



Full wwPDB EM Validation Report ⓘ

Aug 7, 2024 – 04:30 pm BST

PDB ID : 8PJ3
EMDB ID : EMD-17698
Title : Structure of human 48S translation initiation complex upon transfer of initiator tRNA to eIF5B (48S-3)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 3.70 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:

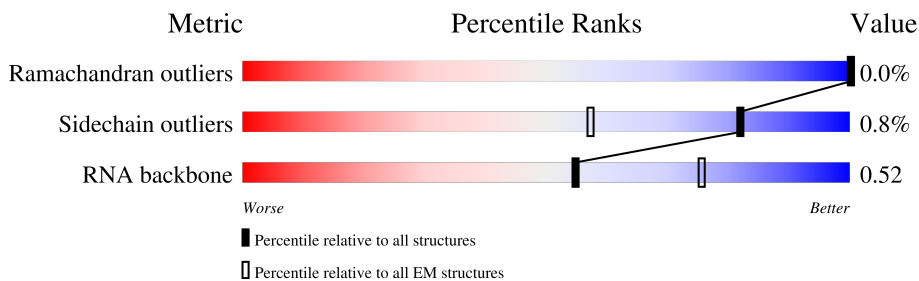
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 3.70 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	0	1220	
2	1	814	
3	2	325	
4	3	218	
5	4	357	
6	5	564	
7	6	374	
8	7	255	



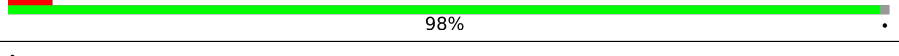
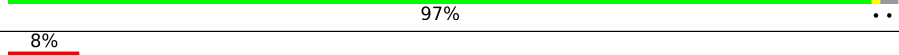
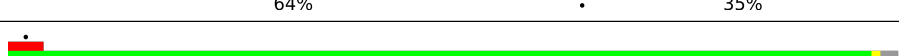
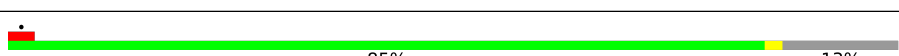
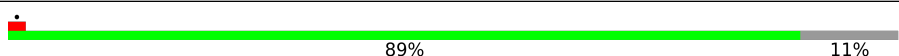

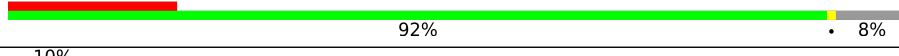
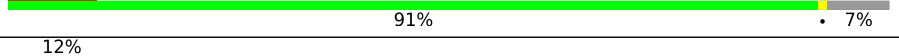
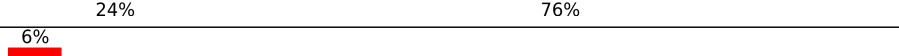

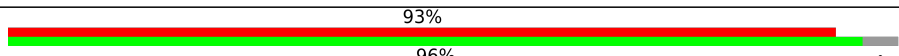

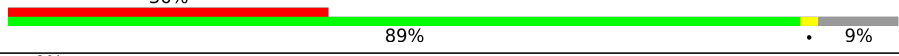



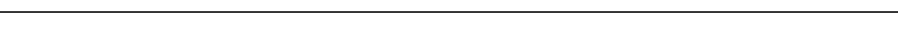


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	8	352	59% 90% 10%
10	9	25	12% 96% .
11	A	1869	69% 23% 6%
12	B	158	89% 10%
13	C	263	96% ..
14	D	194	90% 9%
15	E	143	98% .
16	F	133	44% 56%
17	G	194	90% 9%
18	H	84	96% .
19	I	151	99% ..
20	J	130	98% ..
21	K	83	96% ..
22	L	293	75% 25%
23	M	135	8% 94% ..
24	N	295	69% 30%
25	O	264	78% 20%
26	P	151	87% 12%
27	Q	115	86% 14%
28	R	208	95% 5%
29	S	249	91% 8%
30	T	133	92% 6%
31	V	204	92% 7%
32	Y	146	95% ..
33	Z	243	92% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	a	165	
35	b	145	
36	c	317	
37	d	145	
38	e	125	
39	f	152	
40	h	119	
41	i	56	
42	k	156	
43	m	132	
44	n	69	
45	o	320	
46	q	144	
47	r	315	
48	t	472	
49	u	1382	
50	v	445	
51	w	75	
52	x	548	
53	y	913	
54	z	430	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 123641 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 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	621	4920	3135	850	913	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	588	3258	1986	633	634	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	2	304	1493	885	304	304	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	213	1057	631	213	213	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	4	257	1272	757	257	258	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	520	4347	2814	721	793	19	0	0

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	362	2196	1348	414	427	7	0	0

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	57	1218	547	231	383	57	0	0

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	8	317	1574	937	318	319	0	0

- Molecule 10 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	24	230	139	62	26	3	0	0

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	A	1754	37429	16718	6714	12244	1753	0	0

- Molecule 12 is a protein called 40S ribosomal protein S11.

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

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 14 is a protein called 40S ribosomal protein S9.

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

- Molecule 15 is a protein called 40S ribosomal protein S23.

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

- Molecule 16 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	59	461	285	100	75	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	PRO	LYS	conflict	UNP P62861

- Molecule 17 is a protein called 40S ribosomal protein S7.

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

- Molecule 18 is a protein called 40S ribosomal protein S27.

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

- Molecule 19 is a protein called 40S ribosomal protein S13.

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

- Molecule 20 is a protein called 40S ribosomal protein S15a.

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

- Molecule 21 is a protein called 40S ribosomal protein S21.

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

- Molecule 22 is a protein called 40S ribosomal protein S2.

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

- Molecule 23 is a protein called 40S ribosomal protein S17.

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

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

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

- Molecule 25 is a protein called 40S ribosomal protein S3a.

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

- Molecule 26 is a protein called 40S ribosomal protein S14.

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

- Molecule 27 is a protein called 40S ribosomal protein S26.

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

- Molecule 28 is a protein called 40S ribosomal protein S8.

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

- Molecule 29 is a protein called 40S ribosomal protein S6.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

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

- Molecule 31 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	V	189	1495	934	284	270	7	0	0

- Molecule 32 is a protein called 40S ribosomal protein S16.

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

- Molecule 33 is a protein called 40S ribosomal protein S3.

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

- Molecule 34 is a protein called 40S ribosomal protein S10.

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

- Molecule 35 is a protein called 40S ribosomal protein S15.

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

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a protein called 40S ribosomal protein S19.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 39 is a protein called 40S ribosomal protein S18.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein S29.

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

- Molecule 42 is a protein called Ubiquitin.

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

- Molecule 43 is a protein called 40S ribosomal protein S12.

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

- Molecule 44 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

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

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	117	Total	C	N	O	S	0	0
			943	585	180	174	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	t	455	3439	2179	599	643	18	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	v	405	2740	1720	498	510	12	0	0

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	w	75	1604	717	298	515	74	0	0

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	x	423	2842	1752	523	557	10	0	0

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	y	656	5263	3312	939	977	35	0	0

- Molecule 54 is a protein called Eukaryotic translation initiation factor 5.

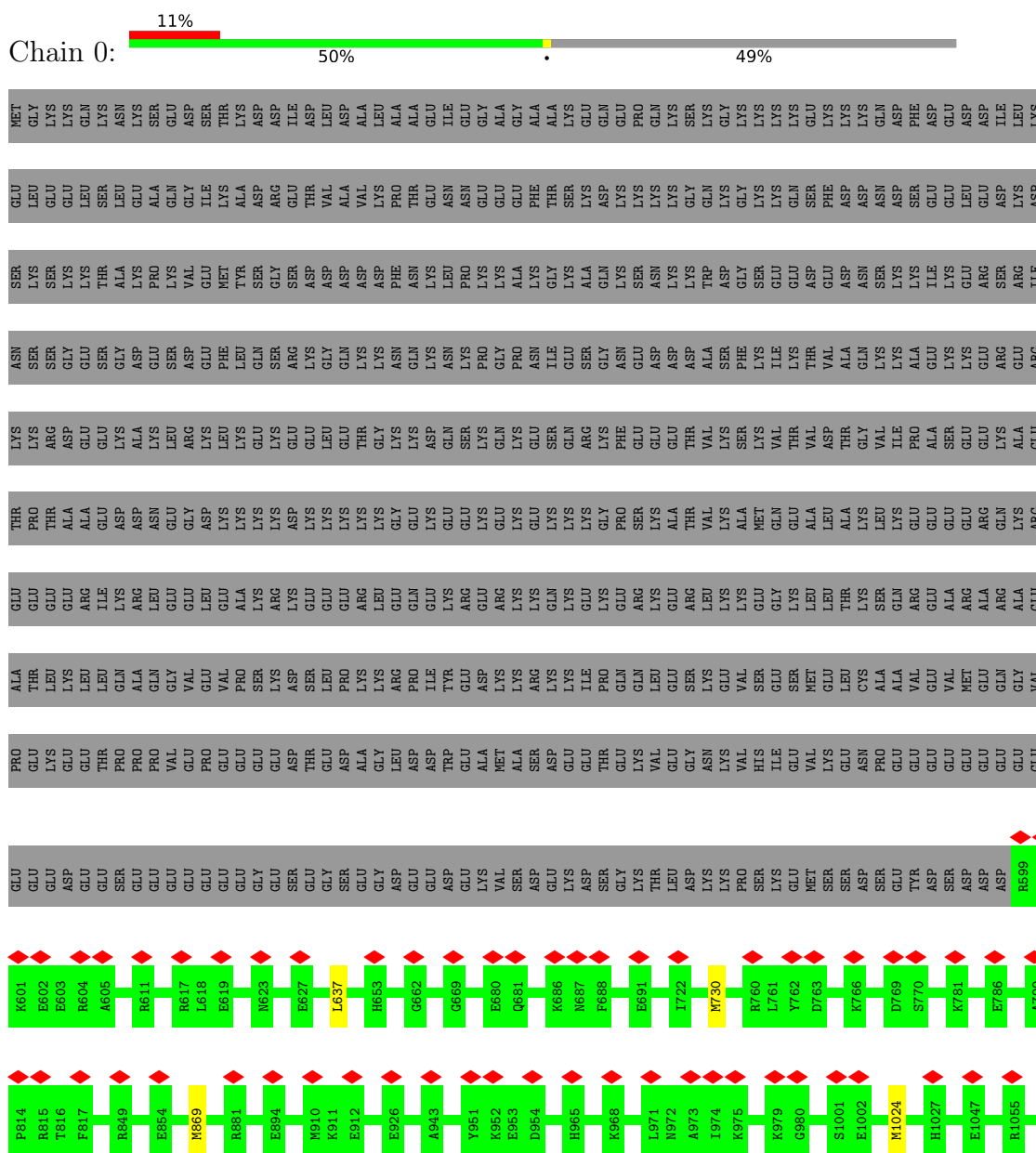
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	z	132	1044	662	184	188	10	0	0

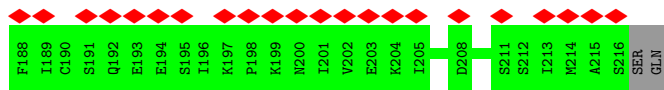
- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

3 Residue-property plots

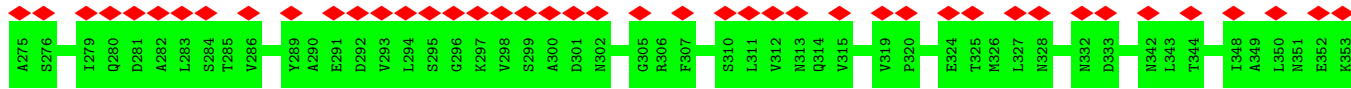
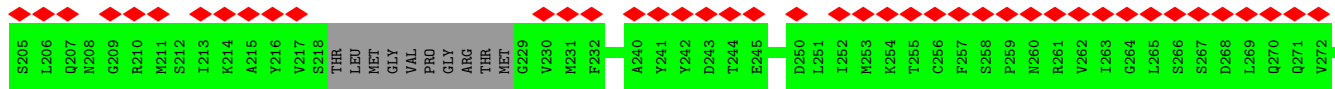
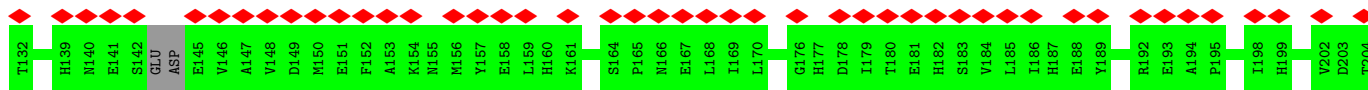
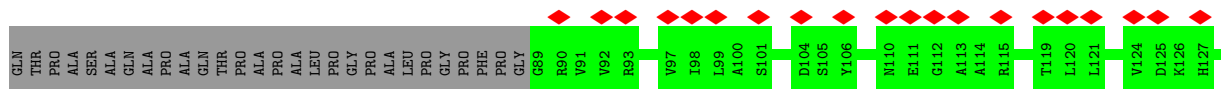
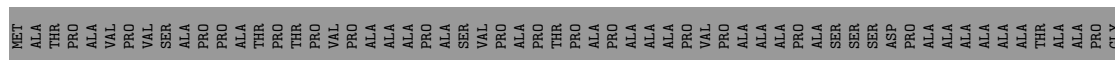
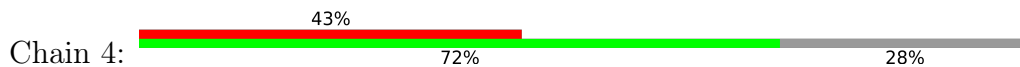
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Eukaryotic translation initiation factor 5B

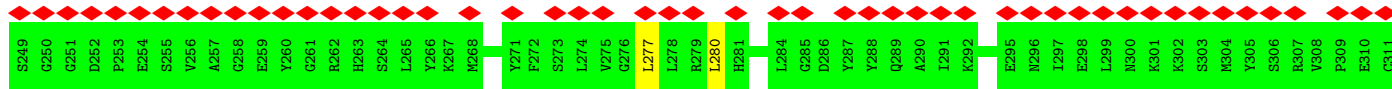
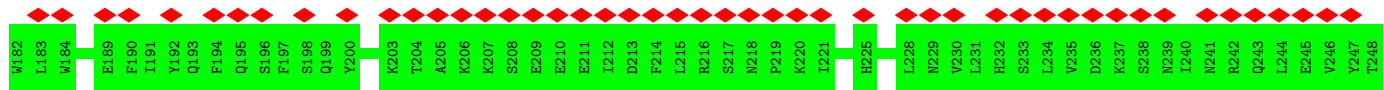
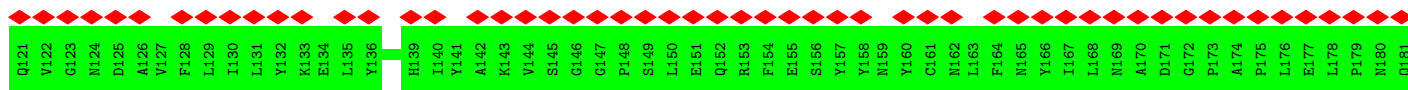
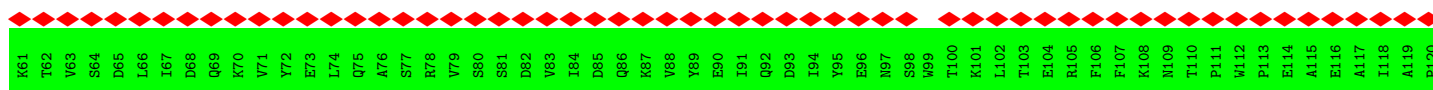
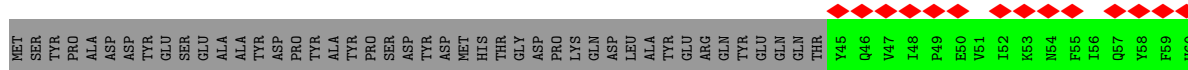
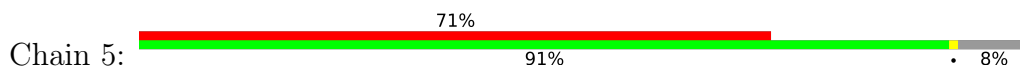


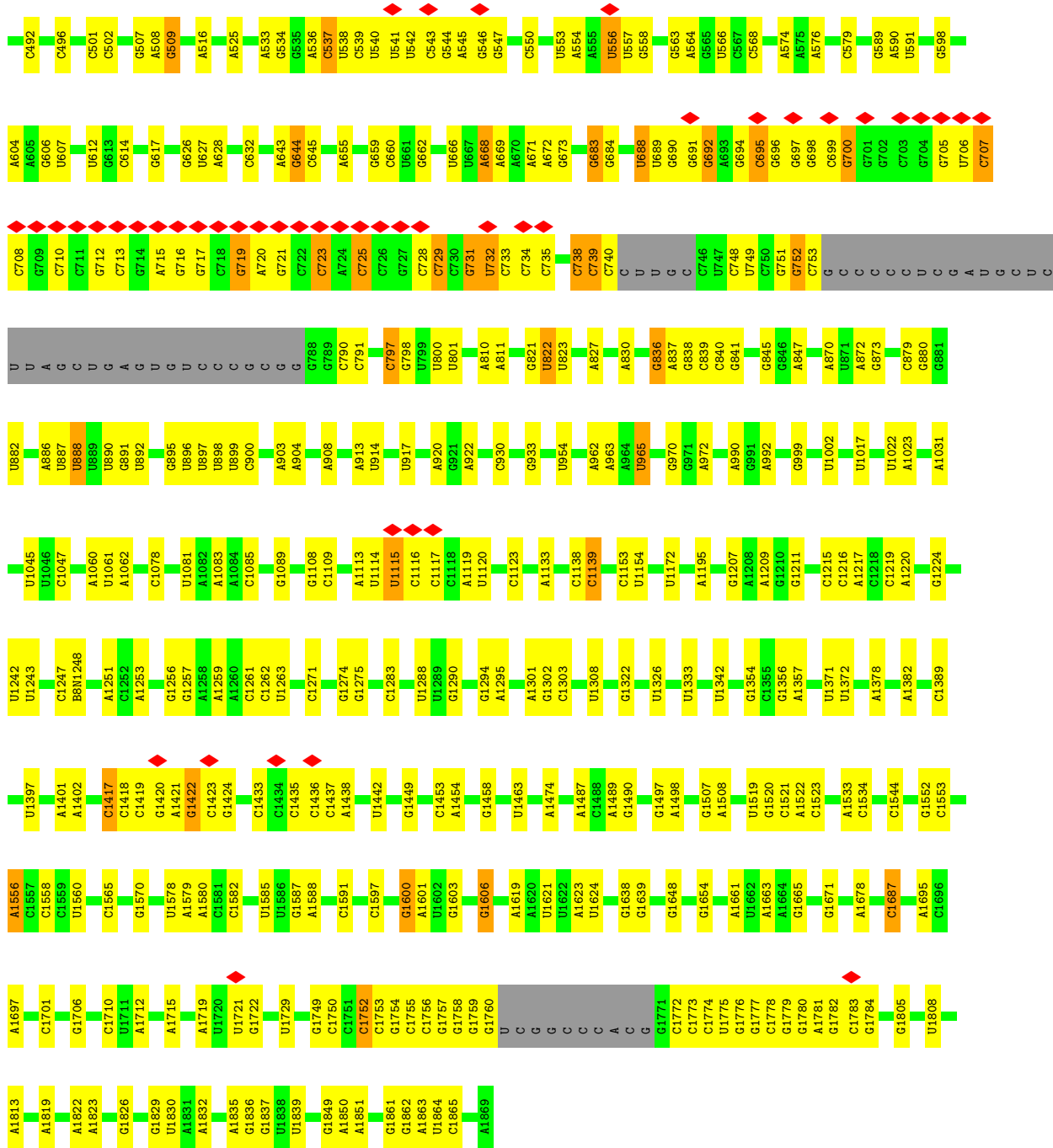


• Molecule 5: Eukaryotic translation initiation factor 3 subunit F

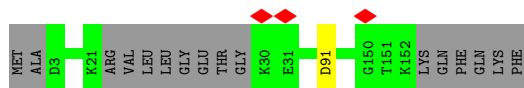
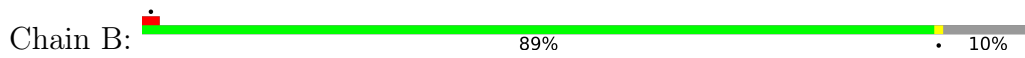


• Molecule 6: Eukaryotic translation initiation factor 3 subunit L





• Molecule 12: 40S ribosomal protein S11

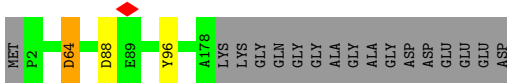
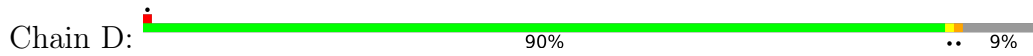


• Molecule 13: 40S ribosomal protein S4, X isoform

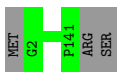




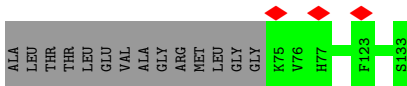
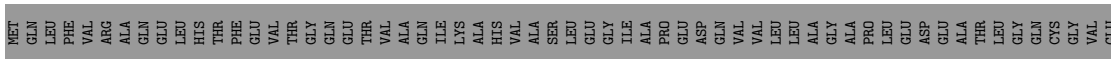
- Molecule 14: 40S ribosomal protein S9



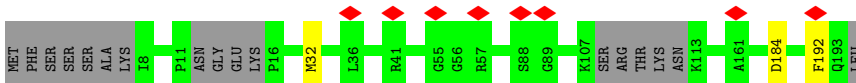
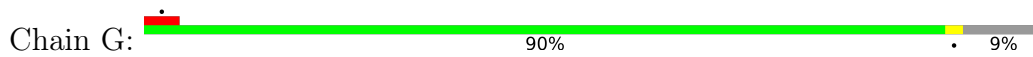
- Molecule 15: 40S ribosomal protein S23



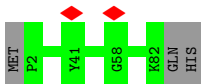
- Molecule 16: Small ribosomal subunit protein eS30



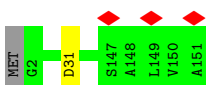
- Molecule 17: 40S ribosomal protein S7



- Molecule 18: 40S ribosomal protein S27




- Molecule 19: 40S ribosomal protein S13




GLY
TYR
GLU
PRO
ARG
LYS
VAL
GLN
GLU
SER
VAL

- Molecule 26: 40S ribosomal protein S14

Chain P:  87% 12%

MET ALA PRO ARG LYS GLY VAL GLN GLU SER VAL
P19 Q20 V21 A22 E23 G24 M60 L116 L151

- Molecule 27: 40S ribosomal protein S26

Chain Q:  86% 14%


MET T12 A48 R100 PHE ARG PRO PRO LYS ALA GLY ALA ALA PRO ARG PRO PRO PRO LYS MET

- Molecule 28: 40S ribosomal protein S8

Chain R:  95% 5%

MET G2 K124 LYS GLY ALA LYS LEU THR PRO GLU E133 G207 LYS

- Molecule 29: 40S ribosomal protein S6

Chain S:  91% 8%

K1 D19 R25 T26 F27 E43 R98 G166 K218 K230 ARG ARG ARG LEU SER SER LEU ARG ALA SER THR SER LYS SER SER SER SER SER SER LYS

- Molecule 30: 40S ribosomal protein S24

Chain T:  92% 6%

MET ASN ASP T4 M23 M74 K101 G128 LYS LYS PRO LYS GLU

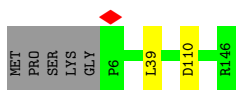
- Molecule 31: 40S ribosomal protein S5

Chain V:  92% 7%

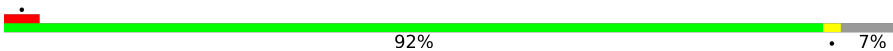
MET THR GLU TRP GLU THR ALA ALA PRO ALA VAL ALA GLU THR PRO D16 D32 E43 M76 A131 R204

- Molecule 32: 40S ribosomal protein S16

Chain Y:  95%



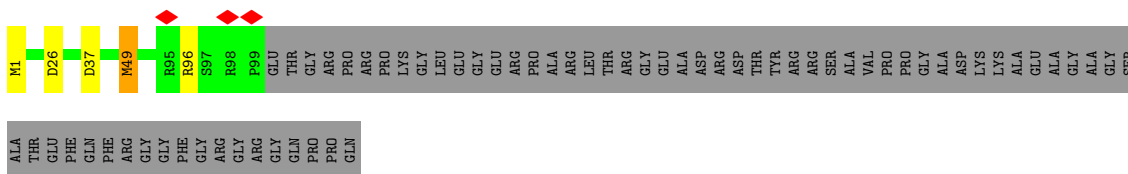
- Molecule 33: 40S ribosomal protein S3

Chain Z:  92%




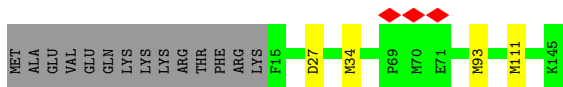
- Molecule 34: 40S ribosomal protein S10

Chain a:  57%



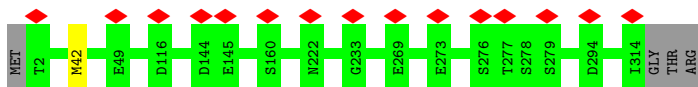
- Molecule 35: 40S ribosomal protein S15

Chain b:  88%



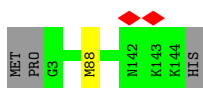
- Molecule 36: Receptor of activated protein C kinase 1

Chain c:  5%



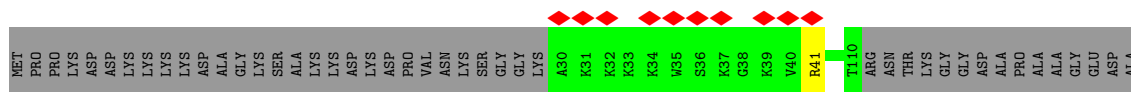
- Molecule 37: 40S ribosomal protein S19

Chain d:  97%

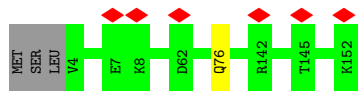


- Molecule 38: 40S ribosomal protein S25

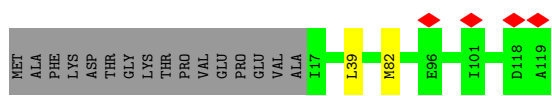
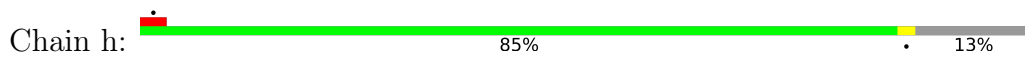
Chain e:  8%



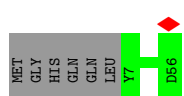
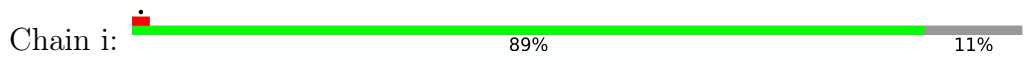
• Molecule 39: 40S ribosomal protein S18



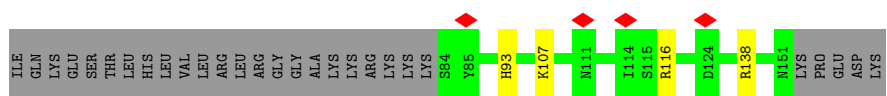
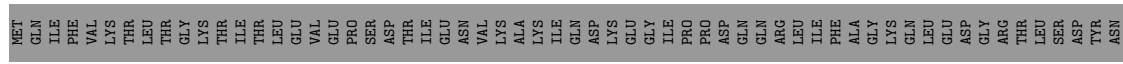
• Molecule 40: 40S ribosomal protein S20



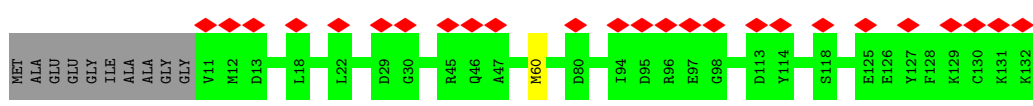
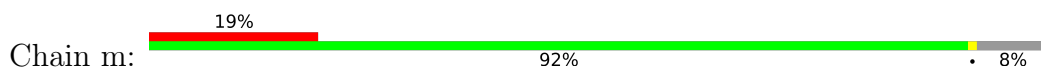
• Molecule 41: 40S ribosomal protein S29



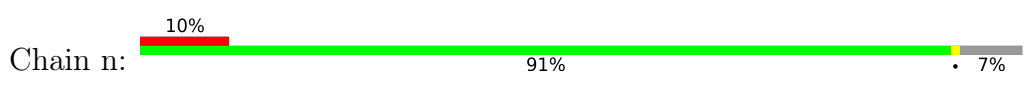
• Molecule 42: Ubiquitin

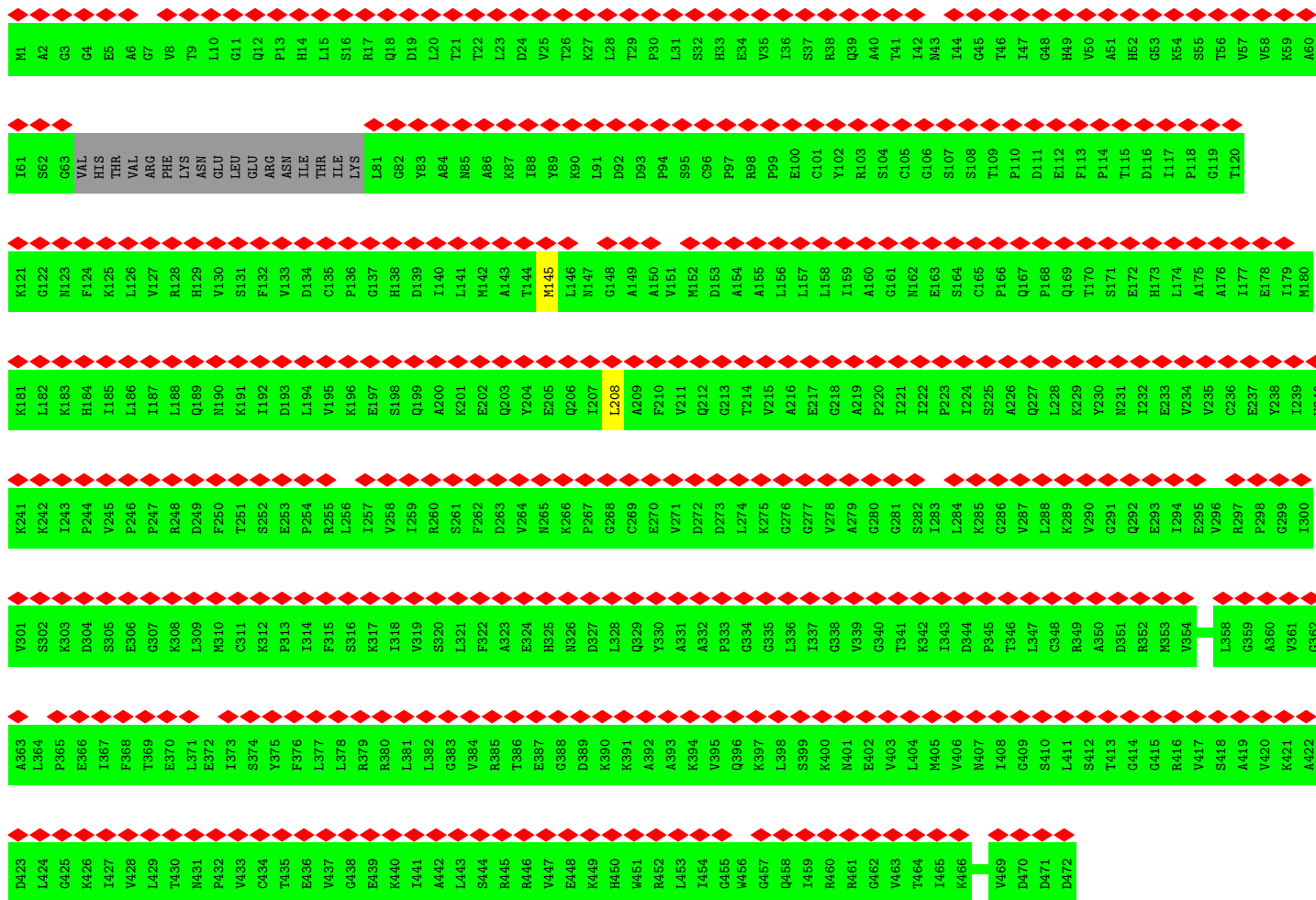


• Molecule 43: 40S ribosomal protein S12

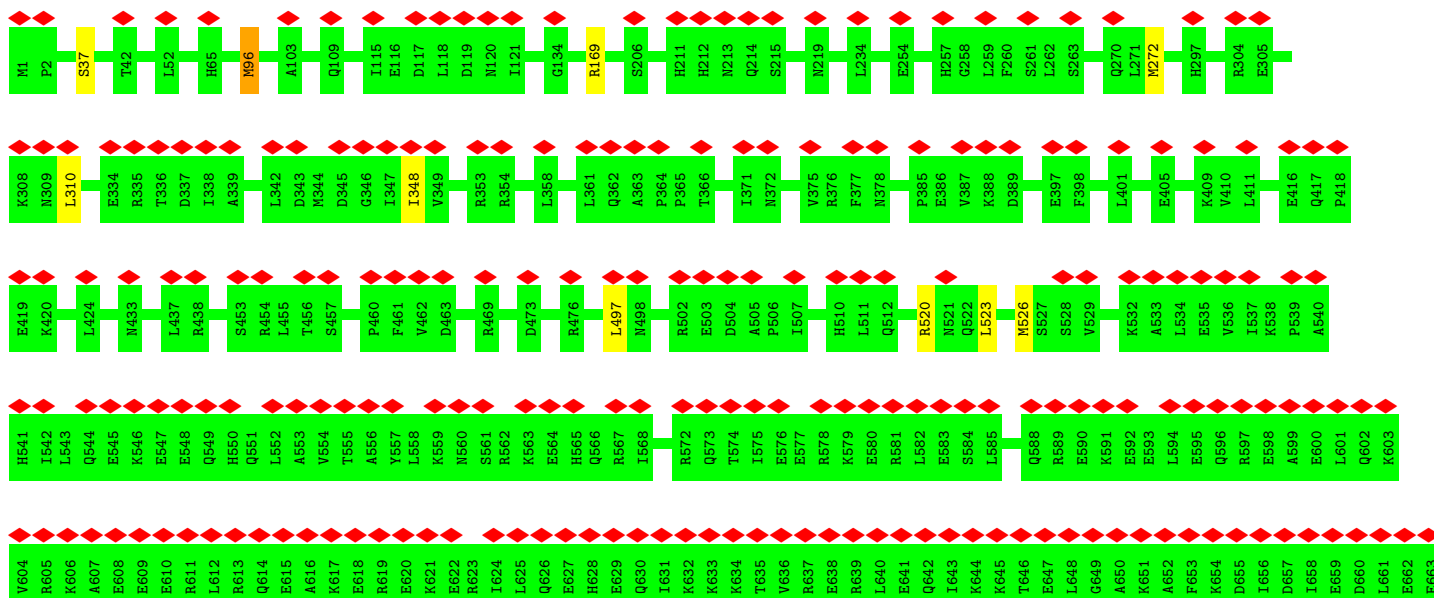


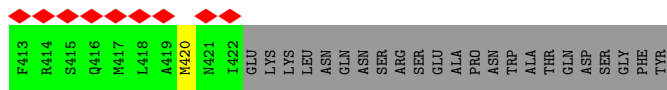
• Molecule 44: 40S ribosomal protein S28



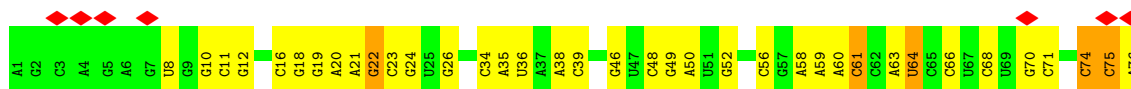


• Molecule 49: Eukaryotic translation initiation factor 3 subunit A

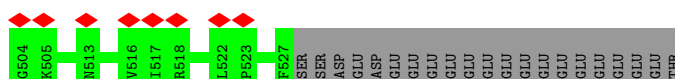
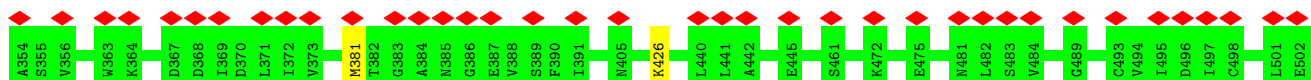
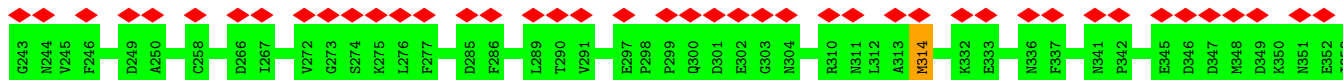
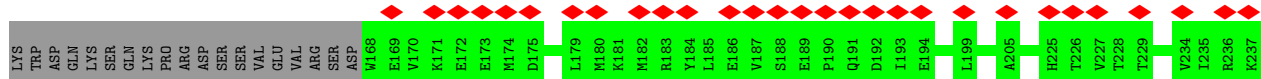
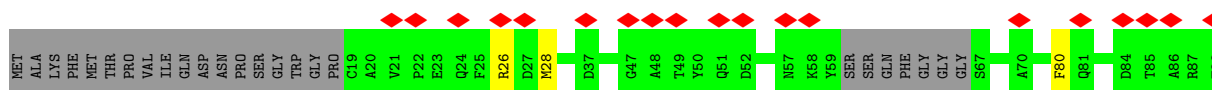
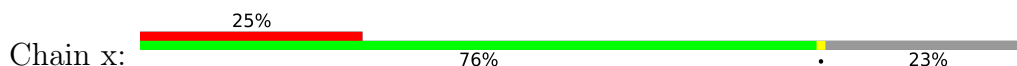




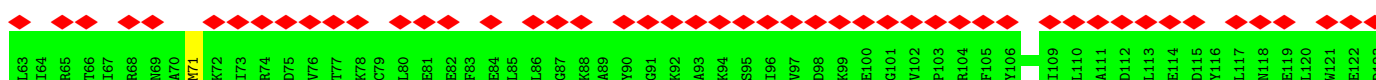
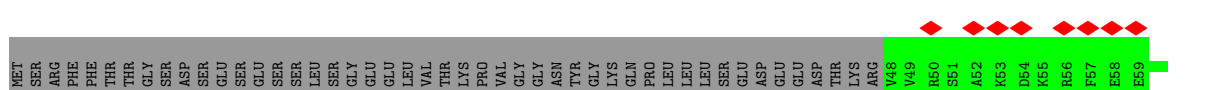
• Molecule 51: Initiator Met-tRNA-i



• Molecule 52: Eukaryotic translation initiation factor 3 subunit D



• Molecule 53: Eukaryotic translation initiation factor 3 subunit C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25632	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	20.786	Depositor
Minimum map value	-9.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: ZN, OMC, UR3, GTP, MG, PSU, NA, MA6, JMH, B8N, A2M, 5MU, 6MZ, OMU, 5MC, OMG

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	0	0.30	0/5002	0.67	6/6743 (0.1%)
2	1	0.27	0/3279	0.57	0/4534
3	2	0.25	0/1491	0.49	0/2068
4	3	0.24	0/1055	0.37	0/1469
5	4	0.25	0/1269	0.40	0/1762
6	5	0.28	0/4458	0.61	7/6027 (0.1%)
7	6	0.28	0/2212	0.57	3/3034 (0.1%)
8	7	0.31	0/1365	0.99	10/2124 (0.5%)
9	8	0.25	0/1572	0.42	0/2187
10	9	0.32	0/231	0.82	0/294
11	A	0.40	0/41130	1.01	146/64100 (0.2%)
12	B	0.30	0/1186	0.58	0/1585
13	C	0.30	0/2077	0.67	3/2796 (0.1%)
14	D	0.32	0/1502	0.71	2/2008 (0.1%)
15	E	0.31	0/1105	0.59	0/1476
16	F	0.30	0/468	0.66	0/618
17	G	0.30	0/1451	0.63	2/1942 (0.1%)
18	H	0.30	0/644	0.60	0/864
19	I	0.34	0/1232	0.61	0/1656
20	J	0.32	0/1051	0.69	1/1406 (0.1%)
21	K	0.30	0/623	0.63	0/833
22	L	0.32	0/1743	0.63	0/2354
23	M	0.33	0/1078	0.76	3/1447 (0.2%)
24	N	0.30	0/1670	0.64	2/2271 (0.1%)
25	O	0.31	0/1742	0.67	2/2330 (0.1%)
26	P	0.34	0/1010	0.75	2/1353 (0.1%)
27	Q	0.32	0/805	0.65	0/1079
28	R	0.28	0/1654	0.57	0/2203
29	S	0.29	0/1885	0.61	0/2510
30	T	0.32	0/1032	0.68	1/1371 (0.1%)
31	V	0.29	0/1516	0.63	1/2037 (0.0%)
32	Y	0.31	0/1142	0.70	2/1528 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.31	0/1793	0.67	3/2414 (0.1%)
34	a	0.33	0/859	0.71	2/1159 (0.2%)
35	b	0.34	0/1094	0.78	3/1464 (0.2%)
36	c	0.29	0/2493	0.62	1/3394 (0.0%)
37	d	0.28	0/1123	0.61	1/1504 (0.1%)
38	e	0.30	0/657	0.68	0/878
39	f	0.30	0/1245	0.66	0/1665
40	h	0.32	0/827	0.69	1/1110 (0.1%)
41	i	0.32	0/429	0.61	0/568
42	k	0.38	0/566	0.72	0/753
43	m	0.29	0/960	0.63	0/1286
44	n	0.32	0/508	0.83	1/680 (0.1%)
45	o	0.28	0/628	0.63	0/846
46	q	0.31	0/954	0.65	1/1268 (0.1%)
47	r	0.31	0/2167	0.63	2/2943 (0.1%)
48	t	0.29	0/3494	0.59	1/4726 (0.0%)
49	u	0.31	0/5475	0.69	5/7432 (0.1%)
50	v	0.32	1/2778 (0.0%)	0.69	4/3797 (0.1%)
51	w	0.50	0/1795	1.32	18/2798 (0.6%)
52	x	0.28	0/2885	0.62	4/3940 (0.1%)
53	y	0.35	2/5350 (0.0%)	0.73	11/7215 (0.2%)
54	z	0.30	0/1066	0.66	1/1436 (0.1%)
All	All	0.34	3/128826 (0.0%)	0.81	252/183285 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	y	824	LYS	C-N	7.04	1.50	1.34
50	v	362	MET	C-N	6.29	1.48	1.34
53	y	825	MET	C-N	-5.50	1.21	1.34

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1453	C	N1-C2-O2	10.54	125.22	118.90
11	A	1453	C	C2-N1-C1'	9.77	129.55	118.80
11	A	882	U	N1-C2-O2	9.63	129.54	122.80
11	A	888	U	C2-N1-C1'	9.53	129.14	117.70
49	u	96	MET	CA-CB-CG	9.41	129.29	113.30
11	A	1115	U	N1-C2-O2	9.20	129.24	122.80
11	A	501	C	N1-C2-O2	9.10	124.36	118.90
35	b	34	MET	CA-CB-CG	9.09	128.75	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	537	C	N3-C2-O2	-9.08	115.55	121.90
14	D	64	ASP	CB-CG-OD1	9.08	126.47	118.30
11	A	1115	U	C2-N1-C1'	8.87	128.34	117.70
11	A	1115	U	N3-C2-O2	-8.76	116.07	122.20
11	A	1597	C	N3-C2-O2	-8.72	115.80	121.90
51	w	34	C	C6-N1-C2	-8.60	116.86	120.30
11	A	888	U	N1-C2-O2	8.58	128.81	122.80
11	A	556	U	C2-N1-C1'	8.42	127.80	117.70
11	A	501	C	C2-N1-C1'	8.41	128.06	118.80
11	A	882	U	N3-C2-O2	-8.39	116.33	122.20
11	A	1752	C	N1-C2-O2	8.33	123.90	118.90
32	Y	110	ASP	CB-CG-OD1	8.25	125.73	118.30
44	n	37	ASP	CB-CG-OD1	8.21	125.69	118.30
11	A	1597	C	N1-C2-O2	8.20	123.82	118.90
11	A	1752	C	C2-N1-C1'	8.20	127.82	118.80
51	w	34	C	C5-C6-N1	8.20	125.10	121.00
11	A	888	U	N3-C2-O2	-8.18	116.47	122.20
13	C	19	MET	CA-CB-CG	8.12	127.11	113.30
11	A	740	C	N3-C2-O2	-8.10	116.23	121.90
11	A	706	U	N1-C2-O2	8.04	128.43	122.80
11	A	537	C	N1-C2-O2	8.02	123.71	118.90
11	A	1453	C	N3-C2-O2	-7.99	116.31	121.90
33	Z	169	ASP	CB-CG-OD1	7.92	125.43	118.30
11	A	706	U	C2-N1-C1'	7.66	126.89	117.70
11	A	1139	C	C2-N1-C1'	7.65	127.21	118.80
11	A	1022	U	C2-N1-C1'	7.62	126.84	117.70
11	A	556	U	N3-C2-O2	-7.53	116.93	122.20
47	r	170	ASP	CB-CG-OD1	7.52	125.06	118.30
11	A	168	C	N1-C2-O2	7.48	123.39	118.90
11	A	501	C	N3-C2-O2	-7.48	116.66	121.90
11	A	1520	G	C4-N9-C1'	7.44	136.17	126.50
14	D	88	ASP	CB-CG-OD1	7.40	124.96	118.30
11	A	556	U	N1-C2-O2	7.38	127.97	122.80
7	6	352	ASP	CB-CG-OD1	7.34	124.91	118.30
11	A	706	U	N3-C2-O2	-7.34	117.06	122.20
11	A	882	U	C2-N1-C1'	7.33	126.50	117.70
24	N	44	ASP	CB-CG-OD1	7.33	124.90	118.30
13	C	21	ASP	CB-CG-OD1	7.29	124.86	118.30
23	M	108	LEU	CA-CB-CG	7.20	131.85	115.30
53	y	726	LEU	CA-CB-CG	7.20	131.86	115.30
23	M	110	ASP	CB-CG-OD1	7.20	124.78	118.30
6	5	388	LEU	CA-CB-CG	7.15	131.75	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	h	39	LEU	CA-CB-CG	7.12	131.68	115.30
6	5	398	MET	CA-CB-CG	7.11	125.38	113.30
11	A	1139	C	N1-C2-O2	7.08	123.15	118.90
8	7	-31	C	N1-C2-O2	7.08	123.14	118.90
51	w	66	C	C6-N1-C2	-7.03	117.49	120.30
8	7	-21	A	P-O3'-C3'	7.02	128.12	119.70
6	5	481	LEU	CA-CB-CG	6.97	131.33	115.30
11	A	731	G	P-O3'-C3'	6.97	128.06	119.70
11	A	1422	G	N3-C4-N9	6.96	130.18	126.00
11	A	729	C	C5-C6-N1	6.95	124.47	121.00
11	A	1520	G	N3-C4-N9	6.93	130.16	126.00
11	A	1261	C	N1-C2-O2	6.90	123.04	118.90
11	A	739	C	N1-C2-O2	6.87	123.02	118.90
30	T	74	MET	CG-SD-CE	-6.85	89.24	100.20
49	u	310	LEU	CA-CB-CG	6.84	131.03	115.30
35	b	27	ASP	CB-CG-OD1	6.79	124.41	118.30
11	A	836	G	C4-N9-C1'	6.78	135.32	126.50
53	y	591	MET	CA-CB-CG	6.78	124.83	113.30
11	A	1422	G	N3-C4-C5	-6.75	125.22	128.60
1	0	1110	MET	CA-CB-CG	6.75	124.77	113.30
11	A	1453	C	C6-N1-C1'	-6.73	112.72	120.80
26	P	60	MET	CA-CB-CG	6.73	124.75	113.30
11	A	739	C	N3-C2-O2	-6.68	117.22	121.90
8	7	-31	C	OP2-P-O3'	6.66	119.84	105.20
20	J	4	MET	CA-CB-CG	6.65	124.61	113.30
33	Z	154	ASP	CB-CG-OD1	6.64	124.27	118.30
11	A	707	C	C6-N1-C2	-6.60	117.66	120.30
11	A	1520	G	C8-N9-C1'	-6.59	118.44	127.00
51	w	22	G	P-O3'-C3'	6.57	127.59	119.70
11	A	723	C	N1-C2-O2	6.56	122.84	118.90
11	A	962	A	P-O3'-C3'	6.53	127.54	119.70
52	x	314	MET	CA-CB-CG	6.53	124.40	113.30
11	A	836	G	N3-C4-N9	6.49	129.89	126.00
11	A	537	C	C6-N1-C2	-6.48	117.71	120.30
49	u	523	LEU	CA-CB-CG	6.48	130.20	115.30
11	A	501	C	C6-N1-C2	-6.46	117.72	120.30
11	A	836	G	N3-C4-C5	-6.45	125.38	128.60
11	A	1453	C	C6-N1-C2	-6.44	117.72	120.30
11	A	1389	C	C6-N1-C2	-6.43	117.73	120.30
11	A	706	U	C5-C6-N1	6.41	125.91	122.70
11	A	739	C	C6-N1-C2	-6.37	117.75	120.30
50	v	411	LEU	CA-CB-CG	6.37	129.94	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1687	C	C6-N1-C2	-6.37	117.75	120.30
11	A	1422	G	C4-N9-C1'	6.32	134.72	126.50
11	A	1591	C	N1-C2-O2	6.32	122.69	118.90
11	A	1752	C	N3-C2-O2	-6.32	117.47	121.90
23	M	126	MET	CA-CB-CG	6.31	124.03	113.30
37	d	88	MET	CA-CB-CG	6.30	124.01	113.30
47	r	167	LEU	CA-CB-CG	6.30	129.78	115.30
11	A	537	C	C2-N1-C1'	6.25	125.68	118.80
11	A	965	U	N1-C2-O2	6.25	127.17	122.80
8	7	-31	C	P-O3'-C3'	6.18	127.11	119.70
11	A	1139	C	N3-C2-O2	-6.18	117.58	121.90
51	w	61	C	C5-C6-N1	6.17	124.08	121.00
51	w	61	C	C6-N1-C2	-6.15	117.84	120.30
11	A	739	C	O5'-P-OP1	-6.14	100.17	105.70
34	a	26	ASP	CB-CG-OD1	6.14	123.83	118.30
11	A	1687	C	C5-C6-N1	6.14	124.07	121.00
17	G	32	MET	CA-CB-CG	6.12	123.70	113.30
11	A	1687	C	C2-N1-C1'	6.11	125.52	118.80
11	A	888	U	C6-N1-C1'	-6.06	112.72	121.20
11	A	1453	C	C5-C6-N1	6.05	124.03	121.00
50	v	420	MET	CG-SD-CE	6.05	109.88	100.20
11	A	1	U	OP1-P-O3'	6.05	118.51	105.20
53	y	634	LEU	CA-CB-CG	6.05	129.21	115.30
46	q	50	MET	CB-CG-SD	6.04	130.52	112.40
7	6	283	MET	CA-CB-CG	6.04	123.56	113.30
11	A	710	C	C5-C6-N1	6.03	124.01	121.00
51	w	74	C	O4'-C1'-N1	6.00	113.00	108.20
11	A	688	U	P-O3'-C3'	5.99	126.89	119.70
31	V	76	MET	CB-CG-SD	5.98	130.35	112.40
52	x	28	MET	CA-CB-CG	5.98	123.46	113.30
11	A	1261	C	N3-C2-O2	-5.97	117.72	121.90
11	A	1752	C	C6-N1-C1'	-5.94	113.67	120.80
53	y	445	LEU	CB-CG-CD1	-5.94	100.90	111.00
11	A	1116	C	N1-C2-O2	5.92	122.45	118.90
11	A	1606	G	O4'-C1'-N9	5.92	112.94	108.20
11	A	965	U	N3-C2-O2	-5.90	118.07	122.20
11	A	1271	C	N1-C2-O2	5.90	122.44	118.90
8	7	-31	C	N3-C2-O2	-5.87	117.79	121.90
8	7	-22	C	N1-C2-O2	5.86	122.42	118.90
11	A	732	U	O5'-P-OP1	-5.84	100.44	105.70
51	w	64	U	C2-N1-C1'	5.84	124.71	117.70
11	A	291	G	P-O3'-C3'	5.84	126.70	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	201	C	N1-C2-O2	5.81	122.39	118.90
11	A	1600	G	P-O3'-C3'	5.79	126.65	119.70
24	N	10	MET	CG-SD-CE	5.79	109.46	100.20
25	O	172	MET	CA-CB-CG	5.79	123.14	113.30
51	w	61	C	C2-N1-C1'	5.79	125.17	118.80
11	A	1520	G	N3-C4-C5	-5.77	125.72	128.60
51	w	66	C	C5-C6-N1	5.77	123.88	121.00
53	y	824	LYS	O-C-N	5.77	131.93	122.70
11	A	168	C	N3-C2-O2	-5.76	117.87	121.90
11	A	178	C	N1-C2-O2	5.76	122.36	118.90
51	w	64	U	C5-C6-N1	5.76	125.58	122.70
13	C	87	MET	CA-CB-CG	5.75	123.07	113.30
11	A	836	G	C8-N9-C1'	-5.74	119.53	127.00
11	A	708	C	C2-N1-C1'	5.70	125.07	118.80
11	A	735	C	C5-C6-N1	5.69	123.85	121.00
11	A	666	U	C2-N1-C1'	5.68	124.51	117.70
51	w	75	C	N1-C2-O2	5.67	122.30	118.90
11	A	797	C	P-O3'-C3'	5.66	126.49	119.70
11	A	1262	C	N1-C2-O2	5.63	122.28	118.90
53	y	832	MET	CA-CB-CG	5.63	122.87	113.30
52	x	26	ARG	CA-CB-CG	5.62	125.76	113.40
8	7	-22	C	C6-N1-C2	-5.62	118.05	120.30
11	A	168	C	C2-N1-C1'	5.62	124.98	118.80
51	w	71	C	C6-N1-C2	-5.61	118.06	120.30
34	a	49	MET	CB-CG-SD	5.61	129.22	112.40
53	y	831	LEU	CA-CB-CG	5.60	128.19	115.30
11	A	719	G	N7-C8-N9	5.59	115.89	113.10
11	A	1022	U	C6-N1-C1'	-5.59	113.38	121.20
11	A	659	G	C4-N9-C1'	5.58	133.76	126.50
11	A	1600	G	OP1-P-O3'	5.57	117.45	105.20
32	Y	39	LEU	CA-CB-CG	5.56	128.10	115.30
11	A	1115	U	C6-N1-C1'	-5.55	113.43	121.20
11	A	888	U	C5-C6-N1	5.54	125.47	122.70
8	7	-31	C	C6-N1-C2	-5.52	118.09	120.30
6	5	560	MET	CA-CB-CG	5.51	122.66	113.30
53	y	402	LEU	CA-CB-CG	5.51	127.97	115.30
6	5	277	LEU	CA-CB-CG	5.50	127.95	115.30
11	A	501	C	C6-N1-C1'	-5.49	114.22	120.80
11	A	700	G	C6-C5-N7	-5.48	127.11	130.40
11	A	130	G	C4-N9-C1'	5.46	133.60	126.50
1	0	1024	MET	CB-CG-SD	5.46	128.77	112.40
11	A	700	G	N3-C4-N9	5.45	129.27	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	695	C	N3-C2-O2	-5.42	118.11	121.90
11	A	130	G	N3-C4-C5	-5.41	125.90	128.60
54	z	46	LEU	CA-CB-CG	5.40	127.72	115.30
36	c	42	MET	CB-CG-SD	5.39	128.58	112.40
51	w	24	G	C6-C5-N7	-5.39	127.17	130.40
11	A	1115	U	C5-C6-N1	5.39	125.39	122.70
17	G	184	ASP	CB-CG-OD1	5.39	123.15	118.30
53	y	589	MET	CA-CB-CG	5.39	122.46	113.30
53	y	826	ILE	O-C-N	-5.38	114.09	122.70
11	A	1022	U	N1-C2-O2	5.37	126.56	122.80
11	A	707	C	C5-C6-N1	5.36	123.68	121.00
11	A	501	C	C5-C6-N1	5.35	123.67	121.00
11	A	719	G	C8-N9-C4	-5.35	104.26	106.40
11	A	1422	G	C8-N9-C1'	-5.35	120.05	127.00
1	0	1071	LYS	CA-CB-CG	5.34	125.15	113.40
52	x	381	MET	CA-CB-CG	5.34	122.38	113.30
25	O	113	MET	CG-SD-CE	-5.34	91.66	100.20
11	A	1578	U	N3-C2-O2	-5.33	118.47	122.20
7	6	326	ASP	CB-CG-OD1	5.33	123.09	118.30
11	A	729	C	C6-N1-C2	-5.32	118.17	120.30
50	v	420	MET	CA-CB-CG	5.32	122.34	113.30
11	A	879	C	C2-N1-C1'	5.31	124.64	118.80
11	A	1556	A	C2-N3-C4	5.31	113.25	110.60
11	A	710	C	C6-N1-C2	-5.30	118.18	120.30
11	A	579	C	N1-C2-O2	5.30	122.08	118.90
51	w	75	C	C2-N1-C1'	5.30	124.63	118.80
11	A	731	G	OP1-P-O3'	5.29	116.83	105.20
11	A	738	C	N3-C2-O2	-5.28	118.20	121.90
33	Z	1	MET	CA-CB-CG	5.28	122.27	113.30
8	7	-22	C	N3-C2-O2	-5.28	118.21	121.90
35	b	93	MET	CA-CB-CG	5.25	122.22	113.30
11	A	725	C	C5-C6-N1	5.24	123.62	121.00
11	A	1139	C	C6-N1-C1'	-5.24	114.51	120.80
11	A	130	G	N3-C4-N9	5.23	129.14	126.00
11	A	740	C	N1-C2-O2	5.23	122.04	118.90
11	A	752	G	C4-N9-C1'	5.23	133.30	126.50
11	A	1591	C	N3-C2-O2	-5.21	118.25	121.90
11	A	1600	G	N3-C4-N9	5.21	129.13	126.00
1	0	1125	MET	CA-CB-CG	5.21	122.16	113.30
11	A	1417	C	N3-C2-O2	-5.20	118.26	121.90
11	A	1756	C	N1-C2-O2	5.20	122.02	118.90
51	w	24	G	N7-C8-N9	5.20	115.70	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	632	C	C2-N1-C1'	5.18	124.50	118.80
11	A	692	G	N1-C2-N2	-5.18	111.54	116.20
11	A	723	C	C2-N1-C1'	5.16	124.48	118.80
1	0	637	LEU	CA-CB-CG	5.16	127.17	115.30
6	5	484	GLN	CA-CB-CG	5.16	124.75	113.40
1	0	869	MET	CA-CB-CG	5.15	122.06	113.30
11	A	882	U	C5-C6-N1	5.15	125.28	122.70
11	A	556	U	C6-N1-C1'	-5.14	114.00	121.20
11	A	1261	C	C2-N1-C1'	5.14	124.45	118.80
11	A	1139	C	C6-N1-C2	-5.12	118.25	120.30
49	u	497	LEU	CA-CB-CG	5.12	127.08	115.30
11	A	327	G	O5'-P-OP1	5.11	116.84	110.70
11	A	708	C	C5-C6-N1	5.11	123.55	121.00
11	A	1389	C	C2-N1-C1'	5.10	124.41	118.80
49	u	348	ILE	CG1-CB-CG2	-5.10	100.18	111.40
6	5	280	LEU	CA-CB-CG	5.10	127.02	115.30
11	A	725	C	C6-N1-C2	-5.10	118.26	120.30
50	v	374	LEU	CA-CB-CG	5.09	127.02	115.30
11	A	1520	G	C6-C5-N7	-5.09	127.35	130.40
11	A	1078	C	N3-C2-O2	-5.08	118.34	121.90
51	w	64	U	N1-C2-O2	5.08	126.35	122.80
11	A	706	U	C6-N1-C2	-5.08	117.95	121.00
11	A	752	G	N3-C4-C5	-5.07	126.06	128.60
53	y	71	MET	CG-SD-CE	5.07	108.31	100.20
11	A	168	C	C6-N1-C2	-5.07	118.27	120.30
11	A	1578	U	N1-C2-O2	5.07	126.35	122.80
11	A	644	OMG	O3'-P-O5'	5.06	113.62	104.00
26	P	60	MET	CB-CG-SD	5.06	127.57	112.40
8	7	-31	C	C2-N1-C1'	5.05	124.36	118.80
11	A	965	U	C2-N1-C1'	5.04	123.75	117.70
48	t	208	LEU	CA-CB-CG	5.04	126.89	115.30
11	A	738	C	C6-N1-C2	-5.03	118.29	120.30
51	w	34	C	C2-N1-C1'	5.03	124.33	118.80
11	A	556	U	C5-C6-N1	5.01	125.21	122.70

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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	619/1220 (51%)	593 (96%)	26 (4%)	0	100	100
2	1	584/814 (72%)	544 (93%)	40 (7%)	0	100	100
3	2	300/325 (92%)	291 (97%)	9 (3%)	0	100	100
4	3	209/218 (96%)	203 (97%)	6 (3%)	0	100	100
5	4	251/357 (70%)	237 (94%)	14 (6%)	0	100	100
6	5	518/564 (92%)	500 (96%)	18 (4%)	0	100	100
7	6	360/374 (96%)	342 (95%)	18 (5%)	0	100	100
9	8	313/352 (89%)	289 (92%)	24 (8%)	0	100	100
10	9	22/25 (88%)	22 (100%)	0	0	100	100
12	B	138/158 (87%)	133 (96%)	5 (4%)	0	100	100
13	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
14	D	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
15	E	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
16	F	57/133 (43%)	51 (90%)	6 (10%)	0	100	100
17	G	171/194 (88%)	163 (95%)	8 (5%)	0	100	100
18	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
19	I	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
20	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
21	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
22	L	218/293 (74%)	211 (97%)	7 (3%)	0	100	100
23	M	129/135 (96%)	120 (93%)	9 (7%)	0	100	100
24	N	205/295 (70%)	198 (97%)	7 (3%)	0	100	100
25	O	209/264 (79%)	202 (97%)	7 (3%)	0	100	100
26	P	131/151 (87%)	121 (92%)	10 (8%)	0	100	100
27	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
29	S	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
30	T	123/133 (92%)	123 (100%)	0	0	100	100
31	V	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
32	Y	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
33	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
34	a	97/165 (59%)	91 (94%)	6 (6%)	0	100	100
35	b	129/145 (89%)	122 (95%)	7 (5%)	0	100	100
36	c	311/317 (98%)	290 (93%)	21 (7%)	0	100	100
37	d	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
38	e	79/125 (63%)	76 (96%)	3 (4%)	0	100	100
39	f	147/152 (97%)	139 (95%)	8 (5%)	0	100	100
40	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
41	i	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
42	k	66/156 (42%)	59 (89%)	6 (9%)	1 (2%)	10	44
43	m	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
44	n	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
45	o	75/320 (23%)	72 (96%)	3 (4%)	0	100	100
46	q	115/144 (80%)	108 (94%)	7 (6%)	0	100	100
47	r	294/315 (93%)	276 (94%)	18 (6%)	0	100	100
48	t	451/472 (96%)	443 (98%)	8 (2%)	0	100	100
49	u	705/1382 (51%)	659 (94%)	46 (6%)	0	100	100
50	v	403/445 (91%)	371 (92%)	32 (8%)	0	100	100
52	x	417/548 (76%)	390 (94%)	27 (6%)	0	100	100
53	y	650/913 (71%)	621 (96%)	29 (4%)	0	100	100
54	z	130/430 (30%)	123 (95%)	7 (5%)	0	100	100
All	All	11167/14768 (76%)	10648 (95%)	518 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	k	93	HIS

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	0	546/1081 (50%)	541 (99%)	5 (1%)	78	88
2	1	97/702 (14%)	97 (100%)	0	100	100
6	5	477/515 (93%)	476 (100%)	1 (0%)	93	97
7	6	112/335 (33%)	112 (100%)	0	100	100
9	8	1/310 (0%)	1 (100%)	0	100	100
10	9	23/24 (96%)	23 (100%)	0	100	100
12	B	129/142 (91%)	128 (99%)	1 (1%)	81	89
13	C	220/225 (98%)	219 (100%)	1 (0%)	88	94
14	D	158/168 (94%)	156 (99%)	2 (1%)	69	83
15	E	112/115 (97%)	112 (100%)	0	100	100
16	F	47/104 (45%)	47 (100%)	0	100	100
17	G	159/174 (91%)	158 (99%)	1 (1%)	86	93
18	H	73/76 (96%)	73 (100%)	0	100	100
19	I	130/131 (99%)	129 (99%)	1 (1%)	81	89
20	J	112/113 (99%)	112 (100%)	0	100	100
21	K	65/67 (97%)	64 (98%)	1 (2%)	65	81
22	L	186/225 (83%)	185 (100%)	1 (0%)	88	94
23	M	119/122 (98%)	118 (99%)	1 (1%)	81	89
24	N	173/243 (71%)	171 (99%)	2 (1%)	71	84
25	O	192/231 (83%)	190 (99%)	2 (1%)	76	86
26	P	104/119 (87%)	103 (99%)	1 (1%)	76	86
27	Q	86/98 (88%)	86 (100%)	0	100	100
28	R	172/180 (96%)	172 (100%)	0	100	100
29	S	200/218 (92%)	197 (98%)	3 (2%)	65	81
30	T	107/115 (93%)	106 (99%)	1 (1%)	78	88
31	V	159/170 (94%)	159 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	117/121 (97%)	117 (100%)	0	100	100
33	Z	190/202 (94%)	189 (100%)	1 (0%)	88	94
34	a	90/136 (66%)	86 (96%)	4 (4%)	28	58
35	b	117/130 (90%)	116 (99%)	1 (1%)	78	88
36	c	272/275 (99%)	272 (100%)	0	100	100
37	d	112/115 (97%)	112 (100%)	0	100	100
38	e	71/103 (69%)	70 (99%)	1 (1%)	67	82
39	f	129/132 (98%)	128 (99%)	1 (1%)	81	89
40	h	94/107 (88%)	93 (99%)	1 (1%)	73	85
41	i	44/49 (90%)	44 (100%)	0	100	100
42	k	61/140 (44%)	58 (95%)	3 (5%)	25	56
43	m	104/108 (96%)	103 (99%)	1 (1%)	76	86
44	n	57/62 (92%)	57 (100%)	0	100	100
45	o	64/277 (23%)	64 (100%)	0	100	100
46	q	99/123 (80%)	97 (98%)	2 (2%)	55	74
47	r	190/280 (68%)	188 (99%)	2 (1%)	73	85
48	t	380/397 (96%)	379 (100%)	1 (0%)	92	96
49	u	528/1259 (42%)	522 (99%)	6 (1%)	73	85
50	v	206/406 (51%)	201 (98%)	5 (2%)	49	71
52	x	207/494 (42%)	204 (99%)	3 (1%)	67	82
53	y	562/811 (69%)	559 (100%)	3 (0%)	88	94
54	z	116/388 (30%)	113 (97%)	3 (3%)	46	69
All	All	7769/12118 (64%)	7707 (99%)	62 (1%)	82	89

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	730	MET
1	0	1080	LYS
1	0	1090	PHE
1	0	1102	PHE
1	0	1197	TRP
6	5	480	ASP
12	B	91	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	C	216	ASN
14	D	64	ASP
14	D	96	TYR
17	G	192	PHE
19	I	31	ASP
21	K	71	ARG
22	L	152	ARG
23	M	92	ASP
24	N	39	TYR
24	N	40	LYS
25	O	38	MET
25	O	211	PHE
26	P	116	LEU
29	S	27	PHE
29	S	98	ARG
29	S	218	LYS
30	T	23	MET
33	Z	214	LYS
34	a	1	MET
34	a	37	ASP
34	a	49	MET
34	a	96	ARG
35	b	111	MET
38	e	41	ARG
39	f	76	GLN
40	h	82	MET
42	k	107	LYS
42	k	116	ARG
42	k	138	ARG
43	m	60	MET
46	q	50	MET
46	q	87	ASN
47	r	51	SER
47	r	234	TYR
48	t	145	MET
49	u	37	SER
49	u	96	MET
49	u	169	ARG
49	u	272	MET
49	u	520	ARG
49	u	526	MET
50	v	238	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	v	249	MET
50	v	355	MET
50	v	362	MET
50	v	407	LYS
52	x	80	PHE
52	x	314	MET
52	x	426	LYS
53	y	662	GLN
53	y	701	HIS
53	y	844	MET
54	z	15	ARG
54	z	77	ASN
54	z	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	1074	GLN
7	6	366	ASN
17	G	165	ASN
31	V	29	GLN
37	d	51	ASN
48	t	206	GLN
50	v	377	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1741/1869 (93%)	421 (24%)	15 (0%)
51	w	74/75 (98%)	33 (44%)	0
8	7	56/255 (21%)	40 (71%)	3 (5%)
All	All	1871/2199 (85%)	494 (26%)	18 (0%)

All (494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-34	C
8	7	-32	A
8	7	-31	C
8	7	-30	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	-29	A
8	7	-28	C
8	7	-27	A
8	7	-26	A
8	7	-23	A
8	7	-22	C
8	7	-21	A
8	7	-20	A
8	7	-15	C
8	7	-13	A
8	7	-12	A
8	7	-11	A
8	7	-10	A
8	7	-8	A
8	7	-7	G
8	7	-6	A
8	7	-5	C
8	7	-4	C
8	7	-3	A
8	7	-2	C
8	7	-1	C
8	7	1	A
8	7	3	G
8	7	4	G
8	7	6	A
8	7	7	C
8	7	10	U
8	7	11	U
8	7	13	A
8	7	14	A
8	7	15	G
8	7	18	U
8	7	19	U
8	7	20	G
8	7	21	A
8	7	22	G
11	A	2	A
11	A	4	C
11	A	14	C
11	A	17	C
11	A	26	U
11	A	33	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	42	A
11	A	46	A
11	A	56	G
11	A	58	C
11	A	59	U
11	A	62	G
11	A	64	A
11	A	67	C
11	A	68	A
11	A	73	C
11	A	74	G
11	A	76	U
11	A	78	C
11	A	103	A
11	A	115	U
11	A	126	G
11	A	129	C
11	A	130	G
11	A	140	U
11	A	142	C
11	A	143	U
11	A	155	G
11	A	158	A
11	A	160	U
11	A	163	U
11	A	173	A
11	A	182	C
11	A	184	G
11	A	190	G
11	A	197	U
11	A	198	U
11	A	199	C
11	A	200	G
11	A	202	G
11	A	203	G
11	A	204	G
11	A	206	G
11	A	208	G
11	A	291	G
11	A	292	A
11	A	294	U
11	A	295	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	306	C
11	A	307	G
11	A	308	G
11	A	314	U
11	A	318	A
11	A	319	C
11	A	321	C
11	A	323	C
11	A	324	C
11	A	325	C
11	A	326	C
11	A	327	G
11	A	329	G
11	A	332	G
11	A	339	A
11	A	347	G
11	A	351	G
11	A	362	C
11	A	364	A
11	A	368	U
11	A	369	C
11	A	370	G
11	A	381	C
11	A	384	U
11	A	385	G
11	A	386	C
11	A	409	C
11	A	418	A
11	A	421	G
11	A	448	A
11	A	450	C
11	A	452	G
11	A	455	A
11	A	465	A
11	A	467	G
11	A	471	G
11	A	472	C
11	A	473	A
11	A	474	G
11	A	476	A
11	A	482	G
11	A	487	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	492	C
11	A	496	C
11	A	502	C
11	A	507	G
11	A	508	A
11	A	509	OMG
11	A	516	A
11	A	525	A
11	A	533	A
11	A	534	G
11	A	536	A
11	A	537	C
11	A	538	U
11	A	539	C
11	A	540	U
11	A	541	U
11	A	542	U
11	A	543	C
11	A	544	G
11	A	545	A
11	A	546	G
11	A	547	G
11	A	550	C
11	A	553	U
11	A	554	A
11	A	556	U
11	A	557	U
11	A	558	G
11	A	563	G
11	A	564	A
11	A	566	U
11	A	568	C
11	A	574	A
11	A	576	A
11	A	589	G
11	A	590	A
11	A	591	U
11	A	598	G
11	A	604	A
11	A	606	G
11	A	607	U
11	A	614	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	617	G
11	A	626	G
11	A	627	U
11	A	628	A
11	A	643	A
11	A	644	OMG
11	A	645	C
11	A	655	A
11	A	660	C
11	A	662	G
11	A	668	A2M
11	A	669	A
11	A	671	A
11	A	672	A
11	A	673	G
11	A	683	OMG
11	A	684	G
11	A	688	U
11	A	689	U
11	A	690	G
11	A	691	G
11	A	692	G
11	A	695	C
11	A	696	G
11	A	697	G
11	A	698	G
11	A	699	C
11	A	700	G
11	A	705	G
11	A	707	C
11	A	712	G
11	A	713	C
11	A	715	A
11	A	717	G
11	A	719	G
11	A	720	A
11	A	721	G
11	A	723	C
11	A	725	C
11	A	728	C
11	A	729	C
11	A	731	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	732	U
11	A	733	C
11	A	734	C
11	A	738	C
11	A	739	C
11	A	748	C
11	A	749	U
11	A	751	G
11	A	752	G
11	A	753	C
11	A	790	C
11	A	791	C
11	A	797	C
11	A	798	G
11	A	800	U
11	A	801	U
11	A	810	A
11	A	811	A
11	A	821	G
11	A	822	PSU
11	A	827	A
11	A	830	A
11	A	836	G
11	A	837	A
11	A	838	G
11	A	839	C
11	A	840	C
11	A	841	G
11	A	845	G
11	A	847	A
11	A	870	A
11	A	872	A
11	A	873	G
11	A	880	G
11	A	886	A
11	A	887	U
11	A	888	U
11	A	890	U
11	A	891	G
11	A	892	U
11	A	895	G
11	A	896	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	897	U
11	A	898	U
11	A	899	U
11	A	900	C
11	A	903	A
11	A	904	A
11	A	908	A
11	A	913	A
11	A	914	U
11	A	917	U
11	A	920	A
11	A	922	A
11	A	930	C
11	A	933	G
11	A	954	U
11	A	963	A
11	A	965	U
11	A	970	G
11	A	972	A
11	A	990	A
11	A	992	A
11	A	999	G
11	A	1002	U
11	A	1017	U
11	A	1023	A
11	A	1045	U
11	A	1047	C
11	A	1060	A
11	A	1061	U
11	A	1062	A
11	A	1083	A
11	A	1085	C
11	A	1089	G
11	A	1108	G
11	A	1109	C
11	A	1113	A
11	A	1114	U
11	A	1115	U
11	A	1117	C
11	A	1119	A
11	A	1120	U
11	A	1123	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1133	A
11	A	1138	C
11	A	1139	C
11	A	1153	C
11	A	1154	U
11	A	1172	U
11	A	1195	A
11	A	1207	G
11	A	1209	A
11	A	1211	G
11	A	1215	C
11	A	1216	C
11	A	1217	A
11	A	1220	A
11	A	1224	G
11	A	1242	U
11	A	1247	C
11	A	1251	A
11	A	1253	A
11	A	1256	G
11	A	1257	G
11	A	1259	A
11	A	1263	U
11	A	1274	G
11	A	1275	G
11	A	1283	C
11	A	1288	U
11	A	1290	G
11	A	1294	G
11	A	1295	A
11	A	1301	A
11	A	1302	G
11	A	1303	C
11	A	1308	U
11	A	1322	G
11	A	1326	U
11	A	1333	U
11	A	1342	U
11	A	1354	G
11	A	1356	G
11	A	1357	A
11	A	1371	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1372	U
11	A	1378	A
11	A	1382	A
11	A	1397	U
11	A	1401	A
11	A	1402	A
11	A	1417	C
11	A	1418	C
11	A	1419	C
11	A	1420	G
11	A	1421	A
11	A	1422	G
11	A	1423	C
11	A	1424	G
11	A	1433	C
11	A	1435	C
11	A	1436	C
11	A	1437	C
11	A	1438	A
11	A	1442	U
11	A	1449	G
11	A	1454	A
11	A	1458	G
11	A	1463	U
11	A	1474	A
11	A	1487	A
11	A	1489	A
11	A	1490	G
11	A	1497	G
11	A	1498	A
11	A	1507	G
11	A	1508	A
11	A	1519	U
11	A	1521	C
11	A	1522	A
11	A	1523	C
11	A	1533	A
11	A	1534	C
11	A	1544	C
11	A	1552	G
11	A	1553	C
11	A	1556	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1558	C
11	A	1560	U
11	A	1565	C
11	A	1570	G
11	A	1579	A
11	A	1580	A
11	A	1582	C
11	A	1585	U
11	A	1587	G
11	A	1588	A
11	A	1600	G
11	A	1601	A
11	A	1603	G
11	A	1606	G
11	A	1619	A
11	A	1621	U
11	A	1623	A
11	A	1624	U
11	A	1638	G
11	A	1639	G
11	A	1648	G
11	A	1654	G
11	A	1661	A
11	A	1663	A
11	A	1665	G
11	A	1671	G
11	A	1687	C
11	A	1695	A
11	A	1697	A
11	A	1701	C
11	A	1706	G
11	A	1710	C
11	A	1712	A
11	A	1715	A
11	A	1719	A
11	A	1721	U
11	A	1722	G
11	A	1729	U
11	A	1749	G
11	A	1750	C
11	A	1752	C
11	A	1753	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1754	G
11	A	1755	C
11	A	1757	G
11	A	1758	G
11	A	1759	G
11	A	1760	G
11	A	1772	C
11	A	1773	C
11	A	1774	C
11	A	1775	U
11	A	1776	G
11	A	1777	G
11	A	1778	C
11	A	1779	G
11	A	1780	G
11	A	1781	A
11	A	1782	G
11	A	1783	C
11	A	1784	G
11	A	1805	G
11	A	1808	U
11	A	1813	A
11	A	1819	A
11	A	1822	A
11	A	1823	A
11	A	1826	G
11	A	1829	G
11	A	1835	A
11	A	1836	G
11	A	1837	G
11	A	1839	U
11	A	1849	G
11	A	1861	G
11	A	1862	G
11	A	1863	A
11	A	1864	U
11	A	1865	C
51	w	8	U
51	w	10	G
51	w	11	C
51	w	12	G
51	w	16	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	w	18	G
51	w	19	G
51	w	20	A
51	w	21	A
51	w	22	G
51	w	23	C
51	w	26	G
51	w	35	A
51	w	36	U
51	w	38	A
51	w	39	C
51	w	46	G
51	w	48	C
51	w	49	G
51	w	50	A
51	w	52	G
51	w	56	C
51	w	58	A
51	w	59	A
51	w	60	A
51	w	61	C
51	w	63	A
51	w	64	U
51	w	68	C
51	w	70	G
51	w	74	C
51	w	75	C
51	w	76	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-31	C
8	7	-21	A
8	7	13	A
11	A	1	U
11	A	291	G
11	A	367	U
11	A	368	U
11	A	509	OMG
11	A	626	G
11	A	644	OMG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	683	OMG
11	A	688	U
11	A	694	G
11	A	716	G
11	A	731	G
11	A	797	C
11	A	1600	G
11	A	1836	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
11	5MU	A	814	11	19,22,23	0.23	0	28,32,35	0.32	0
11	JMH	A	1219	11,57	18,22,23	2.93	5 (27%)	21,32,35	1.76	5 (23%)
11	PSU	A	1243	11	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
11	A2M	A	1031	11	18,25,26	4.33	7 (38%)	18,36,39	3.74	4 (22%)
11	PSU	A	823	11	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
11	OMC	A	517	11	19,22,23	0.58	0	26,31,34	0.80	0
11	PSU	A	612	11	18,21,22	1.03	1 (5%)	22,30,33	1.81	5 (22%)
11	PSU	A	822	11	18,21,22	1.03	1 (5%)	22,30,33	1.78	5 (22%)
11	OMC	A	174	11,57	19,22,23	0.55	0	26,31,34	0.68	0
11	OMU	A	121	11	19,22,23	3.01	6 (31%)	26,31,34	1.67	5 (19%)
11	A2M	A	668	11,57	18,25,26	4.22	8 (44%)	18,36,39	3.79	6 (33%)
11	MA6	A	1851	11	18,26,27	1.36	3 (16%)	19,38,41	3.36	2 (10%)
11	A2M	A	159	11	18,25,26	4.31	8 (44%)	18,36,39	3.85	5 (27%)
11	A2M	A	166	11	18,25,26	4.31	9 (50%)	18,36,39	3.77	4 (22%)
11	OMC	A	1703	11	19,22,23	0.58	0	26,31,34	0.65	0
11	OMU	A	116	11	19,22,23	3.00	6 (31%)	26,31,34	1.58	4 (15%)
11	OMG	A	644	11	18,26,27	2.42	8 (44%)	19,38,41	2.62	8 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	A2M	A	484	11	18,25,26	4.25	9 (50%)	18,36,39	3.85	4 (22%)
11	OMG	A	683	11	18,26,27	2.56	8 (44%)	19,38,41	2.95	11 (57%)
11	B8N	A	1248	11	24,29,30	3.06	6 (25%)	29,42,45	1.72	6 (20%)
11	A2M	A	27	11,57	18,25,26	4.30	8 (44%)	18,36,39	3.81	5 (27%)
11	UR3	A	1830	11	19,22,23	2.82	7 (36%)	26,32,35	1.47	4 (15%)
11	A2M	A	1678	11	18,25,26	4.34	9 (50%)	18,36,39	3.88	4 (22%)
11	PSU	A	1081	11	18,21,22	1.01	1 (5%)	22,30,33	1.82	3 (13%)
11	OMG	A	509	11,57	18,26,27	2.63	8 (44%)	19,38,41	2.66	8 (42%)
11	6MZ	A	1832	11,57	18,25,26	1.74	3 (16%)	16,36,39	2.09	3 (18%)
11	PSU	A	119	11	18,21,22	1.01	1 (5%)	22,30,33	1.61	4 (18%)
11	5MC	A	1374	11	18,22,23	0.59	0	26,32,35	0.64	0
11	MA6	A	1850	11	18,26,27	1.36	3 (16%)	19,38,41	3.13	2 (10%)

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
11	5MU	A	814	11	-	0/7/25/26	0/2/2/2
11	JMH	A	1219	11,57	-	1/7/25/26	0/2/2/2
11	PSU	A	1243	11	-	0/7/25/26	0/2/2/2
11	A2M	A	1031	11	-	1/5/27/28	0/3/3/3
11	PSU	A	823	11	-	0/7/25/26	0/2/2/2
11	OMC	A	517	11	-	0/9/27/28	0/2/2/2
11	PSU	A	612	11	-	0/7/25/26	0/2/2/2
11	PSU	A	822	11	-	2/7/25/26	0/2/2/2
11	OMC	A	174	11,57	-	0/9/27/28	0/2/2/2
11	OMU	A	121	11	-	0/9/27/28	0/2/2/2
11	A2M	A	668	11,57	-	2/5/27/28	0/3/3/3
11	MA6	A	1851	11	-	6/7/29/30	0/3/3/3
11	A2M	A	159	11	-	1/5/27/28	0/3/3/3
11	A2M	A	166	11	-	1/5/27/28	0/3/3/3
11	OMC	A	1703	11	-	0/9/27/28	0/2/2/2
11	OMU	A	116	11	-	1/9/27/28	0/2/2/2
11	OMG	A	644	11	-	4/5/27/28	0/3/3/3
11	A2M	A	484	11	-	1/5/27/28	0/3/3/3
11	OMG	A	683	11	-	2/5/27/28	0/3/3/3
11	B8N	A	1248	11	-	3/16/34/35	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	A	27	11,57	-	1/5/27/28	0/3/3/3
11	UR3	A	1830	11	-	2/7/25/26	0/2/2/2
11	A2M	A	1678	11	-	1/5/27/28	0/3/3/3
11	PSU	A	1081	11	-	1/7/25/26	0/2/2/2
11	OMG	A	509	11,57	-	3/5/27/28	0/3/3/3
11	6MZ	A	1832	11,57	-	2/5/27/28	0/3/3/3
11	PSU	A	119	11	-	2/7/25/26	0/2/2/2
11	5MC	A	1374	11	-	0/7/25/26	0/2/2/2
11	MA6	A	1850	11	-	3/7/29/30	0/3/3/3

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1031	A2M	C3'-C2'	-12.96	1.24	1.52
11	A	27	A2M	C3'-C2'	-12.90	1.24	1.52
11	A	1678	A2M	C3'-C2'	-12.77	1.24	1.52
11	A	166	A2M	C3'-C2'	-12.76	1.24	1.52
11	A	159	A2M	C3'-C2'	-12.66	1.24	1.52
11	A	484	A2M	C3'-C2'	-12.51	1.25	1.52
11	A	668	A2M	C3'-C2'	-12.40	1.25	1.52
11	A	1219	JMH	C2-N1	8.43	1.50	1.38
11	A	1248	B8N	C4-N3	-8.31	1.25	1.40
11	A	159	A2M	O4'-C1'	7.80	1.52	1.41
11	A	1678	A2M	O4'-C1'	7.63	1.51	1.41
11	A	1830	UR3	C2-N1	7.63	1.49	1.38
11	A	166	A2M	O4'-C1'	7.61	1.51	1.41
11	A	1248	B8N	C6-N1	7.56	1.55	1.36
11	A	27	A2M	O4'-C1'	7.54	1.51	1.41
11	A	1031	A2M	O4'-C1'	7.53	1.51	1.41
11	A	484	A2M	O4'-C1'	7.53	1.51	1.41
11	A	116	OMU	C2-N1	7.06	1.49	1.38
11	A	121	OMU	C2-N1	7.06	1.49	1.38
11	A	116	OMU	C2-N3	7.04	1.50	1.38
11	A	121	OMU	C2-N3	6.98	1.50	1.38
11	A	668	A2M	O4'-C4'	-6.93	1.29	1.45
11	A	668	A2M	O4'-C1'	6.89	1.50	1.41
11	A	1678	A2M	O4'-C4'	-6.68	1.30	1.45
11	A	159	A2M	O4'-C4'	-6.46	1.30	1.45
11	A	166	A2M	O4'-C4'	-6.43	1.30	1.45
11	A	1031	A2M	O4'-C4'	-6.43	1.30	1.45
11	A	484	A2M	O4'-C4'	-6.30	1.30	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	27	A2M	O4'-C4'	-6.24	1.31	1.45
11	A	121	OMU	C6-C5	6.20	1.49	1.35
11	A	116	OMU	C6-C5	6.13	1.49	1.35
11	A	1830	UR3	C6-C5	6.10	1.49	1.35
11	A	1219	JMH	C6-C5	5.98	1.49	1.35
11	A	1248	B8N	C6-C5	5.53	1.42	1.34
11	A	1832	6MZ	C6-N6	5.35	1.43	1.35
11	A	509	OMG	C2-N3	5.22	1.45	1.33
11	A	1678	A2M	C3'-C4'	5.21	1.66	1.53
11	A	509	OMG	C4-N3	5.17	1.49	1.37
11	A	159	A2M	C3'-C4'	5.14	1.66	1.53
11	A	1219	JMH	C2-N3	5.12	1.48	1.39
11	A	484	A2M	C3'-C4'	5.09	1.66	1.53
11	A	509	OMG	C2-N2	5.09	1.46	1.34
11	A	1830	UR3	C2-N3	5.04	1.48	1.39
11	A	683	OMG	C2-N3	5.01	1.45	1.33
11	A	1031	A2M	C3'-C4'	5.01	1.65	1.53
11	A	683	OMG	C2-N2	5.01	1.46	1.34
11	A	1248	B8N	C2-N1	5.00	1.54	1.39
11	A	166	A2M	C3'-C4'	4.99	1.65	1.53
11	A	27	A2M	C3'-C4'	4.98	1.65	1.53
11	A	668	A2M	C3'-C4'	4.97	1.65	1.53
11	A	644	OMG	C2-N2	4.94	1.45	1.34
11	A	644	OMG	C4-N3	4.88	1.49	1.37
11	A	683	OMG	C4-N3	4.80	1.49	1.37
11	A	644	OMG	C2-N3	4.78	1.44	1.33
11	A	121	OMU	C4-N3	4.09	1.45	1.38
11	A	116	OMU	C4-N3	4.04	1.45	1.38
11	A	1248	B8N	C1'-C5	3.68	1.58	1.50
11	A	683	OMG	C6-N1	3.56	1.43	1.37
11	A	509	OMG	C6-N1	3.50	1.43	1.37
11	A	1248	B8N	O2-C2	-3.46	1.16	1.22
11	A	484	A2M	O2'-C2'	3.45	1.51	1.42
11	A	1031	A2M	O2'-C2'	3.44	1.51	1.42
11	A	823	PSU	C6-C5	3.42	1.39	1.35
11	A	119	PSU	C6-C5	3.42	1.39	1.35
11	A	166	A2M	O2'-C2'	3.42	1.51	1.42
11	A	27	A2M	O2'-C2'	3.41	1.51	1.42
11	A	159	A2M	O2'-C2'	3.39	1.51	1.42
11	A	1678	A2M	O2'-C2'	3.37	1.51	1.42
11	A	1243	PSU	C6-C5	3.36	1.39	1.35
11	A	668	A2M	O2'-C2'	3.31	1.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1851	MA6	C2-N3	3.17	1.37	1.32
11	A	822	PSU	C6-C5	3.17	1.39	1.35
11	A	1850	MA6	C2-N3	3.17	1.37	1.32
11	A	484	A2M	C6-N6	3.14	1.45	1.34
11	A	1678	A2M	C6-N6	3.12	1.45	1.34
11	A	159	A2M	C6-N6	3.12	1.45	1.34
11	A	166	A2M	C6-N6	3.10	1.45	1.34
11	A	1031	A2M	C6-N6	3.10	1.45	1.34
11	A	668	A2M	C6-N6	3.09	1.45	1.34
11	A	1081	PSU	C6-C5	3.08	1.38	1.35
11	A	27	A2M	C6-N6	3.07	1.45	1.34
11	A	1830	UR3	C6-N1	3.02	1.45	1.38
11	A	612	PSU	C6-C5	2.98	1.38	1.35
11	A	509	OMG	C5-C6	2.91	1.53	1.47
11	A	1851	MA6	C5-C4	-2.90	1.33	1.40
11	A	644	OMG	C6-N1	2.90	1.42	1.37
11	A	668	A2M	C5-C4	-2.86	1.33	1.40
11	A	1219	JMH	C6-N1	2.82	1.44	1.38
11	A	1850	MA6	C5-C4	-2.82	1.33	1.40
11	A	1031	A2M	C5-C4	-2.80	1.33	1.40
11	A	166	A2M	C5-C4	-2.79	1.33	1.40
11	A	1678	A2M	C5-C4	-2.79	1.33	1.40
11	A	27	A2M	C5-C4	-2.76	1.33	1.40
11	A	484	A2M	C5-C4	-2.71	1.33	1.40
11	A	683	OMG	C5-C6	2.69	1.52	1.47
11	A	159	A2M	C5-C4	-2.68	1.33	1.40
11	A	121	OMU	C6-N1	2.59	1.44	1.38
11	A	116	OMU	C6-N1	2.59	1.44	1.38
11	A	683	OMG	C2-N1	2.54	1.44	1.37
11	A	1219	JMH	C5-C4	2.49	1.48	1.42
11	A	509	OMG	O6-C6	-2.47	1.18	1.23
11	A	644	OMG	C5-C6	2.45	1.52	1.47
11	A	683	OMG	C5-C4	-2.44	1.36	1.43
11	A	644	OMG	O6-C6	-2.44	1.18	1.23
11	A	1832	6MZ	C5-C4	-2.42	1.34	1.40
11	A	644	OMG	C5-C4	-2.40	1.37	1.43
11	A	683	OMG	O6-C6	-2.39	1.18	1.23
11	A	509	OMG	C2-N1	2.36	1.43	1.37
11	A	509	OMG	C5-C4	-2.34	1.37	1.43
11	A	1830	UR3	O4-C4	-2.32	1.18	1.23
11	A	1832	6MZ	C9-N6	-2.27	1.41	1.45
11	A	644	OMG	C2-N1	2.22	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1830	UR3	O2-C2	-2.21	1.18	1.22
11	A	1830	UR3	C5-C4	2.21	1.49	1.43
11	A	484	A2M	C2-N3	2.21	1.35	1.32
11	A	121	OMU	C5-C4	2.17	1.48	1.43
11	A	166	A2M	O3'-C3'	2.10	1.47	1.43
11	A	27	A2M	C2-N3	2.10	1.35	1.32
11	A	668	A2M	O3'-C3'	2.09	1.47	1.43
11	A	159	A2M	C2-N3	2.09	1.35	1.32
11	A	1678	A2M	C2-N3	2.09	1.35	1.32
11	A	116	OMU	C5-C4	2.07	1.48	1.43
11	A	1678	A2M	O3'-C3'	2.06	1.47	1.43
11	A	166	A2M	C2-N3	2.04	1.35	1.32
11	A	1851	MA6	C4-N3	2.03	1.38	1.35
11	A	484	A2M	O3'-C3'	2.03	1.47	1.43
11	A	1850	MA6	C4-N3	2.01	1.38	1.35

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1851	MA6	N1-C6-N6	-13.20	103.17	117.06
11	A	1850	MA6	N1-C6-N6	-12.41	103.99	117.06
11	A	1678	A2M	C1'-N9-C4	10.39	144.89	126.64
11	A	484	A2M	C1'-N9-C4	10.33	144.79	126.64
11	A	27	A2M	C1'-N9-C4	10.24	144.64	126.64
11	A	159	A2M	C1'-N9-C4	10.17	144.50	126.64
11	A	166	A2M	C1'-N9-C4	9.75	143.77	126.64
11	A	1031	A2M	C1'-N9-C4	9.75	143.77	126.64
11	A	668	A2M	C1'-N9-C4	9.62	143.54	126.64
11	A	668	A2M	C5-C6-N6	9.09	134.16	120.35
11	A	1678	A2M	C5-C6-N6	9.07	134.14	120.35
11	A	166	A2M	C5-C6-N6	8.96	133.96	120.35
11	A	1031	A2M	C5-C6-N6	8.93	133.93	120.35
11	A	159	A2M	C5-C6-N6	8.92	133.91	120.35
11	A	484	A2M	C5-C6-N6	8.77	133.69	120.35
11	A	27	A2M	C5-C6-N6	8.76	133.66	120.35
11	A	683	OMG	O2'-C2'-C1'	7.54	124.04	109.09
11	A	644	OMG	O2'-C2'-C1'	6.16	121.31	109.09
11	A	668	A2M	N6-C6-N1	-6.09	105.93	118.57
11	A	1678	A2M	N6-C6-N1	-6.06	105.99	118.57
11	A	159	A2M	N6-C6-N1	-6.03	106.06	118.57
11	A	509	OMG	O2'-C2'-C1'	6.01	121.02	109.09
11	A	1031	A2M	N6-C6-N1	-5.98	106.17	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	166	A2M	N6-C6-N1	-5.97	106.17	118.57
11	A	484	A2M	N6-C6-N1	-5.96	106.20	118.57
11	A	27	A2M	N6-C6-N1	-5.89	106.34	118.57
11	A	1832	6MZ	N3-C2-N1	-5.81	119.60	128.68
11	A	166	A2M	N3-C2-N1	-5.80	119.61	128.68
11	A	1851	MA6	N3-C2-N1	-5.75	119.70	128.68
11	A	1678	A2M	N3-C2-N1	-5.71	119.76	128.68
11	A	644	OMG	O3'-C3'-C4'	5.68	127.46	111.05
11	A	27	A2M	N3-C2-N1	-5.66	119.83	128.68
11	A	1031	A2M	N3-C2-N1	-5.63	119.88	128.68
11	A	484	A2M	N3-C2-N1	-5.61	119.91	128.68
11	A	159	A2M	N3-C2-N1	-5.44	120.18	128.68
11	A	668	A2M	N3-C2-N1	-5.40	120.24	128.68
11	A	1850	MA6	N3-C2-N1	-5.24	120.48	128.68
11	A	121	OMU	C4-N3-C2	-5.13	119.82	126.58
11	A	509	OMG	O3'-C3'-C4'	5.07	125.71	111.05
11	A	1248	B8N	C5-C4-N3	4.90	125.25	116.17
11	A	1081	PSU	C4-N3-C2	-4.80	119.43	126.34
11	A	1243	PSU	N1-C2-N3	4.80	120.56	115.13
11	A	683	OMG	O3'-C3'-C2'	4.66	124.39	111.17
11	A	1243	PSU	C4-N3-C2	-4.64	119.65	126.34
11	A	116	OMU	C4-N3-C2	-4.63	120.47	126.58
11	A	822	PSU	C4-N3-C2	-4.59	119.72	126.34
11	A	1081	PSU	N1-C2-N3	4.57	120.31	115.13
11	A	823	PSU	C4-N3-C2	-4.55	119.78	126.34
11	A	612	PSU	N1-C2-N3	4.55	120.29	115.13
11	A	822	PSU	N1-C2-N3	4.50	120.22	115.13
11	A	823	PSU	N1-C2-N3	4.47	120.20	115.13
11	A	612	PSU	C4-N3-C2	-4.47	119.90	126.34
11	A	1830	UR3	C4-N3-C2	-4.46	120.36	124.56
11	A	1832	6MZ	C2-N1-C6	4.40	120.36	116.59
11	A	119	PSU	N1-C2-N3	4.19	119.88	115.13
11	A	119	PSU	C4-N3-C2	-4.10	120.43	126.34
11	A	1219	JMH	C1'-N1-C2	4.08	123.88	116.99
11	A	1248	B8N	C4-N3-C2	-4.05	120.33	125.46
11	A	1219	JMH	C6-N1-C2	-3.87	118.32	121.79
11	A	509	OMG	O3'-C3'-C2'	3.86	122.12	111.17
11	A	644	OMG	O3'-C3'-C2'	3.78	121.89	111.17
11	A	121	OMU	N3-C2-N1	3.71	119.82	114.89
11	A	683	OMG	O3'-C3'-C4'	3.71	121.77	111.05
11	A	1219	JMH	O2-C2-N3	-3.71	116.12	121.34
11	A	683	OMG	C5-C6-N1	3.69	120.48	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	683	OMG	CM2-O2'-C2'	3.69	124.20	114.52
11	A	509	OMG	C5-C6-N1	3.65	120.40	113.95
11	A	1832	6MZ	C1'-N9-C4	-3.44	120.60	126.64
11	A	116	OMU	N3-C2-N1	3.39	119.38	114.89
11	A	1830	UR3	C1'-N1-C2	3.38	122.69	116.99
11	A	509	OMG	C2-N1-C6	-3.37	118.89	125.10
11	A	121	OMU	C5-C4-N3	3.29	119.76	114.84
11	A	683	OMG	C2-N1-C6	-3.26	119.09	125.10
11	A	116	OMU	C5-C4-N3	3.19	119.62	114.84
11	A	683	OMG	C5'-C4'-C3'	3.14	126.96	115.18
11	A	509	OMG	C5'-C4'-C3'	3.11	126.82	115.18
11	A	1248	B8N	C31-N3-C4	3.10	121.88	117.31
11	A	1248	B8N	N3-C2-N1	3.09	121.12	116.76
11	A	612	PSU	O2-C2-N1	-2.94	119.55	122.79
11	A	116	OMU	O4-C4-C5	-2.81	120.22	125.16
11	A	823	PSU	O2-C2-N1	-2.76	119.75	122.79
11	A	1830	UR3	C6-N1-C2	-2.75	119.32	121.79
11	A	1243	PSU	O2-C2-N1	-2.73	119.78	122.79
11	A	121	OMU	O4-C4-C5	-2.73	120.36	125.16
11	A	644	OMG	C5-C6-N1	2.68	118.68	113.95
11	A	1081	PSU	O2-C2-N1	-2.61	119.92	122.79
11	A	644	OMG	O5'-C5'-C4'	2.60	117.85	108.99
11	A	159	A2M	C2'-C3'-C4'	2.55	107.53	101.99
11	A	822	PSU	O2-C2-N1	-2.52	120.01	122.79
11	A	612	PSU	C6-N1-C2	-2.50	120.13	122.68
11	A	509	OMG	C8-N7-C5	2.49	107.74	102.99
11	A	1219	JMH	O3'-C3'-C2'	2.45	119.73	111.82
11	A	1248	B8N	O4-C4-N3	-2.40	115.90	119.98
11	A	823	PSU	C6-N1-C2	-2.36	120.27	122.68
11	A	683	OMG	N2-C2-N1	2.36	121.73	116.71
11	A	1830	UR3	O2-C2-N3	-2.34	118.05	121.34
11	A	509	OMG	O6-C6-C5	-2.32	119.83	124.37
11	A	119	PSU	C6-N1-C2	-2.32	120.31	122.68
11	A	1243	PSU	C6-N1-C2	-2.31	120.32	122.68
11	A	683	OMG	O6-C6-C5	-2.31	119.86	124.37
11	A	644	OMG	C5'-C4'-C3'	2.31	123.83	115.18
11	A	644	OMG	N1-C2-N3	-2.25	119.12	123.32
11	A	119	PSU	O2-C2-N1	-2.23	120.34	122.79
11	A	668	A2M	C3'-C2'-C1'	2.20	107.03	102.89
11	A	822	PSU	O4'-C1'-C2'	2.19	108.23	105.14
11	A	822	PSU	C6-N1-C2	-2.17	120.46	122.68
11	A	612	PSU	O4'-C1'-C2'	2.14	108.16	105.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	27	A2M	O4'-C1'-C2'	-2.10	102.95	106.59
11	A	1219	JMH	O3'-C3'-C4'	2.09	117.09	111.05
11	A	668	A2M	C2'-C3'-C4'	2.08	106.52	101.99
11	A	644	OMG	O4'-C4'-C5'	2.07	116.19	109.37
11	A	1248	B8N	O4'-C1'-C2'	2.06	108.05	105.14
11	A	683	OMG	C8-N7-C5	2.05	106.90	102.99
11	A	683	OMG	N1-C2-N3	-2.04	119.51	123.32
11	A	121	OMU	O2-C2-N1	-2.02	120.10	122.79
11	A	1243	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	27	A2M	C1'-C2'-O2'-CM'
11	A	116	OMU	C1'-C2'-O2'-CM2
11	A	166	A2M	C1'-C2'-O2'-CM'
11	A	484	A2M	C1'-C2'-O2'-CM'
11	A	509	OMG	C1'-C2'-O2'-CM2
11	A	644	OMG	C4'-C5'-O5'-P
11	A	644	OMG	C3'-C4'-C5'-O5'
11	A	644	OMG	C1'-C2'-O2'-CM2
11	A	1031	A2M	C1'-C2'-O2'-CM'
11	A	1678	A2M	C1'-C2'-O2'-CM'
11	A	1832	6MZ	N1-C6-N6-C9
11	A	1850	MA6	C5-C6-N6-C9
11	A	1850	MA6	C5-C6-N6-C10
11	A	1851	MA6	O4'-C4'-C5'-O5'
11	A	1851	MA6	C5-C6-N6-C10
11	A	683	OMG	C1'-C2'-O2'-CM2
11	A	1248	B8N	C31-C32-C33-C34
11	A	1248	B8N	C31-C32-C33-N34
11	A	1830	UR3	O4'-C1'-N1-C2
11	A	509	OMG	C3'-C4'-C5'-O5'
11	A	668	A2M	O4'-C4'-C5'-O5'
11	A	1851	MA6	C3'-C4'-C5'-O5'
11	A	668	A2M	C3'-C4'-C5'-O5'
11	A	822	PSU	C3'-C4'-C5'-O5'
11	A	822	PSU	O4'-C4'-C5'-O5'
11	A	683	OMG	C3'-C4'-C5'-O5'
11	A	1850	MA6	N1-C6-N6-C10
11	A	1830	UR3	O4'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1851	MA6	N1-C6-N6-C10
11	A	644	OMG	O4'-C4'-C5'-O5'
11	A	1851	MA6	C5-C6-N6-C9
11	A	159	A2M	C3'-C4'-C5'-O5'
11	A	119	PSU	O4'-C4'-C5'-O5'
11	A	1832	6MZ	C5-C6-N6-C9
11	A	1851	MA6	C4'-C5'-O5'-P
11	A	1248	B8N	O4'-C1'-C5-C4
11	A	1081	PSU	C4'-C5'-O5'-P
11	A	509	OMG	O4'-C4'-C5'-O5'
11	A	119	PSU	C3'-C4'-C5'-O5'
11	A	1219	JMH	C2'-C1'-N1-C2

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 93 ligands modelled in this entry, 92 are monoatomic - 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
55	GTP	0	2001	57,56	26,34,34	1.12	2 (7%)	32,54,54	1.78	6 (18%)

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
55	GTP	0	2001	57,56	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	0	2001	GTP	C5-C6	-3.92	1.39	1.47
55	0	2001	GTP	C2-N3	2.08	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	0	2001	GTP	PA-O3A-PB	-5.04	115.52	132.83
55	0	2001	GTP	PB-O3B-PG	-3.25	121.67	132.83
55	0	2001	GTP	C5-C6-N1	3.24	119.67	113.95
55	0	2001	GTP	C8-N7-C5	3.09	108.87	102.99
55	0	2001	GTP	C2-N1-C6	-2.88	119.79	125.10
55	0	2001	GTP	C3'-C2'-C1'	2.71	105.06	100.98

There are no chirality outliers.

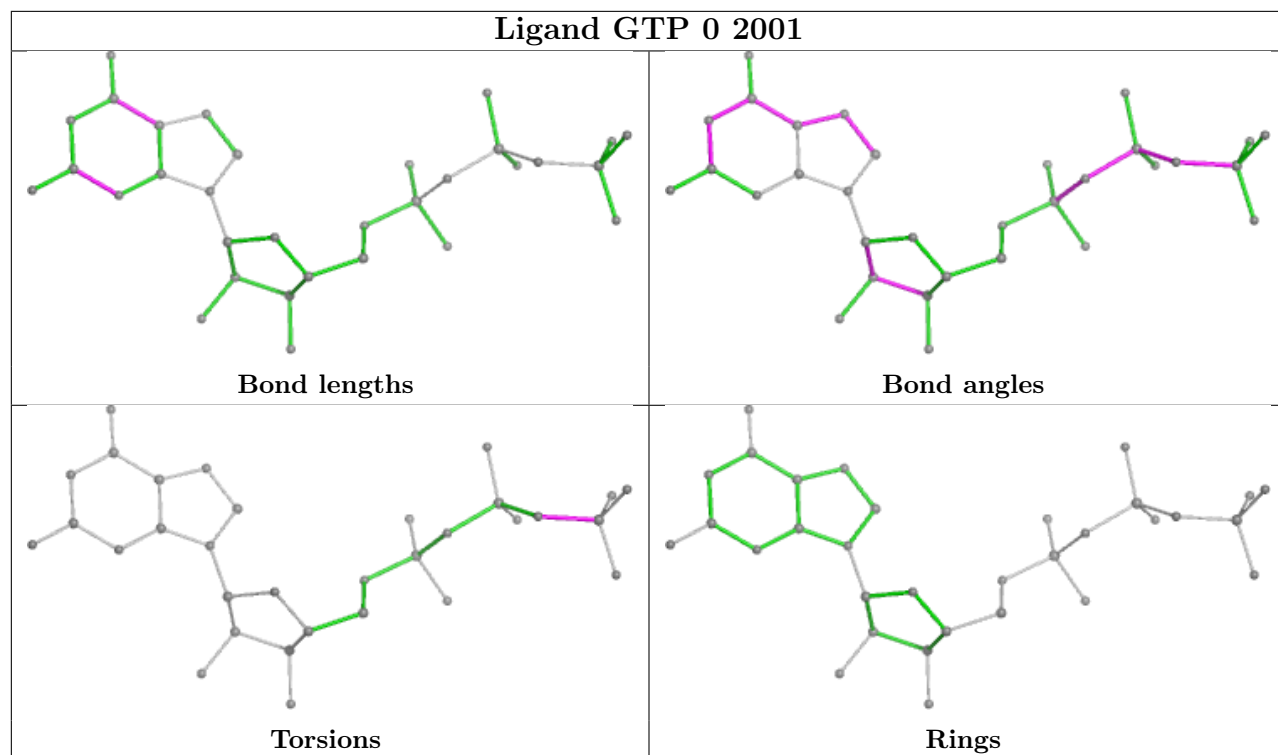
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	0	2001	GTP	PB-O3B-PG-O2G

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

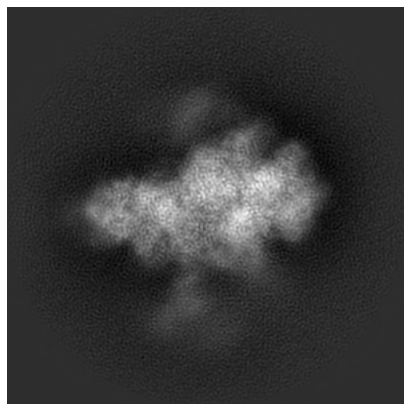
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17698. These allow visual inspection of the internal detail of the map and identification of artifacts.

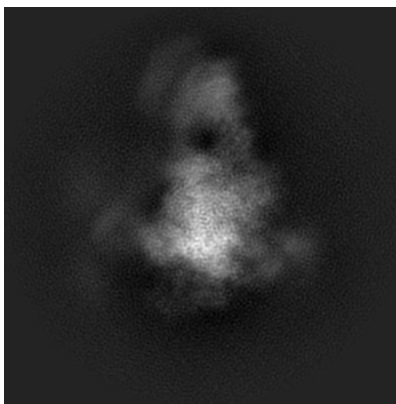
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

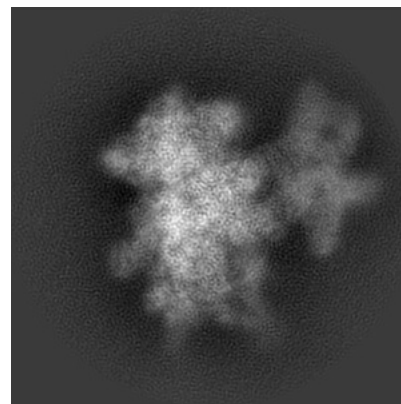
6.1.1 Primary map



X

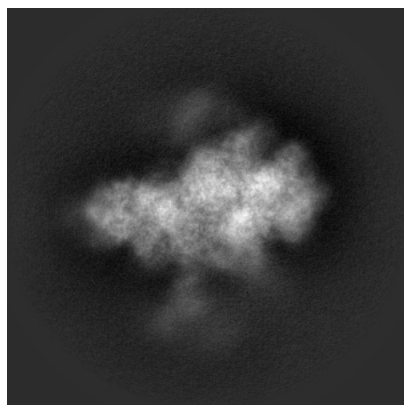


Y

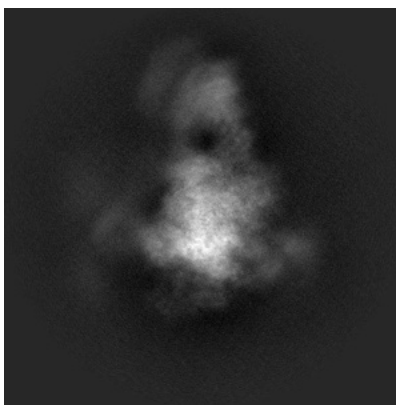


Z

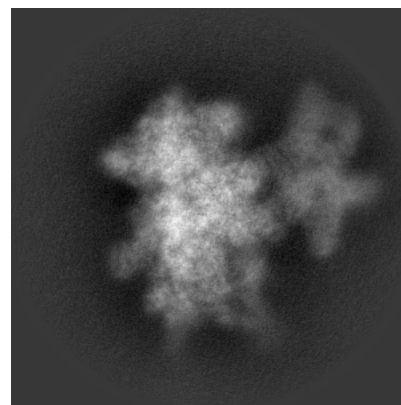
6.1.2 Raw map



X



Y

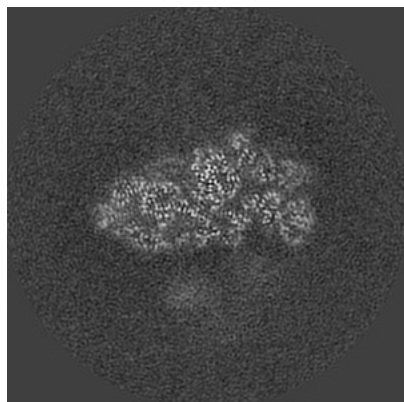


Z

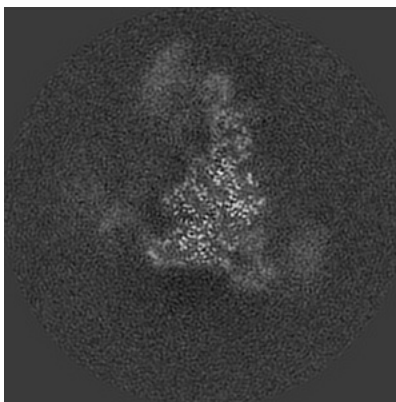
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

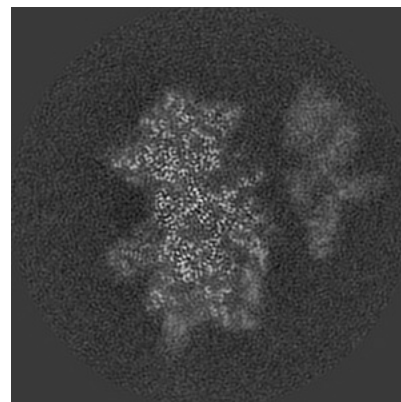
6.2.1 Primary map



X Index: 180

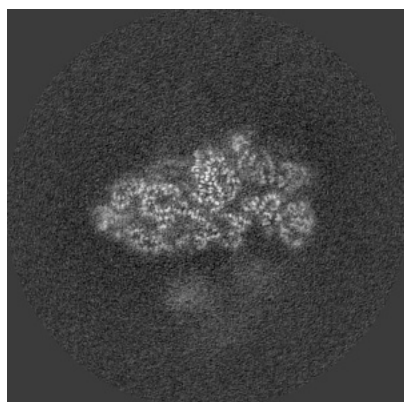


Y Index: 180

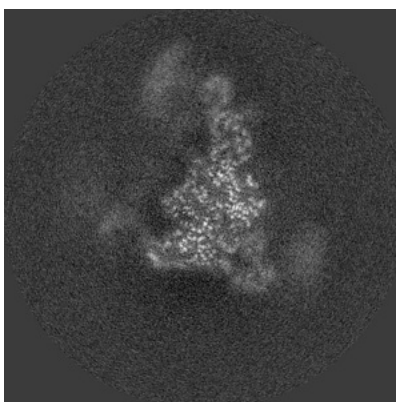


Z Index: 180

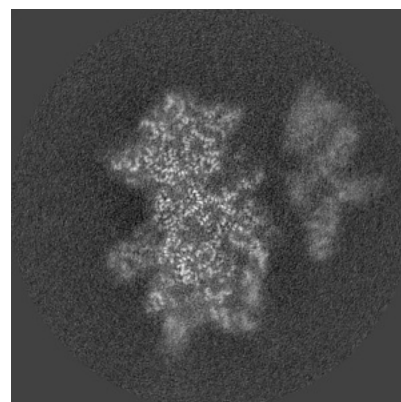
6.2.2 Raw map



X Index: 180



Y Index: 180

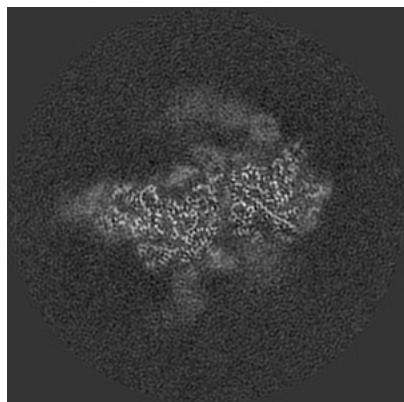


Z Index: 180

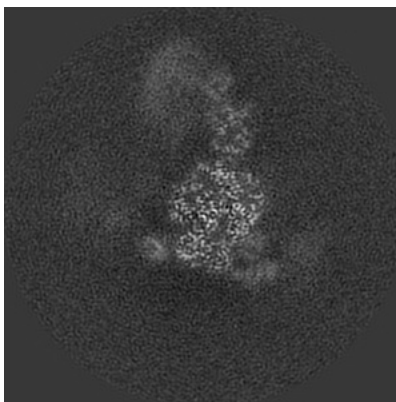
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

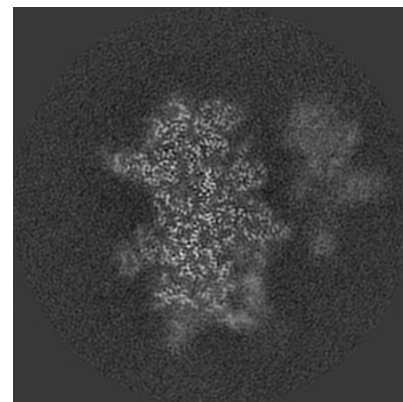
6.3.1 Primary map



X Index: 147

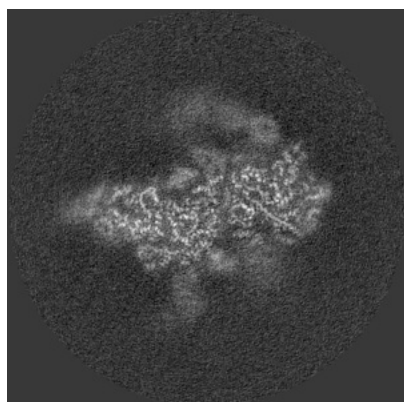


Y Index: 185

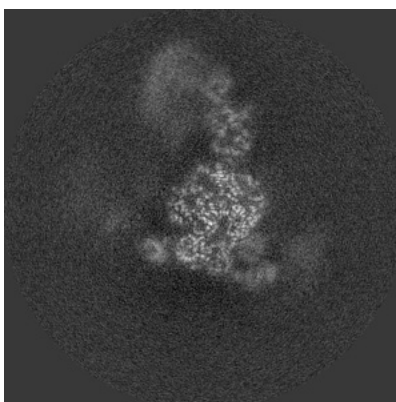


Z Index: 174

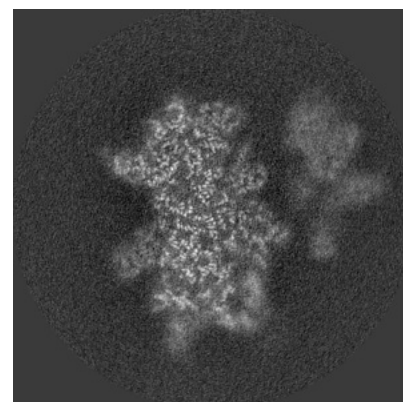
6.3.2 Raw map



X Index: 147



Y Index: 185

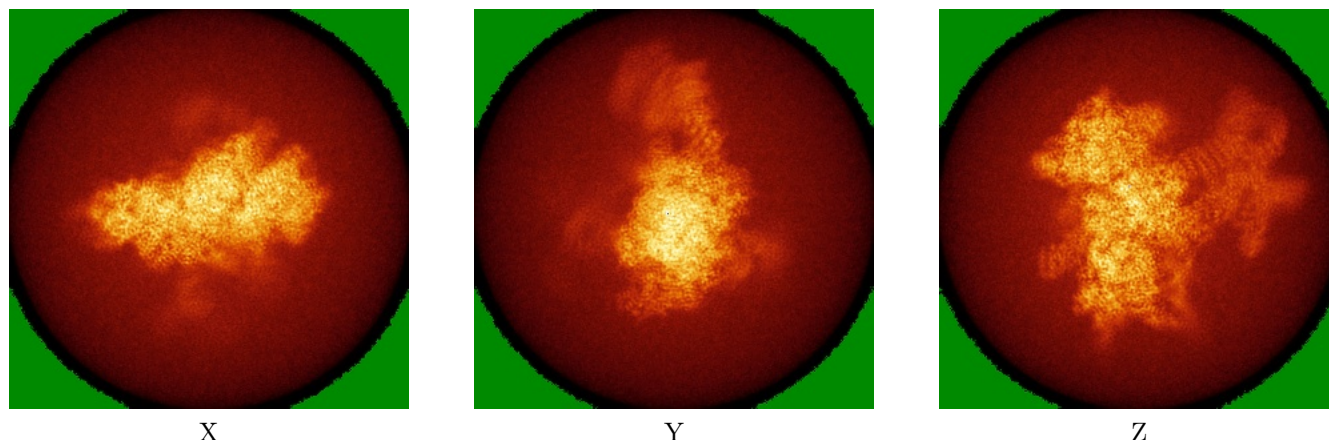


Z Index: 175

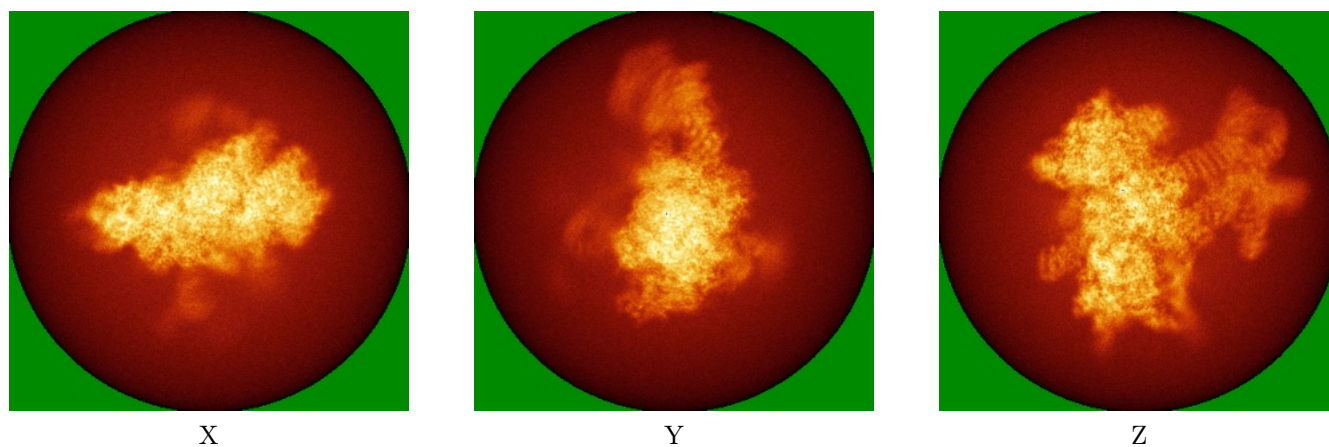
The images above show the largest variance slices of the map in three orthogonal directions.

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

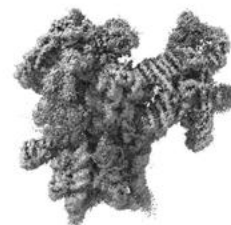
6.5.2 Raw map



X



Y



Z

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

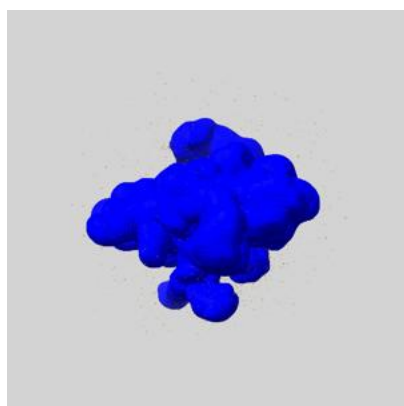
6.6 Mask visualisation [i](#)

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

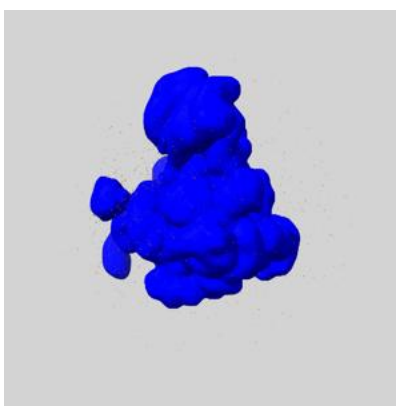
A mask typically either:

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

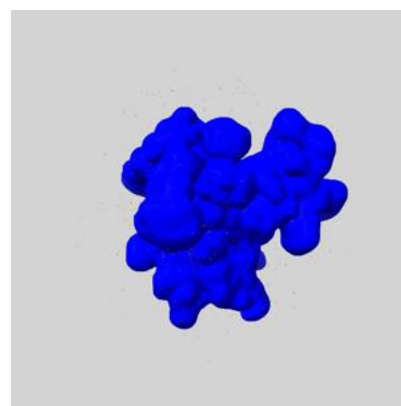
6.6.1 emd_17698_msk_1.map [i](#)



X



Y

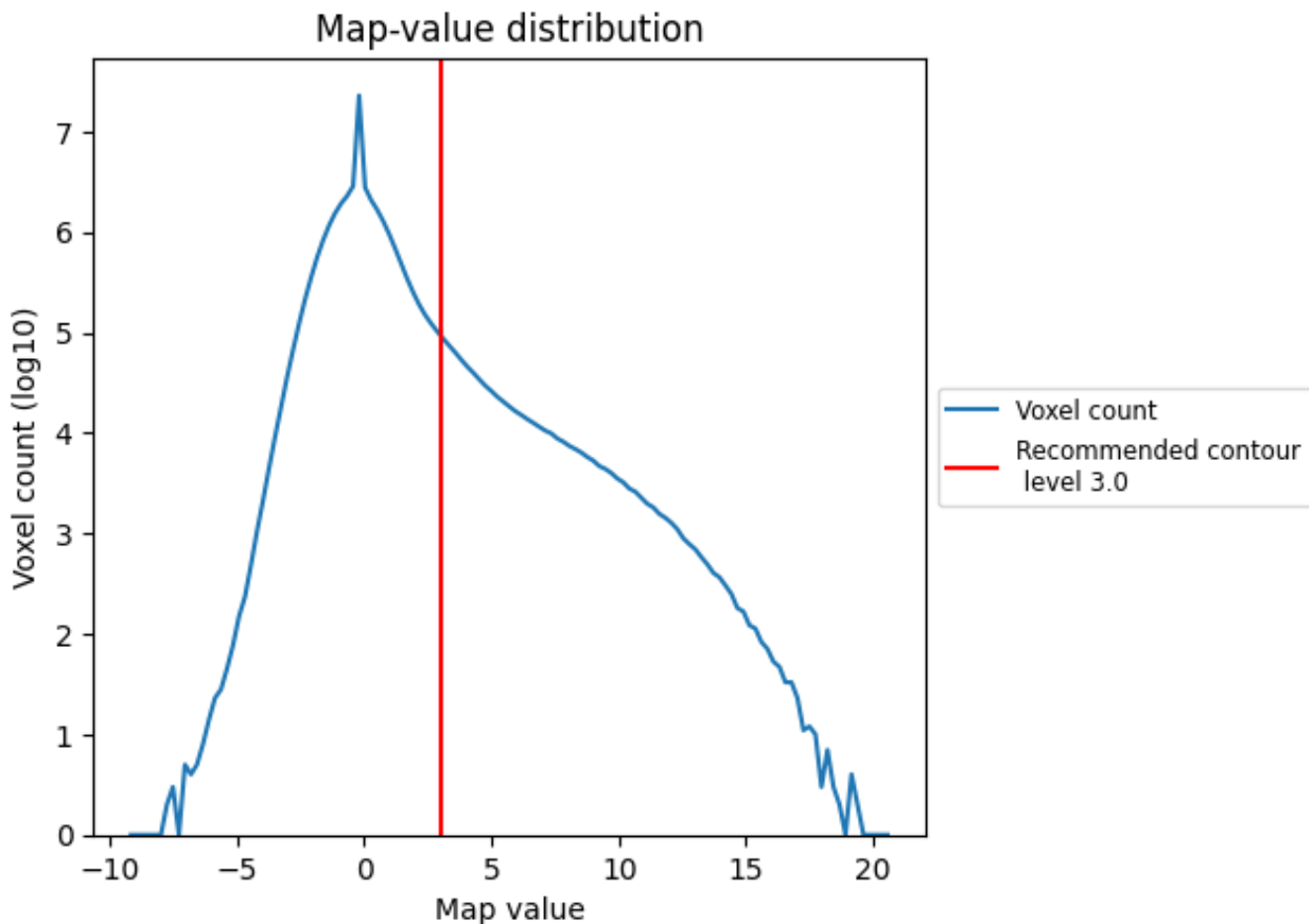


Z

7 Map analysis [i](#)

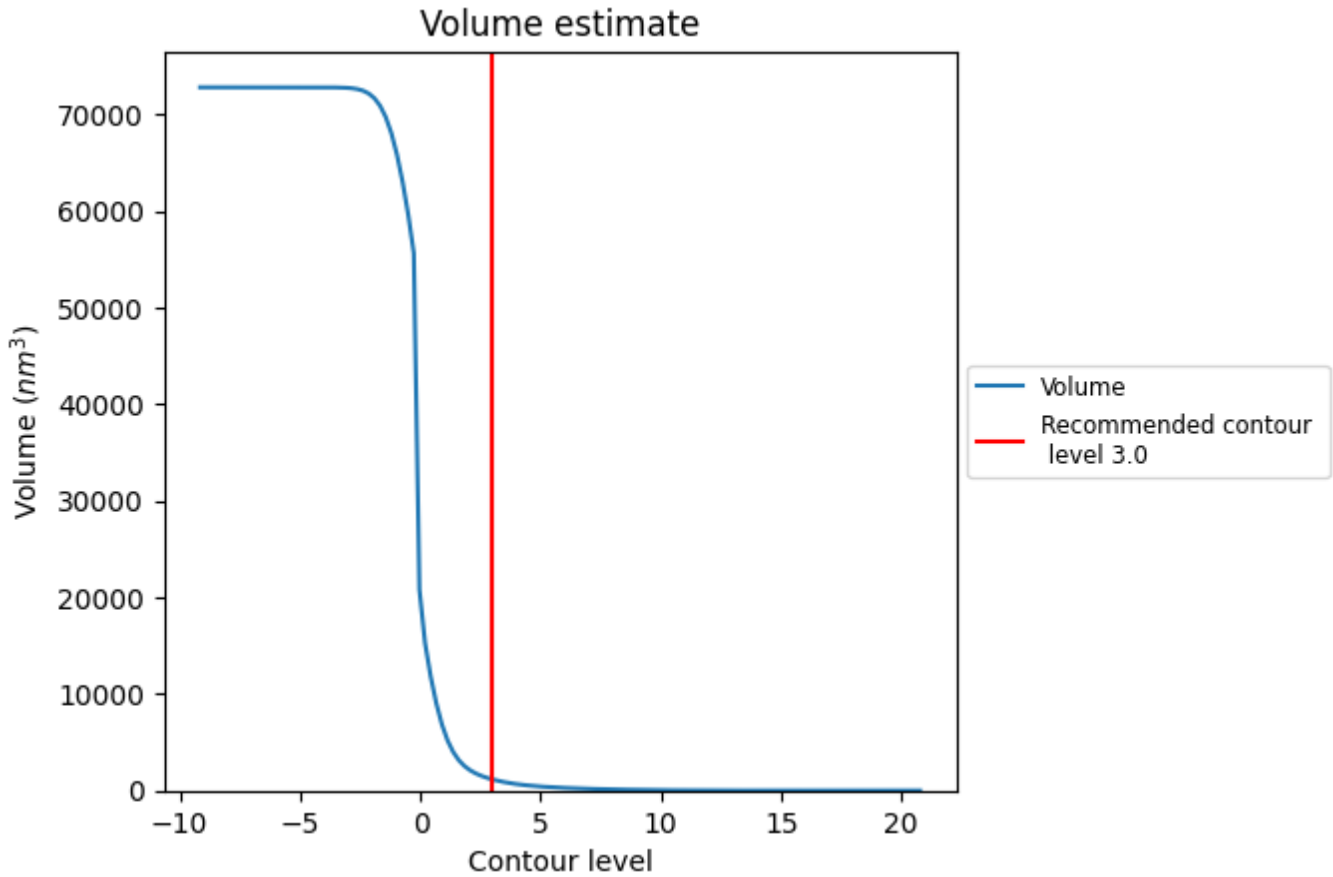
This section contains the results of statistical analysis of the map.

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.

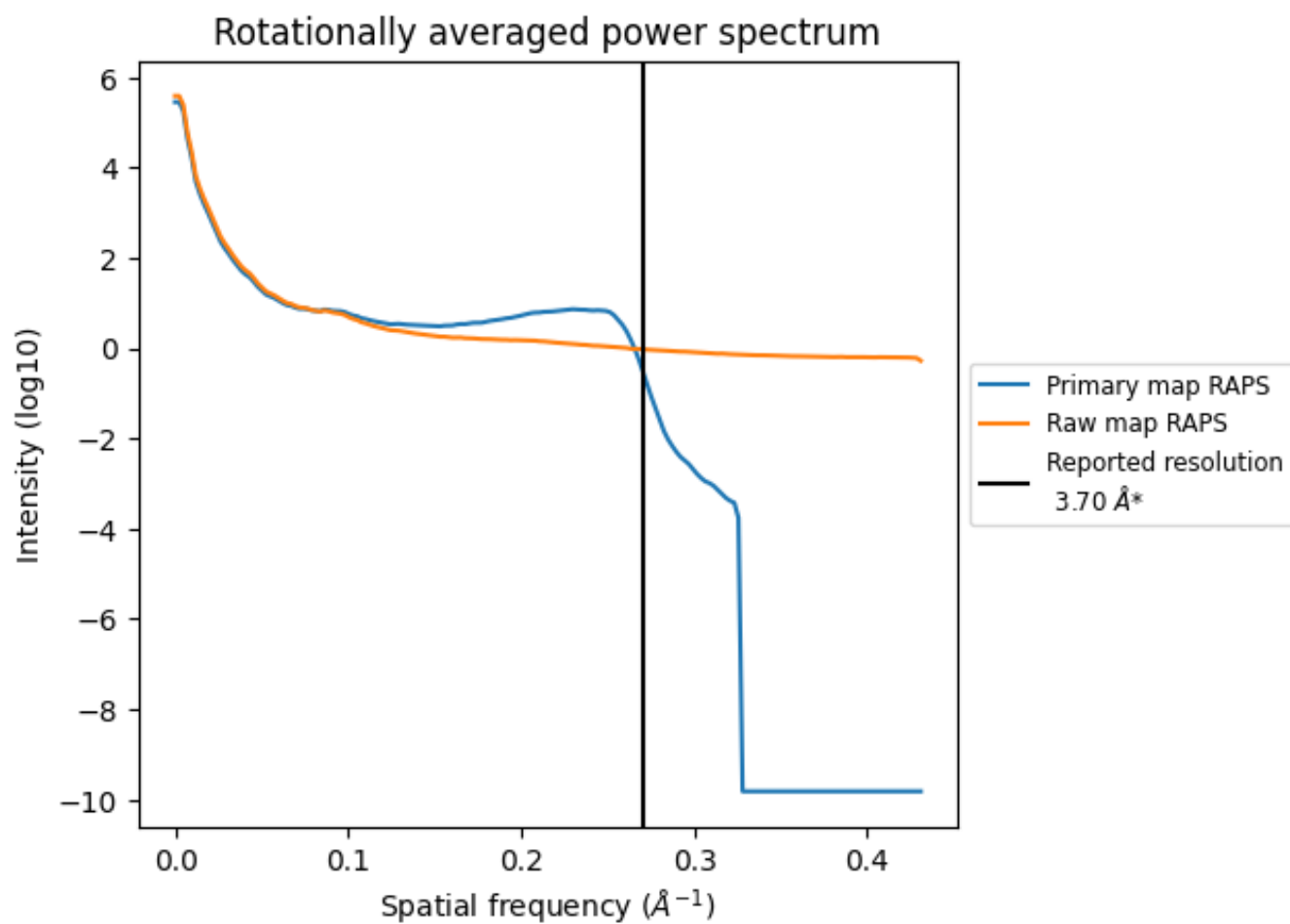
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1159 nm³; this corresponds to an approximate mass of 1047 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](#)

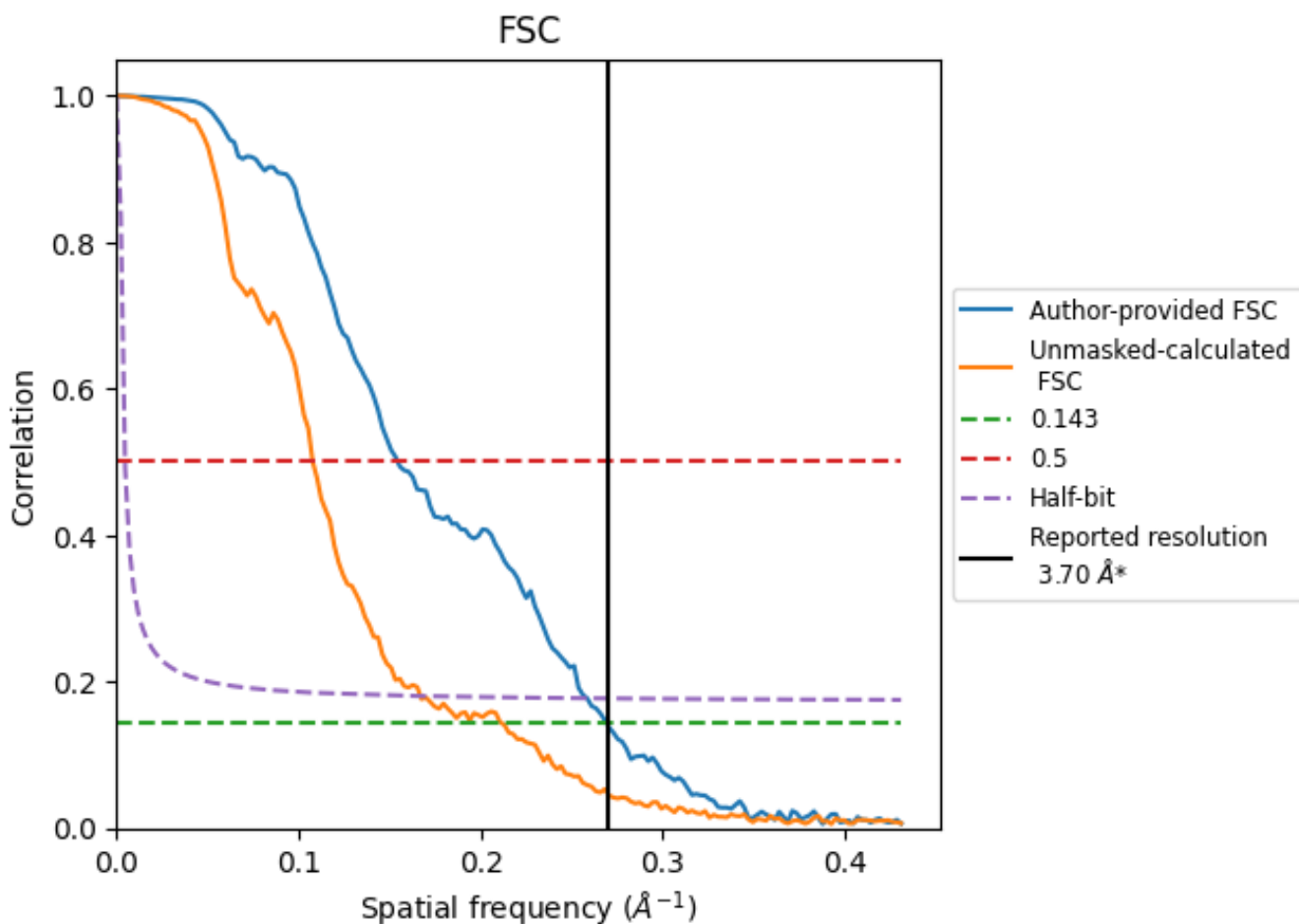


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

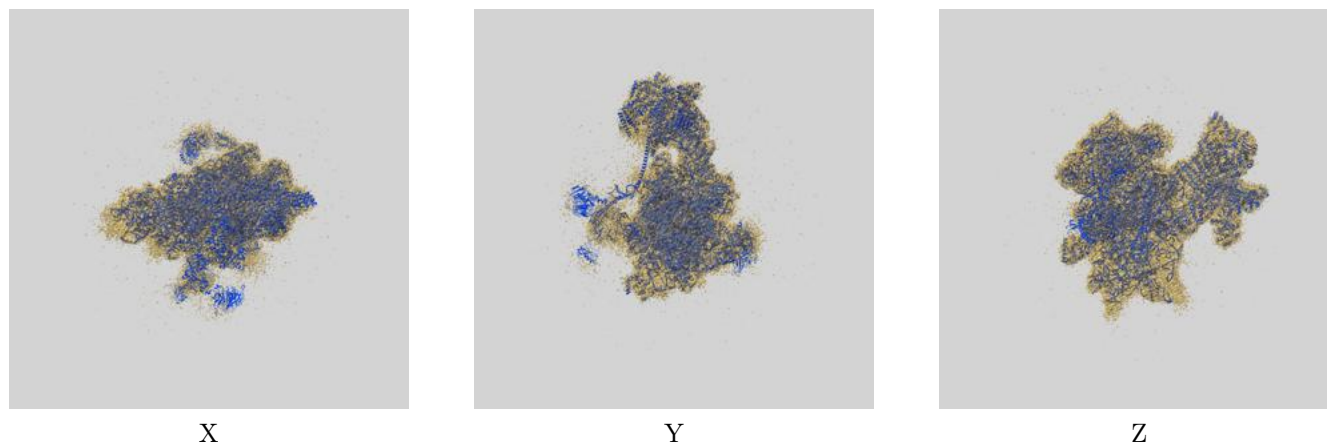
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	6.47	3.87
Unmasked-calculated*	4.73	9.28	5.99

*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 4.73 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

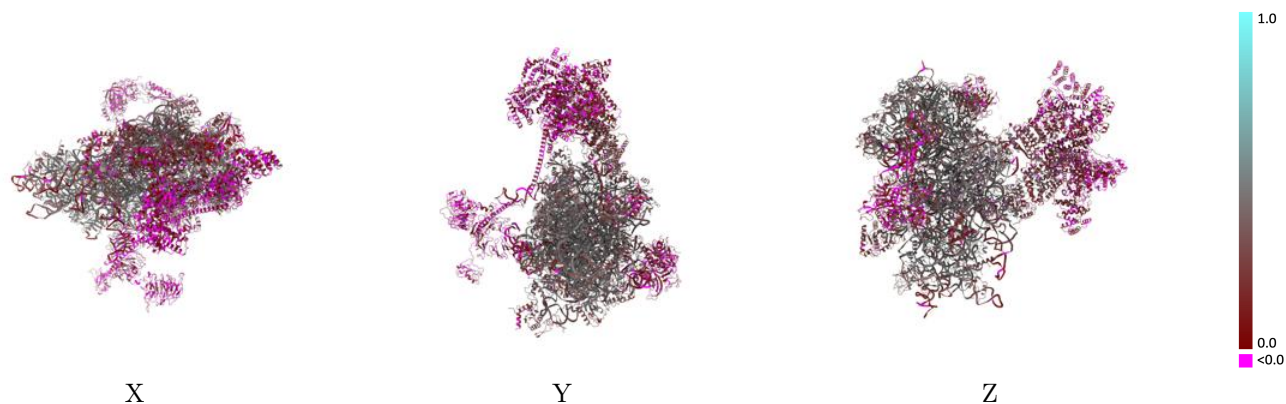
This section contains information regarding the fit between EMDB map EMD-17698 and PDB model 8PJ3. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



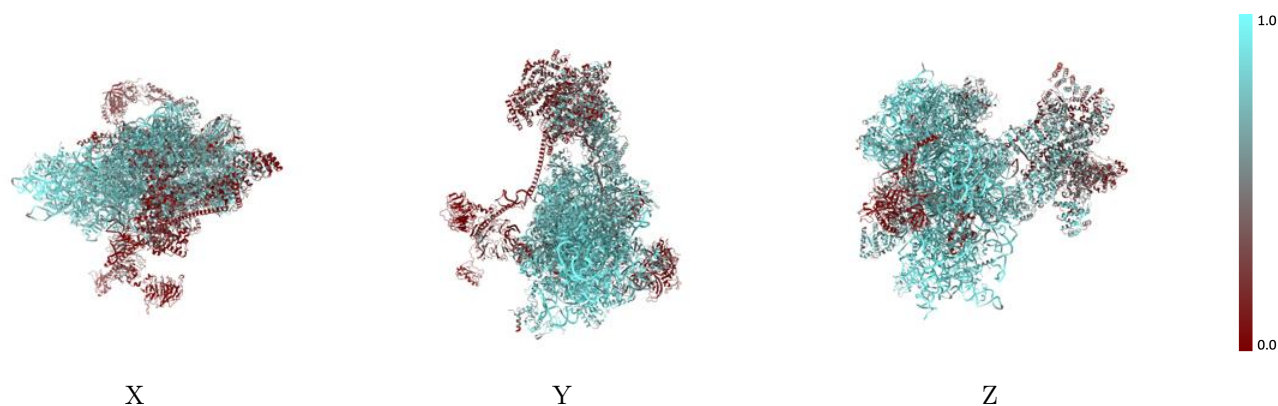
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



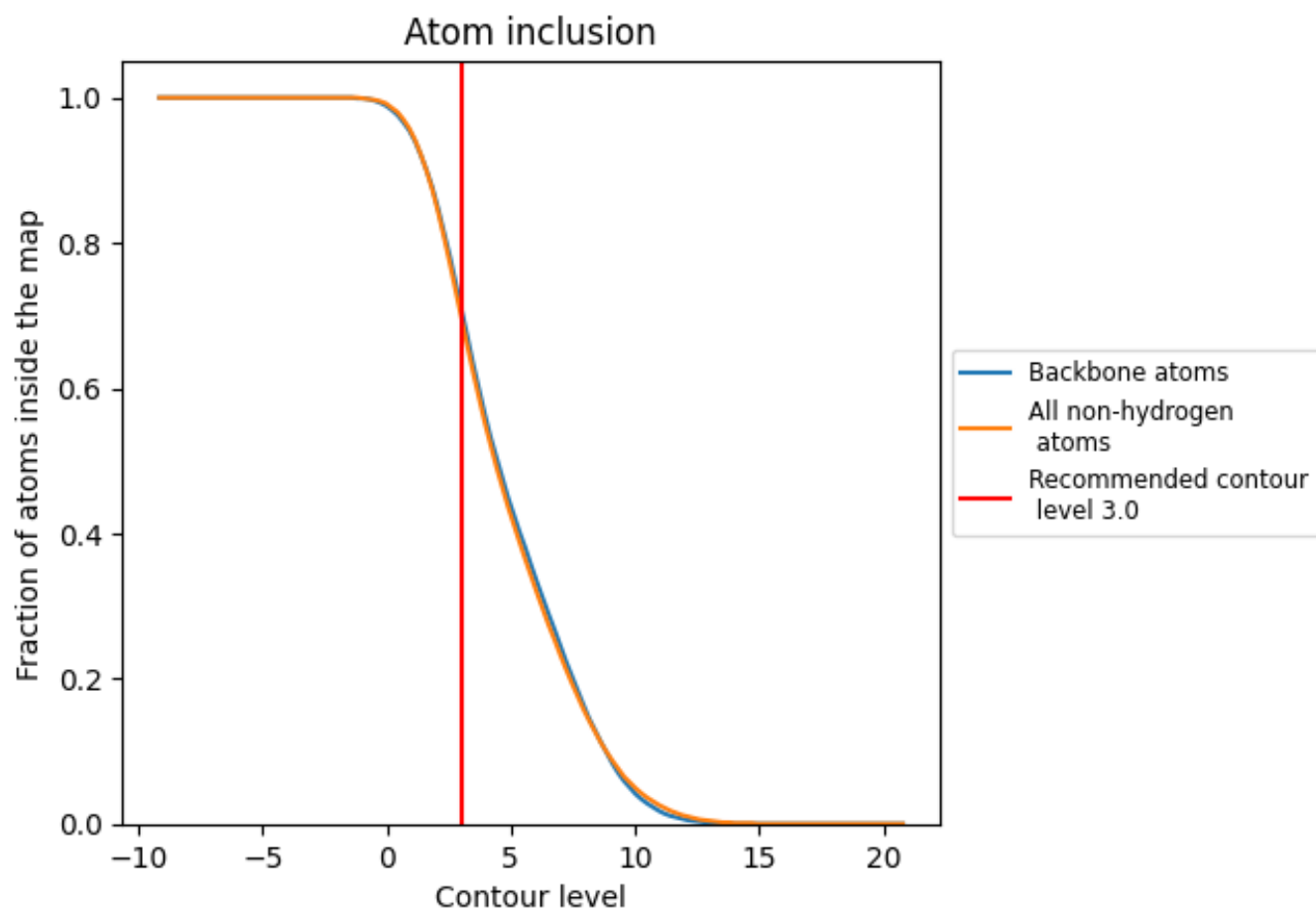
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.3120
0	 0.5780	 0.2760
1	 0.1450	 0.0790
2	 0.0030	 0.0290
3	 0.2580	 0.0400
4	 0.4140	 0.0820
5	 0.2490	 0.0460
6	 0.3860	 0.0960
7	 0.4730	 0.1680
8	 0.3820	 0.0720
9	 0.7270	 0.3710
A	 0.9310	 0.3970
B	 0.8420	 0.4530
C	 0.8670	 0.4520
D	 0.8370	 0.4350
E	 0.8560	 0.4640
F	 0.7600	 0.4010
G	 0.7550	 0.3780
H	 0.7950	 0.4370
I	 0.8260	 0.4360
J	 0.8550	 0.4620
K	 0.8080	 0.4430
L	 0.7980	 0.4370
M	 0.7350	 0.3970
N	 0.8300	 0.4350
O	 0.7990	 0.4200
P	 0.8050	 0.4220
Q	 0.8710	 0.4590
R	 0.8690	 0.4210
S	 0.8370	 0.3790
T	 0.8720	 0.4300
V	 0.8130	 0.4360
Y	 0.8710	 0.4420
Z	 0.7560	 0.4070
a	 0.8200	 0.4240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.8100	 0.4010
c	 0.8010	 0.3880
d	 0.8800	 0.4330
e	 0.7170	 0.3790
f	 0.8050	 0.3940
h	 0.7810	 0.3970
i	 0.9080	 0.4610
k	 0.6870	 0.2650
m	 0.6080	 0.2420
n	 0.7160	 0.4150
o	 0.3860	 0.1630
q	 0.7190	 0.4110
r	 0.5270	 0.2080
t	 0.0800	 0.0790
u	 0.5210	 0.2010
v	 0.4960	 0.1120
w	 0.7200	 0.1600
x	 0.5450	 0.2260
y	 0.5770	 0.2550
z	 0.4810	 0.2130