32,32,32	0
57	MG	AL15	201	1/1	0.94	0.12	74,74,74,74	0
57	MG	A16S	1628	1/1	0.94	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B23S	2970	1/1	0.95	0.07	57,57,57,57	0
57	MG	B23S	2934	1/1	0.95	0.20	24,24,24,24	0
57	MG	B5S	204	1/1	0.95	0.07	55,55,55,55	0
57	MG	B23S	2993	1/1	0.95	0.09	43,43,43,43	0
57	MG	B23S	2974	1/1	0.95	0.26	45,45,45,45	0
57	MG	B23S	3017	1/1	0.95	0.07	46,46,46,46	0
57	MG	B23S	2995	1/1	0.95	0.13	57,57,57,57	0
57	MG	A23S	2966	1/1	0.95	0.18	46,46,46,46	0
57	MG	B23S	2906	1/1	0.95	0.09	37,37,37,37	0
57	MG	AL33	101	1/1	0.95	0.10	60,60,60,60	0
57	MG	BL28	102	1/1	0.95	0.10	41,41,41,41	0
57	MG	A23S	2941	1/1	0.95	0.29	46,46,46,46	0
57	MG	A23S	2950	1/1	0.95	0.06	34,34,34,34	0
57	MG	B23S	2985	1/1	0.95	0.11	42,42,42,42	0
57	MG	A23S	2954	1/1	0.95	0.12	40,40,40,40	0
57	MG	B23S	2920	1/1	0.95	0.09	31,31,31,31	0
57	MG	B23S	3008	1/1	0.95	0.12	53,53,53,53	0
57	MG	B23S	3030	1/1	0.95	0.07	61,61,61,61	0
57	MG	B23S	2942	1/1	0.95	0.10	41,41,41,41	0
57	MG	BL16	203	1/1	0.95	0.05	69,69,69,69	0
57	MG	BL34	101	1/1	0.95	0.34	41,41,41,41	0
57	MG	AL27	101	1/1	0.95	0.09	40,40,40,40	0
57	MG	A23S	2960	1/1	0.95	0.16	56,56,56,56	0
57	MG	AL20	201	1/1	0.96	0.13	75,75,75,75	0
57	MG	A23S	2931	1/1	0.96	0.18	40,40,40,40	0
57	MG	AL23	101	1/1	0.96	0.11	57,57,57,57	0
57	MG	A23S	2924	1/1	0.96	0.06	46,46,46,46	0
57	MG	B23S	2967	1/1	0.96	0.08	64,64,64,64	0
57	MG	B23S	2905	1/1	0.96	0.15	31,31,31,31	0
57	MG	B23S	2929	1/1	0.96	0.14	38,38,38,38	0
57	MG	A16S	1621	1/1	0.96	0.07	63,63,63,63	0
57	MG	A23S	2971	1/1	0.96	0.04	102,102,102,102	0
57	MG	B23S	2972	1/1	0.96	0.14	62,62,62,62	0
57	MG	A16S	1615	1/1	0.96	0.08	51,51,51,51	0
57	MG	A23S	2958	1/1	0.96	0.07	50,50,50,50	0
57	MG	B23S	2978	1/1	0.96	0.16	39,39,39,39	0
57	MG	B23S	2979	1/1	0.96	0.10	51,51,51,51	0
57	MG	B16S	1620	1/1	0.96	0.05	76,76,76,76	0
57	MG	BL33	103	1/1	0.96	0.06	61,61,61,61	0
57	MG	B23S	2998	1/1	0.96	0.05	51,51,51,51	0
57	MG	B23S	2999	1/1	0.96	0.08	35,35,35,35	0
57	MG	BL36	101	1/1	0.96	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BS16	101	1/1	0.96	0.11	71,71,71,71	0
57	MG	BS17	201	1/1	0.96	0.16	66,66,66,66	0
57	MG	A23S	2952	1/1	0.96	0.07	43,43,43,43	0
57	MG	AL21	203	1/1	0.97	0.08	86,86,86,86	0
57	MG	A23S	2934	1/1	0.97	0.12	39,39,39,39	0
57	MG	A23S	2968	1/1	0.97	0.16	51,51,51,51	0
57	MG	B23S	3019	1/1	0.97	0.09	51,51,51,51	0
57	MG	A23S	2955	1/1	0.97	0.07	58,58,58,58	0
57	MG	BL33	101	1/1	0.97	0.17	57,57,57,57	0
57	MG	B23S	2984	1/1	0.97	0.25	41,41,41,41	0
57	MG	A23S	2922	1/1	0.97	0.05	58,58,58,58	0
57	MG	AL21	202	1/1	0.97	0.05	77,77,77,77	0
57	MG	BL34	102	1/1	0.97	0.08	38,38,38,38	0
57	MG	B23S	2975	1/1	0.97	0.05	37,37,37,37	0
57	MG	B23S	2909	1/1	0.97	0.24	32,32,32,32	0
57	MG	B23S	3013	1/1	0.97	0.08	77,77,77,77	0
57	MG	B23S	2947	1/1	0.97	0.11	41,41,41,41	0
57	MG	B23S	2931	1/1	0.97	0.18	33,33,33,33	0
58	SF4	AS04	501	8/8	0.97	0.06	60,86,91,92	0
57	MG	B23S	3020	1/1	0.98	0.05	53,53,53,53	0
57	MG	B16S	1609	1/1	0.98	0.05	65,65,65,65	0
57	MG	B23S	2973	1/1	0.98	0.12	54,54,54,54	0
57	MG	A23S	2929	1/1	0.98	0.05	52,52,52,52	0
57	MG	AL02	301	1/1	0.98	0.05	51,51,51,51	0
57	MG	BL18	203	1/1	0.98	0.06	80,80,80,80	0
57	MG	BL02	305	1/1	0.98	0.06	59,59,59,59	0
57	MG	A23S	2965	1/1	0.98	0.06	62,62,62,62	0
57	MG	B23S	3007	1/1	0.98	0.09	34,34,34,34	0
57	MG	B16S	1621	1/1	0.98	0.13	38,38,38,38	0
57	MG	B23S	2965	1/1	0.98	0.03	43,43,43,43	0
57	MG	B23S	3001	1/1	0.98	0.05	32,32,32,32	0
58	SF4	BS04	501	8/8	0.98	0.07	76,98,101,103	0
57	MG	B5S	202	1/1	0.99	0.03	58,58,58,58	0
57	MG	B23S	2977	1/1	0.99	0.02	63,63,63,63	0
57	MG	A23S	2915	1/1	0.99	0.11	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.