



Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 10:25 pm BST

PDB ID : 7O81
EMDB ID : EMD-12759
Title : Rabbit 80S ribosome colliding in another ribosome stalled by the SARS-CoV-2 pseudoknot
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on : 2021-04-14
Resolution : 3.10 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:

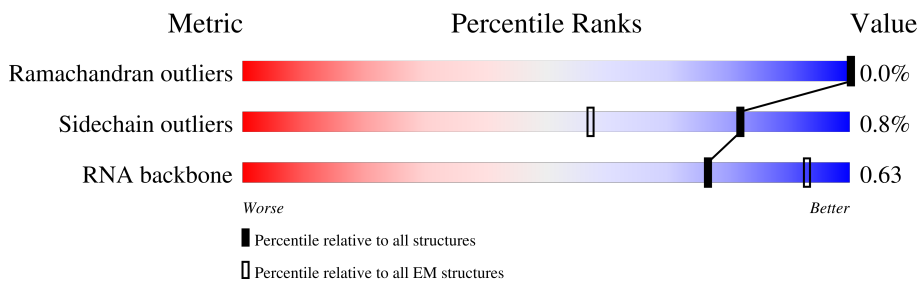
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



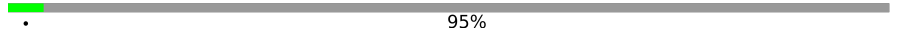







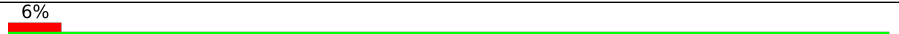

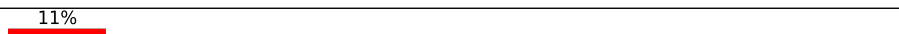
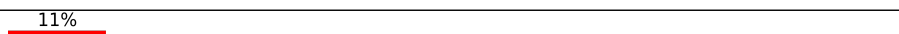
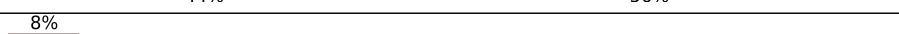
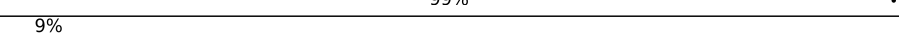
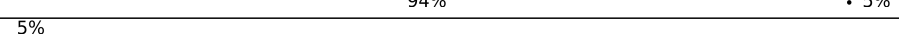

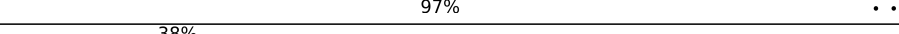

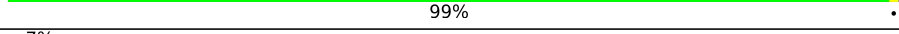



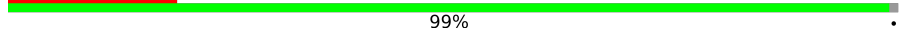
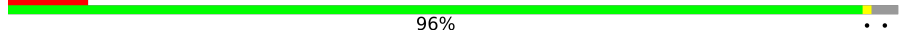
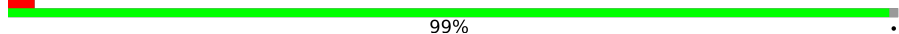
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	A2	1870	
2	AA	84	
3	AB	69	
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	

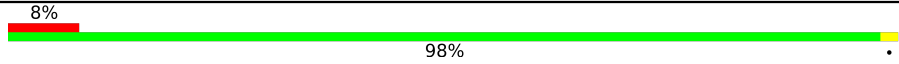
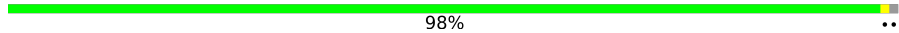
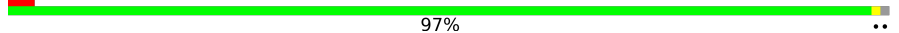
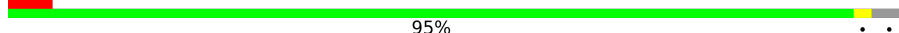

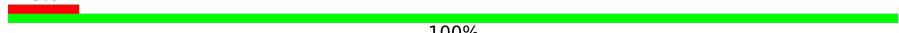









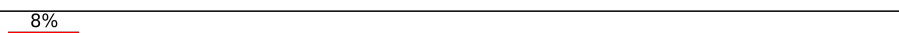
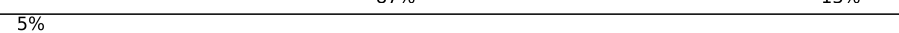
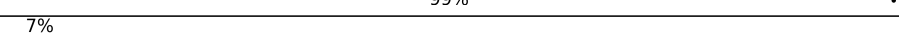
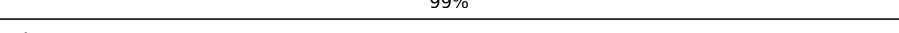
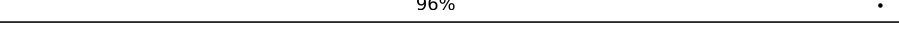
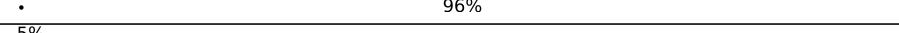
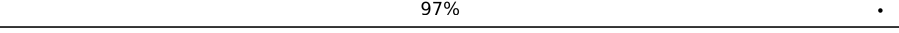

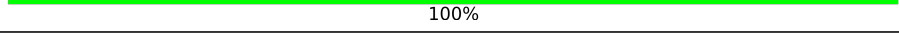
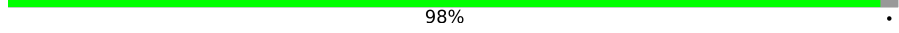
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Mol	Chain	Length	Quality of chain
9	AH	217	 95%
10	AJ	76	 38% 78% 22%
11	AT	75	 80% 20%
12	AU	148	 57% 72% 26%
13	AZ	295	 8% 74% 25%
14	Aa	264	 5% 80% 19%
15	Ab	293	 74% 25%
16	Ac	281	 9% 79% 20%
17	Ad	263	 6% 99%
18	Ae	204	 6% 94% 6%
19	Af	249	 11% 95% 5%
20	Ag	432	 11% 44% 56%
21	Ah	208	 8% 99%
22	Ai	194	 9% 94% 5%
23	Aj	165	 5% 58% 42%
24	Ak	158	 15% 97%
25	Al	132	 38% 90% 6%
26	Am	151	 5% 99%
27	An	151	 7% 89% 10%
28	Ao	145	 10% 88% 12%
29	Ap	172	 5% 82% 18%
30	Aq	135	 19% 99%
31	Ar	152	 9% 96%
32	As	145	 99%
33	At	119	 21% 87% 13%

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Mol	Chain	Length	Quality of chain
34	Au	83	 8% 98%
35	Av	130	 98%
36	Aw	143	 97%
37	Ax	130	 5% 95%
38	Ay	124	 8% 58% 41%
39	Az	25	 8% 100%
40	B5	4808	 5% 66% 12% 22%
41	B7	120	 92% 8%
42	B8	158	 8% 87% 12%
43	BA	257	 8% 98%
44	BB	403	 8% 99%
45	BC	413	 8% 87% 12%
46	BD	297	 8% 99%
47	BE	291	 9% 83% 16%
48	BF	247	 91% 9%
49	BG	266	 8% 87% 13%
50	BH	192	 5% 99%
51	BI	214	 7% 99%
52	BJ	178	 8% 96%
53	BK	1071	 8% 96%
54	BL	211	 5% 97%
55	BM	218	 8% 63% 37%
56	BN	204	 100%
57	BO	203	 8% 98%
58	BP	184	 8% 86% 14%



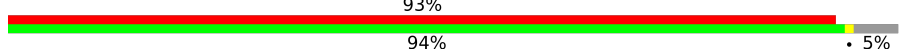
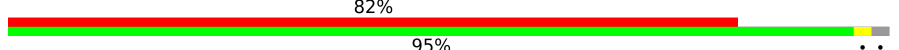
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Mol	Chain	Length	Quality of chain
59	BQ	188	99%
60	BR	196	91% 8%
61	BS	176	99%
62	BT	160	99%
63	BU	128	6% 77% 23%
64	BV	140	9% 99%
65	BW	157	31% 77% 23%
66	BX	156	78% 22%
67	BY	145	90% 8%
68	BZ	136	99%
69	Ba	148	99%
70	Bb	245	11% 44% 56%
71	Bc	115	14% 94% 6%
72	Bd	125	86% 14%
73	Be	135	96%
74	Bf	110	99%
75	Bg	117	7% 97%
76	Bh	123	5% 98%
77	Bi	105	95%
78	Bj	97	89% 11%
79	Bk	70	9% 99%
80	Bl	51	6% 96%
81	Bm	128	41% 59%
82	Bo	106	7% 97%
83	Bp	92	99%

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Mol	Chain	Length	Quality of chain
84	Br	137	 91% 8%
85	Bs	318	 59% 61% 38%
86	Bt	165	 93% 94% 5%
87	Bv	217	 82% 95%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 228361 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	1770	37833	16911	6781	12371	1770	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AA	83	651	408	121	115	7	0	0

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	63	495	302	98	93	2	0	0

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AC	74	610	385	117	101	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AD	45	369	228	84	56	1	0	0

- Molecule 6 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AE	101	814	507	170	132	5	0	0

- Molecule 7 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AF	313	2436	1535	424	465	12	0	0

- Molecule 8 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AG	55	459	286	94	74	5	0	0

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AH	10	212	95	39	68	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called A-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	AJ	76	1622	724	290	532	76	0	0

- Molecule 11 is a RNA chain called P-site tRNA(Pro).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AT	75	1604	714	284	531	75	0	0

- Molecule 12 is a protein called EDF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AU	110	Total	C	N	O	0	0
			864	529	169	166		

- Molecule 13 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 14 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Aa	214	Total	C	N	O	S	0	0
			1738	1104	311	309	14		

- Molecule 15 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 16 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 17 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ad	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 18 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 19 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Af	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 20 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 21 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 22 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ai	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 23 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 24 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 26 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 27 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 28 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 29 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 30 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 31 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 32 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 33 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 34 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 35 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Av	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 36 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 37 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ay	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Az	25	239	145	64	27	3	0	0

- Molecule 40 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	B5	3764	80772	36003	14762	26243	3764	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	B7	120	2570	1141	456	851	122	0	0

- Molecule 42 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	B8	156	3319	1481	585	1097	156	0	0

- Molecule 43 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BA	253	1940	1214	396	324	6	0	0

- Molecule 44 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BB	398	3206	2042	605	546	13	0	0

- Molecule 45 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BC	362	2886	1814	577	481	14	0	0

- Molecule 46 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BD	294	2398	1516	439	429	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BE	243	1960	1258	378	321	3	0	0

- Molecule 48 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BF	226	1886	1211	362	304	9	0	0

- Molecule 49 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BG	232	1868	1191	359	314	4	0	0

- Molecule 50 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BH	190	1516	954	284	272	6	0	0

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 52 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 53 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	39	Total	C	N	O	S	0	0
			290	180	48	55	7		

- Molecule 54 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 55 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 56 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 57 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 58 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	BP	159	1289	809	249	222	9	0	0

- Molecule 59 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BQ	187	1515	946	315	250	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	BR	180	1508	933	328	238	9	0	0

- Molecule 61 is a protein called Ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	BS	176	1457	924	288	234	11	0	0

- Molecule 62 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	BT	159	1298	823	252	217	6	0	0

- Molecule 63 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	BU	99	806	516	141	147	2	0	0

- Molecule 64 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BV	139	1034	648	199	182	5	0	0

- Molecule 65 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 66 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BX	122	Total	C	N	O	S	0	0
			1004	642	190	171	1		

- Molecule 67 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 68 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 69 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 70 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 71 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 72 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bd	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 73 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 74 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 75 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 76 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 77 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 78 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 79 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Bk	69	569	366	103	99	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 80 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Bl	50	447	286	96	64	1	0	0

- Molecule 81 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Bm	52	432	269	90	67	6	0	0

- Molecule 82 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Bo	105	863	543	175	139	6	0	0

- Molecule 83 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Bp	91	708	445	136	120	7	0	0

- Molecule 84 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Br	126	1014	629	209	170	6	0	0

- Molecule 85 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bs	196	1507	959	263	276	9	0	0

- Molecule 86 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Bt	156	1178	733	221	220	4	0	0

- Molecule 87 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	Bv	212	1707	1092	308	299	8	0	0

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A2	84	Total 84	Mg 84	0
88	B5	250	Total 250	Mg 250	0
88	B7	7	Total 7	Mg 7	0
88	B8	5	Total 5	Mg 5	0
88	BP	1	Total 1	Mg 1	0
88	BV	1	Total 1	Mg 1	0
88	Ba	1	Total 1	Mg 1	0

- Molecule 89 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
89	A2	62	Total 62	X 62	0
89	AT	1	Total 1	X 1	0
89	An	1	Total 1	X 1	0

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Mol	Chain	Residues	Atoms		AltConf
89	B5	175	Total 175	X 175	0
89	B7	6	Total 6	X 6	0
89	B8	4	Total 4	X 4	0
89	BA	4	Total 4	X 4	0
89	BB	1	Total 1	X 1	0
89	BH	1	Total 1	X 1	0
89	BI	1	Total 1	X 1	0
89	BL	1	Total 1	X 1	0
89	BN	3	Total 3	X 3	0
89	BO	1	Total 1	X 1	0
89	BT	2	Total 2	X 2	0
89	Be	1	Total 1	X 1	0
89	Bf	1	Total 1	X 1	0
89	Bg	1	Total 1	X 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

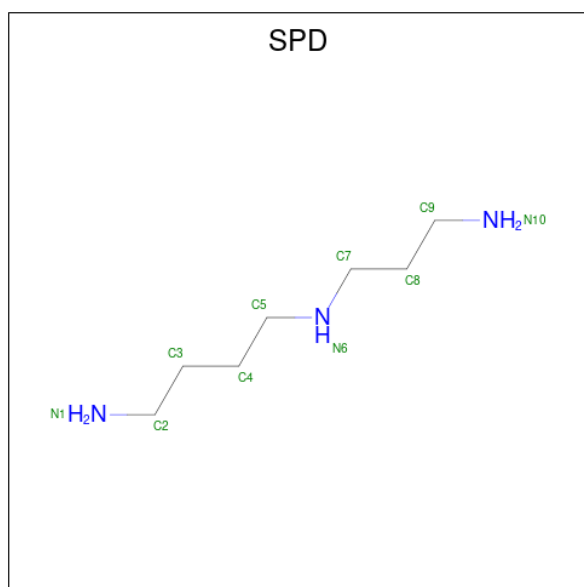
Mol	Chain	Residues	Atoms		AltConf
90	AC	1	Total 1	Zn 1	0
90	AE	1	Total 1	Zn 1	0
90	AG	1	Total 1	Zn 1	0
90	Bg	1	Total 1	Zn 1	0
90	Bj	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
90	Bm	1	Total	Zn	0
			1	1	
90	Bo	1	Total	Zn	0
			1	1	
90	Bp	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
91	B5	1	Total	C	N	0
			10	7	3	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	391	Total	O	0
			391	391	
92	AE	1	Total	O	0
			1	1	
92	Ab	1	Total	O	0
			1	1	
92	Af	1	Total	O	0
			1	1	
92	Ak	2	Total	O	0
			2	2	

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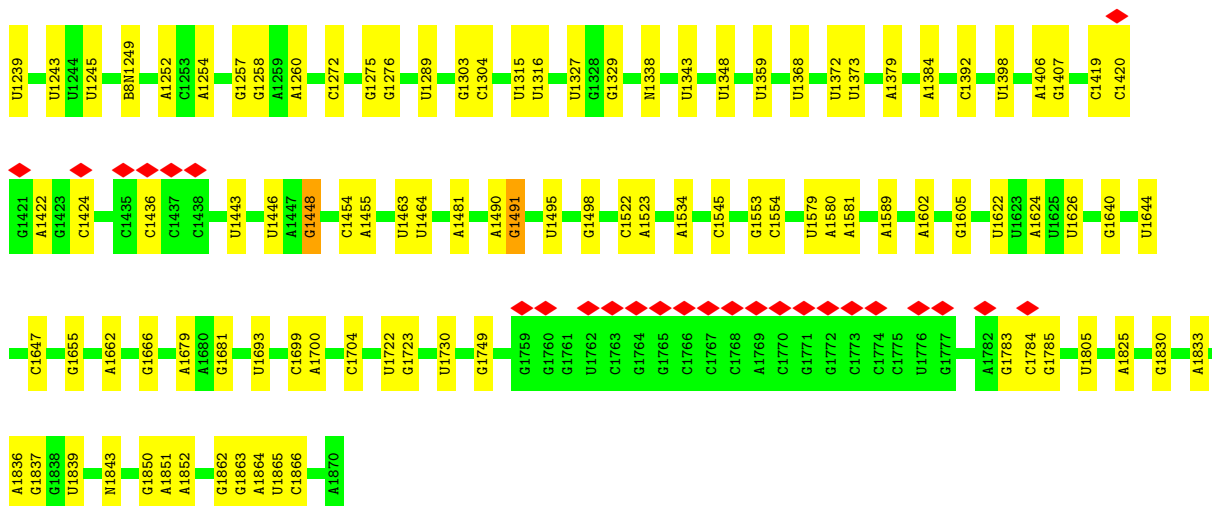
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Mol	Chain	Residues	Atoms		AltConf
92	An	1	Total 1	O 1	0
92	Ap	2	Total 2	O 2	0
92	Ar	1	Total 1	O 1	0
92	As	2	Total 2	O 2	0
92	Aw	5	Total 5	O 5	0
92	B5	1197	Total 1197	O 1197	0
92	B7	35	Total 35	O 35	0
92	B8	35	Total 35	O 35	0
92	BA	4	Total 4	O 4	0
92	BB	3	Total 3	O 3	0
92	BC	3	Total 3	O 3	0
92	BD	1	Total 1	O 1	0
92	BF	2	Total 2	O 2	0
92	BH	1	Total 1	O 1	0
92	BI	1	Total 1	O 1	0
92	BL	1	Total 1	O 1	0
92	BN	2	Total 2	O 2	0
92	BO	1	Total 1	O 1	0
92	BP	3	Total 3	O 3	0
92	BR	5	Total 5	O 5	0
92	BV	3	Total 3	O 3	0

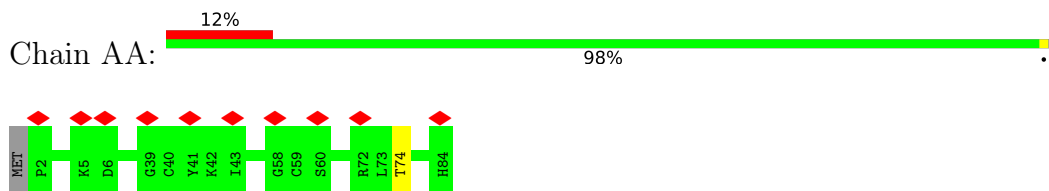
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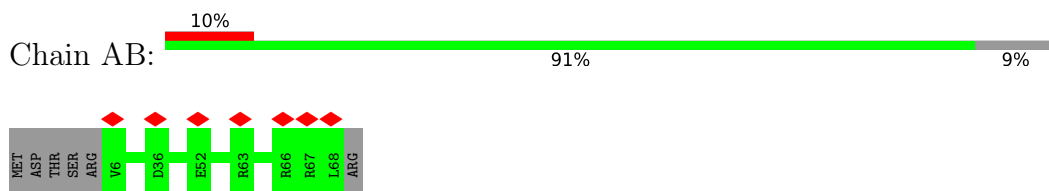
Mol	Chain	Residues	Atoms		AltConf
92	BX	2	Total 2	O 2	0
92	BY	1	Total 1	O 1	0
92	Ba	7	Total 7	O 7	0
92	Bb	1	Total 1	O 1	0
92	Be	4	Total 4	O 4	0
92	Bg	2	Total 2	O 2	0
92	Bj	3	Total 3	O 3	0
92	Bm	1	Total 1	O 1	0



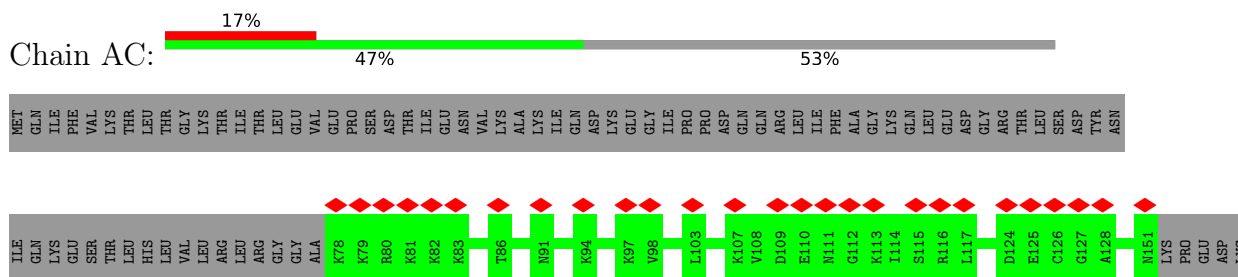
• Molecule 2: 40S ribosomal protein S27



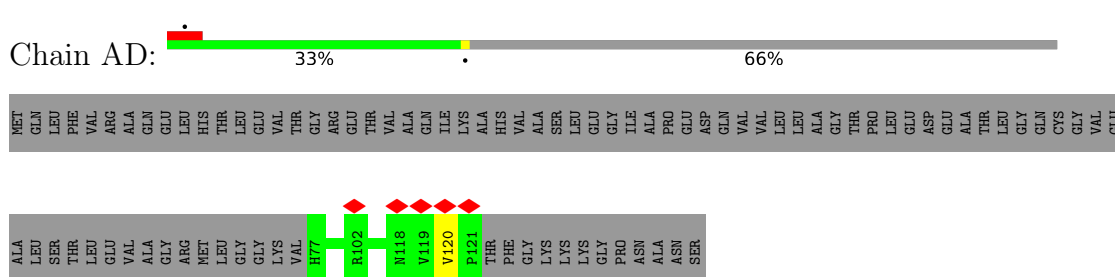
• Molecule 3: Ribosomal protein S28

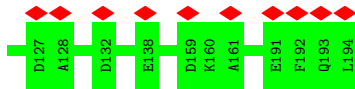


• Molecule 4: Ribosomal protein S27a

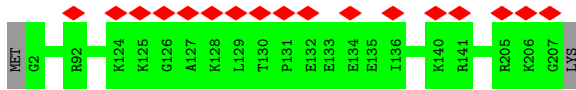


• Molecule 5: 40S ribosomal protein S30

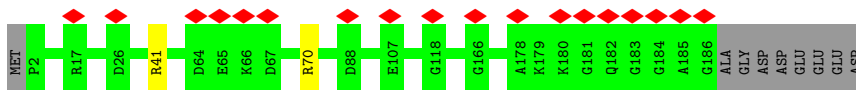




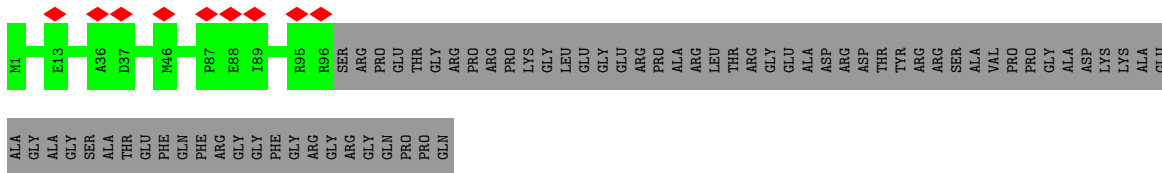
- Molecule 21: 40S ribosomal protein S8



- Molecule 22: Ribosomal protein S9 (Predicted)



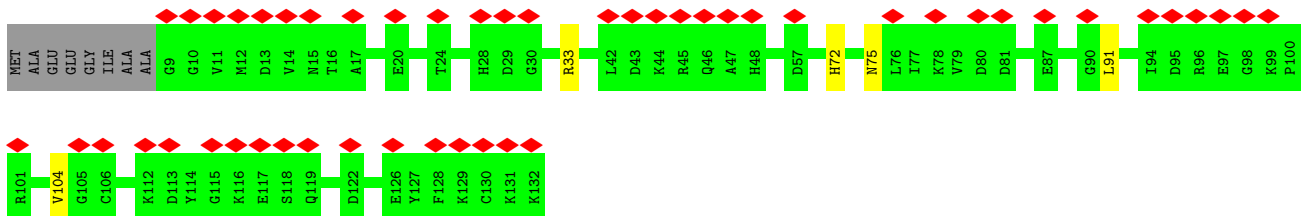
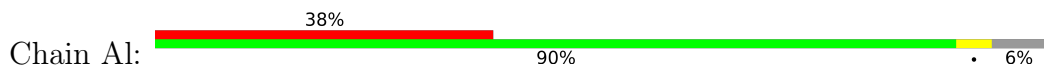
- Molecule 23: Ribosomal protein eS10



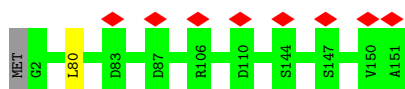
- Molecule 24: 40S ribosomal protein S11



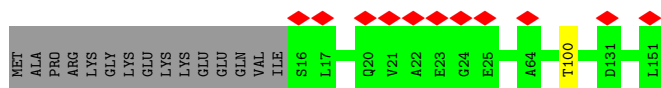
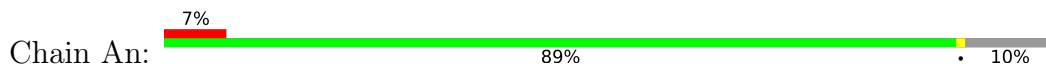
- Molecule 25: 40S ribosomal protein S12



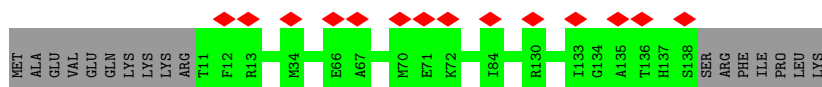
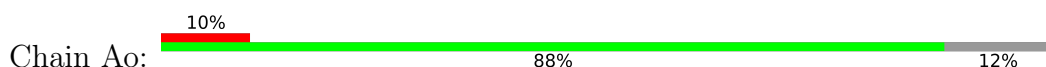
- Molecule 26: uS15



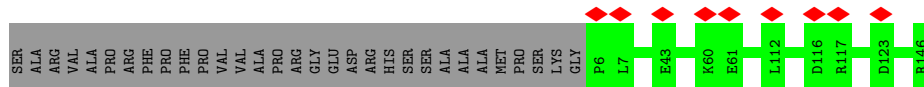
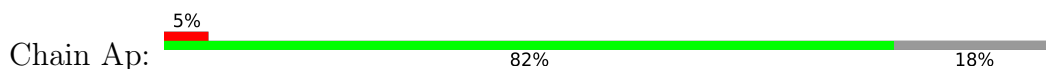
- Molecule 27: 40S ribosomal protein uS11



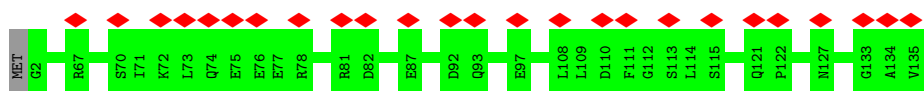
- Molecule 28: 40S ribosomal protein uS19



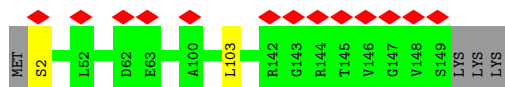
- Molecule 29: uS9



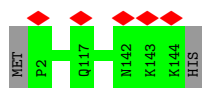
- Molecule 30: 40S ribosomal protein eS17



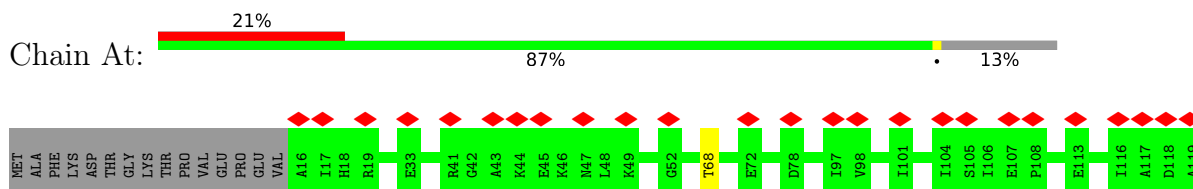
- Molecule 31: 40S ribosomal protein S18



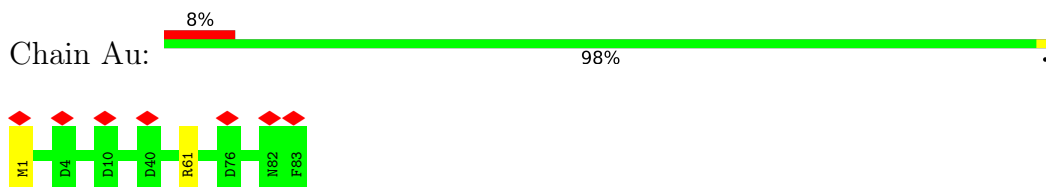
- Molecule 32: Ribosomal protein eS19



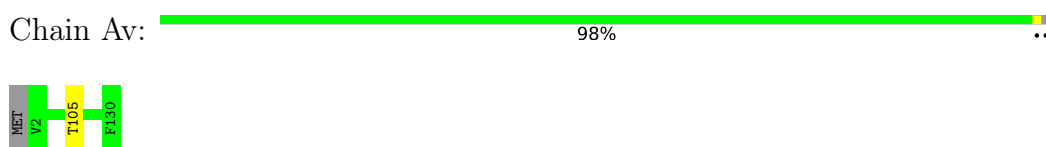
- Molecule 33: 40S ribosomal protein uS10



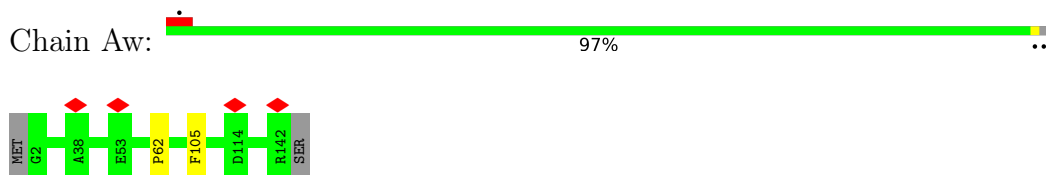
- Molecule 34: Ribosomal protein eS21



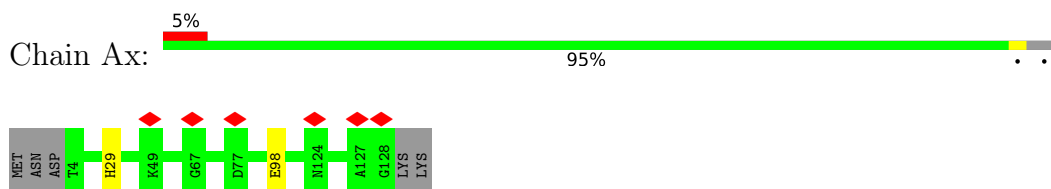
- Molecule 35: Ribosomal protein S15a



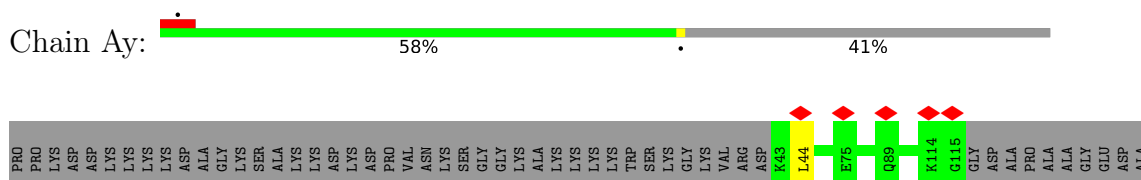
- Molecule 36: 40S ribosomal protein S23



- Molecule 37: 40S ribosomal protein S24

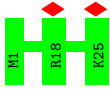


- Molecule 38: 40S ribosomal protein S25

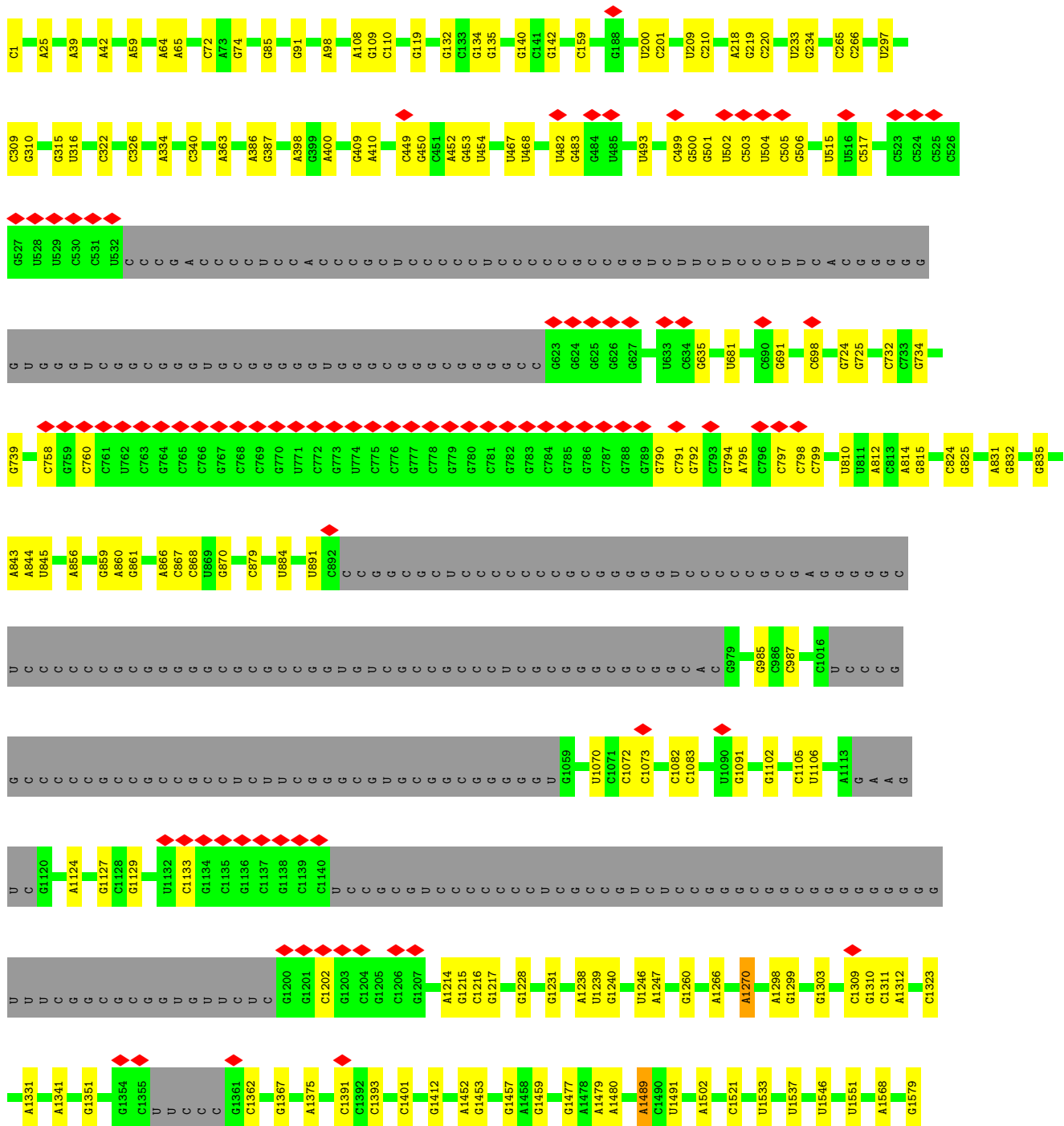


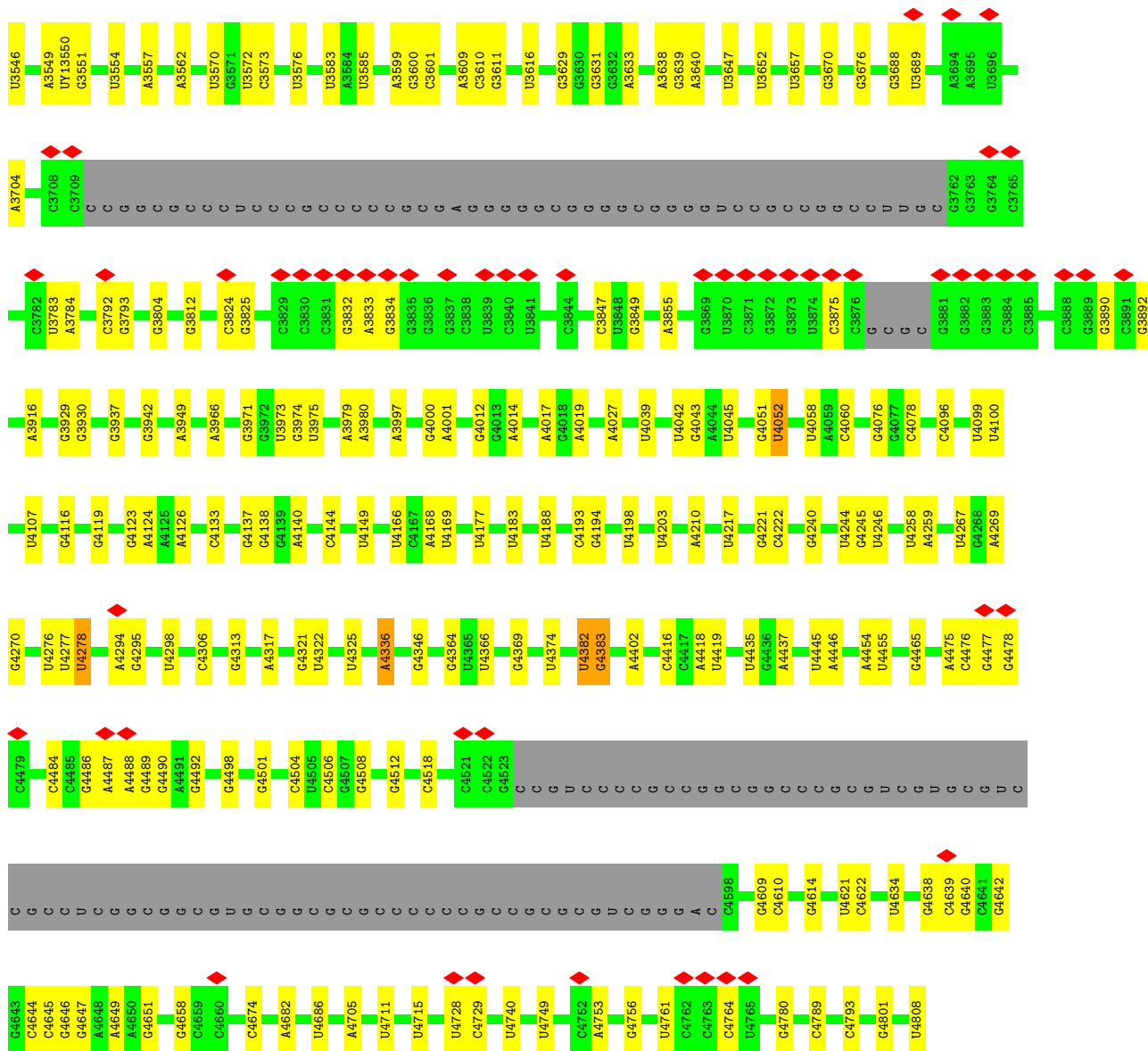
- Molecule 39: 60s ribosomal protein l41

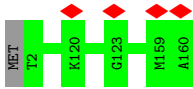




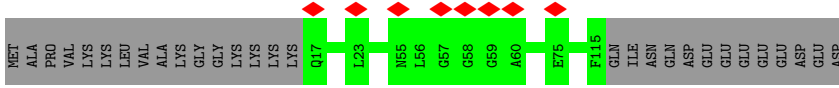
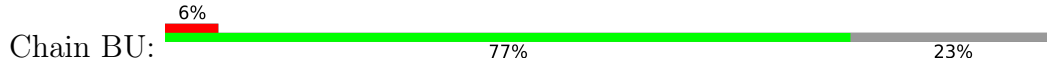
• Molecule 40: 28S rRNA



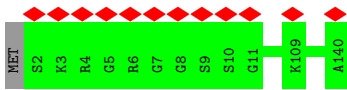




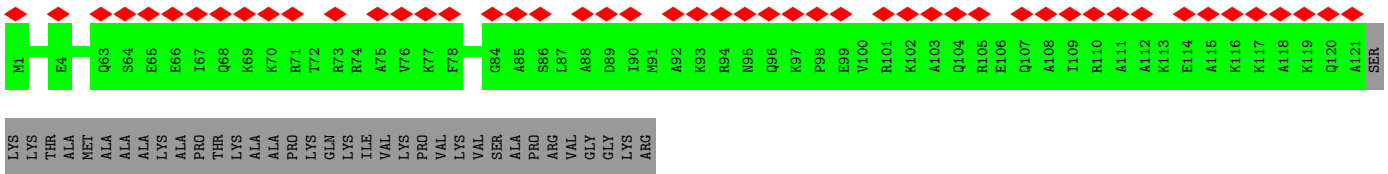
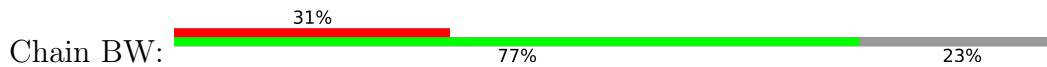
- Molecule 63: Ribosomal protein eL22



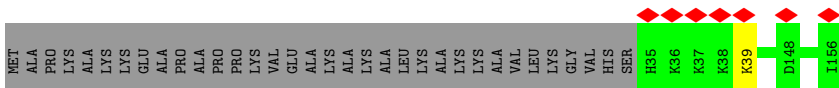
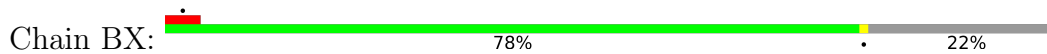
- Molecule 64: Ribosomal protein L23



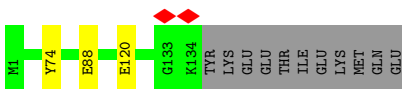
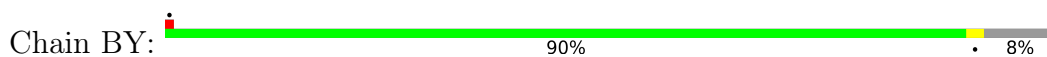
- Molecule 65: eL24



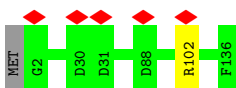
- Molecule 66: uL23



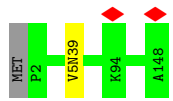
- Molecule 67: Ribosomal protein L26



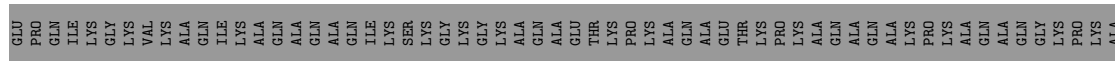
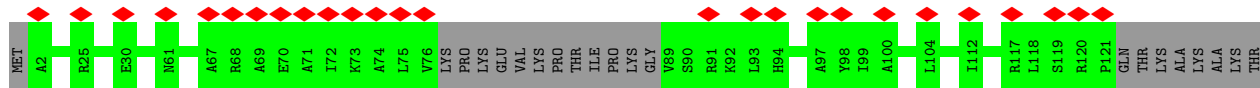
- Molecule 68: 60S ribosomal protein L27



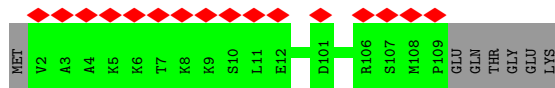
• Molecule 69: 60S ribosomal protein L27a



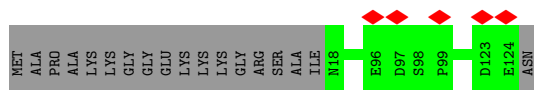
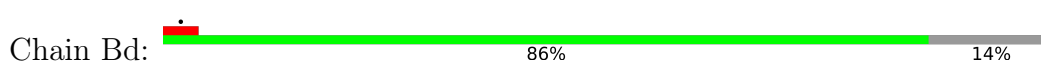
• Molecule 70: 60S ribosomal protein L29



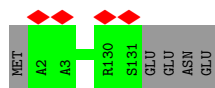
• Molecule 71: eL30



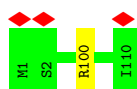
• Molecule 72: eL31



• Molecule 73: eL32



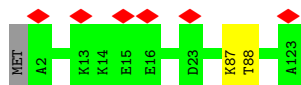
• Molecule 74: eL33



• Molecule 75: 60S ribosomal protein L34



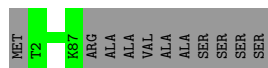
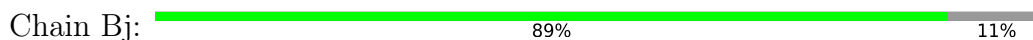
• Molecule 76: uL29



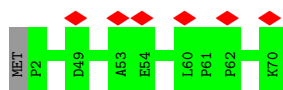
• Molecule 77: 60S ribosomal protein L36



• Molecule 78: Ribosomal protein L37



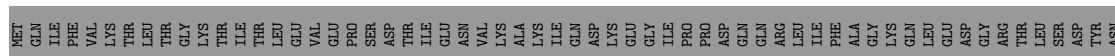
• Molecule 79: eL38

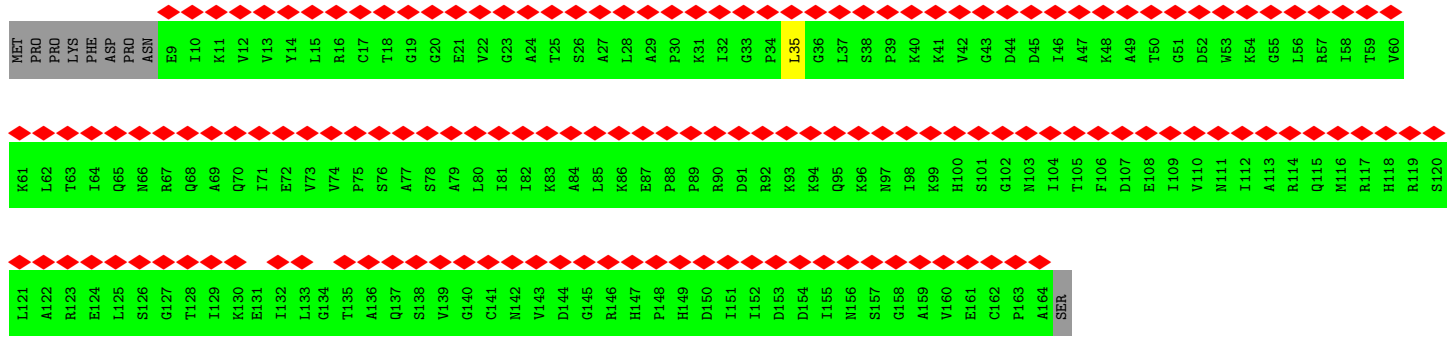


• Molecule 80: eL39

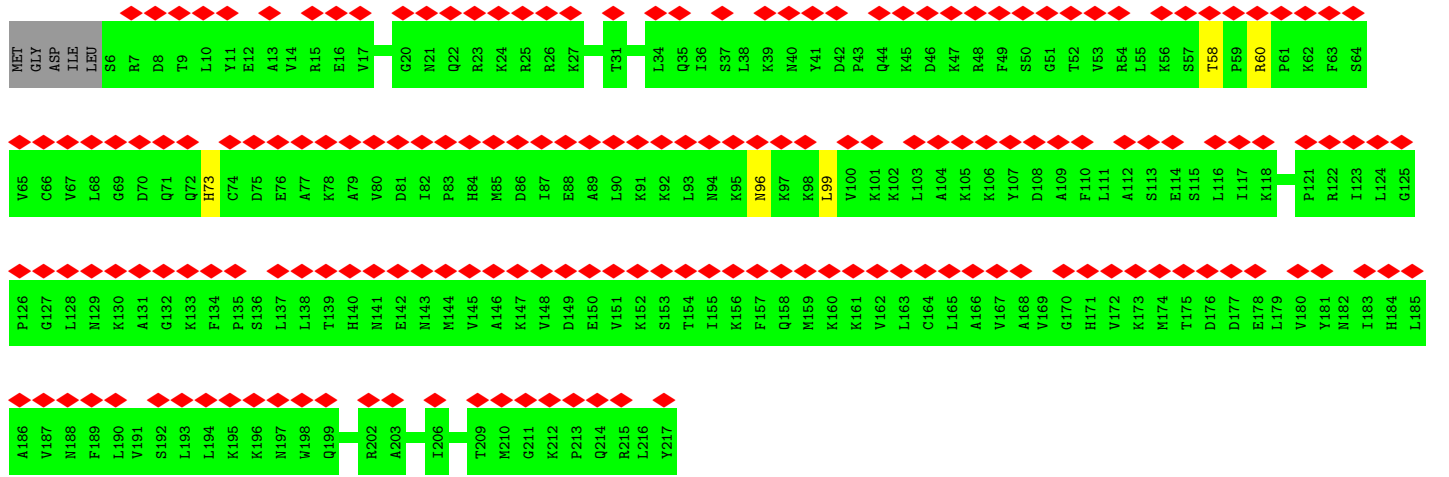
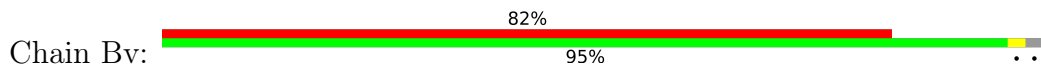


• Molecule 81: 60S ribosomal protein L40





• Molecule 87: Ribosomal protein uL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19009	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.676	Depositor
Minimum map value	-1.120	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, NMM, A2M, 5MU, AAC, SPD, M3L, 6MZ, OMU, UNX, MA6, HY3, PSU, V5N, AME, MG, AYA, MLZ, 4AC, B8N, OMG, UY1, 5MC, UR3, SAC, G7M, OMC, 1MA, HIC

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	A2	0.17	1/40342 (0.0%)	0.68	8/62877 (0.0%)
2	AA	0.24	0/665	0.45	0/891
3	AB	0.23	0/497	0.57	0/666
4	AC	0.25	0/622	0.48	0/822
5	AD	0.23	0/372	0.55	0/489
6	AE	0.24	0/828	0.53	0/1109
7	AF	0.23	0/2493	0.46	0/3394
8	AG	0.24	0/470	0.51	0/623
9	AH	0.15	0/236	0.66	0/365
10	AJ	0.28	1/1767 (0.1%)	0.65	0/2751
11	AT	0.29	1/1746 (0.1%)	0.65	0/2720
12	AU	0.24	0/871	0.46	0/1166
13	AZ	0.24	0/1771	0.46	0/2406
14	Aa	0.23	0/1765	0.45	0/2361
15	Ab	0.24	0/1742	0.45	0/2354
16	Ac	0.24	0/1779	0.49	0/2395
17	Ad	0.24	0/2118	0.49	0/2849
18	Ae	0.23	0/1531	0.47	0/2059
19	Af	0.24	0/1946	0.52	0/2590
20	Ag	0.24	0/1552	0.47	0/2079
21	Ah	0.24	0/1715	0.51	0/2287
22	Ai	0.23	0/1550	0.53	0/2069
23	Aj	0.24	0/834	0.42	0/1125
24	Ak	0.25	0/1284	0.51	0/1717
25	Al	0.23	0/968	0.42	0/1296
26	Am	0.23	0/1232	0.47	0/1656
27	An	0.24	0/1029	0.52	0/1380
28	Ao	0.24	0/1069	0.48	0/1429
29	Ap	0.24	0/1142	0.49	0/1528
30	Aq	0.24	0/1094	0.48	0/1469
31	Ar	0.23	0/1226	0.52	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	As	0.24	0/1119	0.46	0/1498
33	At	0.23	0/831	0.51	0/1115
34	Au	0.25	0/636	0.47	0/852
35	Av	0.24	0/1051	0.48	0/1406
36	Aw	0.24	0/1107	0.49	0/1475
37	Ax	0.24	0/1032	0.50	0/1371
38	Ay	0.23	0/585	0.46	0/785
39	Az	0.22	0/240	0.65	0/305
40	B5	0.18	3/87403 (0.0%)	0.67	14/136359 (0.0%)
41	B7	0.16	0/2835	0.65	0/4418
42	B8	0.24	1/3635 (0.0%)	0.66	0/5661
43	BA	0.25	0/1965	0.53	0/2633
44	BB	0.24	0/3261	0.49	0/4364
45	BC	0.24	0/2932	0.50	0/3939
46	BD	0.24	0/2437	0.47	0/3264
47	BE	0.24	0/1998	0.49	0/2673
48	BF	0.24	0/1922	0.48	0/2563
49	BG	0.24	0/1899	0.47	0/2555
50	BH	0.24	0/1535	0.49	0/2063
51	BI	0.24	0/1756	0.50	0/2346
52	BJ	0.24	0/1385	0.50	0/1852
53	BK	0.52	1/296 (0.3%)	0.49	0/402
54	BL	0.24	0/1733	0.53	0/2316
55	BM	0.24	0/1158	0.49	0/1547
56	BN	0.24	0/1746	0.54	0/2338
57	BO	0.24	0/1662	0.48	0/2222
58	BP	0.23	0/1317	0.48	0/1768
59	BQ	0.24	0/1539	0.56	0/2054
60	BR	0.23	0/1524	0.52	0/2013
61	BS	0.25	0/1497	0.52	0/2008
62	BT	0.25	0/1326	0.49	0/1770
63	BU	0.24	0/820	0.45	0/1100
64	BV	0.25	0/1048	0.52	0/1402
65	BW	0.24	0/1006	0.50	0/1334
66	BX	0.24	0/1022	0.47	0/1371
67	BY	0.23	0/1132	0.52	0/1504
68	BZ	0.25	0/1130	0.48	0/1507
69	Ba	0.24	0/1179	0.50	0/1572
70	Bb	0.23	0/884	0.50	0/1169
71	Bc	0.23	0/847	0.44	0/1134
72	Bd	0.24	0/903	0.52	0/1216
73	Be	0.23	0/1088	0.51	0/1451
74	Bf	0.25	0/903	0.53	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Bg	0.24	0/916	0.53	0/1220
76	Bh	0.23	0/1021	0.49	0/1348
77	Bi	0.23	0/841	0.52	0/1112
78	Bj	0.24	0/720	0.56	0/952
79	Bk	0.24	0/575	0.44	0/761
80	Bl	0.23	0/459	0.51	0/608
81	Bm	0.23	0/426	0.50	0/564
82	Bo	0.25	0/866	0.50	0/1141
83	Bp	0.24	0/718	0.49	0/953
84	Br	0.23	0/1020	0.53	0/1366
85	Bs	0.24	0/1530	0.45	0/2064
86	Bt	0.23	0/1193	0.47	0/1609
87	Bv	0.24	0/1735	0.45	0/2328
All	All	0.21	8/237600 (0.0%)	0.61	22/348494 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
82	Bo	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4761	U	C4-O4	12.87	1.33	1.23
11	AT	1	G	OP3-P	-10.62	1.48	1.61
42	B8	1	C	OP3-P	-10.61	1.48	1.61
40	B5	1	C	OP3-P	-10.57	1.48	1.61
1	A2	1	U	OP3-P	-10.52	1.48	1.61
10	AJ	1	G	OP3-P	-10.50	1.48	1.61
53	BK	4353	PRO	N-CD	6.94	1.57	1.47
40	B5	4761	U	N3-C4	-5.22	1.33	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4761	U	N3-C4-C5	12.14	121.89	114.60
40	B5	4761	U	C2-N3-C4	-11.53	120.08	127.00
40	B5	4761	U	C5-C4-O4	-9.57	120.16	125.90
1	A2	1454	C	C2-N1-C1'	8.64	128.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	2312	C	C2-N1-C1'	8.47	128.12	118.80
1	A2	1454	C	N1-C2-O2	8.26	123.86	118.90
40	B5	2312	C	N1-C2-O2	8.22	123.83	118.90
40	B5	4761	U	N1-C2-N3	7.29	119.27	114.90
40	B5	2312	C	N3-C2-O2	-6.53	117.33	121.90
1	A2	1454	C	N3-C2-O2	-6.49	117.36	121.90
40	B5	1594	U	C2-N1-C1'	6.22	125.16	117.70
40	B5	2252	U	C2-N1-C1'	6.00	124.90	117.70
1	A2	1454	C	C6-N1-C1'	-5.99	113.61	120.80
40	B5	2312	C	C6-N1-C1'	-5.95	113.66	120.80
1	A2	1454	C	C6-N1-C2	-5.61	118.06	120.30
1	A2	854	C	C2-N1-C1'	5.46	124.81	118.80
40	B5	4761	U	N1-C2-O2	-5.40	119.02	122.80
40	B5	1070	U	C2-N1-C1'	5.31	124.07	117.70
40	B5	2312	C	C6-N1-C2	-5.24	118.20	120.30
1	A2	1315	U	C2-N1-C1'	5.12	123.84	117.70
1	A2	1454	C	C5-C6-N1	5.05	123.53	121.00
40	B5	2252	U	N1-C2-O2	5.04	126.33	122.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	Bo	53	MLZ	Mainchain

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	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	43/133 (32%)	43 (100%)	0	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AU	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
13	AZ	219/295 (74%)	215 (98%)	4 (2%)	0	100	100
14	Aa	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
15	Ab	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
16	Ac	223/281 (79%)	221 (99%)	1 (0%)	1 (0%)	34	69
17	Ad	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
18	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
19	Af	235/249 (94%)	235 (100%)	0	0	100	100
20	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
21	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
22	Ai	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
23	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
24	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
25	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
26	Am	148/151 (98%)	148 (100%)	0	0	100	100
27	An	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
28	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
29	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
30	Aq	132/135 (98%)	132 (100%)	0	0	100	100
31	Ar	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
32	As	140/145 (97%)	140 (100%)	0	0	100	100
33	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
34	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
35	Av	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
36	Aw	138/143 (96%)	138 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Ax	123/130 (95%)	123 (100%)	0	0	100	100
38	Ay	71/124 (57%)	69 (97%)	2 (3%)	0	100	100
39	Az	23/25 (92%)	23 (100%)	0	0	100	100
43	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
44	BB	395/403 (98%)	393 (100%)	2 (0%)	0	100	100
45	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
46	BD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
47	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
48	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
49	BG	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
50	BH	188/192 (98%)	188 (100%)	0	0	100	100
51	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
52	BJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
53	BK	37/1071 (4%)	32 (86%)	4 (11%)	1 (3%)	5	25
54	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
55	BM	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
56	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
57	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
58	BP	157/184 (85%)	154 (98%)	3 (2%)	0	100	100
59	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
60	BR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
61	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
62	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
63	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
64	BV	137/140 (98%)	137 (100%)	0	0	100	100
65	BW	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
66	BX	120/156 (77%)	119 (99%)	1 (1%)	0	100	100
67	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
68	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
69	Ba	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
70	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	Bc	106/115 (92%)	106 (100%)	0	0	100	100
72	Bd	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
73	Be	128/135 (95%)	128 (100%)	0	0	100	100
74	Bf	108/110 (98%)	108 (100%)	0	0	100	100
75	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
76	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
77	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
78	Bj	84/97 (87%)	84 (100%)	0	0	100	100
79	Bk	67/70 (96%)	67 (100%)	0	0	100	100
80	Bl	48/51 (94%)	48 (100%)	0	0	100	100
81	Bm	49/128 (38%)	49 (100%)	0	0	100	100
82	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
83	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
84	Br	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
85	Bs	194/318 (61%)	187 (96%)	7 (4%)	0	100	100
86	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
87	Bv	210/217 (97%)	204 (97%)	6 (3%)	0	100	100
All	All	12026/15056 (80%)	11848 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Ac	211	VAL
53	BK	4388	GLU

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	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AB	56/62 (90%)	56 (100%)	0	100	100
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	38/106 (36%)	37 (97%)	1 (3%)	46	74
6	AE	88/98 (90%)	88 (100%)	0	100	100
7	AF	272/275 (99%)	269 (99%)	3 (1%)	73	89
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AU	92/121 (76%)	89 (97%)	3 (3%)	38	69
13	AZ	182/243 (75%)	180 (99%)	2 (1%)	73	89
14	Aa	195/231 (84%)	192 (98%)	3 (2%)	65	85
15	Ab	185/223 (83%)	181 (98%)	4 (2%)	52	78
16	Ac	189/232 (82%)	187 (99%)	2 (1%)	73	89
17	Ad	224/225 (100%)	223 (100%)	1 (0%)	91	96
18	Ae	161/170 (95%)	161 (100%)	0	100	100
19	Af	207/218 (95%)	206 (100%)	1 (0%)	88	94
20	Ag	170/360 (47%)	168 (99%)	2 (1%)	71	88
21	Ah	178/180 (99%)	178 (100%)	0	100	100
22	Ai	161/168 (96%)	159 (99%)	2 (1%)	71	88
23	Aj	87/136 (64%)	87 (100%)	0	100	100
24	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	93
25	Al	104/108 (96%)	99 (95%)	5 (5%)	25	58
26	Am	130/131 (99%)	129 (99%)	1 (1%)	81	92
27	An	106/119 (89%)	105 (99%)	1 (1%)	78	91
28	Ao	114/130 (88%)	114 (100%)	0	100	100
29	Ap	117/140 (84%)	117 (100%)	0	100	100
30	Aq	120/121 (99%)	120 (100%)	0	100	100
31	Ar	127/131 (97%)	126 (99%)	1 (1%)	81	92
32	As	112/114 (98%)	112 (100%)	0	100	100
33	At	94/107 (88%)	93 (99%)	1 (1%)	73	89
34	Au	67/67 (100%)	66 (98%)	1 (2%)	65	85
35	Av	112/113 (99%)	111 (99%)	1 (1%)	78	91
36	Aw	112/114 (98%)	111 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Ax	107/112 (96%)	105 (98%)	2 (2%)	57	81
38	Ay	64/102 (63%)	63 (98%)	1 (2%)	62	84
39	Az	24/24 (100%)	24 (100%)	0	100	100
43	BA	194/198 (98%)	193 (100%)	1 (0%)	88	94
44	BB	344/347 (99%)	343 (100%)	1 (0%)	92	96
45	BC	302/337 (90%)	301 (100%)	1 (0%)	92	96
46	BD	247/250 (99%)	247 (100%)	0	100	100
47	BE	216/251 (86%)	214 (99%)	2 (1%)	78	91
48	BF	197/215 (92%)	197 (100%)	0	100	100
49	BG	198/223 (89%)	198 (100%)	0	100	100
50	BH	169/171 (99%)	169 (100%)	0	100	100
51	BI	180/181 (99%)	179 (99%)	1 (1%)	86	94
52	BJ	143/149 (96%)	143 (100%)	0	100	100
53	BK	34/936 (4%)	31 (91%)	3 (9%)	10	36
54	BL	175/176 (99%)	170 (97%)	5 (3%)	42	72
55	BM	117/161 (73%)	116 (99%)	1 (1%)	78	91
56	BN	171/172 (99%)	171 (100%)	0	100	100
57	BO	171/173 (99%)	170 (99%)	1 (1%)	86	94
58	BP	140/163 (86%)	139 (99%)	1 (1%)	84	93
59	BQ	164/165 (99%)	164 (100%)	0	100	100
60	BR	159/175 (91%)	158 (99%)	1 (1%)	86	94
61	BS	154/154 (100%)	153 (99%)	1 (1%)	86	94
62	BT	139/140 (99%)	139 (100%)	0	100	100
63	BU	88/113 (78%)	88 (100%)	0	100	100
64	BV	106/107 (99%)	106 (100%)	0	100	100
65	BW	100/126 (79%)	100 (100%)	0	100	100
66	BX	110/134 (82%)	109 (99%)	1 (1%)	78	91
67	BY	124/135 (92%)	121 (98%)	3 (2%)	49	76
68	BZ	117/118 (99%)	116 (99%)	1 (1%)	78	91
69	Ba	118/119 (99%)	118 (100%)	0	100	100
70	Bb	87/183 (48%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Bc	92/98 (94%)	92 (100%)	0	100	100
72	Bd	98/110 (89%)	98 (100%)	0	100	100
73	Be	116/121 (96%)	116 (100%)	0	100	100
74	Bf	89/89 (100%)	88 (99%)	1 (1%)	73	89
75	Bg	98/100 (98%)	97 (99%)	1 (1%)	76	90
76	Bh	109/110 (99%)	107 (98%)	2 (2%)	59	82
77	Bi	86/89 (97%)	84 (98%)	2 (2%)	50	77
78	Bj	73/80 (91%)	73 (100%)	0	100	100
79	Bk	64/65 (98%)	64 (100%)	0	100	100
80	Bl	47/48 (98%)	46 (98%)	1 (2%)	53	79
81	Bm	47/115 (41%)	47 (100%)	0	100	100
82	Bo	92/93 (99%)	91 (99%)	1 (1%)	73	89
83	Bp	74/75 (99%)	74 (100%)	0	100	100
84	Br	109/120 (91%)	109 (100%)	0	100	100
85	Bs	164/258 (64%)	163 (99%)	1 (1%)	86	94
86	Bt	128/137 (93%)	127 (99%)	1 (1%)	81	92
87	Bv	191/195 (98%)	186 (97%)	5 (3%)	46	74
All	All	10465/12763 (82%)	10385 (99%)	80 (1%)	82	92

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
5	AD	120	VAL
7	AF	113	PHE
7	AF	143	GLN
7	AF	159	ASN
12	AU	55	THR
12	AU	73	VAL
12	AU	126	ARG
13	AZ	121	LEU
13	AZ	206	ASP
14	Aa	170	GLU
14	Aa	178	THR
14	Aa	219	LYS
15	Ab	79	GLU

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Mol	Chain	Res	Type
15	Ab	121	ARG
15	Ab	236	PHE
15	Ab	248	TYR
16	Ac	46	THR
16	Ac	105	LEU
17	Ad	139	LEU
19	Af	7	PHE
20	Ag	18	GLU
20	Ag	109	ARG
22	Ai	41	ARG
22	Ai	70	ARG
24	Ak	69	ARG
25	Al	33	ARG
25	Al	72	HIS
25	Al	75	ASN
25	Al	91	LEU
25	Al	104	VAL
26	Am	80	LEU
27	An	100	THR
31	Ar	103	LEU
33	At	68	THR
34	Au	61	ARG
35	Av	105	THR
36	Aw	105	PHE
37	Ax	29	HIS
37	Ax	98	GLU
38	Ay	44	LEU
43	BA	246	LEU
44	BB	340	THR
45	BC	122	TYR
47	BE	107	THR
47	BE	109	VAL
51	BI	38	ARG
53	BK	4377	LYS
53	BK	4386	LEU
53	BK	4390	MET
54	BL	63	THR
54	BL	67	HIS
54	BL	115	GLN
54	BL	129	ARG
54	BL	200	LYS
55	BM	126	GLU

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Mol	Chain	Res	Type
57	BO	117	ARG
58	BP	140	MET
60	BR	106	LEU
61	BS	6	THR
66	BX	39	LYS
67	BY	74	TYR
67	BY	88	GLU
67	BY	120	GLU
68	BZ	102	ARG
74	Bf	100	ARG
75	Bg	73	HIS
76	Bh	87	LYS
76	Bh	88	THR
77	Bi	29	ARG
77	Bi	35	LYS
80	Bl	47	THR
82	Bo	97	LYS
85	Bs	61	MET
86	Bt	35	LEU
87	Bv	58	THR
87	Bv	60	ARG
87	Bv	73	HIS
87	Bv	96	ASN
87	Bv	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	19	HIS
2	AA	29	ASN
2	AA	51	GLN
5	AD	89	GLN
7	AF	62	HIS
7	AF	159	ASN
7	AF	296	GLN
8	AG	16	GLN
8	AG	37	ASN
12	AU	51	GLN
12	AU	86	GLN
13	AZ	113	GLN
13	AZ	193	HIS
15	Ab	178	HIS

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Mol	Chain	Res	Type
17	Ad	98	ASN
17	Ad	142	HIS
18	Ae	65	GLN
20	Ag	68	GLN
20	Ag	91	HIS
21	Ah	7	ASN
21	Ah	165	GLN
21	Ah	167	GLN
23	Aj	77	GLN
24	Ak	11	GLN
25	Al	28	HIS
26	Am	5	HIS
26	Am	36	GLN
27	An	113	GLN
28	Ao	103	ASN
29	Ap	80	GLN
29	Ap	86	GLN
29	Ap	97	GLN
30	Aq	121	GLN
32	As	12	GLN
34	Au	2	GLN
36	Aw	23	HIS
36	Aw	39	ASN
36	Aw	110	HIS
37	Ax	19	GLN
37	Ax	85	ASN
37	Ax	89	HIS
43	BA	50	HIS
43	BA	139	HIS
43	BA	140	ASN
44	BB	184	GLN
45	BC	38	ASN
45	BC	48	ASN
45	BC	61	GLN
46	BD	122	GLN
46	BD	202	GLN
47	BE	131	HIS
48	BF	57	HIS
49	BG	43	GLN
49	BG	64	GLN
49	BG	81	ASN
50	BH	42	ASN

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Mol	Chain	Res	Type
51	BI	59	GLN
51	BI	163	GLN
51	BI	166	HIS
52	BJ	112	HIS
53	BK	4385	GLN
55	BM	33	GLN
55	BM	34	ASN
57	BO	180	GLN
58	BP	75	GLN
60	BR	39	GLN
60	BR	40	GLN
61	BS	125	GLN
61	BS	173	ASN
62	BT	131	GLN
63	BU	17	GLN
63	BU	38	ASN
65	BW	63	GLN
65	BW	120	GLN
66	BX	107	HIS
67	BY	14	ASN
67	BY	56	GLN
69	Ba	60	HIS
69	Ba	62	HIS
69	Ba	66	ASN
70	Bb	50	ASN
71	Bc	33	GLN
75	Bg	112	GLN
75	Bg	114	GLN
78	Bj	13	ASN
80	Bl	4	HIS
82	Bo	102	GLN
83	Bp	92	GLN
84	Br	4	HIS
84	Br	6	GLN
85	Bs	34	ASN
85	Bs	41	GLN
85	Bs	58	ASN
85	Bs	179	ASN
86	Bt	70	GLN
86	Bt	100	HIS
87	Bv	96	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	241 (13%)	2 (0%)
10	AJ	75/76 (98%)	14 (18%)	0
11	AT	74/75 (98%)	12 (16%)	0
40	B5	3750/4808 (77%)	475 (12%)	2 (0%)
41	B7	118/120 (98%)	8 (6%)	0
42	B8	155/158 (98%)	15 (9%)	0
9	AH	9/217 (4%)	1 (11%)	0
All	All	5939/7324 (81%)	766 (12%)	4 (0%)

All (766) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C
1	A2	26	U
1	A2	33	G
1	A2	41	G
1	A2	44	U
1	A2	46	A
1	A2	56	G
1	A2	58	C
1	A2	67	C
1	A2	68	A
1	A2	73	C
1	A2	74	G
1	A2	76	U
1	A2	77	A
1	A2	79	A
1	A2	103	A
1	A2	113	G
1	A2	115	U
1	A2	126	G
1	A2	129	C
1	A2	130	G
1	A2	143	U
1	A2	147	A
1	A2	155	G
1	A2	158	A
1	A2	168	C
1	A2	178	C

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Mol	Chain	Res	Type
1	A2	180	G
1	A2	184	G
1	A2	188	C
1	A2	189	U
1	A2	190	G
1	A2	192	C
1	A2	204	G
1	A2	226	A
1	A2	227	U
1	A2	228	C
1	A2	283	G
1	A2	287	U
1	A2	288	U
1	A2	303	A
1	A2	306	U
1	A2	308	G
1	A2	310	G
1	A2	313	G
1	A2	321	G
1	A2	324	C
1	A2	325	U
1	A2	327	C
1	A2	328	G
1	A2	333	G
1	A2	334	G
1	A2	348	G
1	A2	363	C
1	A2	365	A
1	A2	369	U
1	A2	370	C
1	A2	386	G
1	A2	387	C
1	A2	401	C
1	A2	410	C
1	A2	417	U
1	A2	449	A
1	A2	450	A
1	A2	451	C
1	A2	465	A
1	A2	472	G
1	A2	473	C
1	A2	474	A

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Mol	Chain	Res	Type
1	A2	475	G
1	A2	477	A
1	A2	483	G
1	A2	488	U
1	A2	493	C
1	A2	494	A
1	A2	502	C
1	A2	509	A
1	A2	535	G
1	A2	537	A
1	A2	544	C
1	A2	545	G
1	A2	556	A
1	A2	557	U
1	A2	565	A
1	A2	577	A2M
1	A2	588	A
1	A2	590	G
1	A2	592	U
1	A2	607	G
1	A2	609	C
1	A2	615	C
1	A2	629	A
1	A2	632	U
1	A2	644	A
1	A2	645	OMG
1	A2	656	A
1	A2	661	C
1	A2	669	A2M
1	A2	670	A
1	A2	672	A
1	A2	673	A
1	A2	674	G
1	A2	689	U
1	A2	697	G
1	A2	746	C
1	A2	747	C
1	A2	749	C
1	A2	754	C
1	A2	755	G
1	A2	757	C
1	A2	759	C

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Mol	Chain	Res	Type
1	A2	789	G
1	A2	800	U
1	A2	809	A
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G
1	A2	837	G
1	A2	838	A
1	A2	839	G
1	A2	840	C
1	A2	841	C
1	A2	842	G
1	A2	848	A
1	A2	870	A
1	A2	871	A
1	A2	872	U
1	A2	873	A
1	A2	879	G
1	A2	892	G
1	A2	902	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
1	A2	931	C
1	A2	934	G
1	A2	944	U
1	A2	956	A
1	A2	957	G
1	A2	964	A
1	A2	971	G
1	A2	972	G
1	A2	986	G
1	A2	991	A
1	A2	993	A
1	A2	1000	G
1	A2	1003	U
1	A2	1024	A
1	A2	1062	U
1	A2	1063	A

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Mol	Chain	Res	Type
1	A2	1084	A
1	A2	1086	C
1	A2	1116	U
1	A2	1117	C
1	A2	1118	C
1	A2	1119	C
1	A2	1122	G
1	A2	1134	A
1	A2	1145	A
1	A2	1154	C
1	A2	1155	U
1	A2	1196	A
1	A2	1216	C
1	A2	1243	U
1	A2	1252	A
1	A2	1254	A
1	A2	1257	G
1	A2	1258	G
1	A2	1260	A
1	A2	1272	C
1	A2	1275	G
1	A2	1276	G
1	A2	1303	G
1	A2	1304	C
1	A2	1316	U
1	A2	1343	U
1	A2	1359	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1398	U
1	A2	1406	A
1	A2	1407	G
1	A2	1419	C
1	A2	1420	C
1	A2	1422	A
1	A2	1424	C
1	A2	1436	C
1	A2	1448	OMG
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U

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Mol	Chain	Res	Type
1	A2	1481	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1495	U
1	A2	1498	G
1	A2	1522	C
1	A2	1523	A
1	A2	1534	A
1	A2	1545	C
1	A2	1553	G
1	A2	1554	C
1	A2	1579	U
1	A2	1580	A
1	A2	1581	A
1	A2	1589	A
1	A2	1602	A
1	A2	1605	G
1	A2	1622	U
1	A2	1624	A
1	A2	1647	C
1	A2	1655	G
1	A2	1662	A
1	A2	1666	G
1	A2	1681	G
1	A2	1699	C
1	A2	1700	A
1	A2	1722	U
1	A2	1723	G
1	A2	1730	U
1	A2	1749	G
1	A2	1783	G
1	A2	1784	C
1	A2	1785	G
1	A2	1825	A
1	A2	1830	G
1	A2	1836	A
1	A2	1837	G
1	A2	1839	U
1	A2	1850	G
1	A2	1862	G
1	A2	1863	G
1	A2	1864	A

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Mol	Chain	Res	Type
1	A2	1865	U
1	A2	1866	C
9	AH	3430	C
10	AJ	5	U
10	AJ	9	A
10	AJ	17	A
10	AJ	18	G
10	AJ	19	G
10	AJ	20	C
10	AJ	21	A
10	AJ	22	G
10	AJ	36	U
10	AJ	46	G
10	AJ	48	C
10	AJ	49	C
10	AJ	73	A
10	AJ	74	C
11	AT	9	G
11	AT	16	G
11	AT	17	G
11	AT	18	G
11	AT	19	U
11	AT	20	A
11	AT	45	G
11	AT	46	U
11	AT	47	C
11	AT	48	C
11	AT	58	A
11	AT	75	A
40	B5	25	A
40	B5	39	A
40	B5	42	A
40	B5	59	A
40	B5	64	A
40	B5	65	A
40	B5	72	C
40	B5	74	G
40	B5	85	G
40	B5	91	G
40	B5	98	A
40	B5	108	A
40	B5	109	G

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Mol	Chain	Res	Type
40	B5	110	C
40	B5	119	G
40	B5	132	G
40	B5	134	G
40	B5	135	G
40	B5	140	G
40	B5	142	G
40	B5	159	C
40	B5	200	U
40	B5	201	C
40	B5	209	U
40	B5	210	C
40	B5	218	A
40	B5	219	G
40	B5	220	C
40	B5	233	U
40	B5	234	G
40	B5	265	C
40	B5	266	C
40	B5	297	U
40	B5	309	C
40	B5	310	G
40	B5	315	G
40	B5	316	U
40	B5	322	C
40	B5	326	C
40	B5	334	A
40	B5	340	C
40	B5	363	A
40	B5	386	A
40	B5	387	G
40	B5	409	G
40	B5	410	A
40	B5	449	C
40	B5	450	G
40	B5	452	A
40	B5	453	G
40	B5	454	U
40	B5	467	U
40	B5	468	U
40	B5	482	U
40	B5	483	G

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Mol	Chain	Res	Type
40	B5	493	U
40	B5	499	C
40	B5	500	G
40	B5	501	G
40	B5	502	U
40	B5	503	C
40	B5	504	U
40	B5	505	C
40	B5	506	G
40	B5	515	U
40	B5	517	C
40	B5	635	G
40	B5	681	U
40	B5	691	G
40	B5	698	C
40	B5	724	G
40	B5	725	G
40	B5	732	C
40	B5	734	G
40	B5	739	G
40	B5	758	C
40	B5	760	C
40	B5	790	G
40	B5	791	C
40	B5	792	G
40	B5	794	G
40	B5	795	A
40	B5	797	C
40	B5	798	C
40	B5	799	C
40	B5	810	U
40	B5	812	A
40	B5	814	A
40	B5	815	G
40	B5	824	C
40	B5	825	G
40	B5	831	A
40	B5	832	G
40	B5	835	G
40	B5	843	A
40	B5	844	A
40	B5	845	U

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Mol	Chain	Res	Type
40	B5	856	A
40	B5	859	G
40	B5	860	A
40	B5	861	G
40	B5	866	A
40	B5	867	C
40	B5	868	C
40	B5	870	G
40	B5	879	C
40	B5	884	U
40	B5	891	U
40	B5	985	G
40	B5	987	C
40	B5	1072	C
40	B5	1073	C
40	B5	1082	C
40	B5	1083	C
40	B5	1091	G
40	B5	1102	G
40	B5	1105	C
40	B5	1106	U
40	B5	1124	A
40	B5	1127	G
40	B5	1129	G
40	B5	1133	C
40	B5	1202	C
40	B5	1214	A
40	B5	1215	G
40	B5	1216	C
40	B5	1217	G
40	B5	1228	G
40	B5	1231	G
40	B5	1238	A
40	B5	1239	U
40	B5	1240	G
40	B5	1246	U
40	B5	1247	A
40	B5	1270	A2M
40	B5	1298	A
40	B5	1299	G
40	B5	1303	G
40	B5	1309	C

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Mol	Chain	Res	Type
40	B5	1310	G
40	B5	1311	C
40	B5	1312	A
40	B5	1323	C
40	B5	1331	A
40	B5	1341	A
40	B5	1351	G
40	B5	1362	C
40	B5	1367	G
40	B5	1375	A
40	B5	1391	C
40	B5	1393	C
40	B5	1401	C
40	B5	1412	G
40	B5	1452	A
40	B5	1453	G
40	B5	1457	G
40	B5	1459	G
40	B5	1480	A
40	B5	1489	A2M
40	B5	1502	A
40	B5	1521	C
40	B5	1533	U
40	B5	1546	U
40	B5	1551	U
40	B5	1568	A
40	B5	1579	G
40	B5	1580	OMG
40	B5	1586	A
40	B5	1588	G
40	B5	1589	A
40	B5	1609	G
40	B5	1616	C
40	B5	1631	C
40	B5	1632	PSU
40	B5	1646	G
40	B5	1653	C
40	B5	1657	C
40	B5	1658	C
40	B5	1694	C
40	B5	1695	U
40	B5	1700	G

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Mol	Chain	Res	Type
40	B5	1704	A
40	B5	1705	A
40	B5	1707	C
40	B5	1720	PSU
40	B5	1726	A
40	B5	1743	A
40	B5	1745	G
40	B5	1754	G
40	B5	1767	C
40	B5	1774	G
40	B5	1775	G
40	B5	1776	A
40	B5	1781	G
40	B5	1794	G
40	B5	1808	G
40	B5	1831	A
40	B5	1832	C
40	B5	1836	A
40	B5	1857	U
40	B5	1859	C
40	B5	1860	C
40	B5	1861	G
40	B5	1870	C
40	B5	1871	A
40	B5	1879	G
40	B5	1887	G
40	B5	1890	G
40	B5	1898	U
40	B5	1899	A
40	B5	1900	G
40	B5	1913	U
40	B5	1914	G
40	B5	1922	A
40	B5	1923	A
40	B5	1924	G
40	B5	1925	U
40	B5	1926	C
40	B5	1936	U
40	B5	1940	G
40	B5	1942	G
40	B5	1943	U
40	B5	1963	G

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Mol	Chain	Res	Type
40	B5	1965	A
40	B5	1985	G
40	B5	1987	U
40	B5	1994	G
40	B5	1995	G
40	B5	2008	A
40	B5	2023	U
40	B5	2024	G
40	B5	2032	G
40	B5	2034	A
40	B5	2037	G
40	B5	2041	G
40	B5	2043	A
40	B5	2044	A
40	B5	2045	G
40	B5	2046	A
40	B5	2101	C
40	B5	2132	C
40	B5	2143	A
40	B5	2144	G
40	B5	2156	A
40	B5	2157	G
40	B5	2191	G
40	B5	2194	OMC
40	B5	2203	A
40	B5	2207	OMG
40	B5	2238	A
40	B5	2240	G
40	B5	2242	G
40	B5	2264	G
40	B5	2268	U
40	B5	2269	U
40	B5	2296	A
40	B5	2318	G
40	B5	2331	C
40	B5	2332	C
40	B5	2338	U
40	B5	2346	G
40	B5	2349	G
40	B5	2356	A
40	B5	2372	A
40	B5	2380	A

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Mol	Chain	Res	Type
40	B5	2386	A
40	B5	2387	G
40	B5	2388	U
40	B5	2390	G
40	B5	2397	U
40	B5	2409	G
40	B5	2416	A
40	B5	2429	G
40	B5	2430	A
40	B5	2444	A
40	B5	2483	G
40	B5	2496	C
40	B5	2503	A
40	B5	2504	U
40	B5	2512	C
40	B5	2530	U
40	B5	2537	G
40	B5	2538	A
40	B5	2539	A
40	B5	2551	U
40	B5	2552	C
40	B5	2554	G
40	B5	2564	G
40	B5	2586	A
40	B5	2606	U
40	B5	2612	U
40	B5	2630	A2M
40	B5	2631	U
40	B5	2633	U
40	B5	2641	A
40	B5	2649	A
40	B5	2657	C
40	B5	2669	U
40	B5	2670	G
40	B5	2672	U
40	B5	2698	G
40	B5	2745	G
40	B5	3329	G
40	B5	3350	C
40	B5	3358	G
40	B5	3367	A
40	B5	3380	A

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Mol	Chain	Res	Type
40	B5	3385	A
40	B5	3394	A
40	B5	3405	C
40	B5	3428	C
40	B5	3441	U
40	B5	3442	G
40	B5	3444	A
40	B5	3445	U
40	B5	3478	A
40	B5	3493	C
40	B5	3498	A
40	B5	3506	A
40	B5	3507	A
40	B5	3508	G
40	B5	3509	G
40	B5	3510	U
40	B5	3516	A
40	B5	3541	G
40	B5	3542	C
40	B5	3543	G
40	B5	3546	U
40	B5	3549	A
40	B5	3551	G
40	B5	3570	U
40	B5	3572	U
40	B5	3600	G
40	B5	3609	A
40	B5	3610	C
40	B5	3611	G
40	B5	3629	G
40	B5	3633	A
40	B5	3638	A
40	B5	3639	G
40	B5	3640	A
40	B5	3647	U
40	B5	3670	G
40	B5	3688	G
40	B5	3689	U
40	B5	3704	A
40	B5	3783	U
40	B5	3784	A
40	B5	3792	C

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Mol	Chain	Res	Type
40	B5	3793	G
40	B5	3804	G
40	B5	3812	G
40	B5	3824	C
40	B5	3825	G
40	B5	3832	G
40	B5	3833	A
40	B5	3834	G
40	B5	3847	C
40	B5	3849	G
40	B5	3855	A
40	B5	3875	C
40	B5	3890	G
40	B5	3892	G
40	B5	3916	A
40	B5	3929	G
40	B5	3930	G
40	B5	3937	G
40	B5	3949	A
40	B5	3971	G
40	B5	3975	U
40	B5	3979	A
40	B5	3980	A
40	B5	3997	A
40	B5	4000	G
40	B5	4001	A
40	B5	4012	G
40	B5	4014	A
40	B5	4017	A
40	B5	4019	A
40	B5	4027	A
40	B5	4043	G
40	B5	4051	G
40	B5	4052	OMU
40	B5	4060	C
40	B5	4076	G
40	B5	4078	C
40	B5	4096	C
40	B5	4100	U
40	B5	4119	G
40	B5	4123	G
40	B5	4124	A

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Mol	Chain	Res	Type
40	B5	4126	A
40	B5	4133	C
40	B5	4137	G
40	B5	4140	A
40	B5	4144	C
40	B5	4168	A
40	B5	4183	U
40	B5	4194	G
40	B5	4198	U
40	B5	4210	A
40	B5	4221	G
40	B5	4222	C
40	B5	4258	U
40	B5	4259	A
40	B5	4270	G
40	B5	4277	U
40	B5	4278	PSU
40	B5	4294	A
40	B5	4295	G
40	B5	4306	C
40	B5	4313	G
40	B5	4321	G
40	B5	4336	A2M
40	B5	4346	G
40	B5	4382	PSU
40	B5	4383	OMG
40	B5	4402	A
40	B5	4416	C
40	B5	4418	A
40	B5	4437	A
40	B5	4446	A
40	B5	4454	A
40	B5	4455	U
40	B5	4465	G
40	B5	4475	A
40	B5	4476	C
40	B5	4477	G
40	B5	4478	G
40	B5	4484	C
40	B5	4486	G
40	B5	4487	A
40	B5	4488	A

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Mol	Chain	Res	Type
40	B5	4489	G
40	B5	4490	G
40	B5	4492	G
40	B5	4498	G
40	B5	4501	G
40	B5	4504	C
40	B5	4506	C
40	B5	4508	G
40	B5	4512	G
40	B5	4518	C
40	B5	4609	G
40	B5	4610	C
40	B5	4614	G
40	B5	4621	U
40	B5	4622	C
40	B5	4634	U
40	B5	4638	G
40	B5	4639	C
40	B5	4640	G
40	B5	4642	G
40	B5	4644	C
40	B5	4645	C
40	B5	4646	G
40	B5	4647	G
40	B5	4649	A
40	B5	4651	G
40	B5	4658	G
40	B5	4674	C
40	B5	4682	A
40	B5	4686	U
40	B5	4705	A
40	B5	4715	U
40	B5	4728	U
40	B5	4729	C
40	B5	4753	A
40	B5	4756	G
40	B5	4764	C
40	B5	4780	G
40	B5	4789	C
40	B5	4793	C
40	B5	4801	G
40	B5	4808	U

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Mol	Chain	Res	Type
41	B7	7	G
41	B7	53	U
41	B7	54	A
41	B7	63	C
41	B7	64	G
41	B7	102	U
41	B7	110	G
41	B7	120	U
42	B8	23	C
42	B8	34	U
42	B8	35	C
42	B8	59	A
42	B8	62	A
42	B8	63	U
42	B8	81	C
42	B8	84	A
42	B8	87	G
42	B8	94	G
42	B8	103	A
42	B8	105	C
42	B8	110	U
42	B8	114	G
42	B8	127	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	745	G
1	A2	871	A
40	B5	4294	A
40	B5	4445	U

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	B5	1632	40	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
40	1MA	B5	1266	40,88	16,25,26	1.55	2 (12%)	18,37,40	1.06	3 (16%)
40	A2M	B5	1489	40,88	18,25,26	0.99	1 (5%)	18,36,39	1.34	2 (11%)
1	PSU	A2	1644	1,88	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	OMC	A2	518	1	19,22,23	0.82	0	26,31,34	0.83	0
40	OMU	B5	4366	40	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
40	PSU	B5	1801	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	119	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
69	V5N	Ba	39	69	4,11,12	0.76	0	5,14,16	1.54	1 (20%)
1	PSU	A2	967	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
32	NMM	As	67	32	9,11,12	0.59	0	6,12,14	0.40	0
40	OMG	B5	2267	40	18,26,27	0.91	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	A2	1233	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.89	1 (3%)
40	A2M	B5	4336	40	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
11	5MU	AT	53	11	19,22,23	1.42	6 (31%)	28,32,35	2.07	7 (25%)
40	OMC	B5	2208	40	19,22,23	0.80	0	26,31,34	0.77	0
40	A2M	B5	3450	40	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	A2	823	1	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
40	OMG	B5	2207	40	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
40	OMU	B5	2680	40	19,22,23	1.21	2 (10%)	26,31,34	1.71	5 (19%)
1	A2M	A2	669	1,88	18,25,26	0.98	1 (5%)	18,36,39	1.35	2 (11%)
40	PSU	B5	3502	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	A2M	B5	400	40	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	A2M	A2	99	1,88	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
1	OMU	A2	172	1	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
1	A2M	A2	513	1	18,25,26	1.01	1 (5%)	18,36,39	1.19	2 (11%)
1	OMU	A2	116	1	19,22,23	1.20	2 (10%)	26,31,34	1.69	4 (15%)
40	PSU	B5	4740	40	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
40	OMU	B5	3657	40	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
40	UR3	B5	4276	40	19,22,23	0.97	0	26,32,35	1.42	1 (3%)
40	OMG	B5	3524	40	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
40	OMG	B5	4364	40	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A2	27	1,88	18,25,26	1.00	1 (5%)	18,36,39	1.19	2 (11%)
1	OMU	A2	1443	1,88	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	3427	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1047	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	A2M	B5	3562	40	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
1	OMG	A2	510	1,88	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	OMG	A2	1491	1,88	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	A2M	A2	1384	1	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	OMC	A2	174	1,88	19,22,23	0.82	0	26,31,34	0.82	0
40	OMC	B5	3433	40	19,22,23	0.80	0	26,31,34	0.74	0
40	OMG	B5	4240	40	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
40	PSU	B5	4419	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	OMU	B5	4244	40	19,22,23	1.20	2 (10%)	26,31,34	1.72	5 (19%)
40	OMC	B5	1284	40	19,22,23	0.81	0	26,31,34	0.79	0
10	5MU	AJ	54	10	19,22,23	1.42	6 (31%)	28,32,35	1.99	6 (21%)
1	A2M	A2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
40	OMC	B5	2647	40	19,22,23	0.82	0	26,31,34	0.82	0
1	PSU	A2	109	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
40	OMC	B5	2265	40,88	19,22,23	0.82	0	26,31,34	0.89	1 (3%)
40	5MC	B5	3514	40,88	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
40	PSU	B5	4246	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4298	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	A2	355	1	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
40	PSU	B5	3490	40	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
45	AYA	BC	2	45	6,7,8	0.71	0	5,8,10	0.43	0
1	OMU	A2	1327	1	19,22,23	1.18	2 (10%)	26,31,34	1.72	5 (19%)
40	PSU	B5	3494	40	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
40	OMC	B5	3573	40	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
40	PSU	B5	4217	40	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1693	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1175	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
13	SAC	AZ	2	13	7,8,9	0.52	0	8,9,11	0.87	1 (12%)
40	A2M	B5	3492	40	18,25,26	1.01	1 (5%)	18,36,39	1.34	2 (11%)
40	UY1	B5	3550	40	19,22,23	1.38	3 (15%)	22,31,34	1.83	4 (18%)
1	OMG	A2	437	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMC	B5	2667	40	19,22,23	0.81	0	26,31,34	0.82	0
40	OMG	B5	4116	40	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
40	PSU	B5	1491	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	4711	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
42	OMG	B8	75	42	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
82	MLZ	Bo	53	82	8,9,10	0.49	0	4,9,11	0.08	0
40	PSU	B5	4166	40	18,21,22	1.39	3 (16%)	22,30,33	1.80	4 (18%)
1	A2M	A2	166	1	18,25,26	1.06	1 (5%)	18,36,39	1.28	2 (11%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
40	OMG	B5	3942	40	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
40	PSU	B5	1720	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	OMC	B5	4202	40	19,22,23	0.81	0	26,31,34	0.79	0
40	5MC	B5	4193	40	18,22,23	0.99	2 (11%)	26,32,35	1.19	2 (7%)
40	PSU	B5	4188	40	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
40	PSU	B5	4203	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	577	1	18,25,26	1.01	1 (5%)	18,36,39	1.18	2 (11%)
1	OMG	A2	602	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
43	V5N	BA	216	43	4,11,12	0.78	0	5,14,16	1.55	1 (20%)
40	A2M	B5	4317	40	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	4AC	A2	1338	1	21,24,25	1.07	2 (9%)	29,34,37	1.26	3 (10%)
1	PSU	A2	210	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
40	A2M	B5	3517	40	18,25,26	0.95	1 (5%)	18,36,39	1.33	2 (11%)
40	A2M	B5	2244	40	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
40	OMG	B5	3631	40	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
40	PSU	B5	2475	40	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
40	OMC	B5	2704	40	19,22,23	0.82	0	26,31,34	0.82	0
40	OMG	B5	1260	40	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
44	HIC	BB	245	44	8,11,12	0.87	0	6,14,16	0.84	0
40	OMG	B5	3359	40	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
40	PSU	B5	3462	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	A2M	B5	398	40	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	868	1	18,26,27	0.94	1 (5%)	19,38,41	1.05	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	B5	3583	40	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	1718	40	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	1329	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	A2	1289	1	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	PSU	A2	34	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	A2M	B5	3557	40	18,25,26	1.04	1 (5%)	18,36,39	1.21	2 (11%)
40	PSU	B5	4749	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
40	OMG	B5	3676	40	18,26,27	0.94	1 (5%)	19,38,41	1.04	2 (10%)
1	OMU	A2	121	1	19,22,23	1.22	2 (10%)	26,31,34	1.69	4 (15%)
40	6MZ	B5	3966	40	18,25,26	0.88	1 (5%)	16,36,39	2.01	4 (25%)
1	PSU	A2	815	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
1	MA6	A2	1852	1	18,26,27	1.04	2 (11%)	19,38,41	1.50	3 (15%)
40	A2M	B5	2658	40,88	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
40	A2M	B5	3456	40	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
40	PSU	B5	4435	40	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
40	PSU	B5	3371	40	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
40	OMG	B5	4369	40	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	1046	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	3576	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
81	M3L	Bm	98	81	10,11,12	0.84	0	9,14,16	0.53	0
1	A2M	A2	591	1	18,25,26	1.05	1 (5%)	18,36,39	1.23	2 (11%)
40	OMU	B5	3973	40	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
10	PSU	AJ	55	10	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	3652	40,88	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
34	AME	Au	1	34	9,10,11	0.49	0	9,11,13	0.87	1 (11%)
40	A2M	B5	2630	40,88	18,25,26	0.99	1 (5%)	18,36,39	1.39	3 (16%)
42	PSU	B8	55	42	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
40	OMC	B5	4282	40	19,22,23	0.82	0	26,31,34	0.85	0
1	PSU	A2	218	1	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1239	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
42	PSU	B8	69	42	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
36	HY3	Aw	62	36	6,8,9	2.14	1 (16%)	5,10,12	1.08	1 (20%)
1	PSU	A2	1626	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMG	B5	1477	40	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
40	PSU	B5	4267	40,88	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
40	OMG	B5	2719	40	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
40	PSU	B5	4039	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	1537	40	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	1679	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
40	PSU	B5	3554	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1245	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	G7M	A2	1640	1,11	20,26,27	2.63	4 (20%)	17,39,42	0.95	1 (5%)
40	OMC	B5	3619	40	19,22,23	0.82	0	26,31,34	0.86	0
1	4AC	A2	1843	1	21,24,25	1.13	2 (9%)	29,34,37	1.28	3 (10%)
1	PSU	A2	1005	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
40	PSU	B5	4374	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	A2M	B5	3599	40	18,25,26	0.99	1 (5%)	18,36,39	1.19	2 (11%)
40	PSU	B5	4177	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	864	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	3447	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
41	GTP	B7	1	41	26,34,34	0.94	2 (7%)	32,54,54	0.78	0
40	PSU	B5	3466	40	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
40	OMG	B5	1580	40	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	802	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
40	PSU	B5	1799	40	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
40	A2M	B5	1810	40,88	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	3496	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	3585	40,88	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4169	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
40	PSU	B5	4382	40	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
40	PSU	B5	3369	40	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
40	A2M	B5	4269	40,88	18,25,26	1.03	1 (5%)	18,36,39	1.24	2 (11%)
40	OMG	B5	4138	40	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
40	PSU	B5	2351	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	469	1	18,25,26	1.05	1 (5%)	18,36,39	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	682	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	OMC	B5	1820	40,88	19,22,23	0.80	0	26,31,34	0.79	0
1	PSU	A2	105	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	1448	1	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
1	OMU	A2	628	1	19,22,23	1.19	2 (10%)	26,31,34	1.73	5 (19%)
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.85	1 (12%)
40	PSU	B5	4149	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
40	OMC	B5	3601	40	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
40	OMG	B5	4383	40	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
40	A2M	B5	1479	40	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	573	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4322	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1348	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	645	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
40	PSU	B5	4278	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	B8N	A2	1249	1	24,29,30	1.30	3 (12%)	29,42,45	1.28	3 (10%)
40	PSU	B5	1683	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1082	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
40	OMC	B5	3540	40	19,22,23	0.81	0	26,31,34	0.79	0
40	PSU	B5	4107	40	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	A2	463	1	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
11	PSU	AT	54	11	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
40	OMU	B5	2258	40	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
40	PSU	B5	4045	40	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	MA6	A2	1851	1	18,26,27	0.92	1 (5%)	19,38,41	1.55	3 (15%)
1	PSU	A2	1057	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	485	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	OMU	A2	429	1	19,22,23	1.22	4 (21%)	26,31,34	1.69	5 (19%)
40	PSU	B5	3616	40	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
40	OMC	B5	2194	40,88	19,22,23	0.82	0	26,31,34	0.92	1 (3%)
1	PSU	A2	652	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	867	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
40	PSU	B5	4042	40	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
40	A2M	B5	1270	40	18,25,26	0.98	1 (5%)	18,36,39	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	B5	1721	40	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	3500	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	OMG	B5	3974	40	18,26,27	0.91	1 (5%)	19,38,41	1.12	2 (10%)
40	PSU	B5	4325	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
31	SAC	Ar	2	31	7,8,9	0.53	0	8,9,11	0.87	1 (12%)
70	MLZ	Bb	5	70	8,9,10	0.49	0	4,9,11	0.11	0
40	PSU	B5	4058	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	1638	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	1032	1	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
40	A2M	B5	2206	40,88	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
40	OMU	B5	4052	40	19,22,23	1.23	4 (21%)	26,31,34	1.67	4 (15%)
40	PSU	B5	4099	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	6MZ	A2	1833	1,88	18,25,26	0.94	1 (5%)	16,36,39	1.77	3 (18%)
40	OMG	B5	3476	40	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
40	OMG	B5	4245	40,10	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
40	PSU	B5	1731	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)

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
40	PSU	B5	1632	40	-	0/7/25/26	0/2/2/2
40	1MA	B5	1266	40,88	-	0/3/25/26	0/3/3/3
40	A2M	B5	1489	40,88	-	2/5/27/28	0/3/3/3
1	PSU	A2	1644	1,88	-	0/7/25/26	0/2/2/2
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
40	OMU	B5	4366	40	-	1/9/27/28	0/2/2/2
40	PSU	B5	1801	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
69	V5N	Ba	39	69	-	0/5/10/12	0/1/1/1
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
32	NMM	As	67	32	-	0/9/11/13	-
40	OMG	B5	2267	40	-	1/5/27/28	0/3/3/3
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1704	1	-	3/9/27/28	0/2/2/2
40	A2M	B5	4336	40	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	5MU	AT	53	11	-	1/7/25/26	0/2/2/2
40	OMC	B5	2208	40	-	0/9/27/28	0/2/2/2
40	A2M	B5	3450	40	-	2/5/27/28	0/3/3/3
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	2207	40	-	2/5/27/28	0/3/3/3
40	OMU	B5	2680	40	-	1/9/27/28	0/2/2/2
1	A2M	A2	669	1,88	-	2/5/27/28	0/3/3/3
40	PSU	B5	3502	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	400	40	-	0/5/27/28	0/3/3/3
1	A2M	A2	99	1,88	-	1/5/27/28	0/3/3/3
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	513	1	-	2/5/27/28	0/3/3/3
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
40	PSU	B5	4740	40	-	0/7/25/26	0/2/2/2
40	OMU	B5	3657	40	-	1/9/27/28	0/2/2/2
40	UR3	B5	4276	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3524	40	-	0/5/27/28	0/3/3/3
40	OMG	B5	4364	40	-	0/5/27/28	0/3/3/3
1	A2M	A2	27	1,88	-	2/5/27/28	0/3/3/3
1	OMU	A2	1443	1,88	-	0/9/27/28	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3427	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	3562	40	-	0/5/27/28	0/3/3/3
1	OMG	A2	510	1,88	-	1/5/27/28	0/3/3/3
1	OMG	A2	1491	1,88	-	1/5/27/28	0/3/3/3
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
1	OMC	A2	174	1,88	-	0/9/27/28	0/2/2/2
40	OMC	B5	3433	40	-	4/9/27/28	0/2/2/2
40	OMG	B5	4240	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4419	40	-	0/7/25/26	0/2/2/2
40	OMU	B5	4244	40	-	0/9/27/28	0/2/2/2
40	OMC	B5	1284	40	-	1/9/27/28	0/2/2/2
10	5MU	AJ	54	10	-	0/7/25/26	0/2/2/2
1	A2M	A2	159	1	-	0/5/27/28	0/3/3/3
40	OMC	B5	2647	40	-	0/9/27/28	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	2265	40,88	-	0/9/27/28	0/2/2/2
40	5MC	B5	3514	40,88	-	0/7/25/26	0/2/2/2
40	PSU	B5	4246	40	-	1/7/25/26	0/2/2/2
40	PSU	B5	4298	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
40	PSU	B5	3490	40	-	0/7/25/26	0/2/2/2
45	AYA	BC	2	45	-	3/4/6/8	-
1	OMU	A2	1327	1	-	0/9/27/28	0/2/2/2
40	PSU	B5	3494	40	-	2/7/25/26	0/2/2/2
40	OMC	B5	3573	40	-	1/9/27/28	0/2/2/2
40	PSU	B5	4217	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
13	SAC	AZ	2	13	-	2/7/8/10	-
40	A2M	B5	3492	40	-	0/5/27/28	0/3/3/3
40	UY1	B5	3550	40	-	2/9/27/28	0/2/2/2
1	OMG	A2	437	1	-	1/5/27/28	0/3/3/3
40	OMC	B5	2667	40	-	0/9/27/28	0/2/2/2
40	OMG	B5	4116	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	1491	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4711	40	-	0/7/25/26	0/2/2/2
42	OMG	B8	75	42	-	0/5/27/28	0/3/3/3
82	MLZ	B _o	53	82	-	0/7/8/10	-
40	PSU	B5	4166	40	-	2/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	3942	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	1720	40	-	2/7/25/26	0/2/2/2
40	OMC	B5	4202	40	-	0/9/27/28	0/2/2/2
40	5MC	B5	4193	40	-	4/7/25/26	0/2/2/2
40	PSU	B5	4188	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4203	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
1	OMG	A2	602	1	-	0/5/27/28	0/3/3/3
43	V5N	BA	216	43	-	1/5/10/12	0/1/1/1
40	A2M	B5	4317	40	-	0/5/27/28	0/3/3/3
1	4AC	A2	1338	1	-	2/11/29/30	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	3517	40	-	2/5/27/28	0/3/3/3
40	A2M	B5	2244	40	-	0/5/27/28	0/3/3/3
40	OMG	B5	3631	40	-	1/5/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	2475	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	2704	40	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	B5	1260	40	-	1/5/27/28	0/3/3/3
44	HIC	BB	245	44	-	1/5/6/8	0/1/1/1
40	OMG	B5	3359	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3462	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	398	40	-	3/5/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	3/5/27/28	0/3/3/3
40	PSU	B5	3583	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	1718	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	0/5/27/28	0/3/3/3
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	3557	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4749	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3676	40	-	1/5/27/28	0/3/3/3
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
40	6MZ	B5	3966	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	3/5/27/28	0/3/3/3
1	MA6	A2	1852	1	-	1/7/29/30	0/3/3/3
40	A2M	B5	2658	40,88	-	0/5/27/28	0/3/3/3
40	A2M	B5	3456	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4435	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3371	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	4369	40	-	1/5/27/28	0/3/3/3
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3576	40	-	1/7/25/26	0/2/2/2
81	M3L	Bm	98	81	-	0/9/10/12	-
1	A2M	A2	591	1	-	1/5/27/28	0/3/3/3
40	OMU	B5	3973	40	-	0/9/27/28	0/2/2/2
10	PSU	AJ	55	10	-	0/7/25/26	0/2/2/2
40	PSU	B5	3652	40,88	-	0/7/25/26	0/2/2/2
34	AME	Au	1	34	-	2/9/10/12	-
40	A2M	B5	2630	40,88	-	1/5/27/28	0/3/3/3
42	PSU	B8	55	42	-	0/7/25/26	0/2/2/2
40	OMC	B5	4282	40	-	1/9/27/28	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
42	PSU	B8	69	42	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HY3	Aw	62	36	-	0/1/12/14	0/1/1/1
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	1477	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4267	40,88	-	0/7/25/26	0/2/2/2
40	OMG	B5	2719	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4039	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	1537	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
40	PSU	B5	3554	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
1	G7M	A2	1640	1,11	-	0/3/25/26	0/3/3/3
40	OMC	B5	3619	40	-	2/9/27/28	0/2/2/2
1	4AC	A2	1843	1	-	4/11/29/30	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4374	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	3599	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4177	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3447	40	-	0/7/25/26	0/2/2/2
41	GTP	B7	1	41	-	0/18/38/38	0/3/3/3
40	PSU	B5	3466	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	1580	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	1799	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	1810	40,88	-	0/5/27/28	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3496	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3585	40,88	-	0/7/25/26	0/2/2/2
40	PSU	B5	4169	40	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
40	PSU	B5	4382	40	-	4/7/25/26	0/2/2/2
40	PSU	B5	3369	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	4269	40,88	-	0/5/27/28	0/3/3/3
40	OMG	B5	4138	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	2351	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	1820	40,88	-	1/9/27/28	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A2	1448	1	-	3/5/27/28	0/3/3/3
1	OMU	A2	628	1	-	0/9/27/28	0/2/2/2
84	SAC	Br	2	84	-	0/7/8/10	-
40	PSU	B5	4149	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	3601	40	-	0/9/27/28	0/2/2/2
40	OMG	B5	4383	40	-	0/5/27/28	0/3/3/3
40	A2M	B5	1479	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4322	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	645	1	-	3/5/27/28	0/3/3/3
40	PSU	B5	4278	40	-	3/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
40	PSU	B5	1683	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1082	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	3540	40	-	0/9/27/28	0/2/2/2
40	PSU	B5	4107	40	-	0/7/25/26	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
11	PSU	AT	54	11	-	0/7/25/26	0/2/2/2
40	OMU	B5	2258	40	-	0/9/27/28	0/2/2/2
40	PSU	B5	4045	40	-	0/7/25/26	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
40	PSU	B5	3616	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	2194	40,88	-	2/9/27/28	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4042	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	1270	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	1721	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3500	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3974	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4325	40	-	0/7/25/26	0/2/2/2
31	SAC	Ar	2	31	-	0/7/8/10	-
70	MLZ	Bb	5	70	-	0/7/8/10	-
40	PSU	B5	4058	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	1638	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	A2M	B5	2206	40,88	-	0/5/27/28	0/3/3/3
40	OMU	B5	4052	40	-	1/9/27/28	0/2/2/2
40	PSU	B5	4099	40	-	0/7/25/26	0/2/2/2
1	6MZ	A2	1833	1,88	-	0/5/27/28	0/3/3/3
40	OMG	B5	3476	40	-	1/5/27/28	0/3/3/3
40	OMG	B5	4245	40,10	-	0/5/27/28	0/3/3/3
40	PSU	B5	1731	40	-	0/7/25/26	0/2/2/2

All (344) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N9	7.43	1.46	1.33
1	A2	1640	G7M	C8-N7	7.18	1.46	1.33
36	Aw	62	HY3	C3-CA	-4.90	1.50	1.55
40	B5	1266	1MA	C2-N3	4.76	1.34	1.29
1	A2	1640	G7M	C5-C4	4.33	1.47	1.39
40	B5	3550	UY1	C6-C5	3.65	1.39	1.35
11	AT	54	PSU	C6-C5	3.30	1.39	1.35
1	A2	867	PSU	C6-C5	3.27	1.39	1.35
10	AJ	55	PSU	C6-C5	3.27	1.39	1.35
1	A2	93	PSU	C6-C5	3.25	1.39	1.35
1	A2	210	PSU	C6-C5	3.25	1.39	1.35
40	B5	4166	PSU	C6-C5	3.24	1.39	1.35
40	B5	3466	PSU	C6-C5	3.23	1.39	1.35
40	B5	3583	PSU	C6-C5	3.20	1.39	1.35
1	A2	967	PSU	C6-C5	3.20	1.39	1.35
40	B5	1632	PSU	C6-C5	3.20	1.39	1.35
40	B5	1266	1MA	C6-N6	3.19	1.35	1.27
40	B5	3494	PSU	C6-C5	3.19	1.39	1.35
40	B5	3576	PSU	C6-C5	3.19	1.39	1.35
1	A2	1245	PSU	C6-C5	3.18	1.39	1.35
1	A2	823	PSU	C6-C5	3.18	1.39	1.35
40	B5	4188	PSU	C6-C5	3.18	1.39	1.35
40	B5	3490	PSU	C6-C5	3.18	1.39	1.35
40	B5	3427	PSU	C6-C5	3.18	1.39	1.35
1	A2	105	PSU	C6-C5	3.17	1.39	1.35
40	B5	4099	PSU	C6-C5	3.17	1.39	1.35
1	A2	119	PSU	C6-C5	3.17	1.39	1.35
1	A2	1348	PSU	C6-C5	3.17	1.39	1.35
1	A2	652	PSU	C6-C5	3.16	1.39	1.35
40	B5	3447	PSU	C6-C5	3.16	1.39	1.35
1	A2	34	PSU	C6-C5	3.16	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4382	PSU	C6-C5	3.15	1.39	1.35
1	A2	815	PSU	C6-C5	3.15	1.39	1.35
1	A2	1368	PSU	C6-C5	3.15	1.39	1.35
40	B5	4740	PSU	C6-C5	3.15	1.39	1.35
40	B5	1720	PSU	C6-C5	3.15	1.39	1.35
1	A2	816	PSU	C6-C5	3.14	1.39	1.35
1	A2	573	PSU	C6-C5	3.14	1.39	1.35
40	B5	4058	PSU	C6-C5	3.14	1.39	1.35
1	A2	1005	PSU	C6-C5	3.14	1.39	1.35
40	B5	1721	PSU	C6-C5	3.14	1.39	1.35
1	A2	407	PSU	C6-C5	3.14	1.39	1.35
40	B5	3502	PSU	C6-C5	3.14	1.39	1.35
42	B8	69	PSU	C6-C5	3.14	1.39	1.35
40	B5	1683	PSU	C6-C5	3.13	1.39	1.35
40	B5	1731	PSU	C6-C5	3.13	1.39	1.35
1	A2	1178	PSU	C6-C5	3.13	1.39	1.35
1	A2	1047	PSU	C6-C5	3.13	1.39	1.35
1	A2	1057	PSU	C6-C5	3.13	1.39	1.35
40	B5	3496	PSU	C6-C5	3.13	1.39	1.35
40	B5	4711	PSU	C6-C5	3.13	1.39	1.35
40	B5	4169	PSU	C6-C5	3.12	1.39	1.35
1	A2	109	PSU	C6-C5	3.12	1.39	1.35
40	B5	4322	PSU	C6-C5	3.12	1.39	1.35
1	A2	610	PSU	C6-C5	3.12	1.39	1.35
40	B5	4107	PSU	C6-C5	3.12	1.39	1.35
40	B5	3500	PSU	C6-C5	3.12	1.39	1.35
1	A2	687	PSU	C6-C5	3.11	1.38	1.35
40	B5	4749	PSU	C6-C5	3.11	1.38	1.35
40	B5	4278	PSU	C6-C5	3.11	1.38	1.35
40	B5	3462	PSU	C6-C5	3.11	1.38	1.35
40	B5	3554	PSU	C6-C5	3.11	1.38	1.35
1	A2	802	PSU	C6-C5	3.11	1.38	1.35
40	B5	4419	PSU	C6-C5	3.11	1.38	1.35
1	A2	1693	PSU	C6-C5	3.10	1.38	1.35
40	B5	4374	PSU	C6-C5	3.10	1.38	1.35
1	A2	1239	PSU	C6-C5	3.10	1.38	1.35
40	B5	1537	PSU	C6-C5	3.10	1.38	1.35
40	B5	1638	PSU	C6-C5	3.10	1.38	1.35
40	B5	4149	PSU	C6-C5	3.09	1.38	1.35
40	B5	1491	PSU	C6-C5	3.09	1.38	1.35
1	A2	1249	B8N	C4-N3	-3.09	1.34	1.40
1	A2	36	PSU	C6-C5	3.09	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	650	PSU	C6-C5	3.09	1.38	1.35
40	B5	3585	PSU	C6-C5	3.09	1.38	1.35
40	B5	1799	PSU	C6-C5	3.08	1.38	1.35
1	A2	1843	4AC	C4-N4	-3.08	1.35	1.39
40	B5	4039	PSU	C6-C5	3.08	1.38	1.35
40	B5	4267	PSU	C6-C5	3.08	1.38	1.35
1	A2	1175	PSU	C6-C5	3.08	1.38	1.35
1	A2	1644	PSU	C6-C5	3.07	1.38	1.35
40	B5	2475	PSU	C6-C5	3.07	1.38	1.35
1	A2	864	PSU	C6-C5	3.07	1.38	1.35
40	B5	4203	PSU	C6-C5	3.07	1.38	1.35
40	B5	4325	PSU	C6-C5	3.07	1.38	1.35
1	A2	218	PSU	C6-C5	3.07	1.38	1.35
1	A2	1446	PSU	C6-C5	3.07	1.38	1.35
1	A2	1082	PSU	C6-C5	3.06	1.38	1.35
40	B5	1801	PSU	C6-C5	3.06	1.38	1.35
40	B5	1718	PSU	C6-C5	3.06	1.38	1.35
40	B5	4435	PSU	C6-C5	3.06	1.38	1.35
40	B5	4217	PSU	C6-C5	3.06	1.38	1.35
40	B5	4246	PSU	C6-C5	3.06	1.38	1.35
1	A2	1233	PSU	C6-C5	3.05	1.38	1.35
40	B5	3616	PSU	C6-C5	3.05	1.38	1.35
40	B5	4045	PSU	C6-C5	3.05	1.38	1.35
40	B5	4177	PSU	C6-C5	3.04	1.38	1.35
40	B5	2351	PSU	C6-C5	3.04	1.38	1.35
1	A2	1626	PSU	C6-C5	3.04	1.38	1.35
40	B5	3369	PSU	C6-C5	3.04	1.38	1.35
42	B8	55	PSU	C6-C5	3.04	1.38	1.35
40	B5	4042	PSU	C6-C5	3.04	1.38	1.35
1	A2	682	PSU	C6-C5	3.04	1.38	1.35
1	A2	1249	B8N	C6-C5	3.04	1.39	1.34
1	A2	1046	PSU	C6-C5	3.03	1.38	1.35
40	B5	3371	PSU	C6-C5	3.03	1.38	1.35
40	B5	3652	PSU	C6-C5	3.00	1.38	1.35
40	B5	4298	PSU	C6-C5	2.99	1.38	1.35
40	B5	4193	5MC	C6-C5	2.83	1.39	1.34
1	A2	1338	4AC	C4-N4	-2.82	1.35	1.39
40	B5	3616	PSU	C4-N3	-2.79	1.33	1.38
40	B5	3369	PSU	C4-N3	-2.77	1.33	1.38
40	B5	3652	PSU	C4-N3	-2.76	1.33	1.38
40	B5	1799	PSU	C4-N3	-2.76	1.33	1.38
40	B5	4267	PSU	C4-N3	-2.76	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3514	5MC	C6-C5	2.75	1.39	1.34
1	A2	1239	PSU	C4-N3	-2.75	1.33	1.38
40	B5	3490	PSU	C4-N3	-2.75	1.33	1.38
40	B5	4045	PSU	C4-N3	-2.75	1.33	1.38
1	A2	815	PSU	C4-N3	-2.74	1.33	1.38
40	B5	3585	PSU	C4-N3	-2.73	1.33	1.38
11	AT	53	5MU	C6-C5	2.73	1.39	1.34
1	A2	1693	PSU	C4-N3	-2.73	1.33	1.38
40	B5	2351	PSU	C4-N3	-2.73	1.33	1.38
40	B5	4149	PSU	C4-N3	-2.73	1.33	1.38
40	B5	4188	PSU	C4-N3	-2.72	1.33	1.38
42	B8	55	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1446	PSU	C4-N3	-2.72	1.33	1.38
10	AJ	54	5MU	C6-C5	2.72	1.39	1.34
40	B5	1683	PSU	C4-N3	-2.72	1.33	1.38
40	B5	1491	PSU	C4-N3	-2.72	1.33	1.38
40	B5	1638	PSU	C4-N3	-2.72	1.33	1.38
40	B5	4107	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1046	PSU	C4-N3	-2.71	1.33	1.38
40	B5	3502	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.71	1.33	1.38
40	B5	1801	PSU	C4-N3	-2.70	1.33	1.38
40	B5	1721	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4177	PSU	C4-N3	-2.70	1.33	1.38
1	A2	682	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4298	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4203	PSU	C4-N3	-2.70	1.33	1.38
1	A2	867	PSU	C4-N3	-2.69	1.33	1.38
1	A2	652	PSU	C4-N3	-2.69	1.33	1.38
40	B5	3500	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4382	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4711	PSU	C4-N3	-2.69	1.33	1.38
40	B5	3371	PSU	C4-N3	-2.69	1.33	1.38
1	A2	1626	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4042	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4740	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4278	PSU	C4-N3	-2.69	1.33	1.38
40	B5	3496	PSU	C4-N3	-2.69	1.33	1.38
1	A2	802	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1178	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4217	PSU	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	34	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4325	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4039	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4374	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4099	PSU	C4-N3	-2.67	1.33	1.38
1	A2	93	PSU	C4-N3	-2.67	1.33	1.38
40	B5	4435	PSU	C4-N3	-2.67	1.33	1.38
40	B5	4322	PSU	C4-N3	-2.67	1.33	1.38
40	B5	4749	PSU	C4-N3	-2.67	1.33	1.38
40	B5	3583	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1047	PSU	C4-N3	-2.67	1.33	1.38
40	B5	3447	PSU	C4-N3	-2.67	1.33	1.38
1	A2	407	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1175	PSU	C4-N3	-2.67	1.33	1.38
1	A2	573	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.67	1.33	1.38
40	B5	3427	PSU	C4-N3	-2.66	1.33	1.38
40	B5	3554	PSU	C4-N3	-2.66	1.33	1.38
40	B5	1718	PSU	C4-N3	-2.66	1.33	1.38
40	B5	1537	PSU	C4-N3	-2.66	1.33	1.38
1	A2	687	PSU	C4-N3	-2.66	1.33	1.38
1	A2	967	PSU	C4-N3	-2.66	1.33	1.38
1	A2	610	PSU	C4-N3	-2.66	1.33	1.38
40	B5	1632	PSU	C4-N3	-2.66	1.33	1.38
10	AJ	55	PSU	C4-N3	-2.66	1.33	1.38
40	B5	3576	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1368	PSU	C4-N3	-2.66	1.33	1.38
40	B5	3494	PSU	C4-N3	-2.66	1.33	1.38
40	B5	4419	PSU	C4-N3	-2.66	1.33	1.38
1	A2	864	PSU	C4-N3	-2.65	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.65	1.33	1.38
42	B8	69	PSU	C4-N3	-2.65	1.33	1.38
40	B5	3550	UY1	C2-N1	2.65	1.40	1.36
40	B5	1720	PSU	C4-N3	-2.65	1.33	1.38
1	A2	816	PSU	C4-N3	-2.65	1.33	1.38
1	A2	650	PSU	C4-N3	-2.65	1.33	1.38
40	B5	1731	PSU	C4-N3	-2.65	1.33	1.38
1	A2	1348	PSU	C4-N3	-2.65	1.33	1.38
40	B5	3466	PSU	C4-N3	-2.65	1.33	1.38
40	B5	3462	PSU	C4-N3	-2.65	1.33	1.38
1	A2	109	PSU	C4-N3	-2.64	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	36	PSU	C4-N3	-2.64	1.33	1.38
40	B5	4058	PSU	C4-N3	-2.64	1.33	1.38
11	AT	54	PSU	C4-N3	-2.63	1.33	1.38
1	A2	105	PSU	C4-N3	-2.63	1.34	1.38
40	B5	2475	PSU	C4-N3	-2.63	1.34	1.38
1	A2	1245	PSU	C4-N3	-2.62	1.34	1.38
1	A2	210	PSU	C4-N3	-2.62	1.34	1.38
40	B5	4169	PSU	C4-N3	-2.61	1.34	1.38
11	AT	53	5MU	C4-N3	-2.60	1.34	1.38
10	AJ	54	5MU	C4-N3	-2.60	1.34	1.38
1	A2	119	PSU	C4-N3	-2.60	1.34	1.38
1	A2	218	PSU	C4-N3	-2.60	1.34	1.38
40	B5	4166	PSU	C4-N3	-2.59	1.34	1.38
40	B5	3657	OMU	C4-N3	-2.58	1.33	1.38
1	A2	823	PSU	C4-N3	-2.58	1.34	1.38
40	B5	4246	PSU	C4-N3	-2.58	1.34	1.38
40	B5	1260	OMG	C6-N1	-2.56	1.34	1.37
40	B5	4244	OMU	C4-N3	-2.56	1.34	1.38
1	A2	591	A2M	C5-C4	2.56	1.47	1.40
41	B7	1	GTP	C5-C6	-2.55	1.42	1.47
1	A2	1833	6MZ	C5-C4	2.55	1.47	1.40
1	A2	1491	OMG	C6-N1	-2.55	1.34	1.37
1	A2	602	OMG	C6-N1	-2.55	1.34	1.37
40	B5	2680	OMU	C4-N3	-2.55	1.34	1.38
40	B5	4138	OMG	C6-N1	-2.54	1.34	1.37
1	A2	355	OMU	C4-N3	-2.53	1.34	1.38
40	B5	3973	OMU	C4-N3	-2.53	1.34	1.38
40	B5	4052	OMU	C4-N3	-2.52	1.34	1.38
1	A2	1805	OMU	C4-N3	-2.52	1.34	1.38
40	B5	4116	OMG	C6-N1	-2.52	1.34	1.37
1	A2	1443	OMU	C4-N3	-2.52	1.34	1.38
40	B5	3524	OMG	C6-N1	-2.52	1.34	1.37
40	B5	2719	OMG	C6-N1	-2.52	1.34	1.37
40	B5	3359	OMG	C6-N1	-2.51	1.34	1.37
1	A2	121	OMU	C4-N3	-2.51	1.34	1.38
1	A2	469	A2M	C5-C4	2.50	1.47	1.40
40	B5	3631	OMG	C6-N1	-2.50	1.34	1.37
1	A2	628	OMU	C4-N3	-2.50	1.34	1.38
1	A2	1852	MA6	C5-C4	2.50	1.47	1.40
1	A2	868	OMG	C6-N1	-2.50	1.34	1.37
40	B5	2258	OMU	C4-N3	-2.50	1.34	1.38
1	A2	510	OMG	C6-N1	-2.49	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3942	OMG	C6-N1	-2.49	1.34	1.37
1	A2	116	OMU	C4-N3	-2.48	1.34	1.38
1	A2	166	A2M	C5-C4	2.48	1.47	1.40
1	A2	429	OMU	C4-N3	-2.48	1.34	1.38
1	A2	1289	OMU	C4-N3	-2.47	1.34	1.38
40	B5	2207	OMG	C6-N1	-2.47	1.34	1.37
1	A2	1329	OMG	C6-N1	-2.47	1.34	1.37
40	B5	4383	OMG	C6-N1	-2.46	1.34	1.37
1	A2	1327	OMU	C4-N3	-2.46	1.34	1.38
40	B5	3476	OMG	C6-N1	-2.46	1.34	1.37
40	B5	4366	OMU	C4-N3	-2.46	1.34	1.38
40	B5	3676	OMG	C6-N1	-2.46	1.34	1.37
40	B5	400	A2M	C5-C4	2.46	1.47	1.40
40	B5	3456	A2M	C5-C4	2.46	1.47	1.40
1	A2	645	OMG	C6-N1	-2.45	1.34	1.37
1	A2	172	OMU	C4-N3	-2.45	1.34	1.38
40	B5	2658	A2M	C5-C4	2.45	1.47	1.40
1	A2	159	A2M	C5-C4	2.45	1.47	1.40
40	B5	4336	A2M	C5-C4	2.45	1.47	1.40
40	B5	1477	OMG	C6-N1	-2.45	1.34	1.37
42	B8	75	OMG	C6-N1	-2.45	1.34	1.37
40	B5	3450	A2M	C5-C4	2.45	1.47	1.40
40	B5	1580	OMG	C6-N1	-2.45	1.34	1.37
1	A2	1851	MA6	C5-C4	2.44	1.47	1.40
40	B5	4317	A2M	C5-C4	2.44	1.47	1.40
1	A2	684	OMG	C6-N1	-2.44	1.34	1.37
40	B5	3557	A2M	C5-C4	2.44	1.47	1.40
40	B5	4369	OMG	C6-N1	-2.44	1.34	1.37
1	A2	513	A2M	C5-C4	2.44	1.47	1.40
40	B5	4245	OMG	C6-N1	-2.44	1.34	1.37
1	A2	99	A2M	C5-C4	2.44	1.47	1.40
11	AT	53	5MU	C2-N1	2.44	1.42	1.38
40	B5	3599	A2M	C5-C4	2.44	1.47	1.40
1	A2	1249	B8N	C2-N3	-2.44	1.34	1.38
1	A2	437	OMG	C6-N1	-2.43	1.34	1.37
40	B5	4240	OMG	C6-N1	-2.43	1.34	1.37
40	B5	3974	OMG	C6-N1	-2.43	1.34	1.37
40	B5	2244	A2M	C5-C4	2.43	1.47	1.40
1	A2	577	A2M	C5-C4	2.43	1.47	1.40
40	B5	2206	A2M	C5-C4	2.43	1.47	1.40
40	B5	1479	A2M	C5-C4	2.42	1.47	1.40
40	B5	3492	A2M	C5-C4	2.42	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	485	A2M	C5-C4	2.42	1.47	1.40
40	B5	1810	A2M	C5-C4	2.42	1.47	1.40
40	B5	3562	A2M	C5-C4	2.42	1.47	1.40
1	A2	1032	A2M	C5-C4	2.42	1.47	1.40
1	A2	27	A2M	C5-C4	2.41	1.47	1.40
1	A2	1679	A2M	C5-C4	2.41	1.47	1.40
1	A2	1448	OMG	C6-N1	-2.41	1.34	1.37
40	B5	3966	6MZ	C5-C4	2.41	1.47	1.40
40	B5	1270	A2M	C5-C4	2.40	1.47	1.40
1	A2	669	A2M	C5-C4	2.40	1.47	1.40
40	B5	1489	A2M	C5-C4	2.40	1.47	1.40
40	B5	4269	A2M	C5-C4	2.39	1.47	1.40
40	B5	398	A2M	C5-C4	2.39	1.47	1.40
40	B5	2630	A2M	C5-C4	2.39	1.47	1.40
1	A2	1384	A2M	C5-C4	2.39	1.47	1.40
10	AJ	54	5MU	C4-C5	2.39	1.48	1.44
40	B5	2267	OMG	C6-N1	-2.38	1.34	1.37
40	B5	4364	OMG	C6-N1	-2.37	1.34	1.37
40	B5	3517	A2M	C5-C4	2.36	1.47	1.40
11	AT	53	5MU	C4-C5	2.31	1.48	1.44
1	A2	1640	G7M	C6-N1	-2.30	1.34	1.37
40	B5	3514	5MC	C6-N1	-2.29	1.34	1.38
10	AJ	54	5MU	C2-N1	2.28	1.42	1.38
10	AJ	54	5MU	C6-N1	-2.26	1.34	1.38
40	B5	4193	5MC	C6-N1	-2.25	1.34	1.38
1	A2	429	OMU	C2-N1	2.23	1.42	1.38
40	B5	3550	UY1	C6-N1	-2.21	1.32	1.36
1	A2	355	OMU	C2-N3	-2.21	1.34	1.38
1	A2	628	OMU	C2-N3	-2.18	1.34	1.38
1	A2	121	OMU	C2-N3	-2.18	1.34	1.38
40	B5	3657	OMU	C2-N3	-2.17	1.34	1.38
40	B5	4052	OMU	C2-N3	-2.17	1.34	1.38
40	B5	2680	OMU	C2-N3	-2.17	1.34	1.38
1	A2	1843	4AC	C7-N4	-2.16	1.33	1.37
40	B5	4366	OMU	C2-N3	-2.16	1.34	1.38
40	B5	3973	OMU	C2-N3	-2.16	1.34	1.38
40	B5	4244	OMU	C2-N3	-2.15	1.34	1.38
11	AT	53	5MU	C6-N1	-2.15	1.34	1.38
1	A2	1443	OMU	C2-N1	2.14	1.41	1.38
1	A2	1805	OMU	C2-N3	-2.14	1.34	1.38
1	A2	1289	OMU	C2-N1	2.14	1.41	1.38
1	A2	1327	OMU	C2-N3	-2.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	172	OMU	C2-N3	-2.14	1.34	1.38
40	B5	2258	OMU	C2-N1	2.13	1.41	1.38
1	A2	116	OMU	C2-N3	-2.12	1.34	1.38
1	A2	1805	OMU	C2-N1	2.11	1.41	1.38
1	A2	1443	OMU	C2-N3	-2.10	1.34	1.38
1	A2	429	OMU	C2-N3	-2.09	1.34	1.38
1	A2	1289	OMU	C2-N3	-2.08	1.34	1.38
40	B5	4052	OMU	C2-N1	2.05	1.41	1.38
41	B7	1	GTP	C8-N7	-2.05	1.31	1.35
40	B5	4366	OMU	C5-C4	-2.03	1.39	1.43
40	B5	3973	OMU	C2-N1	2.03	1.41	1.38
1	A2	429	OMU	C5-C4	-2.03	1.39	1.43
1	A2	1338	4AC	C7-N4	-2.02	1.33	1.37
40	B5	4052	OMU	C5-C4	-2.02	1.39	1.43
10	AJ	54	5MU	C2-N3	-2.02	1.34	1.38
40	B5	2258	OMU	C5-C4	-2.02	1.39	1.43
40	B5	4166	PSU	C4-C5	2.02	1.49	1.44
1	A2	1852	MA6	C4-N3	-2.02	1.32	1.35
11	AT	53	5MU	C2-N3	-2.01	1.34	1.38

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3369	PSU	N1-C2-N3	6.20	122.16	115.13
40	B5	3616	PSU	N1-C2-N3	6.12	122.07	115.13
40	B5	4045	PSU	N1-C2-N3	6.10	122.04	115.13
40	B5	4435	PSU	N1-C2-N3	6.07	122.01	115.13
40	B5	4188	PSU	N1-C2-N3	6.07	122.01	115.13
40	B5	1720	PSU	N1-C2-N3	6.07	122.01	115.13
1	A2	1057	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	1446	PSU	N1-C2-N3	6.06	122.00	115.13
40	B5	4042	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	815	PSU	N1-C2-N3	6.06	121.99	115.13
1	A2	1233	PSU	N1-C2-N3	6.05	121.98	115.13
40	B5	4278	PSU	N1-C2-N3	6.04	121.98	115.13
40	B5	3494	PSU	N1-C2-N3	6.04	121.98	115.13
40	B5	1491	PSU	N1-C2-N3	6.04	121.97	115.13
40	B5	3500	PSU	N1-C2-N3	6.03	121.97	115.13
40	B5	3554	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	1239	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	682	PSU	N1-C2-N3	6.03	121.96	115.13
40	B5	3490	PSU	N1-C2-N3	6.03	121.96	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3447	PSU	N1-C2-N3	6.02	121.95	115.13
40	B5	3583	PSU	N1-C2-N3	6.02	121.95	115.13
40	B5	3652	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	3427	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4740	PSU	N1-C2-N3	6.01	121.94	115.13
42	B8	55	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	1638	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4325	PSU	N1-C2-N3	6.01	121.94	115.13
10	AJ	55	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	34	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4267	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4711	PSU	N1-C2-N3	6.01	121.93	115.13
40	B5	1731	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	3496	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	650	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	610	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	4419	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	407	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	1693	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	4099	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3502	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3462	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3585	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	1626	PSU	N1-C2-N3	5.99	121.92	115.13
40	B5	1799	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	36	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	652	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	1047	PSU	N1-C2-N3	5.99	121.92	115.13
40	B5	2351	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	4149	PSU	N1-C2-N3	5.99	121.91	115.13
1	A2	105	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	1718	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	4217	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	3576	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	573	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	1046	PSU	N1-C2-N3	5.98	121.91	115.13
40	B5	1801	PSU	N1-C2-N3	5.98	121.90	115.13
1	A2	119	PSU	N1-C2-N3	5.97	121.89	115.13
40	B5	4246	PSU	N1-C2-N3	5.97	121.89	115.13
1	A2	1644	PSU	N1-C2-N3	5.96	121.89	115.13
1	A2	1245	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	3466	PSU	N1-C2-N3	5.96	121.89	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4169	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	4203	PSU	N1-C2-N3	5.96	121.88	115.13
40	B5	4374	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	210	PSU	N1-C2-N3	5.96	121.88	115.13
40	B5	4039	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	1368	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	864	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	967	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	93	PSU	N1-C2-N3	5.95	121.87	115.13
40	B5	4322	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	218	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	1178	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	867	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	1348	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	4298	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	4749	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	4177	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	1721	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	4107	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	4382	PSU	N1-C2-N3	5.93	121.84	115.13
40	B5	2475	PSU	N1-C2-N3	5.92	121.84	115.13
1	A2	823	PSU	N1-C2-N3	5.92	121.84	115.13
40	B5	4058	PSU	N1-C2-N3	5.92	121.84	115.13
40	B5	4276	UR3	C4-N3-C2	-5.92	118.99	124.56
1	A2	816	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	802	PSU	N1-C2-N3	5.91	121.83	115.13
42	B8	69	PSU	N1-C2-N3	5.91	121.83	115.13
40	B5	1537	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	1175	PSU	N1-C2-N3	5.91	121.82	115.13
1	A2	1005	PSU	N1-C2-N3	5.91	121.82	115.13
40	B5	1683	PSU	N1-C2-N3	5.89	121.81	115.13
1	A2	109	PSU	N1-C2-N3	5.89	121.80	115.13
40	B5	1632	PSU	N1-C2-N3	5.88	121.80	115.13
40	B5	3371	PSU	N1-C2-N3	5.88	121.79	115.13
40	B5	3966	6MZ	C2-N1-C6	5.87	121.63	116.59
1	A2	687	PSU	N1-C2-N3	5.86	121.76	115.13
1	A2	1082	PSU	N1-C2-N3	5.85	121.76	115.13
11	AT	54	PSU	N1-C2-N3	5.77	121.67	115.13
40	B5	4166	PSU	N1-C2-N3	5.60	121.48	115.13
1	A2	1833	6MZ	C2-N1-C6	5.56	121.36	116.59
40	B5	3550	UY1	C4-N3-C2	-5.21	118.83	126.34
11	AT	53	5MU	C4-N3-C2	-4.97	120.92	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AJ	54	5MU	C4-N3-C2	-4.94	120.95	127.35
10	AJ	54	5MU	N3-C2-N1	4.80	121.26	114.89
1	A2	1338	4AC	N4-C4-N3	4.77	121.85	113.85
11	AT	53	5MU	N3-C2-N1	4.76	121.21	114.89
1	A2	628	OMU	C4-N3-C2	-4.65	120.44	126.58
1	A2	1843	4AC	N4-C4-N3	4.58	121.54	113.85
1	A2	1851	MA6	N1-C6-N6	4.58	121.88	117.06
1	A2	1327	OMU	C4-N3-C2	-4.58	120.54	126.58
11	AT	53	5MU	C5-C4-N3	4.56	119.21	115.31
1	A2	355	OMU	C4-N3-C2	-4.53	120.60	126.58
40	B5	4244	OMU	C4-N3-C2	-4.51	120.63	126.58
40	B5	2680	OMU	C4-N3-C2	-4.50	120.65	126.58
1	A2	172	OMU	C4-N3-C2	-4.47	120.69	126.58
40	B5	4366	OMU	C4-N3-C2	-4.46	120.70	126.58
40	B5	3657	OMU	C4-N3-C2	-4.45	120.71	126.58
1	A2	116	OMU	C4-N3-C2	-4.41	120.77	126.58
1	A2	121	OMU	C4-N3-C2	-4.37	120.81	126.58
40	B5	4244	OMU	N3-C2-N1	4.35	120.67	114.89
40	B5	3973	OMU	C4-N3-C2	-4.35	120.84	126.58
40	B5	2258	OMU	C4-N3-C2	-4.31	120.90	126.58
40	B5	4052	OMU	C4-N3-C2	-4.29	120.92	126.58
1	A2	1289	OMU	C4-N3-C2	-4.27	120.95	126.58
1	A2	1805	OMU	C4-N3-C2	-4.25	120.97	126.58
1	A2	429	OMU	C4-N3-C2	-4.25	120.97	126.58
1	A2	1443	OMU	C4-N3-C2	-4.24	120.99	126.58
10	AJ	54	5MU	C5-C4-N3	4.23	118.92	115.31
1	A2	355	OMU	N3-C2-N1	4.20	120.46	114.89
40	B5	3550	UY1	N1-C2-N3	4.19	119.88	115.13
40	B5	2258	OMU	N3-C2-N1	4.18	120.43	114.89
40	B5	3657	OMU	N3-C2-N1	4.17	120.42	114.89
1	A2	628	OMU	N3-C2-N1	4.15	120.39	114.89
40	B5	4366	OMU	N3-C2-N1	4.13	120.38	114.89
1	A2	1327	OMU	N3-C2-N1	4.12	120.36	114.89
40	B5	2680	OMU	N3-C2-N1	4.10	120.33	114.89
1	A2	1443	OMU	N3-C2-N1	4.10	120.33	114.89
1	A2	172	OMU	N3-C2-N1	4.09	120.32	114.89
11	AT	53	5MU	O4-C4-C5	-4.09	120.16	124.90
1	A2	116	OMU	N3-C2-N1	4.09	120.32	114.89
1	A2	1852	MA6	N3-C2-N1	-4.08	122.30	128.68
1	A2	121	OMU	N3-C2-N1	4.07	120.30	114.89
40	B5	3616	PSU	C4-N3-C2	-4.05	120.51	126.34
40	B5	3973	OMU	N3-C2-N1	4.04	120.25	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1805	OMU	N3-C2-N1	4.03	120.24	114.89
1	A2	429	OMU	N3-C2-N1	4.02	120.22	114.89
40	B5	4042	PSU	C4-N3-C2	-4.01	120.56	126.34
40	B5	4188	PSU	C4-N3-C2	-4.01	120.57	126.34
40	B5	1799	PSU	C4-N3-C2	-4.00	120.57	126.34
40	B5	4711	PSU	C4-N3-C2	-4.00	120.57	126.34
40	B5	4099	PSU	C4-N3-C2	-3.99	120.59	126.34
40	B5	3490	PSU	C4-N3-C2	-3.99	120.59	126.34
40	B5	4203	PSU	C4-N3-C2	-3.98	120.61	126.34
40	B5	3652	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A2	1446	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A2	1233	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A2	1239	PSU	C4-N3-C2	-3.96	120.63	126.34
40	B5	3369	PSU	C4-N3-C2	-3.96	120.63	126.34
40	B5	4045	PSU	C4-N3-C2	-3.96	120.63	126.34
40	B5	4052	OMU	N3-C2-N1	3.96	120.15	114.89
40	B5	4149	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	1175	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	407	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	1644	PSU	C4-N3-C2	-3.96	120.64	126.34
40	B5	1801	PSU	C4-N3-C2	-3.95	120.64	126.34
42	B8	69	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	1289	OMU	N3-C2-N1	3.95	120.13	114.89
40	B5	4298	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	4193	5MC	C5-C6-N1	-3.94	119.28	123.34
40	B5	1731	PSU	C4-N3-C2	-3.94	120.66	126.34
42	B8	55	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	218	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	682	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	650	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	4435	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	2351	PSU	C4-N3-C2	-3.94	120.67	126.34
40	B5	1718	PSU	C4-N3-C2	-3.94	120.67	126.34
40	B5	3496	PSU	C4-N3-C2	-3.93	120.67	126.34
40	B5	3502	PSU	C4-N3-C2	-3.93	120.67	126.34
40	B5	3447	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A2	1046	PSU	C4-N3-C2	-3.93	120.68	126.34
40	B5	4267	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A2	573	PSU	C4-N3-C2	-3.92	120.68	126.34
1	A2	93	PSU	C4-N3-C2	-3.92	120.69	126.34
40	B5	3500	PSU	C4-N3-C2	-3.92	120.69	126.34
40	B5	4039	PSU	C4-N3-C2	-3.92	120.69	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	1491	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	1693	PSU	C4-N3-C2	-3.91	120.70	126.34
40	B5	1721	PSU	C4-N3-C2	-3.91	120.70	126.34
40	B5	4749	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	119	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A2	1348	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A2	1057	PSU	C4-N3-C2	-3.90	120.72	126.34
40	B5	4177	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	1626	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	105	PSU	C4-N3-C2	-3.90	120.72	126.34
40	B5	4374	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	652	PSU	C4-N3-C2	-3.90	120.73	126.34
1	A2	36	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	34	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	4322	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	4419	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	1638	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	3583	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	4246	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	4058	PSU	C4-N3-C2	-3.88	120.74	126.34
10	AJ	55	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A2	1047	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A2	864	PSU	C4-N3-C2	-3.88	120.75	126.34
40	B5	4278	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	1368	PSU	C4-N3-C2	-3.88	120.75	126.34
40	B5	4325	PSU	C4-N3-C2	-3.87	120.76	126.34
1	A2	1178	PSU	C4-N3-C2	-3.87	120.76	126.34
40	B5	1720	PSU	C4-N3-C2	-3.87	120.76	126.34
40	B5	3427	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	816	PSU	C4-N3-C2	-3.86	120.77	126.34
40	B5	3585	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	1245	PSU	C4-N3-C2	-3.86	120.77	126.34
40	B5	3462	PSU	C4-N3-C2	-3.86	120.77	126.34
40	B5	3554	PSU	C4-N3-C2	-3.86	120.78	126.34
40	B5	4217	PSU	C4-N3-C2	-3.86	120.78	126.34
40	B5	1683	PSU	C4-N3-C2	-3.85	120.79	126.34
40	B5	3466	PSU	C4-N3-C2	-3.85	120.79	126.34
1	A2	967	PSU	C4-N3-C2	-3.85	120.80	126.34
1	A2	815	PSU	C4-N3-C2	-3.84	120.80	126.34
1	A2	109	PSU	C4-N3-C2	-3.83	120.82	126.34
40	B5	4740	PSU	C4-N3-C2	-3.83	120.83	126.34
1	A2	210	PSU	C4-N3-C2	-3.82	120.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3371	PSU	C4-N3-C2	-3.82	120.83	126.34
40	B5	3576	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A2	610	PSU	C4-N3-C2	-3.82	120.83	126.34
40	B5	1537	PSU	C4-N3-C2	-3.82	120.84	126.34
11	AT	54	PSU	C4-N3-C2	-3.81	120.84	126.34
1	A2	867	PSU	C4-N3-C2	-3.81	120.84	126.34
1	A2	1005	PSU	C4-N3-C2	-3.81	120.86	126.34
40	B5	4169	PSU	C4-N3-C2	-3.80	120.86	126.34
40	B5	4107	PSU	C4-N3-C2	-3.80	120.87	126.34
1	A2	687	PSU	C4-N3-C2	-3.79	120.88	126.34
40	B5	2475	PSU	C4-N3-C2	-3.79	120.88	126.34
40	B5	3494	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A2	802	PSU	C4-N3-C2	-3.77	120.90	126.34
40	B5	4382	PSU	C4-N3-C2	-3.75	120.94	126.34
1	A2	823	PSU	C4-N3-C2	-3.71	120.99	126.34
40	B5	1632	PSU	C4-N3-C2	-3.70	121.01	126.34
1	A2	1082	PSU	C4-N3-C2	-3.69	121.02	126.34
1	A2	628	OMU	C5-C4-N3	3.68	120.34	114.84
10	AJ	54	5MU	O4-C4-C5	-3.66	120.66	124.90
1	A2	1852	MA6	N1-C6-N6	3.64	120.89	117.06
1	A2	1327	OMU	C5-C4-N3	3.60	120.22	114.84
40	B5	3514	5MC	C5-C6-N1	-3.59	119.64	123.34
40	B5	2680	OMU	C5-C4-N3	3.59	120.21	114.84
1	A2	355	OMU	C5-C4-N3	3.57	120.19	114.84
1	A2	116	OMU	C5-C4-N3	3.57	120.19	114.84
40	B5	4366	OMU	C5-C4-N3	3.57	120.17	114.84
1	A2	172	OMU	C5-C4-N3	3.56	120.17	114.84
40	B5	4435	PSU	O2-C2-N1	-3.55	118.88	122.79
40	B5	3657	OMU	C5-C4-N3	3.55	120.15	114.84
1	A2	121	OMU	C5-C4-N3	3.54	120.14	114.84
40	B5	4052	OMU	C5-C4-N3	3.54	120.14	114.84
40	B5	3973	OMU	C5-C4-N3	3.54	120.13	114.84
1	A2	1289	OMU	C5-C4-N3	3.53	120.12	114.84
1	A2	429	OMU	C5-C4-N3	3.52	120.11	114.84
10	AJ	54	5MU	C5-C6-N1	-3.49	119.75	123.34
1	A2	652	PSU	O2-C2-N1	-3.48	118.96	122.79
40	B5	3554	PSU	O2-C2-N1	-3.47	118.97	122.79
42	B8	55	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A2	1368	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A2	1805	OMU	C5-C4-N3	3.46	120.02	114.84
40	B5	4244	OMU	C5-C4-N3	3.46	120.02	114.84
40	B5	3616	PSU	O2-C2-N1	-3.46	118.98	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4278	PSU	O2-C2-N1	-3.46	118.98	122.79
1	A2	210	PSU	O2-C2-N1	-3.45	118.99	122.79
40	B5	1638	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	823	PSU	O2-C2-N1	-3.44	119.00	122.79
40	B5	3496	PSU	O2-C2-N1	-3.44	119.00	122.79
40	B5	1731	PSU	O2-C2-N1	-3.43	119.01	122.79
40	B5	3369	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A2	1057	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A2	650	PSU	O2-C2-N1	-3.43	119.01	122.79
40	B5	1801	PSU	O2-C2-N1	-3.43	119.02	122.79
40	B5	1718	PSU	O2-C2-N1	-3.43	119.02	122.79
40	B5	4749	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	1446	PSU	O2-C2-N1	-3.42	119.03	122.79
40	B5	3585	PSU	O2-C2-N1	-3.42	119.03	122.79
40	B5	2475	PSU	O2-C2-N1	-3.42	119.03	122.79
40	B5	3427	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	1443	OMU	C5-C4-N3	3.41	119.94	114.84
40	B5	2258	OMU	C5-C4-N3	3.41	119.94	114.84
40	B5	1720	PSU	O2-C2-N1	-3.41	119.04	122.79
10	AJ	55	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	815	PSU	O2-C2-N1	-3.41	119.04	122.79
40	B5	4267	PSU	O2-C2-N1	-3.40	119.04	122.79
40	B5	1491	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	3490	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A2	1233	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	4169	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	3966	6MZ	C9-N6-C6	-3.40	119.95	122.87
1	A2	1047	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A2	1626	PSU	O2-C2-N1	-3.39	119.06	122.79
40	B5	3462	PSU	O2-C2-N1	-3.39	119.06	122.79
40	B5	4188	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A2	407	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A2	1005	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4325	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	3494	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1082	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	3447	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1245	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1644	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4374	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4149	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4419	PSU	O2-C2-N1	-3.38	119.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4382	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	119	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1046	PSU	O2-C2-N1	-3.37	119.08	122.79
40	B5	3502	PSU	O2-C2-N1	-3.37	119.08	122.79
40	B5	4740	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	36	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	573	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1239	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	4322	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	682	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	4045	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	109	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	3583	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	4166	PSU	C4-N3-C2	-3.36	121.50	126.34
40	B5	3466	PSU	O2-C2-N1	-3.36	119.10	122.79
40	B5	4042	PSU	O2-C2-N1	-3.36	119.10	122.79
40	B5	4298	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1178	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4217	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4203	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4246	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	967	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4107	PSU	O2-C2-N1	-3.34	119.11	122.79
40	B5	4039	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A2	1693	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A2	864	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	1175	PSU	O2-C2-N1	-3.33	119.12	122.79
40	B5	1537	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	610	PSU	O2-C2-N1	-3.33	119.13	122.79
40	B5	4099	PSU	O2-C2-N1	-3.33	119.13	122.79
40	B5	3652	PSU	O2-C2-N1	-3.32	119.13	122.79
1	A2	218	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	93	PSU	O2-C2-N1	-3.31	119.14	122.79
40	B5	3500	PSU	O2-C2-N1	-3.31	119.14	122.79
40	B5	4177	PSU	O2-C2-N1	-3.31	119.15	122.79
1	A2	1249	B8N	C4-N3-C2	-3.31	121.28	125.46
1	A2	105	PSU	O2-C2-N1	-3.30	119.15	122.79
40	B5	4166	PSU	O2-C2-N1	-3.30	119.15	122.79
1	A2	802	PSU	O2-C2-N1	-3.30	119.16	122.79
40	B5	4058	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A2	867	PSU	O2-C2-N1	-3.29	119.17	122.79
42	B8	69	PSU	O2-C2-N1	-3.29	119.17	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	687	PSU	O2-C2-N1	-3.29	119.17	122.79
40	B5	3371	PSU	O2-C2-N1	-3.29	119.17	122.79
40	B5	1721	PSU	O2-C2-N1	-3.28	119.17	122.79
40	B5	3576	PSU	O2-C2-N1	-3.28	119.18	122.79
40	B5	3517	A2M	N3-C2-N1	-3.28	123.55	128.68
40	B5	1799	PSU	O2-C2-N1	-3.28	119.18	122.79
1	A2	1348	PSU	O2-C2-N1	-3.28	119.18	122.79
40	B5	2630	A2M	N3-C2-N1	-3.27	123.57	128.68
40	B5	2351	PSU	O2-C2-N1	-3.26	119.20	122.79
40	B5	1683	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	34	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	1679	A2M	N3-C2-N1	-3.24	123.61	128.68
40	B5	1489	A2M	N3-C2-N1	-3.23	123.62	128.68
40	B5	398	A2M	N3-C2-N1	-3.23	123.63	128.68
40	B5	4711	PSU	O2-C2-N1	-3.23	119.23	122.79
40	B5	1810	A2M	N3-C2-N1	-3.23	123.63	128.68
11	AT	53	5MU	C5-C6-N1	-3.22	120.03	123.34
40	B5	3492	A2M	N3-C2-N1	-3.21	123.66	128.68
1	A2	1384	A2M	N3-C2-N1	-3.21	123.66	128.68
1	A2	1851	MA6	N3-C2-N1	-3.20	123.68	128.68
1	A2	591	A2M	N3-C2-N1	-3.19	123.69	128.68
1	A2	27	A2M	N3-C2-N1	-3.19	123.69	128.68
40	B5	2244	A2M	N3-C2-N1	-3.19	123.69	128.68
40	B5	4269	A2M	N3-C2-N1	-3.19	123.70	128.68
1	A2	485	A2M	N3-C2-N1	-3.18	123.71	128.68
1	A2	159	A2M	N3-C2-N1	-3.17	123.72	128.68
40	B5	2206	A2M	N3-C2-N1	-3.17	123.73	128.68
1	A2	577	A2M	N3-C2-N1	-3.17	123.73	128.68
1	A2	1032	A2M	N3-C2-N1	-3.17	123.73	128.68
40	B5	3562	A2M	N3-C2-N1	-3.16	123.73	128.68
40	B5	4317	A2M	N3-C2-N1	-3.16	123.74	128.68
1	A2	166	A2M	N3-C2-N1	-3.16	123.74	128.68
1	A2	816	PSU	O2-C2-N1	-3.15	119.32	122.79
11	AT	54	PSU	O2-C2-N1	-3.15	119.32	122.79
40	B5	1270	A2M	N3-C2-N1	-3.15	123.75	128.68
40	B5	4336	A2M	N3-C2-N1	-3.15	123.76	128.68
1	A2	99	A2M	N3-C2-N1	-3.15	123.76	128.68
40	B5	3450	A2M	N3-C2-N1	-3.14	123.77	128.68
40	B5	3557	A2M	N3-C2-N1	-3.14	123.77	128.68
40	B5	1479	A2M	N3-C2-N1	-3.14	123.77	128.68
40	B5	2258	OMU	O4-C4-C5	-3.14	119.64	125.16
40	B5	400	A2M	N3-C2-N1	-3.14	123.78	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3599	A2M	N3-C2-N1	-3.14	123.78	128.68
40	B5	3456	A2M	N3-C2-N1	-3.13	123.78	128.68
1	A2	469	A2M	N3-C2-N1	-3.13	123.79	128.68
40	B5	3966	6MZ	N3-C2-N1	-3.12	123.80	128.68
40	B5	1632	PSU	O2-C2-N1	-3.12	119.36	122.79
40	B5	2658	A2M	N3-C2-N1	-3.12	123.81	128.68
1	A2	513	A2M	N3-C2-N1	-3.11	123.81	128.68
1	A2	669	A2M	N3-C2-N1	-3.11	123.82	128.68
1	A2	429	OMU	O4-C4-C5	-3.05	119.80	125.16
40	B5	2680	OMU	O4-C4-C5	-3.02	119.84	125.16
1	A2	116	OMU	O4-C4-C5	-3.01	119.86	125.16
1	A2	628	OMU	O4-C4-C5	-3.00	119.89	125.16
1	A2	172	OMU	O4-C4-C5	-2.98	119.91	125.16
40	B5	4366	OMU	O4-C4-C5	-2.97	119.94	125.16
1	A2	1851	MA6	C4-C5-N7	-2.96	106.31	109.40
40	B5	3657	OMU	O4-C4-C5	-2.96	119.95	125.16
1	A2	1327	OMU	O4-C4-C5	-2.95	119.96	125.16
1	A2	1249	B8N	N3-C2-N1	2.95	120.93	116.76
40	B5	3973	OMU	O4-C4-C5	-2.95	119.97	125.16
1	A2	121	OMU	O4-C4-C5	-2.95	119.98	125.16
1	A2	1805	OMU	O4-C4-C5	-2.92	120.03	125.16
1	A2	1289	OMU	O4-C4-C5	-2.92	120.03	125.16
1	A2	1443	OMU	O4-C4-C5	-2.91	120.04	125.16
40	B5	4244	OMU	O4-C4-C5	-2.90	120.06	125.16
40	B5	4052	OMU	O4-C4-C5	-2.90	120.06	125.16
1	A2	355	OMU	O4-C4-C5	-2.88	120.09	125.16
40	B5	1489	A2M	C4-C5-N7	-2.86	106.41	109.40
1	A2	1833	6MZ	N3-C2-N1	-2.80	124.30	128.68
1	A2	1852	MA6	C4-C5-N7	-2.80	106.48	109.40
1	A2	669	A2M	C4-C5-N7	-2.75	106.54	109.40
40	B5	4336	A2M	C4-C5-N7	-2.72	106.56	109.40
40	B5	2258	OMU	C1'-N1-C2	2.72	122.49	117.57
1	A2	166	A2M	C4-C5-N7	-2.71	106.57	109.40
40	B5	3456	A2M	C4-C5-N7	-2.70	106.58	109.40
1	A2	159	A2M	C4-C5-N7	-2.70	106.58	109.40
40	B5	3562	A2M	C4-C5-N7	-2.70	106.58	109.40
40	B5	4269	A2M	C4-C5-N7	-2.70	106.59	109.40
1	A2	513	A2M	C4-C5-N7	-2.70	106.59	109.40
40	B5	1270	A2M	C4-C5-N7	-2.70	106.59	109.40
40	B5	2658	A2M	C4-C5-N7	-2.70	106.59	109.40
40	B5	3492	A2M	C4-C5-N7	-2.69	106.60	109.40
40	B5	2244	A2M	C4-C5-N7	-2.68	106.61	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	398	A2M	C4-C5-N7	-2.68	106.61	109.40
1	A2	1032	A2M	C4-C5-N7	-2.68	106.61	109.40
40	B5	4317	A2M	C4-C5-N7	-2.67	106.62	109.40
40	B5	2206	A2M	C4-C5-N7	-2.67	106.62	109.40
40	B5	1810	A2M	C4-C5-N7	-2.67	106.62	109.40
40	B5	3557	A2M	C4-C5-N7	-2.65	106.63	109.40
1	A2	469	A2M	C4-C5-N7	-2.65	106.64	109.40
40	B5	3450	A2M	C4-C5-N7	-2.65	106.64	109.40
1	A2	99	A2M	C4-C5-N7	-2.64	106.64	109.40
1	A2	1679	A2M	C4-C5-N7	-2.64	106.65	109.40
40	B5	400	A2M	C4-C5-N7	-2.64	106.65	109.40
1	A2	27	A2M	C4-C5-N7	-2.64	106.65	109.40
1	A2	485	A2M	C4-C5-N7	-2.63	106.66	109.40
1	A2	1640	G7M	CN7-N7-C8	-2.61	112.86	125.43
40	B5	3599	A2M	C4-C5-N7	-2.61	106.68	109.40
11	AT	53	5MU	C1'-N1-C2	2.60	122.28	117.57
1	A2	1384	A2M	C4-C5-N7	-2.60	106.69	109.40
40	B5	1479	A2M	C4-C5-N7	-2.59	106.70	109.40
1	A2	1338	4AC	C5-C4-N4	-2.56	118.47	122.92
1	A2	577	A2M	C4-C5-N7	-2.56	106.73	109.40
40	B5	2630	A2M	C4-C5-N7	-2.54	106.75	109.40
40	B5	3966	6MZ	C4-C5-N7	-2.54	106.75	109.40
40	B5	4193	5MC	C5-C4-N3	-2.51	118.96	121.67
40	B5	3517	A2M	C4-C5-N7	-2.51	106.78	109.40
40	B5	3514	5MC	C5-C4-N3	-2.51	118.96	121.67
1	A2	591	A2M	C4-C5-N7	-2.49	106.80	109.40
34	Au	1	AME	O-C-CA	-2.48	118.28	124.78
43	BA	216	V5N	O-C-CA	-2.47	118.30	124.78
1	A2	1843	4AC	C6-C5-C4	2.45	119.96	116.96
40	B5	4166	PSU	C6-C5-C4	-2.43	116.50	118.20
1	A2	1338	4AC	C6-C5-C4	2.42	119.93	116.96
69	Ba	39	V5N	O-C-CA	-2.41	118.45	124.78
40	B5	4244	OMU	O2-C2-N1	-2.41	119.59	122.79
1	A2	1843	4AC	C5-C4-N4	-2.40	118.75	122.92
40	B5	2719	OMG	C5-C6-N1	2.39	118.18	113.95
40	B5	2207	OMG	C5-C6-N1	2.38	118.16	113.95
1	A2	868	OMG	C8-N7-C5	2.38	107.52	102.99
40	B5	4116	OMG	C5-C6-N1	2.37	118.14	113.95
1	A2	1448	OMG	C8-N7-C5	2.37	107.51	102.99
40	B5	4138	OMG	C5-C6-N1	2.37	118.14	113.95
13	AZ	2	SAC	O-C-CA	-2.36	118.59	124.78
40	B5	3550	UY1	C6-C5-C4	2.36	119.85	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1833	6MZ	C4-C5-N7	-2.36	106.94	109.40
40	B5	1260	OMG	C8-N7-C5	2.36	107.48	102.99
31	Ar	2	SAC	O-C-CA	-2.36	118.61	124.78
40	B5	3550	UY1	O2-C2-N1	-2.36	120.20	122.79
40	B5	4383	OMG	C8-N7-C5	2.35	107.47	102.99
1	A2	628	OMU	O2-C2-N1	-2.35	119.66	122.79
1	A2	645	OMG	C8-N7-C5	2.34	107.45	102.99
1	A2	602	OMG	C5-C6-N1	2.34	118.08	113.95
1	A2	1491	OMG	C5-C6-N1	2.34	118.08	113.95
1	A2	1329	OMG	C8-N7-C5	2.33	107.44	102.99
40	B5	4240	OMG	C5-C6-N1	2.33	118.07	113.95
40	B5	1477	OMG	C8-N7-C5	2.33	107.44	102.99
40	B5	3974	OMG	C8-N7-C5	2.33	107.43	102.99
42	B8	75	OMG	C8-N7-C5	2.33	107.43	102.99
40	B5	4245	OMG	C8-N7-C5	2.33	107.43	102.99
40	B5	2267	OMG	C8-N7-C5	2.33	107.42	102.99
40	B5	2207	OMG	C8-N7-C5	2.32	107.42	102.99
40	B5	4369	OMG	C8-N7-C5	2.32	107.41	102.99
40	B5	1477	OMG	C5-C6-N1	2.32	118.04	113.95
40	B5	4116	OMG	C8-N7-C5	2.32	107.40	102.99
40	B5	3359	OMG	C8-N7-C5	2.31	107.40	102.99
40	B5	1260	OMG	C5-C6-N1	2.31	118.04	113.95
40	B5	2267	OMG	C5-C6-N1	2.31	118.03	113.95
40	B5	3974	OMG	C5-C6-N1	2.31	118.03	113.95
40	B5	3676	OMG	C8-N7-C5	2.31	107.39	102.99
40	B5	3359	OMG	C5-C6-N1	2.31	118.03	113.95
1	A2	510	OMG	C5-C6-N1	2.31	118.03	113.95
40	B5	4245	OMG	C5-C6-N1	2.31	118.03	113.95
40	B5	1580	OMG	C8-N7-C5	2.30	107.38	102.99
40	B5	4364	OMG	C8-N7-C5	2.30	107.38	102.99
1	A2	1491	OMG	C8-N7-C5	2.30	107.38	102.99
1	A2	868	OMG	C5-C6-N1	2.30	118.02	113.95
1	A2	1329	OMG	C5-C6-N1	2.30	118.02	113.95
40	B5	3524	OMG	C5-C6-N1	2.30	118.02	113.95
40	B5	4369	OMG	C5-C6-N1	2.30	118.01	113.95
1	A2	645	OMG	C5-C6-N1	2.30	118.01	113.95
40	B5	2719	OMG	C8-N7-C5	2.30	107.37	102.99
40	B5	4383	OMG	C5-C6-N1	2.30	118.01	113.95
40	B5	3476	OMG	C5-C6-N1	2.29	118.00	113.95
42	B8	75	OMG	C5-C6-N1	2.29	118.00	113.95
40	B5	4138	OMG	C8-N7-C5	2.29	107.36	102.99
1	A2	437	OMG	C8-N7-C5	2.29	107.35	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4240	OMG	C8-N7-C5	2.29	107.35	102.99
40	B5	1266	1MA	C8-N7-C5	2.28	107.34	102.99
40	B5	1266	1MA	C5-C6-N1	2.28	117.30	113.90
40	B5	3631	OMG	C8-N7-C5	2.28	107.34	102.99
40	B5	4364	OMG	C5-C6-N1	2.28	117.98	113.95
40	B5	3524	OMG	C8-N7-C5	2.28	107.33	102.99
40	B5	2194	OMC	O2-C2-N3	-2.28	118.63	122.33
1	A2	437	OMG	C5-C6-N1	2.28	117.97	113.95
40	B5	3942	OMG	C5-C6-N1	2.28	117.97	113.95
11	AT	53	5MU	C1'-N1-C6	-2.28	117.33	121.12
1	A2	510	OMG	C8-N7-C5	2.27	107.32	102.99
40	B5	3631	OMG	C5-C6-N1	2.27	117.97	113.95
84	Br	2	SAC	O-C-CA	-2.27	118.82	124.78
1	A2	684	OMG	C5-C6-N1	2.27	117.96	113.95
40	B5	3476	OMG	C8-N7-C5	2.25	107.28	102.99
40	B5	2630	A2M	C2'-C3'-C4'	2.25	106.88	101.99
40	B5	3676	OMG	C5-C6-N1	2.25	117.92	113.95
1	A2	602	OMG	C8-N7-C5	2.24	107.27	102.99
1	A2	684	OMG	C8-N7-C5	2.24	107.27	102.99
40	B5	3942	OMG	C8-N7-C5	2.24	107.26	102.99
40	B5	2265	OMC	O2-C2-N3	-2.24	118.68	122.33
40	B5	1580	OMG	C5-C6-N1	2.24	117.91	113.95
40	B5	3514	5MC	O2-C2-N3	-2.22	118.71	122.33
1	A2	1448	OMG	C5-C6-N1	2.22	117.87	113.95
1	A2	1249	B8N	C5-C4-N3	2.22	120.28	116.17
1	A2	429	OMU	C1'-N1-C2	2.20	121.56	117.57
1	A2	1327	OMU	O2-C2-N1	-2.20	119.86	122.79
1	A2	1704	OMC	O2-C2-N3	-2.18	118.78	122.33
1	A2	463	OMC	O2-C2-N3	-2.16	118.82	122.33
40	B5	2680	OMU	O2-C2-N1	-2.14	119.94	122.79
36	Aw	62	HY3	O-C-CA	-2.13	118.90	124.83
1	A2	1443	OMU	C1'-N1-C2	2.13	121.42	117.57
40	B5	1632	PSU	O4'-C1'-C2'	2.10	108.11	105.14
40	B5	3573	OMC	O2-C2-N3	-2.10	118.92	122.33
40	B5	3601	OMC	O2-C2-N3	-2.09	118.93	122.33
1	A2	1392	OMC	O2-C2-N3	-2.09	118.93	122.33
40	B5	1799	PSU	C5-C6-N1	-2.08	118.99	122.11
10	AJ	54	5MU	O2-C2-N1	-2.08	120.02	122.79
40	B5	1266	1MA	N1-C2-N3	-2.06	123.62	126.02
40	B5	4188	PSU	C5-C6-N1	-2.04	119.05	122.11
40	B5	4711	PSU	C5-C6-N1	-2.04	119.05	122.11
1	A2	1239	PSU	C5-C6-N1	-2.03	119.06	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1289	OMU	C1'-N1-C2	2.03	121.24	117.57
1	A2	1644	PSU	C5-C6-N1	-2.02	119.08	122.11
1	A2	1175	PSU	C5-C6-N1	-2.01	119.10	122.11

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	O4'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	429	OMU	O4'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	684	OMG	C3'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'
40	B5	1720	PSU	C3'-C4'-C5'-O5'
40	B5	2207	OMG	O4'-C4'-C5'-O5'
40	B5	2630	A2M	C1'-C2'-O2'-CM'
40	B5	3433	OMC	C2'-C1'-N1-C2
40	B5	3433	OMC	C2'-C1'-N1-C6
40	B5	4166	PSU	C2'-C1'-C5-C4
40	B5	4166	PSU	C2'-C1'-C5-C6
40	B5	4278	PSU	O4'-C4'-C5'-O5'
40	B5	4336	A2M	C4'-C5'-O5'-P
40	B5	4382	PSU	O4'-C1'-C5-C4
40	B5	4382	PSU	O4'-C1'-C5-C6
40	B5	4382	PSU	C3'-C4'-C5'-O5'
44	BB	245	HIC	CA-CB-CG-ND1
1	A2	1249	B8N	N34-C33-C34-O35
1	A2	1338	4AC	N3-C4-N4-C7
1	A2	1338	4AC	C5-C4-N4-C7
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1843	4AC	C5-C4-N4-C7
1	A2	1843	4AC	O7-C7-N4-C4
1	A2	1843	4AC	CM7-C7-N4-C4
43	BA	216	V5N	O-C-CA-CB
45	BC	2	AYA	CM-CT-N-CA
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	684	OMG	O4'-C4'-C5'-O5'
40	B5	1489	A2M	O4'-C4'-C5'-O5'
40	B5	3517	A2M	O4'-C4'-C5'-O5'
40	B5	3517	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	B5	4278	PSU	C3'-C4'-C5'-O5'
45	BC	2	AYA	OT-CT-N-CA
1	A2	1249	B8N	N34-C33-C34-O36
34	Au	1	AME	CT2-CT1-N-CA
34	Au	1	AME	OT-CT1-N-CA
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	C3'-C4'-C5'-O5'
1	A2	669	A2M	C3'-C4'-C5'-O5'
40	B5	2207	OMG	C3'-C4'-C5'-O5'
40	B5	4382	PSU	O4'-C4'-C5'-O5'
40	B5	3550	UY1	C1'-C2'-O2'-CM2
1	A2	1448	OMG	O4'-C4'-C5'-O5'
40	B5	4193	5MC	C2'-C1'-N1-C6
40	B5	398	A2M	O4'-C4'-C5'-O5'
40	B5	1489	A2M	C3'-C4'-C5'-O5'
40	B5	1720	PSU	O4'-C4'-C5'-O5'
40	B5	3450	A2M	O4'-C4'-C5'-O5'
1	A2	513	A2M	C3'-C4'-C5'-O5'
40	B5	3631	OMG	C3'-C2'-O2'-CM2
40	B5	4193	5MC	O4'-C1'-N1-C6
40	B5	4193	5MC	C2'-C1'-N1-C2
45	BC	2	AYA	C-CA-N-CT
1	A2	645	OMG	C4'-C5'-O5'-P
40	B5	3550	UY1	C4'-C5'-O5'-P
13	AZ	2	SAC	C-CA-N-C1A
13	AZ	2	SAC	CB-CA-N-C1A
1	A2	437	OMG	C3'-C2'-O2'-CM2
40	B5	4282	OMC	C3'-C2'-O2'-CM2
40	B5	3676	OMG	C4'-C5'-O5'-P
1	A2	27	A2M	O4'-C4'-C5'-O5'
1	A2	868	OMG	C3'-C4'-C5'-O5'
40	B5	3494	PSU	C3'-C4'-C5'-O5'
1	A2	1249	B8N	C32-C33-C34-O36
1	A2	868	OMG	C4'-C5'-O5'-P
1	A2	1852	MA6	C4'-C5'-O5'-P
40	B5	3576	PSU	C4'-C5'-O5'-P
40	B5	4246	PSU	C4'-C5'-O5'-P
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	116	OMU	O4'-C4'-C5'-O5'
1	A2	469	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	B5	1284	OMC	O4'-C4'-C5'-O5'
40	B5	4193	5MC	O4'-C1'-N1-C2
40	B5	3619	OMC	C4'-C5'-O5'-P
1	A2	510	OMG	C3'-C2'-O2'-CM2
1	A2	1289	OMU	C3'-C2'-O2'-CM2
1	A2	1491	OMG	C3'-C2'-O2'-CM2
40	B5	2267	OMG	C3'-C2'-O2'-CM2
40	B5	3657	OMU	C3'-C2'-O2'-CM2
40	B5	4052	OMU	C3'-C2'-O2'-CM2
40	B5	4369	OMG	C3'-C2'-O2'-CM2
1	A2	1249	B8N	C32-C33-C34-O35
40	B5	3433	OMC	O4'-C1'-N1-C6
40	B5	4278	PSU	C4'-C5'-O5'-P
1	A2	684	OMG	C3'-C2'-O2'-CM2
40	B5	1820	OMC	C3'-C2'-O2'-CM2
40	B5	2680	OMU	C3'-C2'-O2'-CM2
40	B5	4366	OMU	C3'-C2'-O2'-CM2
1	A2	1704	OMC	O4'-C4'-C5'-O5'
1	A2	868	OMG	O4'-C4'-C5'-O5'
1	A2	1032	A2M	O4'-C4'-C5'-O5'
40	B5	398	A2M	C3'-C4'-C5'-O5'
40	B5	3450	A2M	C3'-C4'-C5'-O5'
1	A2	1704	OMC	C1'-C2'-O2'-CM2
1	A2	1704	OMC	C3'-C2'-O2'-CM2
40	B5	3573	OMC	C3'-C2'-O2'-CM2
40	B5	3433	OMC	O4'-C1'-N1-C2
1	A2	591	A2M	C3'-C4'-C5'-O5'
40	B5	2194	OMC	O4'-C4'-C5'-O5'
40	B5	3494	PSU	O4'-C4'-C5'-O5'
11	AT	53	5MU	C2'-C1'-N1-C2
40	B5	398	A2M	C3'-C2'-O2'-CM'
40	B5	1260	OMG	C3'-C2'-O2'-CM2
40	B5	3476	OMG	C3'-C2'-O2'-CM2
40	B5	3619	OMC	C3'-C2'-O2'-CM2
1	A2	27	A2M	C3'-C4'-C5'-O5'
40	B5	2194	OMC	C2'-C1'-N1-C2
1	A2	1448	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 624 ligands modelled in this entry, 357 are monoatomic and 266 are unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
91	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	SPD	B5	4901	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	1249:B8N	O3'	1250:C	P	3.10

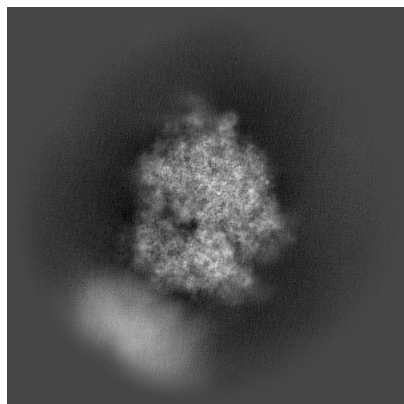
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12759. These allow visual inspection of the internal detail of the map and identification of artifacts.

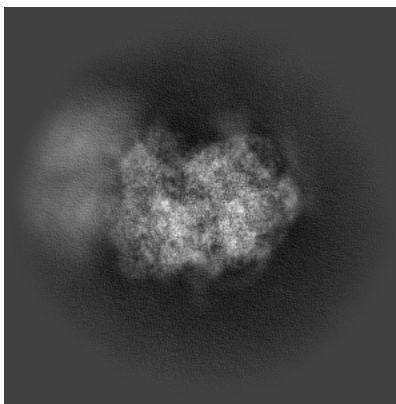
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

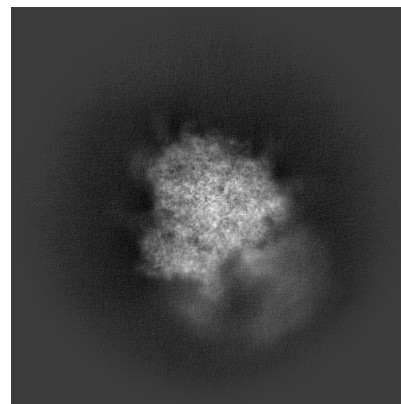
6.1.1 Primary map



X

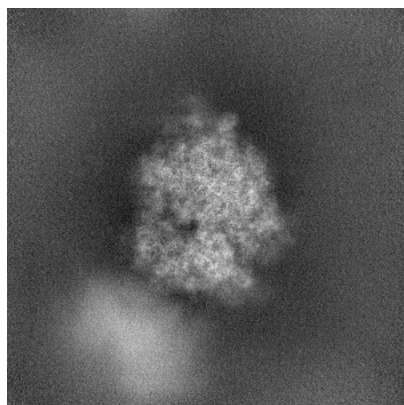


Y

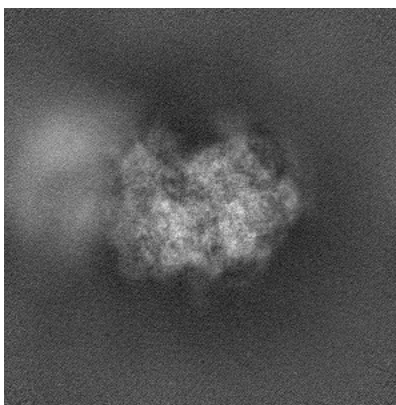


Z

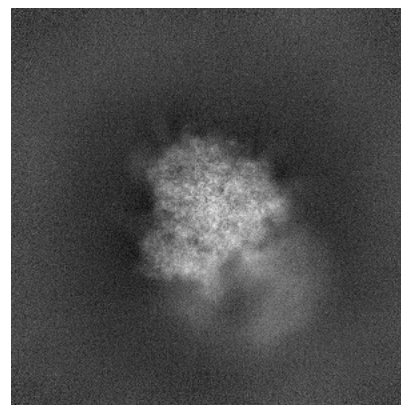
6.1.2 Raw map



X



Y

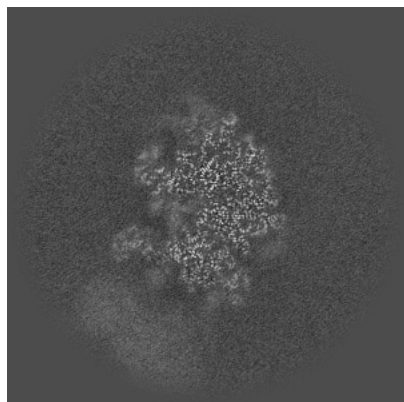


Z

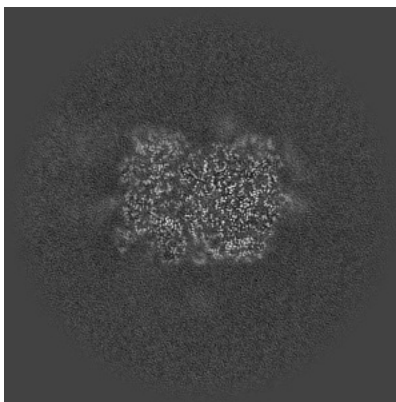
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

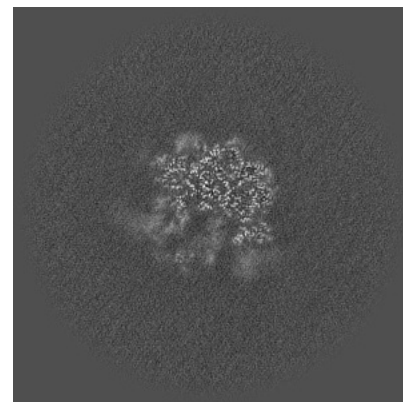
6.2.1 Primary map



X Index: 280

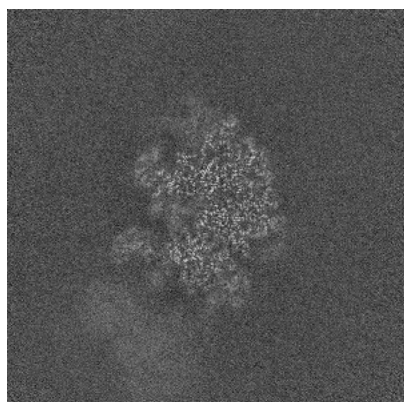


Y Index: 280

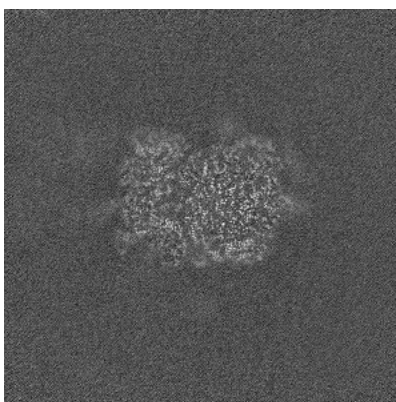


Z Index: 280

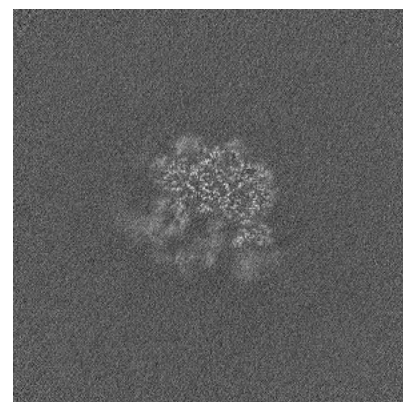
6.2.2 Raw map



X Index: 280



Y Index: 280

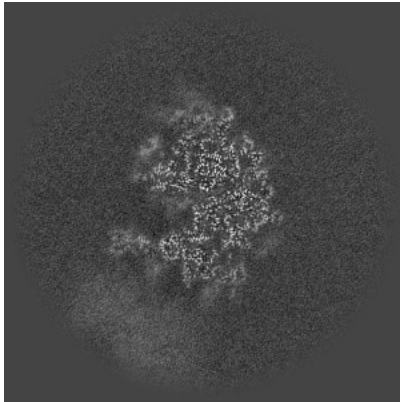


Z Index: 280

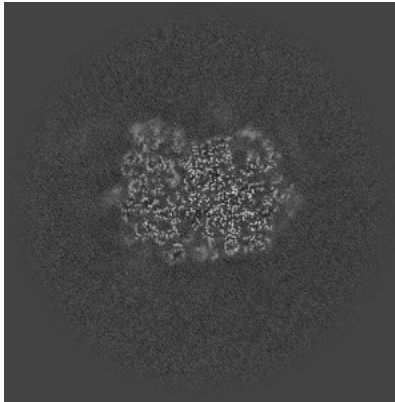
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

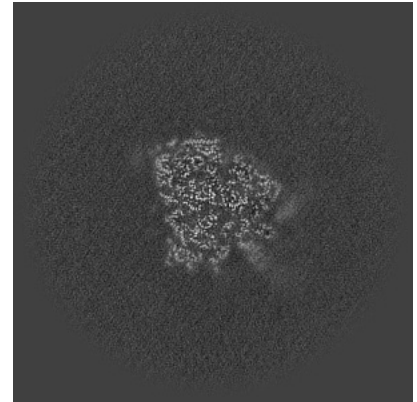
6.3.1 Primary map



X Index: 285

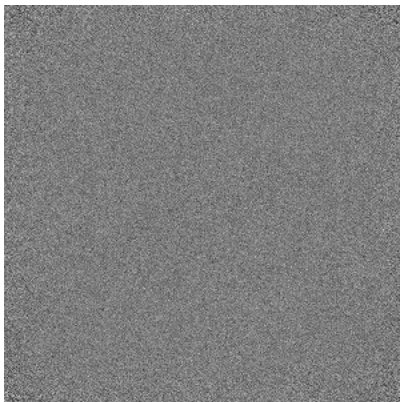


Y Index: 290

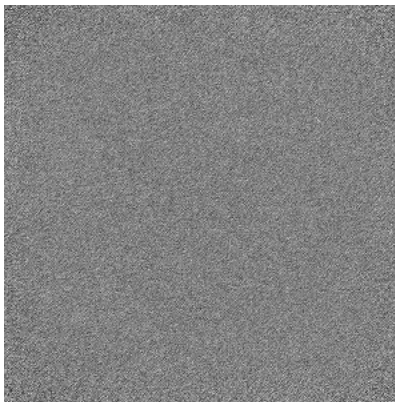


Z Index: 314

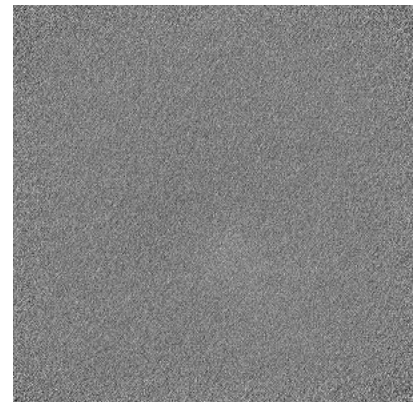
6.3.2 Raw map



X Index: 0



Y Index: 0

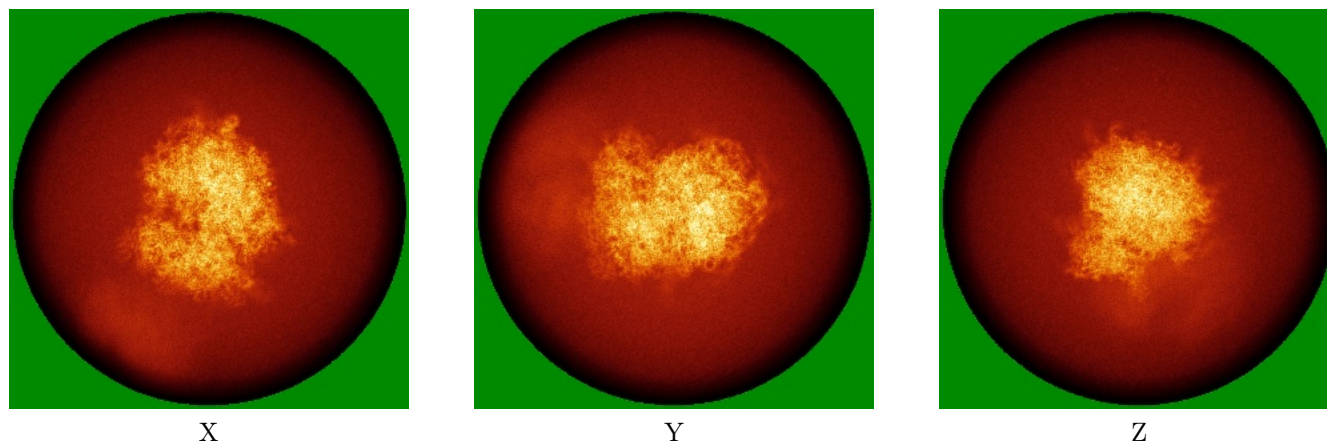


Z Index: 0

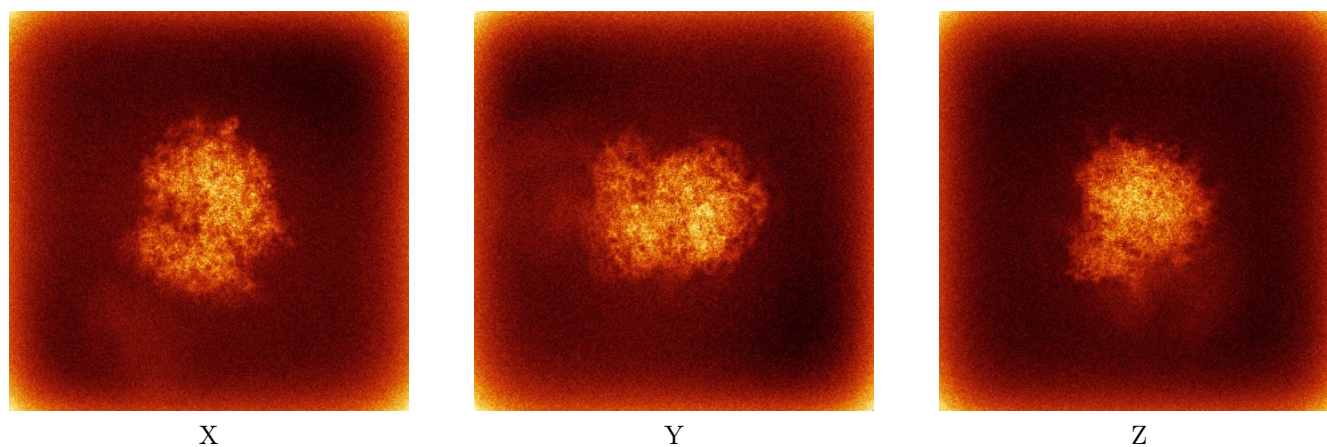
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



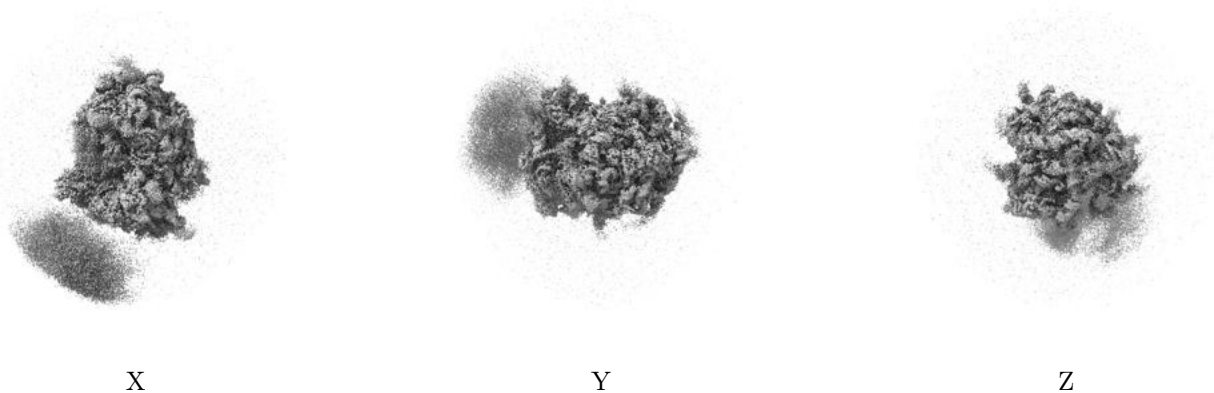
6.4.2 Raw map



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.

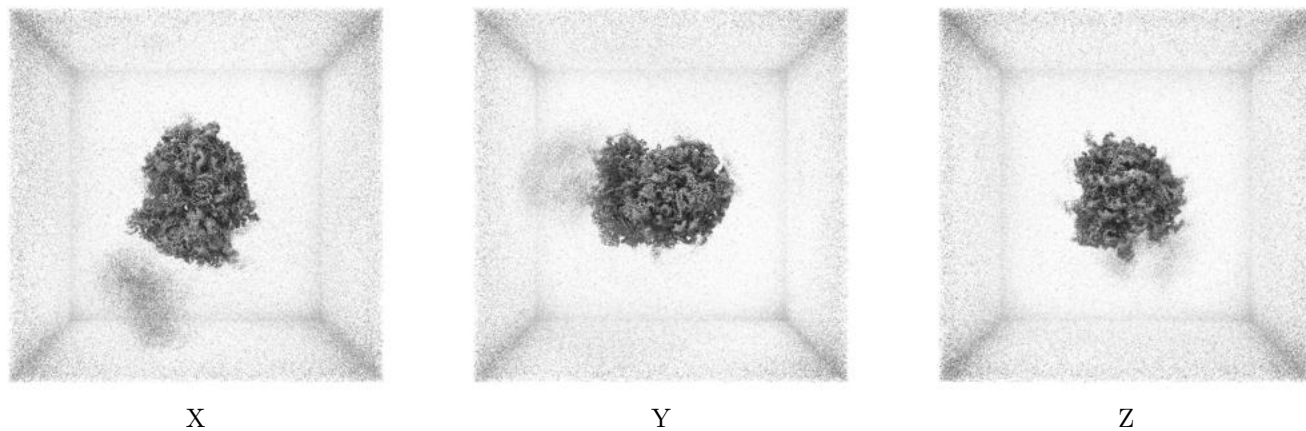
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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



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.

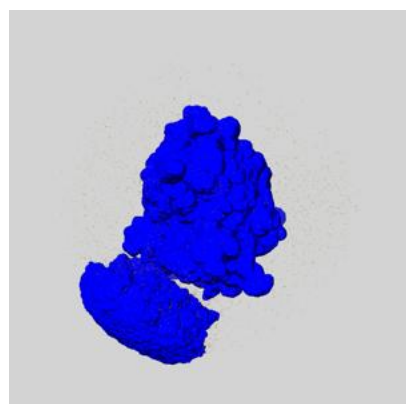
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

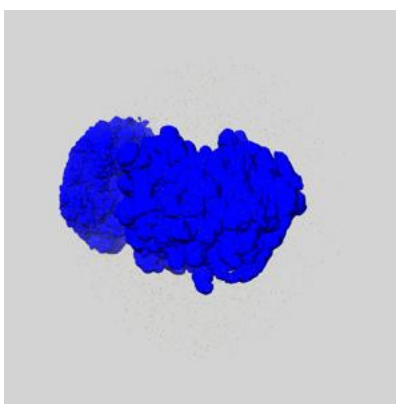
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

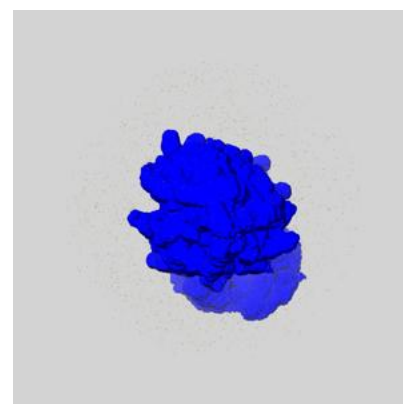
6.6.1 emd_12759_msk_1.map [i](#)



X

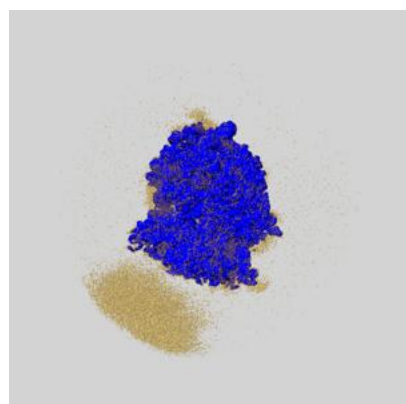


Y

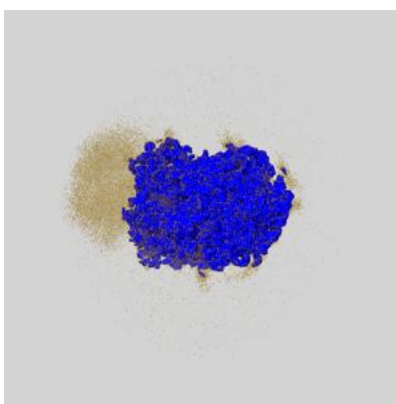


Z

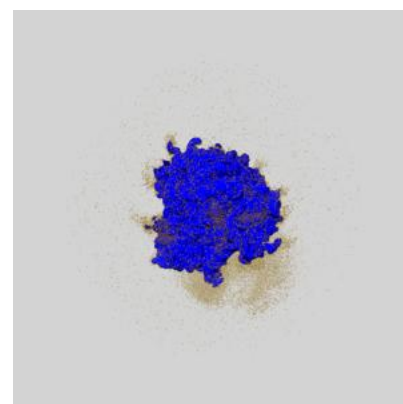
6.6.2 emd_12759_msk_2.map [i](#)



X



Y

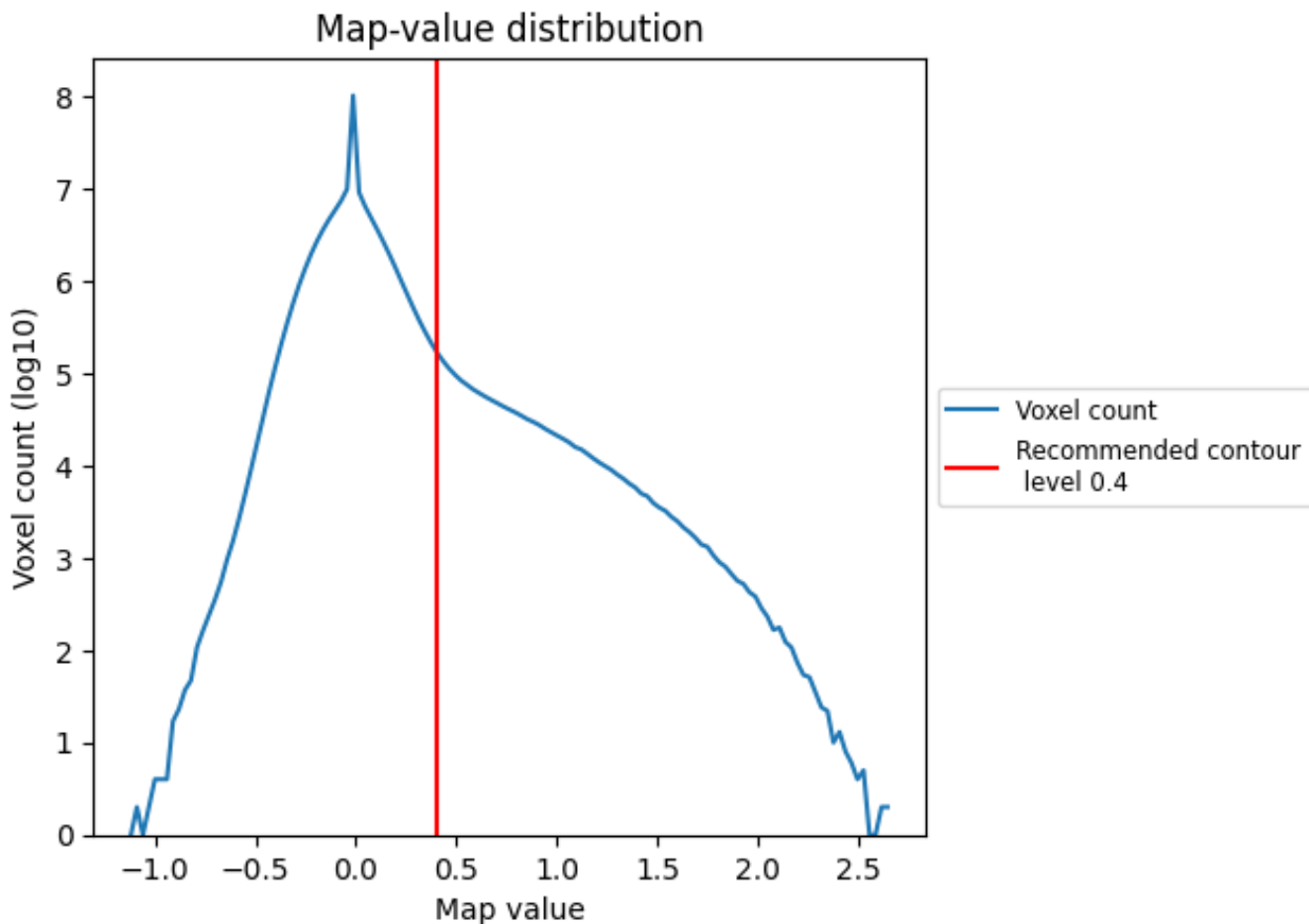


Z

7 Map analysis [i](#)

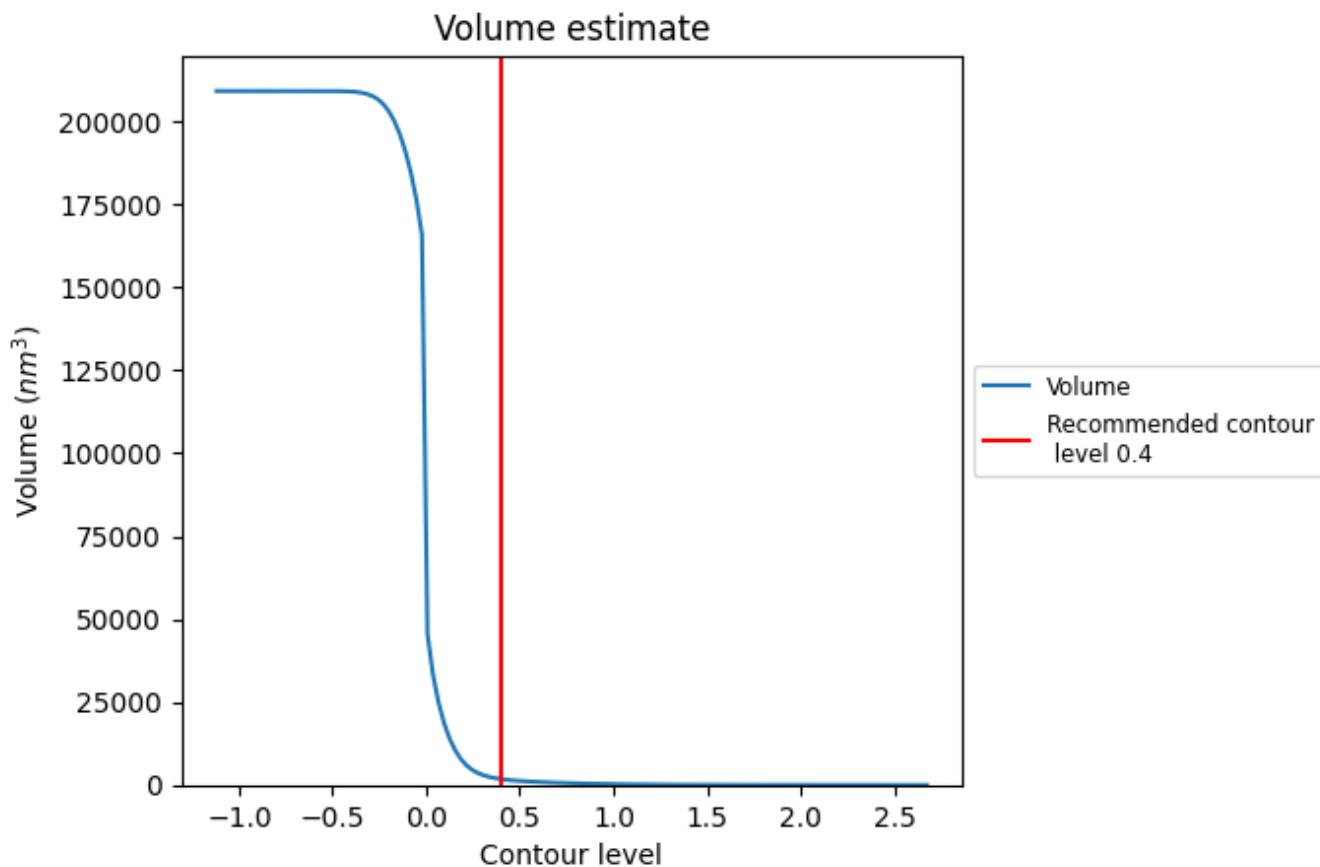
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

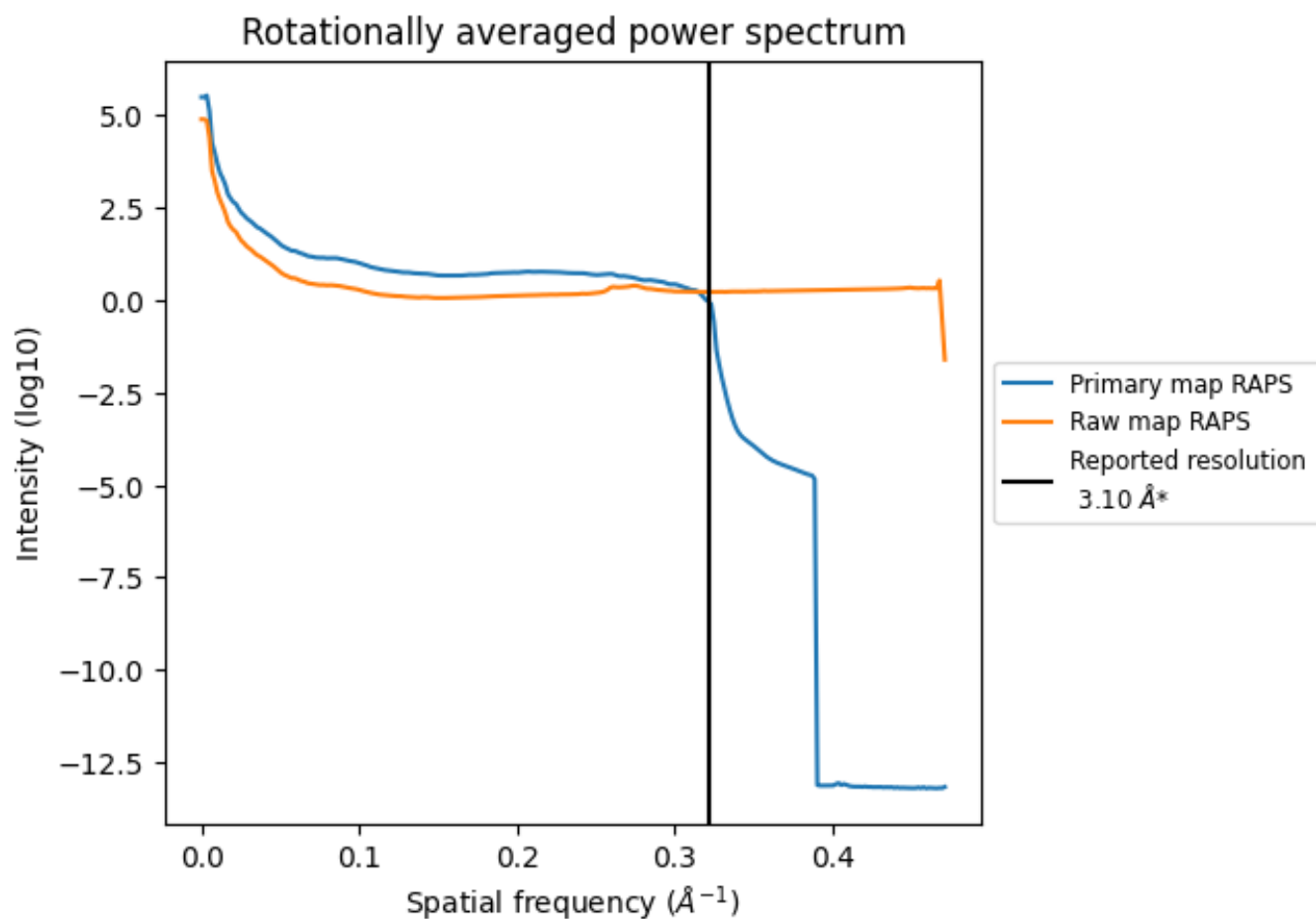
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771 nm^3 ; this corresponds to an approximate mass of 1600 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](#)

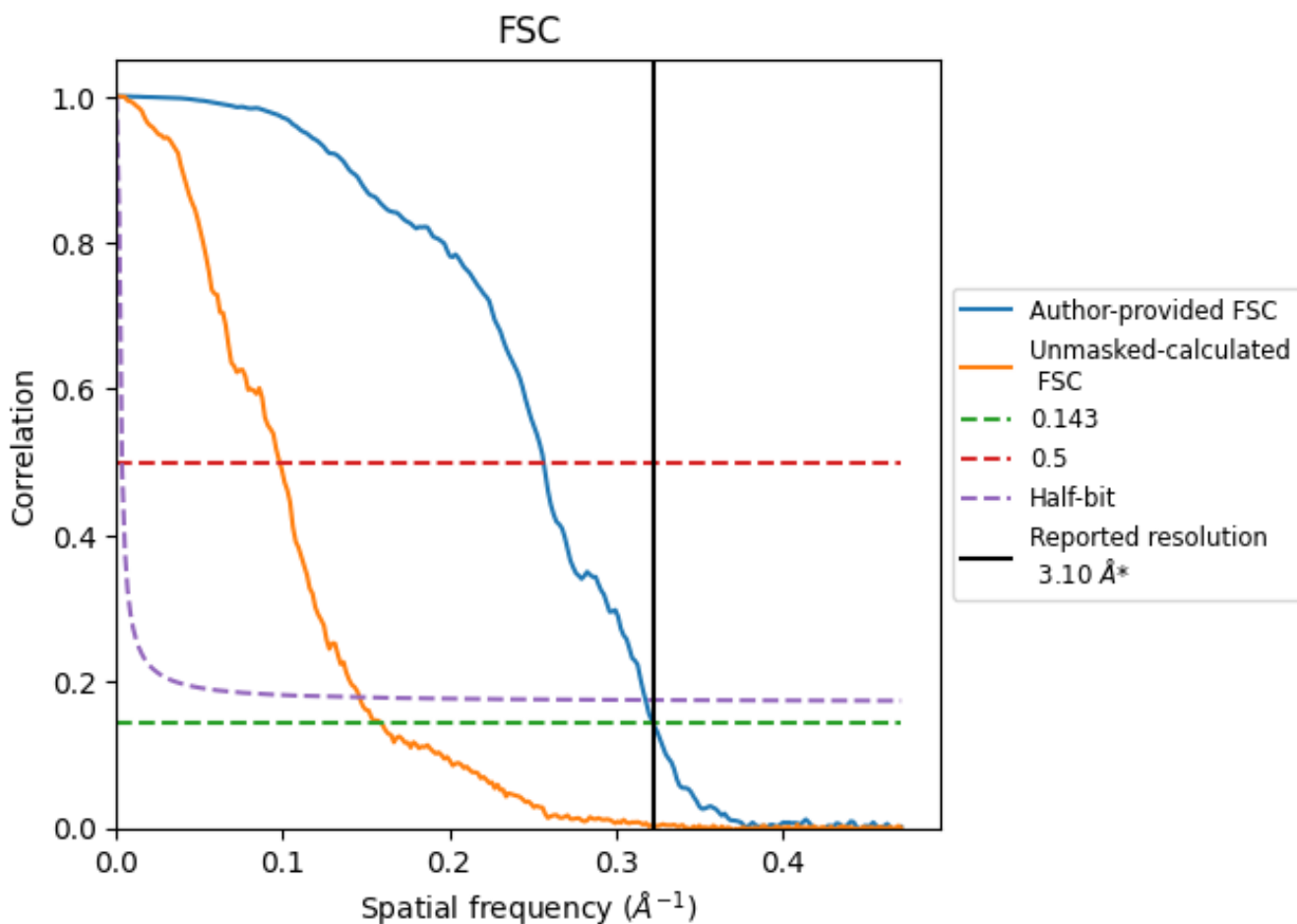


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

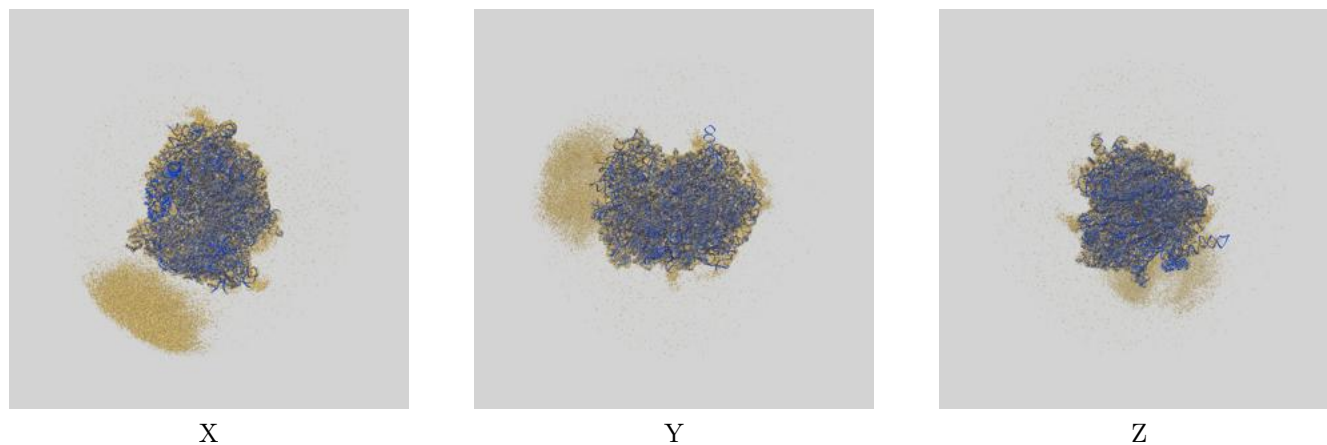
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.89	3.14
Unmasked-calculated*	6.29	10.19	6.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

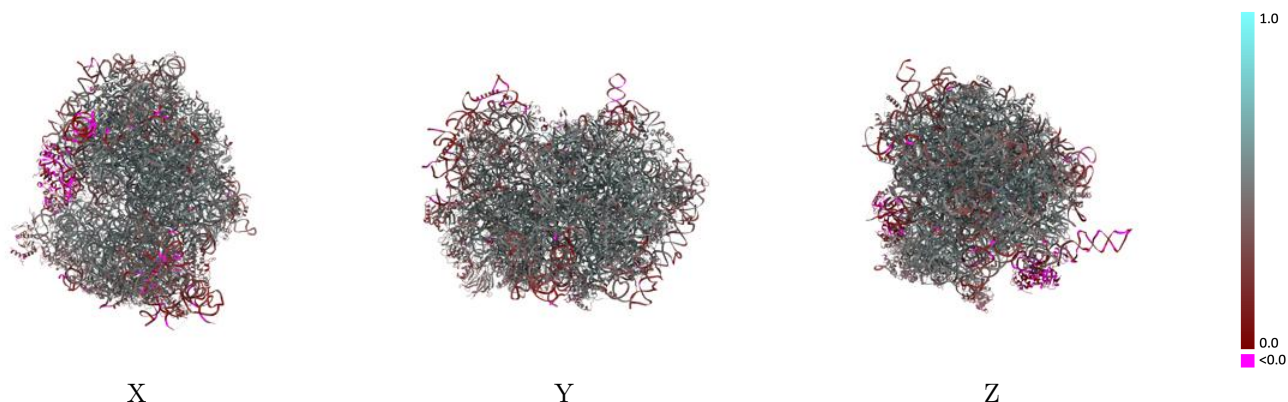
This section contains information regarding the fit between EMDB map EMD-12759 and PDB model 7O81. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



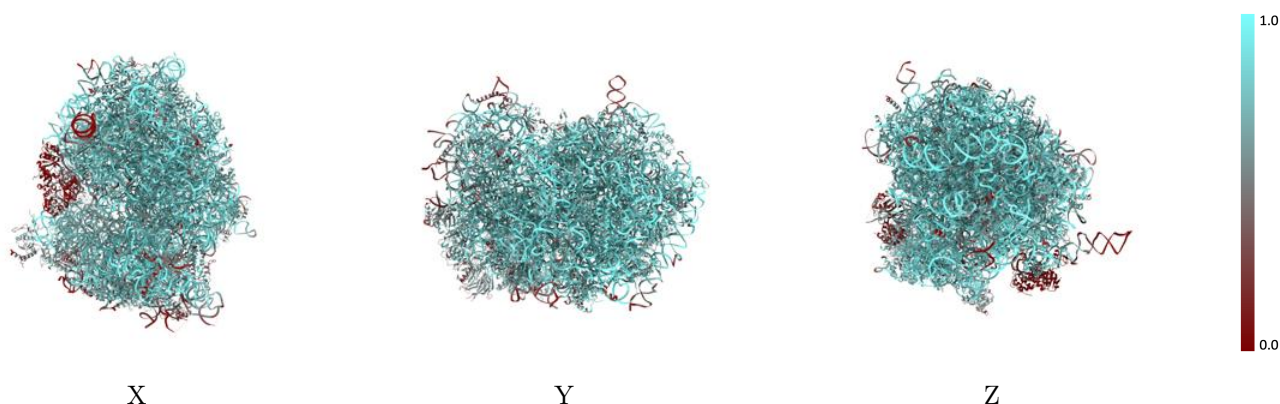
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



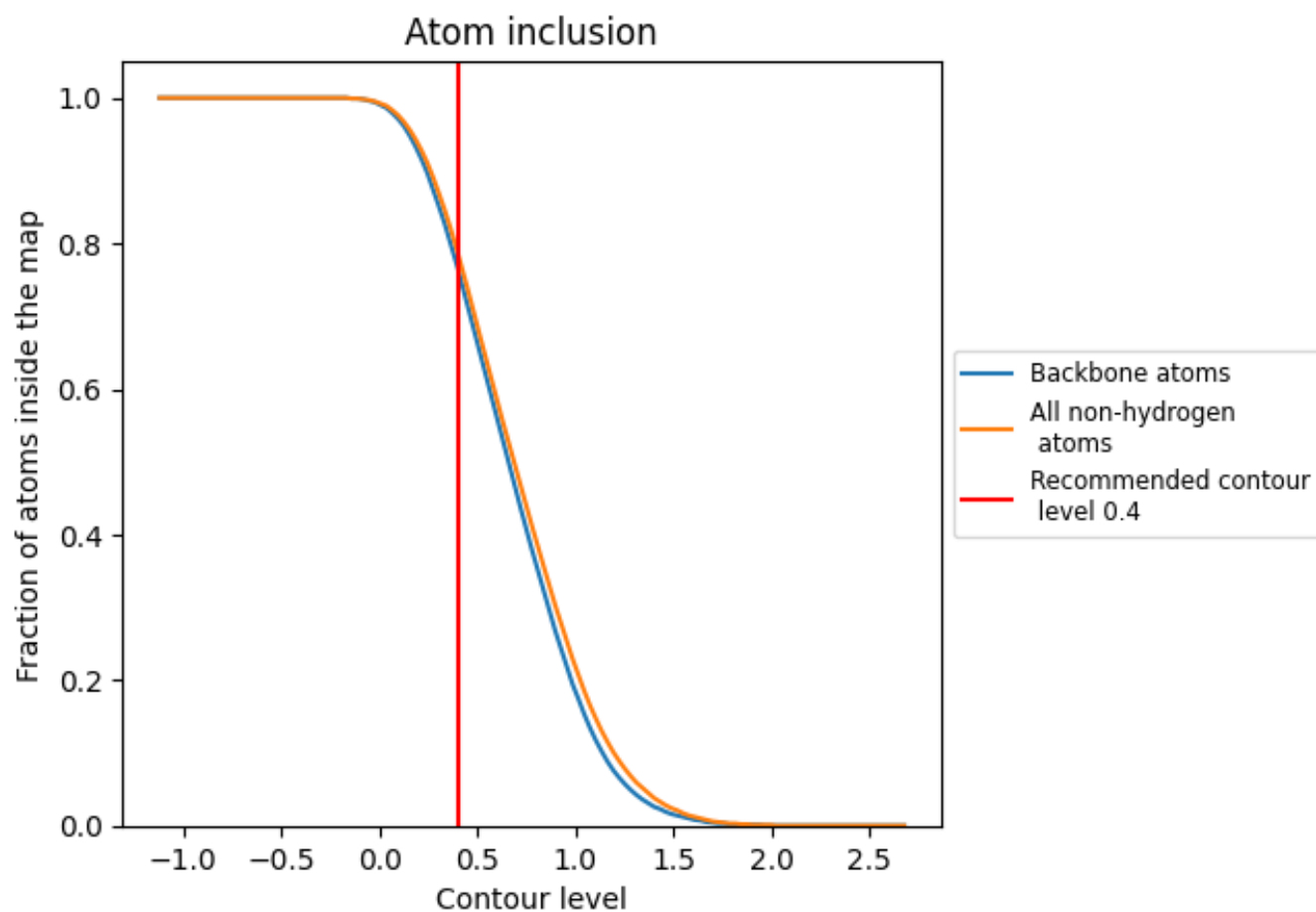
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 79% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.4470
A2	 0.8610	 0.4500
AA	 0.6510	 0.4030
AB	 0.6060	 0.4100
AC	 0.5030	 0.2740
AD	 0.6880	 0.4360
AE	 0.7290	 0.4640
AF	 0.5730	 0.3350
AG	 0.7990	 0.4900
AH	 0.9100	 0.5100
AJ	 0.5190	 0.3100
AT	 0.8180	 0.3800
AU	 0.2870	 0.3270
AZ	 0.6660	 0.4230
Aa	 0.6940	 0.4550
Ab	 0.6920	 0.4640
Ac	 0.6220	 0.4060
Ad	 0.6980	 0.4520
Ae	 0.6660	 0.4080
Af	 0.6690	 0.3720
Ag	 0.5450	 0.3460
Ah	 0.6880	 0.4030
Ai	 0.6760	 0.4340
Aj	 0.6700	 0.4060
Ak	 0.6540	 0.4370
Al	 0.4140	 0.2160
Am	 0.6910	 0.4330
An	 0.6950	 0.4630
Ao	 0.6900	 0.4250
Ap	 0.7050	 0.4220
Aq	 0.5920	 0.3810
Ar	 0.7100	 0.4130
As	 0.7550	 0.4270
At	 0.5940	 0.3480
Au	 0.6760	 0.4520

























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Chain	Atom inclusion	Q-score
Av	 0.7530	 0.4940
Aw	 0.7430	 0.4900
Ax	 0.6790	 0.4110
Ay	 0.6730	 0.3960
Az	 0.7250	 0.4940
B5	 0.8740	 0.4620
B7	 0.9670	 0.5200
B8	 0.9050	 0.4870
BA	 0.7610	 0.5240
BB	 0.8050	 0.4950
BC	 0.8020	 0.5040
BD	 0.8140	 0.4660
BE	 0.7020	 0.4330
BF	 0.7910	 0.5060
BG	 0.7210	 0.4440
BH	 0.7530	 0.4680
BI	 0.7520	 0.4850
BJ	 0.7470	 0.4480
BK	 0.3640	 0.3750
BL	 0.7690	 0.4740
BM	 0.7780	 0.4670
BN	 0.8320	 0.5350
BO	 0.8050	 0.5010
BP	 0.7850	 0.5010
BQ	 0.8010	 0.5100
BR	 0.7720	 0.4650
BS	 0.8210	 0.5110
BT	 0.7830	 0.4990
BU	 0.7260	 0.3990
BV	 0.7290	 0.4920
BW	 0.5320	 0.3520
BX	 0.7470	 0.4700
BY	 0.8070	 0.4820
BZ	 0.7620	 0.4560
Ba	 0.8310	 0.5290
Bb	 0.6490	 0.4040
Bc	 0.6530	 0.4050
Bd	 0.7820	 0.4760
Be	 0.7800	 0.5130
Bf	 0.8160	 0.5190
Bg	 0.7340	 0.4710
Bh	 0.7670	 0.4630

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Chain	Atom inclusion	Q-score
Bi	 0.7520	 0.4550
Bj	 0.8540	 0.5300
Bk	 0.6770	 0.4010
Bl	 0.7820	 0.4920
Bm	 0.7830	 0.4980
Bo	 0.7570	 0.4880
Bp	 0.7460	 0.5070
Br	 0.8030	 0.4970
Bs	 0.0690	 0.0450
Bt	 0.0330	 0.0840
Bv	 0.1970	 0.0930