



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 10:51 am BST

PDB ID : 8PPL
EMDB ID : EMD-17805
Title : MERS-CoV Nsp1 bound to the human 43S pre-initiation complex
Authors : Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on : 2023-07-07
Resolution : 2.65 Å (reported)
Based on initial models : 6ZOL, 6ZOK

This is a wwPDB EM Validation Summary 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:

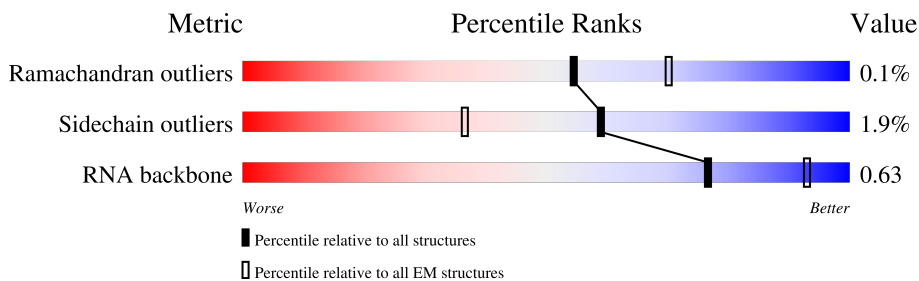
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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	I3	218	
2	I4	357	
3	I5	564	
4	I6	374	
5	I8	352	
6	Io	320	
7	Ip	113	
8	Iq	144	

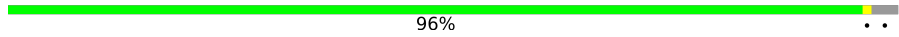
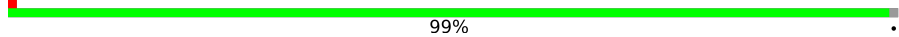

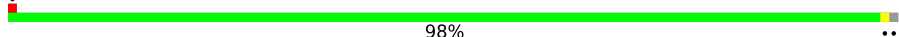

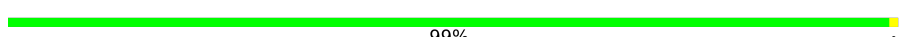
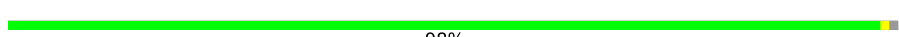



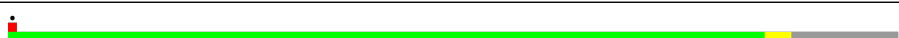


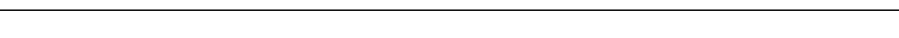
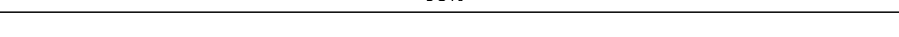
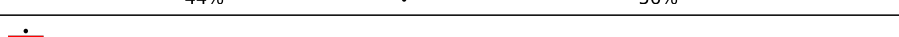

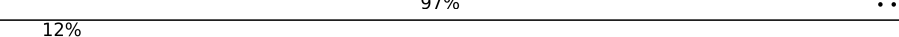
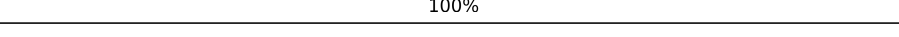
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Mol	Chain	Length	Quality of chain
9	Ir	315	13% 88% 5% 7%
10	Is	333	46% 52%
11	It	472	17% 94%
12	Iu	1382	16% 42% 58%
13	Iv	445	76% 95%
14	Iw	75	73% 23%
15	Ix	548	73% 82% 17%
16	Iy	913	20% 68% 31%
17	A2	1869	79% 16% 5%
18	AA	295	72% 27%
19	AB	264	84% 15%
20	AC	293	73% 26%
21	AD	243	92% 7%
22	AE	263	98%
23	AF	204	94% 6%
24	AG	249	96%
25	AH	194	97%
26	AI	208	99%
27	AJ	194	92% 7%
28	AK	165	58% 41%
29	AL	158	6% 94%
30	AM	132	19% 91% 7%
31	AN	151	99%
32	AO	151	88% 11%
33	AP	145	90% 10%

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Mol	Chain	Length	Quality of chain
34	AQ	146	 96%
35	AR	135	 99%
36	AS	152	 93% 5%
37	AT	145	 98%
38	AU	119	 84% 15%
39	AV	83	 99%
40	AW	130	 98%
41	AX	143	 97%
42	AY	133	 93% 7%
43	AZ	125	 57% 42%
44	Aa	115	 85% 12%
45	Ab	84	 96%
46	Ac	69	 94% 6%
47	Ad	56	 98%
48	Ae	133	 44% 56%
49	Af	156	 46% 53%
50	Ag	317	 97%
51	Ah	25	 100% 12%
52	Aj	216	 13% 87%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 118236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I3	217	1750	1116	288	334	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I4	268	2087	1315	355	405	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I5	372	3111	2011	520	563	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I6	345	2751	1753	464	517	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I8	318	2594	1641	444	494	15	0	0

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

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

- Molecule 7 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ip	105	797	501	145	149	2	0	0

- Molecule 8 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Iq	103	835	525	148	158	4	0	0

- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Ir	293	2368	1486	415	454	13	0	0

- Molecule 10 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Is	159	1288	813	238	228	9	0	0

- Molecule 11 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	It	451	3445	2191	605	632	17	0	0

- Molecule 12 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Iu	587	4830	3048	869	891	22	0	0

- Molecule 13 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Iv	430	3553	2272	602	658	21	0	0

- Molecule 14 is a RNA chain called Met-tRNAⁱ(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Iw	75	Total	C	N	O	P	0	0
			1624	728	299	522	75		

- Molecule 15 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ix	455	Total	C	N	O	S	0	0
			3680	2311	640	707	22		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Iy	633	Total	C	N	O	S	0	0
			4949	3102	886	928	33		

- Molecule 17 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A2	1780	Total	C	N	O	P	0	0
			38049	17008	6822	12439	1780		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AA	216	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

- Molecule 19 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 20 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AC	218	Total	C	N	O	S	1	0
			1698	1099	292	297	10		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AD	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 22 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AF	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AG	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 25 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AH	188	Total	C	N	O	S	0	0
			1515	966	279	269	1		

- Molecule 26 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AI	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 27 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 28 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AK	97	816	533	144	133	6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AL	151	1229	782	230	211	6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AM	123	953	598	169	177	9	0	0

- Molecule 31 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AN	149	1202	770	228	203	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AO	135	1010	618	198	188	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 33 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	AP	131	1075	682	204	182	7	0	0

- Molecule 34 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AQ	142	1128	717	213	195	3	0	0

- Molecule 35 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AR	134	1082	680	201	197	4	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AS	145	1200	753	242	204	1	0	0

- Molecule 37 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AT	144	1123	704	217	199	3	0	0

- Molecule 38 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AU	101	803	504	153	142	4	0	0

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	AV	83	639	395	117	122	5	0	0

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

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

- Molecule 41 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AX	141	1112	703	222	184	3	2	0

- Molecule 42 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AY	124	1014	641	198	170	5	0	0

- Molecule 43 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	AZ	72	574	368	104	101	1	0	0

- Molecule 44 is a protein called 40S ribosomal protein S26.

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

- Molecule 45 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Ab	83	650	408	121	114	7	0	0

- Molecule 46 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Ac	65	512	311	103	96	2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Ad	55	458	286	94	73	5	0	0

- Molecule 48 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Ae	59	467	290	102	74	1	0	0

- Molecule 49 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 50 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ag	314	2440	1537	425	466	12	0	0

- Molecule 51 is a protein called 60S ribosomal protein L41.

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

- Molecule 52 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Aj	29	227	145	36	44	2	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-22	MET	-	initiating methionine	UNP K9N7C7
Aj	-21	ALA	-	expression tag	UNP K9N7C7
Aj	-20	ASP	-	expression tag	UNP K9N7C7
Aj	-19	TYR	-	expression tag	UNP K9N7C7
Aj	-18	LYS	-	expression tag	UNP K9N7C7
Aj	-17	ASP	-	expression tag	UNP K9N7C7
Aj	-16	HIS	-	expression tag	UNP K9N7C7
Aj	-15	ASP	-	expression tag	UNP K9N7C7
Aj	-14	GLY	-	expression tag	UNP K9N7C7
Aj	-13	ASP	-	expression tag	UNP K9N7C7
Aj	-12	TYR	-	expression tag	UNP K9N7C7
Aj	-11	LYS	-	expression tag	UNP K9N7C7

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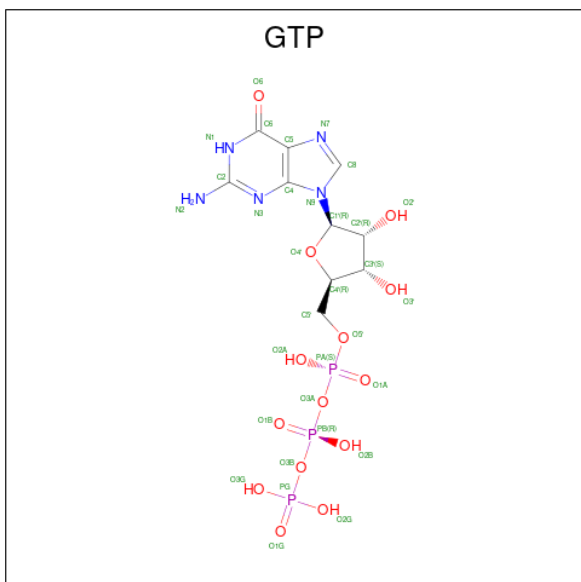
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Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-10	ASP	-	expression tag	UNP K9N7C7
Aj	-9	HIS	-	expression tag	UNP K9N7C7
Aj	-8	ASP	-	expression tag	UNP K9N7C7
Aj	-7	ILE	-	expression tag	UNP K9N7C7
Aj	-6	ASP	-	expression tag	UNP K9N7C7
Aj	-5	TYR	-	expression tag	UNP K9N7C7
Aj	-4	LYS	-	expression tag	UNP K9N7C7
Aj	-3	ASP	-	expression tag	UNP K9N7C7
Aj	-2	ASP	-	expression tag	UNP K9N7C7
Aj	-1	ASP	-	expression tag	UNP K9N7C7
Aj	0	ASP	-	expression tag	UNP K9N7C7
Aj	1	LYS	-	expression tag	UNP K9N7C7

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	Is	1	Total Zn 1 1	0
53	Aa	1	Total Zn 1 1	0
53	Ad	1	Total Zn 1 1	0
53	Af	1	Total Zn 1 1	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

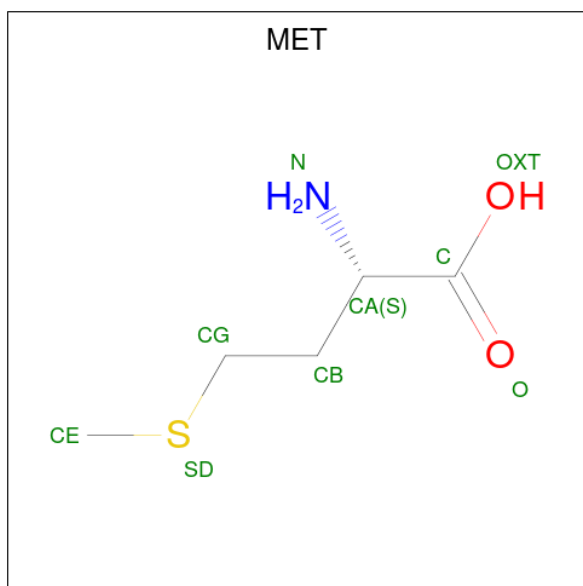


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	It	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	It	1	1	1	0
55	A2	110	110	110	0
55	AG	1	1	1	0
55	AS	2	2	2	0
55	AT	1	1	1	0
55	AX	1	1	1	0

- Molecule 56 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



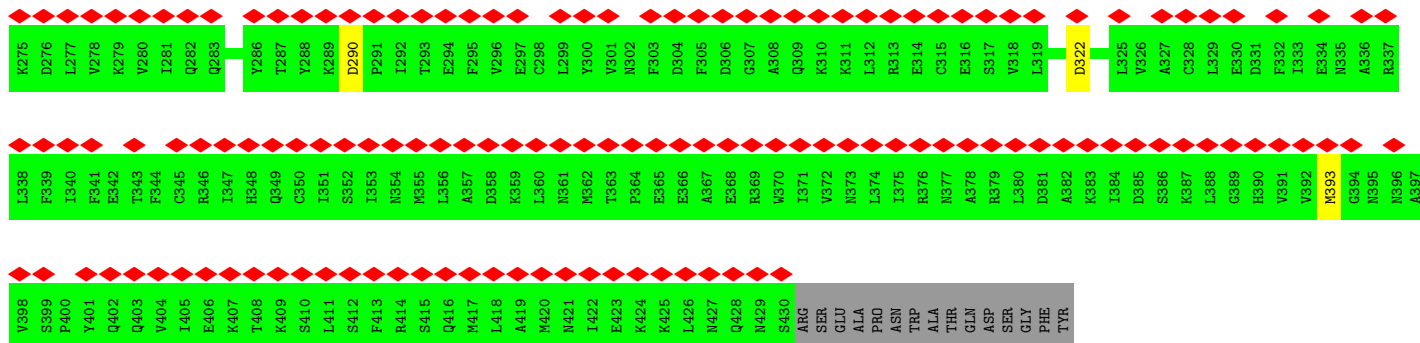
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
56	Iw	1	8	5	1	1	1	0

- Molecule 57 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

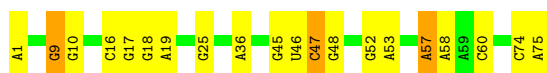
Mol	Chain	Residues	Atoms	AltConf
57	Iw	2	Total X 2 2	0
57	A2	122	Total X 122 122	0
57	AJ	1	Total X 1 1	0
57	AN	1	Total X 1 1	0
57	AO	2	Total X 2 2	0
57	Ad	1	Total X 1 1	0

- Molecule 58 is water.

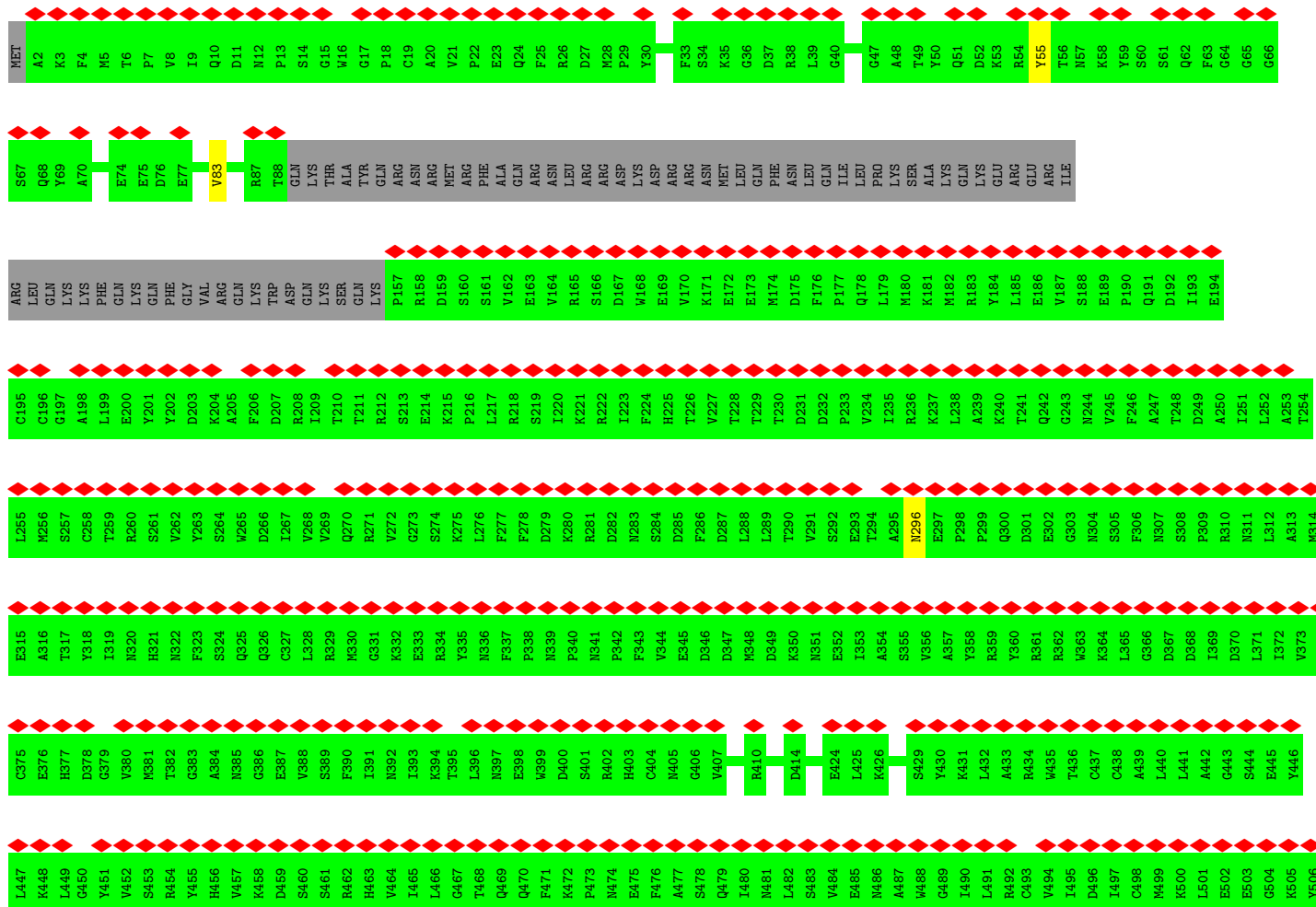
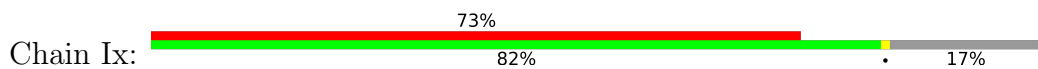
Mol	Chain	Residues	Atoms	AltConf
58	It	2	Total O 2 2	0




• Molecule 14: Met-tRNA_i(Met)

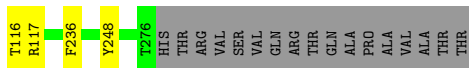
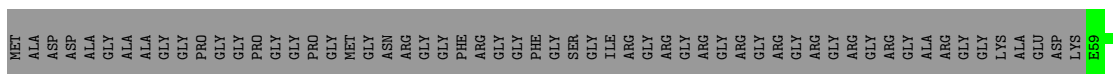


• Molecule 15: Eukaryotic translation initiation factor 3 subunit D



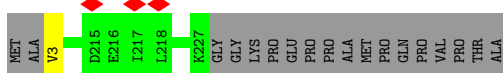
- Molecule 20: 40S ribosomal protein S2

Chain AC:  73% 26%



- Molecule 21: 40S ribosomal protein S3

Chain AD:  92% 7%



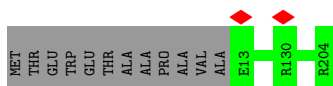
- Molecule 22: 40S ribosomal protein S4, X isoform

Chain AE:  98%



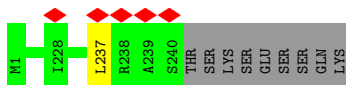
- Molecule 23: 40S ribosomal protein S5

Chain AF:  94% 6%



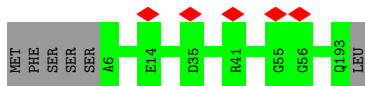
- Molecule 24: 40S ribosomal protein S6

Chain AG:  96%



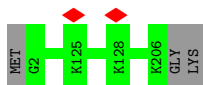
- Molecule 25: 40S ribosomal protein S7

Chain AH:  97%



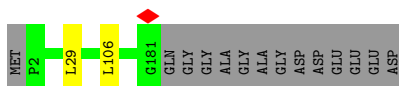
- Molecule 26: 40S ribosomal protein S8

Chain AI:  99%



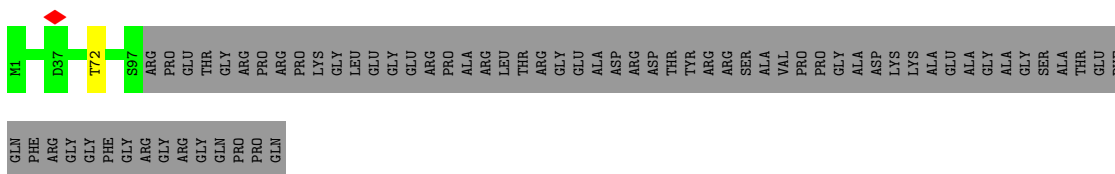
- Molecule 27: 40S ribosomal protein S9

Chain AJ:  92% 7%



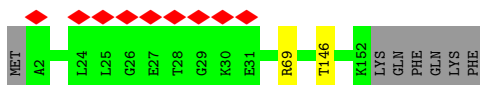
- Molecule 28: 40S ribosomal protein S10

Chain AK:  58% 41%



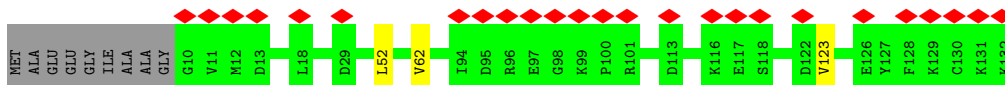
- Molecule 29: 40S ribosomal protein S11

Chain AL:  6% 94%



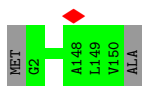
- Molecule 30: 40S ribosomal protein S12

Chain AM:  19% 91% 7%

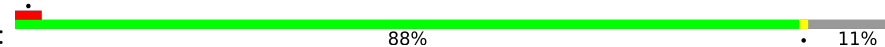


- Molecule 31: 40S ribosomal protein S13

Chain AN:  99%



- Molecule 32: 40S ribosomal protein S14

Chain AO:  88% 11%

Chain AV:  99%



- Molecule 40: 40S ribosomal protein S15a

Chain AW:  98%



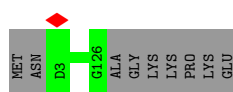
- Molecule 41: 40S ribosomal protein S23

Chain AX:  97%



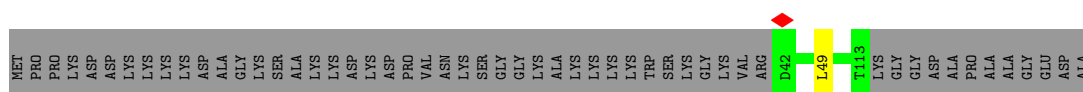
- Molecule 42: 40S ribosomal protein S24

Chain AY:  93%




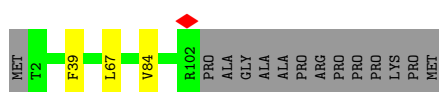
- Molecule 43: 40S ribosomal protein S25

Chain AZ:  57%



- Molecule 44: 40S ribosomal protein S26

Chain Aa:  85%

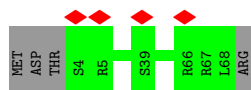


- Molecule 45: 40S ribosomal protein S27

Chain Ab:  96%



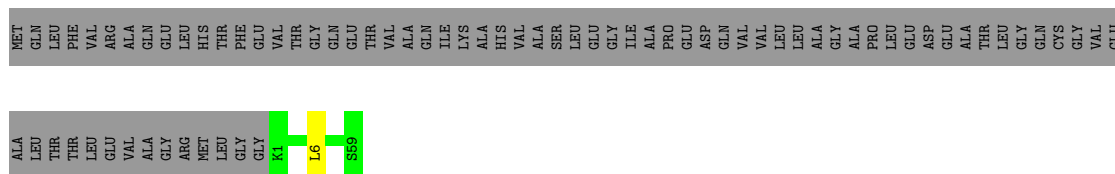
- Molecule 46: 40S ribosomal protein S28



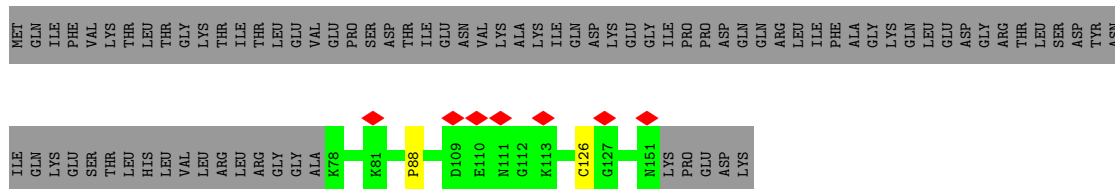
- Molecule 47: 40S ribosomal protein S29



- Molecule 48: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



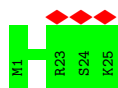
- Molecule 49: Ubiquitin-40S ribosomal protein S27a



- Molecule 50: Receptor of activated protein C kinase 1



- Molecule 51: 60S ribosomal protein L41



- Molecule 52: Host translation inhibitor nsp1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.615	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, OMU, G7M, A2M, PSU, 1MG, NMM, 1MA, 5MC, 6MZ, OMG, B8N, MA6, IAS, SAC, AME, MG, UNX, H2U, OMC, ZN, HY3, 4AC, T6A, 2MG

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	I3	0.23	0/1785	0.43	0/2414
2	I4	0.24	0/2123	0.44	0/2885
3	I5	0.24	0/3187	0.44	0/4299
4	I6	0.23	0/2793	0.41	0/3770
5	I8	0.23	0/2645	0.41	0/3570
6	Io	0.25	0/628	0.52	0/846
7	Ip	0.25	0/808	0.52	1/1085 (0.1%)
8	Iq	0.24	0/845	0.48	0/1128
9	Ir	0.24	0/2400	0.50	0/3234
10	Is	0.25	0/1309	0.48	0/1757
11	It	0.24	0/3502	0.46	0/4739
12	Iu	0.23	0/4919	0.43	0/6647
13	Iv	0.23	0/3626	0.42	0/4902
14	Iw	0.37	1/1601 (0.1%)	0.70	0/2492
15	Ix	0.24	0/3763	0.46	0/5089
16	Iy	0.25	0/5032	0.45	2/6800 (0.0%)
17	A2	0.28	1/40497 (0.0%)	0.70	15/63121 (0.0%)
18	AA	0.26	0/1736	0.47	0/2359
19	AB	0.25	0/1841	0.47	0/2459
20	AC	0.26	0/1737	0.47	0/2346
21	AD	0.25	0/1780	0.49	0/2397
22	AE	0.26	0/2118	0.51	0/2849
23	AF	0.24	0/1539	0.49	0/2071
24	AG	0.24	0/1968	0.53	0/2619
25	AH	0.25	0/1538	0.47	0/2060
26	AI	0.25	0/1711	0.52	0/2282
27	AJ	0.25	0/1524	0.52	0/2035
28	AK	0.24	0/840	0.44	0/1133
29	AL	0.27	0/1250	0.52	0/1673
30	AM	0.23	0/963	0.42	0/1291
31	AN	0.25	0/1226	0.48	0/1649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AO	0.26	0/1014	0.54	0/1358
33	AP	0.25	0/1097	0.49	0/1467
34	AQ	0.26	0/1146	0.51	0/1534
35	AR	0.25	0/1097	0.48	0/1474
36	AS	0.24	0/1209	0.54	0/1620
37	AT	0.24	0/1130	0.46	0/1513
38	AU	0.24	0/813	0.52	0/1092
39	AV	0.26	0/635	0.49	0/850
40	AW	0.26	0/1051	0.50	0/1406
41	AX	0.25	0/1127	0.50	0/1501
42	AY	0.25	0/1031	0.50	0/1370
43	AZ	0.24	0/580	0.47	0/780
44	Aa	0.26	0/828	0.54	0/1109
45	Ab	0.25	0/664	0.46	0/891
46	Ac	0.24	0/514	0.58	0/688
47	Ad	0.26	0/469	0.52	0/623
48	Ae	0.26	0/473	0.53	0/623
49	Af	0.32	0/622	0.50	0/822
50	Ag	0.24	0/2497	0.48	0/3399
51	Ah	0.22	0/240	0.67	0/305
52	Aj	0.25	0/232	0.36	0/311
All	All	0.26	2/121703 (0.0%)	0.57	18/172737 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	1	U	OP3-P	-10.66	1.48	1.61
14	Iw	1	A	OP3-P	-10.60	1.48	1.61

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	356	C	C2-N1-C1'	8.03	127.63	118.80
17	A2	1453	C	C2-N1-C1'	8.02	127.63	118.80
17	A2	356	C	N1-C2-O2	7.84	123.60	118.90
17	A2	1453	C	N1-C2-O2	7.41	123.34	118.90
7	Ip	12	PRO	N-CA-CB	6.66	111.29	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I3	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	I4	266/357 (74%)	261 (98%)	5 (2%)	0	100	100
3	I5	370/564 (66%)	340 (92%)	30 (8%)	0	100	100
4	I6	339/374 (91%)	326 (96%)	12 (4%)	1 (0%)	41	56
5	I8	316/352 (90%)	308 (98%)	8 (2%)	0	100	100
6	Io	75/320 (23%)	71 (95%)	4 (5%)	0	100	100
7	Ip	103/113 (91%)	99 (96%)	3 (3%)	1 (1%)	15	23
8	Iq	99/144 (69%)	97 (98%)	2 (2%)	0	100	100
9	Ir	291/315 (92%)	278 (96%)	12 (4%)	1 (0%)	41	56
10	Is	157/333 (47%)	151 (96%)	6 (4%)	0	100	100
11	It	447/472 (95%)	443 (99%)	4 (1%)	0	100	100
12	Iu	585/1382 (42%)	570 (97%)	15 (3%)	0	100	100
13	Iv	428/445 (96%)	424 (99%)	2 (0%)	2 (0%)	29	43
15	Ix	451/548 (82%)	443 (98%)	8 (2%)	0	100	100
16	Iy	631/913 (69%)	617 (98%)	13 (2%)	1 (0%)	47	64
18	AA	214/295 (72%)	210 (98%)	4 (2%)	0	100	100
19	AB	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
20	AC	217/293 (74%)	215 (99%)	2 (1%)	0	100	100
21	AD	223/243 (92%)	223 (100%)	0	0	100	100
22	AE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
23	AF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AG	238/249 (96%)	238 (100%)	0	0	100	100
25	AH	186/194 (96%)	183 (98%)	3 (2%)	0	100	100
26	AI	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
27	AJ	178/194 (92%)	176 (99%)	2 (1%)	0	100	100
28	AK	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
29	AL	149/158 (94%)	148 (99%)	1 (1%)	0	100	100
30	AM	121/132 (92%)	114 (94%)	7 (6%)	0	100	100
31	AN	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
32	AO	131/151 (87%)	130 (99%)	1 (1%)	0	100	100
33	AP	129/145 (89%)	128 (99%)	1 (1%)	0	100	100
34	AQ	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
35	AR	132/135 (98%)	132 (100%)	0	0	100	100
36	AS	143/152 (94%)	139 (97%)	4 (3%)	0	100	100
37	AT	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
38	AU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
39	AV	81/83 (98%)	81 (100%)	0	0	100	100
40	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
41	AX	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
42	AY	122/133 (92%)	122 (100%)	0	0	100	100
43	AZ	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
44	Aa	99/115 (86%)	99 (100%)	0	0	100	100
45	Ab	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
46	Ac	63/69 (91%)	63 (100%)	0	0	100	100
47	Ad	53/56 (95%)	53 (100%)	0	0	100	100
48	Ae	57/133 (43%)	56 (98%)	1 (2%)	0	100	100
49	Af	72/156 (46%)	66 (92%)	5 (7%)	1 (1%)	11	16
50	Ag	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
51	Ah	23/25 (92%)	23 (100%)	0	0	100	100
52	Aj	27/216 (12%)	27 (100%)	0	0	100	100
All	All	9656/12641 (76%)	9431 (98%)	218 (2%)	7 (0%)	54	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Ip	12	PRO
9	Ir	202	TYR
13	Iv	265	LYS
13	Iv	264	ASN
16	Iy	301	TRP

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	I3	192/193 (100%)	183 (95%)	9 (5%)	26	40
2	I4	237/289 (82%)	229 (97%)	8 (3%)	37	53
3	I5	342/515 (66%)	323 (94%)	19 (6%)	21	33
4	I6	308/335 (92%)	299 (97%)	9 (3%)	42	60
5	I8	290/310 (94%)	283 (98%)	7 (2%)	49	67
6	Io	64/277 (23%)	61 (95%)	3 (5%)	26	40
7	Ip	77/96 (80%)	75 (97%)	2 (3%)	46	64
8	Iq	88/123 (72%)	83 (94%)	5 (6%)	20	31
9	Ir	264/280 (94%)	248 (94%)	16 (6%)	18	29
10	Is	144/304 (47%)	137 (95%)	7 (5%)	25	38
11	It	384/397 (97%)	378 (98%)	6 (2%)	62	78
12	Iu	540/1259 (43%)	528 (98%)	12 (2%)	52	70
13	Iv	394/406 (97%)	390 (99%)	4 (1%)	76	86
15	Ix	406/494 (82%)	403 (99%)	3 (1%)	84	91
16	Iy	516/811 (64%)	509 (99%)	7 (1%)	67	81
18	AA	179/242 (74%)	177 (99%)	2 (1%)	73	85
19	AB	203/231 (88%)	202 (100%)	1 (0%)	88	94
20	AC	185/225 (82%)	181 (98%)	4 (2%)	52	70
21	AD	189/202 (94%)	188 (100%)	1 (0%)	88	94
22	AE	224/225 (100%)	221 (99%)	3 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AF	162/170 (95%)	162 (100%)	0	100	100
24	AG	209/218 (96%)	208 (100%)	1 (0%)	88	94
25	AH	168/174 (97%)	168 (100%)	0	100	100
26	AI	178/180 (99%)	178 (100%)	0	100	100
27	AJ	160/168 (95%)	158 (99%)	2 (1%)	69	82
28	AK	88/136 (65%)	87 (99%)	1 (1%)	73	85
29	AL	135/142 (95%)	133 (98%)	2 (2%)	65	80
30	AM	104/108 (96%)	101 (97%)	3 (3%)	42	60
31	AN	130/131 (99%)	130 (100%)	0	100	100
32	AO	104/118 (88%)	103 (99%)	1 (1%)	76	86
33	AP	117/130 (90%)	117 (100%)	0	100	100
34	AQ	117/121 (97%)	115 (98%)	2 (2%)	60	77
35	AR	121/122 (99%)	121 (100%)	0	100	100
36	AS	125/131 (95%)	123 (98%)	2 (2%)	62	78
37	AT	113/114 (99%)	112 (99%)	1 (1%)	78	87
38	AU	93/107 (87%)	92 (99%)	1 (1%)	73	85
39	AV	66/66 (100%)	66 (100%)	0	100	100
40	AW	112/113 (99%)	111 (99%)	1 (1%)	78	87
41	AX	114/114 (100%)	112 (98%)	2 (2%)	59	75
42	AY	108/115 (94%)	108 (100%)	0	100	100
43	AZ	64/103 (62%)	63 (98%)	1 (2%)	62	78
44	Aa	88/98 (90%)	85 (97%)	3 (3%)	37	53
45	Ab	75/76 (99%)	73 (97%)	2 (3%)	44	63
46	Ac	58/62 (94%)	58 (100%)	0	100	100
47	Ad	48/49 (98%)	48 (100%)	0	100	100
48	Ae	48/104 (46%)	47 (98%)	1 (2%)	53	72
49	Af	67/140 (48%)	66 (98%)	1 (2%)	65	80
50	Ag	272/275 (99%)	267 (98%)	5 (2%)	59	75
51	Ah	24/24 (100%)	24 (100%)	0	100	100
52	Aj	24/182 (13%)	24 (100%)	0	100	100
All	All	8518/11005 (77%)	8358 (98%)	160 (2%)	59	74

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Iy	745	LYS
38	AU	68	THR
19	AB	228	LEU
27	AJ	106	LEU
44	Aa	84	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
15	Ix	486	ASN
22	AE	50	ASN
16	Iy	415	ASN
16	Iy	713	GLN
23	AF	83	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	Iw	74/75 (98%)	14 (18%)	0
17	A2	1768/1869 (94%)	230 (13%)	0
All	All	1842/1944 (94%)	244 (13%)	0

5 of 244 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	Iw	9	1MG
14	Iw	16	C
14	Iw	17	G
14	Iw	18	G
14	Iw	19	A

There are no RNA pucker outliers to report.

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

100 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
17	PSU	A2	609	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	OMU	A2	116	17	19,22,23	1.19	3 (15%)	26,31,34	1.69	4 (15%)
17	OMG	A2	644	17	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
17	PSU	A2	1445	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
32	IAS	AO	138	32	6,7,8	0.96	0	6,8,10	1.33	1 (16%)
14	2MG	Iw	10	14	18,26,27	0.89	1 (5%)	16,38,41	1.13	2 (12%)
17	PSU	A2	36	17	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
17	OMG	A2	601	17	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
17	PSU	A2	572	17	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
17	OMC	A2	1703	17	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
14	1MA	Iw	57	14	16,25,26	1.62	2 (12%)	18,37,40	1.24	3 (16%)
17	A2M	A2	166	17	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
17	OMC	A2	797	17	19,22,23	0.81	0	26,31,34	0.84	0
14	H2U	Iw	46	14	18,21,22	1.00	2 (11%)	21,30,33	1.72	1 (4%)
17	OMU	A2	1442	55,17	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
17	PSU	A2	1046	17	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
17	OMU	A2	1326	55,17	19,22,23	1.19	3 (15%)	26,31,34	1.72	5 (19%)
17	PSU	A2	1692	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	801	17	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
17	OMU	A2	354	17	19,22,23	1.25	3 (15%)	26,31,34	1.75	4 (15%)
17	PSU	A2	1045	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
17	OMC	A2	517	17	19,22,23	0.81	0	26,31,34	0.83	0
17	PSU	A2	822	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
17	PSU	A2	109	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	1347	17	18,21,22	1.34	2 (11%)	22,30,33	1.95	4 (18%)
17	PSU	A2	34	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1244	17	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
17	A2M	A2	1031	17	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
17	OMG	A2	1447	17	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
17	PSU	A2	686	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	PSU	A2	866	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	OMG	A2	1490	55,17	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
17	OMG	A2	436	17	18,26,27	0.94	1 (5%)	19,38,41	1.13	2 (10%)
17	OMU	A2	1804	17	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
17	OMC	A2	1391	17	19,22,23	0.82	0	26,31,34	0.82	0
17	4AC	A2	1337	17	21,24,25	1.09	2 (9%)	29,34,37	1.00	2 (6%)
17	6MZ	A2	1832	55,17	18,25,26	0.89	1 (5%)	16,36,39	1.75	4 (25%)
17	B8N	A2	1248	17	24,29,30	1.28	3 (12%)	29,42,45	1.28	3 (10%)
17	4AC	A2	1842	17	21,24,25	1.10	2 (9%)	29,34,37	1.17	2 (6%)
17	A2M	A2	1678	17	18,25,26	0.98	1 (5%)	18,36,39	1.24	2 (11%)
17	PSU	A2	814	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	PSU	A2	1136	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
41	HY3	AX	62	41	6,8,9	2.17	1 (16%)	5,10,12	1.13	1 (20%)
17	PSU	A2	218	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1056	17	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	1625	17	18,21,22	1.39	2 (11%)	22,30,33	1.88	3 (13%)
17	OMU	A2	172	17	19,22,23	1.19	2 (10%)	26,31,34	1.73	5 (19%)
17	PSU	A2	105	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	OMU	A2	121	17	19,22,23	1.22	3 (15%)	26,31,34	1.73	5 (19%)
17	A2M	A2	576	17	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
17	PSU	A2	93	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	651	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	OMU	A2	627	17	19,22,23	1.18	2 (10%)	26,31,34	1.72	5 (19%)
17	A2M	A2	668	55,17	18,25,26	0.93	1 (5%)	18,36,39	1.28	2 (11%)
14	5MC	Iw	47	14	18,22,23	0.61	0	26,32,35	0.82	1 (3%)
17	PSU	A2	863	17	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	1177	17	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	296	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	A2M	A2	159	17	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
17	PSU	A2	1004	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1367	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
17	OMU	A2	1288	17	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
37	NMM	AT	67	37	9,11,12	1.63	1 (11%)	6,12,14	3.45	2 (33%)
17	PSU	A2	649	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	119	17	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
17	OMG	A2	683	17	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	A2M	A2	590	17	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
17	PSU	A2	1232	17	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
17	OMU	A2	799	17	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
14	G7M	Iw	45	14	20,26,27	2.96	7 (35%)	17,39,42	1.04	1 (5%)
17	PSU	A2	1174	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	406	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
14	1MG	Iw	9	14	18,26,27	0.79	0	19,39,42	1.10	2 (10%)
14	T6A	Iw	36	14	27,34,35	0.97	2 (7%)	29,49,52	1.64	5 (17%)
17	OMU	A2	428	17	19,22,23	1.20	3 (15%)	26,31,34	1.72	5 (19%)
17	PSU	A2	681	17	18,21,22	1.37	3 (16%)	22,30,33	1.90	3 (13%)
17	A2M	A2	468	17	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
17	MA6	A2	1850	17	18,26,27	1.10	2 (11%)	19,38,41	1.95	3 (15%)
18	SAC	AA	2	18	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
17	PSU	A2	966	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	MA6	A2	1851	17	18,26,27	1.10	2 (11%)	19,38,41	1.93	3 (15%)
17	A2M	A2	1383	17	18,25,26	1.01	1 (5%)	18,36,39	1.29	2 (11%)
17	A2M	A2	512	17	18,25,26	0.98	1 (5%)	18,36,39	1.20	2 (11%)
17	A2M	A2	484	17	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
17	OMC	A2	174	55,17	19,22,23	0.82	0	26,31,34	0.79	0
17	A2M	A2	99	55,17	18,25,26	1.06	1 (5%)	18,36,39	1.23	2 (11%)
17	OMG	A2	1328	17	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
17	PSU	A2	1081	17	18,21,22	1.39	3 (16%)	22,30,33	1.86	3 (13%)
17	G7M	A2	1639	14,17	20,26,27	2.93	7 (35%)	17,39,42	0.97	1 (5%)
17	PSU	A2	815	17	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
17	OMC	A2	1272	17	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
17	PSU	A2	1643	55,17	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
36	SAC	AS	2	36	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
17	PSU	A2	1238	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
14	2MG	Iw	25	14	18,26,27	0.88	1 (5%)	16,38,41	1.17	2 (12%)
17	A2M	A2	27	55,17	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
39	AME	AV	1	39	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
17	OMC	A2	462	17	19,22,23	0.82	0	26,31,34	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PSU	A2	609	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	116	17	-	1/9/27/28	0/2/2/2
17	OMG	A2	644	17	-	4/5/27/28	0/3/3/3
17	PSU	A2	1445	17	-	0/7/25/26	0/2/2/2
32	IAS	AO	138	32	-	2/7/7/8	-
14	2MG	Iw	10	14	-	0/5/27/28	0/3/3/3
17	PSU	A2	36	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	601	17	-	0/5/27/28	0/3/3/3
17	PSU	A2	572	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1703	17	-	1/9/27/28	0/2/2/2
14	1MA	Iw	57	14	-	0/3/25/26	0/3/3/3
17	A2M	A2	166	17	-	0/5/27/28	0/3/3/3
17	OMC	A2	797	17	-	1/9/27/28	0/2/2/2
14	H2U	Iw	46	14	-	1/7/38/39	0/2/2/2
17	OMU	A2	1442	55,17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1046	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	1326	55,17	-	0/9/27/28	0/2/2/2
17	PSU	A2	1692	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	801	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	354	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1045	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	517	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	822	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	109	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1347	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	34	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1244	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	1031	17	-	1/5/27/28	0/3/3/3
17	OMG	A2	1447	17	-	2/5/27/28	0/3/3/3
17	PSU	A2	686	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	866	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	1490	55,17	-	0/5/27/28	0/3/3/3
17	OMG	A2	436	17	-	1/5/27/28	0/3/3/3
17	OMU	A2	1804	17	-	0/9/27/28	0/2/2/2
17	OMC	A2	1391	17	-	0/9/27/28	0/2/2/2
17	4AC	A2	1337	17	-	2/11/29/30	0/2/2/2
17	6MZ	A2	1832	55,17	-	0/5/27/28	0/3/3/3
17	B8N	A2	1248	17	-	4/16/34/35	0/2/2/2
17	4AC	A2	1842	17	-	4/11/29/30	0/2/2/2
17	A2M	A2	1678	17	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PSU	A2	814	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1136	17	-	0/7/25/26	0/2/2/2
41	HY3	AX	62	41	-	0/1/12/14	0/1/1/1
17	PSU	A2	218	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1056	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1625	17	-	2/7/25/26	0/2/2/2
17	OMU	A2	172	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	105	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	121	17	-	0/9/27/28	0/2/2/2
17	A2M	A2	576	17	-	2/5/27/28	0/3/3/3
17	PSU	A2	93	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	651	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	627	17	-	1/9/27/28	0/2/2/2
17	A2M	A2	668	55,17	-	2/5/27/28	0/3/3/3
14	5MC	Iw	47	14	-	3/7/25/26	0/2/2/2
17	PSU	A2	863	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1177	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	296	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	159	17	-	1/5/27/28	0/3/3/3
17	PSU	A2	1004	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1367	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	1288	17	-	1/9/27/28	0/2/2/2
37	NMM	AT	67	37	-	1/9/11/13	-
17	PSU	A2	649	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	119	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	683	17	-	3/5/27/28	0/3/3/3
17	A2M	A2	590	17	-	0/5/27/28	0/3/3/3
17	PSU	A2	1232	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	799	17	-	3/9/27/28	0/2/2/2
14	G7M	Iw	45	14	-	0/3/25/26	0/3/3/3
17	PSU	A2	1174	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	406	17	-	0/7/25/26	0/2/2/2
14	1MG	Iw	9	14	-	2/3/25/26	0/3/3/3
14	T6A	Iw	36	14	-	4/19/41/42	0/3/3/3
17	OMU	A2	428	17	-	4/9/27/28	0/2/2/2
17	PSU	A2	681	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	468	17	-	1/5/27/28	0/3/3/3
17	MA6	A2	1850	17	-	0/7/29/30	0/3/3/3
18	SAC	AA	2	18	-	2/7/8/10	-
17	PSU	A2	966	17	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MA6	A2	1851	17	-	2/7/29/30	0/3/3/3
17	A2M	A2	1383	17	-	0/5/27/28	0/3/3/3
17	A2M	A2	512	17	-	3/5/27/28	0/3/3/3
17	A2M	A2	484	17	-	0/5/27/28	0/3/3/3
17	OMC	A2	174	55,17	-	0/9/27/28	0/2/2/2
17	A2M	A2	99	55,17	-	2/5/27/28	0/3/3/3
17	OMG	A2	1328	17	-	1/5/27/28	0/3/3/3
17	PSU	A2	1081	17	-	0/7/25/26	0/2/2/2
17	G7M	A2	1639	14,17	-	0/3/25/26	0/3/3/3
17	PSU	A2	815	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1272	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	1643	55,17	-	0/7/25/26	0/2/2/2
36	SAC	AS	2	36	-	0/7/8/10	-
17	PSU	A2	1238	17	-	0/7/25/26	0/2/2/2
14	2MG	Iw	25	14	-	0/5/27/28	0/3/3/3
17	A2M	A2	27	55,17	-	0/5/27/28	0/3/3/3
39	AME	AV	1	39	-	2/9/10/12	-
17	OMC	A2	462	17	-	0/9/27/28	0/2/2/2

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Iw	45	G7M	C5-C4	7.34	1.53	1.39
17	A2	1639	G7M	O6-C6	7.23	1.38	1.23
17	A2	1639	G7M	C5-C4	7.22	1.53	1.39
14	Iw	45	G7M	O6-C6	7.19	1.37	1.23
14	Iw	57	1MA	C2-N3	5.05	1.35	1.29

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	AT	67	NMM	NE-CZ-NH2	-7.19	112.89	119.48
14	Iw	46	H2U	C4-N3-C2	-6.91	120.06	125.79
17	A2	1347	PSU	N1-C2-N3	6.18	122.13	115.13
17	A2	1232	PSU	N1-C2-N3	6.14	122.09	115.13
17	A2	651	PSU	N1-C2-N3	6.14	122.09	115.13

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	AT	67	NMM	O-C-CA-CB
14	Iw	9	1MG	O4'-C4'-C5'-O5'
14	Iw	36	T6A	O10-C10-N6-C6
14	Iw	36	T6A	N11-C10-N6-C6
14	Iw	36	T6A	N6-C10-N11-C12

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 251 ligands modelled in this entry, 120 are monoatomic and 129 are unknown - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	MET	Iw	101	14	6,7,8	0.48	0	2,7,9	0.24	0
54	GTP	It	1000	55	26,34,34	0.95	2 (7%)	32,54,54	0.89	2 (6%)

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
56	MET	Iw	101	14	-	0/5/6/8	-
54	GTP	It	1000	55	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	It	1000	GTP	C5-C6	-2.60	1.42	1.47
54	It	1000	GTP	C8-N7	-2.05	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	It	1000	GTP	O4'-C1'-C2'	-2.79	102.85	106.93
54	It	1000	GTP	O6-C6-C5	2.00	128.28	124.37

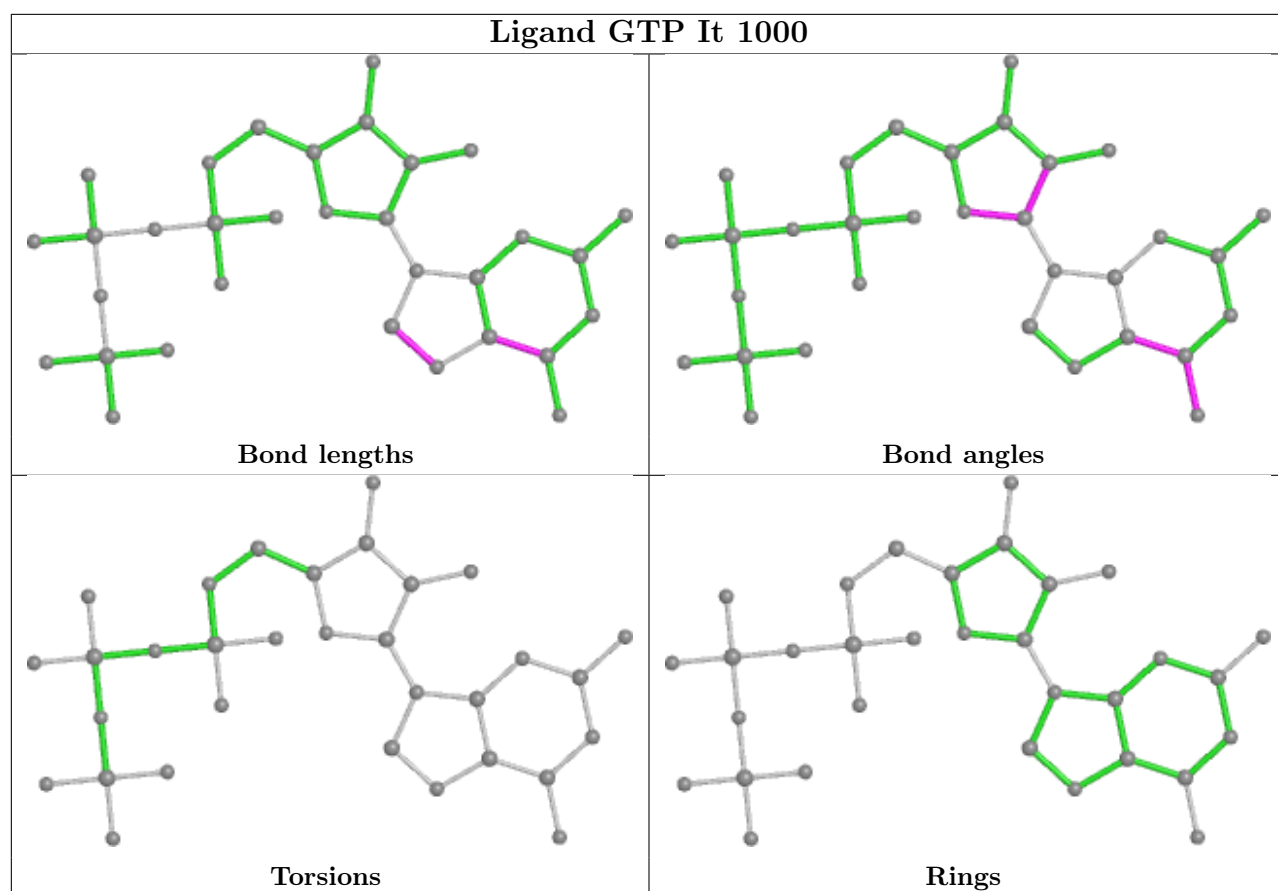
There are no chirality outliers.

There are no torsion outliers.

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.

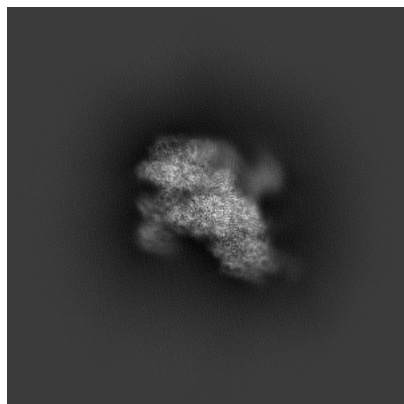
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17805. These allow visual inspection of the internal detail of the map and identification of artifacts.

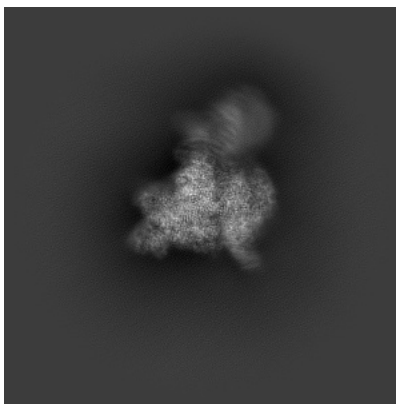
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

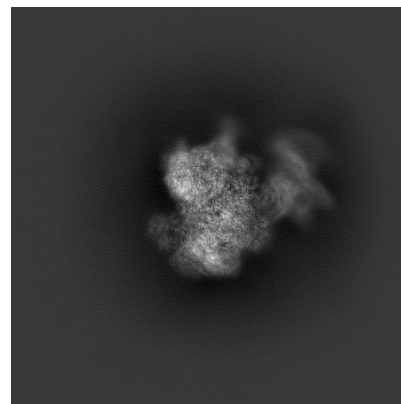
6.1.1 Primary map



X

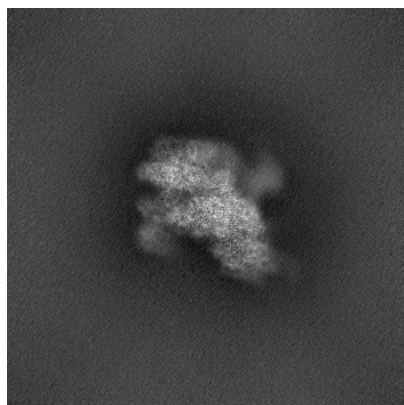


Y

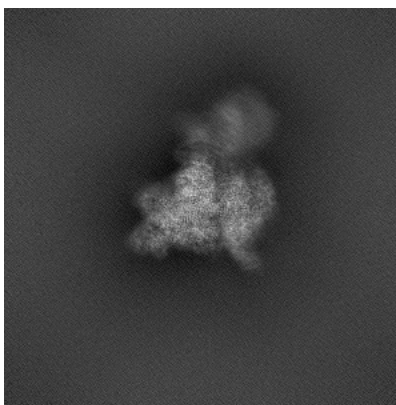


Z

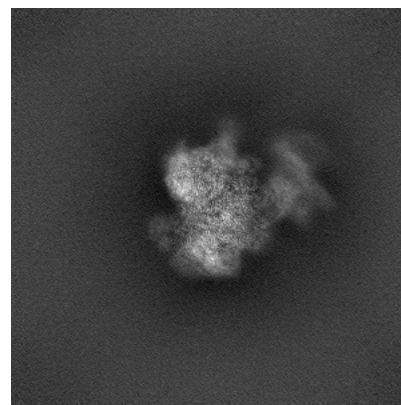
6.1.2 Raw map



X



Y

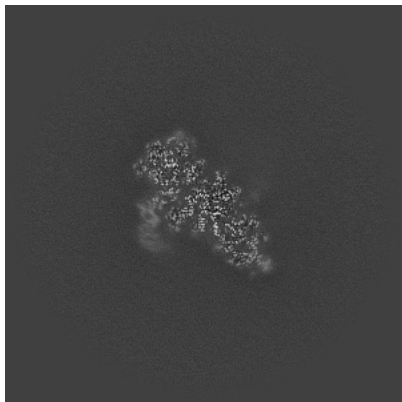


Z

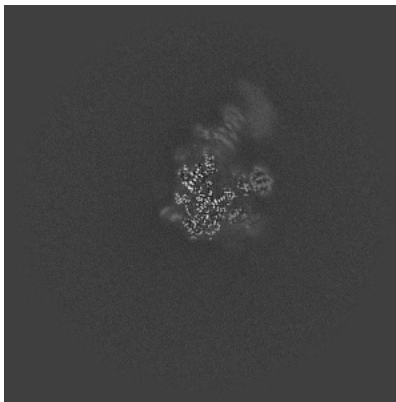
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

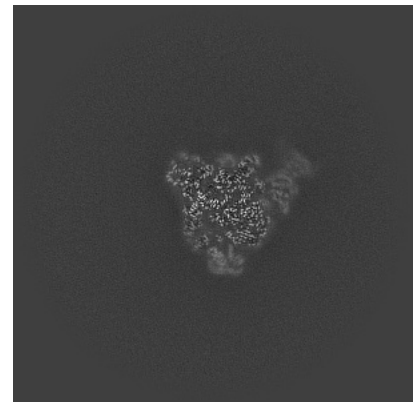
6.2.1 Primary map



X Index: 280

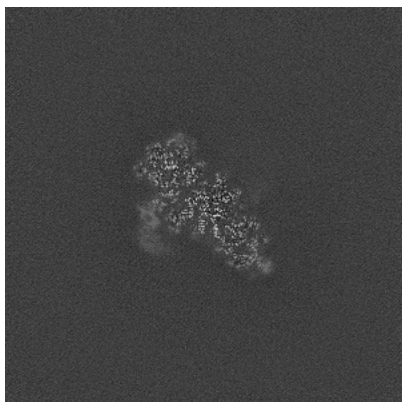


Y Index: 280

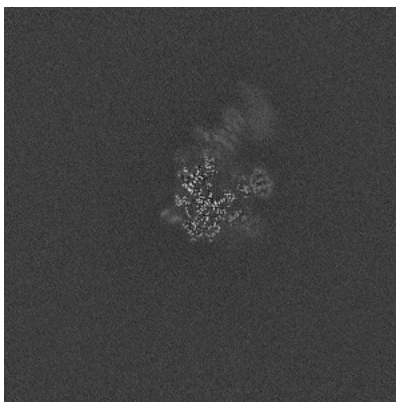


Z Index: 280

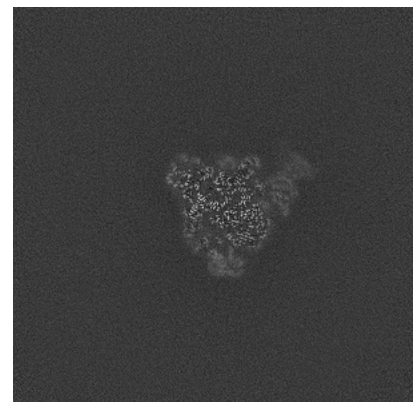
6.2.2 Raw map



X Index: 280



Y Index: 280

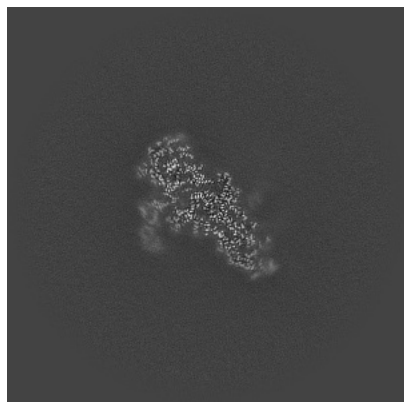


Z Index: 280

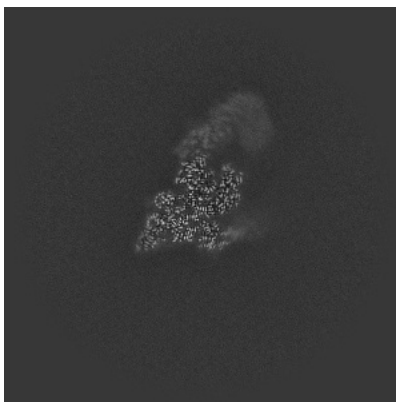
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

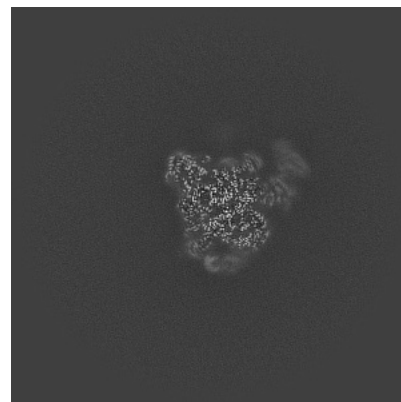
6.3.1 Primary map



X Index: 284

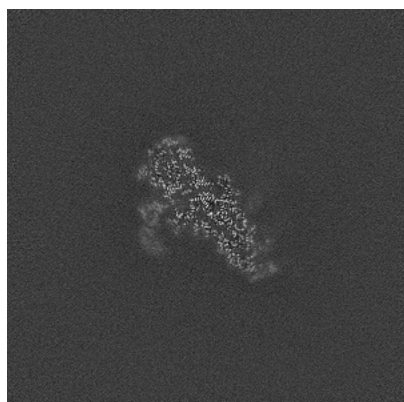


Y Index: 308

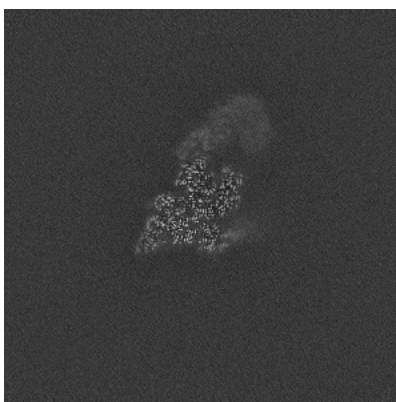


Z Index: 268

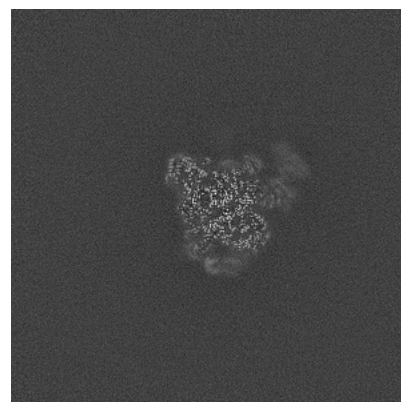
6.3.2 Raw map



X Index: 285



Y Index: 308

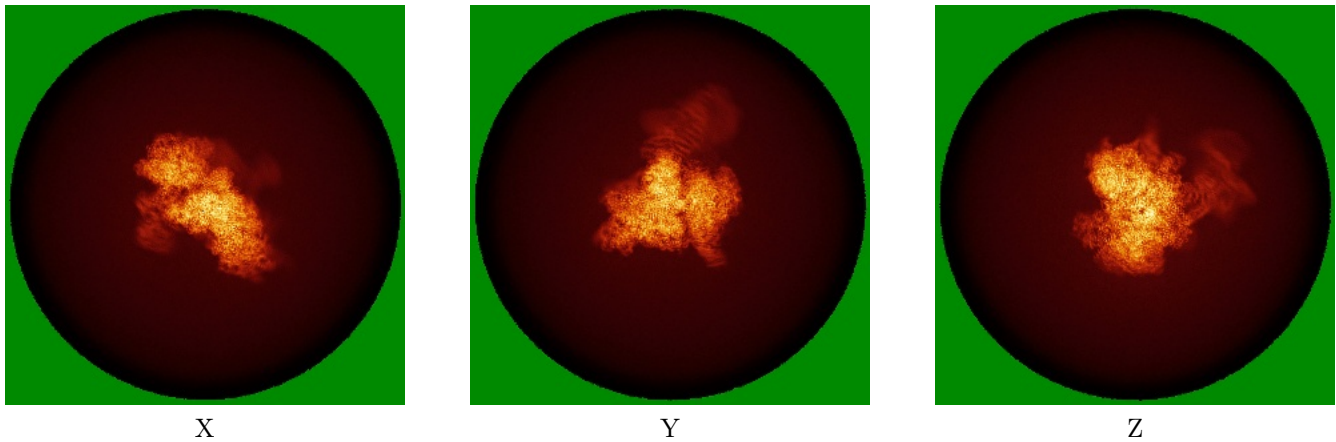


Z Index: 268

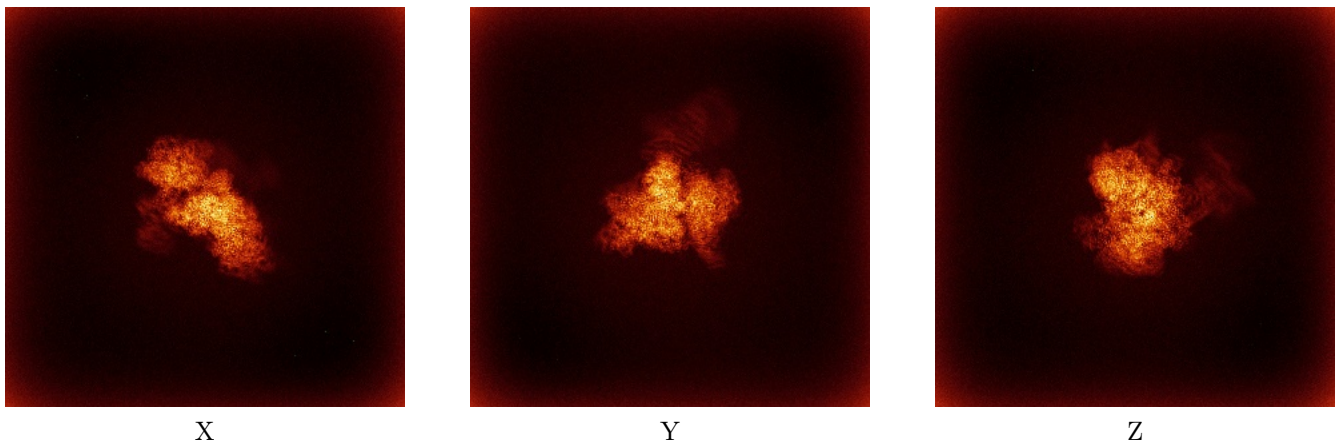
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



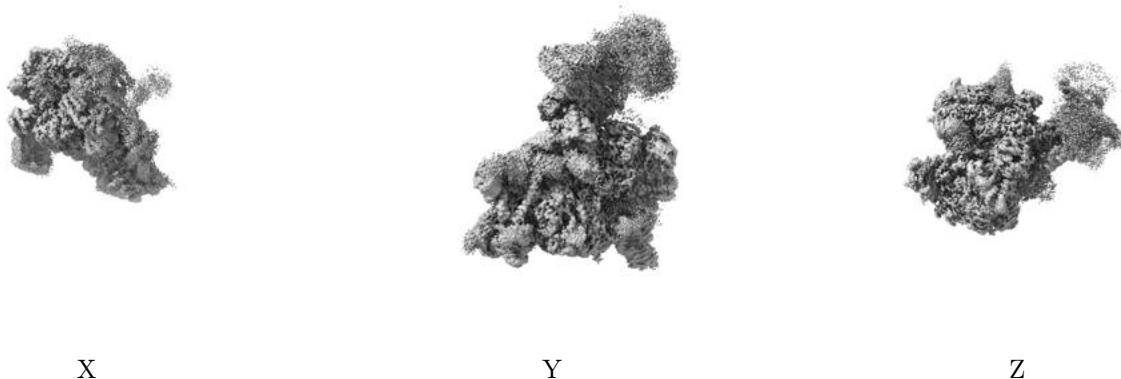
6.4.2 Raw map



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

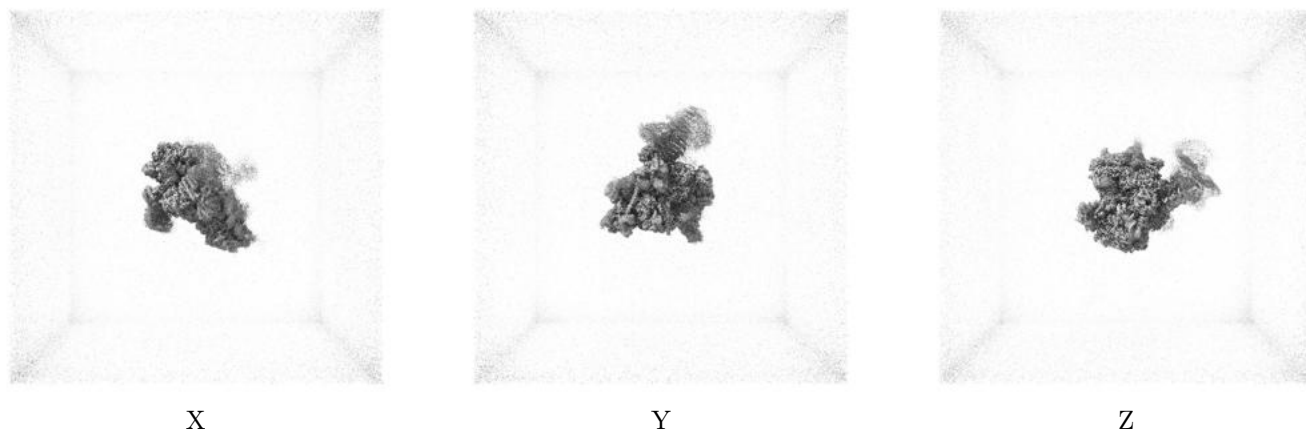
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

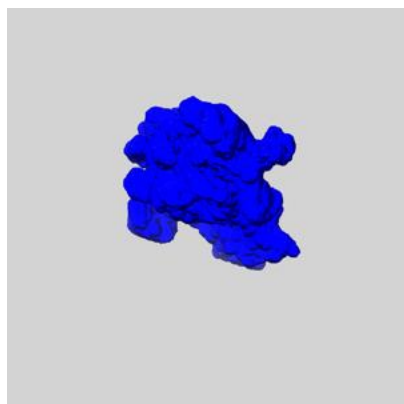
6.6 Mask visualisation [i](#)

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

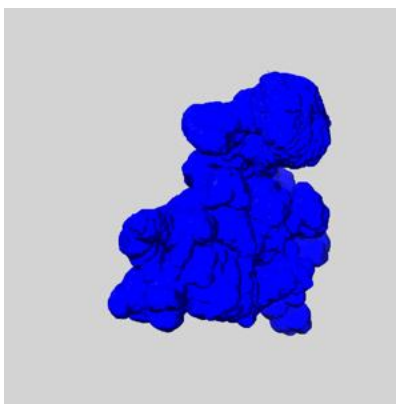
A mask typically either:

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

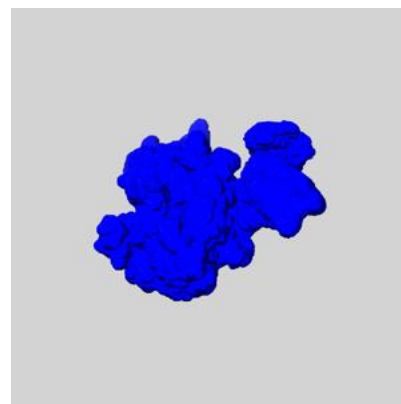
6.6.1 emd_17805_msk_1.map [i](#)



X

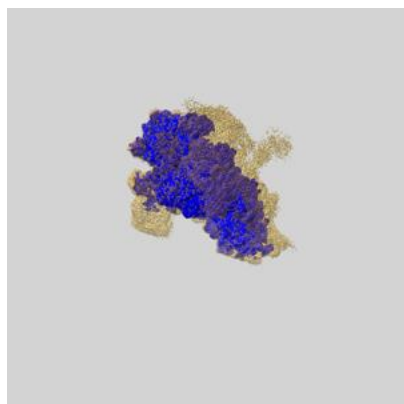


Y

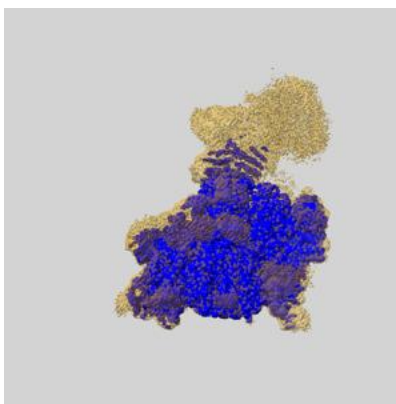


Z

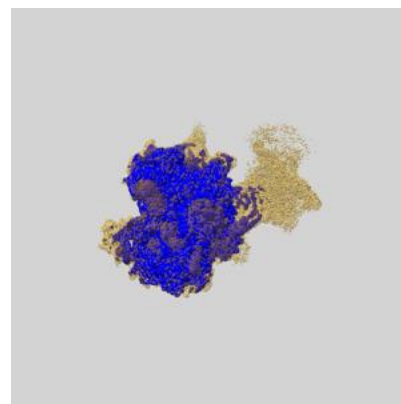
6.6.2 emd_17805_msk_2.map [i](#)



X



Y

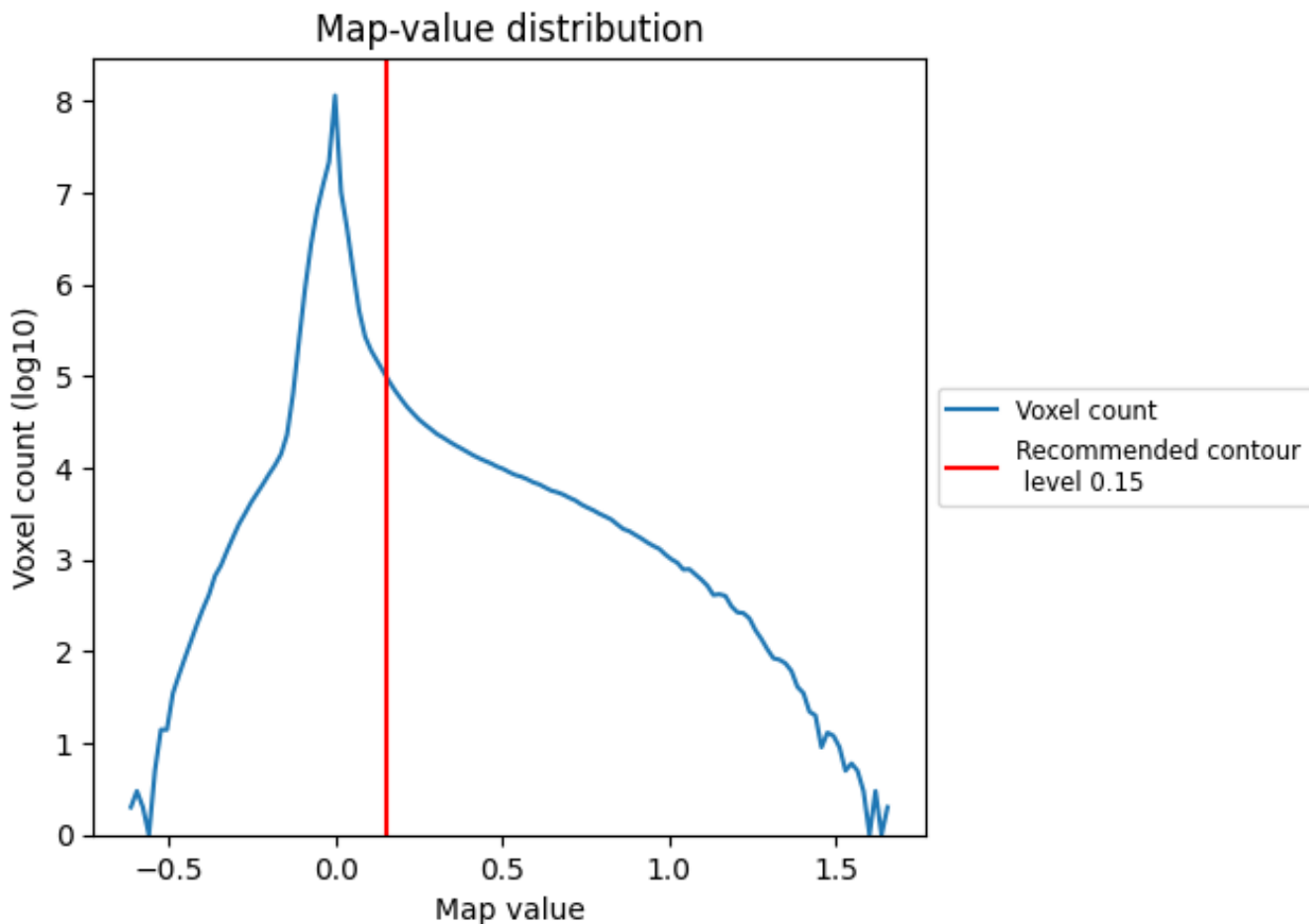


Z

7 Map analysis [i](#)

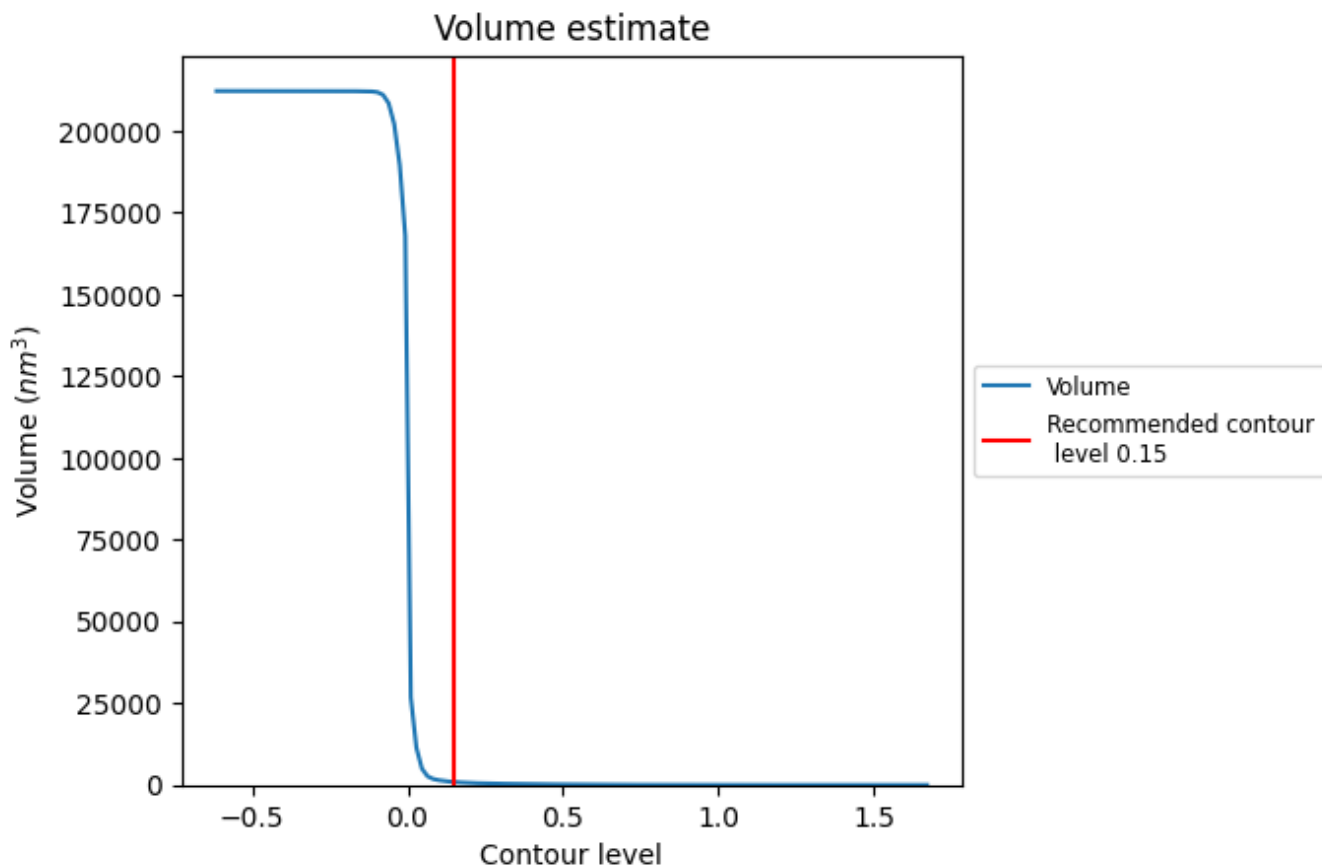
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

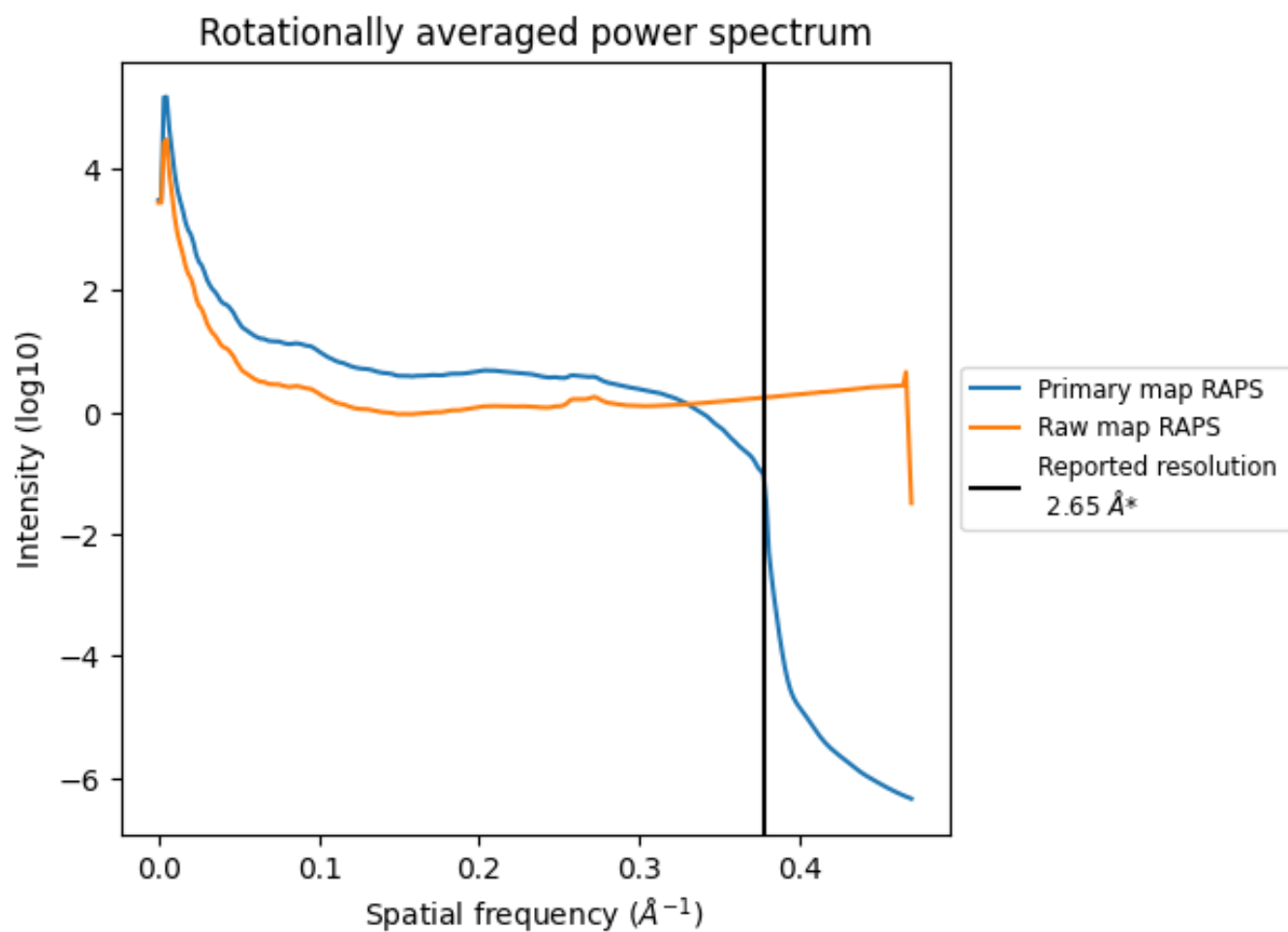
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 907 nm³; this corresponds to an approximate mass of 819 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

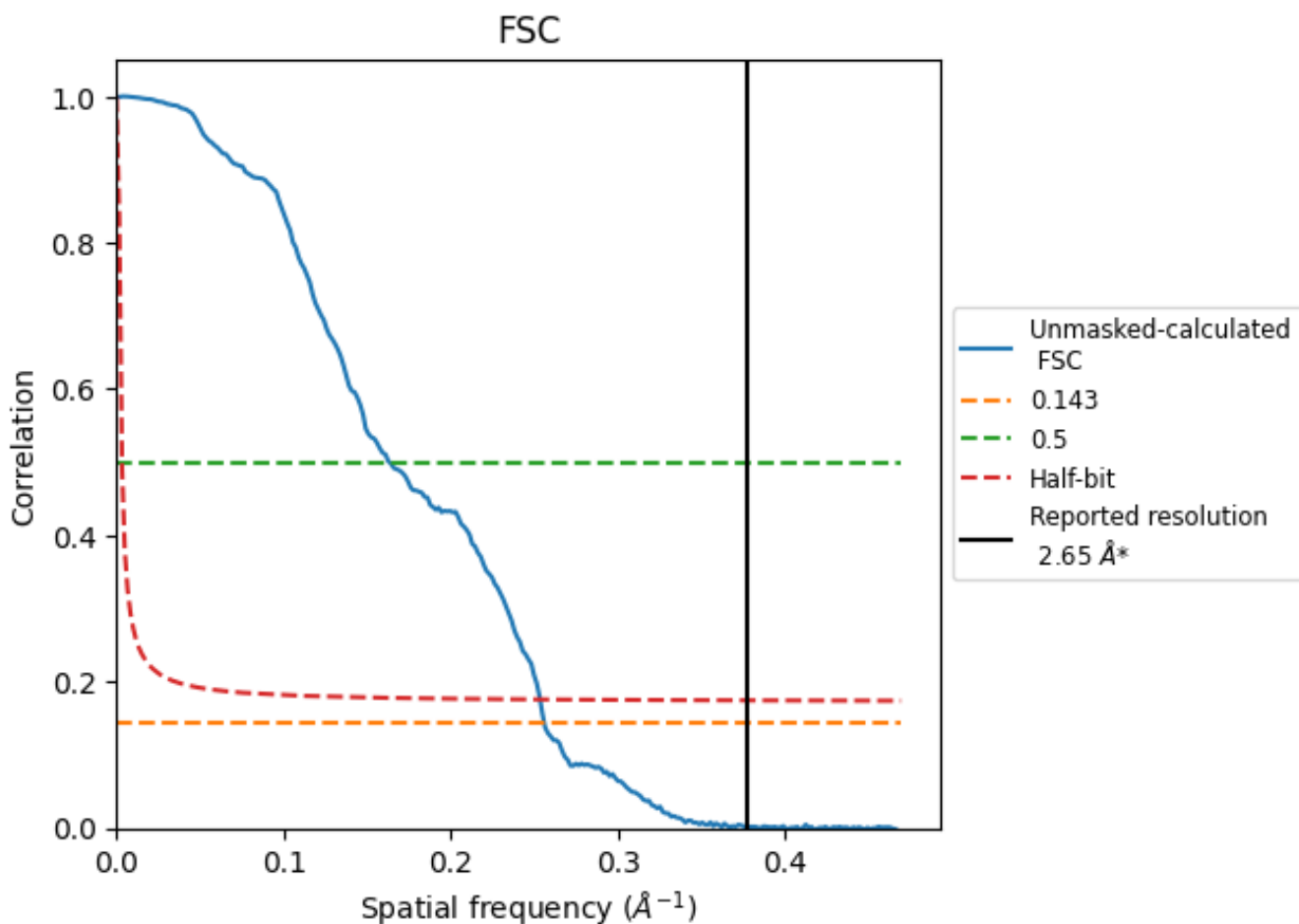


*Reported resolution corresponds to spatial frequency of 0.377 \AA^{-1}

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 0.377 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.12	3.95

*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 3.91 differs from the reported value 2.65 by more than 10 %

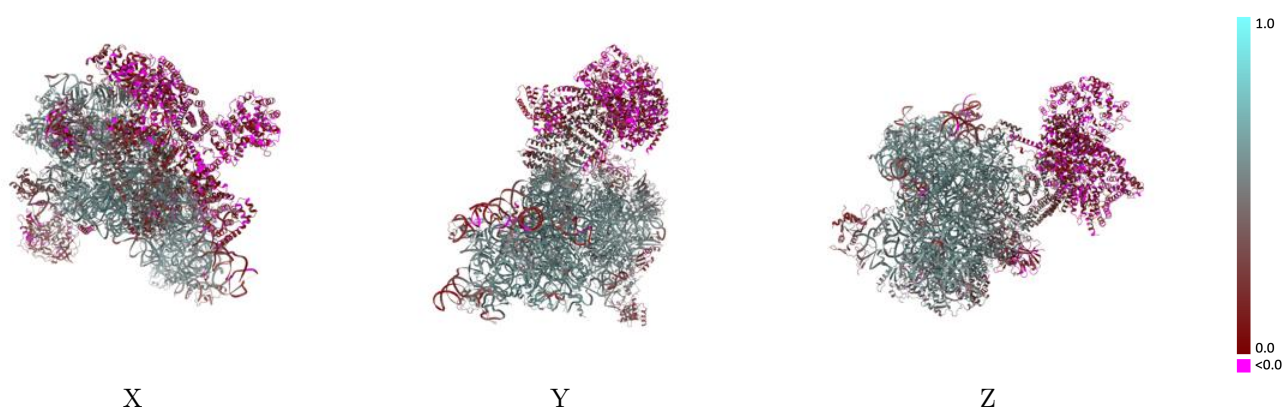
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17805 and PDB model 8PPL. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

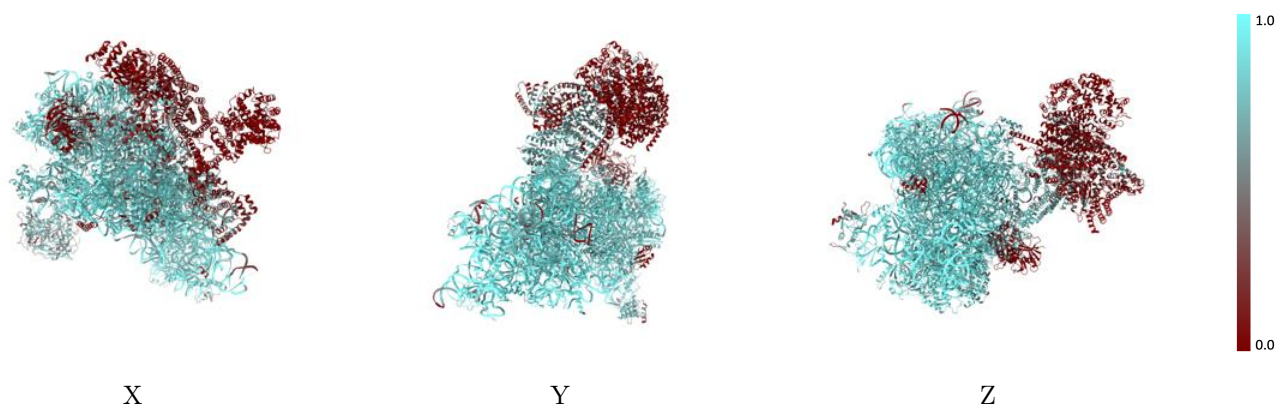
This section was not generated.

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



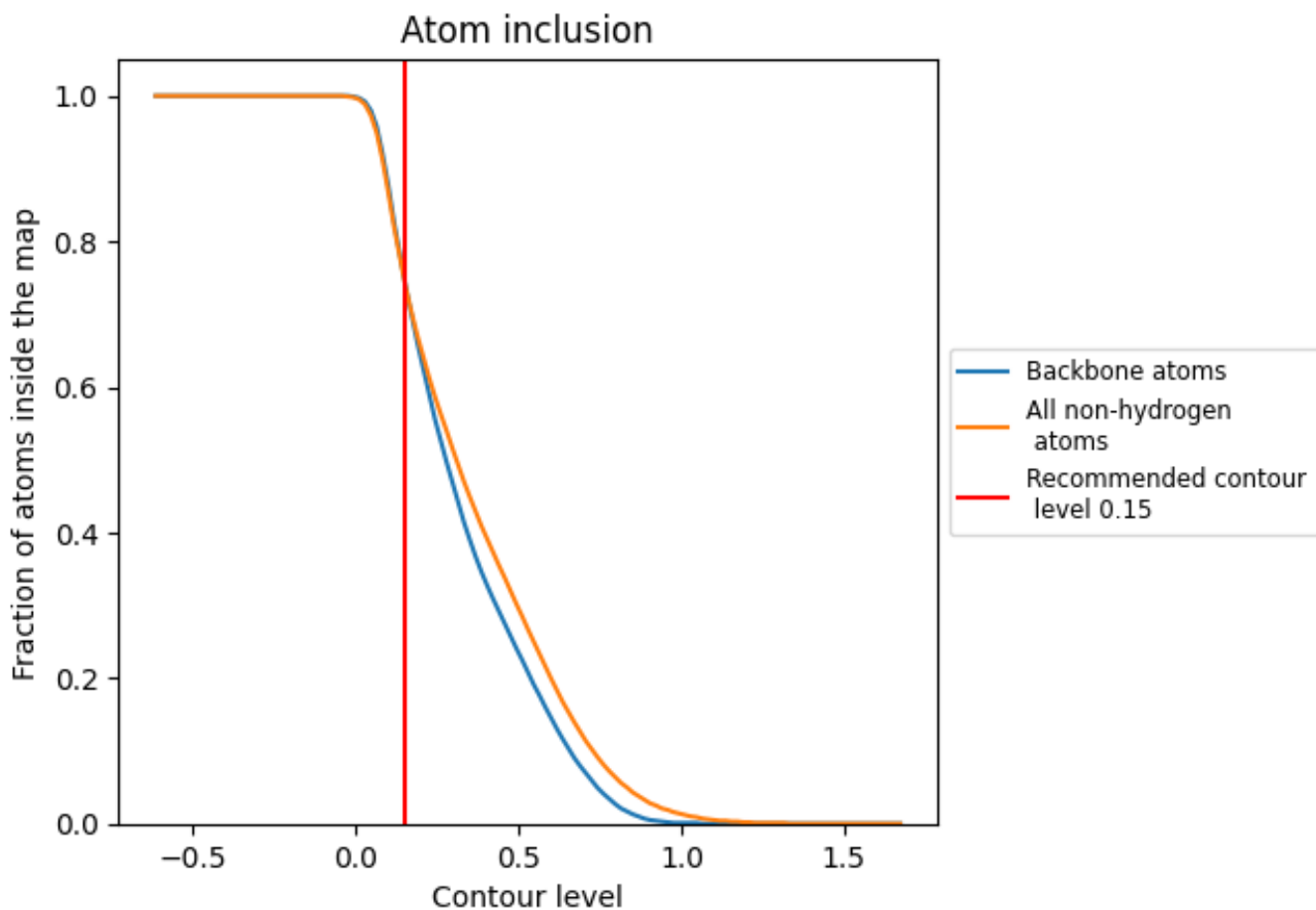
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4270
A2	0.9630	0.5460
AA	0.9230	0.5740
AB	0.9150	0.5600
AC	0.9640	0.6080
AD	0.9120	0.5440
AE	0.9600	0.5900
AF	0.9290	0.5620
AG	0.8860	0.4830
AH	0.8370	0.4640
AI	0.9140	0.5340
AJ	0.9470	0.5870
AK	0.9110	0.5070
AL	0.9080	0.5640
AM	0.6040	0.2490
AN	0.9470	0.5800
AO	0.9260	0.5730
AP	0.8760	0.5200
AQ	0.9620	0.5850
AR	0.9020	0.5520
AS	0.9170	0.5350
AT	0.9310	0.5730
AU	0.8890	0.5310
AV	0.9380	0.5870
AW	0.9770	0.6210
AX	0.9600	0.6050
AY	0.9480	0.5710
AZ	0.8720	0.5110
Aa	0.9460	0.5900
Ab	0.9170	0.5590
Ac	0.8310	0.5210
Ad	0.9550	0.5900
Ae	0.9110	0.5580
Af	0.7220	0.3300
Ag	0.8790	0.4820



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Chain	Atom inclusion	Q-score
Ah	 0.8300	 0.5380
Aj	 0.9070	 0.5640
I3	 0.0100	 0.0450
I4	 0.0660	 0.0650
I5	 0.0280	 0.0790
I6	 0.1460	 0.1010
I8	 0.0440	 0.0650
Io	 0.1820	 0.2490
Ip	 0.8560	 0.5060
Iq	 0.8010	 0.5260
Ir	 0.6910	 0.2930
Is	 0.8090	 0.4270
It	 0.6150	 0.1920
Iu	 0.5100	 0.2280
Iv	 0.2250	 0.1000
Iw	 0.9840	 0.4350
Ix	 0.1410	 0.2120
Iy	 0.5820	 0.2770