Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 01:09 am BST

PDB ID	:	6S47 / pdb_00006s47
EMDB ID	:	EMD-10098
Title	:	Saccharomyces cerevisiae 80S ribosome bound with ABCF protein New1
Authors	:	Kasari, V.; Pochopien, A.A.; Margus, T.; Murina, V.; Turnbull, K.; Zhou, Y.; Nissan, T.; Graf, M.; Novacek, J.; Atkinson, G.C.; Johansson, M.J.O.; Wilson, D.N.; Hauryliuk, V.
Deposited on	:	2019-06-26
Resolution	:	3.28 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

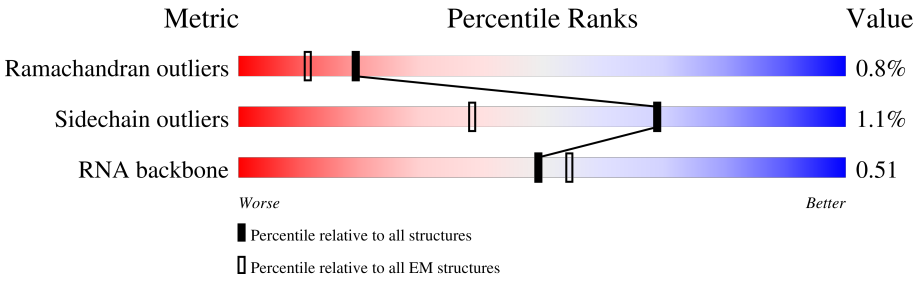
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	3149	5% 75% 22%
2	AB	121	79% 21%
3	AC	158	75% 25%
4	AD	252	99%
5	AE	386	97%
6	AF	361	96%
7	AG	296	7% 98%
8	AH	175	7% 87% 11%

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Mol	Chain	Length	Quality of chain
9	AI	243	88% 9%
10	AJ	233	9% 100%
11	AK	191	6% 98%
12	AL	220	6% 96%
13	AM	169	6% 96%
14	AN	198	9% 94%
15	AO	137	5% 98%
16	AP	203	99%
17	AQ	198	98%
18	AR	183	9% 98%
19	AS	185	6% 99%
20	AT	188	81% 19%
21	AU	172	5% 98%
22	AV	159	6% 99%
23	AW	120	10% 83% 17%
24	AX	136	6% 100%
25	AY	155	39% 61%
26	AZ	141	86% 14%
27	Aa	126	99%
28	Ab	135	99%
29	Ac	148	97%
30	Ad	58	12% 100%
31	Ae	104	92% 7%
32	Af	112	12% 96%
33	Ag	129	5% 98%

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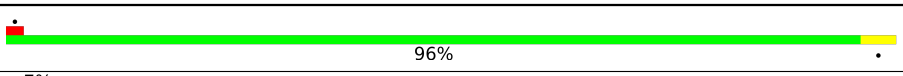
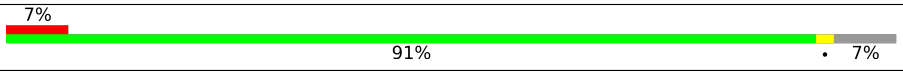
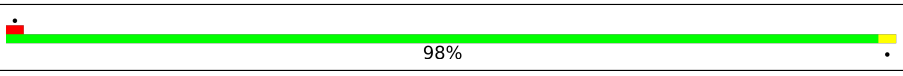
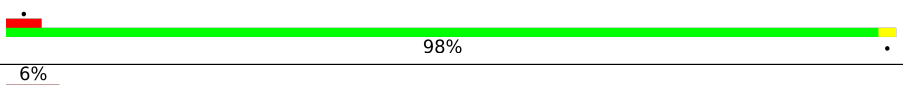
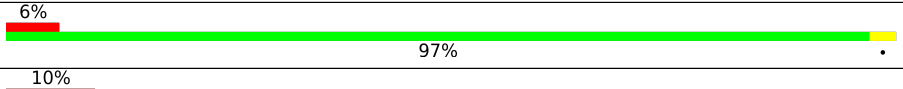
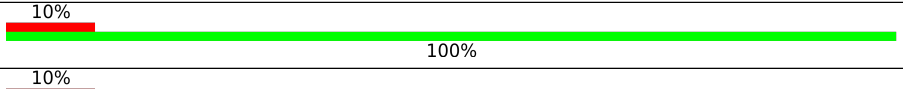
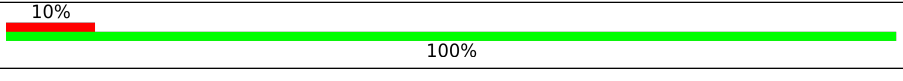
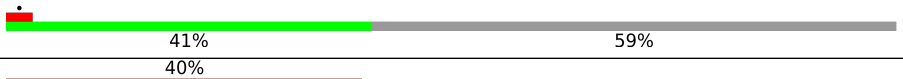
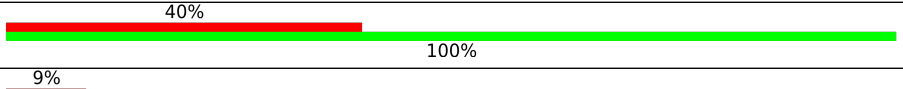
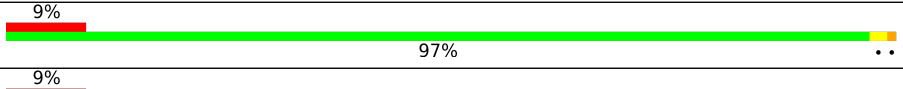
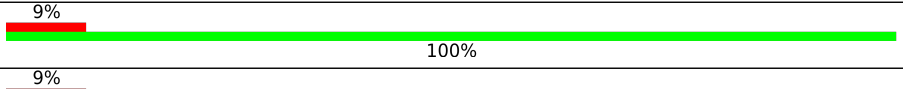
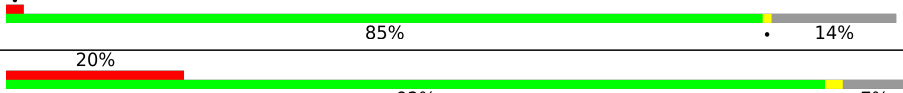
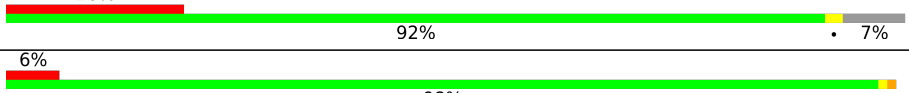
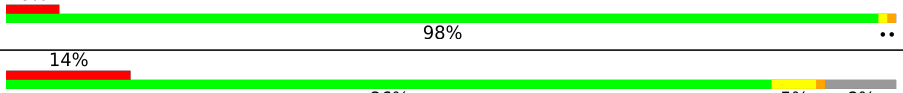
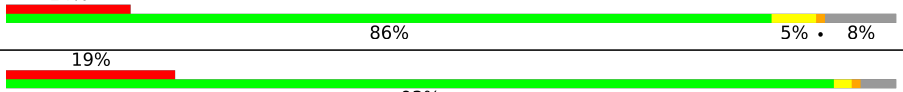
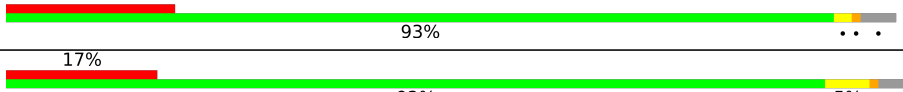
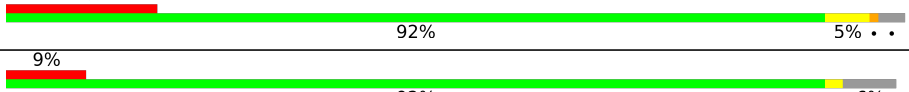
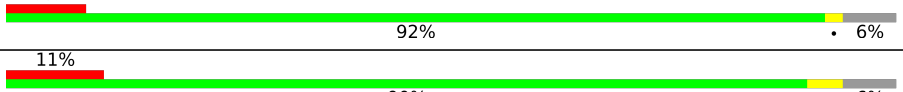
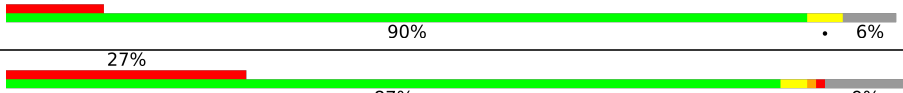
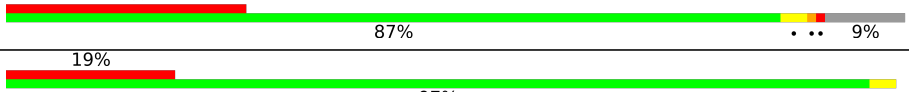
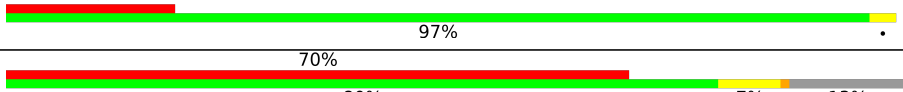
Mol	Chain	Length	Quality of chain
34	Ah	106	
35	Ai	121	
36	Aj	119	
37	Ak	99	
38	Al	87	
39	Am	77	
40	An	50	
41	Ao	127	
42	Ap	25	
43	Aq	105	
44	Ar	91	
45	BA	1707	
46	BB	251	
47	BC	254	
48	BD	253	
49	BE	239	
50	BF	260	
51	BG	224	
52	BH	236	
53	BI	189	
54	BJ	199	
55	BK	196	
56	BL	105	
57	BM	155	
58	BN	142	

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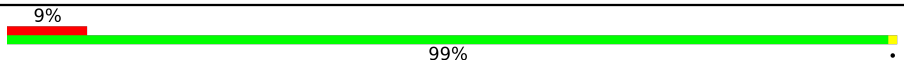
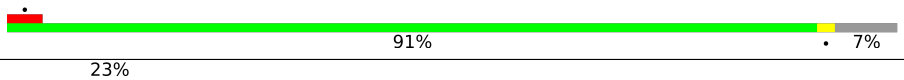
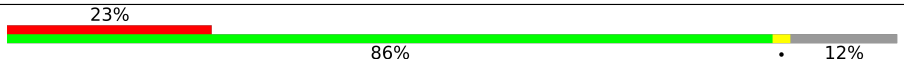
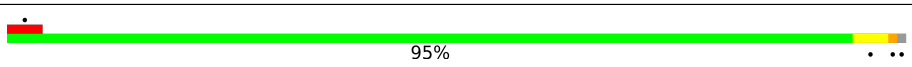
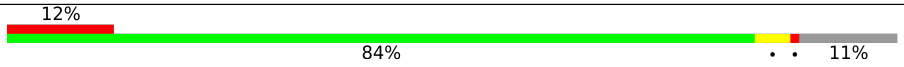
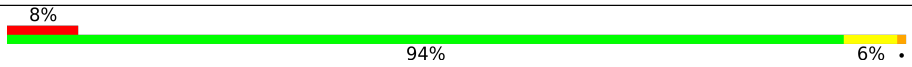
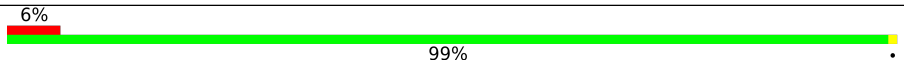
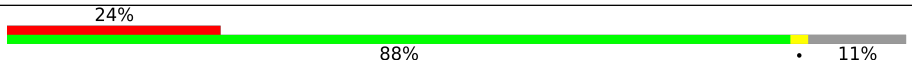
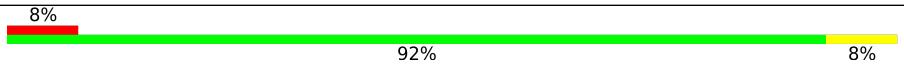
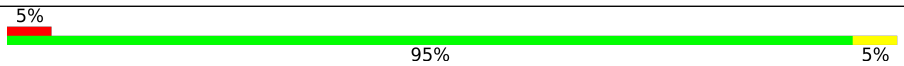
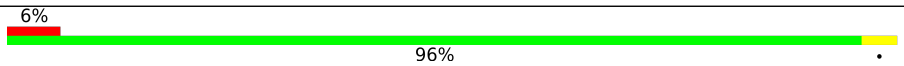
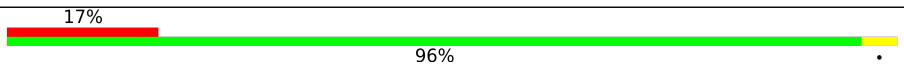
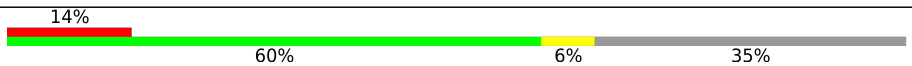
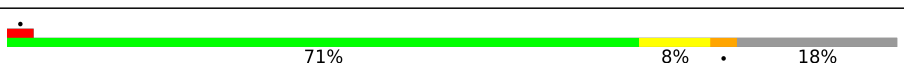
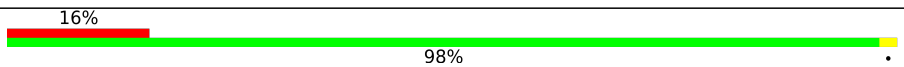
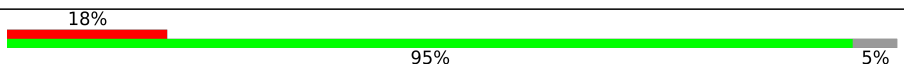
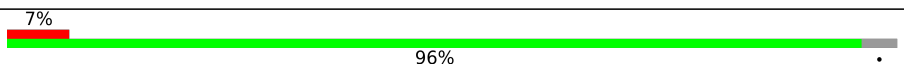
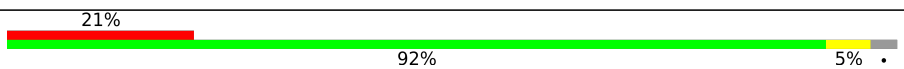
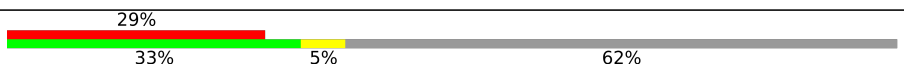
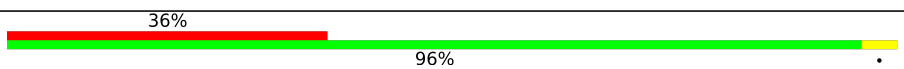
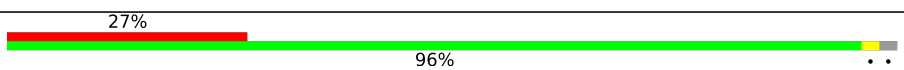
Mol	Chain	Length	Quality of chain
59	BO	150	
60	BP	136	
61	BQ	141	
62	BR	142	
63	BS	135	
64	BT	145	
65	BU	143	
66	BV	120	
67	BW	87	
68	BX	129	
69	BY	144	
70	BZ	134	
71	Ba	107	
72	Bb	118	
73	Bc	81	
74	Bd	66	
75	Be	55	
76	Bf	62	
77	Bg	151	
78	Bh	318	
79	Bi	972	

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 204313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	3149	67355	30086	12142	21978	3149	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	121	2579	1152	461	845	121	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AC	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	252	1914	1191	388	334	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	386	3075	1950	584	533	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	361	2748	1729	522	494	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AN	193	Total 1543	C 962	N 315	O 266	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	136	Total 1053	C 675	N 199	O 177	S 2	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	203	Total 1720	C 1077	N 361	O 281	S 1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	197	Total 1555	C 1003	N 289	O 262	S 1	0	0

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	183	Total 1420	C 882	N 281	O 257	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	185	Total 1441	C 908	N 290	O 241	S 2	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	AT	152	Total 1228	C 763	N 260	O 205	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	AW	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Aa	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Ab	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Ad	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	97	Total 743	C 479	N 124	O 139	S 1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	109	Total 876	C 556	N 167	O 152	S 1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	127	Total 1020	C 647	N 205	O 167	S 1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ah	106	Total 850	C 540	N 165	O 144	S 1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aj	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ak	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Al	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Am	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	An	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ao	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ap	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Aq	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ar	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 45 is a RNA chain called 18S rRNA (1707-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BA	1707	Total	C	N	O	P	0	0
			36375	16263	6440	11965	1707		

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BB	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BC	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 48 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BD	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BF	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 51 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BG	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BH	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	BI	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BJ	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BK	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BL	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BN	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 59 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BO	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 60 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BP	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BQ	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	BR	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BS	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BT	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BU	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 66 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BV	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BW	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BX	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BY	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	BZ	134	Total 1073	C 676	N 208	O 189	0	0

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	Ba	70	Total 563	C 360	N 104	O 99	0	0

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bb	97	Total 769	C 475	N 160	O 129	S 5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bc	81	Total 610	C 382	N 110	O 113	S 5	0	0

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bd	63	Total 497	C 306	N 99	O 91	S 1	0	0

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Be	53	Total 442	C 274	N 92	O 72	S 4	0	0

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bf	60	Total 475	C 299	N 98	O 77	S 1	0	0

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bg	57	Total	C	N	O	S	0	0
			444	281	82	77	4		

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bh	318	Total	C	N	O	S	0	0
			2441	1544	419	470	8		

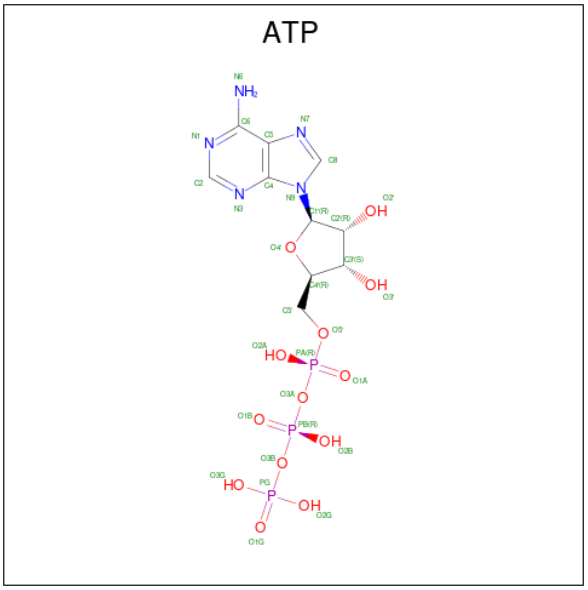
- Molecule 79 is a protein called [NU+] prion formation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bi	952	Total	C	N	O	S	0	0
			7512	4763	1271	1450	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bi	495	ASP	SER	conflict	UNP Q08972
Bi	713	GLN	GLU	conflict	UNP Q08972
Bi	1058	GLN	GLU	conflict	UNP Q08972

- Molecule 80 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
80	Bi	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Continued from previous page...

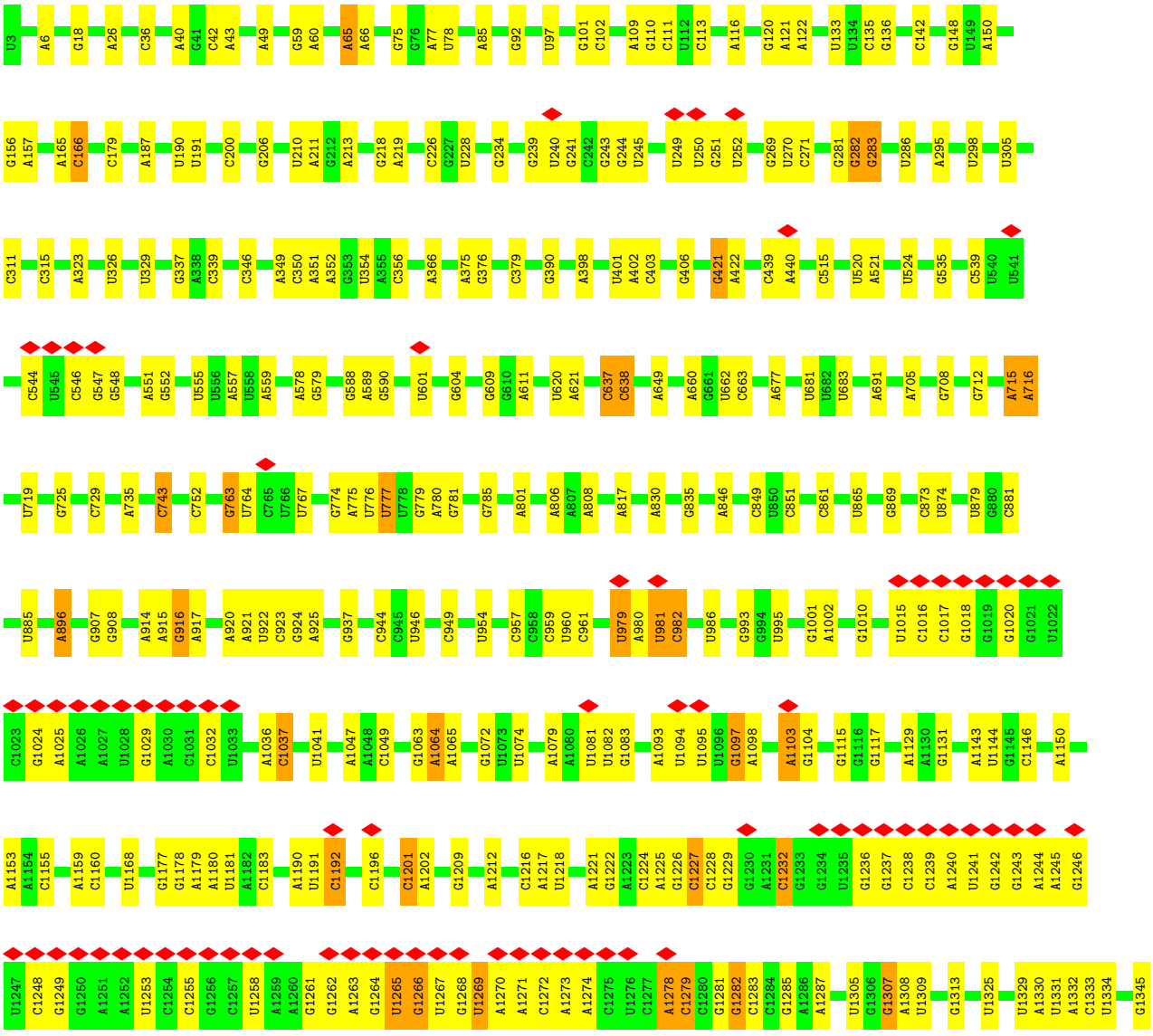
Mol	Chain	Residues	Atoms					AltConf
80	Bi	1	Total	C	N	O	P	0
			31	10	5	13	3	

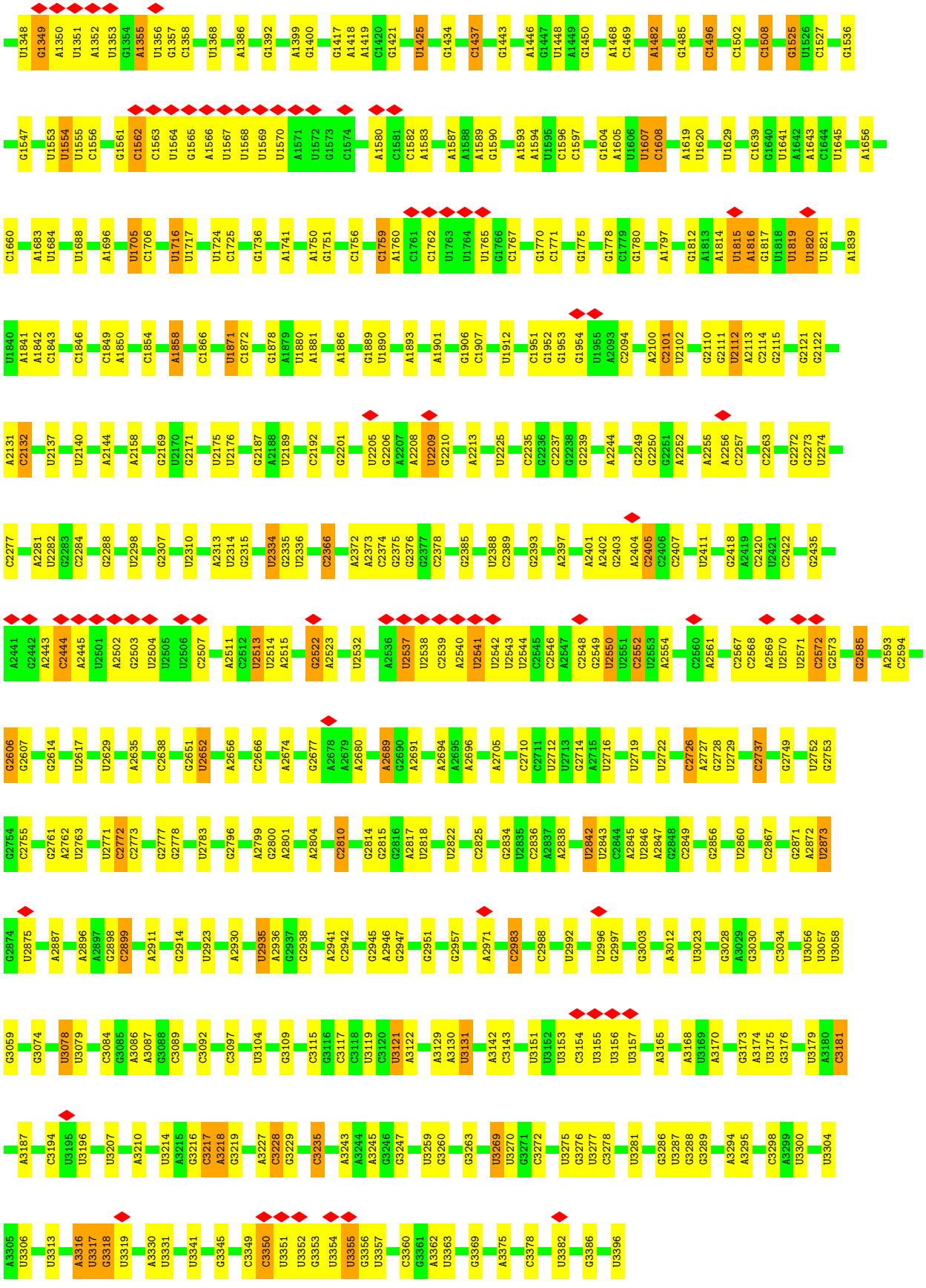
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 28S ribosomal RNA

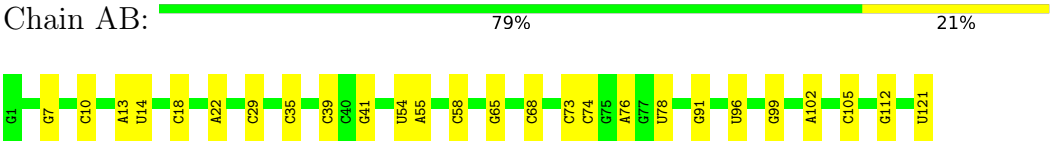
Chain AA: 




U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 U1368 A1386 G1392 A1399 G1400 G1417 A1418 A1419 C1420 G1421 U1425 G1434 C1437 G1443 A1446 G1447 U1448 A1449 G1450 A1468 C1469 A1482 G1485 C1496 C1502 C1508 G1525 U1526 C1527 G1536
G1547 U1553 U1554 U1555 C1556 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1580 C1581 C1582 A1583 A1587 A1588 A1589 G1590 A1593 A1594 U1595 C1596 C1597 G1604 A1605 U1606 U1607 C1608 A1619 U1620 U1629 C1639 G1640 U1641 A1642 A1643 C1644 U1645 A1656
C1660 A1683 U1684 U1688 A1696 U1705 C1706 U1716 U1717 U1724 C1725 G1736 A1741 A1750 G1751 C1756 C1759 A1760 C1761 C1762 U1763 U1764 U1765 G1766 C1767 G1770 C1771 G1775 G1778 C1779 G1780 A1797 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 A1839
U1840 A1841 A1842 C1843 C1846 C1849 A1850 C1854 A1858 C1866 U1871 C1872 G1878 A1879 U1880 A1881 A1886 G1889 U1890 A1893 A1901 G1906 C1907 U1912 C1951 G1952 G1953 G1954 U1955 A2093 C2094 A2100 C2101 U2102 G2110 G2111 U2112 A2113 C2114 G2115 G2121 G2122
A2131 C2132 U2137 U2140 A2144 A2158 G2169 U2170 G2171 U2175 U2176 G2187 A2188 U2189 C2192 G2201 U2205 G2206 A2207 A2208 U2209 G2210 A2213 U2225 C2235 G2236 C2237 G2238 G2239 A2244 G2249 G2250 G2251 A2252 A2255 A2256 C2257 C2263 G2272 G2273 U2274
C2277 A2281 U2282 G2283 C2284 G2288 U2298 G2307 U2310 A2313 U2314 G2315 U2334 G2335 U2336 C2366 A2372 A2373 C2374 G2375 G2376 G2377 C2378 G2385 U2388 C2389 G2393 A2397 A2401 A2402 G2403 A2404 C2405 C2406 C2407 U2411 G2418 A2419 C2420 U2421 C2422 G2435
A2441 G2442 A2443 C2444 A2445 U2501 A2502 G2503 U2504 U2505 U2506 C2507 A2511 C2512 U2513 U2514 A2515 G2522 A2523 U2532 A2536 U2537 U2538 C2539 A2540 U2541 U2542 U2543 U2544 C2545 C2546 A2547 C2548 G2549 U2550 U2551 C2552 U2553 A2554 C2560 A2561 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2585 A2593 C2594
G2606 G2607 G2614 U2617 U2629 A2635 C2638 G2651 U2652 A2656 C2666 A2674 G2677 A2678 A2679 A2680 A2689 C2690 A2691 A2694 A2695 A2696 A2705 C2710 C2711 U2712 U2713 G2714 A2715 U2716 U2719 U2722 C2726 A2727 G2728 U2729 C2737 G2749 U2752 G2753
G2754 C2755 G2761 A2762 U2763 U2771 C2772 C2773 G2777 G2778 U2783 G2796 A2799 G2800 A2801 A2804 C2810 G2814 G2815 G2816 A2817 U2818 U2822 C2825 G2834 U2835 C2836 A2837 A2838 U2842 U2843 C2844 A2845 U2846 A2847 G2848 C2849 G2856 U2860 C2867 G2871 A2872 U2873
G2874 U2875 A2887 A2896 A2897 G2898 C2899 A2911 G2914 U2923 A2930 U2935 A2936 G2937 G2938 A2941 C2942 G2945 A2946 G2947 G2951 G2957 A2971 C2983 C2988 U2992 U2996 G2997 G3003 A3012 U3023 G3028 A3029 G3030 C3034 U3056 U3057 U3058
G3059 G3074 U3078 U3079 C3084 G3085 A3086 A3087 G3088 C3089 C3092 C3097 U3104 G3109 C3115 G3116 C3117 C3118 U3119 C3120 U3121 A3122 A3129 A3130 U3131 A3142 C3143 U3151 U3152 U3153 C3154 U3155 U3156 U3157 A3165 A3168 U3169 A3170 G3173 A3174 U3175 G3176 U3179 A3180 C3181
A3187 C3194 U3195 U3196 U3207 A3210 U3214 A3215 G3216 C3217 A3218 G3219 A3227 G3228 G3229 C3235 A3243 A3244 A3245 G3246 G3247 U3259 G3260 G3263 U3269 U3270 G3271 C3272 U3275 G3276 U3277 C3278 U3281 G3286 U3287 G3288 G3289 A3294 A3295 C3298 A3299 U3300 U3304
A3305 U3306 U3313 A3316 U3317 G3318 U3319 A3330 U3331 U3341 G3345 C3349 C3350 U3351 U3352 G3353 U3354 U3355 G3356 U3357 C3360 G3361 A3362 U3363 G3369 A3375 C3378 U3382 G3386 U3396

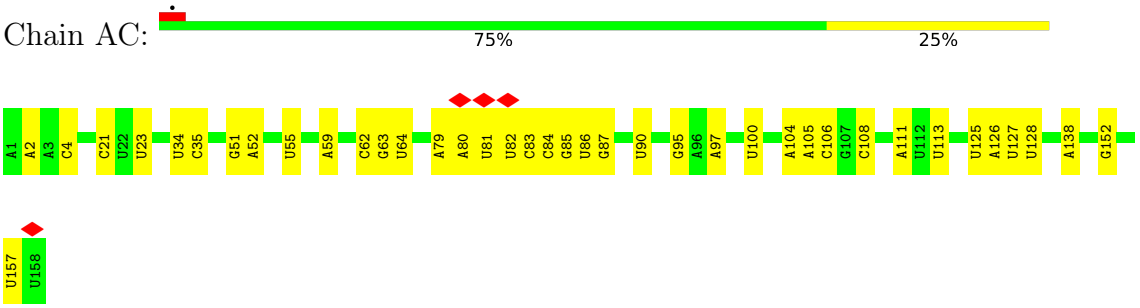
• Molecule 2: 5S ribosomal RNA

Chain AB:



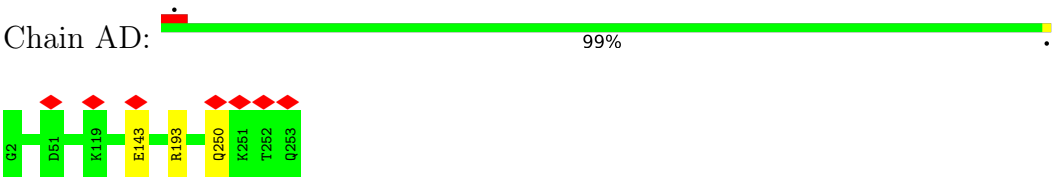
• Molecule 3: 5.8S ribosomal RNA

Chain AC:



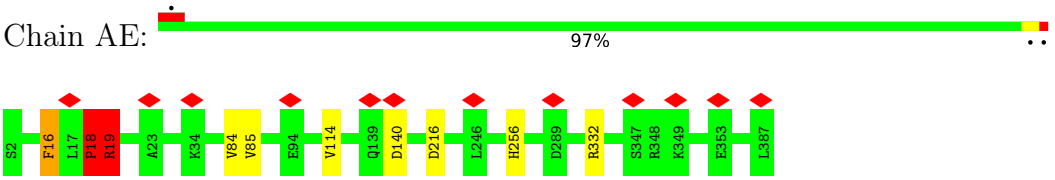
• Molecule 4: 60S ribosomal protein L2-A

Chain AD:



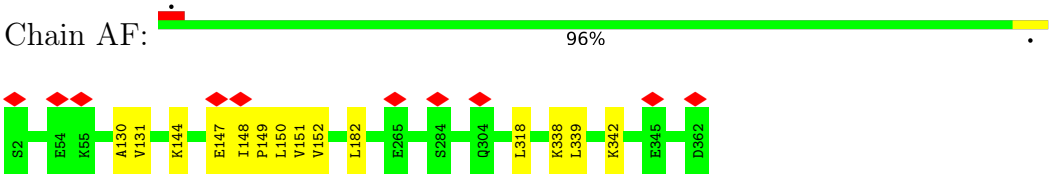
• Molecule 5: 60S ribosomal protein L3

Chain AE:



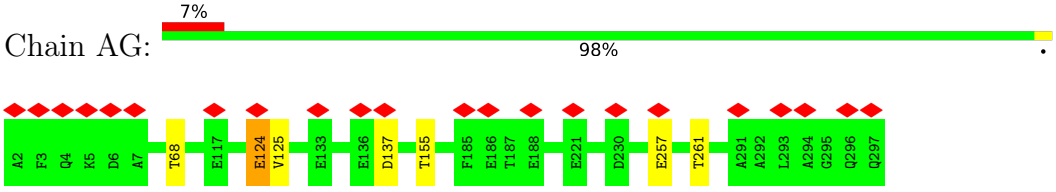
• Molecule 6: 60S ribosomal protein L4-A

Chain AF:

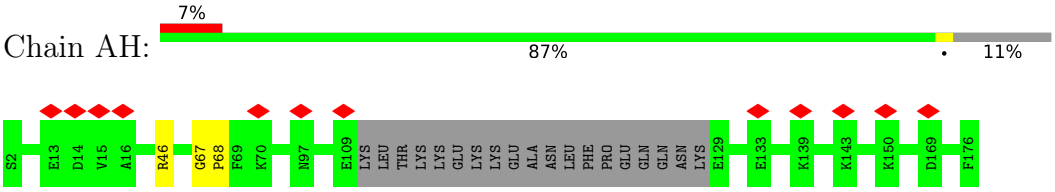


• Molecule 7: 60S ribosomal protein L5

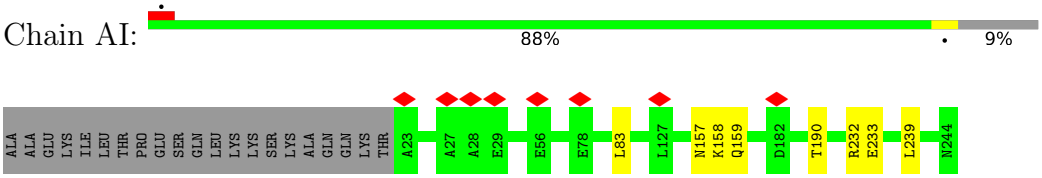
Chain AG:



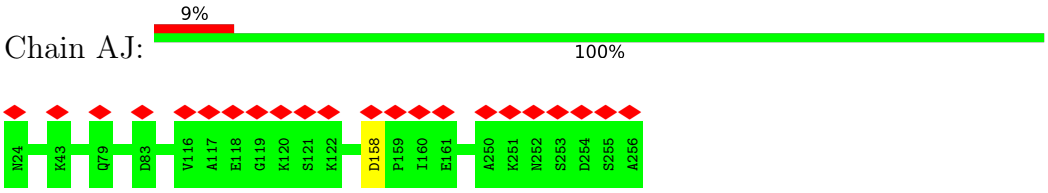
• Molecule 8: 60S ribosomal protein L6-A



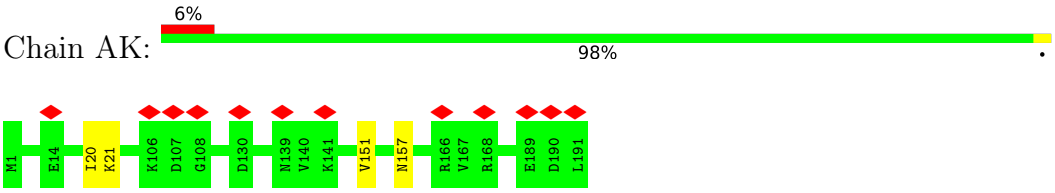
• Molecule 9: 60S ribosomal protein L7-A



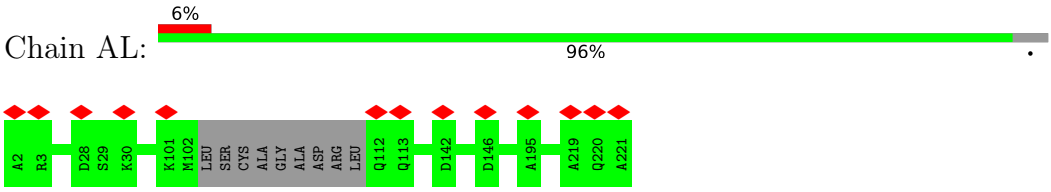
• Molecule 10: 60S ribosomal protein L8-A



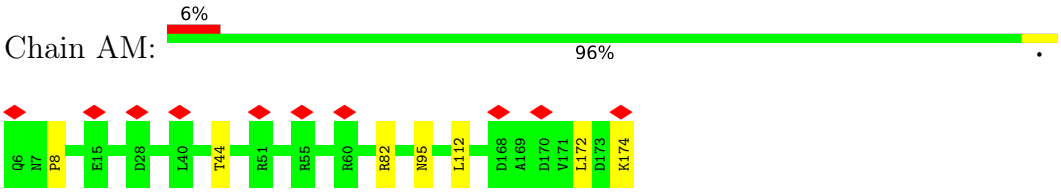
• Molecule 11: 60S ribosomal protein L9-A



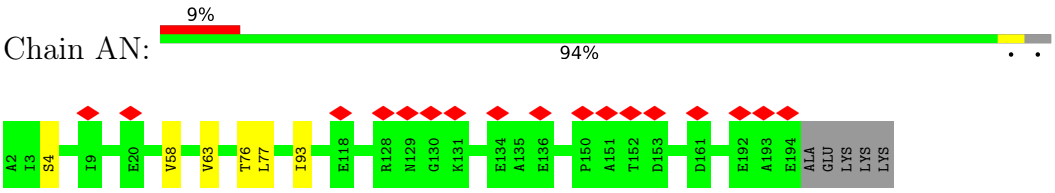
• Molecule 12: 60S ribosomal protein L10



• Molecule 13: 60S ribosomal protein L11-B

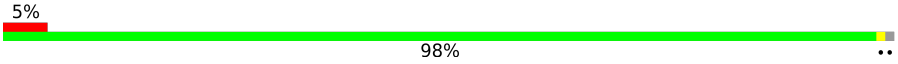


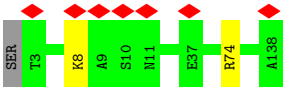
• Molecule 14: 60S ribosomal protein L13-A



• Molecule 15: 60S ribosomal protein L14-A

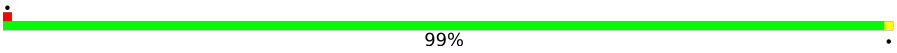
Chain AO:





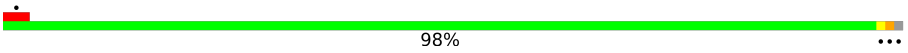
• Molecule 16: 60S ribosomal protein L15-A

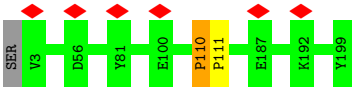
Chain AP:



• Molecule 17: 60S ribosomal protein L16-A

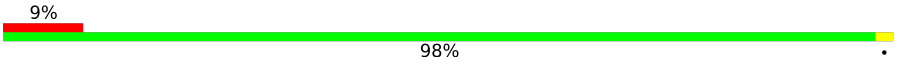
Chain AQ:

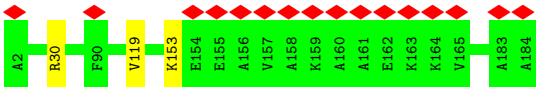




• Molecule 18: 60S ribosomal protein L17-A

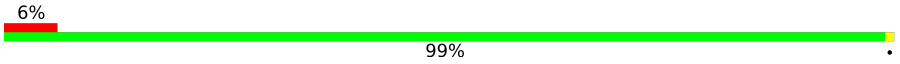
Chain AR:

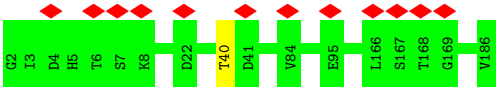




• Molecule 19: 60S ribosomal protein L18-A

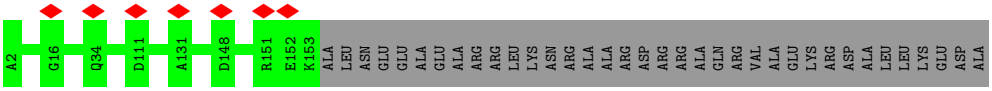
Chain AS:





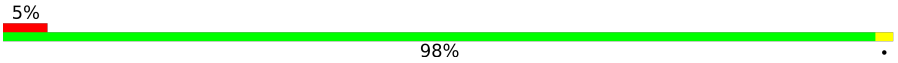
• Molecule 20: 60S ribosomal protein L19-A

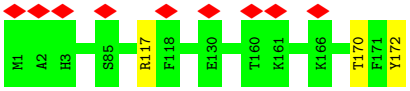
Chain AT:



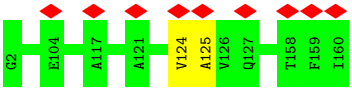
• Molecule 21: 60S ribosomal protein L20-A

Chain AU:

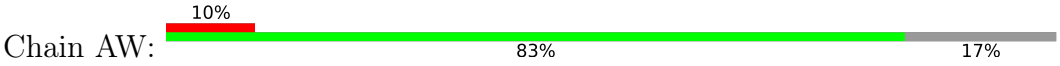


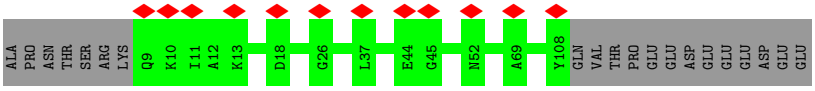


• Molecule 22: 60S ribosomal protein L21-A

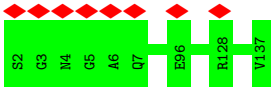


• Molecule 23: 60S ribosomal protein L22-A

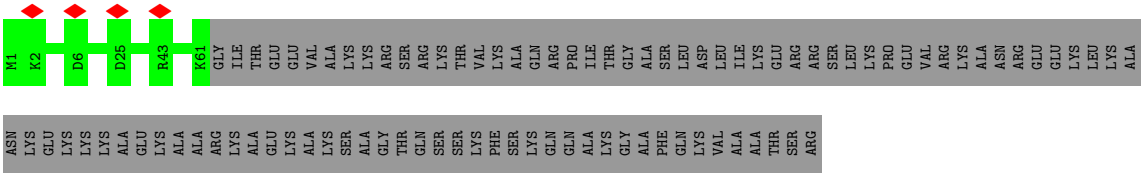




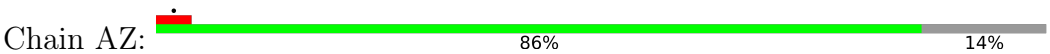
• Molecule 24: 60S ribosomal protein L23-A

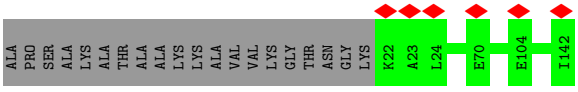


• Molecule 25: 60S ribosomal protein L24-A

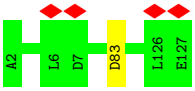


• Molecule 26: 60S ribosomal protein L25



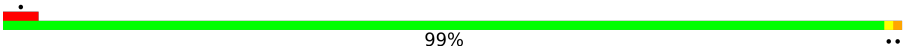


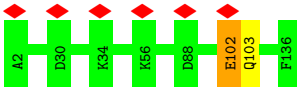
• Molecule 27: 60S ribosomal protein L26-A



• Molecule 28: 60S ribosomal protein L27-A

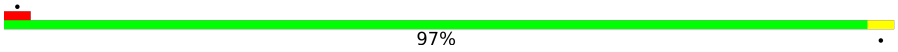
Chain Ab:

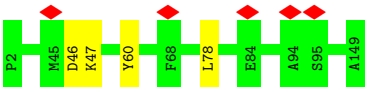




• Molecule 29: 60S ribosomal protein L28

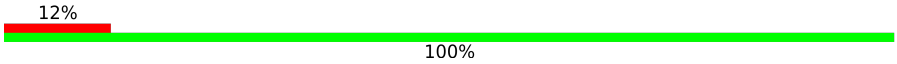
Chain Ac:

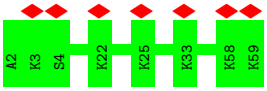




• Molecule 30: 60S ribosomal protein L29

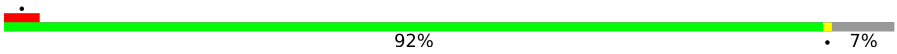
Chain Ad:

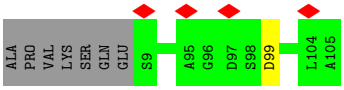




• Molecule 31: 60S ribosomal protein L30

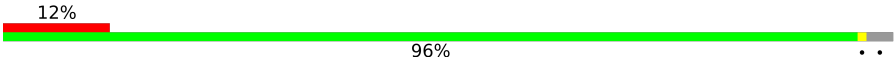
Chain Ae:

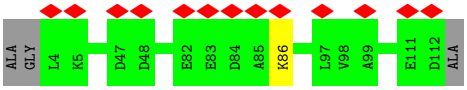




• Molecule 32: 60S ribosomal protein L31-A

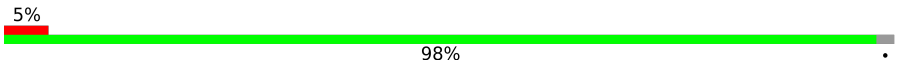
Chain Af:

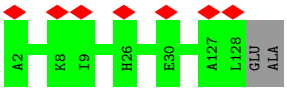




• Molecule 33: 60S ribosomal protein L32

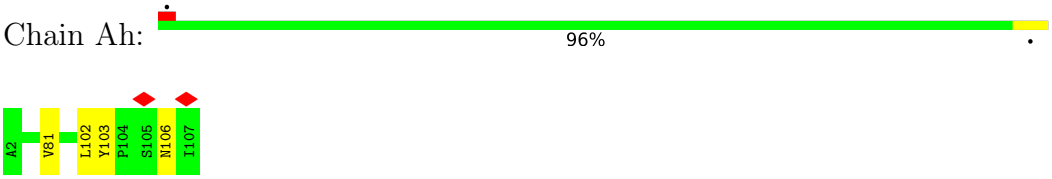
Chain Ag:





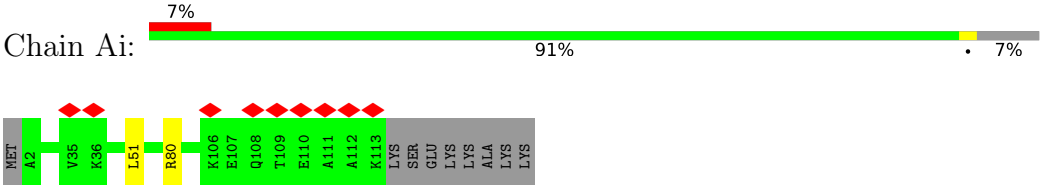
• Molecule 34: 60S ribosomal protein L33-A

Chain Ah:



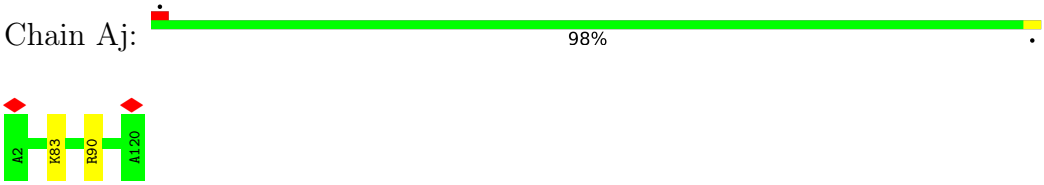
• Molecule 35: 60S ribosomal protein L34-A

Chain Ai:



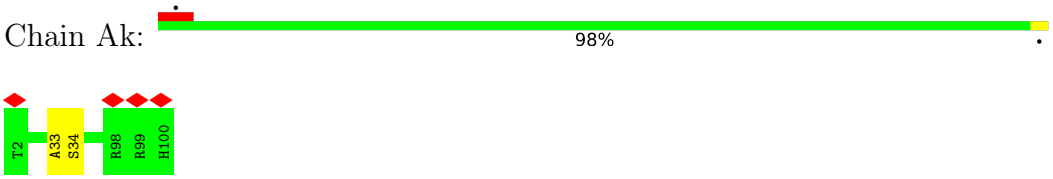
• Molecule 36: 60S ribosomal protein L35-A

Chain Aj:



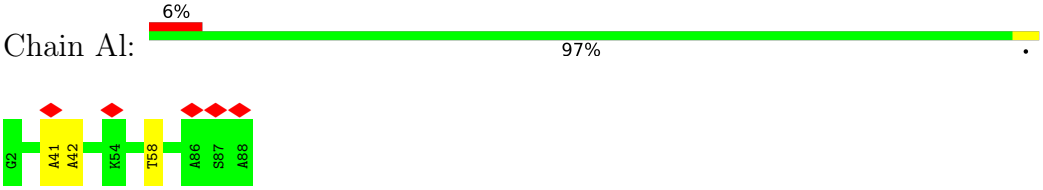
• Molecule 37: 60S ribosomal protein L36-A

Chain Ak:



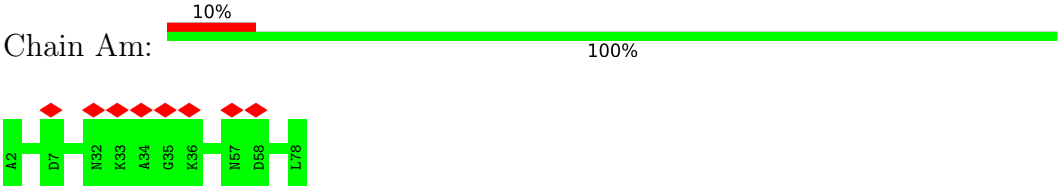
• Molecule 38: 60S ribosomal protein L37-A

Chain Al:



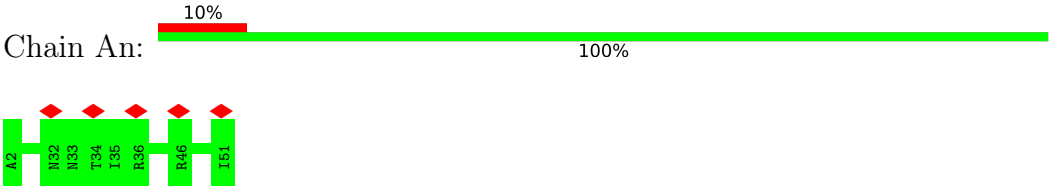
• Molecule 39: 60S ribosomal protein L38

Chain Am:



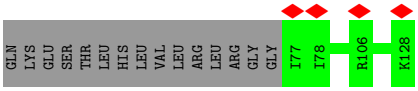
• Molecule 40: 60S ribosomal protein L39

Chain An:



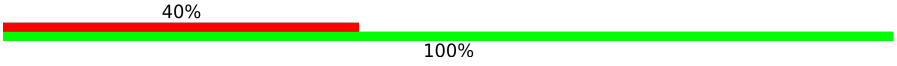
• Molecule 41: Ubiquitin-60S ribosomal protein L40

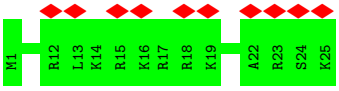
Chain Ao:



• Molecule 42: 60S ribosomal protein L41-B

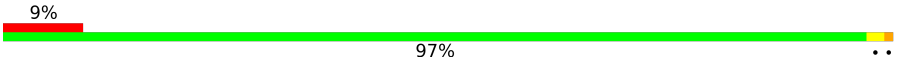
Chain Ap:

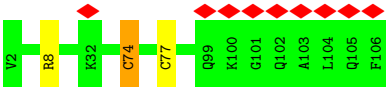




• Molecule 43: 60S ribosomal protein L42-A

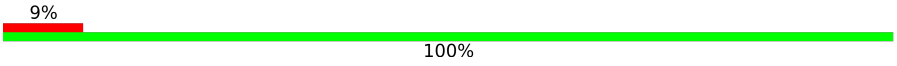
Chain Aq:

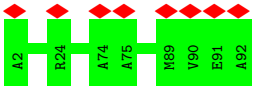




• Molecule 44: 60S ribosomal protein L43-A

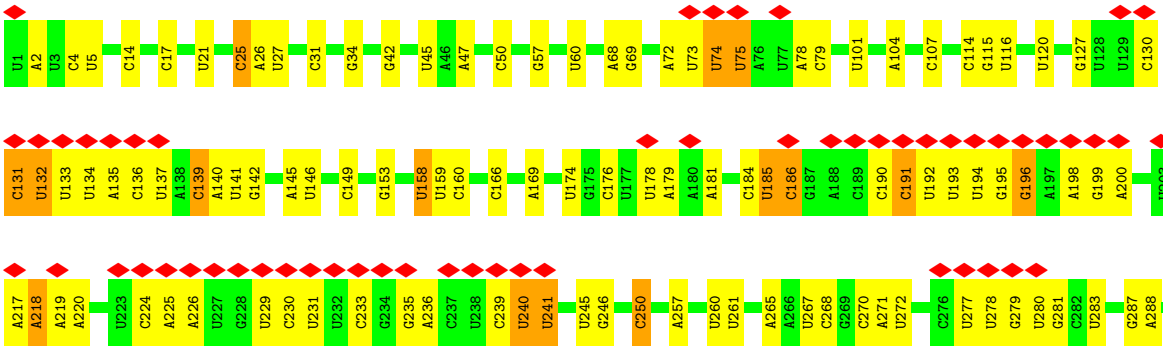
Chain Ar:

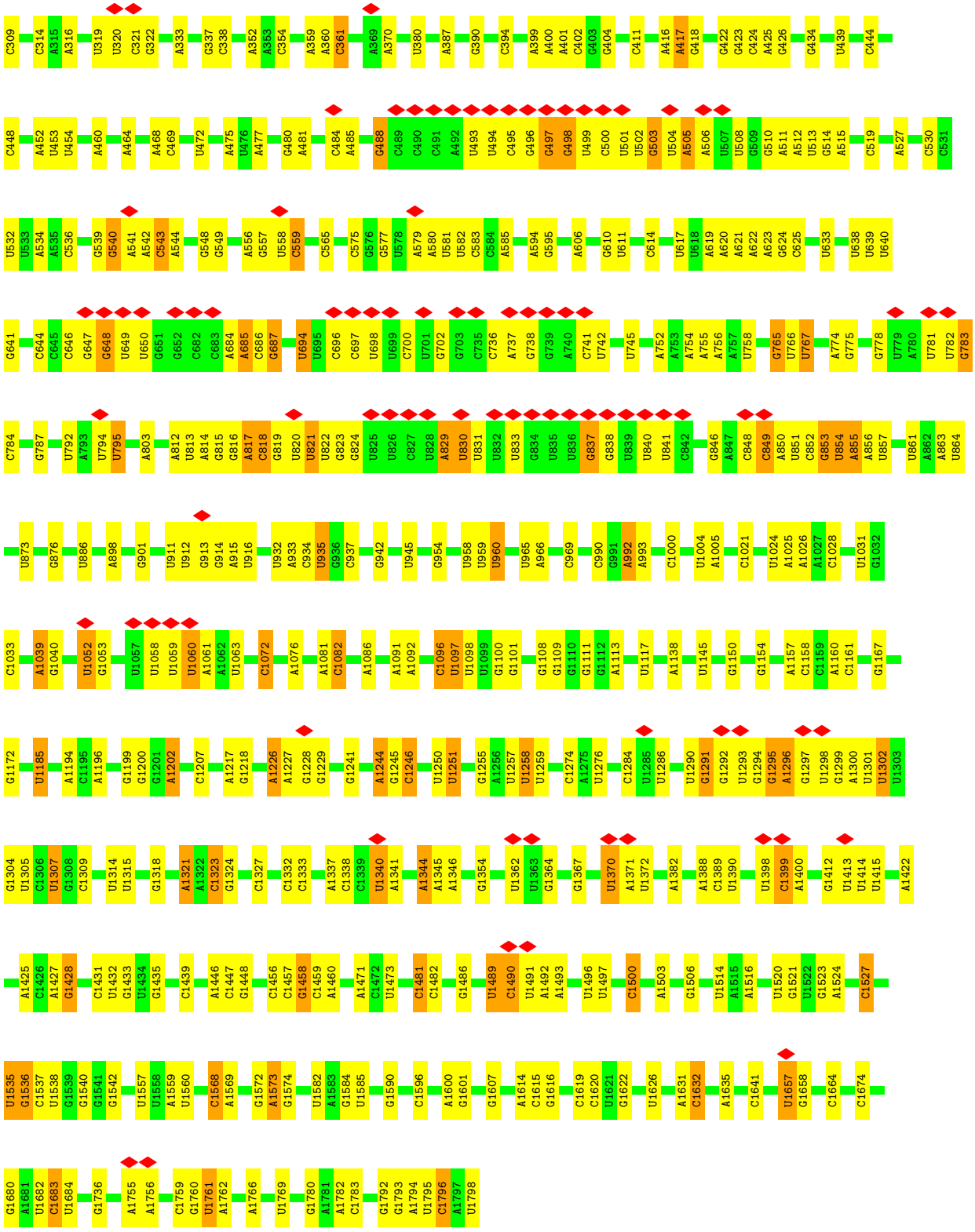




• Molecule 45: 18S rRNA (1707-MER)

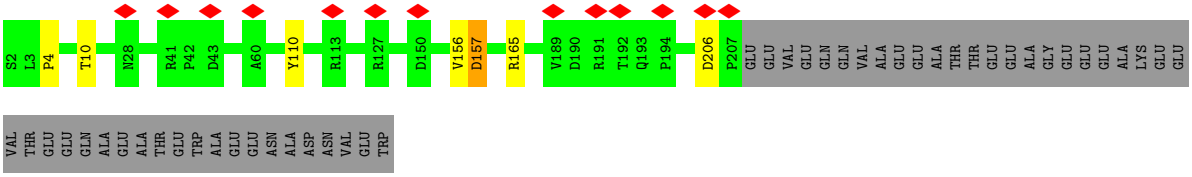
Chain BA:





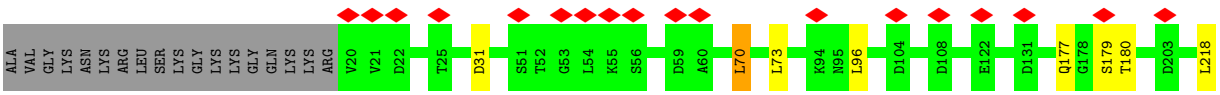
• Molecule 46: 40S ribosomal protein S0-A

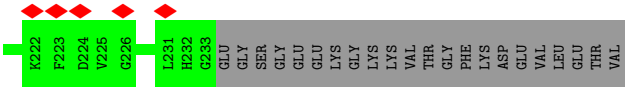
Chain BB:



• Molecule 47: 40S ribosomal protein S1-A

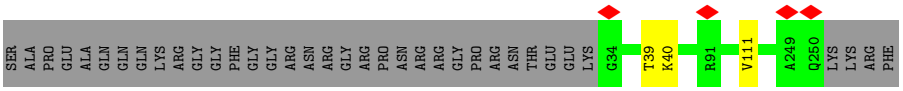
Chain BC:





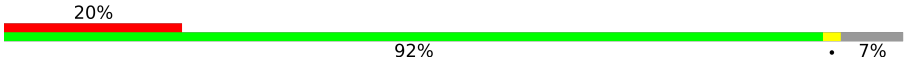
• Molecule 48: 40S ribosomal protein S2

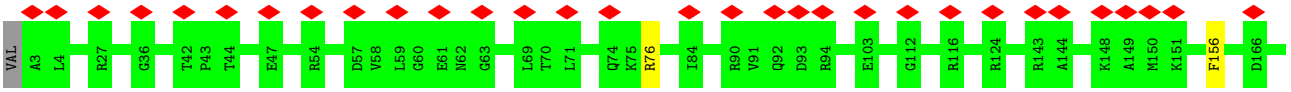
Chain BD:

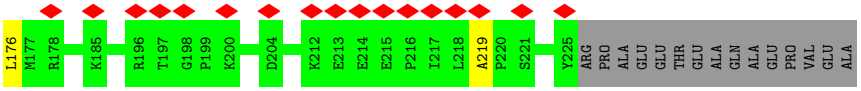


• Molecule 49: 40S ribosomal protein S3

Chain BE:

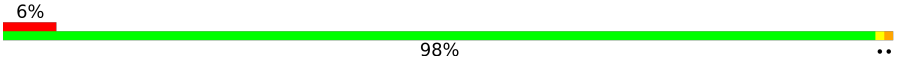


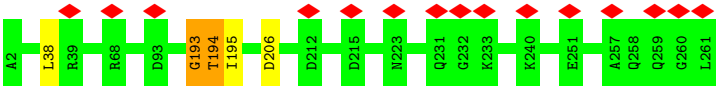




• Molecule 50: 40S ribosomal protein S4-A

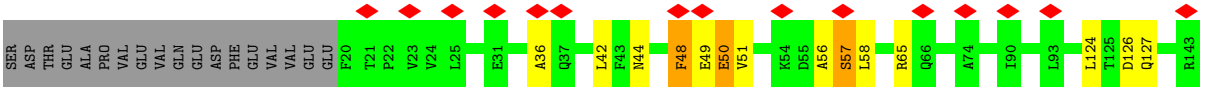
Chain BF:

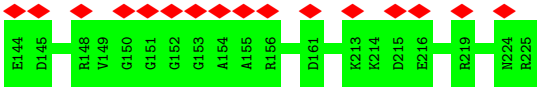




• Molecule 51: Rps5p

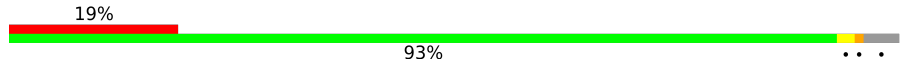
Chain BG:

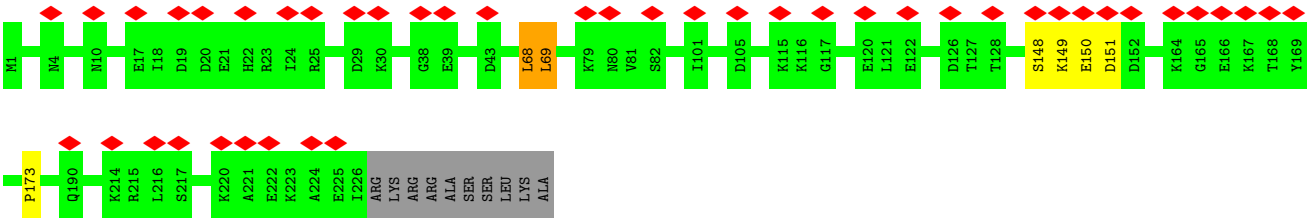




• Molecule 52: 40S ribosomal protein S6-A

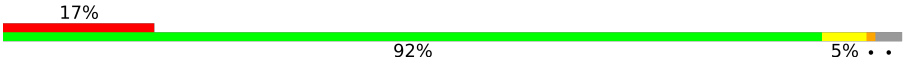
Chain BH:

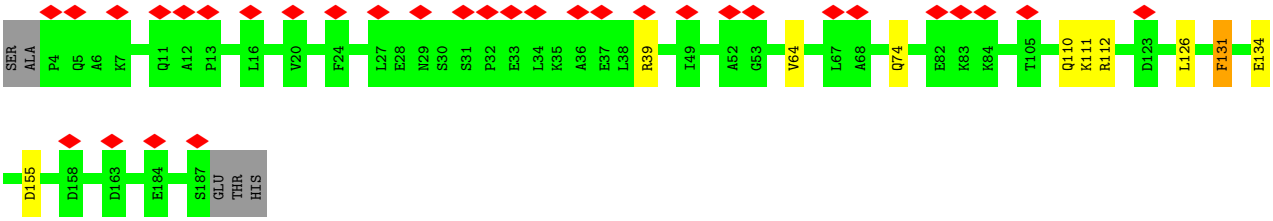




• Molecule 53: 40S ribosomal protein S7-A

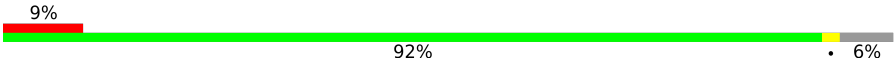
Chain BI:

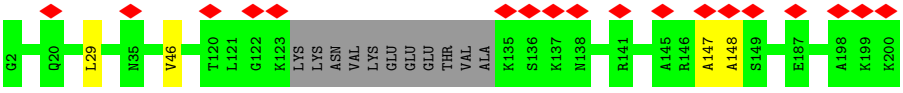




• Molecule 54: 40S ribosomal protein S8-A

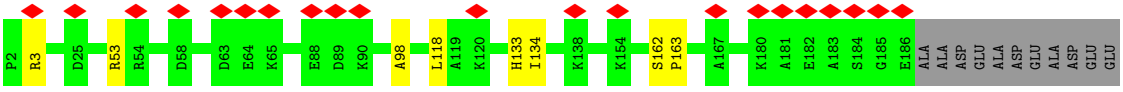
Chain BJ:





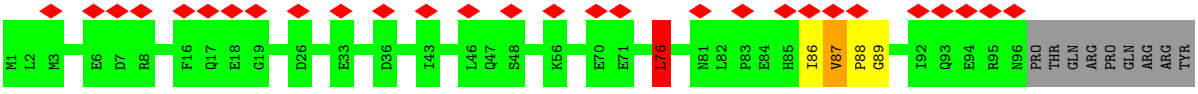
• Molecule 55: 40S ribosomal protein S9-A

Chain BK:



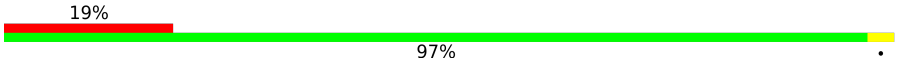
• Molecule 56: 40S ribosomal protein S10-A

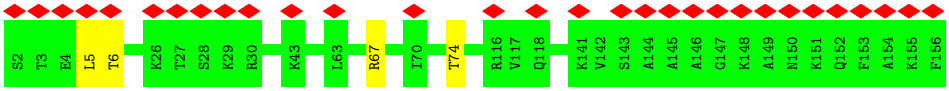
Chain BL:



• Molecule 57: 40S ribosomal protein S11-A

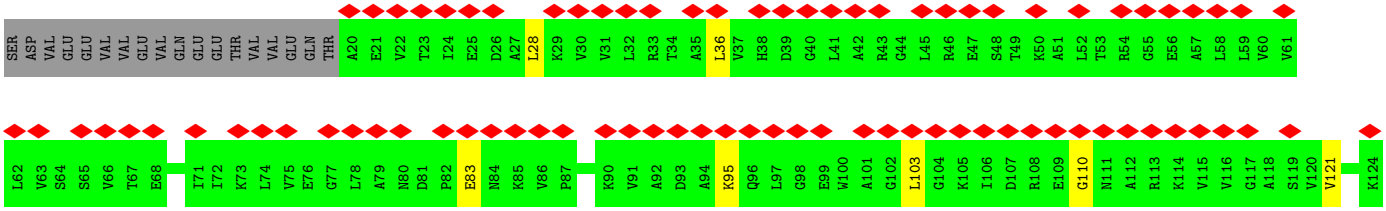
Chain BM:





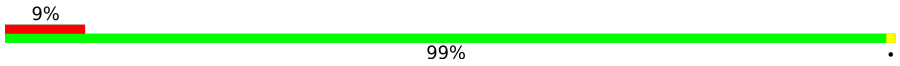
• Molecule 58: 40S ribosomal protein S12

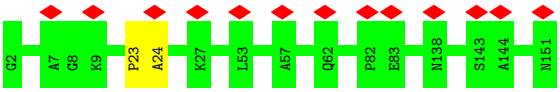
Chain BN:



• Molecule 59: 40S ribosomal protein S13

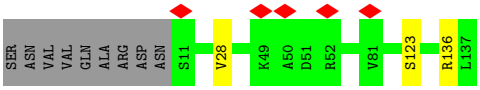
Chain BO:





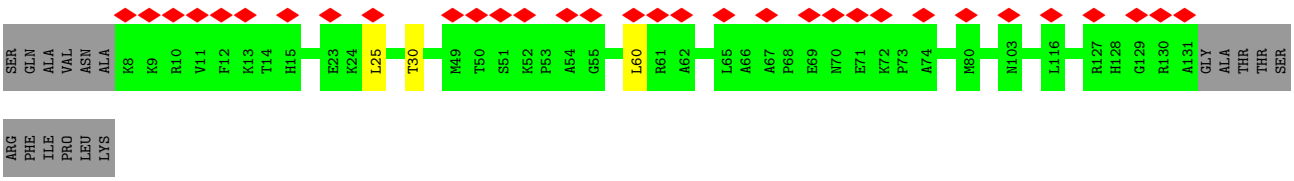
• Molecule 60: 40S ribosomal protein S14-A

Chain BP:



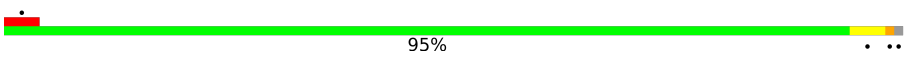
• Molecule 61: 40S ribosomal protein S15

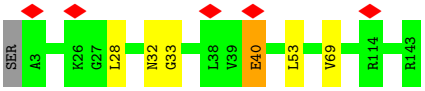
Chain BQ:



• Molecule 62: 40S ribosomal protein S16-A

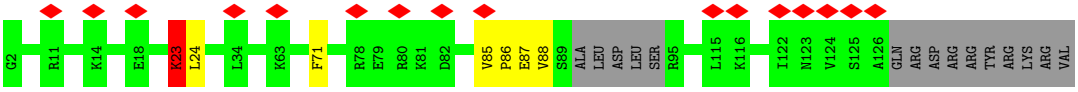
Chain BR:





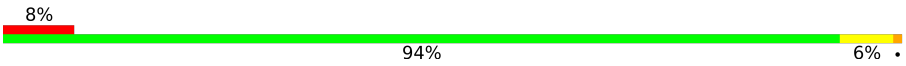
• Molecule 63: 40S ribosomal protein S17-A

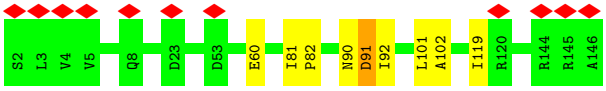
Chain BS:



• Molecule 64: 40S ribosomal protein S18-A

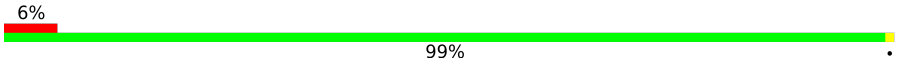
Chain BT:

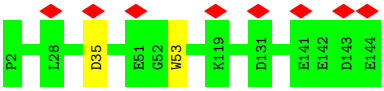




• Molecule 65: 40S ribosomal protein S19-A

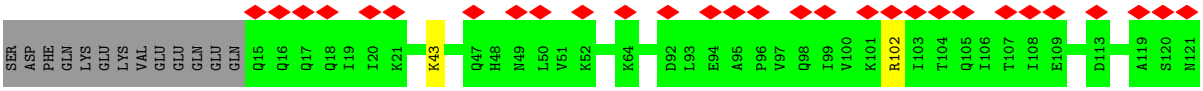
Chain BU:





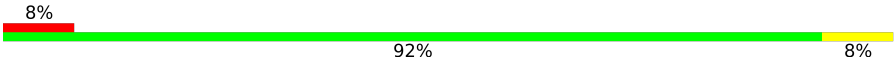
• Molecule 66: 40S ribosomal protein S20

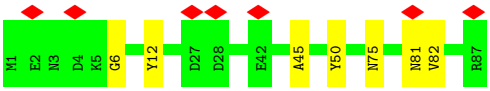
Chain BV:



• Molecule 67: 40S ribosomal protein S21-A

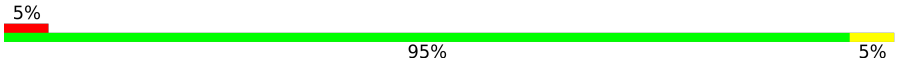
Chain BW:

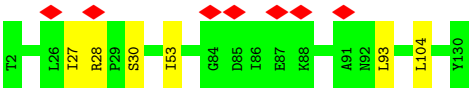




• Molecule 68: 40S ribosomal protein S22-A

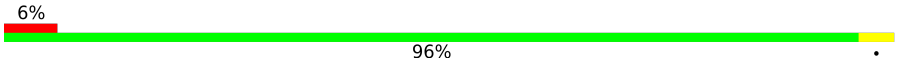
Chain BX:

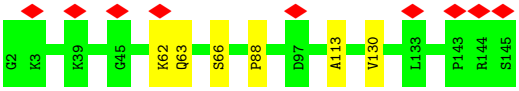




• Molecule 69: 40S ribosomal protein S23-A

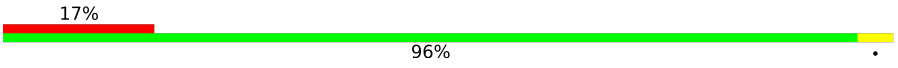
Chain BY:

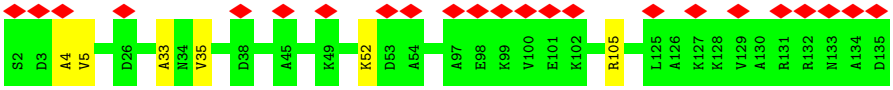




• Molecule 70: 40S ribosomal protein S24-A

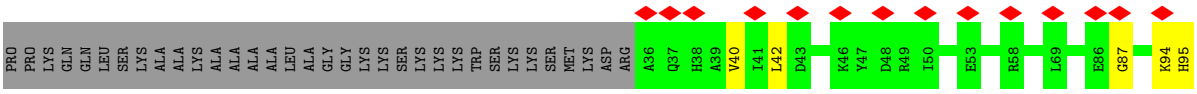
Chain BZ:

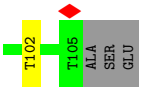




• Molecule 71: 40S ribosomal protein S25-A

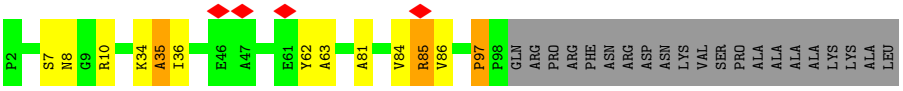
Chain Ba:





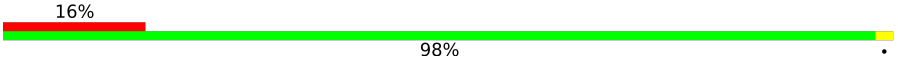
• Molecule 72: 40S ribosomal protein S26-B

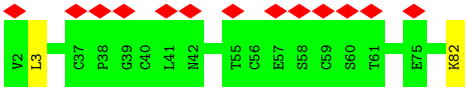
Chain Bb:



• Molecule 73: 40S ribosomal protein S27-A

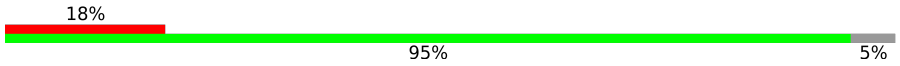
Chain Bc:

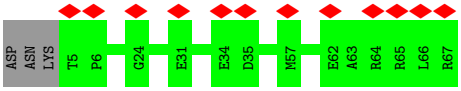




• Molecule 74: 40S ribosomal protein S28-A

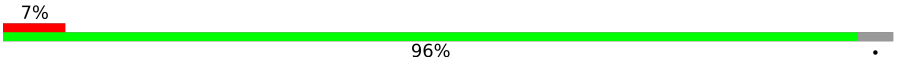
Chain Bd:

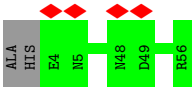




• Molecule 75: 40S ribosomal protein S29-A

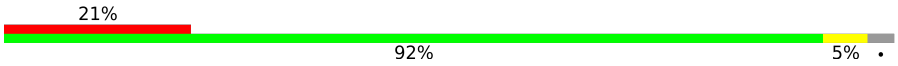
Chain Be:

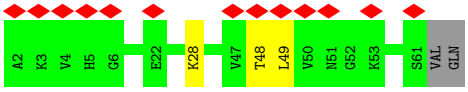




• Molecule 76: 40S ribosomal protein S30-A

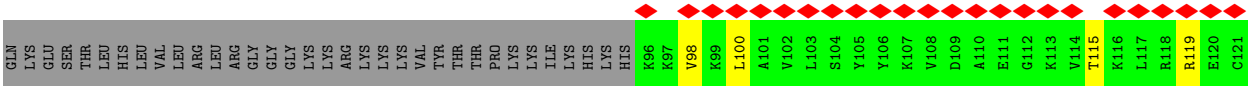
Chain Bf:

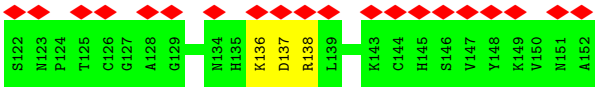




• Molecule 77: Ubiquitin-40S ribosomal protein S31

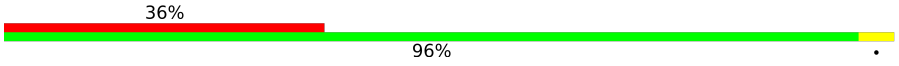
Chain Bg:

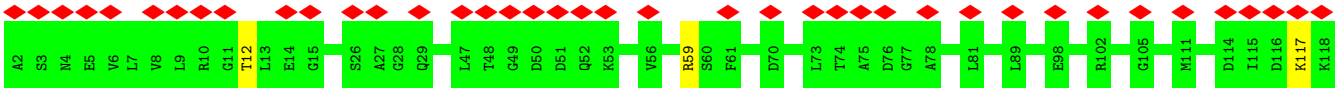


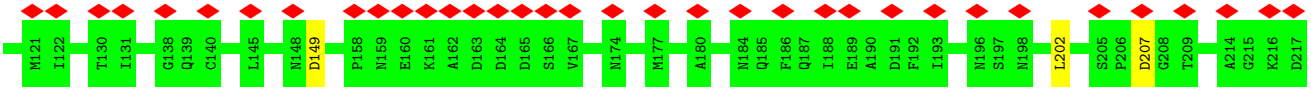


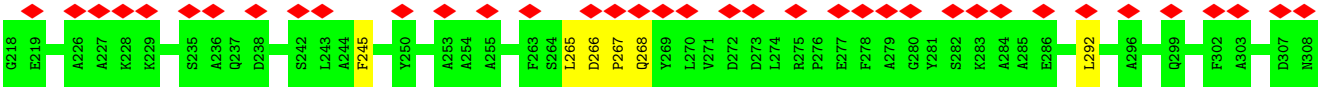
• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein

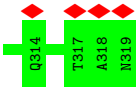
Chain Bh:





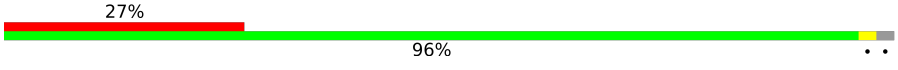


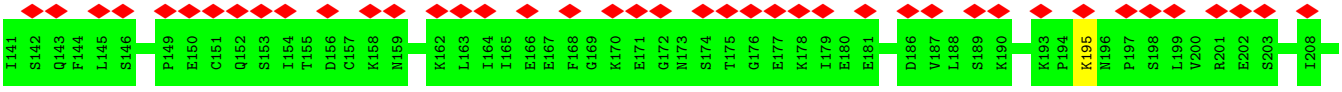


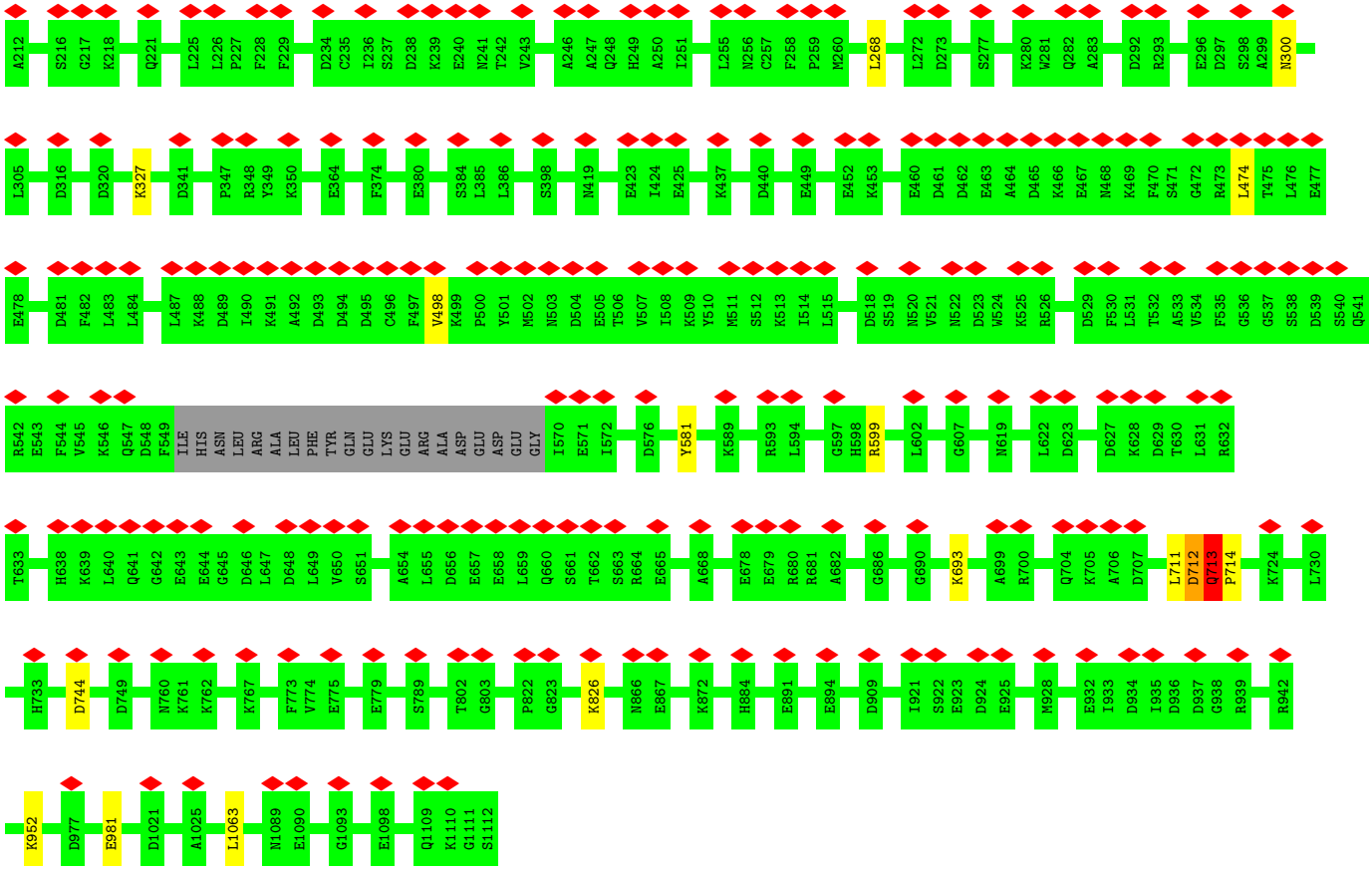


• Molecule 79: [NU+] prion formation protein 1

Chain Bi:






A212 S216 G217 K218 Q221 L225 L226 P227 F228 F229 D234 C235 I236 S237 D238 K239 E240 N241 T242 V243 A246 A247 Q248 H249 A250 I251 L255 N256 C257 F258 P259 M260 L268 L272 D273 S277 K280 W281 Q282 A283 D292 R293 E296 D297 S298 A299 N300
L305 D316 D320 K327 D341 P347 R348 Y349 K350 E364 F374 E380 S384 L385 L386 S398 N419 E423 I424 E425 K437 D440 E449 E452 K453 E460 D461 D462 E463 A464 D465 K466 E467 N468 K469 F470 S471 G472 R473 L474 T475 L476 E477
E478 D481 F482 L483 L484 L487 K488 D489 I490 K491 A492 D493 D494 D495 C496 F497 V498 K499 P500 Y501 M502 N503 D504 E505 T506 V507 I508 K509 Y510 M511 S512 K513 I514 L515 D518 S519 N520 V521 N522 D523 W524 K525 R526 D529 F530 L531 T532 A533 V534 F535 G536 G537 S538 D539 S540 Q541
R542 E543 F544 V545 K546 Q547 D548 F549 ILE HIS ASN LEU ARG ALA LEU PHE TYR GLN GLU LYS GLU ARG ALA ASP GLU ASP GLU GLY I570 E571 I572 D576 Y581 K589 R593 L594 G597 H598 R599 L602 G607 N619 L622 D623 D627 K628 D629 T630 L631 R632
T633 H638 K639 L640 Q641 G642 E643 E644 G645 D646 L647 D648 L649 V650 S651 A654 L655 D656 E657 E658 L659 Q660 S661 T662 S663 R664 E665 A668 E678 E679 R680 R681 A682 G686 G690 K693 A699 R700 Q704 K705 A706 D707 L711 D712 Q713 P714 K724 L730
H733 D744 D749 N760 K761 K762 K767 F773 V774 E775 E779 S789 T802 G803 P822 G823 K826 N866 E867 K872 H884 E891 E894 D909 I921 S922 E923 D924 E925 M928 E932 I933 D934 I935 D936 D937 G938 R939 R942
K952 D977 E981 D1021 A1025 L1063 N1089 E1090 G1093 E1098 Q1109 K1110 G1111 S1112

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.600	Depositor
Minimum map value	-0.343	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	446.46, 446.46, 446.46	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.87	0/75394	1.12	450/117545 (0.4%)
2	AB	0.82	0/2883	1.07	17/4491 (0.4%)
3	AC	0.83	0/3746	1.06	14/5832 (0.2%)
4	AD	0.48	0/1948	0.61	0/2617
5	AE	0.51	2/3146 (0.1%)	0.76	6/4228 (0.1%)
6	AF	0.45	0/2800	0.62	1/3790 (0.0%)
7	AG	0.44	0/2425	0.63	1/3271 (0.0%)
8	AH	0.41	0/1260	0.59	0/1694
9	AI	0.46	0/1821	0.61	0/2451
10	AJ	0.41	0/1836	0.59	0/2481
11	AK	0.44	0/1537	0.56	0/2067
12	AL	0.41	0/1741	0.54	0/2335
13	AM	0.44	1/1374 (0.1%)	0.68	2/1842 (0.1%)
14	AN	0.47	0/1568	0.63	1/2106 (0.0%)
15	AO	0.41	0/1068	0.57	0/1438
16	AP	0.49	0/1757	0.60	1/2354 (0.0%)
17	AQ	0.42	0/1585	0.55	0/2128
18	AR	0.44	0/1443	0.62	0/1944
19	AS	0.42	0/1465	0.54	0/1965
20	AT	0.40	0/1245	0.52	0/1661
21	AU	0.44	0/1481	0.55	0/1990
22	AV	0.46	0/1300	0.56	0/1743
23	AW	0.39	0/812	0.57	0/1099
24	AX	0.42	0/1018	0.58	0/1369
25	AY	0.43	0/521	0.49	0/691
26	AZ	0.45	0/979	0.57	0/1321
27	Aa	0.39	0/1004	0.56	1/1341 (0.1%)
28	Ab	0.42	0/1118	0.58	1/1497 (0.1%)
29	Ac	0.47	0/1204	0.64	1/1612 (0.1%)
30	Ad	0.36	0/473	0.53	0/629
31	Ae	0.44	0/751	0.54	0/1008
32	Af	0.44	0/890	0.55	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ag	0.40	0/1041	0.54	0/1394
34	Ah	0.45	0/868	0.53	0/1168
35	Ai	0.44	0/890	0.56	1/1189 (0.1%)
36	Aj	0.38	0/978	0.51	0/1301
37	Ak	0.39	0/778	0.63	0/1034
38	Al	0.44	0/696	0.59	0/923
39	Am	0.38	0/618	0.60	0/826
40	An	0.42	0/443	0.60	0/588
41	Ao	0.39	0/423	0.57	0/562
42	Ap	0.41	0/234	0.50	0/300
43	Aq	0.49	0/860	0.67	2/1136 (0.2%)
44	Ar	0.49	0/701	0.58	0/934
45	BA	1.01	3/40685 (0.0%)	1.23	400/63392 (0.6%)
46	BB	0.51	0/1617	0.66	0/2215
47	BC	0.51	0/1735	0.77	3/2335 (0.1%)
48	BD	0.55	0/1665	0.65	1/2263 (0.0%)
49	BE	0.63	0/1759	0.69	1/2368 (0.0%)
50	BF	0.55	0/2109	0.68	2/2839 (0.1%)
51	BG	0.62	0/1629	0.77	1/2202 (0.0%)
52	BH	0.44	0/1823	0.62	1/2439 (0.0%)
53	BI	0.46	0/1506	0.71	2/2028 (0.1%)
54	BJ	0.54	0/1514	0.68	1/2021 (0.0%)
55	BK	0.50	0/1519	0.68	1/2035 (0.0%)
56	BL	0.73	0/789	0.76	1/1067 (0.1%)
57	BM	0.56	0/1239	0.60	0/1673
58	BN	0.41	0/898	0.85	1/1220 (0.1%)
59	BO	0.51	0/1215	0.66	0/1638
60	BP	0.54	0/901	0.75	0/1217
61	BQ	0.57	0/998	0.68	2/1341 (0.1%)
62	BR	0.65	0/1125	0.77	3/1510 (0.2%)
63	BS	0.53	0/935	0.73	1/1254 (0.1%)
64	BT	0.53	0/1211	0.66	0/1628
65	BU	0.60	0/1130	0.71	1/1517 (0.1%)
66	BV	0.54	0/865	0.67	0/1169
67	BW	0.62	0/693	0.74	0/935
68	BX	0.58	0/1038	0.69	3/1395 (0.2%)
69	BY	0.55	0/1139	0.68	0/1518
70	BZ	0.50	0/1087	0.64	0/1449
71	Ba	0.57	0/571	0.83	0/768
72	Bb	0.54	0/782	0.75	0/1047
73	Bc	0.52	0/620	0.72	1/838 (0.1%)
74	Bd	0.65	0/499	0.71	0/670
75	Be	0.60	0/452	0.65	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bf	0.49	0/483	0.64	1/643 (0.2%)
77	Bg	0.47	0/451	0.80	1/603 (0.2%)
78	Bh	0.63	0/2494	0.71	2/3393 (0.1%)
79	Bi	0.44	8/7649 (0.1%)	0.67	8/10345 (0.1%)
All	All	0.76	14/218948 (0.0%)	0.98	937/320666 (0.3%)

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
4	AD	0	2
5	AE	0	3
6	AF	0	2
7	AG	0	3
8	AH	0	1
9	AI	0	3
11	AK	0	2
14	AN	0	1
15	AO	0	1
17	AQ	0	1
22	AV	0	1
28	Ab	0	1
35	Ai	0	1
36	Aj	0	2
46	BB	0	4
47	BC	0	2
49	BE	0	1
50	BF	0	2
51	BG	0	10
52	BH	0	3
53	BI	0	1
54	BJ	0	1
55	BK	0	2
56	BL	0	4
57	BM	0	1
58	BN	0	5
60	BP	0	2
62	BR	0	2
63	BS	0	3
64	BT	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	BW	0	2
69	BY	0	3
70	BZ	0	2
71	Ba	0	4
72	Bb	0	9
77	Bg	0	2
79	Bi	0	1
All	All	0	95

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	Bi	712	ASP	C-O	-10.00	1.04	1.23
5	AE	18	PRO	CA-C	8.86	1.70	1.52
79	Bi	712	ASP	N-CA	8.72	1.63	1.46
79	Bi	712	ASP	CG-OD1	-8.20	1.06	1.25
79	Bi	712	ASP	CB-CG	7.90	1.68	1.51
79	Bi	713	GLN	C-O	7.51	1.37	1.23
45	BA	1295	G	N9-C4	6.36	1.43	1.38
45	BA	1296	A	N9-C4	6.34	1.41	1.37
79	Bi	712	ASP	CA-C	6.29	1.69	1.52
79	Bi	714	PRO	N-CD	-5.68	1.39	1.47
79	Bi	711	LEU	C-N	5.62	1.47	1.34
13	AM	82	ARG	CA-CB	-5.59	1.41	1.53
45	BA	855	A	O3'-P	-5.01	1.55	1.61
5	AE	18	PRO	CA-CB	5.00	1.63	1.53

All (937) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AE	18	PRO	CA-C-O	-17.03	79.33	120.20
5	AE	18	PRO	CA-C-N	16.79	154.13	117.20
79	Bi	712	ASP	CB-CG-OD2	15.62	132.36	118.30
1	AA	3217	C	N1-C2-O2	13.23	126.84	118.90
45	BA	1295	G	C8-N9-C4	-12.85	101.26	106.40
45	BA	1473	U	N1-C2-O2	12.07	131.25	122.80
5	AE	18	PRO	O-C-N	-11.64	104.07	122.70
1	AA	3217	C	C2-N1-C1'	11.63	131.60	118.80
1	AA	1279	C	C5-C6-N1	11.39	126.70	121.00
45	BA	1295	G	N3-C4-C5	-11.38	122.91	128.60
45	BA	1473	U	C2-N1-C1'	11.26	131.21	117.70
1	AA	2572	C	N1-C2-O2	11.13	125.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	818	C	N1-C2-O2	10.91	125.44	118.90
1	AA	3217	C	N3-C2-O2	-10.72	114.40	121.90
1	AA	1279	C	C6-N1-C2	-10.65	116.04	120.30
45	BA	453	U	N3-C2-O2	-10.65	114.75	122.20
45	BA	855	A	C4'-C3'-O3'	-10.58	87.19	109.40
45	BA	453	U	N1-C2-O2	10.56	130.19	122.80
45	BA	1473	U	N3-C2-O2	-10.52	114.84	122.20
45	BA	1514	U	N3-C2-O2	-10.28	115.01	122.20
1	AA	3278	C	N1-C2-O2	10.27	125.06	118.90
45	BA	453	U	C2-N1-C1'	10.19	129.93	117.70
1	AA	1228	C	N3-C2-O2	-9.99	114.91	121.90
45	BA	1300	A	C8-N9-C4	-9.88	101.85	105.80
1	AA	3278	C	C2-N1-C1'	9.86	129.65	118.80
1	AA	2842	U	N1-C2-O2	9.73	129.61	122.80
79	Bi	711	LEU	C-N-CA	9.69	145.93	121.70
45	BA	831	U	N3-C2-O2	-9.59	115.49	122.20
45	BA	818	C	C2-N3-C4	9.58	124.69	119.90
1	AA	3057	U	N3-C2-O2	-9.57	115.50	122.20
1	AA	638	C	C5-C6-N1	9.55	125.77	121.00
45	BA	1246	C	N1-C2-O2	9.52	124.61	118.90
45	BA	831	U	N1-C2-O2	9.51	129.46	122.80
45	BA	1514	U	N1-C2-O2	9.50	129.45	122.80
1	AA	2572	C	C2-N1-C1'	9.50	129.25	118.80
1	AA	1269	U	C2-N1-C1'	9.47	129.06	117.70
45	BA	1300	A	N7-C8-N9	9.42	118.51	113.80
65	BU	35	ASP	CB-CG-OD1	9.40	126.76	118.30
1	AA	1269	U	N1-C2-O2	9.36	129.35	122.80
1	AA	2257	C	C2-N1-C1'	9.35	129.08	118.80
45	BA	1389	C	C2-N1-C1'	9.35	129.08	118.80
1	AA	2572	C	N3-C2-O2	-9.31	115.38	121.90
79	Bi	714	PRO	N-CD-CG	-9.30	89.25	103.20
1	AA	2842	U	N3-C2-O2	-9.27	115.71	122.20
1	AA	2257	C	N1-C2-O2	9.22	124.44	118.90
1	AA	1269	U	N3-C2-O2	-9.19	115.77	122.20
45	BA	1072	C	C5-C6-N1	9.19	125.60	121.00
45	BA	864	U	N3-C2-O2	-9.06	115.86	122.20
1	AA	3057	U	N1-C2-O2	9.01	129.11	122.80
45	BA	581	U	N3-C2-O2	-8.99	115.91	122.20
13	AM	82	ARG	N-CA-CB	-8.94	94.51	110.60
1	AA	2842	U	C2-N1-C1'	8.94	128.42	117.70
45	BA	287	G	O4'-C1'-N9	8.91	115.33	108.20
1	AA	3181	C	N1-C2-O2	8.89	124.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1072	C	C6-N1-C2	-8.88	116.75	120.30
45	BA	1292	G	C4-C5-N7	8.84	114.34	110.80
1	AA	3278	C	N3-C2-O2	-8.83	115.72	121.90
45	BA	1295	G	N7-C8-N9	8.81	117.51	113.10
45	BA	1560	U	N3-C2-O2	-8.81	116.04	122.20
45	BA	1024	U	N3-C2-O2	-8.77	116.06	122.20
45	BA	1527	C	C2-N1-C1'	8.74	128.41	118.80
45	BA	1323	C	N1-C2-O2	8.72	124.13	118.90
45	BA	767	U	N3-C2-O2	-8.70	116.11	122.20
45	BA	191	C	C6-N1-C2	-8.69	116.83	120.30
1	AA	922	U	C2-N1-C1'	8.67	128.11	117.70
45	BA	1246	C	C2-N1-C1'	8.65	128.31	118.80
45	BA	736	C	N1-C2-O2	8.64	124.08	118.90
45	BA	1294	G	N3-C2-N2	-8.64	113.85	119.90
45	BA	1527	C	C5-C6-N1	8.56	125.28	121.00
45	BA	1428	G	O5'-P-OP1	-8.54	98.02	105.70
45	BA	1000	C	C2-N1-C1'	8.50	128.15	118.80
45	BA	864	U	N1-C2-O2	8.45	128.71	122.80
45	BA	1258	U	C2-N1-C1'	8.43	127.81	117.70
1	AA	2836	C	N3-C2-O2	-8.42	116.00	121.90
45	BA	543	C	N3-C2-O2	-8.40	116.02	121.90
1	AA	3217	C	C6-N1-C1'	-8.38	110.74	120.80
45	BA	543	C	N1-C2-O2	8.35	123.91	118.90
1	AA	2572	C	C6-N1-C2	-8.35	116.96	120.30
45	BA	581	U	N1-C2-O2	8.34	128.64	122.80
45	BA	361	C	C5-C6-N1	8.31	125.15	121.00
45	BA	1292	G	N3-C4-N9	8.30	130.98	126.00
1	AA	3306	U	N3-C2-O2	-8.30	116.39	122.20
1	AA	2983	C	N3-C2-O2	-8.26	116.12	121.90
45	BA	1246	C	N3-C2-O2	-8.25	116.12	121.90
1	AA	3181	C	C2-N1-C1'	8.23	127.86	118.80
1	AA	1227	C	N1-C2-O2	8.20	123.82	118.90
45	BA	1458	G	C4-N9-C1'	8.19	137.14	126.50
79	Bi	712	ASP	OD1-CG-OD2	-8.17	107.78	123.30
45	BA	31	C	C6-N1-C2	-8.14	117.04	120.30
45	BA	1560	U	C2-N1-C1'	8.12	127.45	117.70
1	AA	102	C	N3-C2-O2	-8.07	116.25	121.90
45	BA	1619	C	N1-C2-O2	8.05	123.73	118.90
45	BA	581	U	C2-N1-C1'	8.03	127.34	117.70
45	BA	1258	U	N3-C2-O2	-8.03	116.58	122.20
1	AA	2836	C	C2-N1-C1'	8.03	127.63	118.80
45	BA	1473	U	C6-N1-C1'	-8.02	109.97	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	102	C	C6-N1-C2	-8.02	117.09	120.30
45	BA	736	C	C2-N1-C1'	8.01	127.61	118.80
45	BA	861	U	C2-N1-C1'	8.00	127.30	117.70
3	AC	127	U	N1-C2-O2	7.99	128.39	122.80
45	BA	116	U	N3-C2-O2	-7.98	116.61	122.20
1	AA	3181	C	N3-C2-O2	-7.96	116.33	121.90
45	BA	1292	G	C6-C5-N7	-7.95	125.63	130.40
1	AA	2836	C	N1-C2-O2	7.94	123.67	118.90
1	AA	2444	C	C2-N1-C1'	7.92	127.52	118.80
56	BL	76	LEU	CA-CB-CG	7.92	133.51	115.30
1	AA	1349	G	N3-C4-C5	-7.92	124.64	128.60
1	AA	1255	C	N1-C2-O2	7.92	123.65	118.90
45	BA	965	U	C2-N1-C1'	7.90	127.18	117.70
68	BX	93	LEU	CA-CB-CG	7.89	133.44	115.30
45	BA	959	U	N3-C2-O2	-7.88	116.69	122.20
1	AA	1349	G	N3-C4-N9	7.88	130.73	126.00
45	BA	142	G	N3-C2-N2	-7.84	114.41	119.90
1	AA	3058	U	N1-C2-O2	7.82	128.28	122.80
45	BA	646	C	C6-N1-C2	-7.79	117.19	120.30
45	BA	1560	U	N1-C2-O2	7.77	128.24	122.80
3	AC	127	U	N3-C2-O2	-7.77	116.76	122.20
1	AA	1448	U	N3-C2-O2	-7.77	116.76	122.20
1	AA	36	C	N1-C2-O2	7.75	123.55	118.90
45	BA	1292	G	N9-C4-C5	-7.75	102.30	105.40
45	BA	1258	U	N1-C2-O2	7.74	128.22	122.80
1	AA	102	C	N1-C2-O2	7.70	123.52	118.90
1	AA	1907	C	N1-C2-O2	7.70	123.52	118.90
45	BA	817	A	N1-C6-N6	7.70	123.22	118.60
45	BA	1294	G	N1-C2-N2	7.69	123.12	116.20
45	BA	1039	A	O4'-C1'-N9	7.68	114.35	108.20
1	AA	3306	U	C2-N1-C1'	7.64	126.86	117.70
45	BA	31	C	C5-C6-N1	7.63	124.82	121.00
1	AA	1368	U	C5-C6-N1	7.61	126.51	122.70
1	AA	1496	C	C2-N1-C1'	7.61	127.17	118.80
5	AE	18	PRO	C-N-CA	7.60	140.70	121.70
1	AA	3214	U	C2-N1-C1'	7.59	126.81	117.70
3	AC	157	U	N1-C2-O2	7.55	128.08	122.80
1	AA	2257	C	N3-C2-O2	-7.53	116.63	121.90
1	AA	981	U	C5-C6-N1	7.52	126.46	122.70
1	AA	1871	U	N3-C2-O2	-7.51	116.94	122.20
1	AA	1871	U	N1-C2-O2	7.50	128.05	122.80
1	AA	922	U	N1-C2-O2	7.50	128.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	817	A	C5-C6-N6	-7.45	117.74	123.70
1	AA	2716	U	N3-C2-O2	-7.45	116.99	122.20
45	BA	1072	C	C2-N1-C1'	7.41	126.95	118.80
1	AA	2541	U	P-O3'-C3'	7.40	128.58	119.70
1	AA	3278	C	C6-N1-C1'	-7.39	111.93	120.80
1	AA	2550	U	N3-C2-O2	-7.39	117.03	122.20
45	BA	1490	C	O5'-P-OP1	-7.38	99.06	105.70
1	AA	1265	U	N1-C2-O2	7.38	127.96	122.80
45	BA	1307	U	N3-C2-O2	-7.36	117.05	122.20
45	BA	583	C	C6-N1-C2	-7.35	117.36	120.30
45	BA	1296	A	N9-C4-C5	-7.35	102.86	105.80
45	BA	783	G	O4'-C1'-N9	7.34	114.07	108.20
45	BA	267	U	N3-C2-O2	-7.32	117.08	122.20
45	BA	488	G	O5'-P-OP1	7.32	119.48	110.70
1	AA	2873	U	N3-C2-O2	-7.28	117.10	122.20
45	BA	849	C	N1-C1'-C2'	-7.28	104.00	112.00
45	BA	1458	G	N3-C4-N9	7.28	130.37	126.00
45	BA	1294	G	P-O3'-C3'	7.26	128.41	119.70
1	AA	1238	C	N1-C2-O2	7.26	123.25	118.90
1	AA	3058	U	C2-N1-C1'	7.25	126.40	117.70
45	BA	1389	C	C5-C6-N1	7.24	124.62	121.00
1	AA	270	U	N1-C2-O2	7.24	127.87	122.80
45	BA	648	G	C4-N9-C1'	7.23	135.90	126.50
1	AA	3078	U	C2-N1-C1'	7.23	126.37	117.70
79	Bi	713	GLN	CB-CA-C	7.22	124.84	110.40
1	AA	524	U	N1-C2-O2	7.22	127.85	122.80
1	AA	1448	U	N1-C2-O2	7.22	127.85	122.80
1	AA	78	U	N3-C2-O2	-7.21	117.15	122.20
1	AA	1307	G	P-O3'-C3'	7.21	128.35	119.70
45	BA	1292	G	C5-C6-O6	-7.19	124.28	128.60
1	AA	1279	C	C2-N1-C1'	7.19	126.71	118.80
45	BA	498	G	P-O3'-C3'	7.19	128.33	119.70
45	BA	648	G	N3-C4-N9	7.19	130.31	126.00
1	AA	2513	U	P-O3'-C3'	7.17	128.30	119.70
45	BA	1370	U	P-O3'-C3'	7.17	128.30	119.70
1	AA	835	G	O4'-C1'-N9	7.16	113.93	108.20
45	BA	583	C	C5-C6-N1	7.16	124.58	121.00
1	AA	3306	U	N1-C2-O2	7.16	127.81	122.80
45	BA	1307	U	C2-N1-C1'	7.16	126.29	117.70
1	AA	406	G	O4'-C1'-N9	7.15	113.92	108.20
1	AA	1227	C	C5-C6-N1	7.14	124.57	121.00
1	AA	1759	C	N1-C2-O2	7.14	123.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2366	C	C2-N1-C1'	7.14	126.65	118.80
45	BA	1296	A	N3-C4-N9	7.14	133.11	127.40
1	AA	1278	A	O4'-C1'-N9	7.12	113.90	108.20
45	BA	817	A	N9-C4-C5	-7.12	102.95	105.80
45	BA	864	U	C2-N1-C1'	7.10	126.22	117.70
1	AA	524	U	N3-C2-O2	-7.09	117.23	122.20
1	AA	36	C	N3-C2-O2	-7.08	116.94	121.90
1	AA	2983	C	C6-N1-C2	-7.08	117.47	120.30
45	BA	1297	G	N7-C8-N9	7.08	116.64	113.10
45	BA	1619	C	N3-C2-O2	-7.07	116.95	121.90
1	AA	1604	G	C4-N9-C1'	7.07	135.69	126.50
1	AA	1815	U	P-O3'-C3'	7.06	128.17	119.70
45	BA	831	U	C2-N1-C1'	7.05	126.16	117.70
1	AA	979	U	P-O3'-C3'	7.04	128.15	119.70
45	BA	1324	G	C8-N9-C4	-7.04	103.58	106.40
1	AA	315	C	C2-N1-C1'	7.03	126.54	118.80
79	Bi	474	LEU	CA-CB-CG	7.03	131.47	115.30
1	AA	2513	U	OP1-P-O3'	7.03	120.66	105.20
45	BA	901	G	O4'-C1'-N9	7.03	113.82	108.20
45	BA	1458	G	N3-C4-C5	-7.02	125.09	128.60
45	BA	1332	C	C2-N1-C1'	7.02	126.52	118.80
1	AA	270	U	N3-C2-O2	-7.01	117.29	122.20
1	AA	1645	U	N3-C2-O2	-7.01	117.29	122.20
1	AA	2132	C	C6-N1-C2	-7.01	117.50	120.30
1	AA	2137	U	C2-N1-C1'	6.99	126.08	117.70
45	BA	1060	U	C2-N1-C1'	6.98	126.08	117.70
45	BA	224	C	C6-N1-C2	-6.98	117.51	120.30
1	AA	1561	G	N3-C4-N9	-6.96	121.82	126.00
45	BA	1664	C	C2-N1-C1'	6.96	126.46	118.80
1	AA	3131	U	C2-N1-C1'	6.95	126.04	117.70
45	BA	959	U	N1-C2-O2	6.95	127.67	122.80
45	BA	191	C	N1-C2-O2	6.94	123.07	118.90
1	AA	113	C	C2-N1-C1'	6.94	126.43	118.80
3	AC	157	U	N3-C2-O2	-6.93	117.35	122.20
1	AA	3058	U	N3-C2-O2	-6.92	117.36	122.20
3	AC	64	U	N3-C2-O2	-6.92	117.36	122.20
45	BA	1202	A	C2-N3-C4	6.92	114.06	110.60
1	AA	2407	C	C5-C6-N1	6.91	124.46	121.00
1	AA	865	U	N3-C2-O2	-6.90	117.37	122.20
1	AA	3350	C	N1-C2-O2	6.90	123.04	118.90
45	BA	916	U	N1-C2-O2	6.89	127.62	122.80
45	BA	901	G	C6-C5-N7	-6.88	126.27	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1295	G	C4-N9-C1'	6.88	135.45	126.50
45	BA	241	U	O5'-P-OP2	-6.88	99.51	105.70
1	AA	3217	C	C6-N1-C2	-6.87	117.55	120.30
45	BA	1458	G	C8-N9-C1'	-6.87	118.07	127.00
45	BA	1295	G	N3-C4-N9	6.87	130.12	126.00
1	AA	954	U	N3-C2-O2	-6.86	117.39	122.20
1	AA	1604	G	N3-C4-N9	6.86	130.12	126.00
45	BA	935	U	N1-C2-O2	6.85	127.60	122.80
45	BA	139	C	P-O3'-C3'	6.85	127.92	119.70
1	AA	957	C	C6-N1-C2	-6.83	117.57	120.30
1	AA	1333	C	C5-C6-N1	6.83	124.41	121.00
45	BA	185	U	N1-C2-O2	6.81	127.57	122.80
45	BA	818	C	C5-C6-N1	6.81	124.40	121.00
1	AA	2652	U	N3-C2-O2	-6.80	117.44	122.20
45	BA	184	C	C2-N1-C1'	6.80	126.28	118.80
45	BA	79	C	C6-N1-C2	-6.80	117.58	120.30
45	BA	990	C	C5-C6-N1	6.79	124.39	121.00
1	AA	2522	G	C4-N9-C1'	6.77	135.30	126.50
45	BA	283	U	N1-C2-O2	6.76	127.53	122.80
1	AA	1349	G	C4-N9-C1'	6.76	135.29	126.50
45	BA	633	U	N3-C2-O2	-6.76	117.47	122.20
45	BA	817	A	C4-C5-N7	6.73	114.06	110.70
1	AA	881	C	N1-C2-O2	6.72	122.93	118.90
45	BA	1596	C	C2-N1-C1'	6.72	126.19	118.80
45	BA	1298	U	N3-C2-O2	-6.72	117.50	122.20
1	AA	2716	U	N1-C2-O2	6.71	127.50	122.80
45	BA	1683	C	O4'-C1'-N1	6.71	113.57	108.20
45	BA	354	C	C5-C6-N1	6.70	124.35	121.00
62	BR	28	LEU	CA-CB-CG	6.70	130.71	115.30
45	BA	1573	A	OP2-P-O3'	6.70	119.94	105.20
1	AA	2652	U	N1-C2-O2	6.69	127.48	122.80
1	AA	2983	C	C2-N1-C1'	6.68	126.15	118.80
45	BA	736	C	N3-C2-O2	-6.68	117.22	121.90
1	AA	1858	A	O4'-C1'-N9	6.65	113.52	108.20
45	BA	1297	G	C8-N9-C4	-6.65	103.74	106.40
1	AA	2873	U	C2-N1-C1'	6.65	125.68	117.70
45	BA	14	C	N3-C2-O2	-6.64	117.25	121.90
45	BA	1000	C	C6-N1-C1'	-6.64	112.84	120.80
45	BA	1307	U	N1-C2-O2	6.63	127.44	122.80
45	BA	830	U	O4'-C1'-N1	6.62	113.50	108.20
3	AC	127	U	C2-N1-C1'	6.62	125.64	117.70
45	BA	14	C	C6-N1-C2	-6.62	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2873	U	N1-C2-O2	6.62	127.43	122.80
45	BA	829	A	P-O3'-C3'	6.61	127.63	119.70
43	Aq	74	CYS	CA-CB-SG	6.60	125.88	114.00
1	AA	270	U	C2-N1-C1'	6.60	125.62	117.70
45	BA	575	C	C6-N1-C2	-6.60	117.66	120.30
1	AA	922	U	N3-C2-O2	-6.59	117.58	122.20
1	AA	3214	U	N3-C2-O2	-6.59	117.59	122.20
45	BA	158	U	P-O3'-C3'	6.58	127.60	119.70
45	BA	1761	U	P-O3'-C3'	6.58	127.60	119.70
45	BA	394	C	C5-C6-N1	6.58	124.29	121.00
1	AA	2101	C	P-O3'-C3'	6.57	127.59	119.70
3	AC	100	U	C2-N1-C1'	6.57	125.58	117.70
1	AA	1238	C	N3-C2-O2	-6.56	117.31	121.90
1	AA	1097	G	P-O3'-C3'	6.56	127.57	119.70
45	BA	1082	C	C6-N1-C2	-6.56	117.68	120.30
1	AA	2783	U	N3-C2-O2	-6.55	117.61	122.20
45	BA	1573	A	P-O3'-C3'	6.55	127.56	119.70
45	BA	648	G	C8-N9-C1'	-6.54	118.50	127.00
1	AA	3057	U	C2-N1-C1'	6.54	125.55	117.70
1	AA	65	A	P-O3'-C3'	6.53	127.53	119.70
45	BA	614	C	C5-C6-N1	6.51	124.26	121.00
1	AA	3298	C	C6-N1-C2	-6.51	117.70	120.30
1	AA	865	U	N1-C2-O2	6.51	127.36	122.80
45	BA	625	C	C6-N1-C2	-6.51	117.70	120.30
45	BA	380	U	N1-C2-O2	6.50	127.35	122.80
45	BA	1535	U	N3-C2-O2	-6.49	117.66	122.20
1	AA	2112	U	OP2-P-O3'	6.49	119.47	105.20
45	BA	1657	U	P-O3'-C3'	6.48	127.48	119.70
45	BA	1096	C	N1-C2-O2	6.48	122.79	118.90
45	BA	1332	C	C6-N1-C2	-6.47	117.71	120.30
47	BC	70	LEU	CA-CB-CG	6.47	130.19	115.30
1	AA	2522	G	N3-C4-N9	6.47	129.88	126.00
45	BA	1274	C	N1-C2-O2	6.46	122.78	118.90
45	BA	505	A	C2-N3-C4	6.46	113.83	110.60
1	AA	2726	C	C2-N1-C1'	6.46	125.90	118.80
45	BA	1527	C	C6-N1-C2	-6.45	117.72	120.30
45	BA	1389	C	C6-N1-C1'	-6.44	113.07	120.80
1	AA	3078	U	N1-C2-O2	6.44	127.31	122.80
1	AA	1716	U	P-O3'-C3'	6.43	127.42	119.70
62	BR	40	GLU	C-N-CD	-6.43	106.46	120.60
1	AA	954	U	N1-C2-O2	6.42	127.30	122.80
45	BA	1489	U	C2-N1-C1'	6.42	125.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1597	C	C5-C6-N1	6.41	124.21	121.00
1	AA	995	U	N1-C2-O2	6.41	127.29	122.80
1	AA	1224	C	N3-C2-O2	-6.41	117.41	121.90
1	AA	1227	C	C6-N1-C2	-6.41	117.74	120.30
1	AA	42	C	C6-N1-C2	-6.41	117.74	120.30
1	AA	2257	C	C6-N1-C1'	-6.40	113.11	120.80
1	AA	946	U	C5-C6-N1	6.40	125.90	122.70
2	AB	58	C	C5-C6-N1	6.40	124.20	121.00
2	AB	73	C	N1-C2-O2	6.40	122.74	118.90
6	AF	182	LEU	CA-CB-CG	6.40	130.02	115.30
1	AA	2112	U	P-O3'-C3'	6.40	127.38	119.70
1	AA	2846	U	N3-C2-O2	-6.39	117.73	122.20
45	BA	855	A	C5'-C4'-O4'	6.36	116.73	109.10
1	AA	42	C	C5-C6-N1	6.36	124.18	121.00
45	BA	79	C	C2-N1-C1'	6.36	125.80	118.80
1	AA	2444	C	N1-C2-O2	6.36	122.71	118.90
2	AB	78	U	C5-C6-N1	6.36	125.88	122.70
45	BA	191	C	N3-C2-O2	-6.35	117.45	121.90
45	BA	934	C	C2-N1-C1'	6.35	125.78	118.80
1	AA	777	U	N3-C2-O2	-6.35	117.76	122.20
1	AA	1645	U	N1-C2-O2	6.35	127.24	122.80
1	AA	1227	C	C2-N3-C4	6.35	123.07	119.90
45	BA	1298	U	O4'-C1'-N1	6.35	113.28	108.20
1	AA	922	U	C6-N1-C1'	-6.34	112.32	121.20
1	AA	1437	C	C2-N1-C1'	6.34	125.78	118.80
1	AA	1604	G	C8-N9-C1'	-6.33	118.77	127.00
45	BA	818	C	N3-C2-O2	-6.33	117.47	121.90
1	AA	601	U	C2-N1-C1'	6.32	125.29	117.70
45	BA	830	U	C2-N1-C1'	6.32	125.28	117.70
1	AA	729	C	C5-C6-N1	6.31	124.15	121.00
45	BA	1527	C	N1-C2-O2	6.30	122.68	118.90
45	BA	1796	C	N3-C2-O2	-6.30	117.49	121.90
1	AA	1255	C	N3-C2-O2	-6.29	117.49	121.90
1	AA	637	C	P-O3'-C3'	6.29	127.25	119.70
45	BA	1024	U	N1-C2-O2	6.29	127.21	122.80
1	AA	2407	C	C6-N1-C2	-6.29	117.78	120.30
45	BA	795	U	N3-C2-O2	-6.29	117.80	122.20
45	BA	543	C	C2-N1-C1'	6.29	125.72	118.80
1	AA	2585	G	N3-C4-C5	-6.28	125.46	128.60
1	AA	3275	U	C5-C6-N1	6.27	125.84	122.70
45	BA	224	C	N3-C2-O2	-6.27	117.51	121.90
45	BA	185	U	C2-N1-C1'	6.27	125.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1146	C	C2-N1-C1'	6.26	125.69	118.80
1	AA	2522	G	N3-C4-C5	-6.26	125.47	128.60
1	AA	1146	C	C6-N1-C2	-6.25	117.80	120.30
45	BA	1291	G	C4-N9-C1'	6.25	134.62	126.50
45	BA	250	C	C5-C6-N1	6.25	124.12	121.00
45	BA	530	C	N1-C2-O2	6.25	122.65	118.90
45	BA	354	C	C6-N1-C2	-6.25	117.80	120.30
45	BA	191	C	C5-C6-N1	6.25	124.12	121.00
1	AA	2257	C	C6-N1-C2	-6.24	117.80	120.30
45	BA	453	U	C6-N1-C1'	-6.24	112.46	121.20
1	AA	113	C	C6-N1-C2	-6.24	117.81	120.30
1	AA	2444	C	C6-N1-C1'	-6.24	113.32	120.80
1	AA	916	G	P-O3'-C3'	6.23	127.18	119.70
1	AA	3362	A	N7-C8-N9	6.23	116.91	113.80
45	BA	1456	C	N3-C2-O2	-6.23	117.54	121.90
1	AA	1608	C	C2-N1-C1'	6.22	125.65	118.80
45	BA	765	G	O4'-C1'-N9	-6.22	103.22	108.20
45	BA	1456	C	C2-N1-C1'	6.22	125.64	118.80
45	BA	1572	G	C4-N9-C1'	6.22	134.58	126.50
1	AA	846	A	C5-C6-N6	-6.21	118.73	123.70
45	BA	536	C	C2-N1-C1'	6.20	125.62	118.80
1	AA	1255	C	C6-N1-C2	-6.20	117.82	120.30
1	AA	1283	C	N3-C2-O2	-6.20	117.56	121.90
1	AA	2366	C	C5-C6-N1	6.19	124.10	121.00
1	AA	1448	U	C2-N1-C1'	6.18	125.12	117.70
1	AA	3228	C	P-O3'-C3'	6.18	127.12	119.70
2	AB	58	C	C6-N1-C2	-6.18	117.83	120.30
1	AA	1907	C	N3-C2-O2	-6.18	117.57	121.90
1	AA	1368	U	C2-N1-C1'	6.17	125.11	117.70
1	AA	2572	C	C6-N1-C1'	-6.17	113.39	120.80
1	AA	2176	U	N3-C2-O2	-6.17	117.88	122.20
1	AA	2572	C	C5-C6-N1	6.17	124.08	121.00
45	BA	530	C	C6-N1-C2	-6.17	117.83	120.30
45	BA	901	G	C4-N9-C1'	6.16	134.50	126.50
1	AA	981	U	C6-N1-C2	-6.16	117.31	121.00
45	BA	841	U	N3-C2-O2	-6.15	117.89	122.20
45	BA	267	U	N1-C2-O2	6.14	127.10	122.80
45	BA	1246	C	C6-N1-C2	-6.14	117.84	120.30
45	BA	1323	C	N3-C2-O2	-6.14	117.60	121.90
45	BA	1060	U	N3-C2-O2	-6.14	117.90	122.20
45	BA	1327	C	C6-N1-C2	-6.14	117.84	120.30
45	BA	1389	C	C6-N1-C2	-6.14	117.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	3034	C	C6-N1-C2	-6.13	117.85	120.30
16	AP	75	VAL	CA-CB-CG1	6.13	120.10	110.90
1	AA	1269	U	C6-N1-C1'	-6.13	112.62	121.20
1	AA	601	U	C5-C6-N1	6.13	125.77	122.70
45	BA	911	U	N1-C2-O2	6.13	127.09	122.80
1	AA	637	C	C2-N1-C1'	-6.12	112.07	118.80
1	AA	1064	A	P-O3'-C3'	6.12	127.04	119.70
1	AA	1265	U	N3-C2-O2	-6.12	117.92	122.20
1	AA	1349	G	C2-N3-C4	6.11	114.96	111.90
1	AA	2537	U	P-O3'-C3'	6.11	127.03	119.70
1	AA	1608	C	N1-C2-O2	6.10	122.56	118.90
45	BA	361	C	C6-N1-C2	-6.09	117.86	120.30
45	BA	149	C	C2-N1-C1'	6.08	125.48	118.80
45	BA	1674	C	C6-N1-C2	-6.08	117.87	120.30
1	AA	3117	C	N1-C2-O2	6.08	122.55	118.90
45	BA	1274	C	C2-N1-C1'	6.07	125.48	118.80
1	AA	2405	C	N1-C2-O2	6.07	122.54	118.90
45	BA	230	C	C6-N1-C2	-6.07	117.87	120.30
45	BA	116	U	N1-C2-O2	6.06	127.04	122.80
1	AA	244	G	N3-C4-N9	6.05	129.63	126.00
45	BA	1761	U	N3-C2-O2	-6.04	117.97	122.20
5	AE	140	ASP	CB-CG-OD1	6.04	123.73	118.30
1	AA	1228	C	C6-N1-C2	-6.03	117.89	120.30
1	AA	1820	U	P-O3'-C3'	6.03	126.94	119.70
1	AA	2334	U	N3-C2-O2	-6.03	117.98	122.20
45	BA	1568	C	P-O3'-C3'	6.02	126.93	119.70
45	BA	911	U	N3-C2-O2	-6.01	117.99	122.20
1	AA	1604	G	N3-C4-C5	-6.00	125.60	128.60
1	AA	2638	C	N1-C2-O2	6.00	122.50	118.90
45	BA	283	U	N3-C2-O2	-6.00	118.00	122.20
3	AC	21	C	N1-C2-O2	6.00	122.50	118.90
45	BA	575	C	C2-N1-C1'	6.00	125.39	118.80
45	BA	142	G	N1-C2-N2	6.00	121.59	116.20
1	AA	1216	C	C2-N1-C1'	5.99	125.39	118.80
1	AA	846	A	C4-C5-N7	5.99	113.69	110.70
45	BA	1309	C	C6-N1-C2	-5.99	117.91	120.30
1	AA	2550	U	C2-N1-C1'	5.98	124.87	117.70
45	BA	1619	C	C6-N1-C2	-5.98	117.91	120.30
45	BA	855	A	C1'-O4'-C4'	-5.97	105.12	109.90
1	AA	2606	G	N3-C4-C5	-5.97	125.61	128.60
45	BA	644	C	N1-C2-O2	5.96	122.48	118.90
1	AA	1103	A	O4'-C1'-N9	5.96	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1155	C	C5-C6-N1	5.96	123.98	121.00
2	AB	105	C	N1-C2-O2	5.96	122.47	118.90
45	BA	1302	U	N3-C2-O2	-5.96	118.03	122.20
1	AA	1115	G	C4-N9-C1'	5.96	134.25	126.50
45	BA	648	G	C6-C5-N7	-5.95	126.83	130.40
45	BA	990	C	C6-N1-C2	-5.95	117.92	120.30
45	BA	1481	C	C6-N1-C2	-5.95	117.92	120.30
1	AA	1525	G	C4-N9-C1'	5.94	134.22	126.50
1	AA	1706	C	N1-C2-O2	5.93	122.46	118.90
45	BA	1324	G	N9-C4-C5	5.93	107.77	105.40
1	AA	1227	C	C2-N1-C1'	5.93	125.32	118.80
1	AA	3277	U	C2-N1-C1'	5.93	124.81	117.70
1	AA	3034	C	N1-C2-O2	5.92	122.45	118.90
45	BA	79	C	C5-C6-N1	5.92	123.96	121.00
1	AA	2846	U	C2-N1-C1'	5.92	124.80	117.70
1	AA	283	G	N3-C4-N9	5.91	129.54	126.00
1	AA	282	G	C8-N9-C4	-5.90	104.04	106.40
45	BA	1327	C	C5-C6-N1	5.90	123.95	121.00
1	AA	1238	C	C6-N1-C2	-5.90	117.94	120.30
1	AA	729	C	C6-N1-C2	-5.90	117.94	120.30
45	BA	417	A	P-O3'-C3'	5.89	126.77	119.70
45	BA	965	U	N1-C2-O2	5.89	126.92	122.80
45	BA	1344	A	P-O3'-C3'	5.89	126.76	119.70
3	AC	100	U	C5-C6-N1	5.88	125.64	122.70
45	BA	160	C	N3-C2-O2	-5.88	117.78	121.90
45	BA	25	C	P-O3'-C3'	5.88	126.76	119.70
45	BA	935	U	N3-C2-O2	-5.88	118.08	122.20
45	BA	1527	C	C6-N1-C1'	-5.88	113.75	120.80
1	AA	638	C	C6-N1-C2	-5.87	117.95	120.30
45	BA	75	U	N1-C2-O2	5.87	126.91	122.80
1	AA	1037	C	N1-C2-O2	5.86	122.42	118.90
50	BF	193	GLY	C-N-CA	5.86	136.35	121.70
45	BA	818	C	C6-N1-C2	-5.86	117.96	120.30
1	AA	982	C	C2-N1-C1'	5.86	125.24	118.80
1	AA	3214	U	N1-C2-O2	5.86	126.90	122.80
45	BA	1664	C	C6-N1-C2	-5.86	117.96	120.30
1	AA	2638	C	C6-N1-C2	-5.86	117.96	120.30
45	BA	916	U	N3-C2-O2	-5.86	118.10	122.20
1	AA	3350	C	N3-C2-O2	-5.85	117.81	121.90
1	AA	1608	C	C6-N1-C2	-5.85	117.96	120.30
1	AA	3298	C	C5-C6-N1	5.85	123.92	121.00
35	Ai	51	LEU	CA-CB-CG	5.85	128.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1238	C	C2-N1-C1'	5.84	125.23	118.80
3	AC	157	U	C2-N1-C1'	5.84	124.71	117.70
1	AA	1953	G	O4'-C1'-N9	-5.84	103.53	108.20
45	BA	1497	U	N1-C2-O2	5.84	126.89	122.80
45	BA	380	U	N3-C2-O2	-5.84	118.11	122.20
45	BA	497	G	P-O3'-C3'	5.84	126.71	119.70
45	BA	736	C	C6-N1-C1'	-5.83	113.80	120.80
1	AA	1355	A	P-O3'-C3'	5.83	126.70	119.70
45	BA	1246	C	C6-N1-C1'	-5.83	113.80	120.80
1	AA	1103	A	P-O3'-C3'	5.83	126.69	119.70
1	AA	2935	U	N1-C2-O2	5.83	126.88	122.80
1	AA	2137	U	C5-C6-N1	5.83	125.61	122.70
29	Ac	47	LYS	C-N-CA	5.82	136.25	121.70
1	AA	3316	A	P-O3'-C3'	5.82	126.68	119.70
1	AA	1816	A	P-O3'-C3'	5.81	126.67	119.70
1	AA	2132	C	C2-N1-C1'	5.81	125.19	118.80
1	AA	3181	C	C6-N1-C1'	-5.81	113.83	120.80
45	BA	647	G	N7-C8-N9	5.81	116.00	113.10
1	AA	1358	C	C5-C6-N1	5.80	123.90	121.00
49	BE	176	LEU	CA-CB-CG	5.80	128.65	115.30
1	AA	1190	A	C4-N9-C1'	5.80	136.74	126.30
45	BA	767	U	C2-N1-C1'	5.80	124.66	117.70
1	AA	1597	C	C6-N1-C2	-5.79	117.98	120.30
1	AA	2773	C	C6-N1-C2	-5.79	117.98	120.30
47	BC	96	LEU	CA-CB-CG	5.79	128.62	115.30
45	BA	583	C	C2-N1-C1'	5.79	125.17	118.80
45	BA	937	C	C6-N1-C2	-5.78	117.99	120.30
1	AA	2726	C	N3-C2-O2	-5.78	117.85	121.90
45	BA	959	U	C2-N1-C1'	5.78	124.64	117.70
1	AA	3269	U	N3-C2-O2	-5.77	118.16	122.20
45	BA	1000	C	N3-C2-O2	-5.77	117.86	121.90
1	AA	2209	U	P-O3'-C3'	5.77	126.62	119.70
45	BA	1000	C	N1-C2-O2	5.77	122.36	118.90
45	BA	1145	U	N3-C2-O2	-5.77	118.16	122.20
1	AA	379	C	C6-N1-C2	-5.76	117.99	120.30
50	BF	194	THR	N-CA-C	5.76	126.56	111.00
45	BA	132	U	P-O3'-C3'	5.76	126.61	119.70
1	AA	1349	G	C8-N9-C1'	-5.75	119.52	127.00
1	AA	1889	G	C4-N9-C1'	5.75	133.97	126.50
45	BA	530	C	C2-N1-C1'	5.75	125.12	118.80
45	BA	75	U	C2-N1-C1'	5.74	124.59	117.70
45	BA	1301	U	C2-N1-C1'	5.74	124.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	530	C	C5-C6-N1	5.74	123.87	121.00
1	AA	2737	C	C6-N1-C2	-5.74	118.00	120.30
1	AA	1554	U	P-O3'-C3'	5.74	126.58	119.70
45	BA	648	G	N3-C4-C5	-5.73	125.73	128.60
45	BA	1274	C	N3-C2-O2	-5.73	117.89	121.90
1	AA	1333	C	C6-N1-C2	-5.73	118.01	120.30
1	AA	1265	U	C2-N1-C1'	5.72	124.57	117.70
1	AA	3034	C	N3-C2-O2	-5.72	117.90	121.90
45	BA	610	G	C4-N9-C1'	5.72	133.94	126.50
2	AB	35	C	N1-C2-O2	5.71	122.33	118.90
45	BA	453	U	C6-N1-C2	-5.71	117.57	121.00
1	AA	97	U	N3-C2-O2	-5.71	118.20	122.20
1	AA	539	C	C6-N1-C2	-5.71	118.02	120.30
45	BA	685	A	P-O3'-C3'	5.71	126.55	119.70
45	BA	1300	A	C5-N7-C8	-5.70	101.05	103.90
45	BA	14	C	N1-C2-O2	5.70	122.32	118.90
45	BA	965	U	C6-N1-C1'	-5.70	113.22	121.20
1	AA	1508	C	N1-C2-O2	5.70	122.32	118.90
1	AA	2378	C	N1-C2-O2	5.70	122.32	118.90
1	AA	3269	U	P-O3'-C3'	5.70	126.54	119.70
45	BA	1033	C	C6-N1-C2	-5.70	118.02	120.30
45	BA	1305	U	C2-N1-C1'	5.70	124.54	117.70
45	BA	131	C	P-O3'-C3'	5.69	126.53	119.70
45	BA	1324	G	N3-C2-N2	-5.69	115.92	119.90
1	AA	3349	C	C6-N1-C2	-5.68	118.03	120.30
1	AA	102	C	C2-N1-C1'	5.68	125.05	118.80
1	AA	881	C	N3-C2-O2	-5.68	117.92	121.90
1	AA	2522	G	C8-N9-C1'	-5.68	119.62	127.00
1	AA	3218	A	P-O3'-C3'	5.68	126.51	119.70
1	AA	282	G	P-O3'-C3'	5.67	126.50	119.70
1	AA	1155	C	C6-N1-C2	-5.67	118.03	120.30
1	AA	2420	C	C6-N1-C2	-5.67	118.03	120.30
1	AA	3217	C	C5-C6-N1	5.67	123.83	121.00
1	AA	1854	C	C6-N1-C2	-5.66	118.03	120.30
45	BA	861	U	C6-N1-C1'	-5.66	113.27	121.20
45	BA	1063	U	N3-C2-O2	-5.66	118.24	122.20
45	BA	1321	A	C2-N3-C4	5.66	113.43	110.60
1	AA	2366	C	N1-C2-O2	5.66	122.30	118.90
45	BA	700	C	C6-N1-C2	-5.66	118.04	120.30
1	AA	1283	C	N1-C2-O2	5.65	122.29	118.90
1	AA	2507	C	C2-N1-C1'	5.65	125.02	118.80
1	AA	715	A	P-O3'-C3'	5.65	126.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2585	G	N3-C4-N9	5.65	129.39	126.00
1	AA	3097	C	C6-N1-C2	-5.65	118.04	120.30
1	AA	2237	C	C6-N1-C2	-5.63	118.05	120.30
1	AA	3362	A	O4'-C1'-N9	5.63	112.70	108.20
45	BA	1332	C	C5-C6-N1	5.63	123.81	121.00
45	BA	1226	A	P-O3'-C3'	5.63	126.45	119.70
45	BA	1291	G	N3-C4-C5	-5.63	125.78	128.60
1	AA	763	G	P-O3'-C3'	5.63	126.45	119.70
1	AA	2899	C	C2-N1-C1'	5.63	124.99	118.80
45	BA	472	U	N3-C2-O2	-5.63	118.26	122.20
1	AA	1482	A	C2-N3-C4	5.62	113.41	110.60
1	AA	1607	U	P-O3'-C3'	5.62	126.44	119.70
1	AA	1279	C	N1-C2-O2	5.62	122.27	118.90
1	AA	1759	C	N3-C2-O2	-5.62	117.97	121.90
1	AA	1561	G	C8-N9-C1'	5.62	134.30	127.00
1	AA	2836	C	C6-N1-C1'	-5.61	114.06	120.80
45	BA	1021	C	C2-N1-C1'	5.61	124.97	118.80
45	BA	107	C	C5-C6-N1	5.60	123.80	121.00
45	BA	1296	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1155	C	C2-N1-C1'	5.59	124.95	118.80
45	BA	1063	U	N1-C2-O2	5.59	126.71	122.80
1	AA	2666	C	C6-N1-C2	-5.59	118.06	120.30
45	BA	1572	G	N3-C4-C5	-5.59	125.81	128.60
68	BX	93	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	AA	1224	C	N1-C2-O2	5.58	122.25	118.90
1	AA	2550	U	N1-C2-O2	5.58	126.71	122.80
1	AA	2842	U	C6-N1-C1'	-5.58	113.39	121.20
1	AA	3349	C	C5-C6-N1	5.58	123.79	121.00
1	AA	1525	G	C8-N9-C1'	-5.58	119.75	127.00
1	AA	2652	U	C2-N1-C1'	5.58	124.39	117.70
2	AB	96	U	N3-C2-O2	-5.58	118.30	122.20
5	AE	19	ARG	N-CA-C	5.57	126.03	111.00
51	BG	42	LEU	CA-CB-CG	5.57	128.11	115.30
45	BA	302	U	N3-C2-O2	-5.56	118.31	122.20
1	AA	1425	U	N3-C2-O2	-5.56	118.31	122.20
1	AA	3089	C	C6-N1-C2	-5.56	118.08	120.30
45	BA	559	C	C2-N1-C1'	5.56	124.91	118.80
45	BA	1251	U	O4'-C1'-N1	5.56	112.65	108.20
45	BA	1456	C	N1-C2-O2	5.55	122.23	118.90
1	AA	101	G	O4'-C1'-N9	5.55	112.64	108.20
1	AA	1496	C	N1-C2-O2	5.55	122.23	118.90
1	AA	3350	C	P-O3'-C3'	5.55	126.36	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	Aq	77	CYS	CA-CB-SG	5.55	123.98	114.00
45	BA	992	A	O4'-C1'-N9	5.54	112.64	108.20
1	AA	915	A	C4-N9-C1'	5.54	136.28	126.30
2	AB	14	U	N3-C2-O2	-5.54	118.32	122.20
13	AM	112	LEU	CA-CB-CG	5.54	128.05	115.30
1	AA	2617	U	C2-N1-C1'	5.54	124.34	117.70
45	BA	1258	U	C6-N1-C1'	-5.54	113.45	121.20
58	BN	103	LEU	CA-CB-CG	5.54	128.04	115.30
1	AA	2507	C	C6-N1-C2	-5.54	118.09	120.30
45	BA	837	G	N3-C4-C5	-5.54	125.83	128.60
47	BC	73	LEU	CA-CB-CG	5.53	128.03	115.30
45	BA	1096	C	N3-C2-O2	-5.53	118.03	121.90
1	AA	3300	U	N3-C2-O2	-5.53	118.33	122.20
45	BA	160	C	C6-N1-C2	-5.53	118.09	120.30
1	AA	2567	C	N1-C2-O2	5.53	122.22	118.90
1	AA	3300	U	N1-C2-O2	5.53	126.67	122.80
28	Ab	102	GLU	C-N-CA	5.52	135.51	121.70
1	AA	2606	G	N3-C4-N9	5.52	129.31	126.00
1	AA	995	U	N3-C2-O2	-5.52	118.34	122.20
1	AA	2585	G	C4-N9-C1'	5.52	133.67	126.50
1	AA	846	A	N1-C6-N6	5.51	121.91	118.60
45	BA	1292	G	C8-N9-C1'	-5.51	119.83	127.00
1	AA	2567	C	C2-N1-C1'	5.51	124.86	118.80
45	BA	1632	C	N3-C2-O2	-5.51	118.05	121.90
45	BA	1333	C	C5-C6-N1	5.50	123.75	121.00
55	BK	118	LEU	CA-CB-CG	5.50	127.95	115.30
45	BA	614	C	C6-N1-C2	-5.50	118.10	120.30
1	AA	1255	C	C2-N1-C1'	5.49	124.84	118.80
45	BA	1324	G	N7-C8-N9	5.49	115.85	113.10
1	AA	311	C	C6-N1-C2	-5.49	118.10	120.30
45	BA	79	C	N1-C2-O2	5.49	122.19	118.90
45	BA	758	U	N3-C2-O2	-5.49	118.36	122.20
1	AA	78	U	N1-C2-O2	5.49	126.64	122.80
1	AA	1660	C	C5-C6-N1	5.49	123.74	121.00
1	AA	354	U	N1-C2-O2	5.48	126.64	122.80
1	AA	1878	G	C4-N9-C1'	5.48	133.63	126.50
45	BA	837	G	N1-C6-O6	-5.48	116.61	119.90
45	BA	1333	C	C6-N1-C2	-5.48	118.11	120.30
1	AA	1562	C	P-O3'-C3'	5.48	126.27	119.70
45	BA	1060	U	N1-C2-O2	5.47	126.63	122.80
45	BA	1572	G	N3-C4-N9	5.47	129.28	126.00
45	BA	270	C	C2-N1-C1'	5.47	124.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	113	C	C5-C6-N1	5.46	123.73	121.00
1	AA	179	C	C5-C6-N1	5.46	123.73	121.00
1	AA	1097	G	OP2-P-O3'	5.46	117.20	105.20
1	AA	954	U	C5-C6-N1	5.45	125.43	122.70
1	AA	3104	U	N3-C2-O2	-5.45	118.38	122.20
1	AA	1064	A	N1-C6-N6	-5.45	115.33	118.60
1	AA	1508	C	C6-N1-C2	-5.45	118.12	120.30
1	AA	1232	C	N1-C2-O2	5.45	122.17	118.90
1	AA	2638	C	N3-C2-O2	-5.45	118.08	121.90
45	BA	302	U	N1-C2-O2	5.45	126.61	122.80
2	AB	105	C	N3-C2-O2	-5.45	118.09	121.90
53	BI	131	PHE	N-CA-C	5.44	125.70	111.00
1	AA	1684	U	C5-C6-N1	5.44	125.42	122.70
45	BA	960	U	N3-C2-O2	-5.44	118.39	122.20
1	AA	282	G	C2'-C3'-O3'	5.44	122.40	113.70
45	BA	1340	U	N1-C2-O2	5.43	126.60	122.80
1	AA	379	C	C5-C6-N1	5.43	123.72	121.00
45	BA	1298	U	C6-N1-C2	-5.43	117.74	121.00
45	BA	1514	U	C5-C4-O4	5.43	129.16	125.90
1	AA	1115	G	C8-N9-C1'	-5.43	119.94	127.00
1	AA	957	C	C5-C6-N1	5.43	123.71	121.00
45	BA	792	U	N3-C2-O2	-5.43	118.40	122.20
1	AA	915	A	N7-C8-N9	5.42	116.51	113.80
1	AA	2189	U	N1-C2-O2	5.42	126.59	122.80
1	AA	3317	U	C2-N1-C1'	5.42	124.20	117.70
3	AC	108	C	C6-N1-C2	-5.41	118.14	120.30
1	AA	3084	C	C6-N1-C2	-5.41	118.14	120.30
54	BJ	29	LEU	CA-CB-CG	5.41	127.73	115.30
61	BQ	60	LEU	CB-CG-CD2	-5.41	101.81	111.00
45	BA	1340	U	N3-C2-O2	-5.40	118.42	122.20
1	AA	283	G	C4-N9-C1'	5.40	133.52	126.50
45	BA	1244	A	P-O3'-C3'	5.40	126.18	119.70
1	AA	283	G	C8-N9-C1'	-5.39	119.99	127.00
79	Bi	713	GLN	CA-C-O	5.39	131.43	120.10
1	AA	356	C	C6-N1-C2	-5.39	118.14	120.30
45	BA	1292	G	C4-N9-C1'	5.39	133.50	126.50
1	AA	3104	U	N1-C2-O2	5.39	126.57	122.80
45	BA	639	U	N3-C2-O2	-5.38	118.43	122.20
79	Bi	712	ASP	N-CA-C	5.38	125.54	111.00
1	AA	1425	U	N1-C2-O2	5.38	126.57	122.80
1	AA	142	C	C6-N1-C2	-5.38	118.15	120.30
45	BA	1489	U	N3-C2-O2	-5.38	118.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	857	U	N1-C2-O2	5.38	126.56	122.80
1	AA	1889	G	C8-N9-C1'	-5.37	120.02	127.00
45	BA	687	G	C8-N9-C4	-5.37	104.25	106.40
1	AA	315	C	C5-C6-N1	5.37	123.68	121.00
1	AA	1232	C	C6-N1-C2	-5.37	118.15	120.30
1	AA	3078	U	N3-C2-O2	-5.37	118.44	122.20
1	AA	1437	C	C5-C6-N1	5.37	123.68	121.00
45	BA	1296	A	C4-C5-N7	5.37	113.38	110.70
1	AA	315	C	C6-N1-C2	-5.37	118.15	120.30
1	AA	1759	C	C2-N1-C1'	5.36	124.70	118.80
1	AA	2935	U	N3-C2-O2	-5.36	118.45	122.20
1	AA	2263	C	C5-C6-N1	5.36	123.68	121.00
1	AA	3131	U	N1-C2-O2	5.36	126.55	122.80
1	AA	3318	G	C6-C5-N7	-5.36	127.19	130.40
1	AA	3318	G	N3-C4-N9	5.36	129.21	126.00
1	AA	637	C	O4'-C1'-N1	5.35	112.48	108.20
1	AA	2552	C	C2-N1-C1'	5.35	124.69	118.80
1	AA	3355	U	N3-C2-O2	-5.35	118.45	122.20
45	BA	1481	C	P-O3'-C3'	5.35	126.12	119.70
1	AA	1872	C	N1-C2-O2	5.35	122.11	118.90
77	Bg	136	LYS	C-N-CA	5.35	135.08	121.70
45	BA	853	G	N9-C1'-C2'	5.35	120.95	114.00
1	AA	1706	C	N3-C2-O2	-5.34	118.16	121.90
1	AA	2983	C	N1-C2-O2	5.34	122.11	118.90
45	BA	687	G	N3-C2-N2	-5.34	116.16	119.90
1	AA	851	C	C6-N1-C2	-5.34	118.16	120.30
1	AA	2189	U	N3-C2-O2	-5.34	118.46	122.20
45	BA	1185	U	C2-N1-C1'	5.34	124.11	117.70
1	AA	851	C	N1-C2-O2	5.34	122.10	118.90
1	AA	1819	U	N1-C2-O2	5.34	126.54	122.80
1	AA	2783	U	N1-C2-O2	5.34	126.54	122.80
45	BA	185	U	N3-C2-O2	-5.34	118.47	122.20
45	BA	453	U	C5-C6-N1	5.34	125.37	122.70
1	AA	2825	C	N1-C2-O2	5.33	122.10	118.90
1	AA	3317	U	N3-C2-O2	-5.33	118.47	122.20
1	AA	846	A	N9-C4-C5	-5.33	103.67	105.80
45	BA	817	A	C6-C5-N7	-5.33	128.57	132.30
45	BA	149	C	C6-N1-C2	-5.33	118.17	120.30
45	BA	184	C	C6-N1-C2	-5.33	118.17	120.30
45	BA	702	G	O4'-C1'-N9	5.33	112.46	108.20
45	BA	901	G	C8-N9-C1'	-5.32	120.08	127.00
45	BA	965	U	N3-C2-O2	-5.32	118.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1323	C	C5-C6-N1	5.32	123.66	121.00
45	BA	1796	C	C6-N1-C2	-5.32	118.17	120.30
14	AN	93	ILE	CG1-CB-CG2	-5.31	99.71	111.40
45	BA	1759	C	C2-N1-C1'	5.31	124.64	118.80
1	AA	2334	U	N1-C2-O2	5.31	126.52	122.80
1	AA	2405	C	C2-N1-C1'	5.31	124.64	118.80
45	BA	700	C	C2-N1-C1'	5.31	124.64	118.80
45	BA	1585	U	C2-N1-C1'	5.31	124.07	117.70
1	AA	226	C	C6-N1-C2	-5.30	118.18	120.30
1	AA	715	A	OP1-P-O3'	5.30	116.86	105.20
1	AA	896	A	O4'-C1'-N9	5.30	112.44	108.20
48	BD	39	THR	CA-CB-CG2	5.29	119.80	112.40
1	AA	2132	C	C5-C6-N1	5.29	123.64	121.00
1	AA	873	C	P-O3'-C3'	5.29	126.04	119.70
1	AA	1496	C	C6-N1-C2	-5.29	118.19	120.30
45	BA	361	C	C4-C5-C6	-5.29	114.76	117.40
45	BA	1620	C	C6-N1-C2	-5.29	118.19	120.30
45	BA	1291	G	N7-C8-N9	5.28	115.74	113.10
45	BA	1489	U	N1-C2-O2	5.28	126.50	122.80
2	AB	96	U	N1-C2-O2	5.28	126.50	122.80
45	BA	795	U	C2-N1-C1'	5.28	124.04	117.70
1	AA	1237	G	C4-N9-C1'	5.27	133.35	126.50
45	BA	1600	A	C4-N9-C1'	5.27	135.79	126.30
1	AA	1561	G	C4-N9-C1'	-5.27	119.65	126.50
45	BA	841	U	N1-C2-O2	5.27	126.49	122.80
45	BA	1161	C	C5-C6-N1	5.26	123.63	121.00
1	AA	1168	U	N1-C2-O2	5.26	126.48	122.80
1	AA	1819	U	N3-C2-O2	-5.26	118.52	122.20
45	BA	166	C	N1-C2-O2	5.26	122.06	118.90
76	Bf	49	LEU	CA-CB-CG	5.26	127.39	115.30
1	AA	716	A	O5'-P-OP1	-5.26	100.97	105.70
1	AA	515	C	C2-N1-C1'	5.25	124.58	118.80
1	AA	3058	U	C6-N1-C1'	-5.25	113.85	121.20
45	BA	1362	U	C5-C6-N1	5.25	125.33	122.70
1	AA	1266	G	N3-C4-C5	-5.25	125.98	128.60
1	AA	637	C	C6-N1-C1'	5.24	127.09	120.80
78	Bh	292	LEU	CA-CB-CG	5.24	127.36	115.30
45	BA	240	U	OP2-P-O3'	5.24	116.72	105.20
45	BA	1024	U	C6-N1-C2	-5.24	117.86	121.00
45	BA	1052	U	C2-N1-C1'	5.23	123.98	117.70
1	AA	2763	U	N1-C2-O2	5.23	126.46	122.80
45	BA	1296	A	C6-C5-N7	-5.23	128.64	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1585	U	N1-C2-O2	5.23	126.46	122.80
1	AA	1561	G	N9-C4-C5	5.23	107.49	105.40
45	BA	74	U	N3-C2-O2	-5.23	118.54	122.20
1	AA	1192	C	N1-C2-O2	5.23	122.04	118.90
1	AA	2546	C	N1-C2-O2	5.23	122.04	118.90
1	AA	2617	U	N3-C2-O2	-5.23	118.54	122.20
45	BA	225	A	N1-C6-N6	5.23	121.74	118.60
45	BA	1620	C	N3-C2-O2	-5.23	118.24	121.90
2	AB	73	C	N3-C2-O2	-5.22	118.24	121.90
1	AA	2235	C	C6-N1-C2	-5.22	118.21	120.30
3	AC	64	U	N1-C2-O2	5.22	126.46	122.80
1	AA	1496	C	C6-N1-C1'	-5.22	114.54	120.80
1	AA	1660	C	C6-N1-C2	-5.22	118.21	120.30
1	AA	3235	C	N1-C2-O2	5.21	122.03	118.90
45	BA	617	U	C5-C6-N1	5.21	125.31	122.70
45	BA	1241	G	O4'-C1'-N9	5.21	112.37	108.20
45	BA	1456	C	C6-N1-C2	-5.21	118.22	120.30
45	BA	1585	U	N3-C2-O2	-5.21	118.55	122.20
1	AA	2988	C	C6-N1-C2	-5.21	118.22	120.30
45	BA	543	C	C6-N1-C2	-5.21	118.22	120.30
45	BA	610	G	C8-N9-C1'	-5.21	120.23	127.00
1	AA	1266	G	C4-N9-C1'	5.20	133.27	126.50
45	BA	1503	A	O4'-C1'-N9	5.20	112.36	108.20
45	BA	268	C	N1-C2-O2	5.20	122.02	118.90
1	AA	752	C	C6-N1-C2	-5.20	118.22	120.30
45	BA	854	U	C1'-C2'-O2'	-5.20	95.00	110.60
45	BA	460	A	C2-N3-C4	5.20	113.20	110.60
45	BA	1632	C	N1-C2-O2	5.19	122.02	118.90
27	Aa	83	ASP	CB-CG-OD1	5.19	122.97	118.30
45	BA	1497	U	N3-C2-O2	-5.19	118.57	122.20
45	BA	224	C	N1-C2-O2	5.19	122.01	118.90
45	BA	1755	A	O4'-C1'-N9	5.19	112.35	108.20
1	AA	2773	C	C2-N1-C1'	5.18	124.50	118.80
3	AC	4	C	N1-C2-O2	5.18	122.01	118.90
1	AA	421	G	C4-N9-C1'	5.18	133.24	126.50
1	AA	743	C	N1-C2-O2	5.18	122.01	118.90
1	AA	1496	C	C5-C6-N1	5.18	123.59	121.00
2	AB	105	C	C6-N1-C2	-5.18	118.23	120.30
45	BA	848	C	C6-N1-C2	-5.18	118.23	120.30
1	AA	2257	C	C5-C6-N1	5.17	123.59	121.00
45	BA	411	C	C2-N1-C1'	5.17	124.49	118.80
45	BA	1632	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	694	U	C2-N1-C1'	5.17	123.90	117.70
1	AA	743	C	N3-C2-O2	-5.16	118.29	121.90
1	AA	601	U	N1-C2-O2	5.16	126.41	122.80
1	AA	1508	C	C5-C6-N1	5.16	123.58	121.00
45	BA	934	C	N1-C2-O2	5.16	122.00	118.90
68	BX	104	LEU	CA-CB-CG	5.16	127.16	115.30
1	AA	2137	U	O4'-C1'-N1	5.16	112.32	108.20
45	BA	166	C	N3-C2-O2	-5.15	118.29	121.90
1	AA	2585	G	C2-N3-C4	5.15	114.47	111.90
2	AB	68	C	C6-N1-C2	-5.15	118.24	120.30
2	AB	18	C	C6-N1-C2	-5.15	118.24	120.30
45	BA	540	G	N3-C4-N9	5.15	129.09	126.00
45	BA	581	U	C6-N1-C1'	-5.14	114.00	121.20
45	BA	174	U	N3-C2-O2	-5.14	118.60	122.20
45	BA	497	G	OP1-P-O3'	5.14	116.51	105.20
1	AA	663	C	C5-C6-N1	5.14	123.57	121.00
1	AA	2822	U	N3-C2-O2	-5.14	118.60	122.20
45	BA	822	U	N3-C2-O2	-5.14	118.60	122.20
1	AA	881	C	C2-N1-C1'	5.14	124.45	118.80
1	AA	2277	C	C6-N1-C2	-5.14	118.24	120.30
45	BA	1291	G	N3-C4-N9	5.14	129.08	126.00
45	BA	1500	C	C2-N1-C1'	5.14	124.45	118.80
1	AA	1907	C	C2-N1-C1'	5.14	124.45	118.80
1	AA	228	U	N3-C2-O2	-5.14	118.61	122.20
1	AA	3277	U	N1-C2-O2	5.14	126.39	122.80
1	AA	326	U	N1-C2-O2	5.13	126.39	122.80
45	BA	1641	C	C6-N1-C2	-5.13	118.25	120.30
1	AA	339	C	N3-C2-O2	-5.13	118.31	121.90
1	AA	2726	C	N1-C2-O2	5.13	121.98	118.90
73	Bc	3	LEU	CA-CB-CG	5.13	127.09	115.30
1	AA	777	U	N1-C2-O2	5.12	126.39	122.80
2	AB	18	C	C2-N1-C1'	5.12	124.44	118.80
45	BA	1626	U	C2-N1-C1'	5.12	123.84	117.70
1	AA	885	U	N3-C2-O2	-5.12	118.62	122.20
45	BA	821	U	N1-C2-O2	5.12	126.38	122.80
1	AA	1437	C	C6-N1-C2	-5.11	118.25	120.30
45	BA	503	G	P-O3'-C3'	5.11	125.84	119.70
62	BR	40	GLU	C-N-CA	5.11	143.48	122.00
1	AA	244	G	C4-N9-C1'	5.11	133.14	126.50
61	BQ	25	LEU	CA-CB-CG	5.11	127.05	115.30
1	AA	166	C	C6-N1-C2	-5.11	118.26	120.30
1	AA	1608	C	C5-C6-N1	5.11	123.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2815	G	N1-C6-O6	-5.10	116.84	119.90
45	BA	969	C	N1-C2-O2	5.10	121.96	118.90
2	AB	14	U	N1-C2-O2	5.10	126.37	122.80
1	AA	1261	G	C2-N3-C4	5.09	114.45	111.90
45	BA	1620	C	N1-C2-O2	5.09	121.96	118.90
1	AA	1183	C	C6-N1-C2	-5.09	118.26	120.30
1	AA	2422	C	C2-N1-C1'	5.09	124.40	118.80
45	BA	120	U	C5-C6-N1	5.09	125.24	122.70
45	BA	1626	U	C5-C6-N1	5.09	125.24	122.70
1	AA	179	C	C6-N1-C2	-5.08	118.27	120.30
1	AA	915	A	C8-N9-C4	-5.08	103.77	105.80
1	AA	1705	U	N1-C2-O2	5.08	126.36	122.80
1	AA	2836	C	C6-N1-C2	-5.08	118.27	120.30
1	AA	3181	C	C6-N1-C2	-5.08	118.27	120.30
1	AA	1216	C	C6-N1-C2	-5.08	118.27	120.30
1	AA	2689	A	C2-N3-C4	5.08	113.14	110.60
45	BA	530	C	N3-C2-O2	-5.08	118.34	121.90
1	AA	271	C	N1-C2-O2	5.08	121.95	118.90
45	BA	160	C	N1-C2-O2	5.08	121.95	118.90
45	BA	901	G	C4-C5-N7	5.08	112.83	110.80
45	BA	1439	C	C5-C6-N1	5.08	123.54	121.00
1	AA	1912	U	N3-C2-O2	-5.08	118.65	122.20
1	AA	2389	C	C6-N1-C2	-5.08	118.27	120.30
53	BI	126	LEU	CA-CB-CG	5.08	126.97	115.30
1	AA	1228	C	N1-C2-O2	5.07	121.94	118.90
45	BA	1117	U	C5-C6-N1	5.07	125.24	122.70
45	BA	1344	A	C3'-C2'-C1'	5.07	105.56	101.50
45	BA	211	U	N3-C2-O2	-5.07	118.65	122.20
1	AA	1168	U	N3-C2-O2	-5.07	118.65	122.20
1	AA	1688	U	N3-C2-O2	-5.07	118.65	122.20
1	AA	2277	C	C5-C6-N1	5.07	123.53	121.00
1	AA	1684	U	N3-C2-O2	-5.07	118.66	122.20
45	BA	1619	C	C2-N1-C1'	5.06	124.37	118.80
1	AA	270	U	C5-C6-N1	5.06	125.23	122.70
45	BA	196	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	949	C	C6-N1-C2	-5.06	118.28	120.30
45	BA	1560	U	C6-N1-C1'	-5.06	114.11	121.20
45	BA	536	C	C6-N1-C2	-5.06	118.28	120.30
1	AA	1620	U	N1-C2-O2	5.06	126.34	122.80
1	AA	2722	U	N3-C2-O2	-5.06	118.66	122.20
1	AA	1843	C	C6-N1-C2	-5.05	118.28	120.30
45	BA	21	U	N3-C2-O2	-5.05	118.66	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1596	C	N1-C2-O2	5.05	121.93	118.90
45	BA	1796	C	C2-N1-C1'	5.05	124.36	118.80
2	AB	39	C	C2-N1-C1'	5.05	124.36	118.80
7	AG	137	ASP	CB-CG-OD1	5.05	122.85	118.30
1	AA	2810	C	N3-C2-O2	-5.05	118.36	121.90
45	BA	186	C	C2-N1-C1'	5.05	124.36	118.80
1	AA	1282	G	N9-C4-C5	5.05	107.42	105.40
45	BA	1302	U	C2-N1-C1'	5.05	123.76	117.70
1	AA	1261	G	N3-C4-C5	-5.05	126.08	128.60
1	AA	2710	C	C6-N1-C2	-5.04	118.28	120.30
1	AA	1201	C	C6-N1-C2	-5.04	118.28	120.30
45	BA	1399	C	C6-N1-C2	-5.04	118.28	120.30
45	BA	1490	C	C2-N1-C1'	5.04	124.34	118.80
63	BS	23	LYS	C-N-CA	5.04	134.30	121.70
1	AA	1037	C	C6-N1-C2	-5.04	118.29	120.30
1	AA	3362	A	C5-N7-C8	-5.04	101.38	103.90
45	BA	1097	U	C2-N1-C1'	5.04	123.74	117.70
1	AA	515	C	C6-N1-C2	-5.03	118.29	120.30
78	Bh	202	LEU	CA-CB-CG	5.03	126.86	115.30
45	BA	218	A	N9-C4-C5	-5.03	103.79	105.80
45	BA	1536	G	C4-N9-C1'	5.03	133.03	126.50
1	AA	1901	A	C4-N9-C1'	5.02	135.34	126.30
1	AA	2274	U	C2-N1-C1'	5.02	123.72	117.70
1	AA	865	U	C2-N1-C1'	5.02	123.72	117.70
1	AA	1265	U	C5-C6-N1	5.02	125.21	122.70
1	AA	1688	U	N1-C2-O2	5.02	126.31	122.80
45	BA	5	U	N3-C2-O2	-5.02	118.69	122.20
45	BA	218	A	P-O3'-C3'	5.02	125.72	119.70
1	AA	2420	C	C5-C6-N1	5.02	123.51	121.00
45	BA	934	C	C6-N1-C1'	-5.01	114.78	120.80
45	BA	1172	G	N7-C8-N9	5.01	115.61	113.10
45	BA	174	U	N1-C2-O2	5.01	126.31	122.80
1	AA	986	U	N3-C2-O2	-5.01	118.69	122.20
45	BA	1226	A	C2'-C3'-O3'	5.01	121.72	113.70
45	BA	831	U	C6-N1-C2	-5.01	118.00	121.00
3	AC	55	U	N1-C2-O2	5.01	126.30	122.80
45	BA	767	U	N1-C2-O2	5.01	126.30	122.80
45	BA	1354	G	C4-N9-C1'	5.01	133.01	126.50
1	AA	3121	U	OP1-P-O3'	5.00	116.21	105.20
52	BH	69	LEU	CA-CB-CG	5.00	126.81	115.30
1	AA	2772	C	C2-N1-C1'	5.00	124.30	118.80
1	AA	995	U	C2-N1-C1'	5.00	123.70	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	1202	A	N3-C4-N9	5.00	131.40	127.40

There are no chirality outliers.

All (95) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	143	GLU	Peptide
4	AD	250	GLN	Peptide
5	AE	16	PHE	Mainchain
5	AE	18	PRO	Mainchain,Peptide
6	AF	318	LEU	Peptide
6	AF	338	LYS	Peptide
7	AG	124	GLU	Peptide
7	AG	257	GLU	Peptide
7	AG	261	THR	Peptide
8	AH	67	GLY	Mainchain
9	AI	157	ASN	Peptide
9	AI	190	THR	Peptide
9	AI	232	ARG	Peptide
11	AK	20	ILE	Peptide
11	AK	21	LYS	Peptide
14	AN	4	SER	Peptide
15	AO	8	LYS	Peptide
17	AQ	110	PRO	Peptide
22	AV	124	VAL	Peptide
28	Ab	102	GLU	Peptide
35	Ai	80	ARG	Peptide
36	Aj	83	LYS	Peptide
36	Aj	90	ARG	Peptide
46	BB	110	TYR	Peptide
46	BB	156	VAL	Peptide
46	BB	157	ASP	Peptide
46	BB	165	ARG	Peptide
47	BC	177	GLN	Peptide
47	BC	179	SER	Peptide
49	BE	219	ALA	Peptide
50	BF	193	GLY	Peptide
50	BF	194	THR	Peptide
51	BG	126	ASP	Peptide
51	BG	36	ALA	Peptide
51	BG	44	ASN	Peptide
51	BG	48	PHE	Peptide

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Mol	Chain	Res	Type	Group
51	BG	49	GLU	Peptide
51	BG	50	GLU	Peptide
51	BG	56	ALA	Peptide
51	BG	57	SER	Peptide
51	BG	58	LEU	Peptide
51	BG	65	ARG	Peptide
52	BH	148	SER	Peptide
52	BH	150	GLU	Peptide
52	BH	68	LEU	Peptide
53	BI	110	GLN	Peptide
54	BJ	147	ALA	Peptide
55	BK	133	HIS	Peptide
55	BK	163	PRO	Peptide
56	BL	76	LEU	Peptide
56	BL	86	ILE	Peptide
56	BL	87	VAL	Peptide
56	BL	89	GLY	Peptide
57	BM	5	LEU	Peptide
58	BN	110	GLY	Peptide
58	BN	126	TRP	Peptide
58	BN	130	THR	Peptide
58	BN	36	LEU	Peptide
58	BN	83	GLU	Peptide
60	BP	123	SER	Peptide
60	BP	28	VAL	Peptide
62	BR	32	ASN	Peptide
62	BR	40	GLU	Peptide
63	BS	23	LYS	Peptide
63	BS	85	VAL	Peptide
63	BS	86	PRO	Peptide
64	BT	101	LEU	Peptide
64	BT	60	GLU	Peptide
64	BT	81	ILE	Peptide
64	BT	90	ASN	Peptide
64	BT	91	ASP	Peptide
67	BW	45	ALA	Peptide
67	BW	75	ASN	Peptide
69	BY	113	ALA	Peptide
69	BY	130	VAL	Peptide
69	BY	88	PRO	Peptide
70	BZ	33	ALA	Peptide
70	BZ	4	ALA	Peptide

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Mol	Chain	Res	Type	Group
71	Ba	40	VAL	Peptide
71	Ba	42	LEU	Peptide
71	Ba	87	GLY	Peptide
71	Ba	94	LYS	Peptide
72	Bb	10	ARG	Peptide
72	Bb	34	LYS	Peptide
72	Bb	35	ALA	Peptide
72	Bb	63	ALA	Peptide
72	Bb	7	SER	Peptide
72	Bb	81	ALA	Peptide
72	Bb	84	VAL	Peptide
72	Bb	85	ARG	Peptide
72	Bb	97	PRO	Peptide
77	Bg	137	ASP	Peptide
77	Bg	98	VAL	Peptide
79	Bi	1063	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	AD	250/252 (99%)	233 (93%)	17 (7%)	0	100 100
5	AE	384/386 (100%)	359 (94%)	23 (6%)	2 (0%)	25 56
6	AF	359/361 (99%)	320 (89%)	33 (9%)	6 (2%)	7 31
7	AG	294/296 (99%)	266 (90%)	26 (9%)	2 (1%)	19 49
8	AH	152/175 (87%)	142 (93%)	9 (6%)	1 (1%)	19 49
9	AI	220/243 (90%)	204 (93%)	13 (6%)	3 (1%)	9 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	231/233 (99%)	214 (93%)	17 (7%)	0	100	100
11	AK	186/191 (97%)	173 (93%)	13 (7%)	0	100	100
12	AL	207/220 (94%)	194 (94%)	13 (6%)	0	100	100
13	AM	167/169 (99%)	144 (86%)	21 (13%)	2 (1%)	11	38
14	AN	191/198 (96%)	169 (88%)	19 (10%)	3 (2%)	8	32
15	AO	134/137 (98%)	123 (92%)	11 (8%)	0	100	100
16	AP	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	13	42
17	AQ	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	13	42
18	AR	181/183 (99%)	165 (91%)	16 (9%)	0	100	100
19	AS	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
20	AT	150/188 (80%)	145 (97%)	5 (3%)	0	100	100
21	AU	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	AV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	22	52
23	AW	98/120 (82%)	90 (92%)	8 (8%)	0	100	100
24	AX	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
25	AY	59/155 (38%)	59 (100%)	0	0	100	100
26	AZ	119/141 (84%)	114 (96%)	5 (4%)	0	100	100
27	Aa	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
28	Ab	133/135 (98%)	121 (91%)	11 (8%)	1 (1%)	16	45
29	Ac	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	19	49
30	Ad	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
31	Ae	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
32	Af	107/112 (96%)	100 (94%)	7 (6%)	0	100	100
33	Ag	125/129 (97%)	122 (98%)	3 (2%)	0	100	100
34	Ah	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	13	42
35	Ai	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
36	Aj	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
37	Ak	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5	27
38	Al	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	5	24
39	Am	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
40	An	48/50 (96%)	44 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	Ao	50/127 (39%)	48 (96%)	2 (4%)	0	100 100
42	Ap	23/25 (92%)	23 (100%)	0	0	100 100
43	Aq	103/105 (98%)	98 (95%)	5 (5%)	0	100 100
44	Ar	89/91 (98%)	84 (94%)	5 (6%)	0	100 100
46	BB	204/251 (81%)	171 (84%)	31 (15%)	2 (1%)	13 42
47	BC	212/254 (84%)	180 (85%)	32 (15%)	0	100 100
48	BD	215/253 (85%)	196 (91%)	18 (8%)	1 (0%)	25 56
49	BE	221/239 (92%)	207 (94%)	14 (6%)	0	100 100
50	BF	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	30 61
51	BG	204/224 (91%)	178 (87%)	22 (11%)	4 (2%)	6 28
52	BH	224/236 (95%)	207 (92%)	13 (6%)	4 (2%)	7 30
53	BI	182/189 (96%)	157 (86%)	18 (10%)	7 (4%)	2 16
54	BJ	184/199 (92%)	157 (85%)	26 (14%)	1 (0%)	25 56
55	BK	183/196 (93%)	156 (85%)	24 (13%)	3 (2%)	8 32
56	BL	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	5 27
57	BM	153/155 (99%)	140 (92%)	12 (8%)	1 (1%)	19 49
58	BN	122/142 (86%)	90 (74%)	29 (24%)	3 (2%)	4 24
59	BO	148/150 (99%)	138 (93%)	8 (5%)	2 (1%)	9 34
60	BP	125/136 (92%)	109 (87%)	16 (13%)	0	100 100
61	BQ	122/141 (86%)	104 (85%)	17 (14%)	1 (1%)	16 45
62	BR	139/142 (98%)	124 (89%)	14 (10%)	1 (1%)	19 49
63	BS	116/135 (86%)	103 (89%)	9 (8%)	4 (3%)	3 18
64	BT	143/145 (99%)	123 (86%)	16 (11%)	4 (3%)	4 22
65	BU	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	19 49
66	BV	105/120 (88%)	92 (88%)	13 (12%)	0	100 100
67	BW	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	3 18
68	BX	127/129 (98%)	121 (95%)	6 (5%)	0	100 100
69	BY	142/144 (99%)	120 (84%)	20 (14%)	2 (1%)	9 34
70	BZ	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	5 25
71	Ba	68/107 (64%)	56 (82%)	12 (18%)	0	100 100
72	Bb	95/118 (80%)	77 (81%)	12 (13%)	6 (6%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Bc	79/81 (98%)	67 (85%)	12 (15%)	0	100	100
74	Bd	61/66 (92%)	54 (88%)	7 (12%)	0	100	100
75	Be	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
76	Bf	58/62 (94%)	48 (83%)	10 (17%)	0	100	100
77	Bg	55/151 (36%)	38 (69%)	15 (27%)	2 (4%)	3	17
78	Bh	316/318 (99%)	288 (91%)	27 (8%)	1 (0%)	37	67
79	Bi	948/972 (98%)	857 (90%)	90 (10%)	1 (0%)	48	77
All	All	11821/12759 (93%)	10708 (91%)	1022 (9%)	91 (1%)	19	45

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	19	ARG
6	AF	152	VAL
6	AF	339	LEU
14	AN	63	VAL
17	AQ	111	PRO
34	Ah	106	ASN
46	BB	206	ASP
50	BF	195	ILE
51	BG	50	GLU
51	BG	51	VAL
53	BI	64	VAL
53	BI	111	LYS
56	BL	87	VAL
56	BL	88	PRO
59	BO	23	PRO
59	BO	24	ALA
63	BS	24	LEU
63	BS	87	GLU
64	BT	91	ASP
67	BW	82	VAL
69	BY	63	GLN
78	Bh	267	PRO
5	AE	18	PRO
6	AF	149	PRO
9	AI	233	GLU
14	AN	77	LEU
29	Ac	78	LEU
51	BG	127	GLN

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Mol	Chain	Res	Type
52	BH	68	LEU
52	BH	149	LYS
52	BH	173	PRO
53	BI	155	ASP
55	BK	134	ILE
58	BN	130	THR
64	BT	92	ILE
67	BW	81	ASN
70	BZ	5	VAL
72	Bb	35	ALA
72	Bb	36	ILE
77	Bg	100	LEU
77	Bg	138	ARG
37	Ak	33	ALA
38	Al	42	ALA
53	BI	74	GLN
53	BI	131	PHE
53	BI	134	GLU
54	BJ	148	ALA
55	BK	98	ALA
61	BQ	30	THR
64	BT	82	PRO
6	AF	151	VAL
7	AG	124	GLU
9	AI	158	LYS
9	AI	159	GLN
14	AN	76	THR
16	AP	74	PRO
37	Ak	34	SER
46	BB	4	PRO
57	BM	6	THR
58	BN	127	GLY
58	BN	131	ASP
62	BR	33	GLY
63	BS	23	LYS
64	BT	102	ALA
69	BY	66	SER
8	AH	68	PRO
17	AQ	110	PRO
38	Al	41	ALA
51	BG	57	SER
65	BU	53	TRP

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Mol	Chain	Res	Type
70	BZ	52	LYS
72	Bb	85	ARG
6	AF	130	ALA
13	AM	172	LEU
22	AV	125	ALA
48	BD	40	LYS
72	Bb	8	ASN
16	AP	75	VAL
28	Ab	103	GLN
79	Bi	713	GLN
7	AG	125	VAL
63	BS	88	VAL
67	BW	6	GLY
72	Bb	86	VAL
6	AF	131	VAL
13	AM	8	PRO
55	BK	162	SER
70	BZ	35	VAL
52	BH	69	LEU
53	BI	112	ARG
72	Bb	97	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	AD	193/194 (100%)	192 (100%)	1 (0%)	86 91
5	AE	319/322 (99%)	311 (98%)	8 (2%)	42 66
6	AF	288/288 (100%)	283 (98%)	5 (2%)	56 74
7	AG	244/244 (100%)	242 (99%)	2 (1%)	79 87
8	AH	134/152 (88%)	133 (99%)	1 (1%)	81 88
9	AI	186/204 (91%)	184 (99%)	2 (1%)	70 82
10	AJ	187/191 (98%)	186 (100%)	1 (0%)	86 91
11	AK	171/171 (100%)	169 (99%)	2 (1%)	67 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	177/186 (95%)	177 (100%)	0	100	100
13	AM	147/147 (100%)	144 (98%)	3 (2%)	50	71
14	AN	154/158 (98%)	153 (99%)	1 (1%)	84	90
15	AO	107/108 (99%)	106 (99%)	1 (1%)	75	85
16	AP	175/175 (100%)	174 (99%)	1 (1%)	84	90
17	AQ	160/161 (99%)	160 (100%)	0	100	100
18	AR	140/145 (97%)	137 (98%)	3 (2%)	48	70
19	AS	150/150 (100%)	149 (99%)	1 (1%)	81	88
20	AT	126/153 (82%)	126 (100%)	0	100	100
21	AU	156/156 (100%)	153 (98%)	3 (2%)	52	72
22	AV	136/136 (100%)	136 (100%)	0	100	100
23	AW	87/106 (82%)	87 (100%)	0	100	100
24	AX	104/104 (100%)	104 (100%)	0	100	100
25	AY	54/129 (42%)	54 (100%)	0	100	100
26	AZ	104/117 (89%)	104 (100%)	0	100	100
27	Aa	109/109 (100%)	109 (100%)	0	100	100
28	Ab	115/115 (100%)	115 (100%)	0	100	100
29	Ac	118/118 (100%)	116 (98%)	2 (2%)	56	74
30	Ad	46/46 (100%)	46 (100%)	0	100	100
31	Ae	81/87 (93%)	80 (99%)	1 (1%)	67	81
32	Af	92/96 (96%)	91 (99%)	1 (1%)	70	82
33	Ag	109/110 (99%)	109 (100%)	0	100	100
34	Ah	90/90 (100%)	87 (97%)	3 (3%)	33	59
35	Ai	95/103 (92%)	95 (100%)	0	100	100
36	Aj	104/104 (100%)	104 (100%)	0	100	100
37	Ak	81/81 (100%)	81 (100%)	0	100	100
38	Al	70/70 (100%)	69 (99%)	1 (1%)	62	78
39	Am	68/68 (100%)	68 (100%)	0	100	100
40	An	45/45 (100%)	45 (100%)	0	100	100
41	Ao	47/115 (41%)	47 (100%)	0	100	100
42	Ap	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Aq	90/90 (100%)	88 (98%)	2 (2%)	47	69
44	Ar	71/71 (100%)	71 (100%)	0	100	100
46	BB	164/209 (78%)	162 (99%)	2 (1%)	67	81
47	BC	191/223 (86%)	187 (98%)	4 (2%)	48	70
48	BD	176/204 (86%)	175 (99%)	1 (1%)	84	90
49	BE	182/194 (94%)	180 (99%)	2 (1%)	70	82
50	BF	221/221 (100%)	219 (99%)	2 (1%)	75	85
51	BG	173/190 (91%)	171 (99%)	2 (1%)	67	81
52	BH	188/201 (94%)	187 (100%)	1 (0%)	86	91
53	BI	165/169 (98%)	164 (99%)	1 (1%)	84	90
54	BJ	150/160 (94%)	149 (99%)	1 (1%)	81	88
55	BK	158/165 (96%)	156 (99%)	2 (1%)	65	79
56	BL	77/98 (79%)	76 (99%)	1 (1%)	65	79
57	BM	129/136 (95%)	127 (98%)	2 (2%)	58	75
58	BN	88/118 (75%)	85 (97%)	3 (3%)	32	58
59	BO	127/127 (100%)	127 (100%)	0	100	100
60	BP	81/104 (78%)	80 (99%)	1 (1%)	67	81
61	BQ	101/117 (86%)	101 (100%)	0	100	100
62	BR	117/118 (99%)	115 (98%)	2 (2%)	56	74
63	BS	94/123 (76%)	93 (99%)	1 (1%)	70	82
64	BT	128/128 (100%)	127 (99%)	1 (1%)	79	87
65	BU	115/115 (100%)	115 (100%)	0	100	100
66	BV	100/113 (88%)	98 (98%)	2 (2%)	50	71
67	BW	74/74 (100%)	72 (97%)	2 (3%)	40	65
68	BX	110/110 (100%)	106 (96%)	4 (4%)	30	57
69	BY	119/119 (100%)	118 (99%)	1 (1%)	79	87
70	BZ	112/112 (100%)	111 (99%)	1 (1%)	75	85
71	Ba	61/88 (69%)	59 (97%)	2 (3%)	33	59
72	Bb	83/99 (84%)	82 (99%)	1 (1%)	67	81
73	Bc	70/70 (100%)	69 (99%)	1 (1%)	62	78
74	Bd	56/59 (95%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
75	Be	47/48 (98%)	47 (100%)	0	100 100
76	Bf	51/53 (96%)	49 (96%)	2 (4%)	27 55
77	Bg	48/134 (36%)	46 (96%)	2 (4%)	25 53
78	Bh	260/261 (100%)	251 (96%)	9 (4%)	31 57
79	Bi	840/857 (98%)	826 (98%)	14 (2%)	56 74
All	All	10009/10755 (93%)	9894 (99%)	115 (1%)	69 82

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AD	193	ARG
5	AE	16	PHE
5	AE	19	ARG
5	AE	84	VAL
5	AE	85	VAL
5	AE	114	VAL
5	AE	216	ASP
5	AE	256	HIS
5	AE	332	ARG
6	AF	144	LYS
6	AF	147	GLU
6	AF	148	ILE
6	AF	150	LEU
6	AF	342	LYS
7	AG	68	THR
7	AG	155	THR
8	AH	46	ARG
9	AI	83	LEU
9	AI	239	LEU
10	AJ	158	ASP
11	AK	151	VAL
11	AK	157	ASN
13	AM	44	THR
13	AM	95	ASN
13	AM	174	LYS
14	AN	58	VAL
15	AO	74	ARG
16	AP	188	ARG
18	AR	30	ARG
18	AR	119	VAL

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Mol	Chain	Res	Type
18	AR	153	LYS
19	AS	40	THR
21	AU	117	ARG
21	AU	170	THR
21	AU	172	TYR
29	Ac	46	ASP
29	Ac	60	TYR
31	Ae	99	ASP
32	Af	86	LYS
34	Ah	81	VAL
34	Ah	102	LEU
34	Ah	103	TYR
38	Al	58	THR
43	Aq	8	ARG
43	Aq	74	CYS
46	BB	10	THR
46	BB	157	ASP
47	BC	31	ASP
47	BC	70	LEU
47	BC	180	THR
47	BC	218	LEU
48	BD	111	VAL
49	BE	76	ARG
49	BE	156	PHE
50	BF	38	LEU
50	BF	206	ASP
51	BG	48	PHE
51	BG	124	LEU
52	BH	151	ASP
53	BI	39	ARG
54	BJ	46	VAL
55	BK	3	ARG
55	BK	53	ARG
56	BL	76	LEU
57	BM	67	ARG
57	BM	74	THR
58	BN	28	LEU
58	BN	95	LYS
58	BN	121	VAL
60	BP	136	ARG
62	BR	53	LEU
62	BR	69	VAL

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Mol	Chain	Res	Type
63	BS	71	PHE
64	BT	119	ILE
66	BV	43	LYS
66	BV	102	ARG
67	BW	12	TYR
67	BW	50	TYR
68	BX	27	ILE
68	BX	28	ARG
68	BX	30	SER
68	BX	53	ILE
69	BY	62	LYS
70	BZ	105	ARG
71	Ba	95	HIS
71	Ba	102	THR
72	Bb	62	TYR
73	Bc	82	LYS
76	Bf	28	LYS
76	Bf	48	THR
77	Bg	115	THR
77	Bg	119	ARG
78	Bh	12	THR
78	Bh	59	ARG
78	Bh	117	LYS
78	Bh	149	ASP
78	Bh	207	ASP
78	Bh	245	PHE
78	Bh	265	LEU
78	Bh	266	ASP
78	Bh	268	GLN
79	Bi	195	LYS
79	Bi	268	LEU
79	Bi	300	ASN
79	Bi	327	LYS
79	Bi	498	VAL
79	Bi	581	TYR
79	Bi	599	ARG
79	Bi	693	LYS
79	Bi	712	ASP
79	Bi	713	GLN
79	Bi	744	ASP
79	Bi	826	LYS
79	Bi	952	LYS

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Mol	Chain	Res	Type
79	Bi	981	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	AD	8	GLN
4	AD	19	HIS
4	AD	97	ASN
4	AD	209	HIS
4	AD	218	HIS
5	AE	139	GLN
6	AF	9	HIS
6	AF	260	GLN
6	AF	304	GLN
7	AG	40	HIS
10	AJ	41	GLN
10	AJ	59	GLN
10	AJ	243	GLN
11	AK	156	GLN
12	AL	59	GLN
12	AL	162	GLN
12	AL	208	ASN
14	AN	19	GLN
14	AN	37	ASN
14	AN	99	HIS
16	AP	175	ASN
17	AQ	26	GLN
17	AQ	29	ASN
17	AQ	50	ASN
18	AR	137	ASN
20	AT	144	GLN
21	AU	108	GLN
24	AX	98	ASN
24	AX	132	ASN
26	AZ	80	ASN
28	Ab	103	GLN
28	Ab	106	GLN
32	Af	57	GLN
36	Aj	59	ASN
37	Ak	92	ASN
38	Al	76	ASN
40	An	32	ASN

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Mol	Chain	Res	Type
40	An	33	ASN
43	Aq	22	GLN
44	Ar	25	GLN
46	BB	46	HIS
46	BB	83	GLN
46	BB	109	ASN
46	BB	163	ASN
47	BC	118	GLN
47	BC	208	GLN
47	BC	232	HIS
48	BD	87	GLN
48	BD	89	GLN
50	BF	258	GLN
51	BG	63	GLN
51	BG	66	GLN
51	BG	104	ASN
52	BH	65	GLN
53	BI	161	GLN
55	BK	123	HIS
55	BK	139	GLN
56	BL	62	GLN
59	BO	36	GLN
60	BP	29	HIS
61	BQ	15	HIS
61	BQ	103	ASN
62	BR	62	ASN
64	BT	8	GLN
64	BT	25	ASN
66	BV	18	GLN
66	BV	33	GLN
67	BW	7	GLN
69	BY	63	GLN
69	BY	65	ASN
69	BY	79	ASN
71	Ba	82	HIS
71	Ba	98	GLN
75	Be	53	ASN
76	Bf	17	GLN
76	Bf	46	ASN
77	Bg	123	ASN
79	Bi	210	ASN
79	Bi	221	GLN

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Mol	Chain	Res	Type
79	Bi	230	ASN
79	Bi	522	ASN
79	Bi	704	GLN
79	Bi	769	ASN
79	Bi	866	ASN
79	Bi	884	HIS
79	Bi	892	HIS
79	Bi	898	ASN
79	Bi	902	GLN
79	Bi	1052	HIS
79	Bi	1087	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3145/3149 (99%)	647 (20%)	42 (1%)
2	AB	120/121 (99%)	16 (13%)	0
3	AC	157/158 (99%)	31 (19%)	1 (0%)
45	BA	1703/1707 (99%)	436 (25%)	37 (2%)
All	All	5125/5135 (99%)	1130 (22%)	80 (1%)

All (1130) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	A
1	AA	18	G
1	AA	26	A
1	AA	40	A
1	AA	43	A
1	AA	49	A
1	AA	59	G
1	AA	60	A
1	AA	65	A
1	AA	66	A
1	AA	75	G
1	AA	77	A
1	AA	85	A
1	AA	92	G
1	AA	109	A
1	AA	110	G
1	AA	111	C

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Mol	Chain	Res	Type
1	AA	116	A
1	AA	120	G
1	AA	121	A
1	AA	122	A
1	AA	133	U
1	AA	135	C
1	AA	136	G
1	AA	148	G
1	AA	150	A
1	AA	156	G
1	AA	157	A
1	AA	165	A
1	AA	166	C
1	AA	187	A
1	AA	190	U
1	AA	191	U
1	AA	200	C
1	AA	206	G
1	AA	210	U
1	AA	211	A
1	AA	213	A
1	AA	218	G
1	AA	219	A
1	AA	234	G
1	AA	240	U
1	AA	241	G
1	AA	243	G
1	AA	245	U
1	AA	249	U
1	AA	250	U
1	AA	251	G
1	AA	252	U
1	AA	269	G
1	AA	281	G
1	AA	283	G
1	AA	286	U
1	AA	295	A
1	AA	298	U
1	AA	305	U
1	AA	323	A
1	AA	329	U
1	AA	337	G

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Mol	Chain	Res	Type
1	AA	346	C
1	AA	349	A
1	AA	350	C
1	AA	351	A
1	AA	352	A
1	AA	366	A
1	AA	375	A
1	AA	376	G
1	AA	390	G
1	AA	398	A
1	AA	401	U
1	AA	402	A
1	AA	403	C
1	AA	421	G
1	AA	422	A
1	AA	439	C
1	AA	440	A
1	AA	520	U
1	AA	521	A
1	AA	535	G
1	AA	544	C
1	AA	546	C
1	AA	547	G
1	AA	548	G
1	AA	551	A
1	AA	552	G
1	AA	555	U
1	AA	557	A
1	AA	559	A
1	AA	578	A
1	AA	579	G
1	AA	589	A
1	AA	590	G
1	AA	604	G
1	AA	609	G
1	AA	611	A
1	AA	620	U
1	AA	621	A
1	AA	637	C
1	AA	638	C
1	AA	649	A
1	AA	660	A

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Mol	Chain	Res	Type
1	AA	662	U
1	AA	677	A
1	AA	681	U
1	AA	683	U
1	AA	691	A
1	AA	705	A
1	AA	708	G
1	AA	712	G
1	AA	715	A
1	AA	716	A
1	AA	719	U
1	AA	725	G
1	AA	735	A
1	AA	743	C
1	AA	764	U
1	AA	767	U
1	AA	774	G
1	AA	775	A
1	AA	776	U
1	AA	777	U
1	AA	779	G
1	AA	780	A
1	AA	781	G
1	AA	785	G
1	AA	801	A
1	AA	806	A
1	AA	808	A
1	AA	817	A
1	AA	830	A
1	AA	849	C
1	AA	861	C
1	AA	869	G
1	AA	874	U
1	AA	879	U
1	AA	896	A
1	AA	907	G
1	AA	908	G
1	AA	914	A
1	AA	916	G
1	AA	917	A
1	AA	920	A
1	AA	921	A

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Mol	Chain	Res	Type
1	AA	923	C
1	AA	924	G
1	AA	925	A
1	AA	937	G
1	AA	944	C
1	AA	959	C
1	AA	960	U
1	AA	961	C
1	AA	979	U
1	AA	980	A
1	AA	981	U
1	AA	982	C
1	AA	1001	G
1	AA	1002	A
1	AA	1010	G
1	AA	1015	U
1	AA	1016	C
1	AA	1017	C
1	AA	1018	G
1	AA	1020	G
1	AA	1024	G
1	AA	1025	A
1	AA	1029	G
1	AA	1032	C
1	AA	1036	A
1	AA	1037	C
1	AA	1041	U
1	AA	1047	A
1	AA	1049	C
1	AA	1063	G
1	AA	1064	A
1	AA	1065	A
1	AA	1072	G
1	AA	1074	U
1	AA	1079	A
1	AA	1081	U
1	AA	1082	U
1	AA	1083	G
1	AA	1093	A
1	AA	1094	U
1	AA	1095	U
1	AA	1097	G

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Mol	Chain	Res	Type
1	AA	1098	A
1	AA	1103	A
1	AA	1104	G
1	AA	1117	G
1	AA	1129	A
1	AA	1131	G
1	AA	1143	A
1	AA	1144	U
1	AA	1150	A
1	AA	1153	A
1	AA	1159	A
1	AA	1160	C
1	AA	1177	G
1	AA	1178	G
1	AA	1179	A
1	AA	1180	A
1	AA	1181	U
1	AA	1191	U
1	AA	1192	C
1	AA	1196	C
1	AA	1201	C
1	AA	1202	A
1	AA	1209	G
1	AA	1212	A
1	AA	1217	A
1	AA	1218	U
1	AA	1221	A
1	AA	1222	G
1	AA	1225	A
1	AA	1226	G
1	AA	1227	C
1	AA	1229	G
1	AA	1232	C
1	AA	1236	G
1	AA	1239	C
1	AA	1240	A
1	AA	1241	U
1	AA	1242	G
1	AA	1243	G
1	AA	1244	A
1	AA	1245	A
1	AA	1246	G

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Mol	Chain	Res	Type
1	AA	1248	C
1	AA	1249	G
1	AA	1253	U
1	AA	1258	U
1	AA	1262	G
1	AA	1263	A
1	AA	1264	G
1	AA	1265	U
1	AA	1266	G
1	AA	1267	U
1	AA	1268	G
1	AA	1269	U
1	AA	1270	A
1	AA	1271	A
1	AA	1272	C
1	AA	1273	A
1	AA	1274	A
1	AA	1278	A
1	AA	1279	C
1	AA	1281	G
1	AA	1282	G
1	AA	1285	G
1	AA	1287	A
1	AA	1305	U
1	AA	1307	G
1	AA	1308	A
1	AA	1309	U
1	AA	1313	G
1	AA	1325	U
1	AA	1330	A
1	AA	1331	U
1	AA	1332	A
1	AA	1334	U
1	AA	1345	G
1	AA	1348	U
1	AA	1349	G
1	AA	1350	A
1	AA	1351	U
1	AA	1352	A
1	AA	1353	U
1	AA	1355	A
1	AA	1356	U

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Mol	Chain	Res	Type
1	AA	1357	G
1	AA	1386	A
1	AA	1392	G
1	AA	1399	A
1	AA	1400	G
1	AA	1417	G
1	AA	1418	A
1	AA	1419	A
1	AA	1421	G
1	AA	1425	U
1	AA	1434	G
1	AA	1437	C
1	AA	1443	G
1	AA	1446	A
1	AA	1450	G
1	AA	1468	A
1	AA	1469	C
1	AA	1482	A
1	AA	1485	G
1	AA	1496	C
1	AA	1502	C
1	AA	1508	C
1	AA	1525	G
1	AA	1527	C
1	AA	1536	G
1	AA	1547	G
1	AA	1553	U
1	AA	1555	U
1	AA	1556	C
1	AA	1562	C
1	AA	1563	C
1	AA	1564	U
1	AA	1565	G
1	AA	1566	A
1	AA	1567	U
1	AA	1568	U
1	AA	1569	U
1	AA	1570	U
1	AA	1580	A
1	AA	1582	C
1	AA	1583	A
1	AA	1587	A

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Mol	Chain	Res	Type
1	AA	1589	A
1	AA	1590	G
1	AA	1593	A
1	AA	1594	A
1	AA	1596	C
1	AA	1605	A
1	AA	1607	U
1	AA	1608	C
1	AA	1619	A
1	AA	1629	U
1	AA	1639	C
1	AA	1641	U
1	AA	1643	A
1	AA	1656	A
1	AA	1683	A
1	AA	1696	A
1	AA	1705	U
1	AA	1716	U
1	AA	1717	U
1	AA	1724	U
1	AA	1725	C
1	AA	1736	G
1	AA	1741	A
1	AA	1750	A
1	AA	1751	G
1	AA	1756	C
1	AA	1759	C
1	AA	1760	A
1	AA	1762	C
1	AA	1765	U
1	AA	1767	C
1	AA	1770	G
1	AA	1771	C
1	AA	1775	G
1	AA	1778	G
1	AA	1780	G
1	AA	1797	A
1	AA	1812	G
1	AA	1814	A
1	AA	1815	U
1	AA	1816	A
1	AA	1817	G

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Mol	Chain	Res	Type
1	AA	1819	U
1	AA	1820	U
1	AA	1821	U
1	AA	1839	A
1	AA	1841	A
1	AA	1842	A
1	AA	1846	C
1	AA	1849	C
1	AA	1850	A
1	AA	1858	A
1	AA	1866	C
1	AA	1871	U
1	AA	1880	U
1	AA	1881	A
1	AA	1886	A
1	AA	1890	U
1	AA	1893	A
1	AA	1906	G
1	AA	1951	C
1	AA	1952	G
1	AA	1954	G
1	AA	2094	C
1	AA	2100	A
1	AA	2101	C
1	AA	2102	U
1	AA	2110	G
1	AA	2111	G
1	AA	2112	U
1	AA	2113	A
1	AA	2114	C
1	AA	2115	G
1	AA	2121	G
1	AA	2122	G
1	AA	2131	A
1	AA	2132	C
1	AA	2140	U
1	AA	2144	A
1	AA	2158	A
1	AA	2169	G
1	AA	2171	G
1	AA	2175	U
1	AA	2187	G

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Mol	Chain	Res	Type
1	AA	2192	C
1	AA	2201	G
1	AA	2205	U
1	AA	2206	G
1	AA	2208	A
1	AA	2210	G
1	AA	2213	A
1	AA	2225	U
1	AA	2239	G
1	AA	2244	A
1	AA	2249	G
1	AA	2250	G
1	AA	2252	A
1	AA	2255	A
1	AA	2256	A
1	AA	2272	G
1	AA	2273	G
1	AA	2281	A
1	AA	2282	U
1	AA	2284	C
1	AA	2288	G
1	AA	2298	U
1	AA	2307	G
1	AA	2310	U
1	AA	2313	A
1	AA	2314	U
1	AA	2315	G
1	AA	2334	U
1	AA	2335	G
1	AA	2336	U
1	AA	2366	C
1	AA	2373	A
1	AA	2374	C
1	AA	2375	G
1	AA	2376	G
1	AA	2385	G
1	AA	2388	U
1	AA	2393	G
1	AA	2397	A
1	AA	2401	A
1	AA	2402	A
1	AA	2403	G

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Mol	Chain	Res	Type
1	AA	2404	A
1	AA	2405	C
1	AA	2411	U
1	AA	2418	G
1	AA	2435	G
1	AA	2443	A
1	AA	2444	C
1	AA	2445	A
1	AA	2502	A
1	AA	2503	G
1	AA	2504	U
1	AA	2511	A
1	AA	2513	U
1	AA	2514	U
1	AA	2515	A
1	AA	2522	G
1	AA	2523	A
1	AA	2532	U
1	AA	2537	U
1	AA	2538	U
1	AA	2539	C
1	AA	2540	A
1	AA	2541	U
1	AA	2542	U
1	AA	2543	U
1	AA	2544	U
1	AA	2548	C
1	AA	2549	G
1	AA	2550	U
1	AA	2552	C
1	AA	2554	A
1	AA	2561	A
1	AA	2568	C
1	AA	2569	A
1	AA	2570	U
1	AA	2571	U
1	AA	2572	C
1	AA	2573	G
1	AA	2585	G
1	AA	2593	A
1	AA	2594	C
1	AA	2606	G

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Mol	Chain	Res	Type
1	AA	2607	G
1	AA	2614	G
1	AA	2629	U
1	AA	2635	A
1	AA	2651	G
1	AA	2652	U
1	AA	2656	A
1	AA	2674	A
1	AA	2677	G
1	AA	2680	A
1	AA	2689	A
1	AA	2691	A
1	AA	2694	A
1	AA	2696	A
1	AA	2705	A
1	AA	2712	U
1	AA	2714	G
1	AA	2719	U
1	AA	2726	C
1	AA	2727	A
1	AA	2728	G
1	AA	2729	U
1	AA	2737	C
1	AA	2749	G
1	AA	2752	U
1	AA	2753	G
1	AA	2755	C
1	AA	2761	G
1	AA	2762	A
1	AA	2772	C
1	AA	2777	G
1	AA	2778	G
1	AA	2796	G
1	AA	2799	A
1	AA	2800	G
1	AA	2801	A
1	AA	2804	A
1	AA	2810	C
1	AA	2814	G
1	AA	2817	A
1	AA	2818	U
1	AA	2834	G

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Mol	Chain	Res	Type
1	AA	2838	A
1	AA	2842	U
1	AA	2843	U
1	AA	2845	A
1	AA	2847	A
1	AA	2849	C
1	AA	2856	G
1	AA	2860	U
1	AA	2867	C
1	AA	2871	G
1	AA	2872	A
1	AA	2873	U
1	AA	2875	U
1	AA	2887	A
1	AA	2896	A
1	AA	2898	G
1	AA	2899	C
1	AA	2911	A
1	AA	2914	G
1	AA	2923	U
1	AA	2930	A
1	AA	2935	U
1	AA	2936	A
1	AA	2938	G
1	AA	2941	A
1	AA	2942	C
1	AA	2945	G
1	AA	2946	A
1	AA	2947	G
1	AA	2951	G
1	AA	2957	G
1	AA	2971	A
1	AA	2983	C
1	AA	2992	U
1	AA	2996	U
1	AA	2997	G
1	AA	3003	G
1	AA	3012	A
1	AA	3023	U
1	AA	3028	G
1	AA	3030	G
1	AA	3056	U

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Mol	Chain	Res	Type
1	AA	3059	G
1	AA	3074	G
1	AA	3078	U
1	AA	3079	U
1	AA	3086	A
1	AA	3087	A
1	AA	3092	C
1	AA	3109	G
1	AA	3115	C
1	AA	3119	U
1	AA	3122	A
1	AA	3129	A
1	AA	3130	A
1	AA	3131	U
1	AA	3142	A
1	AA	3143	C
1	AA	3151	U
1	AA	3153	U
1	AA	3154	C
1	AA	3155	U
1	AA	3156	U
1	AA	3157	U
1	AA	3165	A
1	AA	3168	A
1	AA	3170	A
1	AA	3173	G
1	AA	3174	A
1	AA	3175	U
1	AA	3176	G
1	AA	3179	U
1	AA	3181	C
1	AA	3187	A
1	AA	3194	C
1	AA	3196	U
1	AA	3207	U
1	AA	3210	A
1	AA	3216	G
1	AA	3217	C
1	AA	3218	A
1	AA	3219	G
1	AA	3227	A
1	AA	3229	G

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Mol	Chain	Res	Type
1	AA	3235	C
1	AA	3243	A
1	AA	3245	A
1	AA	3247	G
1	AA	3259	U
1	AA	3260	G
1	AA	3263	G
1	AA	3270	U
1	AA	3272	C
1	AA	3276	G
1	AA	3281	U
1	AA	3286	G
1	AA	3287	U
1	AA	3288	G
1	AA	3289	G
1	AA	3294	A
1	AA	3295	A
1	AA	3304	U
1	AA	3313	U
1	AA	3316	A
1	AA	3317	U
1	AA	3318	G
1	AA	3319	U
1	AA	3330	A
1	AA	3331	U
1	AA	3341	U
1	AA	3345	G
1	AA	3351	U
1	AA	3352	U
1	AA	3353	G
1	AA	3354	U
1	AA	3355	U
1	AA	3356	G
1	AA	3357	U
1	AA	3360	C
1	AA	3363	U
1	AA	3369	G
1	AA	3375	A
1	AA	3378	C
1	AA	3382	U
1	AA	3386	G
1	AA	3396	U

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Mol	Chain	Res	Type
2	AB	7	G
2	AB	10	C
2	AB	13	A
2	AB	22	A
2	AB	29	C
2	AB	41	G
2	AB	54	U
2	AB	55	A
2	AB	65	G
2	AB	74	C
2	AB	76	A
2	AB	91	G
2	AB	99	G
2	AB	102	A
2	AB	112	G
2	AB	121	U
3	AC	2	A
3	AC	23	U
3	AC	34	U
3	AC	35	C
3	AC	51	G
3	AC	52	A
3	AC	59	A
3	AC	62	C
3	AC	63	G
3	AC	79	A
3	AC	80	A
3	AC	81	U
3	AC	82	U
3	AC	83	C
3	AC	84	C
3	AC	85	G
3	AC	86	U
3	AC	87	G
3	AC	90	U
3	AC	95	G
3	AC	97	A
3	AC	104	A
3	AC	105	A
3	AC	106	C
3	AC	111	A
3	AC	113	U

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Mol	Chain	Res	Type
3	AC	125	U
3	AC	126	A
3	AC	128	U
3	AC	138	A
3	AC	152	G
45	BA	2	A
45	BA	4	C
45	BA	17	C
45	BA	25	C
45	BA	26	A
45	BA	27	U
45	BA	34	G
45	BA	42	G
45	BA	45	U
45	BA	47	A
45	BA	50	C
45	BA	57	G
45	BA	60	U
45	BA	68	A
45	BA	69	G
45	BA	72	A
45	BA	73	U
45	BA	74	U
45	BA	75	U
45	BA	78	A
45	BA	101	U
45	BA	104	A
45	BA	114	C
45	BA	115	G
45	BA	127	G
45	BA	130	C
45	BA	131	C
45	BA	132	U
45	BA	133	U
45	BA	134	U
45	BA	135	A
45	BA	136	C
45	BA	137	U
45	BA	140	A
45	BA	141	U
45	BA	145	A
45	BA	146	U

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Mol	Chain	Res	Type
45	BA	153	G
45	BA	158	U
45	BA	159	U
45	BA	169	A
45	BA	176	C
45	BA	178	U
45	BA	179	A
45	BA	181	A
45	BA	185	U
45	BA	186	C
45	BA	190	C
45	BA	191	C
45	BA	192	U
45	BA	193	U
45	BA	194	U
45	BA	195	G
45	BA	196	G
45	BA	198	A
45	BA	199	G
45	BA	200	A
45	BA	217	A
45	BA	218	A
45	BA	219	A
45	BA	220	A
45	BA	226	A
45	BA	229	U
45	BA	231	U
45	BA	233	C
45	BA	235	G
45	BA	236	A
45	BA	239	C
45	BA	240	U
45	BA	241	U
45	BA	245	U
45	BA	246	G
45	BA	250	C
45	BA	257	A
45	BA	260	U
45	BA	261	U
45	BA	265	A
45	BA	271	A
45	BA	272	U

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Mol	Chain	Res	Type
45	BA	277	U
45	BA	278	U
45	BA	279	G
45	BA	280	U
45	BA	281	G
45	BA	288	A
45	BA	299	A
45	BA	309	C
45	BA	314	C
45	BA	316	A
45	BA	319	U
45	BA	320	U
45	BA	321	C
45	BA	322	G
45	BA	333	A
45	BA	337	G
45	BA	338	C
45	BA	352	A
45	BA	359	A
45	BA	360	A
45	BA	361	C
45	BA	370	A
45	BA	387	A
45	BA	390	G
45	BA	399	A
45	BA	400	A
45	BA	401	A
45	BA	402	C
45	BA	404	G
45	BA	416	A
45	BA	417	A
45	BA	418	G
45	BA	422	G
45	BA	423	G
45	BA	424	C
45	BA	425	A
45	BA	426	G
45	BA	434	G
45	BA	439	U
45	BA	444	C
45	BA	448	C
45	BA	452	A

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Mol	Chain	Res	Type
45	BA	454	U
45	BA	464	A
45	BA	468	A
45	BA	469	C
45	BA	475	A
45	BA	477	A
45	BA	480	G
45	BA	481	A
45	BA	484	C
45	BA	485	A
45	BA	488	G
45	BA	493	U
45	BA	494	U
45	BA	495	C
45	BA	496	G
45	BA	497	G
45	BA	498	G
45	BA	499	U
45	BA	500	C
45	BA	501	U
45	BA	502	U
45	BA	504	U
45	BA	505	A
45	BA	506	A
45	BA	508	U
45	BA	510	G
45	BA	511	A
45	BA	513	U
45	BA	514	G
45	BA	515	A
45	BA	519	C
45	BA	527	A
45	BA	532	U
45	BA	534	A
45	BA	539	G
45	BA	540	G
45	BA	541	A
45	BA	542	A
45	BA	543	C
45	BA	544	A
45	BA	548	G
45	BA	549	G

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Mol	Chain	Res	Type
45	BA	556	A
45	BA	557	G
45	BA	558	U
45	BA	559	C
45	BA	565	C
45	BA	577	G
45	BA	579	A
45	BA	580	A
45	BA	582	U
45	BA	585	A
45	BA	594	A
45	BA	595	G
45	BA	606	A
45	BA	611	U
45	BA	619	A
45	BA	620	A
45	BA	621	A
45	BA	622	A
45	BA	623	A
45	BA	624	G
45	BA	638	U
45	BA	640	U
45	BA	641	G
45	BA	648	G
45	BA	649	U
45	BA	650	U
45	BA	684	A
45	BA	686	C
45	BA	687	G
45	BA	694	U
45	BA	696	C
45	BA	697	C
45	BA	698	U
45	BA	737	A
45	BA	738	G
45	BA	741	C
45	BA	742	U
45	BA	745	U
45	BA	752	A
45	BA	754	A
45	BA	755	A
45	BA	756	A

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Mol	Chain	Res	Type
45	BA	765	G
45	BA	766	U
45	BA	767	U
45	BA	774	A
45	BA	775	G
45	BA	778	G
45	BA	781	U
45	BA	782	U
45	BA	783	G
45	BA	784	C
45	BA	787	G
45	BA	794	U
45	BA	795	U
45	BA	803	A
45	BA	812	A
45	BA	813	U
45	BA	814	A
45	BA	815	G
45	BA	816	G
45	BA	817	A
45	BA	818	C
45	BA	819	G
45	BA	820	U
45	BA	821	U
45	BA	823	G
45	BA	824	G
45	BA	829	A
45	BA	830	U
45	BA	833	U
45	BA	837	G
45	BA	838	G
45	BA	840	U
45	BA	846	G
45	BA	849	C
45	BA	850	A
45	BA	851	U
45	BA	852	C
45	BA	853	G
45	BA	854	U
45	BA	855	A
45	BA	856	A
45	BA	863	A

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Mol	Chain	Res	Type
45	BA	873	U
45	BA	876	G
45	BA	886	U
45	BA	898	A
45	BA	912	U
45	BA	913	G
45	BA	914	G
45	BA	915	A
45	BA	932	U
45	BA	933	A
45	BA	935	U
45	BA	942	G
45	BA	945	U
45	BA	954	G
45	BA	958	U
45	BA	960	U
45	BA	966	A
45	BA	992	A
45	BA	993	A
45	BA	1004	U
45	BA	1005	A
45	BA	1025	A
45	BA	1026	A
45	BA	1028	C
45	BA	1031	U
45	BA	1039	A
45	BA	1040	G
45	BA	1052	U
45	BA	1053	G
45	BA	1058	U
45	BA	1059	U
45	BA	1060	U
45	BA	1061	A
45	BA	1072	C
45	BA	1076	A
45	BA	1082	C
45	BA	1086	A
45	BA	1091	A
45	BA	1092	A
45	BA	1096	C
45	BA	1097	U
45	BA	1098	U

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Mol	Chain	Res	Type
45	BA	1100	G
45	BA	1101	G
45	BA	1108	G
45	BA	1109	G
45	BA	1111	G
45	BA	1113	A
45	BA	1138	A
45	BA	1150	G
45	BA	1154	G
45	BA	1158	C
45	BA	1160	A
45	BA	1167	G
45	BA	1185	U
45	BA	1194	A
45	BA	1196	A
45	BA	1199	G
45	BA	1200	G
45	BA	1202	A
45	BA	1207	C
45	BA	1217	A
45	BA	1218	G
45	BA	1227	A
45	BA	1228	G
45	BA	1229	G
45	BA	1244	A
45	BA	1245	G
45	BA	1246	C
45	BA	1250	U
45	BA	1251	U
45	BA	1255	G
45	BA	1257	U
45	BA	1258	U
45	BA	1259	U
45	BA	1276	U
45	BA	1284	C
45	BA	1286	U
45	BA	1290	U
45	BA	1291	G
45	BA	1293	U
45	BA	1295	G
45	BA	1296	A
45	BA	1299	G

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Mol	Chain	Res	Type
45	BA	1302	U
45	BA	1304	G
45	BA	1307	U
45	BA	1314	U
45	BA	1315	U
45	BA	1318	G
45	BA	1321	A
45	BA	1323	C
45	BA	1337	A
45	BA	1338	C
45	BA	1340	U
45	BA	1341	A
45	BA	1344	A
45	BA	1345	A
45	BA	1346	A
45	BA	1364	G
45	BA	1367	G
45	BA	1370	U
45	BA	1371	A
45	BA	1372	U
45	BA	1382	A
45	BA	1388	A
45	BA	1390	U
45	BA	1398	U
45	BA	1399	C
45	BA	1400	A
45	BA	1412	G
45	BA	1413	U
45	BA	1414	U
45	BA	1415	U
45	BA	1422	A
45	BA	1425	A
45	BA	1427	A
45	BA	1428	G
45	BA	1431	C
45	BA	1432	U
45	BA	1433	G
45	BA	1435	G
45	BA	1446	A
45	BA	1447	C
45	BA	1448	G
45	BA	1457	C

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Mol	Chain	Res	Type
45	BA	1458	G
45	BA	1459	C
45	BA	1460	A
45	BA	1471	A
45	BA	1482	C
45	BA	1486	G
45	BA	1489	U
45	BA	1490	C
45	BA	1491	U
45	BA	1492	A
45	BA	1493	A
45	BA	1496	U
45	BA	1500	C
45	BA	1506	G
45	BA	1516	A
45	BA	1520	U
45	BA	1521	G
45	BA	1523	G
45	BA	1524	A
45	BA	1527	C
45	BA	1535	U
45	BA	1536	G
45	BA	1537	C
45	BA	1538	U
45	BA	1540	G
45	BA	1542	G
45	BA	1557	U
45	BA	1559	A
45	BA	1569	A
45	BA	1573	A
45	BA	1574	G
45	BA	1582	U
45	BA	1584	G
45	BA	1590	G
45	BA	1601	G
45	BA	1607	G
45	BA	1614	A
45	BA	1616	G
45	BA	1622	G
45	BA	1631	A
45	BA	1632	C
45	BA	1635	A

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Mol	Chain	Res	Type
45	BA	1657	U
45	BA	1658	G
45	BA	1680	G
45	BA	1682	U
45	BA	1683	C
45	BA	1684	U
45	BA	1736	G
45	BA	1756	A
45	BA	1760	G
45	BA	1762	A
45	BA	1766	A
45	BA	1769	U
45	BA	1780	G
45	BA	1782	A
45	BA	1783	C
45	BA	1792	G
45	BA	1793	G
45	BA	1794	A
45	BA	1795	U
45	BA	1796	C
45	BA	1798	U

All (80) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	65	A
1	AA	239	G
1	AA	282	G
1	AA	547	G
1	AA	588	G
1	AA	637	C
1	AA	715	A
1	AA	763	G
1	AA	916	G
1	AA	979	U
1	AA	993	G
1	AA	1064	A
1	AA	1094	U
1	AA	1097	G
1	AA	1103	A
1	AA	1307	G
1	AA	1329	U

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Mol	Chain	Res	Type
1	AA	1352	A
1	AA	1355	A
1	AA	1554	U
1	AA	1562	C
1	AA	1607	U
1	AA	1716	U
1	AA	1815	U
1	AA	1816	A
1	AA	1820	U
1	AA	2101	C
1	AA	2112	U
1	AA	2209	U
1	AA	2372	A
1	AA	2513	U
1	AA	2537	U
1	AA	2541	U
1	AA	2771	U
1	AA	2801	A
1	AA	3121	U
1	AA	3218	A
1	AA	3228	C
1	AA	3269	U
1	AA	3316	A
1	AA	3350	C
1	AA	3351	U
3	AC	85	G
45	BA	25	C
45	BA	130	C
45	BA	131	C
45	BA	132	U
45	BA	139	C
45	BA	158	U
45	BA	218	A
45	BA	240	U
45	BA	280	U
45	BA	417	A
45	BA	497	G
45	BA	498	G
45	BA	501	U
45	BA	503	G
45	BA	512	A
45	BA	542	A

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Mol	Chain	Res	Type
45	BA	558	U
45	BA	685	A
45	BA	819	G
45	BA	829	A
45	BA	849	C
45	BA	854	U
45	BA	855	A
45	BA	1081	A
45	BA	1108	G
45	BA	1157	A
45	BA	1226	A
45	BA	1244	A
45	BA	1250	U
45	BA	1344	A
45	BA	1370	U
45	BA	1481	C
45	BA	1568	C
45	BA	1573	A
45	BA	1615	C
45	BA	1657	U
45	BA	1761	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\|>2$
80	ATP	Bi	1202	79	26,33,33	0.91	1 (3%)	31,52,52	1.55	5 (16%)
80	ATP	Bi	1201	-	26,33,33	0.93	1 (3%)	31,52,52	1.52	5 (16%)

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
80	ATP	Bi	1202	79	-	3/18/38/38	0/3/3/3
80	ATP	Bi	1201	-	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bi	1202	ATP	C5-C4	2.43	1.47	1.40
80	Bi	1201	ATP	C5-C4	2.41	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
80	Bi	1202	ATP	PB-O3B-PG	-3.76	119.93	132.83
80	Bi	1201	ATP	PA-O3A-PB	-3.54	120.69	132.83
80	Bi	1201	ATP	PB-O3B-PG	-3.24	121.72	132.83
80	Bi	1202	ATP	C3'-C2'-C1'	3.22	105.82	100.98
80	Bi	1201	ATP	N3-C2-N1	-3.20	123.67	128.68
80	Bi	1202	ATP	N3-C2-N1	-3.19	123.70	128.68
80	Bi	1201	ATP	C3'-C2'-C1'	2.94	105.41	100.98
80	Bi	1202	ATP	PA-O3A-PB	-2.91	122.86	132.83
80	Bi	1202	ATP	C4-C5-N7	-2.61	106.68	109.40
80	Bi	1201	ATP	C4-C5-N7	-2.46	106.84	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	Bi	1201	ATP	C5'-O5'-PA-O3A
80	Bi	1202	ATP	PB-O3A-PA-O5'
80	Bi	1201	ATP	C5'-O5'-PA-O1A
80	Bi	1202	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

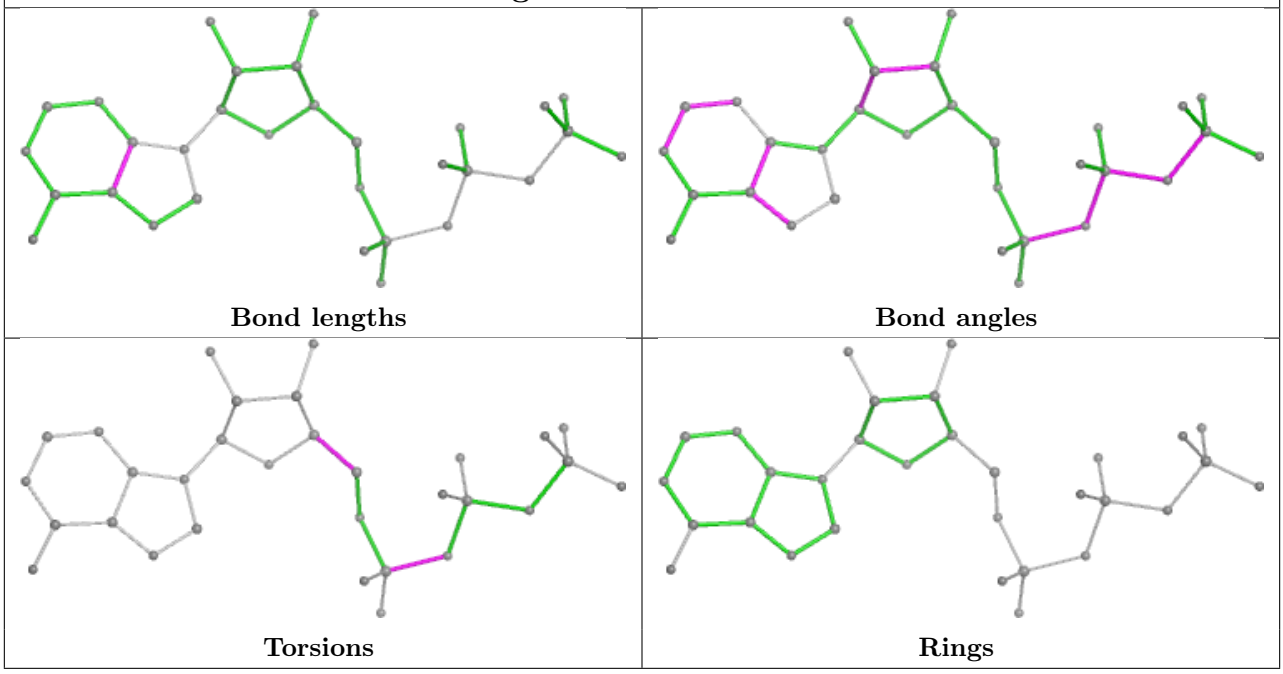
Mol	Chain	Res	Type	Atoms
80	Bi	1202	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

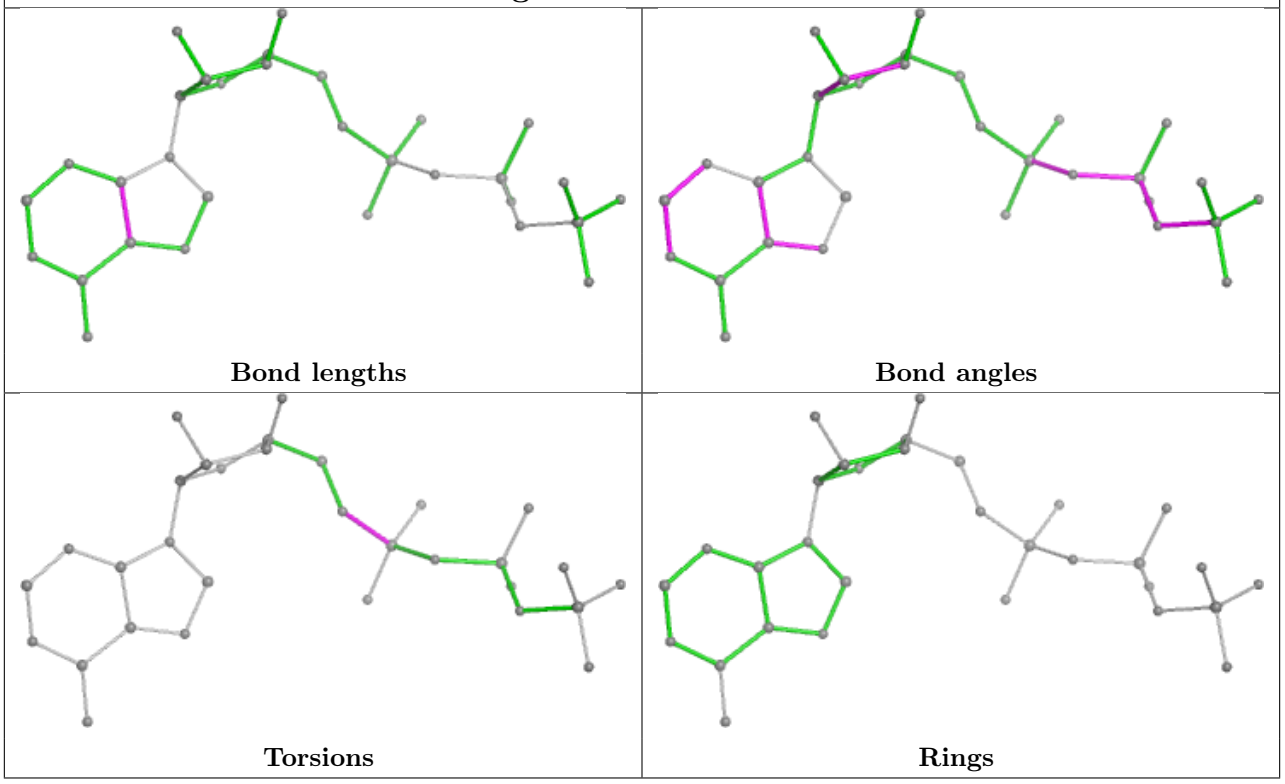
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP Bi 1202



Ligand ATP Bi 1201



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
1	AA	3
45	BA	3
11	AK	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1955:U	O3'	2093:A	P	24.80
1	BA	652:G	O3'	682:C	P	17.82
1	BA	703:G	O3'	735:C	P	16.09
1	BA	1685:G	O3'	1717:G	P	15.70
1	AA	2445:A	O3'	2501:U	P	15.05
1	AA	440:A	O3'	494:G	P	13.22

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AK	167:VAL	C	168:ARG	N	6.38
1	AK	168:ARG	C	169:ASN	N	6.15

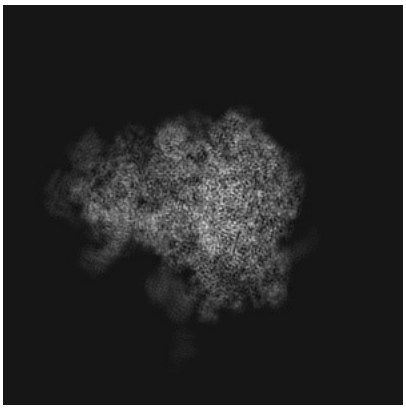
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10098. These allow visual inspection of the internal detail of the map and identification of artifacts.

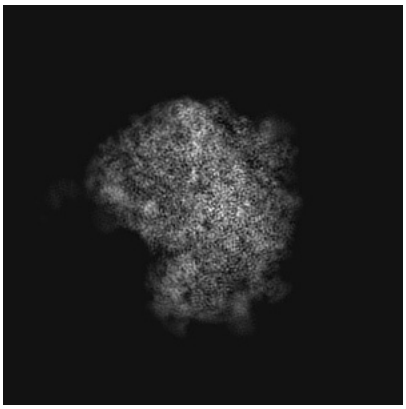
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

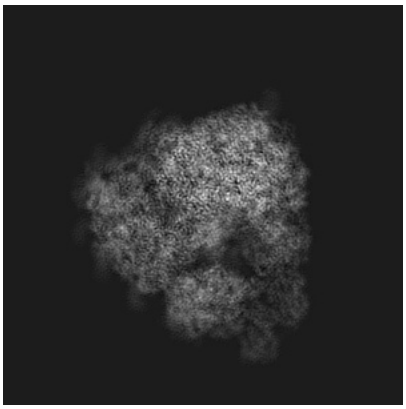
6.1.1 Primary map



X

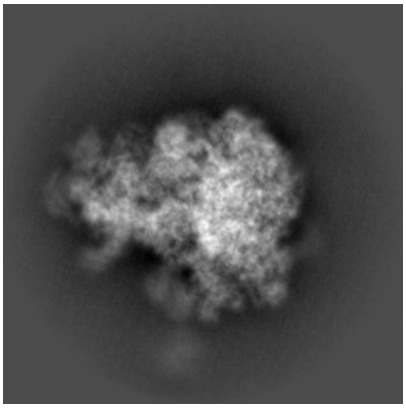


Y

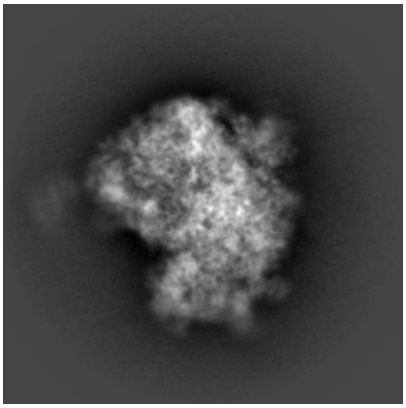


Z

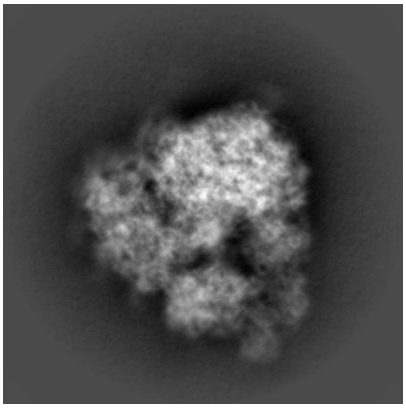
6.1.2 Raw map



X



Y

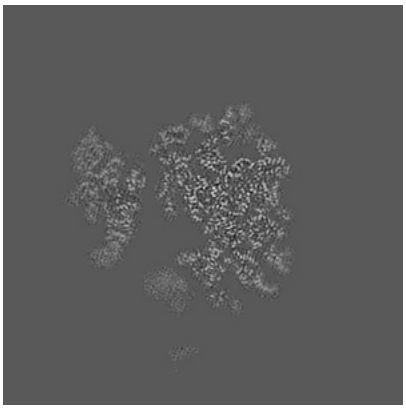


Z

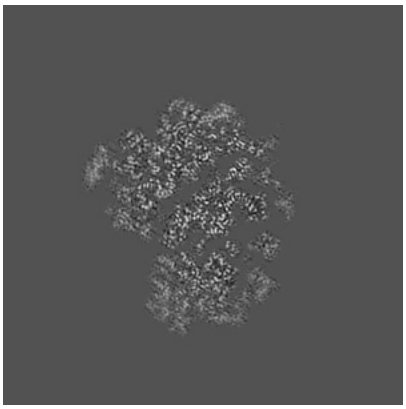
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

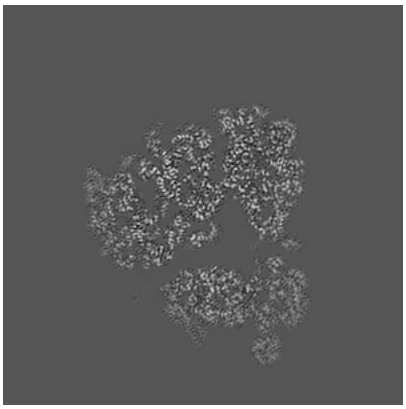
6.2.1 Primary map



X Index: 210

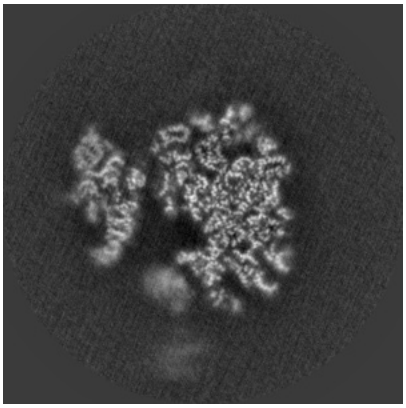


Y Index: 210

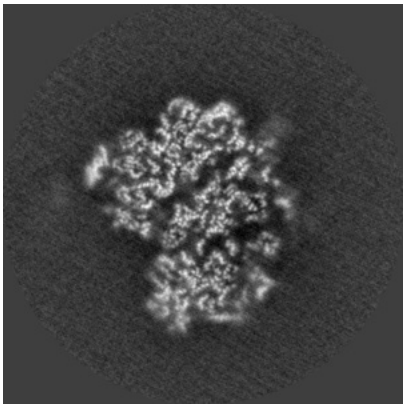


Z Index: 210

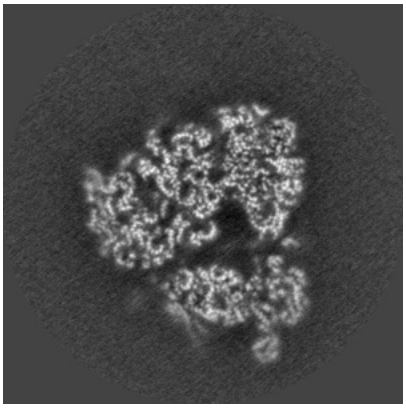
6.2.2 Raw map



X Index: 210



Y Index: 210

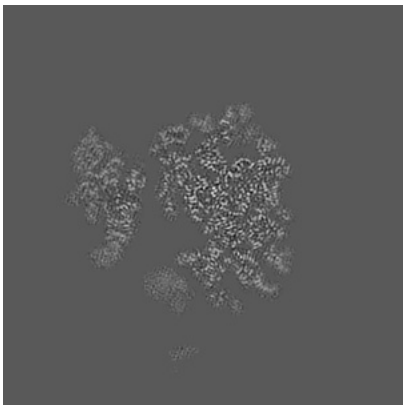


Z Index: 210

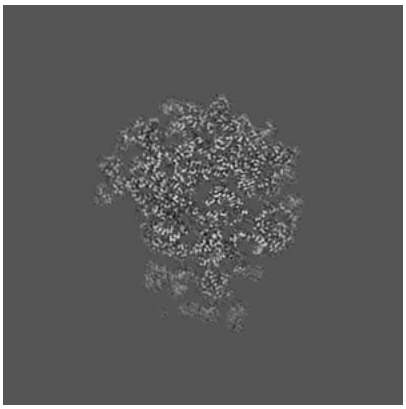
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

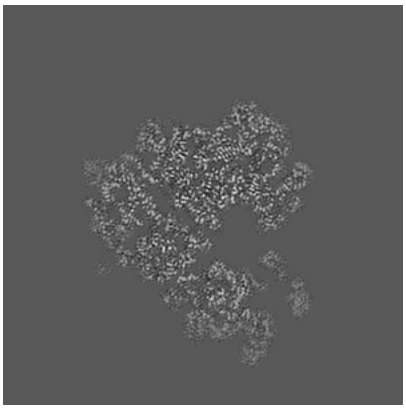
6.3.1 Primary map



X Index: 210

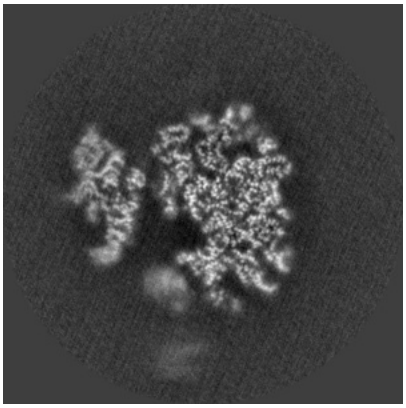


Y Index: 240

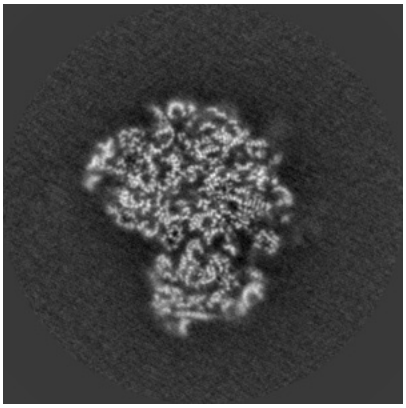


Z Index: 222

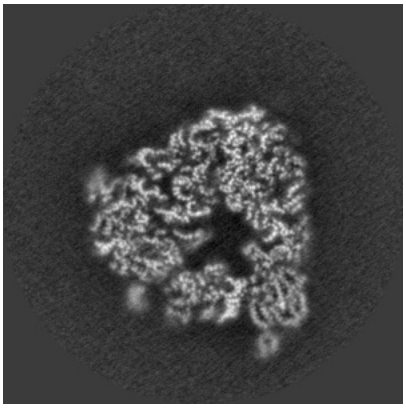
6.3.2 Raw map



X Index: 209



Y Index: 216

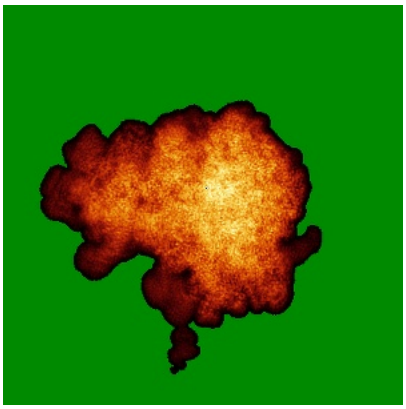


Z Index: 200

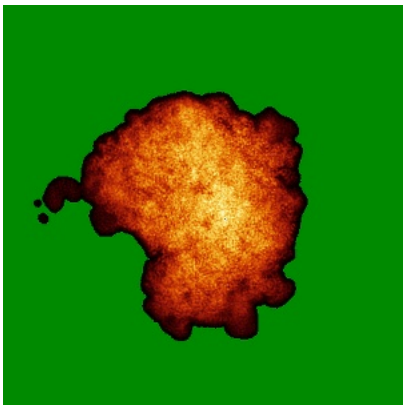
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

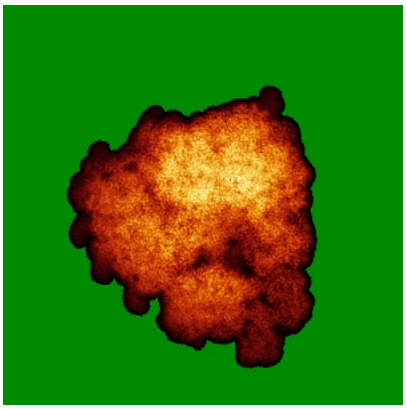
6.4.1 Primary map



X

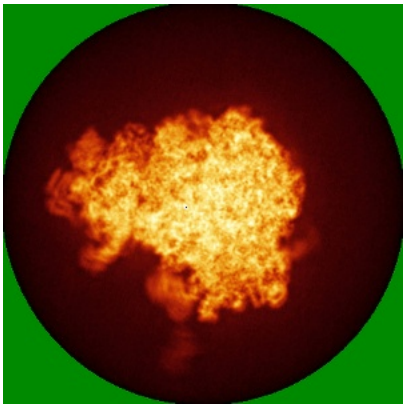


Y

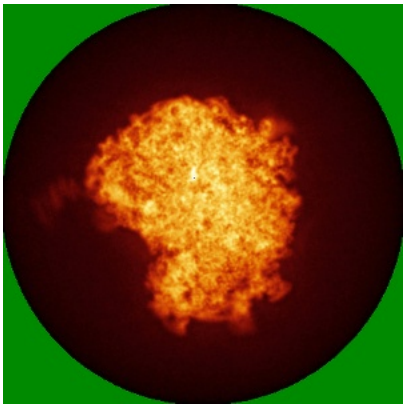


Z

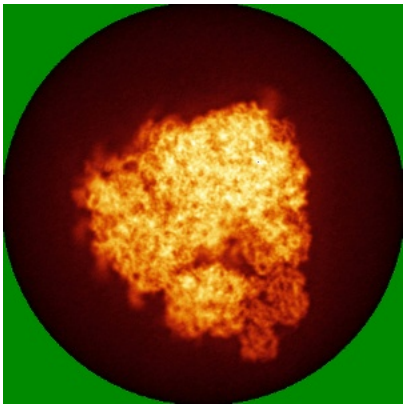
6.4.2 Raw map



X



Y

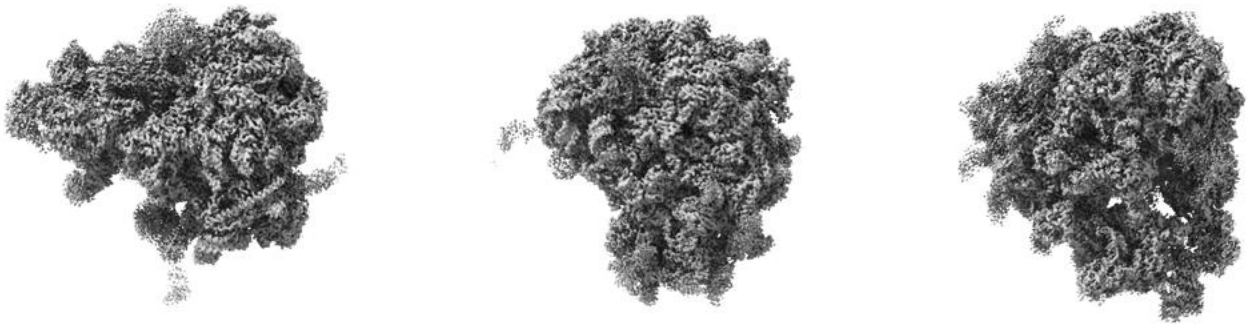


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

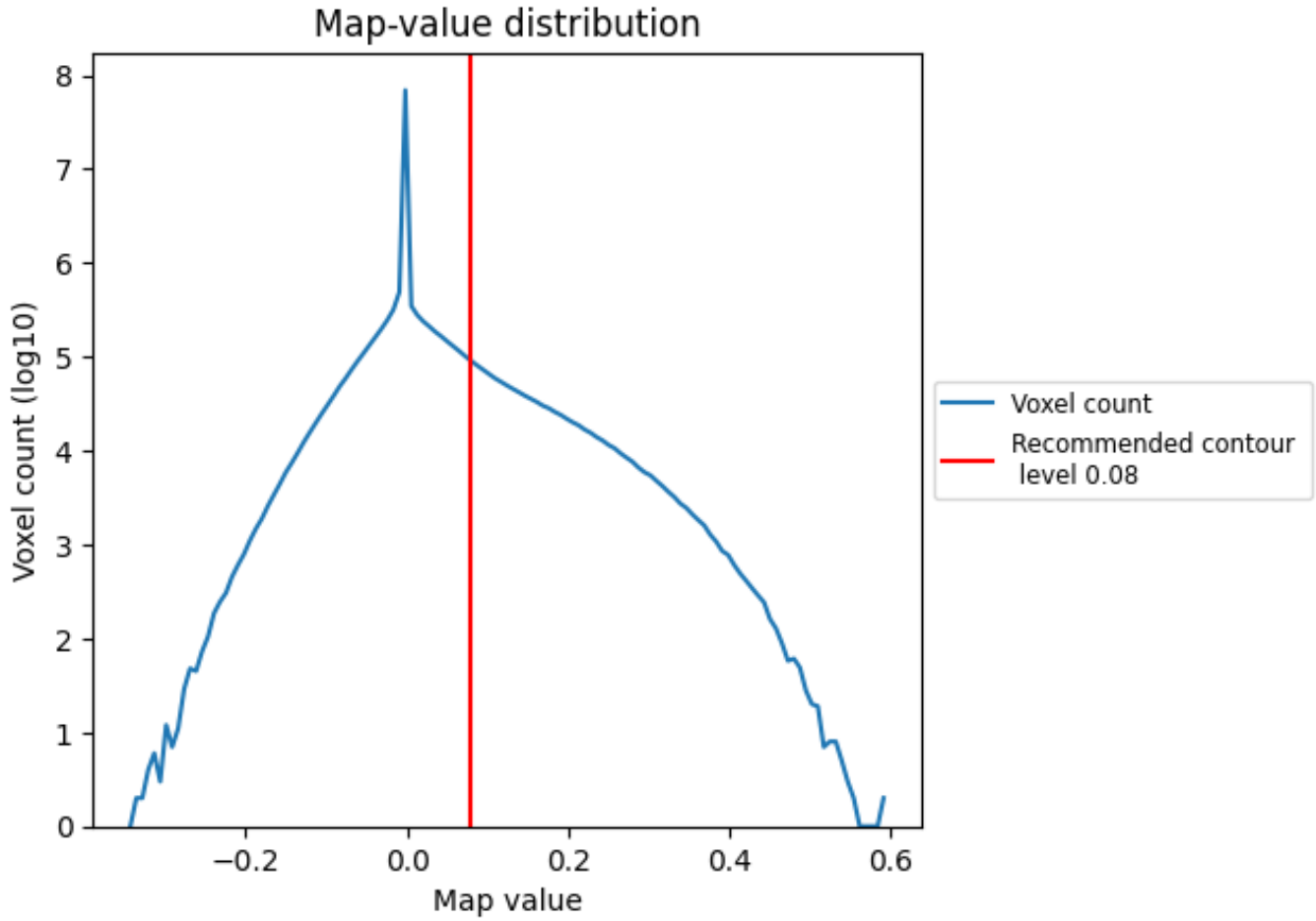
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

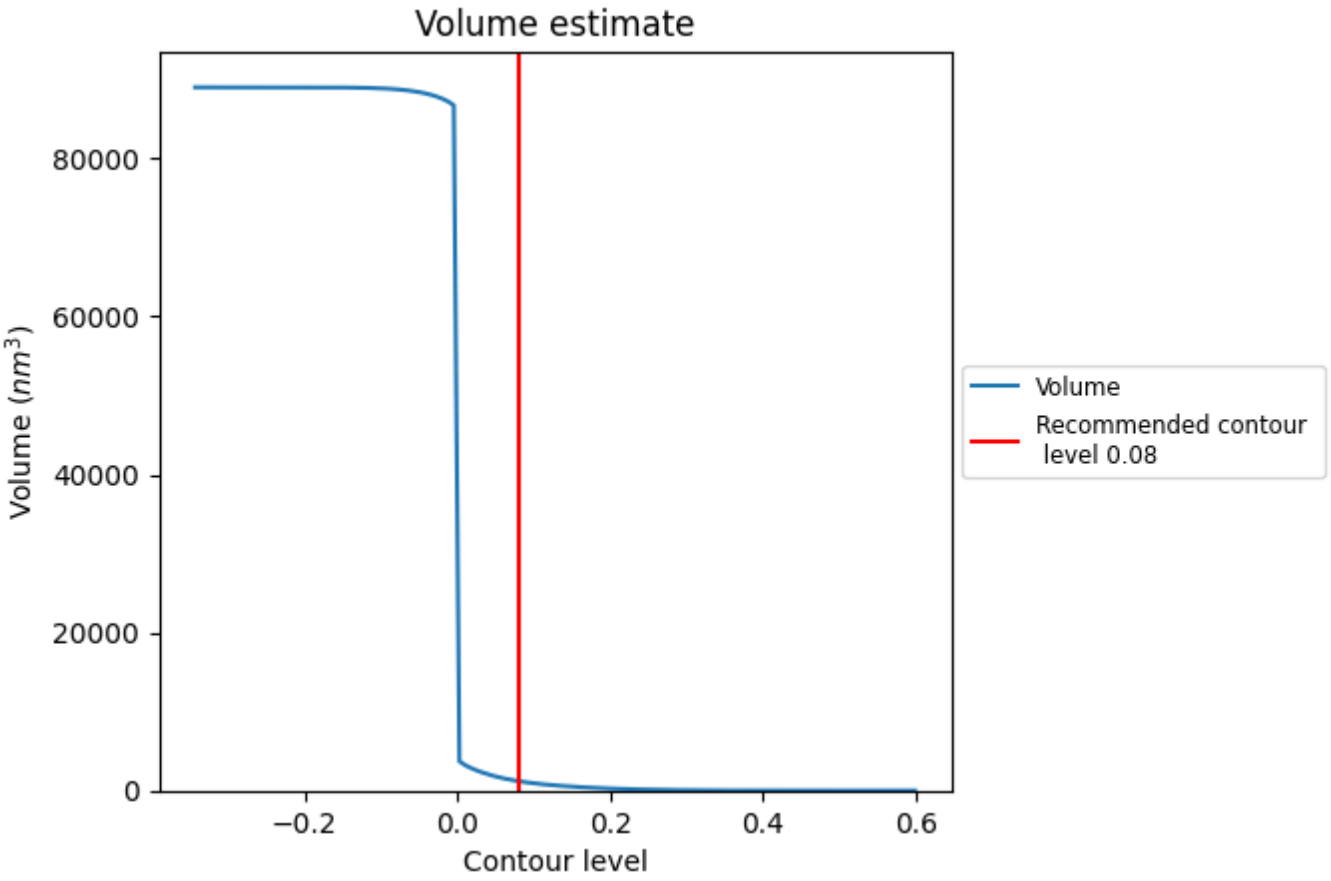
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

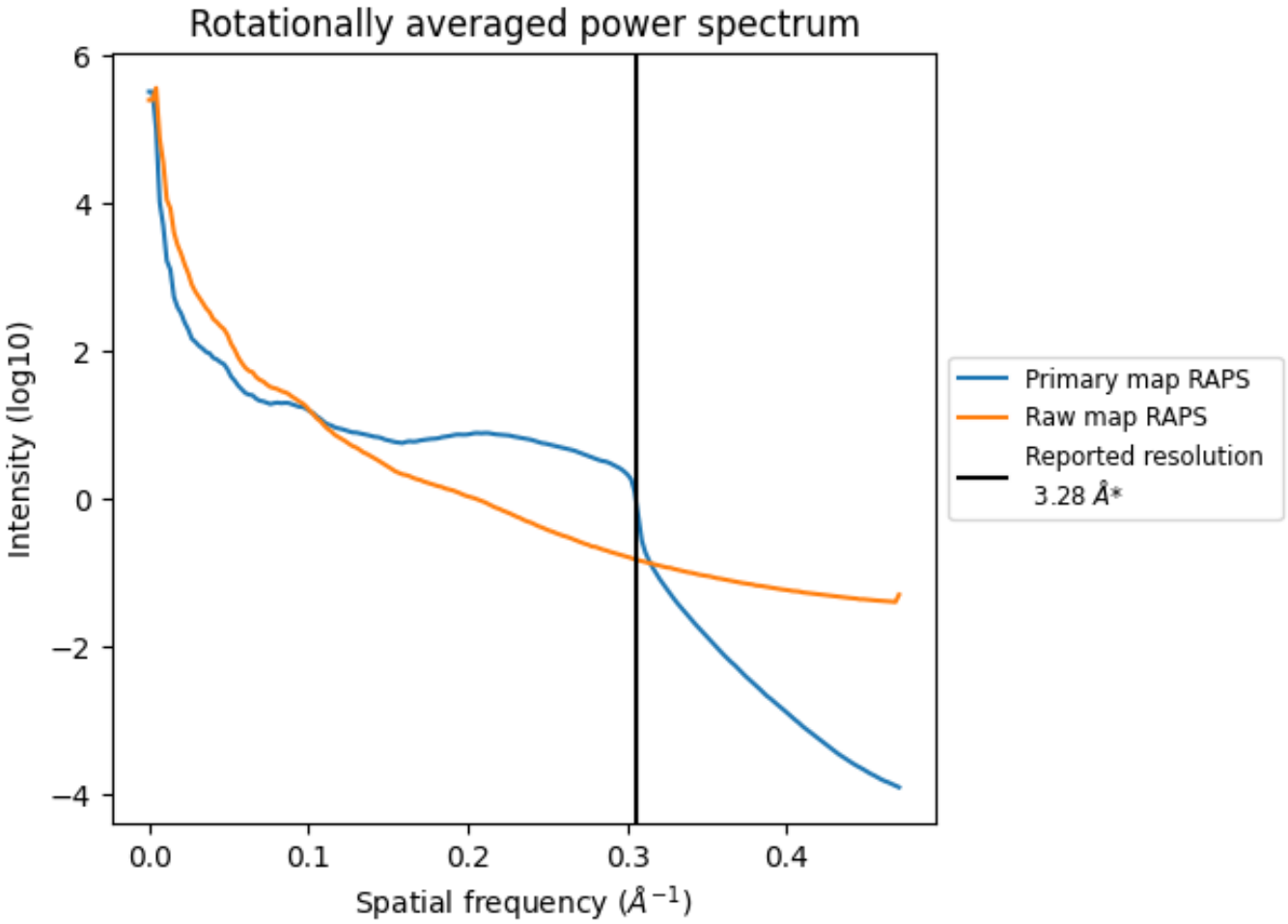
7.2 Volume estimate



The volume at the recommended contour level is 1193 nm^3; this corresponds to an approximate mass of 1078 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

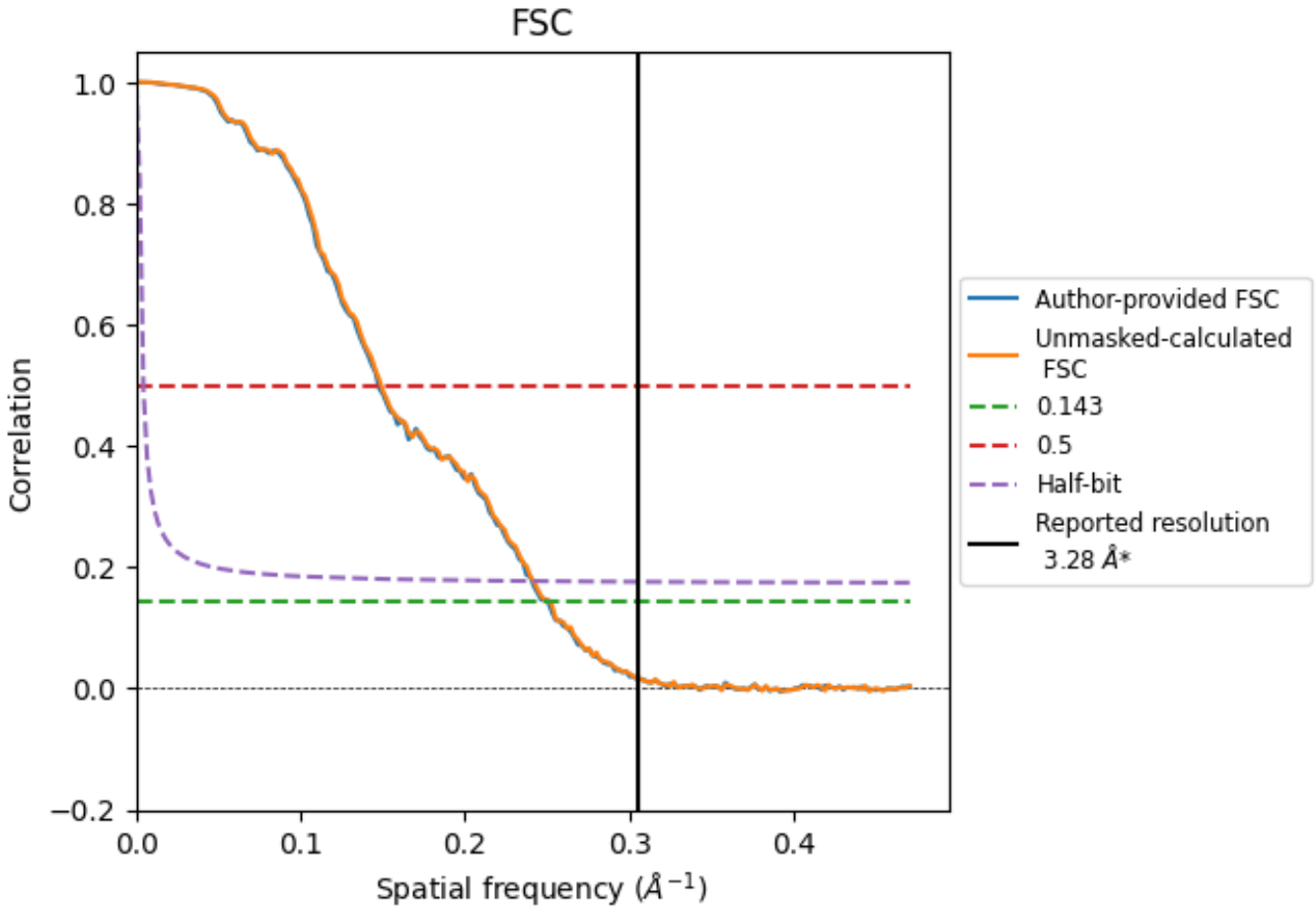


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	4.00	6.78	4.15
Unmasked-calculated*	3.98	6.71	4.14

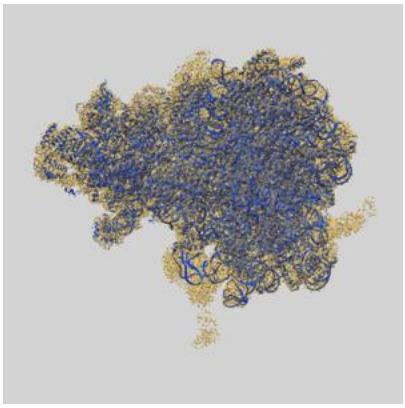
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.28 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.28 by more than 10 %

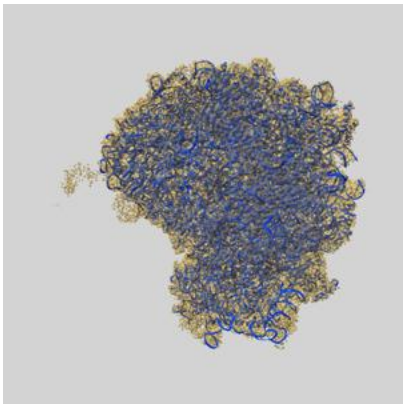
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10098 and PDB model 6S47. Per-residue inclusion information can be found in section 3 on page 19.

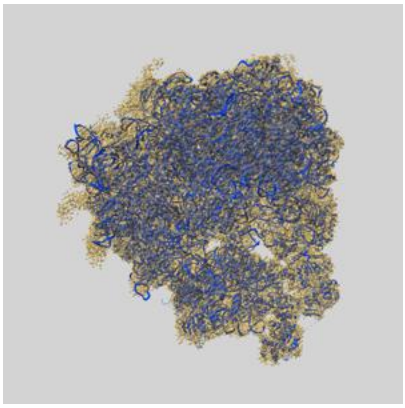
9.1 Map-model overlay



X



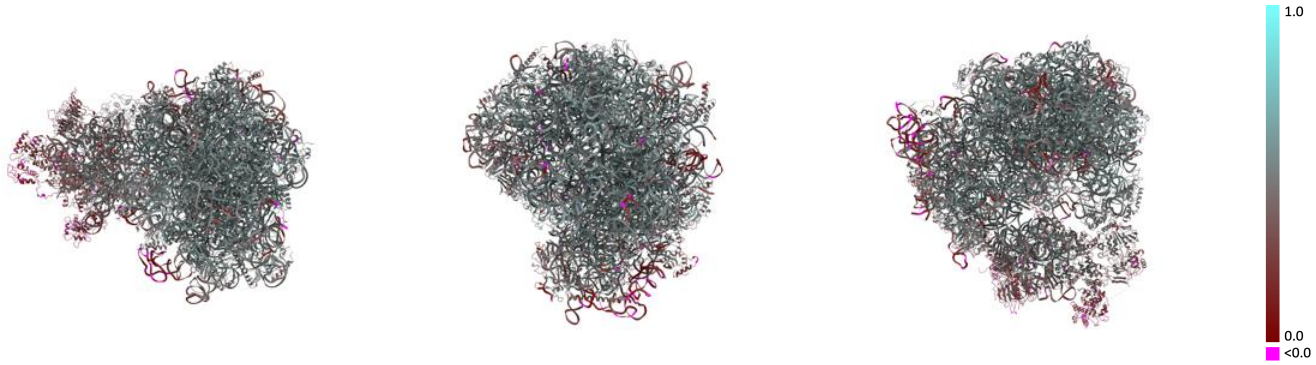
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

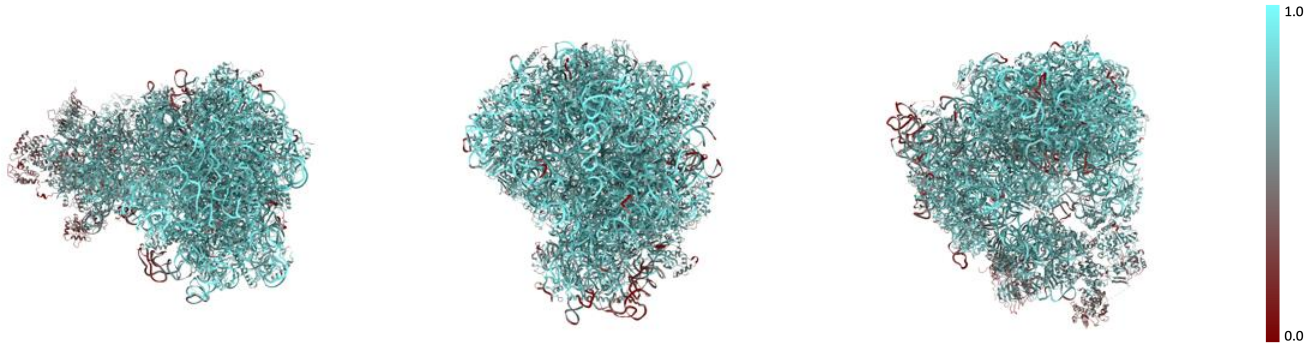
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

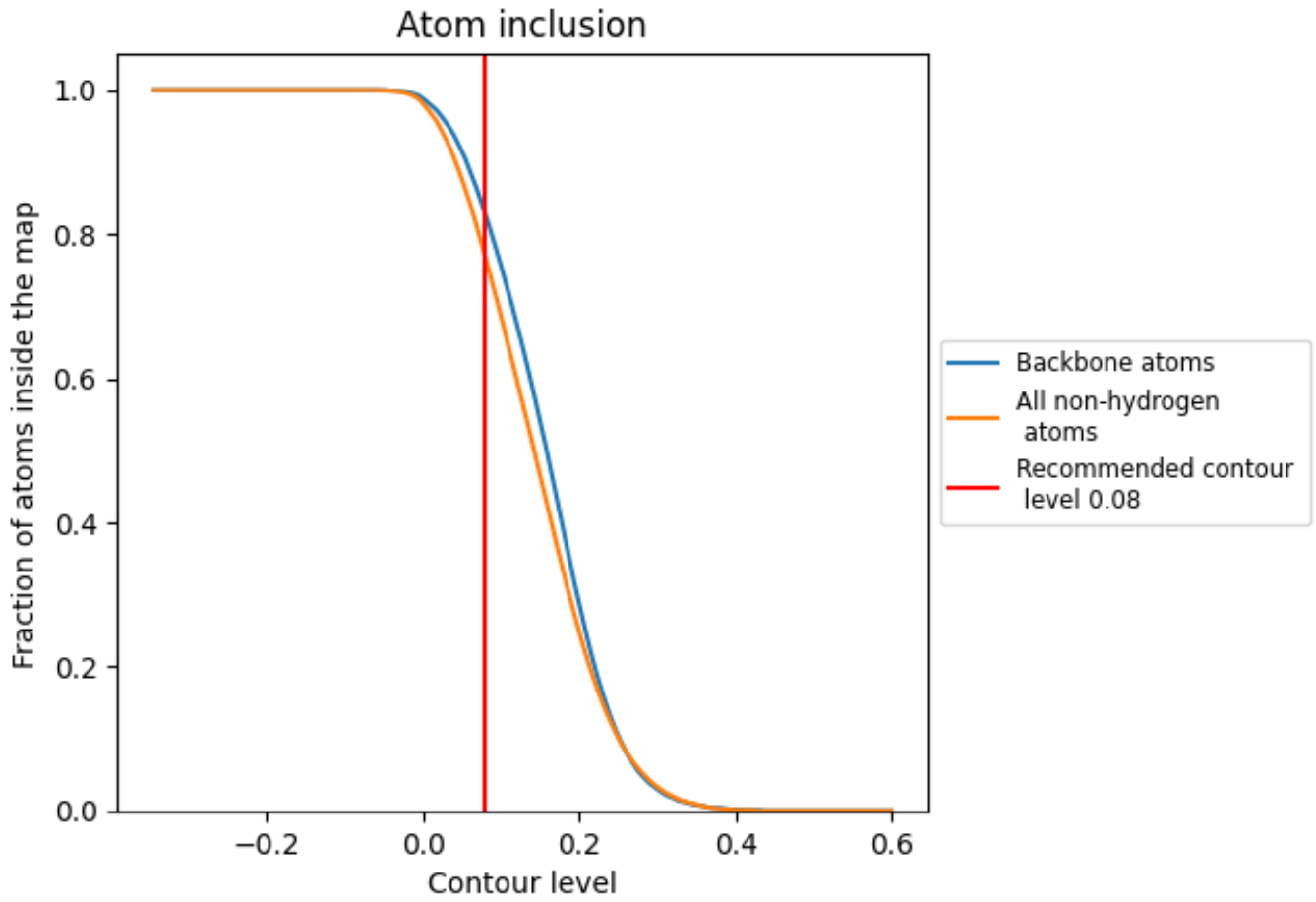
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.4720
AA	0.8610	0.5000
AB	0.9050	0.5110
AC	0.8880	0.5190
AD	0.7740	0.5370
AE	0.7640	0.5160
AF	0.7650	0.5130
AG	0.7260	0.4730
AH	0.6940	0.4770
AI	0.7420	0.5110
AJ	0.6990	0.4720
AK	0.6970	0.4690
AL	0.7310	0.5030
AM	0.6910	0.4680
AN	0.7360	0.5100
AO	0.7370	0.4910
AP	0.7900	0.5500
AQ	0.7540	0.5100
AR	0.7400	0.5050
AS	0.7390	0.5270
AT	0.7780	0.5280
AU	0.7460	0.5130
AV	0.7460	0.5160
AW	0.6830	0.4400
AX	0.7300	0.5130
AY	0.7650	0.5180
AZ	0.7470	0.5130
Aa	0.7590	0.5160
Ab	0.7560	0.4940
Ac	0.7810	0.5340
Ad	0.6900	0.4940
Ae	0.7210	0.4940
Af	0.7190	0.4950
Ag	0.7150	0.5300
Ah	0.7700	0.5280

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Chain	Atom inclusion	Q-score
Ai	0.7320	0.5170
Aj	0.7550	0.5150
Ak	0.7170	0.4850
Al	0.7980	0.5390
Am	0.6660	0.4390
An	0.7450	0.5330
Ao	0.7300	0.4800
Ap	0.4950	0.4850
Aq	0.7070	0.5040
Ar	0.7130	0.5240
BA	0.8040	0.4520
BB	0.7110	0.4680
BC	0.6920	0.4680
BD	0.7300	0.4980
BE	0.5510	0.3770
BF	0.7010	0.4750
BG	0.6230	0.4210
BH	0.5950	0.3870
BI	0.5980	0.3940
BJ	0.6890	0.4720
BK	0.6680	0.4420
BL	0.5130	0.3060
BM	0.6740	0.4720
BN	0.2410	0.1620
BO	0.7130	0.4830
BP	0.7520	0.4880
BQ	0.5670	0.3520
BR	0.6890	0.4470
BS	0.6320	0.4070
BT	0.6780	0.4290
BU	0.7090	0.4500
BV	0.5390	0.3590
BW	0.7110	0.4770
BX	0.7510	0.5260
BY	0.7150	0.5010
BZ	0.6240	0.4210
Ba	0.5580	0.3470
Bb	0.7500	0.4760
Bc	0.6510	0.4590
Bd	0.5810	0.4000
Be	0.7310	0.4490
Bf	0.5770	0.4060

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Chain	Atom inclusion	Q-score
Bg	0.2860	0.1360
Bh	0.4970	0.3120
Bi	0.5360	0.3310