



Full wwPDB EM Validation Report ⓘ

Aug 7, 2024 – 04:03 pm BST

PDB ID : 8PJ6
EMDB ID : EMD-17701
Title : Structure of human 48S translation initiation complex with initiator tRNA, eIF1A and eIF3 (off-pathway)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 2.90 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:

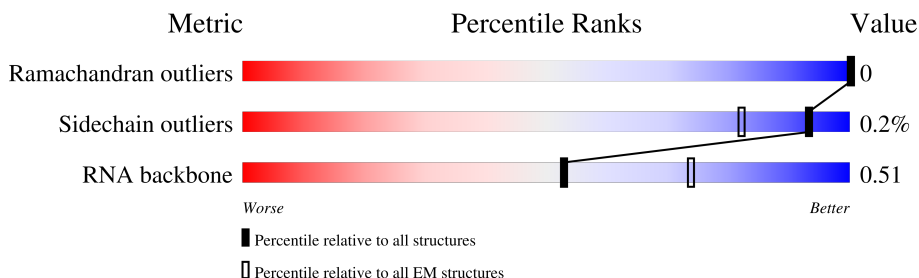
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.



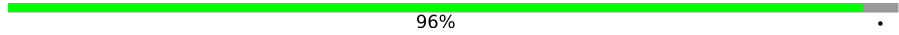


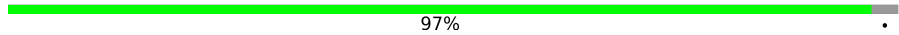

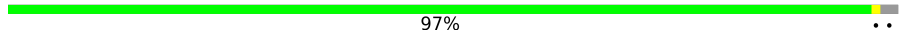
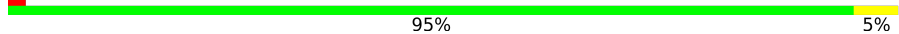

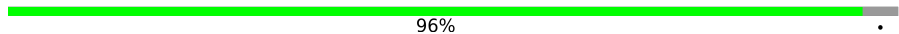
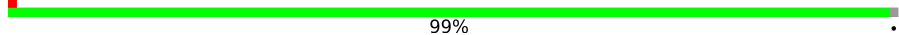
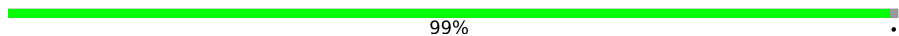
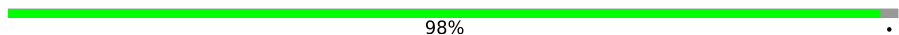

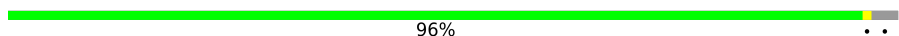




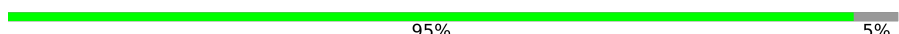

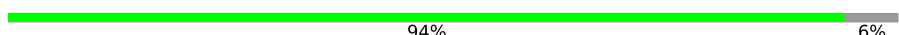

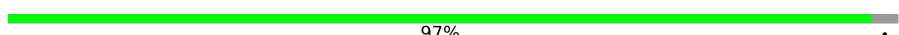


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	814	
2	2	325	
3	3	218	
4	4	357	
5	5	564	
6	6	374	
7	7	255	
8	8	352	


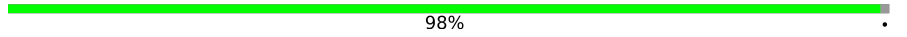
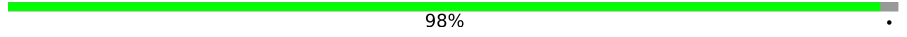

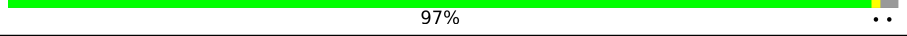



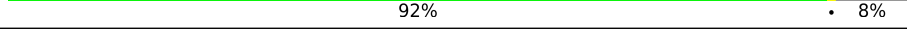

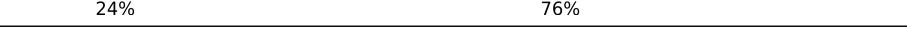
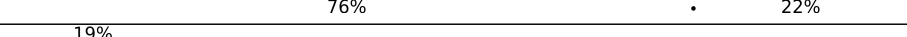

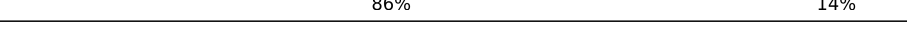



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Mol	Chain	Length	Quality of chain
9	9	25	 96%
10	A	1869	 69% 22% 8%
11	B	158	 89% 10%
12	C	263	 97%
13	D	194	 91% 9%
14	E	143	 97%
15	F	59	 95% 5%
16	G	194	 91% 9%
17	H	84	 96%
18	I	151	 99%
19	J	130	 99%
20	K	83	 98%
21	L	293	 74% 25%
22	M	135	 96%
23	N	295	 70% 30%
24	O	264	 80% 20%
25	P	151	 87% 12%
26	Q	115	 86% 14%
27	R	208	 95% 5%
28	S	249	 92% 8%
29	T	133	 94% 6%
30	V	204	 90% 10%
31	Y	146	 97%
32	Z	243	 93% 7%
33	a	165	 60% 40%

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Mol	Chain	Length	Quality of chain
34	b	145	 90% 10%
35	c	317	 98%
36	d	145	 98%
37	e	125	 53% 47%
38	f	152	 97%
39	h	119	 87% 13%
40	i	56	 89% 11%
41	k	156	 43% 56%
42	m	132	 92% 8%
43	n	69	 91% 9%
44	o	320	 24% 76%
45	q	144	 76% 22%
46	u	1382	 19% 51% 49%
47	v	445	 24% 86% 14%
48	w	75	 59% 35%
49	x	548	 5% 76% 23%
50	y	913	 8% 58% 42%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 106921 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 protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	588	3258	1986	633	634	5	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	2	304	1493	885	304	304	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	213	1057	631	213	213	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	257	1272	757	257	258	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	5	319	1581	943	319	319	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	350	1917	1159	376	380	2	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	7	56	1196	537	226	377	56	0	0

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	8	317	1571	936	317	318	0	0

- Molecule 9 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	24	230	139	62	26	3	0	0

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1719	36678	16385	6575	12000	1718	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	B8N	U	conflict	GB NR_046235.3

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	142	1166	743	218	199	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	256	2035	1302	378	347	8	0	0

- Molecule 13 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 17 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called 40S ribosomal protein S15a.

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

- Molecule 20 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 21 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 22 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 23 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 25 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 26 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 28 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 29 is a protein called 40S ribosomal protein S24.

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

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 31 is a protein called 40S ribosomal protein S16.

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

- Molecule 32 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 33 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 34 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 36 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 38 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 39 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 41 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 42 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 43 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	77	Total	C	N	O	S	0	0
			616	389	111	116			

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	112	Total	C	N	O	S	0	0
			902	560	173	165	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 48 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	w	73	1562	698	290	502	72	0	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	x	420	2826	1743	520	554	9	0	0

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit C.

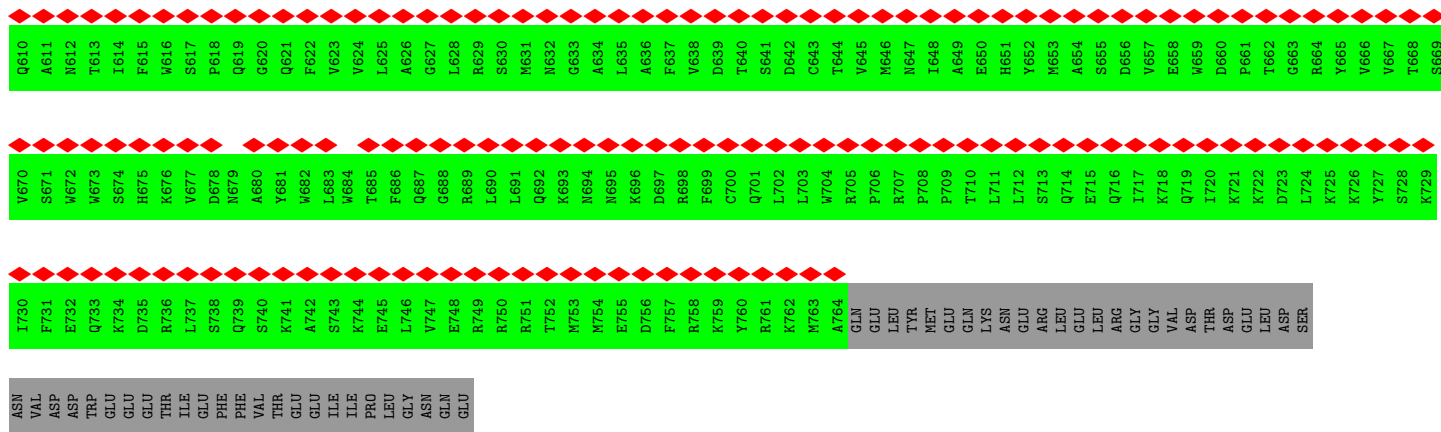
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	y	531	4305	2711	764	797	33	0	0

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

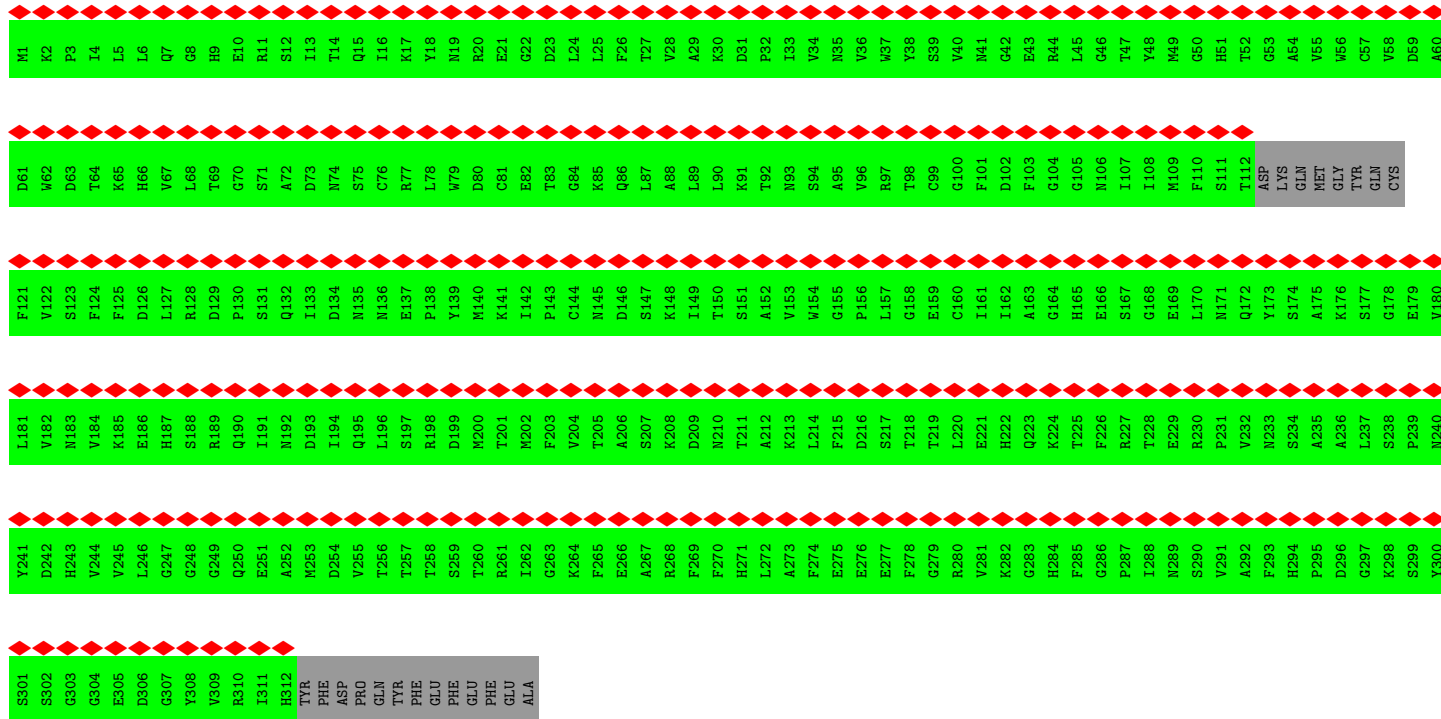
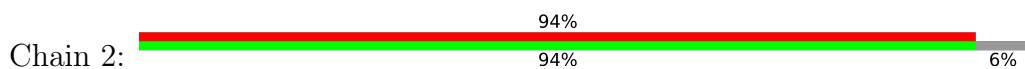
Mol	Chain	Residues	Atoms		AltConf
51	A	82	Total	Mg	0
			82	82	
51	V	1	Total	Mg	0
			1	1	
51	d	1	Total	Mg	0
			1	1	
51	f	1	Total	Mg	0
			1	1	
51	i	2	Total	Mg	0
			2	2	

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

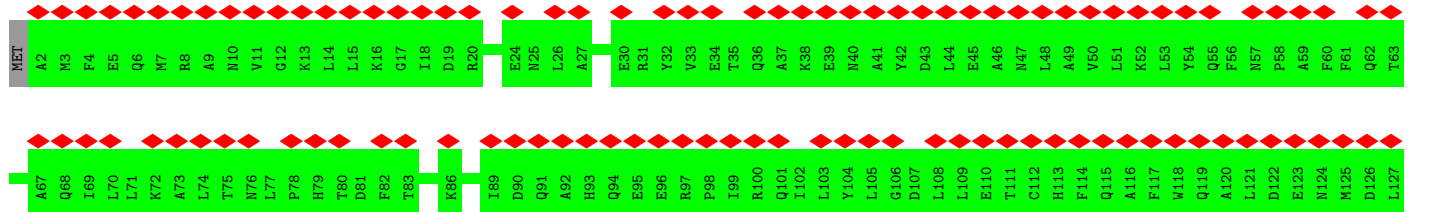
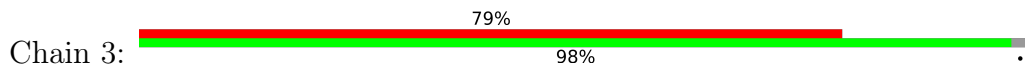
Mol	Chain	Residues	Atoms		AltConf
52	Q	1	Total	Zn	0
			1	1	
52	k	1	Total	Zn	0
			1	1	

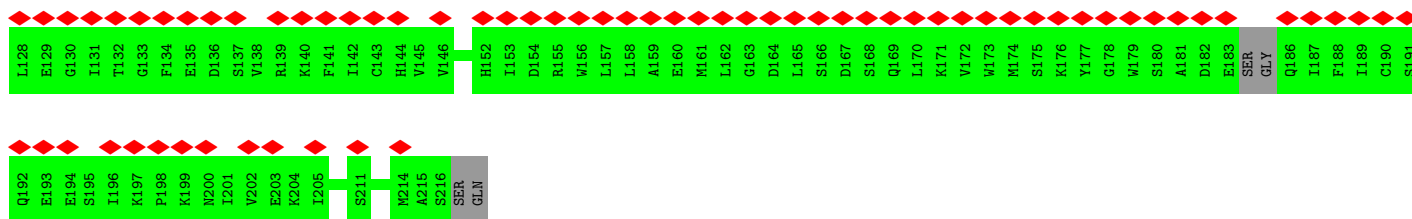


• Molecule 2: Eukaryotic translation initiation factor 3 subunit I

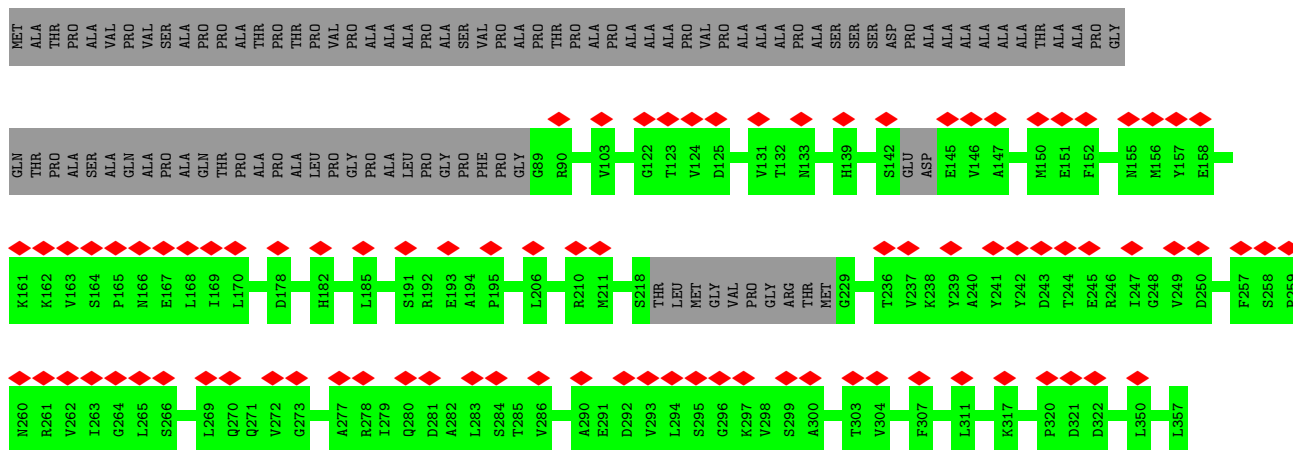


• Molecule 3: Eukaryotic translation initiation factor 3 subunit K

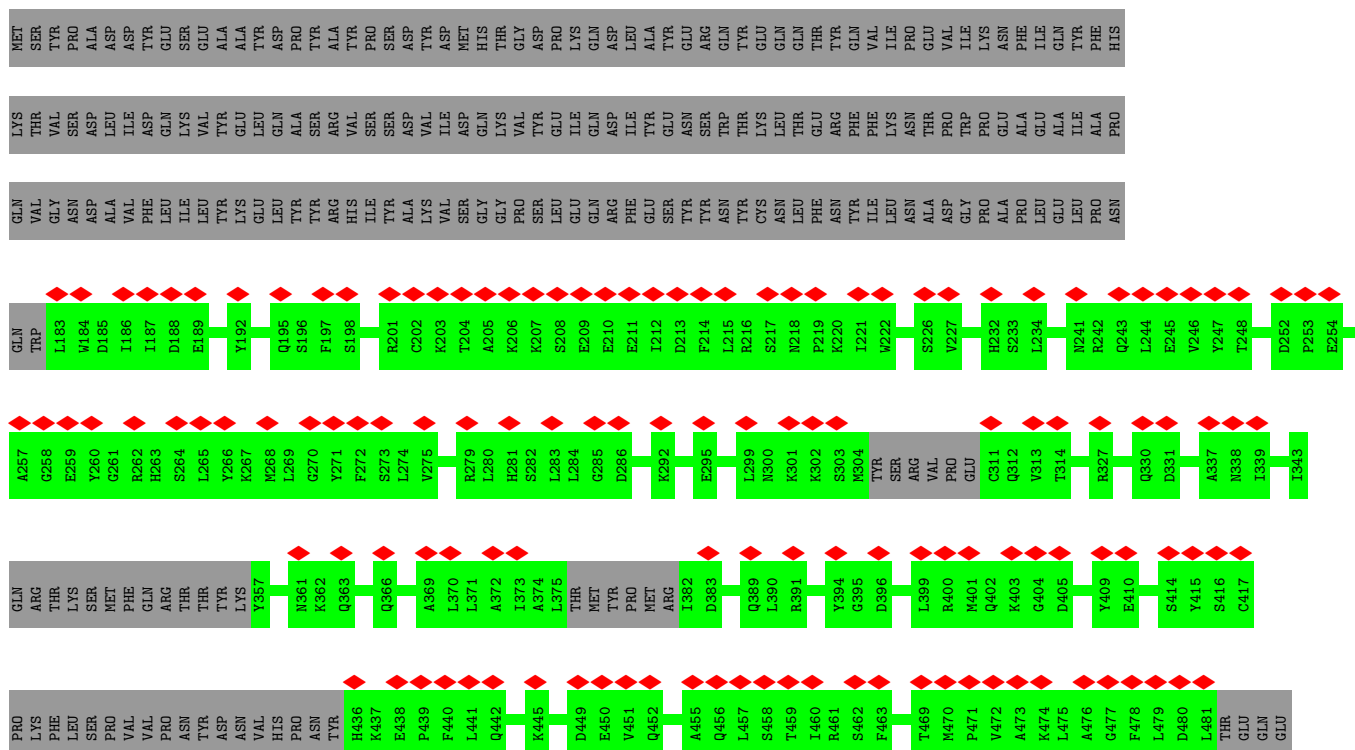


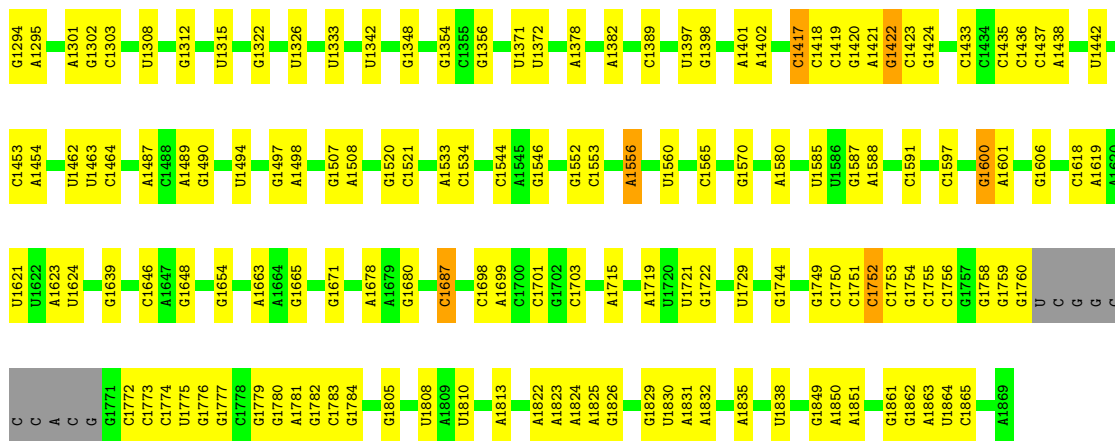


• Molecule 4: Eukaryotic translation initiation factor 3 subunit F

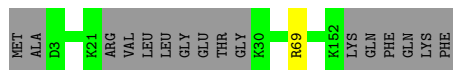
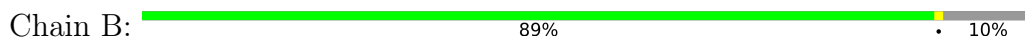


• Molecule 5: Eukaryotic translation initiation factor 3 subunit L





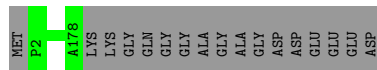
• Molecule 11: 40S ribosomal protein S11



• Molecule 12: 40S ribosomal protein S4, X isoform



• Molecule 13: 40S ribosomal protein S9



• Molecule 14: 40S ribosomal protein S23



• Molecule 15: 40S ribosomal protein S30

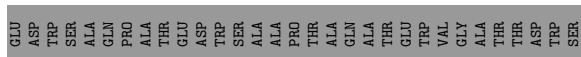
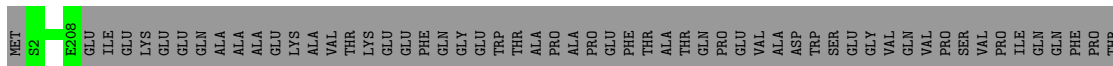


• Molecule 16: 40S ribosomal protein S7



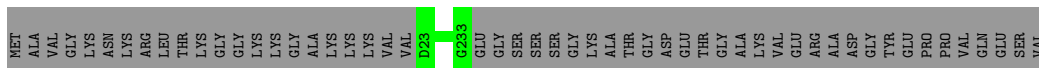
- Molecule 23: 40S ribosomal protein SA

Chain N: 70% 30%



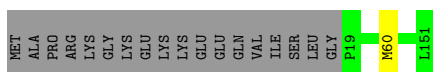
- Molecule 24: 40S ribosomal protein S3a

Chain O: 80% 20%



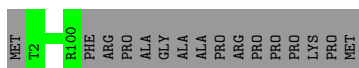
- Molecule 25: 40S ribosomal protein S14

Chain P: 87% 12%



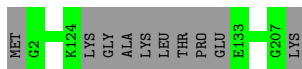
- Molecule 26: 40S ribosomal protein S26

Chain Q: 86% 14%



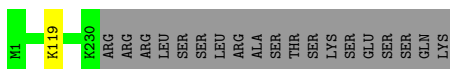
- Molecule 27: 40S ribosomal protein S8

Chain R: 95% 5%

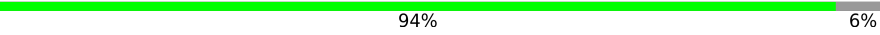


- Molecule 28: 40S ribosomal protein S6

Chain S: 92% 8%




- Molecule 29: 40S ribosomal protein S24

Chain T:  94% 6%



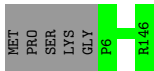
- Molecule 30: 40S ribosomal protein S5

Chain V:  90% 10%



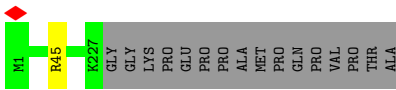
- Molecule 31: 40S ribosomal protein S16

Chain Y:  97% 3%



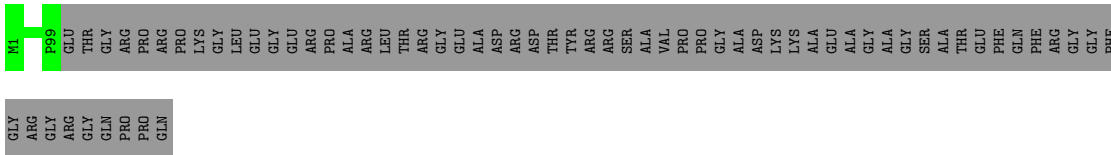
- Molecule 32: 40S ribosomal protein S3

Chain Z:  93% 7%




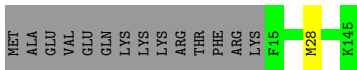
- Molecule 33: 40S ribosomal protein S10

Chain a:  60% 40%



- Molecule 34: 40S ribosomal protein S15

Chain b:  90% 10%

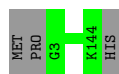


- Molecule 35: Receptor of activated protein C kinase 1

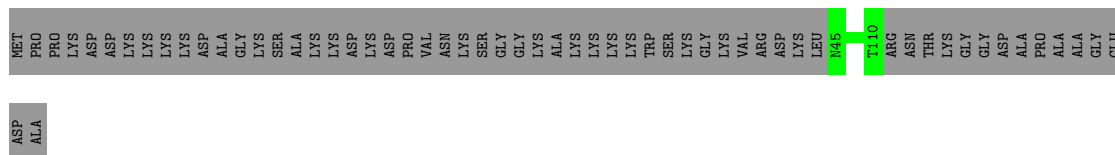
Chain c:  98% 2%



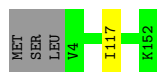
• Molecule 36: 40S ribosomal protein S19



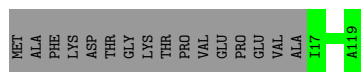
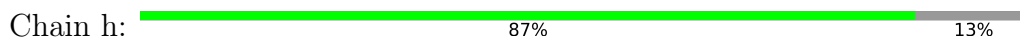
• Molecule 37: 40S ribosomal protein S25



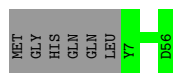
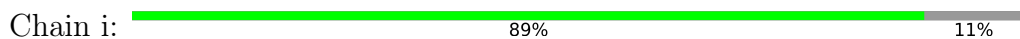
• Molecule 38: 40S ribosomal protein S18



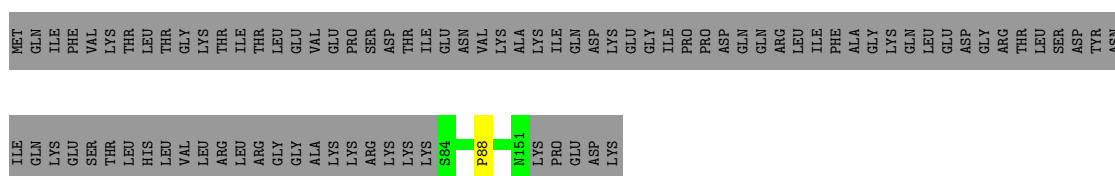
• Molecule 39: 40S ribosomal protein S20



• Molecule 40: 40S ribosomal protein S29



• Molecule 41: Ubiquitin



• Molecule 42: 40S ribosomal protein S12



TRP	GLU	ARG	VAL	ARG	GLY	GLY	VAL	PRO	LEU	VAL	LYS	GLU	LYS	PRO	LYS	M517	F318	G521	T322	E523	I324	T325	H326	A327	V328	E335	Q338	D346	E352	E363	L366	G367	E368	D403	L408	M409	D410	I418	M423	I424	L425	E426	E427	S428	L431	H432	M433		
A434	D435	Q436	P437	L438	R441	R488	E491	E492	R521	Q522	LEU	THR	PRO	PRO	GLU	GLY	SER	SER	LYS	SER	GLU	GLN	ASP	GLN	ALA	GLU	M539	E540	G541	R560	A585	G549	L650	L651	L652	R653	S654	L655	Q656	E657	R658	M659	Q660	E661	Q662	L682	H701	R706	R707
R708	L726	P729	R742	R750	E771	L807	S808	D809	L813	D814	L815	H819	E829	E830	Q837	P838	L859	L863	GLY	SER	LEU	VAL	GLU	ASN	ASN	GLU	ARG	VAL	PHE	ASP	HIS	LYS	GLN	GLY	THR	TYR	GLY	GLY	TYR	PHE	ARG	ASP	GLN	LYS	ASP	GLY	TYR		
ARG	LYS	ASN	GLU	GLY	TYR	MET	ARG	ARG	GLY	GLY	TYR	ARG	GLN	GLN	GLN	SER	GLN	THR	ALA	TYR																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55368	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0102	Depositor
Map size (Å)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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: PSU, OMC, B8N, JMH, OMG, 5MU, 5MC, A2M, OMU, ZN, 6MZ, MG, UR3, MA6

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	1	0.27	0/3279	0.53	0/4534
2	2	0.25	0/1491	0.48	0/2068
3	3	0.23	0/1055	0.36	0/1469
4	4	0.24	0/1269	0.41	0/1762
5	5	0.24	0/1575	0.35	0/2187
6	6	0.24	0/1926	0.45	0/2669
7	7	0.28	0/1340	0.89	3/2085 (0.1%)
8	8	0.24	0/1569	0.43	0/2183
9	9	0.31	0/231	0.78	0/294
10	A	0.47	0/40290	0.94	110/62786 (0.2%)
11	B	0.32	0/1186	0.54	0/1585
12	C	0.32	0/2077	0.59	0/2796
13	D	0.29	0/1502	0.58	0/2008
14	E	0.32	0/1105	0.58	1/1476 (0.1%)
15	F	0.30	0/474	0.65	1/623 (0.2%)
16	G	0.29	0/1451	0.58	0/1942
17	H	0.31	0/644	0.54	0/864
18	I	0.30	0/1232	0.55	0/1656
19	J	0.31	0/1051	0.56	0/1406
20	K	0.36	0/623	0.64	0/833
21	L	0.36	0/1743	0.63	2/2354 (0.1%)
22	M	0.33	0/1078	0.67	0/1447
23	N	0.31	0/1670	0.58	0/2271
24	O	0.33	0/1742	0.61	0/2330
25	P	0.33	0/1010	0.66	1/1353 (0.1%)
26	Q	0.33	0/805	0.60	0/1079
27	R	0.30	0/1654	0.56	0/2203
28	S	0.28	0/1885	0.58	0/2510
29	T	0.30	0/1032	0.59	0/1371
30	V	0.28	0/1481	0.56	1/1988 (0.1%)
31	Y	0.33	0/1142	0.59	0/1528
32	Z	0.29	0/1793	0.53	0/2414

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.31	0/859	0.56	0/1159
34	b	0.30	0/1094	0.63	1/1464 (0.1%)
35	c	0.29	0/2493	0.58	1/3394 (0.0%)
36	d	0.29	0/1123	0.54	0/1504
37	e	0.30	0/529	0.55	0/712
38	f	0.31	0/1245	0.63	1/1665 (0.1%)
39	h	0.36	0/827	0.63	0/1110
40	i	0.31	0/429	0.57	0/568
41	k	0.47	1/566 (0.2%)	0.70	1/753 (0.1%)
42	m	0.27	0/960	0.58	0/1286
43	n	0.32	0/500	0.67	0/669
44	o	0.28	0/628	0.61	0/846
45	q	0.28	0/913	0.69	2/1213 (0.2%)
46	u	0.27	0/5475	0.57	1/7432 (0.0%)
47	v	0.26	0/2672	0.57	0/3647
48	w	0.41	0/1748	1.08	9/2725 (0.3%)
49	x	0.27	0/2869	0.55	2/3918 (0.1%)
50	y	0.27	0/4380	0.59	1/5911 (0.0%)
All	All	0.37	1/111715 (0.0%)	0.75	138/160050 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	k	88	PRO	C-N	5.76	1.47	1.34

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	888	U	N3-C2-O2	-10.50	114.85	122.20
10	A	1453	C	N1-C2-O2	10.48	125.19	118.90
10	A	1453	C	C2-N1-C1'	10.24	130.07	118.80
10	A	888	U	C2-N1-C1'	10.19	129.93	117.70
10	A	882	U	N1-C2-O2	9.75	129.62	122.80
10	A	888	U	N1-C2-O2	9.69	129.58	122.80
10	A	501	C	C2-N1-C1'	9.21	128.93	118.80
10	A	537	C	N3-C2-O2	-9.16	115.49	121.90
10	A	501	C	N1-C2-O2	8.79	124.17	118.90
10	A	882	U	N3-C2-O2	-8.30	116.39	122.20
10	A	1597	C	N3-C2-O2	-8.04	116.28	121.90
10	A	1115	U	C2-N1-C1'	8.01	127.31	117.70
45	q	83	ASP	CB-CG-OD1	7.89	125.40	118.30
10	A	1115	U	N1-C2-O2	7.88	128.31	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	556	U	C2-N1-C1'	7.86	127.13	117.70
10	A	1139	C	N1-C2-O2	7.79	123.58	118.90
10	A	1453	C	N3-C2-O2	-7.75	116.48	121.90
10	A	1139	C	C2-N1-C1'	7.70	127.28	118.80
10	A	882	U	C2-N1-C1'	7.59	126.81	117.70
10	A	537	C	N1-C2-O2	7.54	123.43	118.90
10	A	1687	C	C2-N1-C1'	7.53	127.08	118.80
48	w	36	U	C2-N1-C1'	7.41	126.59	117.70
10	A	965	U	N1-C2-O2	7.41	127.98	122.80
49	x	369	ILE	CG1-CB-CG2	-7.40	95.13	111.40
10	A	168	C	N1-C2-O2	7.37	123.32	118.90
10	A	1115	U	N3-C2-O2	-7.36	117.05	122.20
10	A	1597	C	N1-C2-O2	7.35	123.31	118.90
10	A	1520	G	C4-N9-C1'	7.28	135.96	126.50
48	w	36	U	N3-C2-O2	-7.25	117.13	122.20
10	A	1453	C	C6-N1-C1'	-7.22	112.13	120.80
10	A	1139	C	N3-C2-O2	-7.17	116.88	121.90
10	A	556	U	N1-C2-O2	7.16	127.81	122.80
46	u	385	PRO	CA-N-CD	-7.16	101.47	111.50
10	A	1520	G	N3-C4-N9	7.09	130.25	126.00
10	A	501	C	N3-C2-O2	-7.07	116.95	121.90
10	A	1271	C	N1-C2-O2	6.99	123.10	118.90
10	A	965	U	N3-C2-O2	-6.96	117.33	122.20
14	E	19	ASP	CB-CG-OD1	6.94	124.55	118.30
10	A	1752	C	N1-C2-O2	6.88	123.03	118.90
7	7	-30	C	OP2-P-O3'	6.78	120.11	105.20
10	A	537	C	C6-N1-C2	-6.77	117.59	120.30
10	A	201	C	N1-C2-O2	6.75	122.95	118.90
10	A	1520	G	C8-N9-C1'	-6.73	118.25	127.00
10	A	556	U	N3-C2-O2	-6.63	117.56	122.20
10	A	1422	G	N3-C4-C5	-6.51	125.35	128.60
10	A	501	C	C6-N1-C2	-6.50	117.70	120.30
7	7	-30	C	P-O3'-C3'	6.49	127.48	119.70
7	7	-20	A	P-O3'-C3'	6.49	127.48	119.70
10	A	1422	G	N3-C4-N9	6.49	129.89	126.00
10	A	1453	C	C5-C6-N1	6.46	124.23	121.00
10	A	1422	G	C4-N9-C1'	6.42	134.84	126.50
10	A	888	U	C6-N1-C2	-6.42	117.15	121.00
10	A	1591	C	N1-C2-O2	6.38	122.73	118.90
10	A	1261	C	N1-C2-O2	6.33	122.70	118.90
21	L	104	ASP	CB-CG-OD1	6.29	123.96	118.30
10	A	984	C	N3-C2-O2	-6.28	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	501	C	C6-N1-C1'	-6.26	113.28	120.80
21	L	271	ASP	CB-CG-OD1	6.25	123.92	118.30
10	A	1453	C	C6-N1-C2	-6.25	117.80	120.30
10	A	688	U	P-O3'-C3'	6.23	127.18	119.70
10	A	965	U	C2-N1-C1'	6.21	125.15	117.70
10	A	1078	C	N1-C2-O2	6.17	122.60	118.90
38	f	117	ILE	CG1-CB-CG2	-6.14	97.89	111.40
10	A	1022	U	C2-N1-C1'	6.10	125.02	117.70
10	A	1389	C	C2-N1-C1'	6.08	125.49	118.80
10	A	836	G	C4-N9-C1'	6.02	134.33	126.50
10	A	888	U	C6-N1-C1'	-5.92	112.91	121.20
10	A	888	U	C5-C6-N1	5.90	125.65	122.70
10	A	550	C	C6-N1-C1'	5.87	127.85	120.80
10	A	1565	C	C2-N1-C1'	5.86	125.25	118.80
10	A	1116	C	N1-C2-O2	5.83	122.40	118.90
10	A	1752	C	N3-C2-O2	-5.80	117.84	121.90
10	A	1600	G	N3-C4-N9	5.79	129.47	126.00
10	A	1078	C	C2-N1-C1'	5.78	125.16	118.80
10	A	178	C	N1-C2-O2	5.74	122.35	118.90
10	A	501	C	C5-C6-N1	5.73	123.86	121.00
10	A	1139	C	C6-N1-C2	-5.72	118.01	120.30
10	A	168	C	C2-N1-C1'	5.69	125.06	118.80
10	A	1078	C	N3-C2-O2	-5.66	117.94	121.90
10	A	1417	C	N3-C2-O2	-5.66	117.94	121.90
34	b	28	MET	CA-CB-CG	5.66	122.91	113.30
10	A	659	G	C4-N9-C1'	5.64	133.84	126.50
10	A	836	G	N3-C4-N9	5.64	129.39	126.00
10	A	1520	G	C6-C5-N7	-5.62	127.03	130.40
10	A	1078	C	C6-N1-C2	-5.61	118.06	120.30
10	A	836	G	N3-C4-C5	-5.61	125.80	128.60
10	A	168	C	N3-C2-O2	-5.61	117.97	121.90
10	A	494	C	N1-C2-O2	5.58	122.25	118.90
10	A	130	G	C4-N9-C1'	5.58	133.75	126.50
10	A	537	C	C2-N1-C1'	5.55	124.91	118.80
10	A	1752	C	C2-N1-C1'	5.54	124.90	118.80
50	y	651	LEU	CA-CB-CG	5.54	128.05	115.30
10	A	1289	U	N1-C2-O2	5.54	126.68	122.80
10	A	566	U	N1-C2-O2	5.52	126.67	122.80
48	w	13	C	C2-N1-C1'	5.51	124.86	118.80
48	w	13	C	N1-C2-O2	5.48	122.19	118.90
10	A	1271	C	N3-C2-O2	-5.47	118.07	121.90
48	w	34	C	C2-N1-C1'	5.45	124.80	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1111	U	N3-C2-O2	-5.45	118.39	122.20
10	A	201	C	N3-C2-O2	-5.45	118.09	121.90
10	A	797	C	P-O3'-C3'	5.44	126.23	119.70
48	w	68	C	C2-N1-C1'	5.44	124.79	118.80
48	w	36	U	N1-C2-O2	5.42	126.59	122.80
49	x	22	PRO	CA-N-CD	-5.41	103.93	111.50
10	A	1422	G	C8-N9-C1'	-5.40	119.98	127.00
10	A	1687	C	C6-N1-C2	-5.39	118.14	120.30
10	A	1271	C	C2-N1-C1'	5.35	124.68	118.80
10	A	566	U	N3-C2-O2	-5.33	118.47	122.20
10	A	130	G	N3-C4-N9	5.32	129.19	126.00
35	c	189	ILE	CG1-CB-CG2	-5.30	99.75	111.40
25	P	60	MET	CA-CB-CG	5.29	122.29	113.30
10	A	882	U	C5-C6-N1	5.24	125.32	122.70
10	A	1752	C	C6-N1-C2	-5.23	118.21	120.30
48	w	56	C	C5-C6-N1	5.23	123.62	121.00
10	A	1289	U	N3-C2-O2	-5.22	118.54	122.20
10	A	291	G	P-O3'-C3'	5.20	125.94	119.70
41	k	88	PRO	O-C-N	5.20	131.02	122.70
48	w	32	C	N1-C2-O2	5.19	122.01	118.90
10	A	1591	C	N3-C2-O2	-5.18	118.28	121.90
15	F	121	PRO	CA-N-CD	-5.16	104.27	111.50
10	A	327	G	O5'-P-OP1	5.16	116.89	110.70
45	q	82	ARG	C-N-CA	5.13	134.54	121.70
10	A	550	C	C2-N1-C1'	-5.13	113.15	118.80
10	A	1315	U	N3-C2-O2	-5.13	118.61	122.20
30	V	177	LEU	CA-CB-CG	5.13	127.10	115.30
10	A	1261	C	N3-C2-O2	-5.13	118.31	121.90
10	A	368	U	P-O3'-C3'	5.10	125.81	119.70
10	A	1139	C	C6-N1-C1'	-5.09	114.69	120.80
10	A	1687	C	C6-N1-C1'	-5.09	114.69	120.80
10	A	1	U	OP1-P-O3'	5.08	116.39	105.20
10	A	556	U	C6-N1-C1'	-5.08	114.08	121.20
10	A	201	C	C2-N1-C1'	5.07	124.38	118.80
10	A	1289	U	C2-N1-C1'	5.07	123.79	117.70
10	A	1520	G	N3-C4-C5	-5.06	126.07	128.60
10	A	1115	U	C6-N1-C1'	-5.04	114.14	121.20
10	A	1116	C	C2-N1-C1'	5.03	124.33	118.80
10	A	1261	C	C2-N1-C1'	5.02	124.32	118.80
10	A	1556	A	C2-N3-C4	5.00	113.10	110.60

There are no chirality outliers.

There are no planarity outliers.

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	
1	1	584/814 (72%)	535 (92%)	49 (8%)	0	100	100
2	2	300/325 (92%)	297 (99%)	3 (1%)	0	100	100
3	3	209/218 (96%)	204 (98%)	5 (2%)	0	100	100
4	4	251/357 (70%)	232 (92%)	19 (8%)	0	100	100
5	5	307/564 (54%)	293 (95%)	14 (5%)	0	100	100
6	6	348/374 (93%)	308 (88%)	40 (12%)	0	100	100
8	8	313/352 (89%)	282 (90%)	31 (10%)	0	100	100
9	9	22/25 (88%)	22 (100%)	0	0	100	100
11	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
12	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
13	D	175/194 (90%)	172 (98%)	3 (2%)	0	100	100
14	E	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
15	F	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
16	G	171/194 (88%)	167 (98%)	4 (2%)	0	100	100
17	H	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
18	I	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
19	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
20	K	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
21	L	218/293 (74%)	215 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	M	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
23	N	205/295 (70%)	201 (98%)	4 (2%)	0	100	100
24	O	209/264 (79%)	206 (99%)	3 (1%)	0	100	100
25	P	131/151 (87%)	124 (95%)	7 (5%)	0	100	100
26	Q	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
27	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
28	S	228/249 (92%)	226 (99%)	2 (1%)	0	100	100
29	T	123/133 (92%)	123 (100%)	0	0	100	100
30	V	180/204 (88%)	179 (99%)	1 (1%)	0	100	100
31	Y	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
32	Z	225/243 (93%)	224 (100%)	1 (0%)	0	100	100
33	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
34	b	129/145 (89%)	123 (95%)	6 (5%)	0	100	100
35	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
36	d	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
37	e	64/125 (51%)	63 (98%)	1 (2%)	0	100	100
38	f	147/152 (97%)	142 (97%)	5 (3%)	0	100	100
39	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
40	i	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
41	k	66/156 (42%)	60 (91%)	6 (9%)	0	100	100
42	m	120/132 (91%)	120 (100%)	0	0	100	100
43	n	61/69 (88%)	58 (95%)	3 (5%)	0	100	100
44	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
45	q	110/144 (76%)	100 (91%)	10 (9%)	0	100	100
46	u	705/1382 (51%)	662 (94%)	43 (6%)	0	100	100
47	v	380/445 (85%)	355 (93%)	25 (7%)	0	100	100
49	x	414/548 (76%)	399 (96%)	15 (4%)	0	100	100
50	y	527/913 (58%)	508 (96%)	19 (4%)	0	100	100
All	All	9273/12257 (76%)	8885 (96%)	388 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	1	97/702 (14%)	97 (100%)	0	100	100
6	6	49/335 (15%)	49 (100%)	0	100	100
9	9	23/24 (96%)	23 (100%)	0	100	100
11	B	129/142 (91%)	128 (99%)	1 (1%)	81	94
12	C	220/225 (98%)	220 (100%)	0	100	100
13	D	158/168 (94%)	158 (100%)	0	100	100
14	E	112/115 (97%)	112 (100%)	0	100	100
15	F	48/48 (100%)	46 (96%)	2 (4%)	30	63
16	G	159/174 (91%)	159 (100%)	0	100	100
17	H	73/76 (96%)	73 (100%)	0	100	100
18	I	130/131 (99%)	130 (100%)	0	100	100
19	J	112/113 (99%)	112 (100%)	0	100	100
20	K	65/67 (97%)	65 (100%)	0	100	100
21	L	186/225 (83%)	186 (100%)	0	100	100
22	M	119/122 (98%)	118 (99%)	1 (1%)	81	94
23	N	173/243 (71%)	173 (100%)	0	100	100
24	O	192/231 (83%)	192 (100%)	0	100	100
25	P	104/119 (87%)	104 (100%)	0	100	100
26	Q	86/98 (88%)	86 (100%)	0	100	100
27	R	172/180 (96%)	172 (100%)	0	100	100
28	S	200/218 (92%)	199 (100%)	1 (0%)	88	96
29	T	107/115 (93%)	107 (100%)	0	100	100
30	V	156/170 (92%)	156 (100%)	0	100	100
31	Y	117/121 (97%)	117 (100%)	0	100	100
32	Z	190/202 (94%)	189 (100%)	1 (0%)	88	96
33	a	90/136 (66%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	b	117/130 (90%)	117 (100%)	0	100	100
35	c	272/275 (99%)	272 (100%)	0	100	100
36	d	112/115 (97%)	112 (100%)	0	100	100
37	e	58/103 (56%)	58 (100%)	0	100	100
38	f	129/132 (98%)	129 (100%)	0	100	100
39	h	94/107 (88%)	94 (100%)	0	100	100
40	i	44/49 (90%)	44 (100%)	0	100	100
41	k	61/140 (44%)	61 (100%)	0	100	100
42	m	104/108 (96%)	103 (99%)	1 (1%)	76	92
43	n	56/62 (90%)	56 (100%)	0	100	100
44	o	64/277 (23%)	64 (100%)	0	100	100
45	q	94/123 (76%)	93 (99%)	1 (1%)	73	92
46	u	528/1259 (42%)	527 (100%)	1 (0%)	93	98
47	v	206/406 (51%)	205 (100%)	1 (0%)	88	96
49	x	206/494 (42%)	206 (100%)	0	100	100
50	y	473/811 (58%)	471 (100%)	2 (0%)	91	97
All	All	5885/9091 (65%)	5873 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	69	ARG
15	F	75	LYS
15	F	125	LYS
22	M	80	ARG
28	S	119	LYS
32	Z	45	ARG
42	m	96	ARG
45	q	24	ARG
46	u	62	ARG
47	v	268	ARG
50	y	560	ARG
50	y	658	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
27	R	168	GLN
30	V	83	ASN
46	u	10	ASN
46	u	434	ASN
50	y	840	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1705/1869 (91%)	373 (21%)	6 (0%)
48	w	72/75 (96%)	26 (36%)	0
7	7	55/255 (21%)	34 (61%)	3 (5%)
All	All	1832/2199 (83%)	433 (23%)	9 (0%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	-30	C
7	7	-29	A
7	7	-28	A
7	7	-27	C
7	7	-26	A
7	7	-25	A
7	7	-22	A
7	7	-21	C
7	7	-19	A
7	7	-16	A
7	7	-12	A
7	7	-11	A
7	7	-10	A
7	7	-9	A
7	7	-7	A
7	7	-6	G
7	7	-5	A
7	7	-4	C
7	7	-3	C
7	7	-2	A
7	7	3	G
7	7	4	G
7	7	6	A
7	7	7	C
7	7	8	G

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Mol	Chain	Res	Type
7	7	10	U
7	7	11	U
7	7	14	A
7	7	15	G
7	7	18	U
7	7	19	U
7	7	20	G
7	7	21	A
7	7	22	G
10	A	2	A
10	A	26	U
10	A	33	G
10	A	41	G
10	A	44	U
10	A	45	A
10	A	46	A
10	A	56	G
10	A	58	C
10	A	59	U
10	A	62	G
10	A	65	C
10	A	67	C
10	A	68	A
10	A	73	C
10	A	74	G
10	A	76	U
10	A	78	C
10	A	79	A
10	A	103	A
10	A	114	G
10	A	115	U
10	A	126	G
10	A	129	C
10	A	130	G
10	A	140	U
10	A	142	C
10	A	143	U
10	A	149	A
10	A	155	G
10	A	158	A
10	A	163	U
10	A	173	A

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Mol	Chain	Res	Type
10	A	182	C
10	A	184	G
10	A	190	G
10	A	198	U
10	A	199	C
10	A	200	G
10	A	202	G
10	A	203	G
10	A	204	G
10	A	206	G
10	A	288	G
10	A	291	G
10	A	292	A
10	A	295	C
10	A	306	C
10	A	307	G
10	A	308	G
10	A	309	G
10	A	318	A
10	A	319	C
10	A	321	C
10	A	323	C
10	A	324	C
10	A	325	C
10	A	326	C
10	A	327	G
10	A	329	G
10	A	332	G
10	A	347	G
10	A	362	C
10	A	364	A
10	A	369	C
10	A	370	G
10	A	381	C
10	A	384	U
10	A	385	G
10	A	386	C
10	A	409	C
10	A	418	A
10	A	421	G
10	A	428	U
10	A	448	A

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Mol	Chain	Res	Type
10	A	449	A
10	A	450	C
10	A	452	G
10	A	455	A
10	A	465	A
10	A	467	G
10	A	471	G
10	A	472	C
10	A	473	A
10	A	474	G
10	A	476	A
10	A	482	G
10	A	487	U
10	A	492	C
10	A	502	C
10	A	503	C
10	A	508	A
10	A	517	OMC
10	A	525	A
10	A	536	A
10	A	537	C
10	A	538	U
10	A	539	C
10	A	540	U
10	A	541	U
10	A	542	U
10	A	543	C
10	A	544	G
10	A	545	A
10	A	546	G
10	A	553	U
10	A	554	A
10	A	556	U
10	A	557	U
10	A	558	G
10	A	563	G
10	A	564	A
10	A	566	U
10	A	568	C
10	A	576	A
10	A	587	A
10	A	589	G

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Mol	Chain	Res	Type
10	A	590	A
10	A	591	U
10	A	593	C
10	A	604	A
10	A	606	G
10	A	607	U
10	A	614	C
10	A	617	G
10	A	626	G
10	A	627	U
10	A	643	A
10	A	655	A
10	A	660	C
10	A	662	G
10	A	668	A2M
10	A	669	A
10	A	671	A
10	A	672	A
10	A	673	G
10	A	684	G
10	A	688	U
10	A	689	U
10	A	693	A
10	A	694	G
10	A	734	C
10	A	748	C
10	A	749	U
10	A	751	G
10	A	752	G
10	A	753	C
10	A	791	C
10	A	798	G
10	A	799	U
10	A	808	A
10	A	810	A
10	A	821	G
10	A	822	PSU
10	A	827	A
10	A	830	A
10	A	836	G
10	A	837	A
10	A	838	G

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Mol	Chain	Res	Type
10	A	839	C
10	A	840	C
10	A	841	G
10	A	847	A
10	A	870	A
10	A	872	A
10	A	873	G
10	A	880	G
10	A	887	U
10	A	888	U
10	A	890	U
10	A	894	G
10	A	895	G
10	A	896	U
10	A	897	U
10	A	898	U
10	A	899	U
10	A	901	G
10	A	903	A
10	A	913	A
10	A	914	U
10	A	917	U
10	A	920	A
10	A	922	A
10	A	930	C
10	A	933	G
10	A	934	G
10	A	953	C
10	A	954	U
10	A	955	A
10	A	956	G
10	A	963	A
10	A	969	U
10	A	972	A
10	A	978	G
10	A	990	A
10	A	992	A
10	A	999	G
10	A	1017	U
10	A	1023	A
10	A	1045	U
10	A	1061	U

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Mol	Chain	Res	Type
10	A	1062	A
10	A	1078	C
10	A	1083	A
10	A	1085	C
10	A	1089	G
10	A	1109	C
10	A	1112	U
10	A	1113	A
10	A	1115	U
10	A	1117	C
10	A	1120	U
10	A	1123	C
10	A	1133	A
10	A	1138	C
10	A	1149	A
10	A	1153	C
10	A	1154	U
10	A	1155	U
10	A	1172	U
10	A	1195	A
10	A	1207	G
10	A	1208	A
10	A	1211	G
10	A	1215	C
10	A	1216	C
10	A	1217	A
10	A	1221	G
10	A	1224	G
10	A	1242	U
10	A	1249	C
10	A	1250	A
10	A	1251	A
10	A	1253	A
10	A	1256	G
10	A	1257	G
10	A	1259	A
10	A	1274	G
10	A	1275	G
10	A	1283	C
10	A	1284	A
10	A	1288	U
10	A	1290	G

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Mol	Chain	Res	Type
10	A	1294	G
10	A	1295	A
10	A	1301	A
10	A	1302	G
10	A	1303	C
10	A	1308	U
10	A	1312	G
10	A	1322	G
10	A	1326	U
10	A	1333	U
10	A	1342	U
10	A	1348	G
10	A	1354	G
10	A	1356	G
10	A	1371	U
10	A	1372	U
10	A	1378	A
10	A	1382	A
10	A	1397	U
10	A	1398	G
10	A	1401	A
10	A	1402	A
10	A	1417	C
10	A	1418	C
10	A	1419	C
10	A	1420	G
10	A	1421	A
10	A	1422	G
10	A	1423	C
10	A	1424	G
10	A	1433	C
10	A	1435	C
10	A	1436	C
10	A	1437	C
10	A	1438	A
10	A	1442	U
10	A	1454	A
10	A	1462	U
10	A	1463	U
10	A	1464	C
10	A	1487	A
10	A	1489	A

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Mol	Chain	Res	Type
10	A	1490	G
10	A	1494	U
10	A	1497	G
10	A	1498	A
10	A	1507	G
10	A	1508	A
10	A	1521	C
10	A	1533	A
10	A	1534	C
10	A	1544	C
10	A	1546	G
10	A	1552	G
10	A	1553	C
10	A	1556	A
10	A	1560	U
10	A	1570	G
10	A	1580	A
10	A	1585	U
10	A	1587	G
10	A	1588	A
10	A	1600	G
10	A	1601	A
10	A	1606	G
10	A	1618	C
10	A	1619	A
10	A	1621	U
10	A	1623	A
10	A	1624	U
10	A	1639	G
10	A	1646	C
10	A	1648	G
10	A	1654	G
10	A	1663	A
10	A	1665	G
10	A	1671	G
10	A	1680	G
10	A	1687	C
10	A	1698	C
10	A	1699	A
10	A	1701	C
10	A	1715	A
10	A	1719	A

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Mol	Chain	Res	Type
10	A	1721	U
10	A	1722	G
10	A	1729	U
10	A	1744	G
10	A	1749	G
10	A	1750	C
10	A	1751	C
10	A	1752	C
10	A	1753	C
10	A	1754	G
10	A	1755	C
10	A	1756	C
10	A	1758	G
10	A	1759	G
10	A	1760	G
10	A	1772	C
10	A	1773	C
10	A	1774	C
10	A	1775	U
10	A	1776	G
10	A	1777	G
10	A	1779	G
10	A	1780	G
10	A	1781	A
10	A	1782	G
10	A	1783	C
10	A	1784	G
10	A	1805	G
10	A	1808	U
10	A	1810	U
10	A	1813	A
10	A	1822	A
10	A	1823	A
10	A	1824	A
10	A	1825	A
10	A	1826	G
10	A	1829	G
10	A	1831	A
10	A	1835	A
10	A	1838	U
10	A	1849	G
10	A	1861	G

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Mol	Chain	Res	Type
10	A	1862	G
10	A	1863	A
10	A	1864	U
10	A	1865	C
48	w	2	G
48	w	6	A
48	w	8	U
48	w	9	G
48	w	11	C
48	w	13	C
48	w	16	C
48	w	18	G
48	w	19	G
48	w	20	A
48	w	21	A
48	w	22	G
48	w	34	C
48	w	48	C
48	w	52	G
48	w	53	G
48	w	56	C
48	w	57	G
48	w	58	A
48	w	61	C
48	w	63	A
48	w	64	U
48	w	69	U
48	w	70	G
48	w	71	C
48	w	74	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	7	-30	C
7	7	-20	A
7	7	13	A
10	A	1	U
10	A	291	G
10	A	368	U
10	A	688	U
10	A	797	C

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Mol	Chain	Res	Type
10	A	1600	G

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

29 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
10	A2M	A	668	51,10	18,25,26	4.21	8 (44%)	18,36,39	3.89	5 (27%)
10	PSU	A	823	10	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
10	MA6	A	1850	10	18,26,27	1.32	2 (11%)	19,38,41	3.11	2 (10%)
10	5MU	A	814	10	19,22,23	0.48	0	28,32,35	0.93	2 (7%)
10	OMG	A	683	10	18,26,27	1.20	2 (11%)	19,38,41	0.89	1 (5%)
10	UR3	A	1830	10	19,22,23	2.76	7 (36%)	26,32,35	1.51	4 (15%)
10	A2M	A	1031	10	18,25,26	4.38	8 (44%)	18,36,39	3.85	4 (22%)
10	OMU	A	121	10	19,22,23	2.95	6 (31%)	26,31,34	1.63	5 (19%)
10	OMG	A	509	51,10	18,26,27	1.20	2 (11%)	19,38,41	0.89	1 (5%)
10	MA6	A	1851	10	18,26,27	1.33	2 (11%)	19,38,41	3.17	2 (10%)
10	A2M	A	484	10	18,25,26	4.24	9 (50%)	18,36,39	3.89	5 (27%)
10	PSU	A	612	10	18,21,22	1.00	1 (5%)	22,30,33	1.79	5 (22%)
10	OMG	A	644	10	18,26,27	1.19	2 (11%)	19,38,41	0.85	1 (5%)
10	6MZ	A	1832	51,10	18,25,26	1.77	2 (11%)	16,36,39	2.59	5 (31%)
10	PSU	A	119	10	18,21,22	0.99	1 (5%)	22,30,33	1.59	4 (18%)
10	PSU	A	822	10	18,21,22	1.03	1 (5%)	22,30,33	1.86	6 (27%)
10	A2M	A	27	51,10	18,25,26	4.32	7 (38%)	18,36,39	3.84	4 (22%)
10	JMH	A	1219	10	18,22,23	0.25	0	21,32,35	0.25	0
10	B8N	A	1248	10	24,29,30	0.30	0	29,42,45	0.73	1 (3%)
10	A2M	A	166	10	18,25,26	4.35	7 (38%)	18,36,39	3.82	5 (27%)
10	A2M	A	1678	51,10	18,25,26	4.39	8 (44%)	18,36,39	3.88	4 (22%)
10	PSU	A	1081	10	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PSU	A	1243	10	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
10	OMC	A	517	10	19,22,23	0.59	0	26,31,34	0.66	0
10	A2M	A	159	10	18,25,26	4.26	8 (44%)	18,36,39	3.96	5 (27%)
10	5MC	A	1374	10	18,22,23	0.65	0	26,32,35	0.60	0
10	OMC	A	1703	10	19,22,23	0.61	0	26,31,34	0.77	1 (3%)
10	OMC	A	174	51,10	19,22,23	0.57	0	26,31,34	0.71	1 (3%)
10	OMU	A	116	10	19,22,23	2.97	5 (26%)	26,31,34	1.58	5 (19%)

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
10	A2M	A	668	51,10	-	2/5/27/28	0/3/3/3
10	PSU	A	823	10	-	0/7/25/26	0/2/2/2
10	MA6	A	1850	10	-	0/7/29/30	0/3/3/3
10	5MU	A	814	10	-	0/7/25/26	0/2/2/2
10	OMG	A	683	10	-	2/5/27/28	0/3/3/3
10	UR3	A	1830	10	-	2/7/25/26	0/2/2/2
10	A2M	A	1031	10	-	1/5/27/28	0/3/3/3
10	OMU	A	121	10	-	1/9/27/28	0/2/2/2
10	OMG	A	509	51,10	-	1/5/27/28	0/3/3/3
10	MA6	A	1851	10	-	3/7/29/30	0/3/3/3
10	A2M	A	484	10	-	1/5/27/28	0/3/3/3
10	PSU	A	612	10	-	0/7/25/26	0/2/2/2
10	OMG	A	644	10	-	2/5/27/28	0/3/3/3
10	6MZ	A	1832	51,10	-	0/5/27/28	0/3/3/3
10	PSU	A	119	10	-	0/7/25/26	0/2/2/2
10	PSU	A	822	10	-	2/7/25/26	0/2/2/2
10	A2M	A	27	51,10	-	1/5/27/28	0/3/3/3
10	JMH	A	1219	10	-	0/7/25/26	0/2/2/2
10	B8N	A	1248	10	-	7/16/34/35	0/2/2/2
10	A2M	A	166	10	-	0/5/27/28	0/3/3/3
10	A2M	A	1678	51,10	-	0/5/27/28	0/3/3/3
10	PSU	A	1081	10	-	1/7/25/26	0/2/2/2
10	PSU	A	1243	10	-	2/7/25/26	0/2/2/2
10	OMC	A	517	10	-	2/9/27/28	0/2/2/2
10	A2M	A	159	10	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	5MC	A	1374	10	-	0/7/25/26	0/2/2/2
10	OMC	A	1703	10	-	2/9/27/28	0/2/2/2
10	OMC	A	174	51,10	-	0/9/27/28	0/2/2/2
10	OMU	A	116	10	-	1/9/27/28	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1031	A2M	C3'-C2'	-12.99	1.24	1.52
10	A	1678	A2M	C3'-C2'	-12.96	1.24	1.52
10	A	166	A2M	C3'-C2'	-12.90	1.24	1.52
10	A	27	A2M	C3'-C2'	-12.85	1.24	1.52
10	A	159	A2M	C3'-C2'	-12.45	1.25	1.52
10	A	484	A2M	C3'-C2'	-12.41	1.25	1.52
10	A	668	A2M	C3'-C2'	-12.27	1.25	1.52
10	A	1031	A2M	O4'-C1'	7.93	1.52	1.41
10	A	166	A2M	O4'-C1'	7.84	1.52	1.41
10	A	1678	A2M	O4'-C1'	7.78	1.51	1.41
10	A	27	A2M	O4'-C1'	7.46	1.51	1.41
10	A	1830	UR3	C2-N1	7.36	1.49	1.38
10	A	484	A2M	O4'-C1'	7.24	1.51	1.41
10	A	159	A2M	O4'-C1'	7.21	1.51	1.41
10	A	116	OMU	C2-N3	7.09	1.50	1.38
10	A	668	A2M	O4'-C4'	-7.02	1.29	1.45
10	A	159	A2M	O4'-C4'	-6.95	1.29	1.45
10	A	1678	A2M	O4'-C4'	-6.92	1.29	1.45
10	A	116	OMU	C2-N1	6.91	1.49	1.38
10	A	121	OMU	C2-N1	6.86	1.49	1.38
10	A	121	OMU	C2-N3	6.86	1.50	1.38
10	A	668	A2M	O4'-C1'	6.83	1.50	1.41
10	A	484	A2M	O4'-C4'	-6.62	1.30	1.45
10	A	27	A2M	O4'-C4'	-6.61	1.30	1.45
10	A	166	A2M	O4'-C4'	-6.60	1.30	1.45
10	A	1031	A2M	O4'-C4'	-6.59	1.30	1.45
10	A	121	OMU	C6-C5	6.11	1.49	1.35
10	A	116	OMU	C6-C5	6.04	1.49	1.35
10	A	1830	UR3	C6-C5	6.02	1.49	1.35
10	A	1832	6MZ	C6-N6	5.72	1.44	1.35
10	A	484	A2M	C3'-C4'	5.22	1.66	1.53
10	A	159	A2M	C3'-C4'	5.11	1.66	1.53
10	A	1678	A2M	C3'-C4'	5.05	1.65	1.53
10	A	27	A2M	C3'-C4'	5.03	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	668	A2M	C3'-C4'	4.98	1.65	1.53
10	A	1830	UR3	C2-N3	4.92	1.48	1.39
10	A	1031	A2M	C3'-C4'	4.88	1.65	1.53
10	A	166	A2M	C3'-C4'	4.80	1.65	1.53
10	A	116	OMU	C4-N3	4.05	1.45	1.38
10	A	121	OMU	C4-N3	3.92	1.45	1.38
10	A	159	A2M	O2'-C2'	3.41	1.51	1.42
10	A	484	A2M	O2'-C2'	3.37	1.51	1.42
10	A	1243	PSU	C6-C5	3.37	1.39	1.35
10	A	27	A2M	O2'-C2'	3.34	1.51	1.42
10	A	166	A2M	O2'-C2'	3.33	1.51	1.42
10	A	668	A2M	O2'-C2'	3.33	1.51	1.42
10	A	1678	A2M	O2'-C2'	3.28	1.51	1.42
10	A	823	PSU	C6-C5	3.28	1.39	1.35
10	A	119	PSU	C6-C5	3.27	1.39	1.35
10	A	1031	A2M	O2'-C2'	3.27	1.51	1.42
10	A	822	PSU	C6-C5	3.11	1.38	1.35
10	A	159	A2M	C6-N6	3.10	1.45	1.34
10	A	1031	A2M	C6-N6	3.09	1.45	1.34
10	A	1678	A2M	C6-N6	3.08	1.45	1.34
10	A	166	A2M	C6-N6	3.08	1.45	1.34
10	A	484	A2M	C6-N6	3.08	1.45	1.34
10	A	668	A2M	C6-N6	3.08	1.45	1.34
10	A	27	A2M	C6-N6	3.07	1.45	1.34
10	A	1081	PSU	C6-C5	3.05	1.38	1.35
10	A	1851	MA6	C2-N3	3.02	1.37	1.32
10	A	1830	UR3	C6-N1	2.98	1.45	1.38
10	A	1851	MA6	C5-C4	-2.95	1.33	1.40
10	A	644	OMG	C8-N7	-2.93	1.30	1.35
10	A	1850	MA6	C2-N3	2.92	1.36	1.32
10	A	612	PSU	C6-C5	2.90	1.38	1.35
10	A	509	OMG	C8-N7	-2.90	1.30	1.35
10	A	1031	A2M	C5-C4	-2.89	1.33	1.40
10	A	166	A2M	C5-C4	-2.88	1.33	1.40
10	A	668	A2M	C5-C4	-2.87	1.33	1.40
10	A	1850	MA6	C5-C4	-2.86	1.33	1.40
10	A	1678	A2M	C5-C4	-2.86	1.33	1.40
10	A	683	OMG	C8-N7	-2.83	1.30	1.35
10	A	27	A2M	C5-C4	-2.82	1.33	1.40
10	A	159	A2M	C5-C4	-2.78	1.33	1.40
10	A	484	A2M	C5-C4	-2.76	1.33	1.40
10	A	509	OMG	C5-C6	-2.56	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	644	OMG	C5-C6	-2.54	1.42	1.47
10	A	121	OMU	C6-N1	2.51	1.44	1.38
10	A	683	OMG	C5-C6	-2.51	1.42	1.47
10	A	116	OMU	C6-N1	2.43	1.43	1.38
10	A	1830	UR3	O4-C4	-2.35	1.18	1.23
10	A	1832	6MZ	C5-C4	-2.33	1.34	1.40
10	A	1830	UR3	O2-C2	-2.30	1.18	1.22
10	A	159	A2M	C2-N3	2.17	1.35	1.32
10	A	1678	A2M	C2-N3	2.15	1.35	1.32
10	A	1830	UR3	C5-C4	2.15	1.49	1.43
10	A	484	A2M	O3'-C3'	2.13	1.48	1.43
10	A	668	A2M	O3'-C3'	2.13	1.48	1.43
10	A	484	A2M	C2-N3	2.13	1.35	1.32
10	A	121	OMU	C5-C4	2.10	1.48	1.43
10	A	1031	A2M	C2-N3	2.05	1.35	1.32

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1851	MA6	N1-C6-N6	-12.38	104.03	117.06
10	A	1850	MA6	N1-C6-N6	-12.18	104.24	117.06
10	A	159	A2M	C1'-N9-C4	10.97	145.91	126.64
10	A	1678	A2M	C1'-N9-C4	10.91	145.81	126.64
10	A	484	A2M	C1'-N9-C4	10.64	145.34	126.64
10	A	1031	A2M	C1'-N9-C4	10.32	144.77	126.64
10	A	668	A2M	C1'-N9-C4	10.28	144.70	126.64
10	A	27	A2M	C1'-N9-C4	10.21	144.59	126.64
10	A	166	A2M	C1'-N9-C4	9.69	143.67	126.64
10	A	668	A2M	C5-C6-N6	9.12	134.22	120.35
10	A	166	A2M	C5-C6-N6	9.03	134.08	120.35
10	A	27	A2M	C5-C6-N6	8.97	133.98	120.35
10	A	1031	A2M	C5-C6-N6	8.93	133.93	120.35
10	A	159	A2M	C5-C6-N6	8.86	133.82	120.35
10	A	484	A2M	C5-C6-N6	8.77	133.68	120.35
10	A	1678	A2M	C5-C6-N6	8.75	133.65	120.35
10	A	668	A2M	N6-C6-N1	-6.25	105.61	118.57
10	A	166	A2M	N6-C6-N1	-6.10	105.92	118.57
10	A	1031	A2M	N6-C6-N1	-6.09	105.93	118.57
10	A	166	A2M	N3-C2-N1	-6.05	119.22	128.68
10	A	27	A2M	N6-C6-N1	-6.02	106.07	118.57
10	A	159	A2M	N6-C6-N1	-6.00	106.13	118.57
10	A	1832	6MZ	N3-C2-N1	-5.98	119.33	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1678	A2M	N6-C6-N1	-5.96	106.19	118.57
10	A	484	A2M	N6-C6-N1	-5.95	106.23	118.57
10	A	27	A2M	N3-C2-N1	-5.76	119.68	128.68
10	A	1031	A2M	N3-C2-N1	-5.67	119.81	128.68
10	A	1678	A2M	N3-C2-N1	-5.63	119.88	128.68
10	A	1851	MA6	N3-C2-N1	-5.61	119.91	128.68
10	A	484	A2M	N3-C2-N1	-5.57	119.97	128.68
10	A	1850	MA6	N3-C2-N1	-5.50	120.09	128.68
10	A	159	A2M	N3-C2-N1	-5.49	120.10	128.68
10	A	668	A2M	N3-C2-N1	-5.45	120.16	128.68
10	A	1832	6MZ	C2-N1-C6	5.36	121.19	116.59
10	A	1832	6MZ	C9-N6-C6	4.98	127.17	122.87
10	A	121	OMU	C4-N3-C2	-4.91	120.10	126.58
10	A	1081	PSU	C4-N3-C2	-4.80	119.43	126.34
10	A	822	PSU	N1-C2-N3	4.72	120.47	115.13
10	A	1243	PSU	N1-C2-N3	4.71	120.46	115.13
10	A	822	PSU	C4-N3-C2	-4.66	119.62	126.34
10	A	823	PSU	C4-N3-C2	-4.60	119.71	126.34
10	A	1081	PSU	N1-C2-N3	4.59	120.34	115.13
10	A	612	PSU	C4-N3-C2	-4.57	119.76	126.34
10	A	1243	PSU	C4-N3-C2	-4.56	119.77	126.34
10	A	116	OMU	C4-N3-C2	-4.55	120.58	126.58
10	A	612	PSU	N1-C2-N3	4.55	120.28	115.13
10	A	823	PSU	N1-C2-N3	4.50	120.23	115.13
10	A	1830	UR3	C4-N3-C2	-4.49	120.33	124.56
10	A	119	PSU	N1-C2-N3	4.12	119.79	115.13
10	A	119	PSU	C4-N3-C2	-4.02	120.54	126.34
10	A	121	OMU	N3-C2-N1	3.67	119.77	114.89
10	A	1830	UR3	C1'-N1-C2	3.56	123.00	116.99
10	A	116	OMU	N3-C2-N1	3.48	119.50	114.89
10	A	121	OMU	C5-C4-N3	3.23	119.67	114.84
10	A	116	OMU	C5-C4-N3	3.02	119.36	114.84
10	A	1832	6MZ	C1'-N9-C4	-2.95	121.47	126.64
10	A	822	PSU	O2-C2-N1	-2.94	119.55	122.79
10	A	612	PSU	O2-C2-N1	-2.87	119.63	122.79
10	A	1830	UR3	C6-N1-C2	-2.84	119.25	121.79
10	A	116	OMU	O4-C4-C5	-2.83	120.19	125.16
10	A	1243	PSU	O2-C2-N1	-2.72	119.80	122.79
10	A	121	OMU	O4-C4-C5	-2.70	120.41	125.16
10	A	1832	6MZ	C4-C5-N7	-2.69	106.60	109.40
10	A	1248	B8N	C3'-C2'-C1'	2.63	104.70	101.64
10	A	823	PSU	O2-C2-N1	-2.60	119.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	509	OMG	O6-C6-C5	2.51	129.27	124.37
10	A	644	OMG	O6-C6-C5	2.45	129.16	124.37
10	A	814	5MU	C1'-N1-C2	2.44	122.00	117.57
10	A	1081	PSU	O2-C2-N1	-2.43	120.11	122.79
10	A	1830	UR3	O2-C2-N3	-2.40	117.96	121.34
10	A	1243	PSU	C6-N1-C2	-2.40	120.23	122.68
10	A	823	PSU	C6-N1-C2	-2.35	120.28	122.68
10	A	119	PSU	C6-N1-C2	-2.34	120.29	122.68
10	A	119	PSU	O2-C2-N1	-2.34	120.22	122.79
10	A	822	PSU	C6-N1-C2	-2.33	120.30	122.68
10	A	683	OMG	O6-C6-C5	2.30	128.86	124.37
10	A	668	A2M	C3'-C2'-C1'	2.27	107.16	102.89
10	A	612	PSU	C6-N1-C2	-2.22	120.42	122.68
10	A	121	OMU	O2-C2-N1	-2.21	119.85	122.79
10	A	822	PSU	O4'-C1'-C2'	2.18	108.21	105.14
10	A	484	A2M	C3'-C2'-C1'	2.17	106.97	102.89
10	A	1703	OMC	C1'-N1-C2	2.17	123.26	118.42
10	A	814	5MU	O2-C2-N1	2.14	125.63	122.79
10	A	159	A2M	O4'-C1'-C2'	-2.13	102.89	106.59
10	A	612	PSU	O4'-C1'-C2'	2.11	108.12	105.14
10	A	822	PSU	C6-C5-C4	2.09	119.66	118.20
10	A	166	A2M	C5'-C4'-C3'	-2.07	107.42	115.18
10	A	1081	PSU	O4'-C1'-C2'	2.06	108.05	105.14
10	A	1081	PSU	C6-N1-C2	-2.04	120.60	122.68
10	A	116	OMU	C1'-N1-C2	2.03	121.25	117.57
10	A	174	OMC	C1'-N1-C2	2.01	122.91	118.42

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	27	A2M	C1'-C2'-O2'-CM'
10	A	116	OMU	C1'-C2'-O2'-CM2
10	A	121	OMU	C1'-C2'-O2'-CM2
10	A	159	A2M	C1'-C2'-O2'-CM'
10	A	484	A2M	C1'-C2'-O2'-CM'
10	A	1031	A2M	C1'-C2'-O2'-CM'
10	A	1830	UR3	O4'-C1'-N1-C2
10	A	1851	MA6	O4'-C4'-C5'-O5'
10	A	1248	B8N	C32-C31-N3-C2
10	A	1248	B8N	C32-C31-N3-C4
10	A	1830	UR3	O4'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	668	A2M	O4'-C4'-C5'-O5'
10	A	668	A2M	C3'-C4'-C5'-O5'
10	A	1851	MA6	C3'-C4'-C5'-O5'
10	A	1248	B8N	C32-C33-C34-O36
10	A	517	OMC	C3'-C4'-C5'-O5'
10	A	517	OMC	O4'-C4'-C5'-O5'
10	A	1703	OMC	O4'-C4'-C5'-O5'
10	A	1248	B8N	C32-C33-C34-O35
10	A	644	OMG	C3'-C4'-C5'-O5'
10	A	1703	OMC	C3'-C4'-C5'-O5'
10	A	1248	B8N	N34-C33-C34-O36
10	A	683	OMG	O4'-C4'-C5'-O5'
10	A	822	PSU	C3'-C4'-C5'-O5'
10	A	1243	PSU	O4'-C4'-C5'-O5'
10	A	1248	B8N	N34-C33-C34-O35
10	A	1243	PSU	C3'-C4'-C5'-O5'
10	A	159	A2M	C4'-C5'-O5'-P
10	A	822	PSU	O4'-C4'-C5'-O5'
10	A	1851	MA6	C4'-C5'-O5'-P
10	A	644	OMG	O4'-C4'-C5'-O5'
10	A	1248	B8N	O4'-C1'-C5'-C4
10	A	1081	PSU	C4'-C5'-O5'-P
10	A	683	OMG	C3'-C4'-C5'-O5'
10	A	509	OMG	O4'-C4'-C5'-O5'

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 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

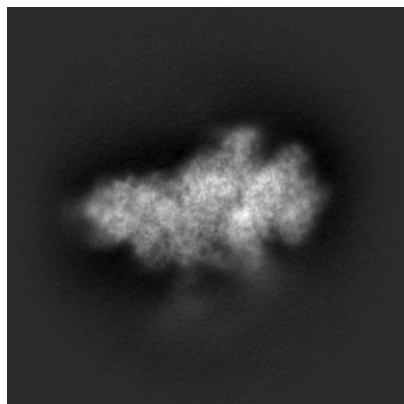
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17701. These allow visual inspection of the internal detail of the map and identification of artifacts.

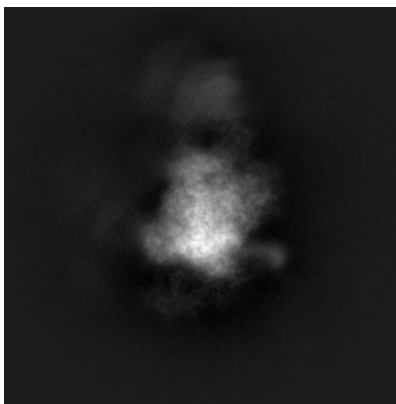
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

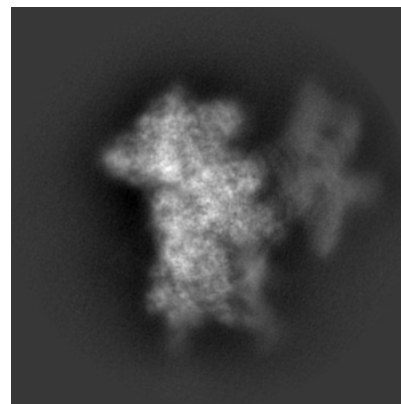
6.1.1 Primary map



X

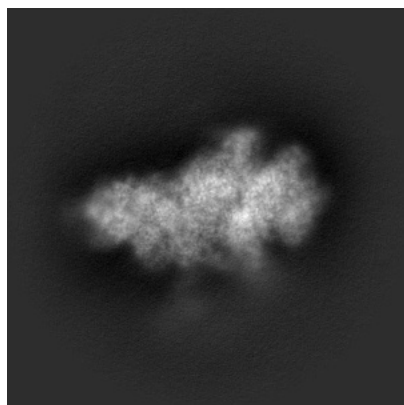


Y

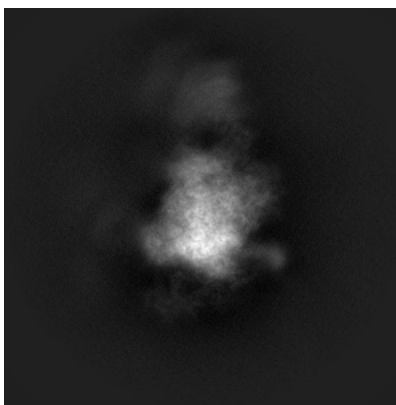


Z

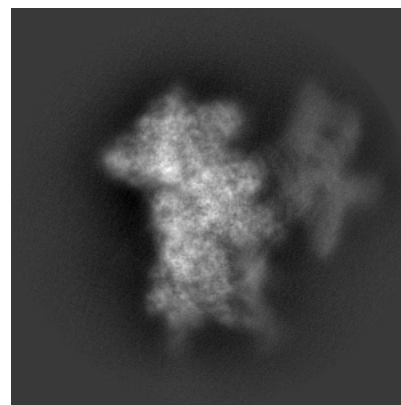
6.1.2 Raw map



X



Y

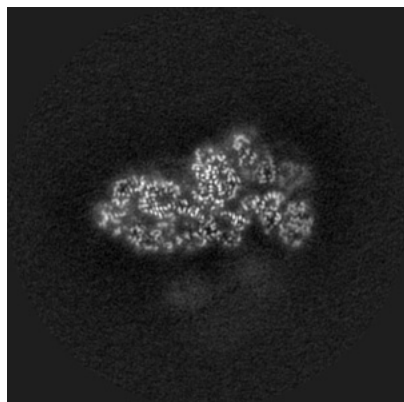


Z

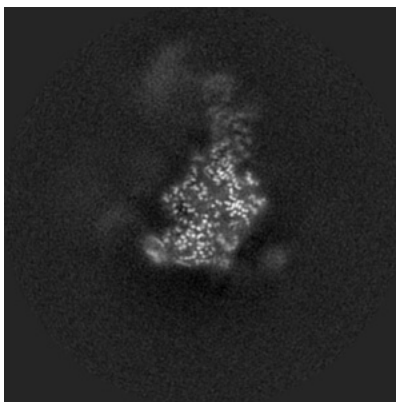
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

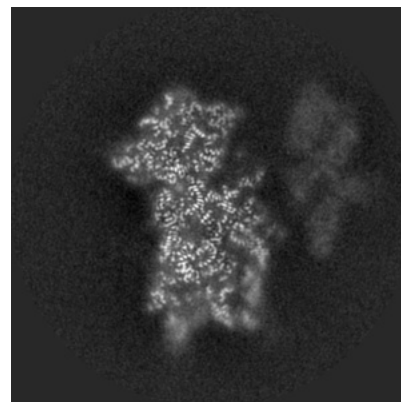
6.2.1 Primary map



X Index: 180

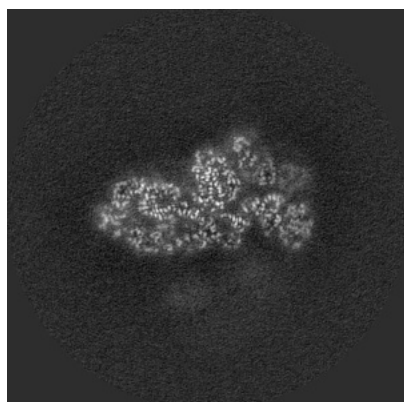


Y Index: 180

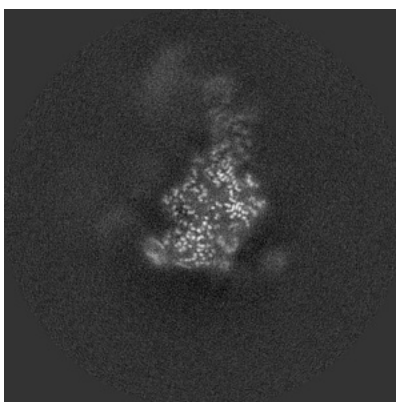


Z Index: 180

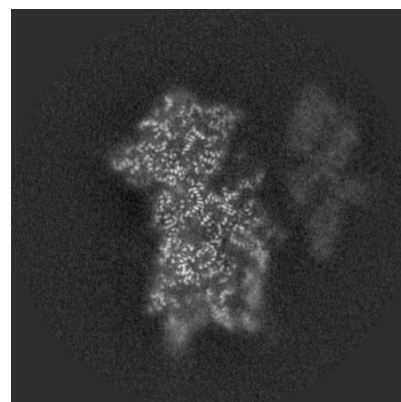
6.2.2 Raw map



X Index: 180



Y Index: 180

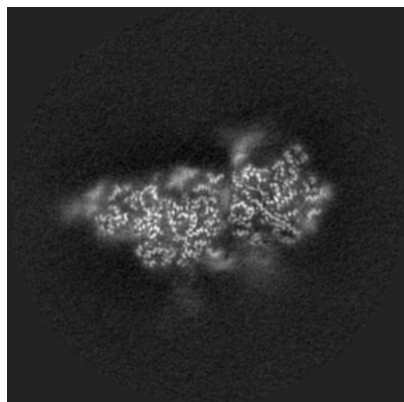


Z Index: 180

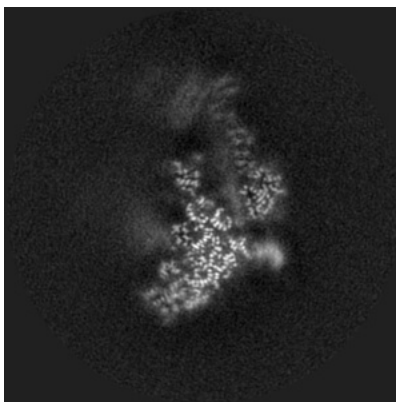
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

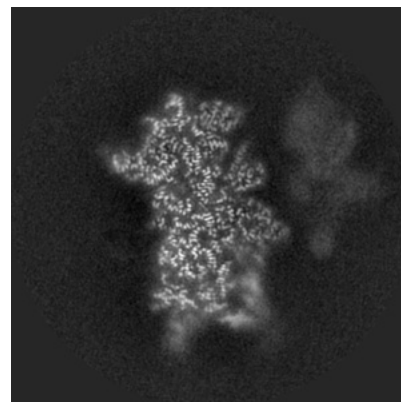
6.3.1 Primary map



X Index: 147

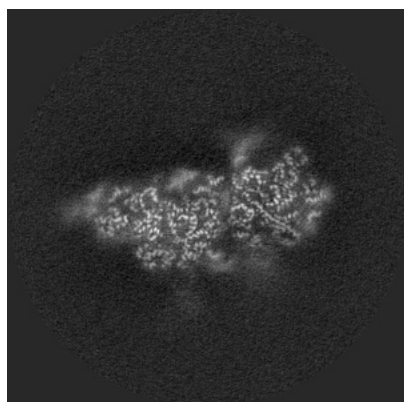


Y Index: 216

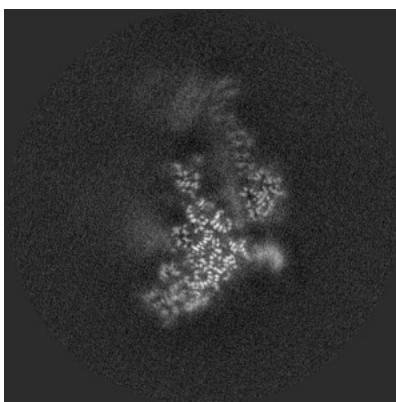


Z Index: 174

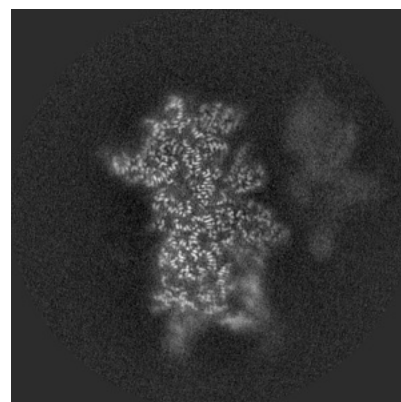
6.3.2 Raw map



X Index: 147



Y Index: 216

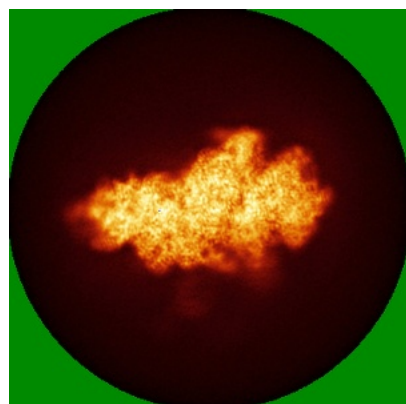


Z Index: 174

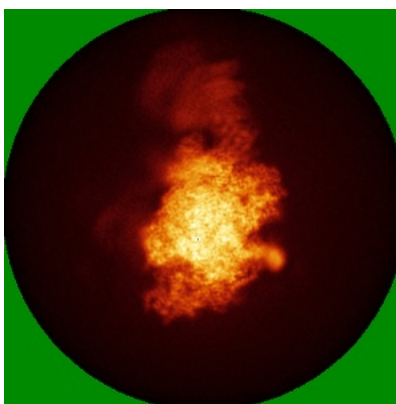
The images above show the largest variance slices of the map in three orthogonal directions.

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

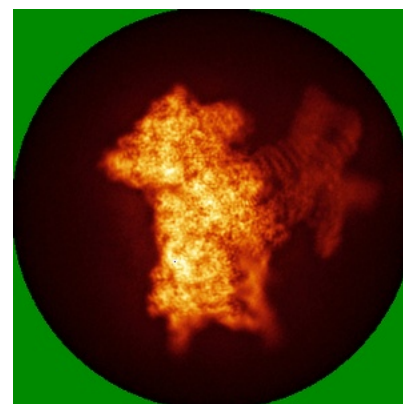
6.4.1 Primary map



X

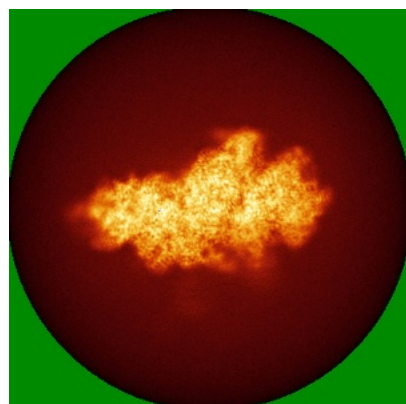


Y

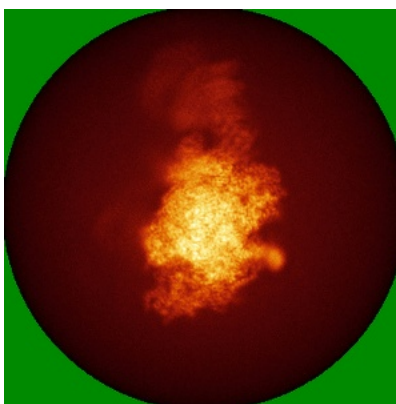


Z

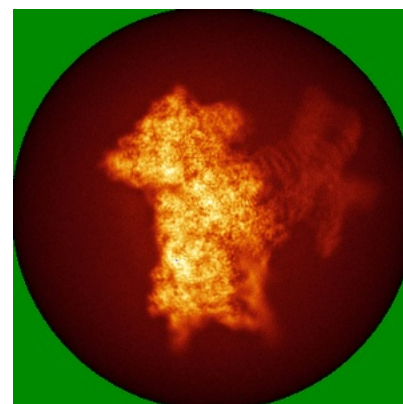
6.4.2 Raw map



X



Y

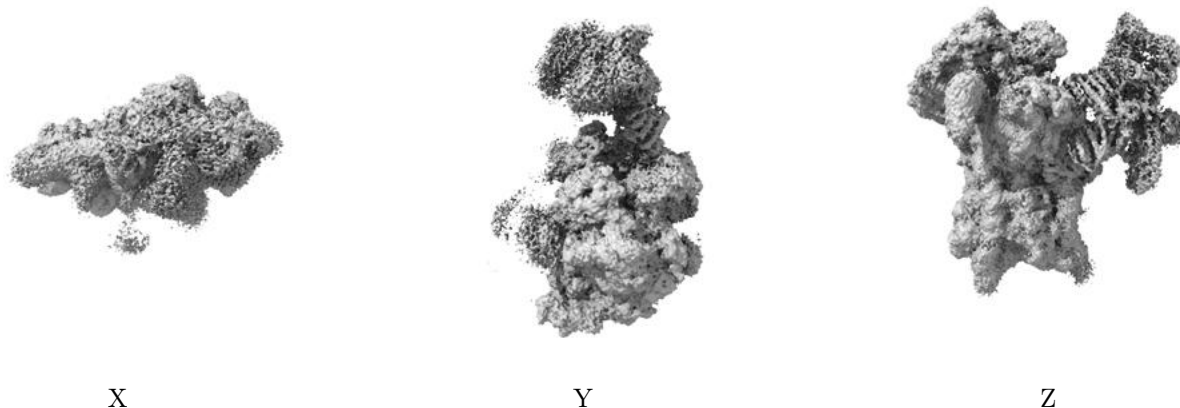


Z

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

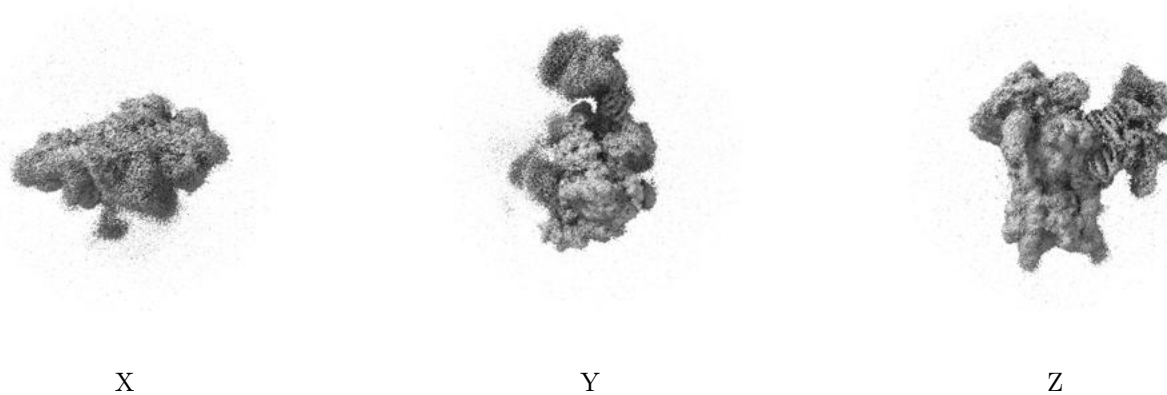
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0102. 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.

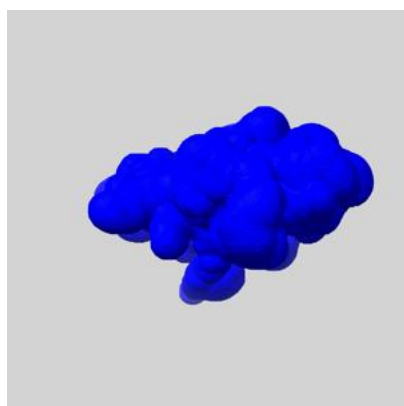
6.6 Mask visualisation [i](#)

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

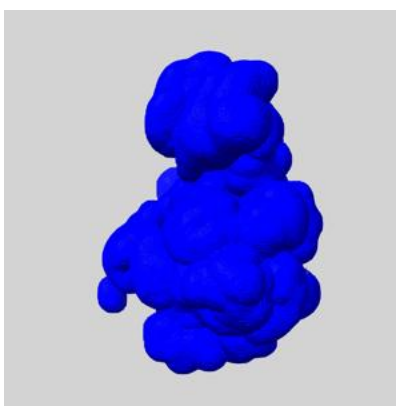
A mask typically either:

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

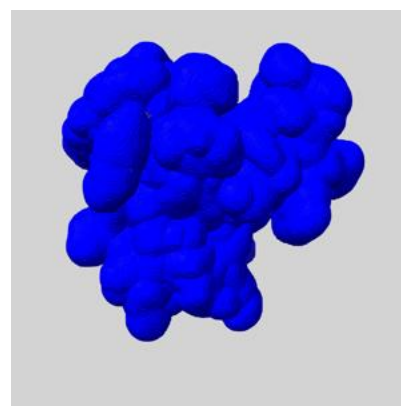
6.6.1 emd_17701_msk_1.map [i](#)



X



Y

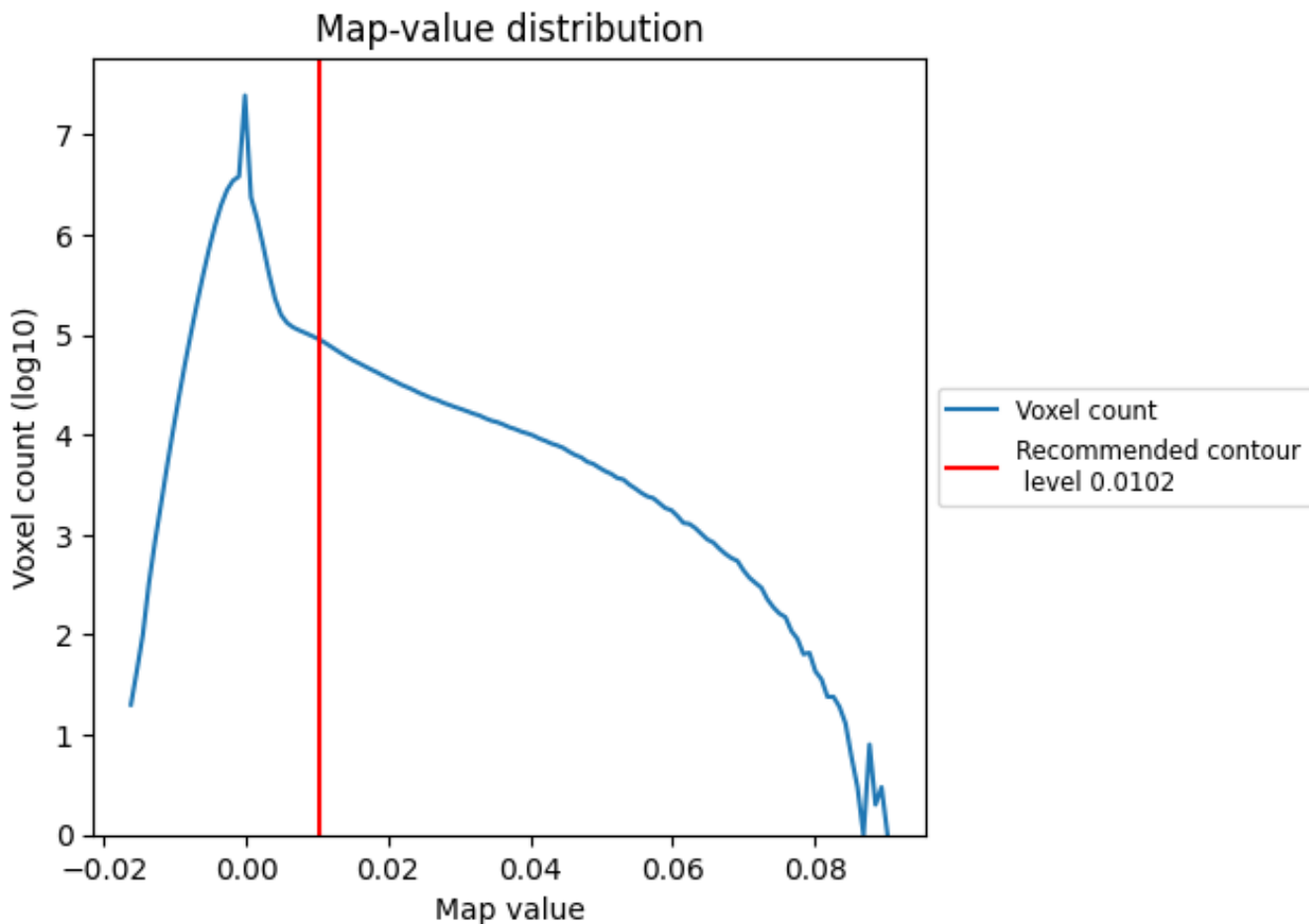


Z

7 Map analysis [i](#)

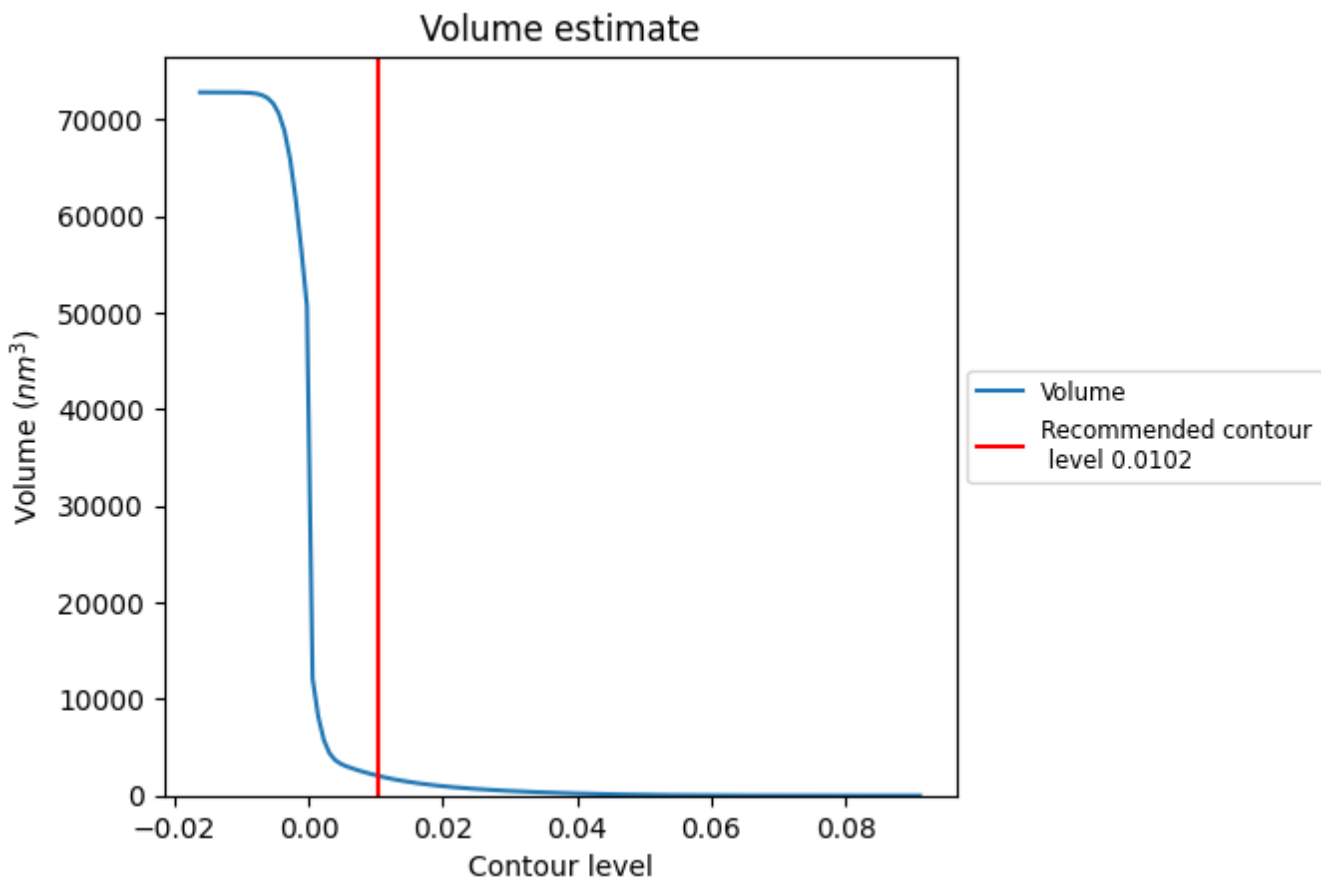
This section contains the results of statistical analysis of the map.

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.

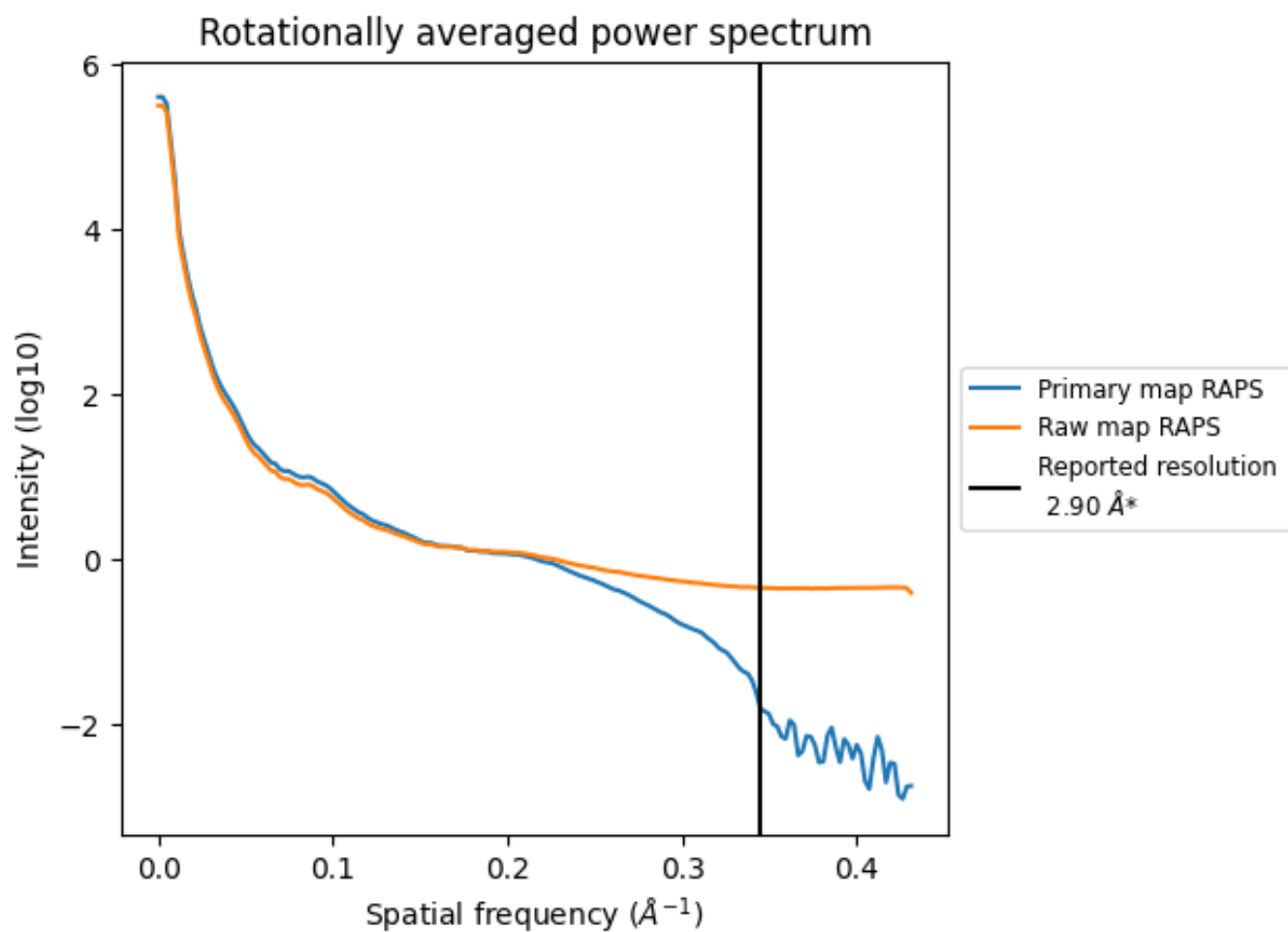
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2072 nm^3 ; this corresponds to an approximate mass of 1872 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

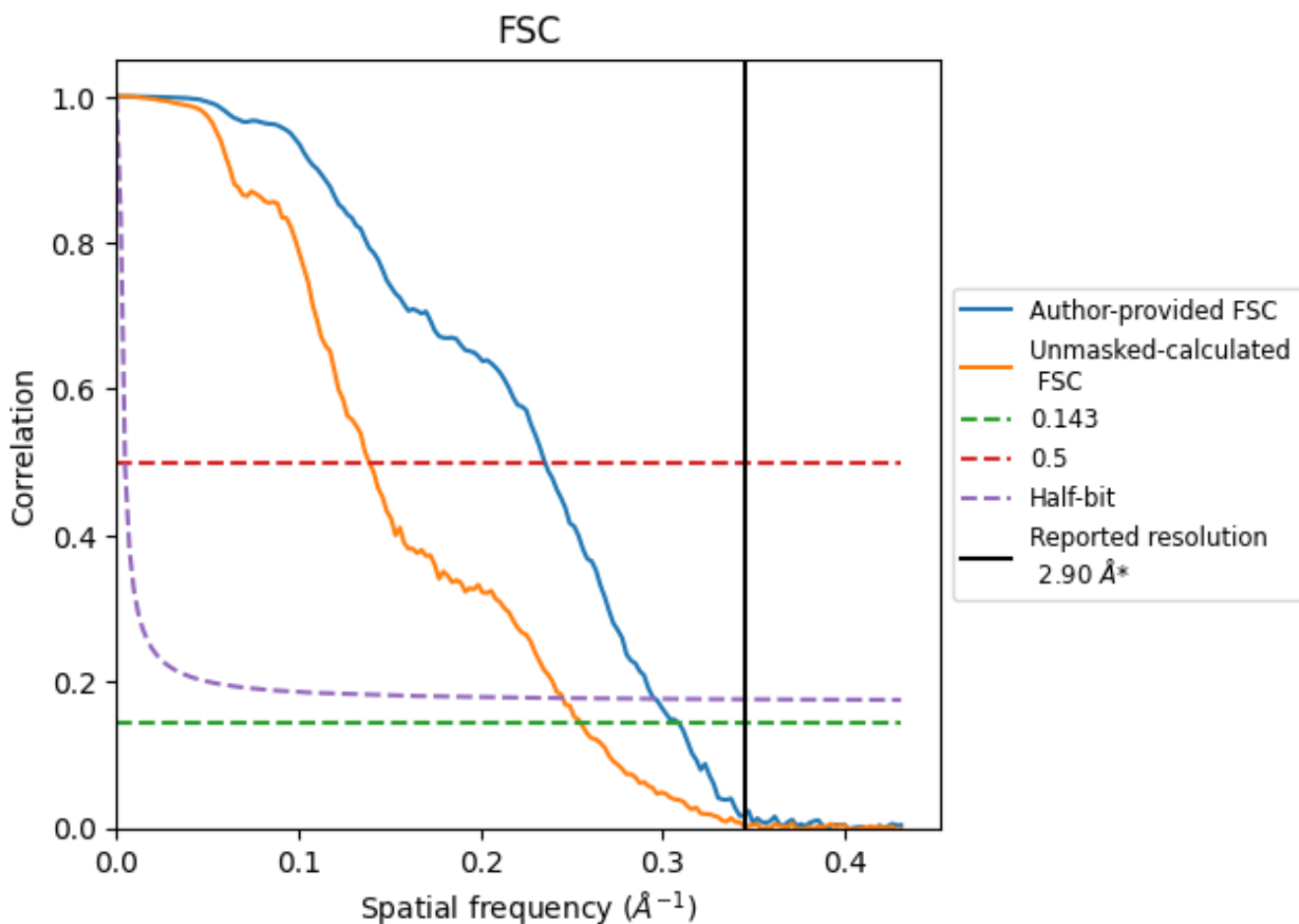


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.24	4.25	3.38
Unmasked-calculated*	3.92	7.21	4.08

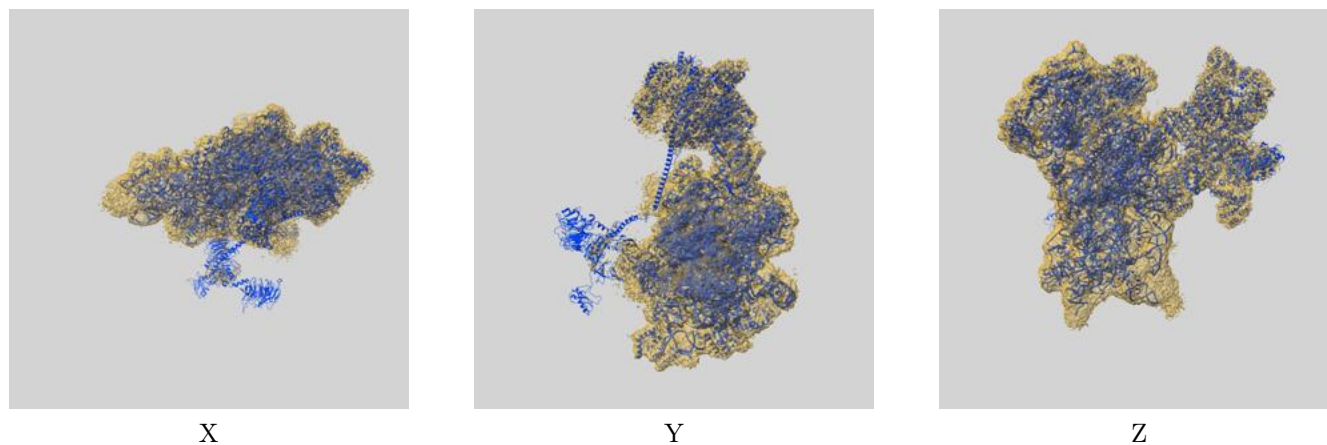
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.24 differs from the reported value 2.9 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

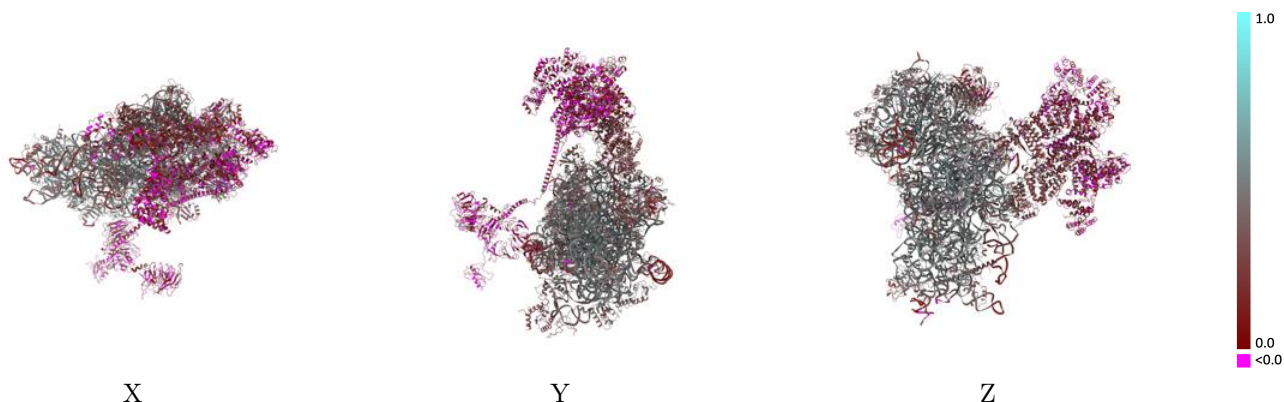
This section contains information regarding the fit between EMDB map EMD-17701 and PDB model 8PJ6. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



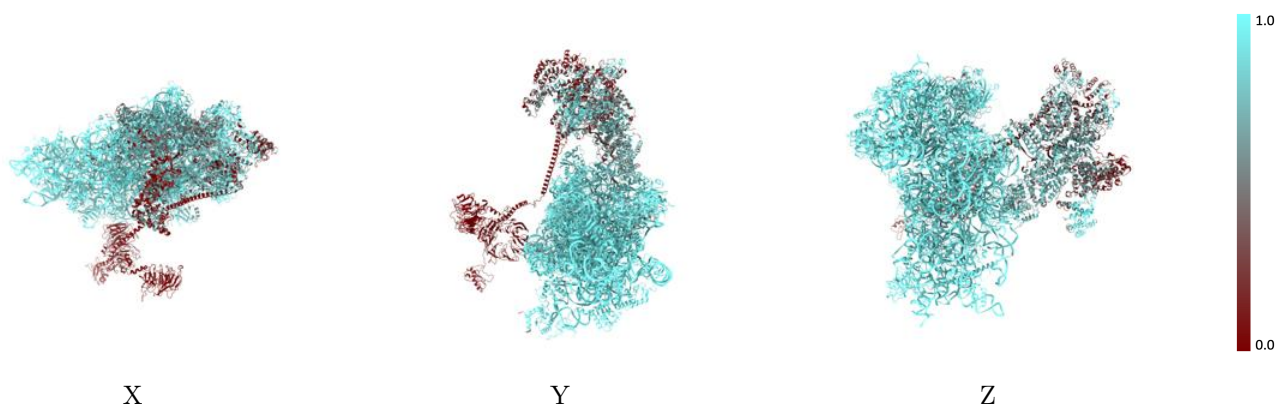
The images above show the 3D surface view of the map at the recommended contour level 0.0102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



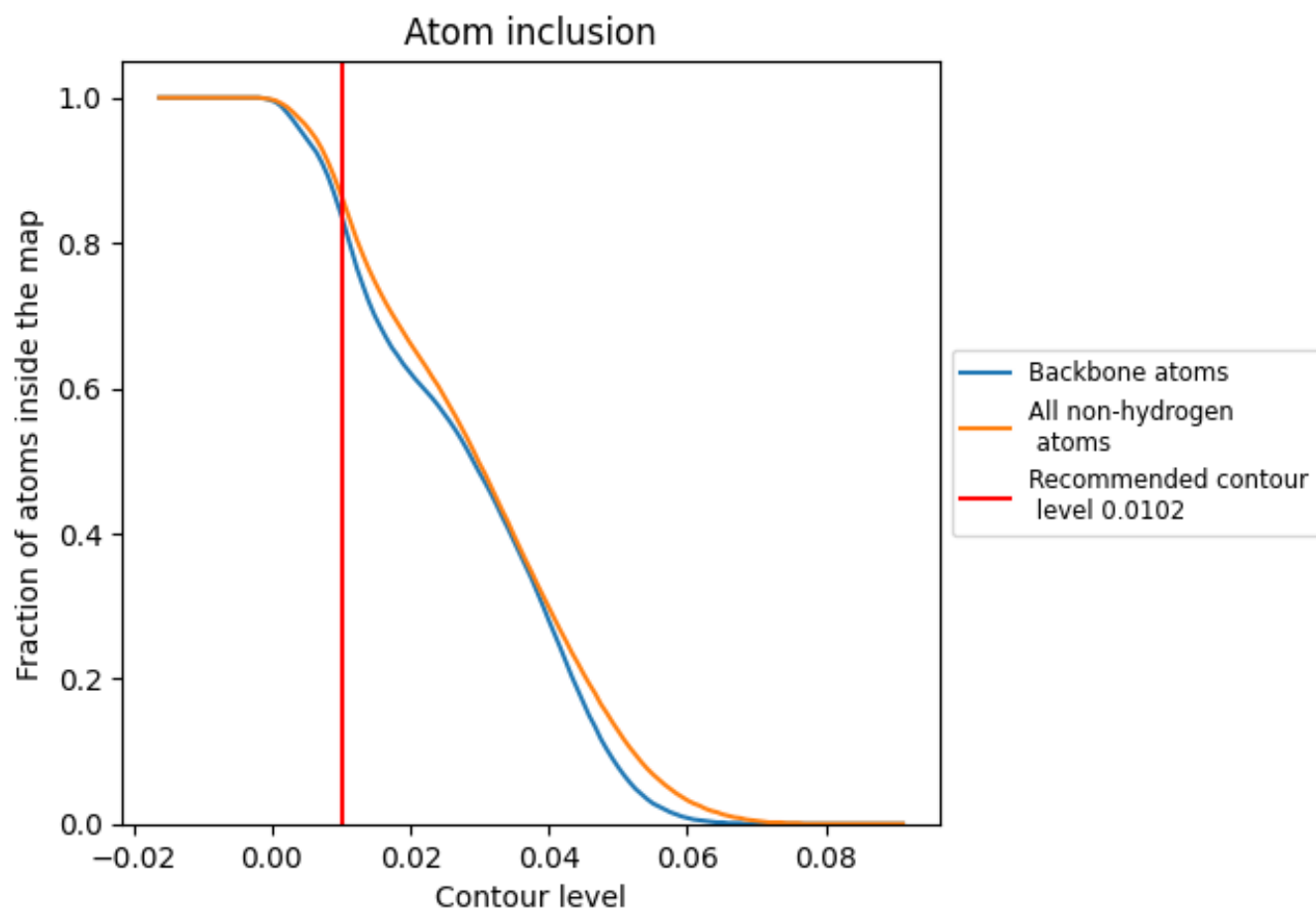
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0102).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.0102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.3740
1	 0.0480	 0.1230
2	 0.0000	 0.1160
3	 0.2540	 0.1220
4	 0.6150	 0.1240
5	 0.4660	 0.1170
6	 0.5550	 0.1380
7	 0.7220	 0.2430
8	 0.5440	 0.1010
9	 1.0000	 0.4250
A	 0.9990	 0.4610
B	 0.9950	 0.4940
C	 0.9970	 0.4780
D	 0.9900	 0.4640
E	 0.9990	 0.4890
F	 0.9760	 0.4130
G	 0.9430	 0.3920
H	 0.9760	 0.4540
I	 0.9860	 0.4500
J	 0.9940	 0.4840
K	 0.9780	 0.4460
L	 0.9730	 0.4710
M	 0.9530	 0.4080
N	 0.9800	 0.4530
O	 0.9890	 0.4390
P	 0.9810	 0.4610
Q	 0.9920	 0.4920
R	 0.9990	 0.4510
S	 0.9930	 0.4000
T	 0.9990	 0.4350
V	 0.9880	 0.4590
Y	 0.9970	 0.4770
Z	 0.9650	 0.4390
a	 0.9830	 0.4270
b	 0.9930	 0.4170



Continued on next page...

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Chain	Atom inclusion	Q-score
c	 0.9910	 0.4260
d	 0.9940	 0.4570
e	 0.9900	 0.4340
f	 0.9920	 0.4300
h	 0.9890	 0.4360
i	 0.9880	 0.5020
k	 0.9960	 0.3130
m	 0.9630	 0.2870
n	 0.9900	 0.4500
o	 0.9110	 0.2080
q	 0.9670	 0.3550
u	 0.5270	 0.2040
v	 0.5880	 0.1420
w	 0.9970	 0.2510
x	 0.8460	 0.2890
y	 0.6840	 0.2590