Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 02:23 PM EST

PDB ID	:	7M2Y
EMDB ID	:	EMD-23637
Title	:	Closed conformation of the Yeast wild-type gamma-TuRC
Authors	:	Brilot, A.F.; Lyon, A.S.; Zelter, A.; Viswanath, S.; Maxwell, A.; MacCoss, M.J.; Muller, E.G.; Sali, A.; Davis, T.N.; Agard, D.A.
Deposited on	:	2021-03-17
Resolution	:	4.03 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:

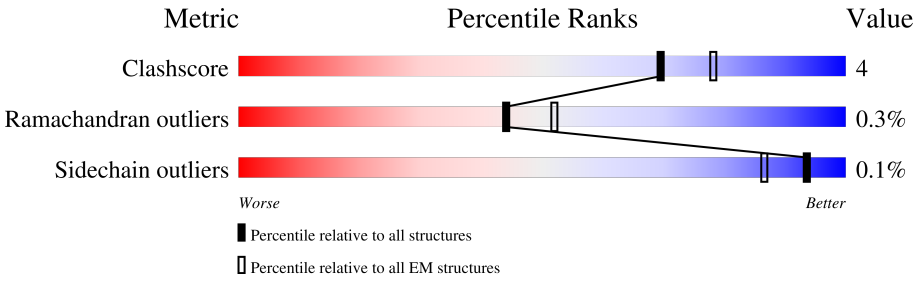
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.03 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	12% 85% 8% 7%
1	B	473	13% 87% 7% • 5%
2	C	846	5% 68% 9% • 22%
3	D	823	• 79% 7% 15%
4	U	220	• 14% 86%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GDP	A	501	-	-	X	-
5	GDP	B	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18560 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 Tubulin gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3447	2156	582	693	16		
1	B	447	Total	C	N	O	S	0	0
			3491	2182	591	701	17		

- Molecule 2 is a protein called Spindle pole body component SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	656	Total	C	N	O	S	0	0
			5435	3518	899	1002	16		

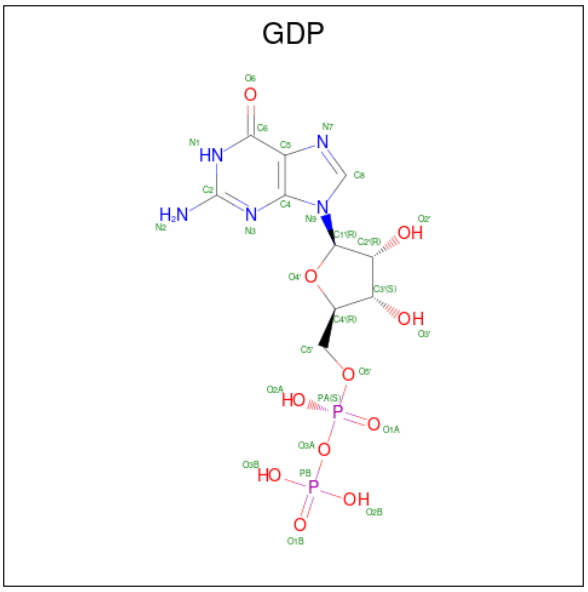
- Molecule 3 is a protein called Spindle pole body component SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	703	Total	C	N	O	S	0	0
			5868	3781	984	1074	29		

- Molecule 4 is a protein called Spindle pole body component 110.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	31	Total	C	N	O	S	0	0
			263	162	49	50	2		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



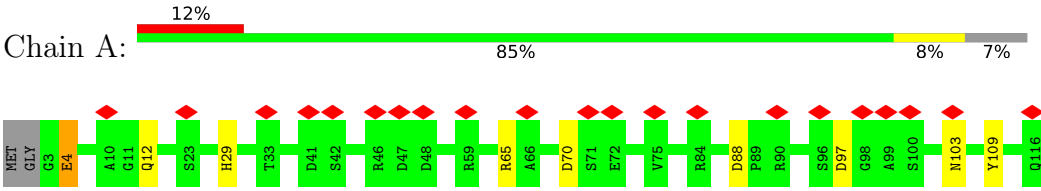
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

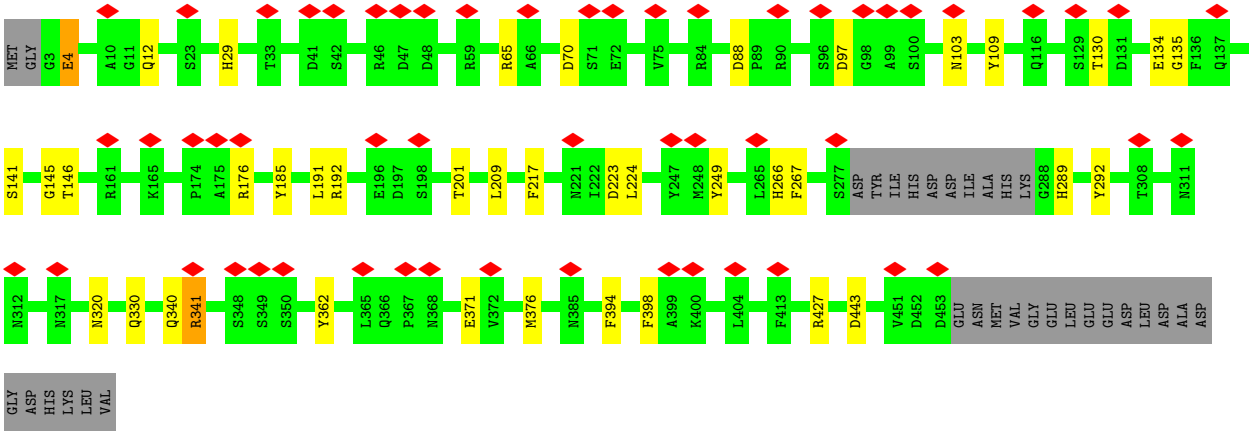
3 Residue-property plots (i)

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

• Molecule 1: Tubulin gamma chain

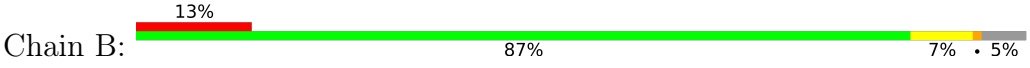
Chain A:

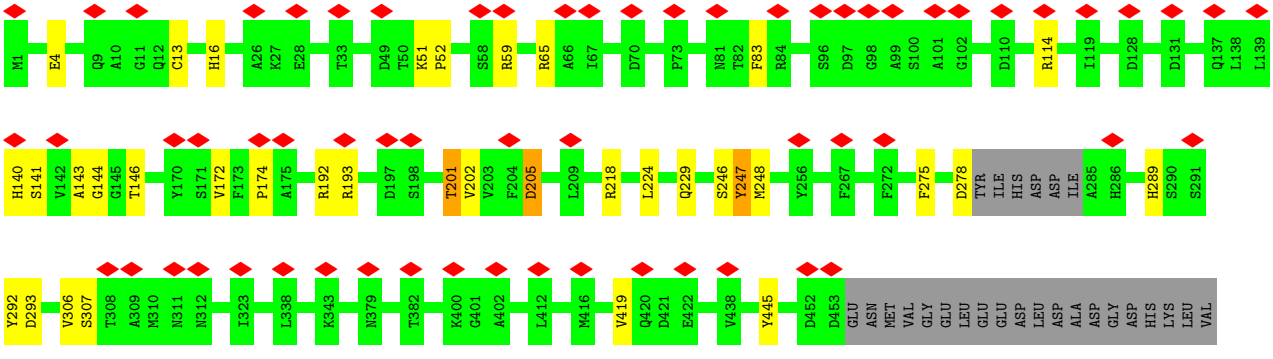




• Molecule 1: Tubulin gamma chain

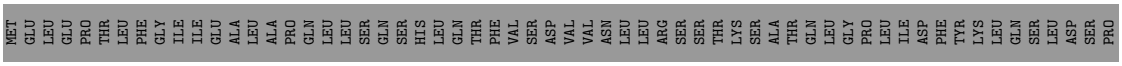
Chain B:

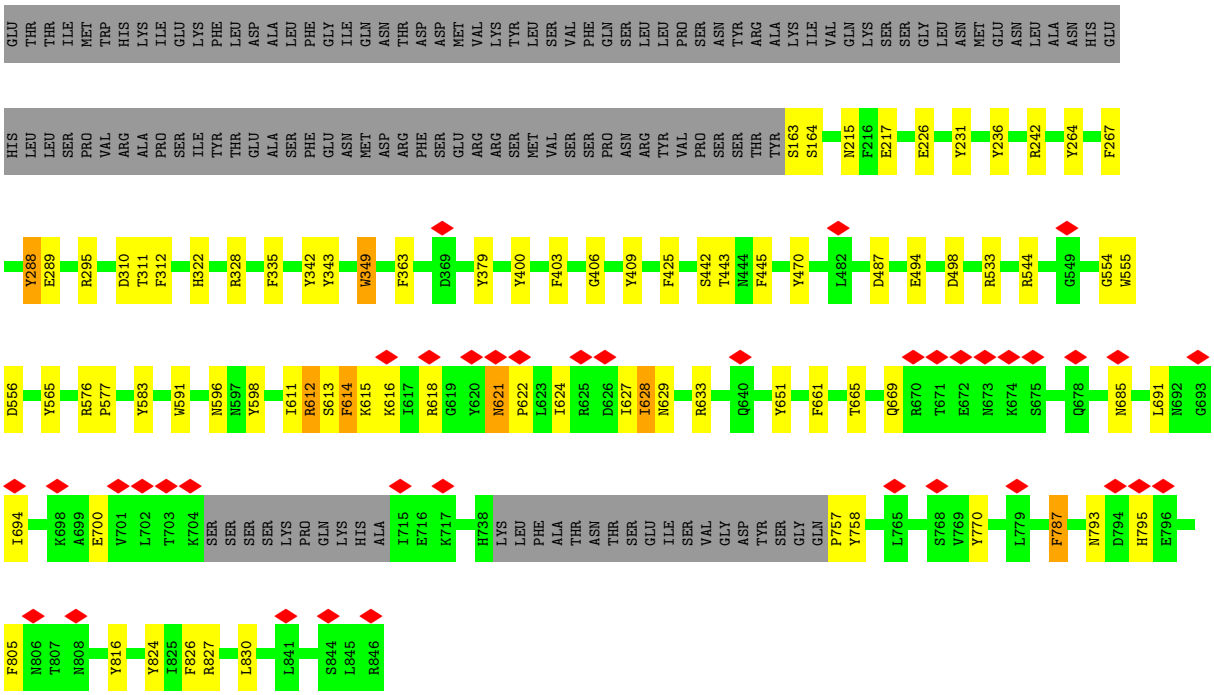




• Molecule 2: Spindle pole body component SPC98

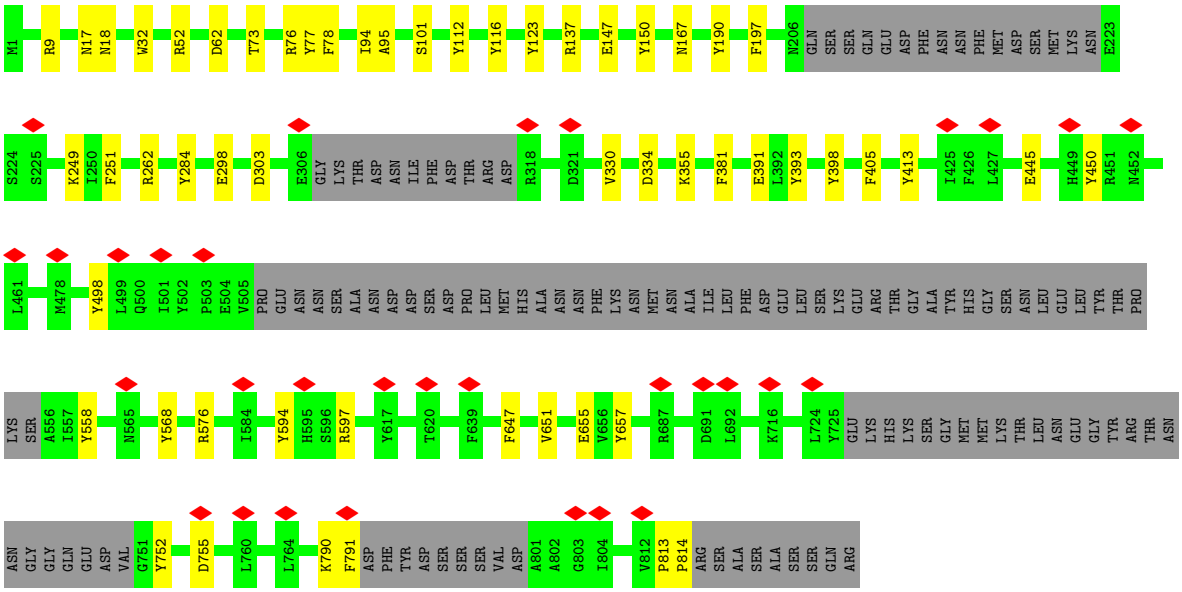
Chain C:





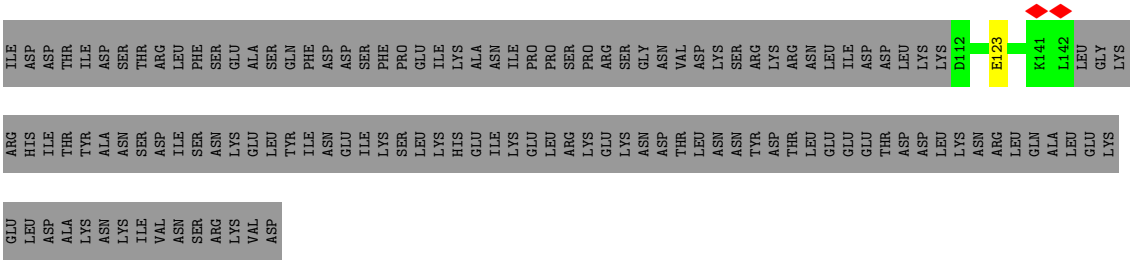
• Molecule 3: Spindle pole body component SPC97

Chain D:



• Molecule 4: Spindle pole body component 110

Chain U:


ILE ASP ASP THR ILE ASP SER THR ARG LEU PHE SER GLU ALA SER GLN PHE ASP ASP SER PHE PRO GLU ILE LYS ALA ASN ILE PRO PRO SER PRO ARG SER GLY ASN VAL ASP LYS SER ARG LYS ARG ASN LEU ILE ASP ASP LEU LYS LYS D112 E123 K141 L142 LEU GLY LYS
ARG HIS ILE THR TYR ALA ASN SER ASP ILE SER ASN LYS GLU LEU TYR ILE ASN GLU ILE LYS SER LEU LYS HIS GLU ILE LYS GLU LEU ARG LYS GLU LYS ASN ASP THR LEU ASN ASN TYR ASP THR LEU GLU GLU GLU THR ASP ASP LEU LYS ASN ARG LEU GLN ALA LEU GLU LYS
GLU LEU ASP ALA LYS ASN LYS ILE VAL ASN SER ARG LYS VAL ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=0.01 Å, axial sym=C1	Depositor
Number of segments used	20420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Final reconstruction in cis-TEM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47214	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	21.845	Depositor
Minimum map value	-11.274	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.822	Depositor
Recommended contour level	3.4	Depositor
Map size (Å)	635.39844, 635.39844, 635.39844	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4183, 1.4183, 1.4183	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	1.10	7/3518 (0.2%)	0.98	6/4778 (0.1%)
1	B	1.07	7/3563 (0.2%)	1.02	11/4837 (0.2%)
2	C	1.28	31/5551 (0.6%)	0.99	20/7500 (0.3%)
3	D	1.22	28/5984 (0.5%)	0.96	12/8078 (0.1%)
4	U	1.21	1/266 (0.4%)	0.86	0/352
All	All	1.19	74/18882 (0.4%)	0.98	49/25545 (0.2%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	190	TYR	CB-CG	-11.62	1.34	1.51
2	C	288	TYR	CB-CG	-10.94	1.35	1.51
3	D	78	PHE	CB-CG	-10.01	1.34	1.51
2	C	349	TRP	CB-CG	-9.95	1.32	1.50
2	C	267	PHE	CB-CG	-9.22	1.35	1.51
3	D	298	GLU	CD-OE2	-8.46	1.16	1.25
1	B	419	VAL	CB-CG2	-8.01	1.36	1.52
3	D	112	TYR	CB-CG	-7.75	1.40	1.51
3	D	197	PHE	CB-CG	-7.45	1.38	1.51
2	C	403	PHE	CB-CG	-7.25	1.39	1.51
2	C	470	TYR	CB-CG	-7.18	1.40	1.51
2	C	651	TYR	CB-CG	-7.14	1.41	1.51
1	A	398	PHE	CB-CG	-7.05	1.39	1.51
2	C	379	TYR	CE1-CZ	-6.98	1.29	1.38
2	C	335	PHE	CB-CG	-6.96	1.39	1.51
1	A	29	HIS	CB-CG	-6.90	1.37	1.50
2	C	425	PHE	CB-CG	-6.81	1.39	1.51
1	B	247	TYR	CB-CG	-6.62	1.41	1.51
2	C	591	TRP	CB-CG	-6.45	1.38	1.50
2	C	312	PHE	CB-CG	-6.39	1.40	1.51
2	C	231	TYR	CB-CG	-6.39	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	568	TYR	CB-CG	-6.23	1.42	1.51
2	C	445	PHE	CB-CG	-6.22	1.40	1.51
3	D	381	PHE	CB-CG	-6.22	1.40	1.51
2	C	661	PHE	CB-CG	-6.19	1.40	1.51
2	C	400	TYR	CB-CG	-6.13	1.42	1.51
2	C	787	PHE	CB-CG	-5.96	1.41	1.51
3	D	413	TYR	CD2-CE2	-5.95	1.30	1.39
3	D	32	TRP	CB-CG	-5.92	1.39	1.50
2	C	583	TYR	CD2-CE2	-5.84	1.30	1.39
2	C	494	GLU	CD-OE2	-5.79	1.19	1.25
1	A	109	TYR	CB-CG	-5.77	1.43	1.51
1	B	278	ASP	CB-CG	5.77	1.63	1.51
3	D	657	TYR	CB-CG	-5.73	1.43	1.51
2	C	758	TYR	CB-CG	-5.70	1.43	1.51
2	C	770	TYR	CB-CG	-5.66	1.43	1.51
3	D	398	TYR	CB-CG	-5.62	1.43	1.51
3	D	391	GLU	CD-OE1	-5.62	1.19	1.25
2	C	757	PRO	N-CD	-5.56	1.40	1.47
3	D	150	TYR	CB-CG	-5.55	1.43	1.51
3	D	393	TYR	CB-CG	-5.54	1.43	1.51
3	D	405	PHE	CB-CG	-5.53	1.42	1.51
1	A	185	TYR	CB-CG	-5.48	1.43	1.51
3	D	568	TYR	CD2-CE2	-5.47	1.31	1.39
1	A	134	GLU	CD-OE1	-5.43	1.19	1.25
3	D	116	TYR	CB-CG	-5.43	1.43	1.51
3	D	398	TYR	CD1-CE1	-5.37	1.31	1.39
3	D	298	GLU	CB-CG	-5.34	1.42	1.52
3	D	330	VAL	CB-CG2	-5.34	1.41	1.52
3	D	251	PHE	CB-CG	-5.32	1.42	1.51
2	C	583	TYR	CE2-CZ	-5.30	1.31	1.38
3	D	752	TYR	CB-CG	-5.24	1.43	1.51
1	B	4	GLU	CG-CD	-5.22	1.44	1.51
3	D	445	GLU	CD-OE1	-5.22	1.20	1.25
1	A	394	PHE	CB-CG	-5.16	1.42	1.51
2	C	816	TYR	CB-CG	-5.16	1.44	1.51
4	U	123	GLU	CD-OE2	-5.16	1.20	1.25
3	D	498	TYR	CB-CG	-5.11	1.44	1.51
2	C	264	TYR	CB-CG	-5.11	1.44	1.51
2	C	363	PHE	CB-CG	-5.10	1.42	1.51
2	C	409	TYR	CB-CG	-5.10	1.44	1.51
2	C	226	GLU	CD-OE1	-5.09	1.20	1.25
2	C	289	GLU	CD-OE2	-5.09	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	217	GLU	CD-OE1	-5.08	1.20	1.25
3	D	147	GLU	CD-OE1	-5.08	1.20	1.25
1	B	247	TYR	CD2-CE2	-5.08	1.31	1.39
1	B	292	TYR	CB-CG	-5.07	1.44	1.51
2	C	700	GLU	CD-OE1	-5.05	1.20	1.25
2	C	596	ASN	CB-CG	-5.05	1.39	1.51
1	B	83	PHE	CB-CG	-5.04	1.42	1.51
3	D	284	TYR	CB-CG	-5.03	1.44	1.51
3	D	62	ASP	CB-CG	-5.03	1.41	1.51
3	D	655	GLU	CD-OE1	-5.02	1.20	1.25
1	A	4	GLU	CD-OE1	-5.00	1.20	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	413	TYR	CB-CG-CD2	-11.02	114.39	121.00
2	C	612	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	C	612	ARG	NE-CZ-NH1	8.36	124.48	120.30
2	C	533	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	217	PHE	CB-CG-CD1	8.11	126.48	120.80
1	B	218	ARG	NE-CZ-NH2	-7.95	116.33	120.30
2	C	544	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	C	242	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	362	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	B	65	ARG	NE-CZ-NH2	-7.59	116.50	120.30
3	D	77	TYR	CB-CG-CD1	-7.57	116.46	121.00
1	A	427	ARG	NE-CZ-NH2	-7.45	116.58	120.30
3	D	413	TYR	CB-CG-CD1	7.38	125.43	121.00
2	C	295	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	C	295	ARG	NE-CZ-NH2	-7.26	116.67	120.30
3	D	568	TYR	CB-CG-CD2	-7.11	116.73	121.00
2	C	342	TYR	CB-CG-CD1	-7.09	116.75	121.00
1	A	217	PHE	CB-CG-CD2	-6.91	115.97	120.80
2	C	805	PHE	CB-CG-CD2	-6.82	116.03	120.80
2	C	805	PHE	CB-CG-CD1	6.59	125.42	120.80
1	B	205	ASP	CB-CG-OD2	6.48	124.14	118.30
2	C	236	TYR	CB-CG-CD2	-6.36	117.19	121.00
3	D	137	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	114	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	C	288	TYR	CB-CG-CD1	-6.13	117.32	121.00
3	D	558	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	B	201	THR	N-CA-C	5.96	127.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	343	TYR	CB-CG-CD1	-5.80	117.52	121.00
2	C	614	PHE	CB-CG-CD2	5.72	124.81	120.80
1	A	65	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	249	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	C	565	TYR	CB-CG-CD2	-5.53	117.68	121.00
2	C	758	TYR	CB-CG-CD1	-5.34	117.80	121.00
3	D	576	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	205	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	B	59	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	C	583	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	D	594	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	B	218	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	247	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	C	312	PHE	CB-CG-CD1	-5.17	117.18	120.80
1	B	193	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	D	9	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	D	450	TYR	CB-CG-CD2	-5.13	117.92	121.00
3	D	262	ARG	NE-CZ-NH2	-5.07	117.77	120.30
3	D	597	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	445	TYR	CB-CG-CD1	-5.04	117.98	121.00
2	C	598	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	C	651	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3305	29	0
1	B	3491	0	3349	40	0
2	C	5435	0	5462	54	0
3	D	5868	0	5932	13	0
4	U	263	0	266	0	0
5	A	28	0	12	13	0
5	B	28	0	11	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18560	0	18337	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:621:ASN:HB3	2:C:622:PRO:CD	1.17	1.46
1:B:174:PRO:CD	5:B:501:GDP:O3'	1.63	1.42
2:C:621:ASN:CB	2:C:622:PRO:CD	2.09	1.25
1:B:174:PRO:HD3	5:B:501:GDP:O3'	1.02	1.18
1:B:143:ALA:HB3	5:B:501:GDP:H4'	1.13	1.11
2:C:621:ASN:CB	2:C:622:PRO:HD2	1.77	1.08
1:B:143:ALA:HB3	5:B:501:GDP:C4'	1.89	1.02
2:C:613:SER:HA	2:C:616:LYS:CD	1.91	1.01
2:C:621:ASN:HB3	2:C:622:PRO:HD2	1.03	1.00
2:C:621:ASN:HB3	2:C:622:PRO:HD3	1.02	0.99
1:A:176:ARG:NH1	5:A:501:GDP:O2'	1.96	0.98
2:C:621:ASN:CB	2:C:622:PRO:HD3	1.85	0.98
1:A:141:SER:OG	5:A:501:GDP:H4'	1.63	0.98
1:B:174:PRO:CG	5:B:501:GDP:O3'	2.13	0.94
2:C:613:SER:HA	2:C:616:LYS:HG3	1.52	0.91
1:B:143:ALA:CB	5:B:501:GDP:H4'	2.00	0.90
2:C:613:SER:HA	2:C:616:LYS:CG	2.01	0.90
2:C:614:PHE:CE2	2:C:628:ILE:HG12	2.09	0.88
1:B:144:GLY:CA	5:B:501:GDP:O5'	2.25	0.85
1:A:141:SER:OG	5:A:501:GDP:C4'	2.24	0.84
1:A:146:THR:OG1	5:A:501:GDP:O1B	1.96	0.81
2:C:612:ARG:O	2:C:616:LYS:HG3	1.83	0.79
1:B:144:GLY:HA2	5:B:501:GDP:O5'	1.83	0.77
2:C:613:SER:HA	2:C:616:LYS:CE	2.15	0.76
2:C:614:PHE:CD2	2:C:628:ILE:HG12	2.22	0.75
1:B:174:PRO:HG3	5:B:501:GDP:O3'	1.88	0.74
1:A:176:ARG:CZ	5:A:501:GDP:O2'	2.36	0.73
1:B:16:HIS:HB2	5:B:501:GDP:O6	1.90	0.72
2:C:613:SER:HA	2:C:616:LYS:HE3	1.70	0.71
2:C:613:SER:CA	2:C:616:LYS:HE3	2.19	0.71
2:C:614:PHE:CE2	2:C:628:ILE:CG1	2.76	0.68
2:C:614:PHE:HE2	2:C:628:ILE:CG1	2.06	0.68
2:C:613:SER:CA	2:C:616:LYS:HG3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:HIS:HB3	1:A:371:GLU:HG3	1.77	0.67
2:C:612:ARG:O	2:C:616:LYS:CG	2.43	0.66
2:C:628:ILE:HG22	2:C:629:ASN:N	2.11	0.66
2:C:613:SER:HA	2:C:616:LYS:HD2	1.75	0.65
1:B:143:ALA:HB3	5:B:501:GDP:C3'	2.28	0.63
1:B:146:THR:HB	5:B:501:GDP:PB	2.38	0.62
1:A:289:HIS:HB3	1:A:371:GLU:CD	2.19	0.62
1:B:143:ALA:CB	5:B:501:GDP:C4'	2.69	0.62
1:B:174:PRO:HB3	5:B:501:GDP:O2'	2.01	0.61
1:A:145:GLY:N	5:A:501:GDP:O2B	2.35	0.60
2:C:576:ARG:HB3	2:C:577:PRO:CD	2.31	0.60
1:B:174:PRO:HG3	5:B:501:GDP:C3'	2.31	0.59
2:C:611:ILE:O	2:C:615:LYS:HG2	2.02	0.59
3:D:52:ARG:NH2	3:D:101:SER:OG	2.36	0.58
1:B:172:VAL:HG21	5:B:501:GDP:HN22	1.68	0.58
2:C:618:ARG:C	2:C:618:ARG:HD2	2.23	0.58
1:A:176:ARG:NH1	5:A:501:GDP:O3'	2.37	0.58
1:B:144:GLY:HA2	5:B:501:GDP:O3A	2.04	0.58
1:A:289:HIS:HB3	1:A:371:GLU:CG	2.34	0.57
1:A:443:ASP:OD1	1:A:443:ASP:N	2.37	0.57
1:A:224:LEU:HD13	5:A:501:GDP:C4	2.41	0.55
2:C:826:PHE:CE2	2:C:830:LEU:HD11	2.41	0.55
1:B:143:ALA:CB	5:B:501:GDP:C3'	2.84	0.55
2:C:614:PHE:HE2	2:C:628:ILE:HG13	1.71	0.54
2:C:576:ARG:HB3	2:C:577:PRO:HD2	1.90	0.54
2:C:288:TYR:OH	3:D:123:TYR:OH	2.26	0.53
1:B:306:VAL:O	1:B:307:SER:C	2.46	0.53
1:A:224:LEU:HD22	5:A:501:GDP:C2	2.44	0.53
1:B:146:THR:N	5:B:501:GDP:O2B	2.34	0.53
1:A:141:SER:HG	5:A:501:GDP:H4'	1.68	0.52
1:B:143:ALA:HB3	5:B:501:GDP:O3'	2.09	0.52
1:B:144:GLY:HA2	5:B:501:GDP:PA	2.49	0.52
2:C:498:ASP:N	2:C:498:ASP:OD1	2.43	0.51
1:B:146:THR:OG1	5:B:501:GDP:O2B	2.29	0.51
1:B:143:ALA:CB	5:B:501:GDP:O3'	2.59	0.50
3:D:167:ASN:OD1	3:D:167:ASN:N	2.44	0.50
2:C:613:SER:OG	2:C:616:LYS:NZ	2.43	0.49
1:A:266:HIS:H	1:A:266:HIS:HD1	1.59	0.49
1:B:146:THR:CB	5:B:501:GDP:O2B	2.59	0.49
2:C:629:ASN:O	2:C:633:ARG:HG2	2.12	0.49
3:D:303:ASP:OD2	3:D:355:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:HB3	1:B:52:PRO:HD3	1.95	0.49
1:B:13:CYS:HA	5:B:501:GDP:C5	2.47	0.49
2:C:665:THR:O	2:C:669:GLN:NE2	2.47	0.48
2:C:487:ASP:N	2:C:487:ASP:OD1	2.46	0.48
2:C:613:SER:N	2:C:616:LYS:HE3	2.29	0.47
2:C:685:ASN:OD1	2:C:685:ASN:N	2.47	0.47
1:B:201:THR:OG1	1:B:202:VAL:N	2.47	0.47
3:D:755:ASP:N	3:D:755:ASP:OD1	2.48	0.47
1:A:209:LEU:HD11	5:A:501:GDP:N2	2.30	0.47
2:C:554:GLY:O	2:C:556:ASP:N	2.48	0.46
1:A:103:ASN:OD1	5:A:501:GDP:O2B	2.34	0.46
2:C:793:ASN:O	2:C:795:HIS:N	2.49	0.45
1:B:246:SER:OG	1:B:247:TYR:N	2.47	0.45
1:B:224:LEU:HD22	5:B:501:GDP:C2	2.52	0.45
2:C:442:SER:OG	2:C:443:THR:N	2.50	0.45
2:C:618:ARG:C	2:C:618:ARG:CD	2.85	0.45
1:A:340:GLN:O	1:A:341:ARG:CB	2.65	0.45
2:C:612:ARG:C	2:C:616:LYS:HE3	2.37	0.45
1:B:229:GLN:OE1	1:B:229:GLN:N	2.47	0.44
2:C:163:SER:OG	2:C:164:SER:N	2.49	0.44
1:A:4:GLU:HG3	1:A:130:THR:HB	1.99	0.44
1:B:205:ASP:N	1:B:205:ASP:OD1	2.46	0.44
2:C:349:TRP:CE2	2:C:406:GLY:HA3	2.53	0.44
1:B:289:HIS:HB3	1:B:293:ASP:HB2	2.00	0.43
1:B:144:GLY:HA3	5:B:501:GDP:O5'	2.15	0.43
2:C:624:ILE:HG23	2:C:628:ILE:CD1	2.49	0.43
3:D:17:ASN:OD1	3:D:17:ASN:N	2.50	0.43
1:B:275:PHE:CD2	1:B:275:PHE:N	2.86	0.43
2:C:215:ASN:OD1	2:C:215:ASN:N	2.48	0.43
2:C:322:HIS:O	2:C:328:ARG:NE	2.52	0.43
2:C:613:SER:OG	2:C:616:LYS:CE	2.66	0.43
2:C:614:PHE:HA	2:C:787:PHE:CD1	2.53	0.43
3:D:249:LYS:NZ	3:D:334:ASP:OD1	2.39	0.43
3:D:790:LYS:O	3:D:791:PHE:C	2.57	0.43
1:A:191:LEU:O	1:A:192:ARG:C	2.57	0.42
2:C:691:LEU:HB2	2:C:694:ILE:HD11	2.01	0.42
1:B:141:SER:OG	5:B:501:GDP:C4'	2.68	0.42
1:B:144:GLY:CA	5:B:501:GDP:PA	3.08	0.42
2:C:624:ILE:HD13	2:C:624:ILE:HA	1.91	0.42
1:A:97:ASP:N	1:A:97:ASP:OD1	2.49	0.42
2:C:624:ILE:HG23	2:C:628:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:813:PRO:HA	3:D:814:PRO:HD3	1.95	0.42
1:B:140:HIS:CG	1:B:141:SER:N	2.87	0.41
2:C:824:TYR:O	2:C:827:ARG:HG2	2.20	0.41
1:A:88:ASP:C	1:A:88:ASP:OD1	2.59	0.41
1:A:292:TYR:HB2	1:A:330:GLN:HB3	2.01	0.41
1:A:320:ASN:HD22	1:A:376:MET:HB2	1.84	0.41
1:B:16:HIS:CB	5:B:501:GDP:O6	2.64	0.41
1:A:12:GLN:OE1	5:A:501:GDP:O3B	2.37	0.41
1:A:201:THR:HG23	1:A:267:PHE:CD2	2.56	0.41
3:D:18:ASN:OD1	3:D:18:ASN:N	2.43	0.41
3:D:647:PHE:O	3:D:651:VAL:HB	2.20	0.41
1:B:146:THR:HB	5:B:501:GDP:O1B	2.20	0.41
1:A:223:ASP:N	1:A:223:ASP:OD1	2.50	0.41
2:C:621:ASN:HB2	2:C:622:PRO:HD2	1.85	0.41
1:A:289:HIS:CB	1:A:371:GLU:HG3	2.47	0.41
3:D:94:ILE:O	3:D:95:ALA:C	2.59	0.41
2:C:310:ASP:OD1	2:C:311:THR:N	2.54	0.40
2:C:576:ARG:CB	2:C:577:PRO:CD	2.96	0.40
1:A:70:ASP:OD1	1:A:70:ASP:N	2.52	0.40
3:D:73:THR:O	3:D:76:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

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	A	437/473 (92%)	420 (96%)	15 (3%)	2 (0%)	29 67
1	B	443/473 (94%)	432 (98%)	11 (2%)	0	100 100
2	C	650/846 (77%)	634 (98%)	12 (2%)	4 (1%)	25 63
3	D	691/823 (84%)	681 (99%)	10 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	U	29/220 (13%)	28 (97%)	1 (3%)	0	100 100
All	All	2250/2835 (79%)	2195 (98%)	49 (2%)	6 (0%)	44 75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	555	TRP
2	C	628	ILE
1	A	135	GLY
1	A	341	ARG
2	C	621	ASN
2	C	627	ILE

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	A	393/420 (94%)	393 (100%)	0	100 100
1	B	397/420 (94%)	395 (100%)	2 (0%)	88 93
2	C	613/787 (78%)	613 (100%)	0	100 100
3	D	659/766 (86%)	659 (100%)	0	100 100
4	U	30/206 (15%)	30 (100%)	0	100 100
All	All	2092/2599 (80%)	2090 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	ARG
1	B	248	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
3	D	485	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GDP	B	501	-	24,30,30	0.96	0	30,47,47	1.17	4 (13%)
5	GDP	A	501	-	24,30,30	0.97	0	30,47,47	1.17	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	B	501	-	-	3/12/32/32	0/3/3/3
5	GDP	A	501	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	GDP	C5-C6-N1	2.71	118.73	113.95
5	A	501	GDP	C5-C6-N1	2.69	118.70	113.95
5	B	501	GDP	PA-O3A-PB	-2.65	123.73	132.83
5	A	501	GDP	PA-O3A-PB	-2.64	123.77	132.83
5	B	501	GDP	C8-N7-C5	2.39	107.55	102.99
5	A	501	GDP	C8-N7-C5	2.38	107.53	102.99
5	B	501	GDP	O3'-C3'-C4'	-2.04	105.14	111.05
5	A	501	GDP	O3'-C3'-C4'	-2.04	105.14	111.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GDP	C5'-O5'-PA-O2A
5	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	C5'-O5'-PA-O1A

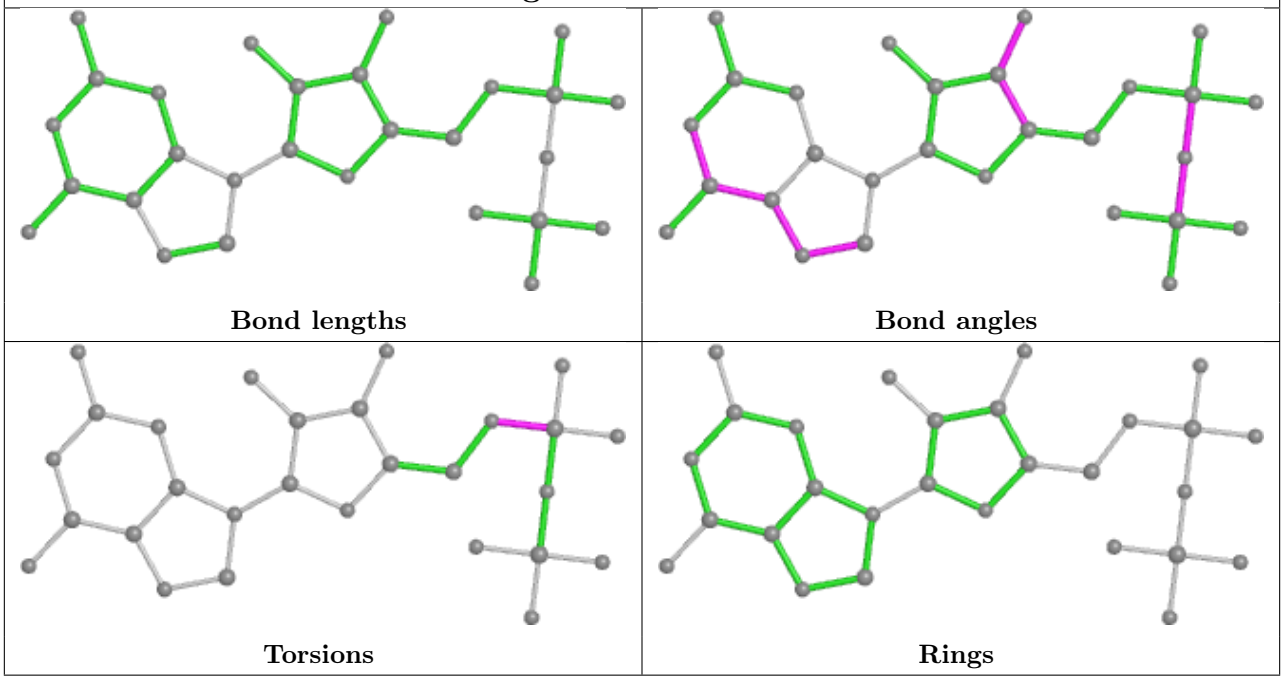
There are no ring outliers.

2 monomers are involved in 44 short contacts:

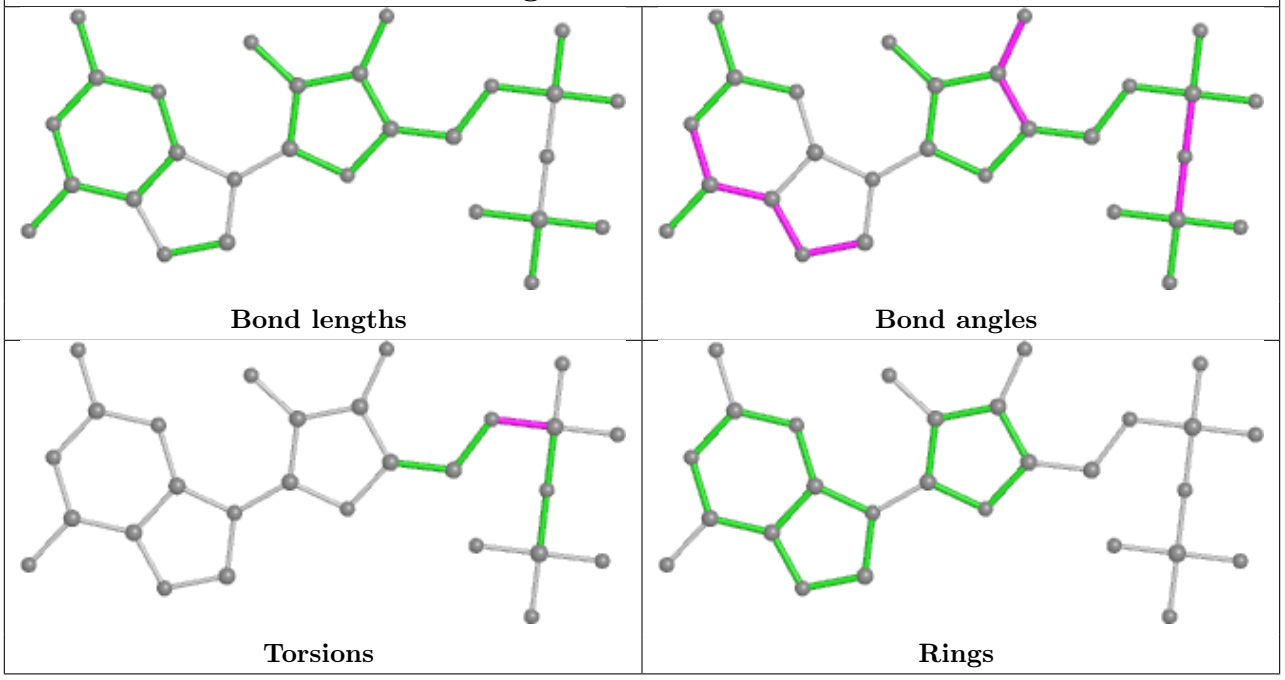
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	31	0
5	A	501	GDP	13	0

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

Ligand GDP B 501



Ligand GDP A 501



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.

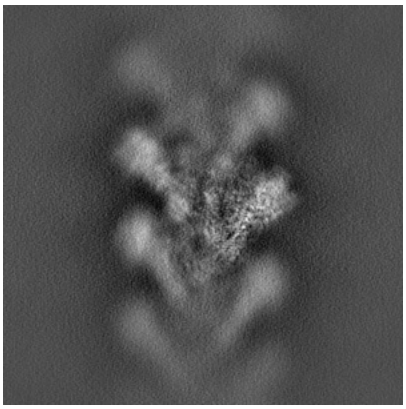
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23637. These allow visual inspection of the internal detail of the map and identification of artifacts.

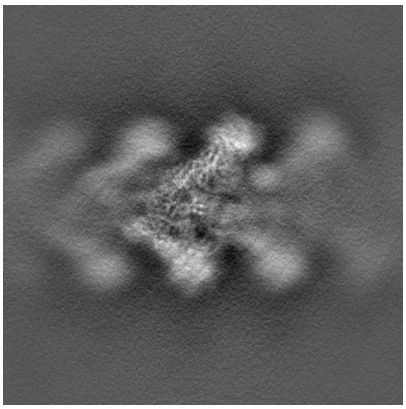
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

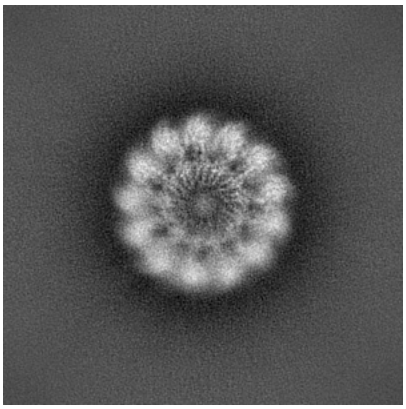
6.1.1 Primary map



X

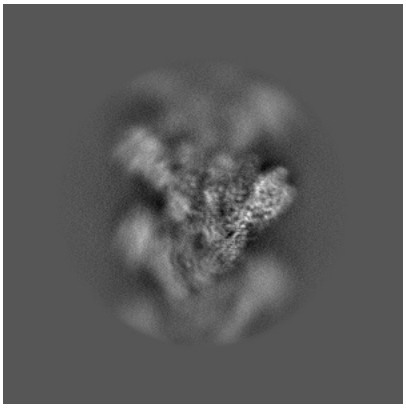


Y

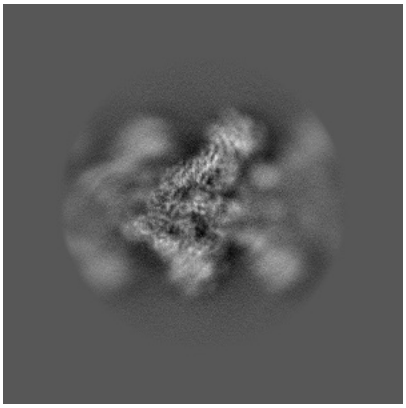


Z

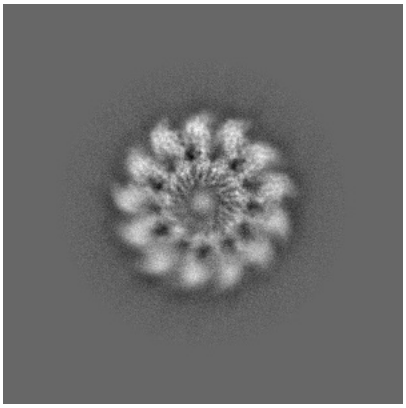
6.1.2 Raw map



X



Y

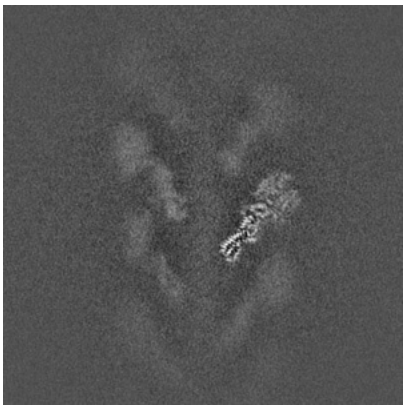


Z

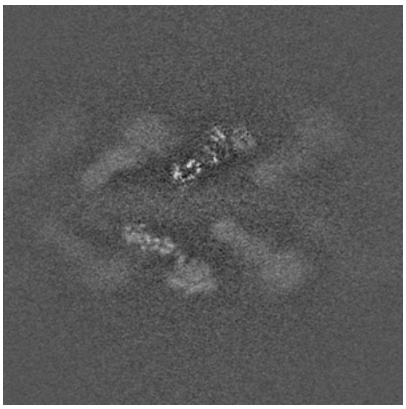
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

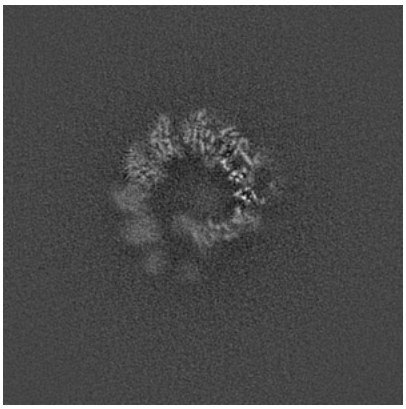
6.2.1 Primary map



X Index: 224

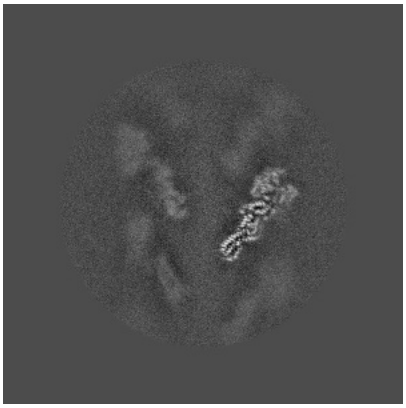


Y Index: 224

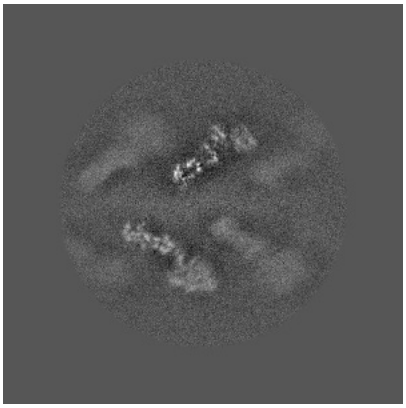


Z Index: 224

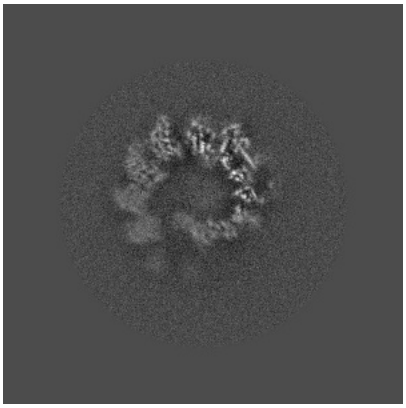
6.2.2 Raw map



X Index: 224



Y Index: 224

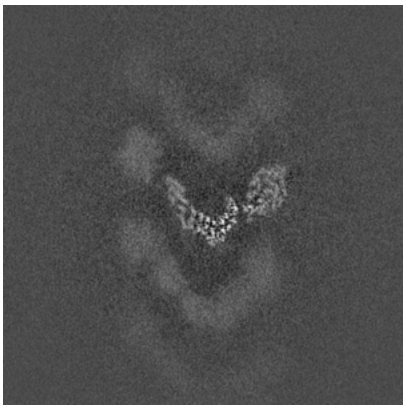


Z Index: 224

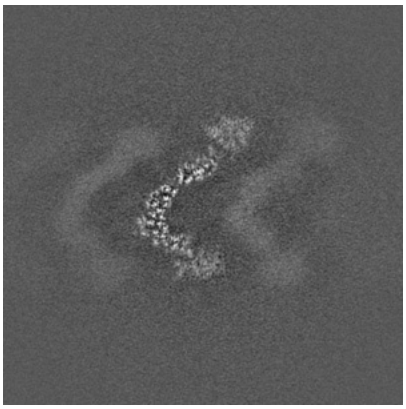
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



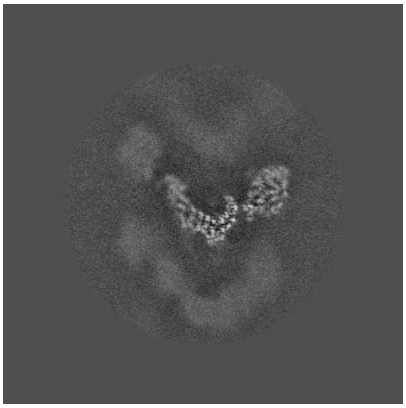
X Index: 256



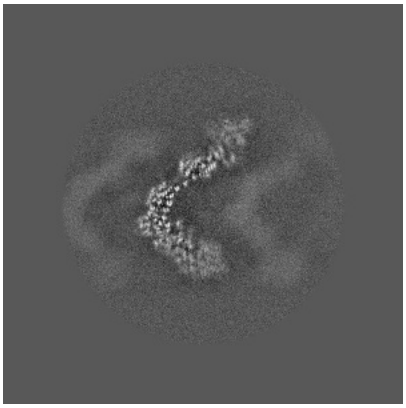
Y Index: 252

Z Index: 213

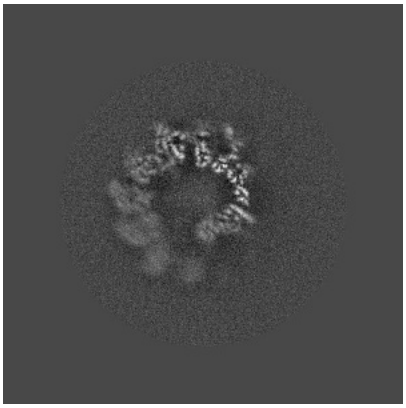
6.3.2 Raw map



X Index: 256



Y Index: 256

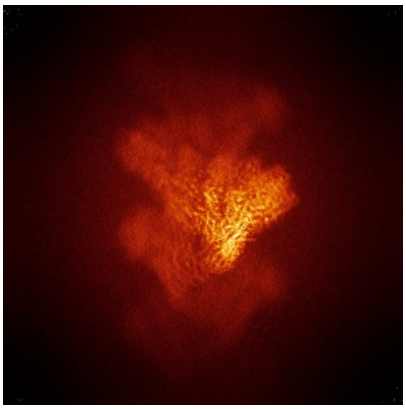


Z Index: 214

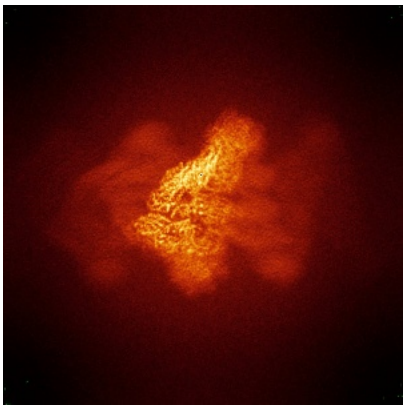
The images above show the largest variance slices of the map in three orthogonal directions.

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

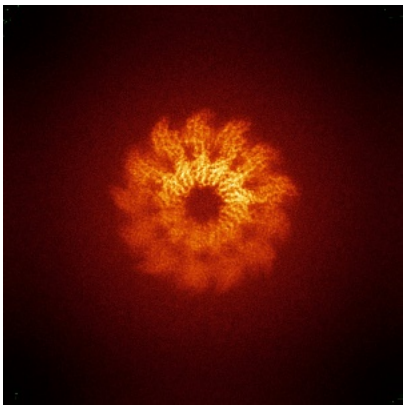
6.4.1 Primary map



X

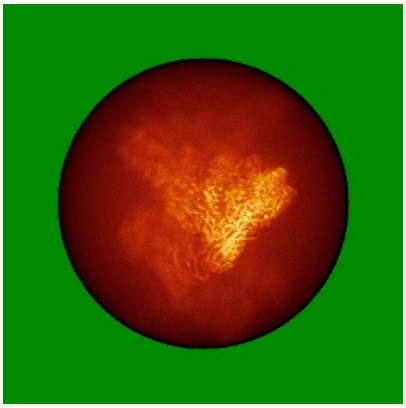


Y

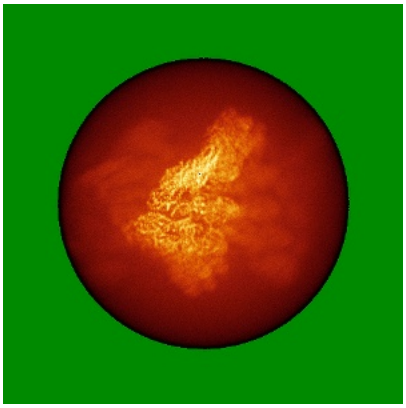


Z

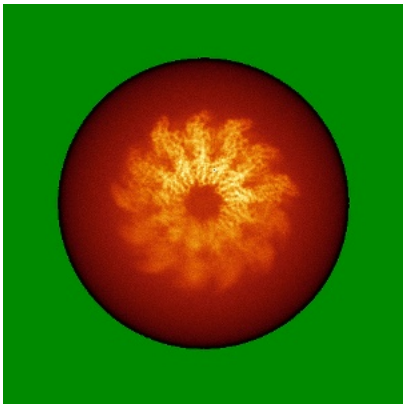
6.4.2 Raw map



X



Y

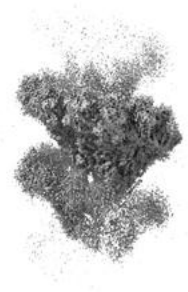


Z

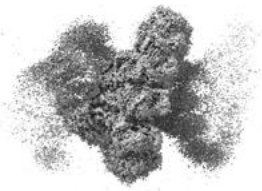
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

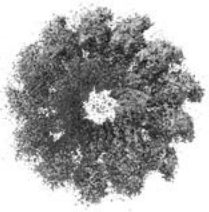
6.5.1 Primary map



X



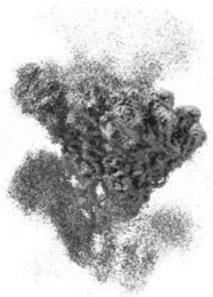
Y



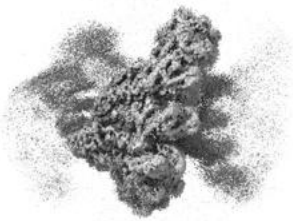
Z

The images above show the 3D surface view of the map at the recommended contour level 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

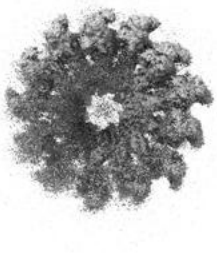
6.5.2 Raw map



X



Y



Z

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

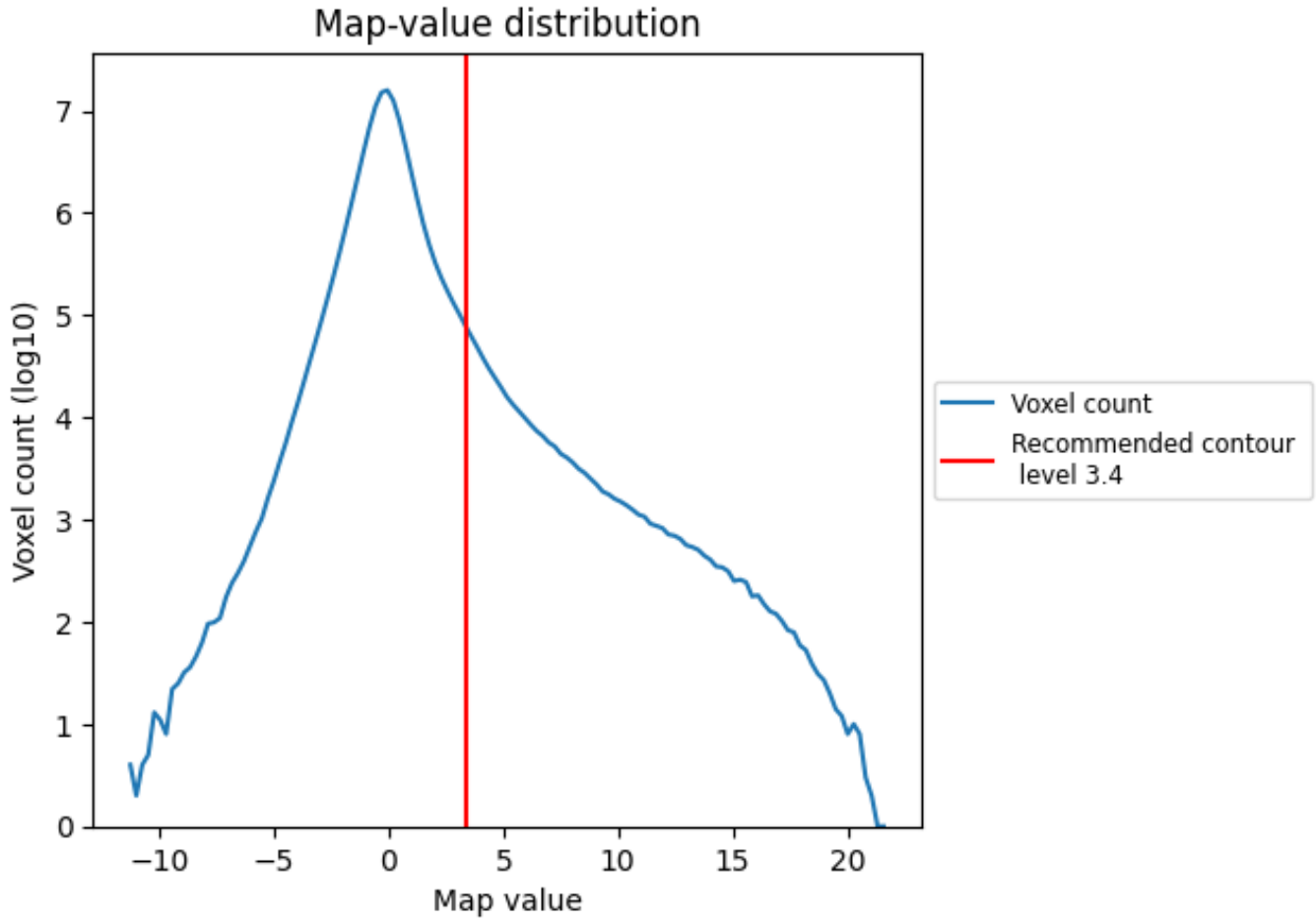
6.6 Mask visualisation (i)

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

7 Map analysis

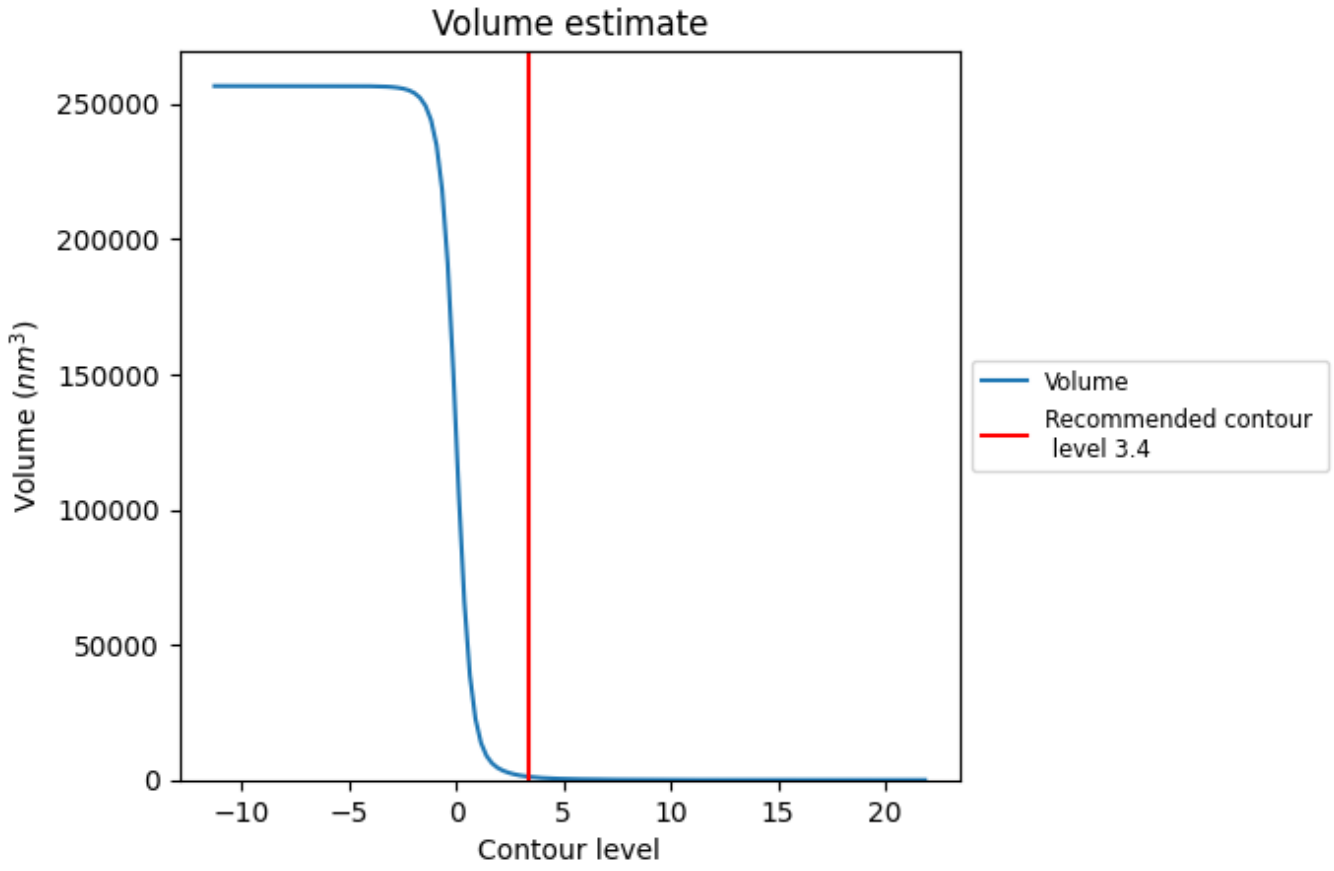
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

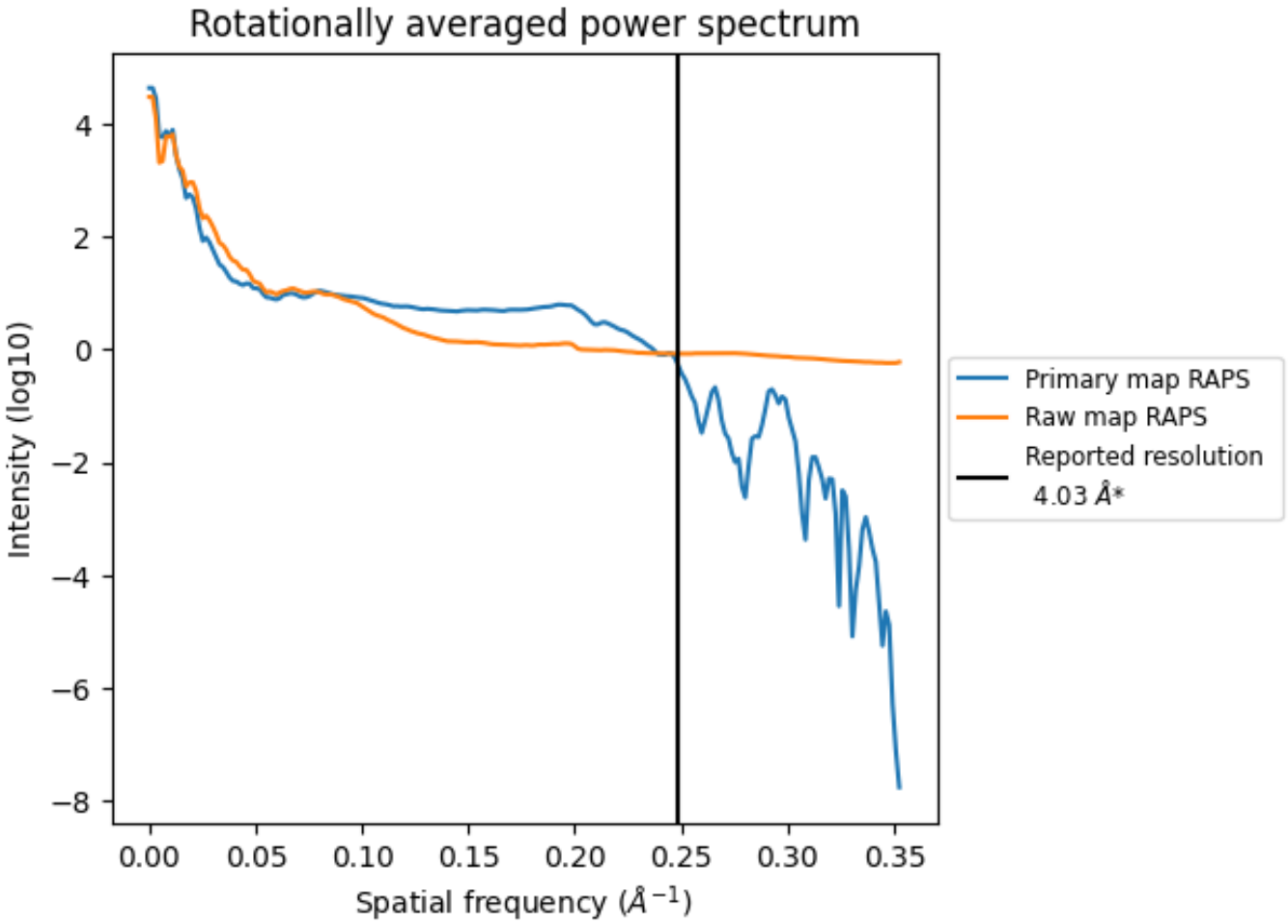
7.2 Volume estimate



The volume at the recommended contour level is 1173 nm^3; this corresponds to an approximate mass of 1060 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)

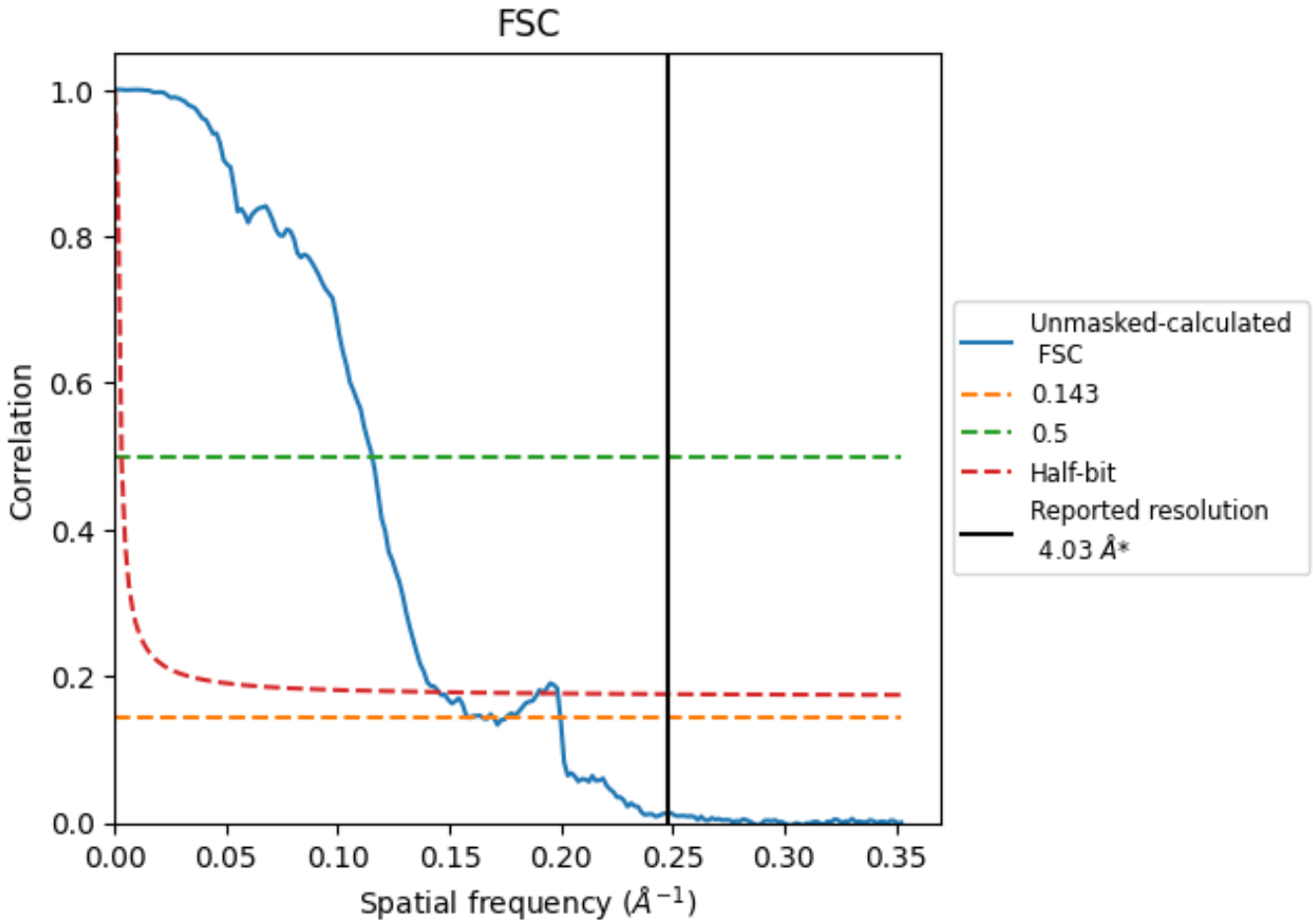


*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8.2 Resolution estimates (i)

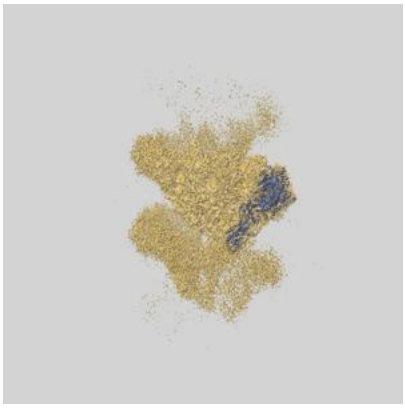
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.29	8.67	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 4.03 by more than 10 %

9 Map-model fit

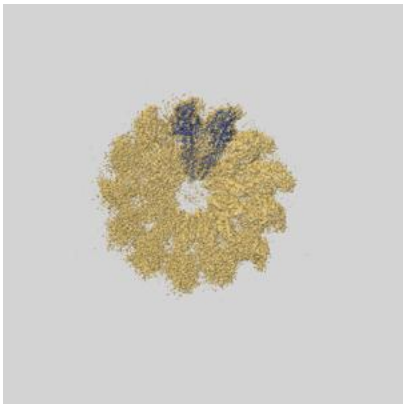
This section contains information regarding the fit between EMDB map EMD-23637 and PDB model 7M2Y. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay



X

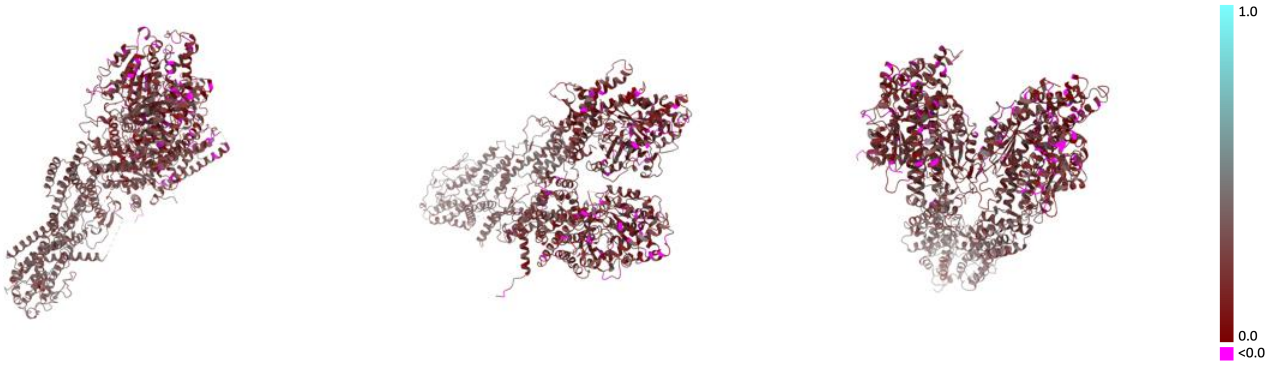
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

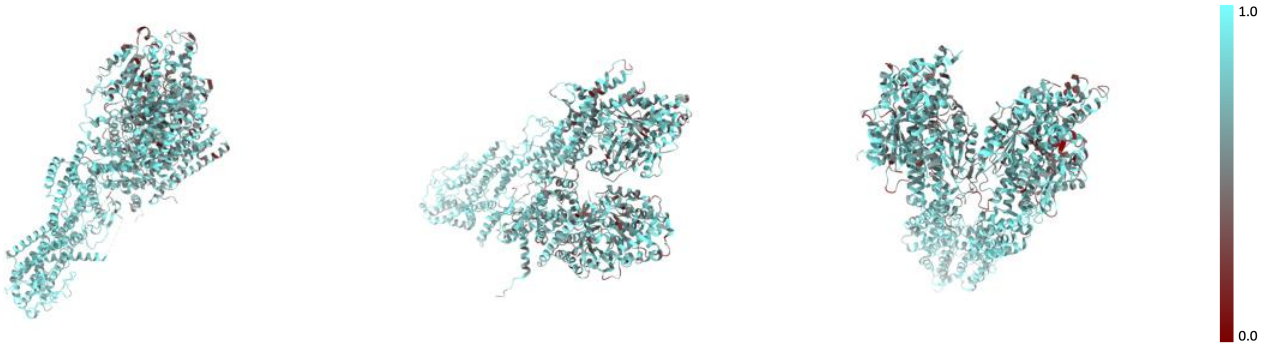
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

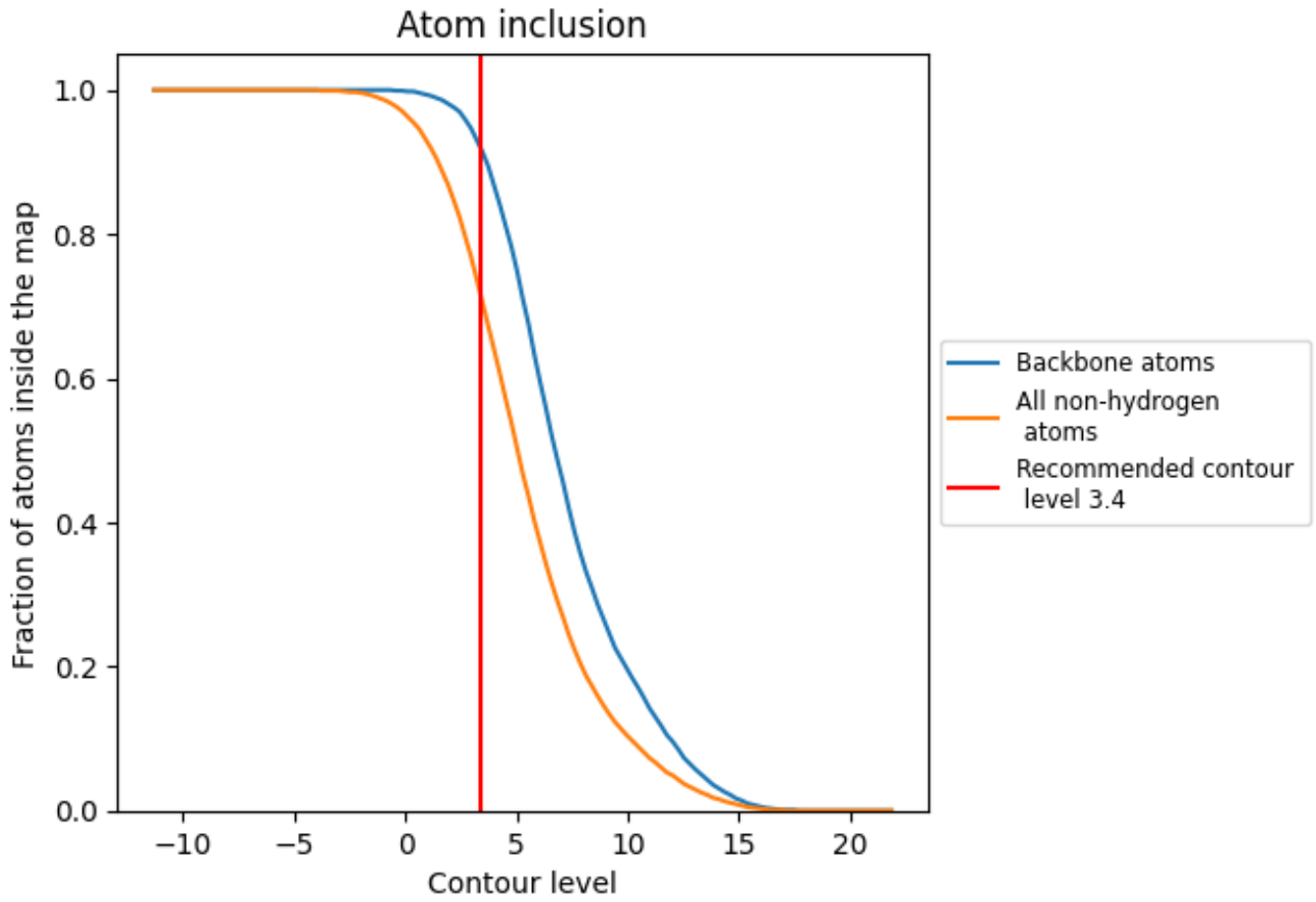
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.4).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 72% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.2490
A	0.6780	0.2060
B	0.6720	0.1950
C	0.7460	0.2780
D	0.7370	0.2830
U	0.6650	0.1940