



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:20 AM UTC

PDB ID : 8XZD / pdb_00008xzd
EMDB ID : EMD-38793
Title : The structure of fox ACE2 and Omicron BF.7 RBD complex
Authors : sun, J.Q.
Deposited on : 2024-01-21
Resolution : 3.47 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:

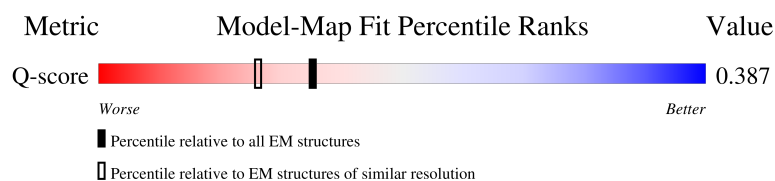
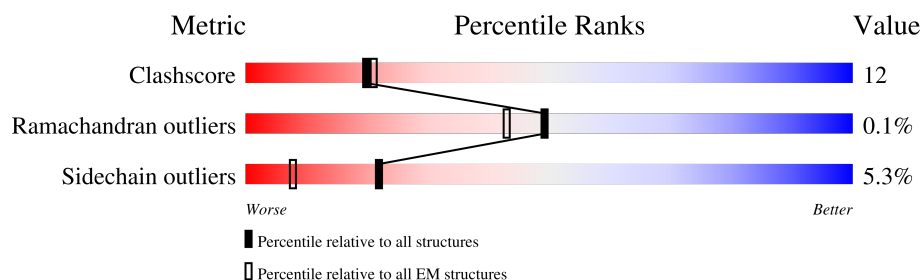
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.47 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	B	247	
2	A	613	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6436 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 Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	195	Total	C	N	O	S	0	0
			1550	999	260	283	8		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P0DTC2
B	302	HIS	-	expression tag	UNP P0DTC2
B	303	SER	-	expression tag	UNP P0DTC2
B	304	SER	-	expression tag	UNP P0DTC2
B	305	ALA	-	expression tag	UNP P0DTC2
B	306	LEU	-	expression tag	UNP P0DTC2
B	307	LEU	-	expression tag	UNP P0DTC2
B	308	CYS	-	expression tag	UNP P0DTC2
B	309	CYS	-	expression tag	UNP P0DTC2
B	310	LEU	-	expression tag	UNP P0DTC2
B	311	VAL	-	expression tag	UNP P0DTC2
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	THR	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	VAL	-	expression tag	UNP P0DTC2
B	317	ARG	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	596	Total	C	N	O	S	0	0
			4885	3123	810	923	29		

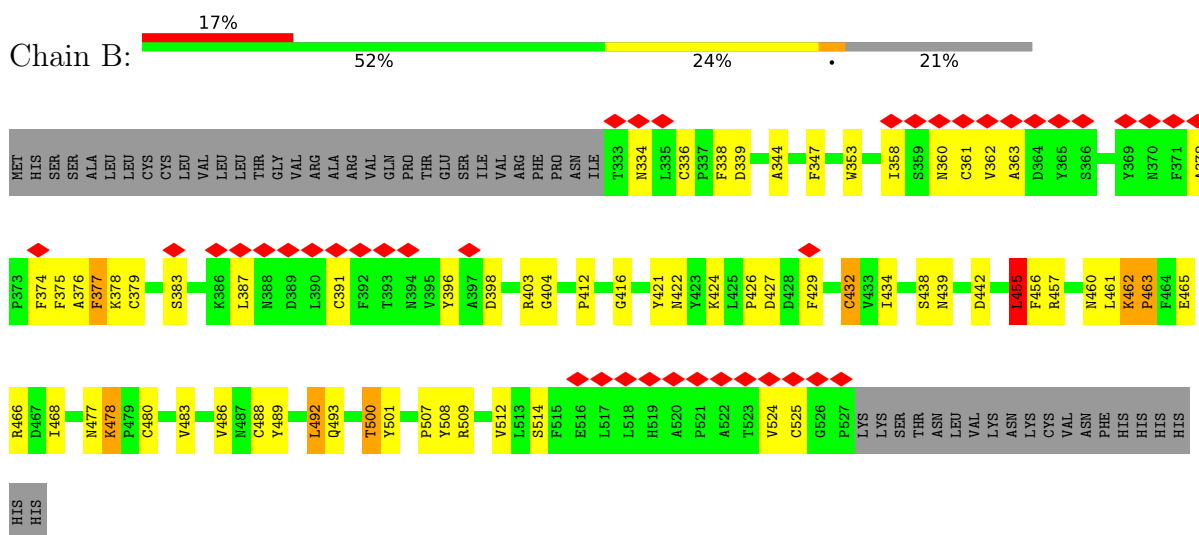
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

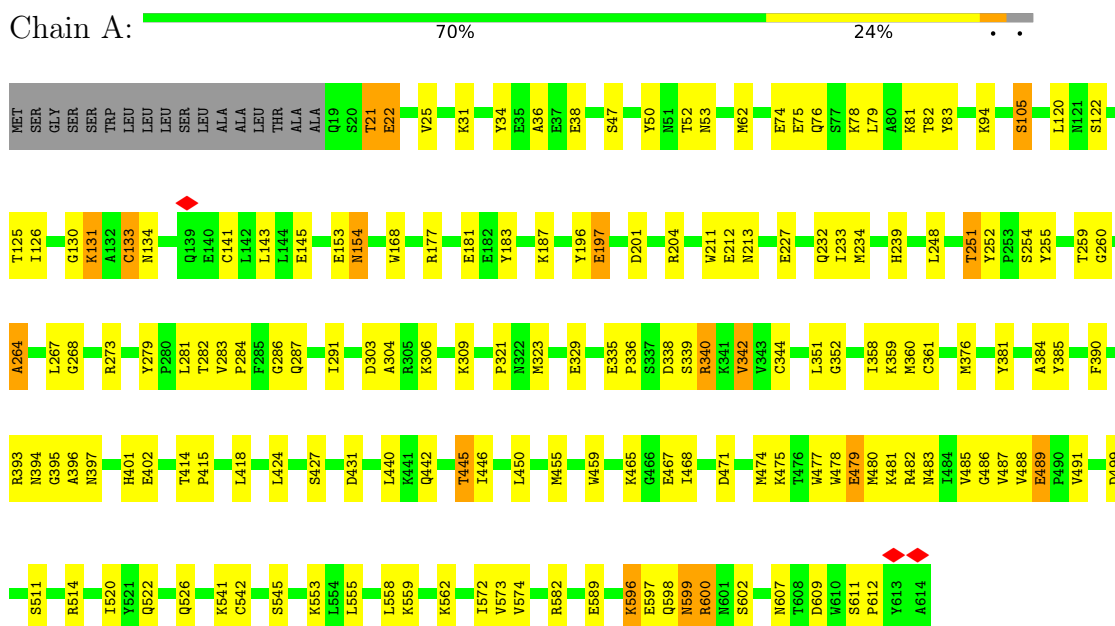
3 Residue-property plots

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

• Molecule 1: Spike protein S1



• Molecule 2: Angiotensin-converting enzyme



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69826	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.675	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.123	Depositor
Map size ($\text{\AA}$)	176.64, 176.64, 176.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.69, 0.69, 0.69	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.57	0/1597	1.01	15/2176 (0.7%)
2	A	1.49	7/5027 (0.1%)	1.26	78/6830 (1.1%)
All	All	1.33	7/6624 (0.1%)	1.20	93/9006 (1.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	522	GLN	CA-C	-5.89	1.45	1.52
2	A	252	TYR	CA-C	-5.81	1.47	1.52
2	A	134	ASN	CA-C	-5.70	1.46	1.53
2	A	477	TRP	CA-C	-5.26	1.46	1.52
2	A	211	TRP	CA-C	-5.24	1.46	1.52
2	A	468	ILE	CA-C	-5.18	1.48	1.53
2	A	459	TRP	CA-C	-5.05	1.46	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	339	SER	N-CA-C	10.71	124.47	111.40
2	A	255	TYR	N-CA-C	10.40	122.70	111.36
2	A	264	ALA	N-CA-C	9.93	122.10	111.28
2	A	286	GLY	N-CA-C	9.92	124.63	112.73
2	A	22	GLU	N-CA-C	-9.49	100.92	111.07
2	A	344	CYS	N-CA-C	9.14	124.43	113.28
2	A	573	VAL	N-CA-C	9.13	119.11	110.53
1	B	377	PHE	N-CA-C	-8.85	101.47	112.88
2	A	329	GLU	N-CA-C	8.47	120.59	111.36
2	A	612	PRO	N-CA-C	-8.28	106.07	114.68
2	A	282	THR	N-CA-C	8.16	122.02	112.72
2	A	609	ASP	N-CA-C	8.07	120.08	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	611	SER	CA-C-N	-7.94	112.73	120.83
2	A	611	SER	C-N-CA	-7.94	112.73	120.83
2	A	131	LYS	N-CA-C	7.70	121.66	109.50
2	A	268	GLY	N-CA-C	7.57	124.76	114.92
2	A	197	GLU	N-CA-C	7.55	119.59	111.36
2	A	483	ASN	N-CA-C	7.54	119.57	111.36
1	B	455	LEU	N-CA-C	7.41	119.43	111.36
2	A	21	THR	N-CA-C	-7.34	103.59	112.54
2	A	598	GLN	N-CA-C	7.30	119.24	111.28
1	B	501	TYR	N-CA-C	7.30	120.16	110.53
2	A	260	GLY	N-CA-C	7.28	124.57	112.85
2	A	342	VAL	N-CA-C	7.24	118.91	108.48
2	A	267	LEU	N-CA-C	7.03	121.45	113.02
2	A	212	GLU	N-CA-C	7.01	122.29	111.56
1	B	442	ASP	N-CA-C	6.90	118.88	111.36
2	A	602	SER	N-CA-C	6.80	119.74	110.55
2	A	397	ASN	N-CA-C	-6.77	99.05	109.14
2	A	599	ASN	CB-CA-C	-6.72	100.64	111.06
2	A	283	VAL	CB-CA-C	-6.71	102.97	110.68
2	A	52	THR	N-CA-C	6.69	118.65	111.36
2	A	574	VAL	N-CA-C	6.62	120.65	113.43
2	A	287	GLN	N-CA-C	6.57	118.10	111.07
2	A	82	THR	N-CA-C	6.51	118.38	111.28
2	A	445	THR	N-CA-C	6.40	118.33	111.36
2	A	177	ARG	CA-C-N	-6.30	112.05	119.05
2	A	177	ARG	C-N-CA	-6.30	112.05	119.05
2	A	338	ASP	N-CA-C	6.27	118.67	108.08
2	A	396	ALA	N-CA-C	6.25	118.09	111.28
2	A	22	GLU	N-CA-CB	6.24	119.05	110.01
2	A	196	TYR	N-CA-C	-6.20	101.30	110.48
2	A	145	GLU	CA-C-N	-6.19	112.10	119.84
2	A	145	GLU	C-N-CA	-6.19	112.10	119.84
2	A	168	TRP	N-CA-C	-6.19	104.53	111.28
2	A	338	ASP	CB-CA-C	-6.08	109.57	116.63
2	A	600	ARG	N-CA-C	-6.08	104.73	111.36
2	A	321	PRO	N-CA-C	6.06	121.01	111.38
1	B	465	GLU	N-CA-C	6.02	119.53	109.95
1	B	463	PRO	N-CA-C	6.02	120.53	111.14
2	A	234	MET	CA-C-N	-6.01	112.38	119.05
2	A	234	MET	C-N-CA	-6.01	112.38	119.05
2	A	340	ARG	N-CA-C	5.90	118.16	110.43
2	A	213	ASN	N-CA-C	5.88	118.44	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	251	THR	N-CA-C	5.87	117.76	111.36
2	A	522	GLN	CB-CA-C	-5.86	101.69	110.88
2	A	259	THR	N-CA-C	5.84	117.73	111.36
1	B	492	LEU	N-CA-C	5.74	119.17	109.76
2	A	133	CYS	N-CA-C	5.65	118.43	109.50
1	B	432	CYS	N-CA-C	5.64	118.09	108.90
1	B	500	THR	N-CA-C	5.61	119.83	113.15
2	A	254	SER	N-CA-C	5.59	117.45	111.36
1	B	374	PHE	N-CA-C	5.52	118.23	110.23
2	A	384	ALA	N-CA-C	5.50	117.28	111.28
2	A	36	ALA	N-CA-C	5.49	117.34	111.36
2	A	589	GLU	CA-C-N	-5.47	112.98	119.05
2	A	589	GLU	C-N-CA	-5.47	112.98	119.05
2	A	427	SER	N-CA-C	5.44	119.55	113.02
2	A	81	LYS	N-CA-C	-5.44	105.91	112.54
2	A	304	ALA	N-CA-C	5.40	117.17	111.28
2	A	154	ASN	N-CA-C	5.39	120.87	113.97
2	A	582	ARG	CA-C-N	-5.37	113.09	119.05
2	A	582	ARG	C-N-CA	-5.37	113.09	119.05
2	A	273	ARG	N-CA-C	5.36	117.12	111.28
2	A	105	SER	N-CA-C	5.35	122.19	110.80
1	B	416	GLY	N-CA-C	-5.30	101.86	110.55
2	A	450	LEU	CA-C-N	-5.27	113.20	119.05
2	A	450	LEU	C-N-CA	-5.27	113.20	119.05
2	A	306	LYS	N-CA-C	-5.23	105.58	111.28
1	B	339	ASP	N-CA-C	5.20	117.37	111.02
2	A	352	GLY	CA-C-O	-5.20	118.58	122.37
2	A	486	GLY	N-CA-C	5.19	123.11	113.76
1	B	478	LYS	CA-C-N	-5.17	114.44	119.76
1	B	478	LYS	C-N-CA	-5.17	114.44	119.76
2	A	279	TYR	CA-C-N	-5.16	113.32	119.05
2	A	279	TYR	C-N-CA	-5.16	113.32	119.05
2	A	130	GLY	N-CA-C	5.08	118.45	111.54
1	B	372	ALA	N-CA-C	5.05	120.98	109.81
2	A	390	PHE	N-CA-C	5.05	116.47	111.07
2	A	83	TYR	CA-C-N	-5.03	114.40	119.83
2	A	83	TYR	C-N-CA	-5.03	114.40	119.83
2	A	134	ASN	CA-C-N	-5.01	113.39	118.85
2	A	134	ASN	C-N-CA	-5.01	113.39	118.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	B	1550	0	1479	54	0
2	A	4885	0	4654	106	0
3	A	1	0	0	0	0
All	All	6436	0	6133	155	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 12.

All (155) 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:A:381:TYR:CE2	2:A:385:TYR:HE2	1.44	1.36
2:A:394:ASN:HB2	2:A:562:LYS:HE3	1.20	1.18
2:A:381:TYR:CE2	2:A:385:TYR:CE2	2.31	1.18
2:A:394:ASN:CB	2:A:562:LYS:HE3	1.73	1.15
2:A:336:PRO:HG2	2:A:342:VAL:HG21	1.16	1.14
2:A:381:TYR:OH	2:A:395:GLY:HA2	1.47	1.13
2:A:47:SER:HA	2:A:62:MET:CE	1.80	1.11
1:B:375:PHE:CE1	1:B:508:TYR:CE2	2.39	1.09
2:A:394:ASN:HB2	2:A:562:LYS:CE	1.82	1.08
2:A:47:SER:CA	2:A:62:MET:HE2	1.89	1.02
2:A:455:MET:HE1	2:A:481:LYS:HG2	1.39	1.02
2:A:47:SER:HA	2:A:62:MET:HE2	1.00	1.00
1:B:396:TYR:HB2	1:B:514:SER:OG	1.61	0.99
2:A:131:LYS:HG2	2:A:143:LEU:HD23	1.40	0.99
1:B:489:TYR:CE1	2:A:31:LYS:HG2	1.98	0.98
1:B:375:PHE:CZ	1:B:508:TYR:CD2	2.51	0.98
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.04	0.98
2:A:455:MET:CE	2:A:481:LYS:HG2	1.96	0.96
2:A:455:MET:HE1	2:A:481:LYS:CG	1.94	0.96
2:A:336:PRO:HG2	2:A:342:VAL:CG2	1.95	0.95
1:B:375:PHE:HZ	1:B:508:TYR:HD2	1.16	0.93
2:A:381:TYR:HE2	2:A:385:TYR:HE2	1.14	0.92
2:A:131:LYS:HG2	2:A:143:LEU:CD2	2.00	0.91
1:B:455:LEU:HD21	2:A:34:TYR:HE2	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:CYS:SG	1:B:363:ALA:CB	2.60	0.90
1:B:375:PHE:CZ	1:B:508:TYR:CE2	2.63	0.86
1:B:375:PHE:CZ	1:B:508:TYR:HD2	1.92	0.85
2:A:381:TYR:HH	2:A:395:GLY:HA2	1.37	0.85
2:A:76:GLN:HE21	2:A:79:LEU:HD12	1.38	0.84
1:B:375:PHE:CE1	1:B:508:TYR:HE2	1.96	0.84
2:A:442:GLN:O	2:A:445:THR:HG22	1.78	0.84
2:A:336:PRO:CG	2:A:342:VAL:HG21	2.05	0.83
1:B:375:PHE:CE1	1:B:508:TYR:CD2	2.69	0.80
2:A:133:CYS:HB3	2:A:141:CYS:SG	2.22	0.80
1:B:379:CYS:HG	1:B:432:CYS:HG	0.92	0.79
2:A:455:MET:HE3	2:A:480:MET:HB3	1.65	0.79
1:B:468:ILE:O	1:B:468:ILE:HG22	1.82	0.78
2:A:485:VAL:HG12	2:A:485:VAL:O	1.83	0.78
2:A:455:MET:HE3	2:A:480:MET:CB	2.14	0.78
2:A:394:ASN:CB	2:A:562:LYS:CE	2.52	0.77
2:A:455:MET:HE1	2:A:481:LYS:N	2.01	0.75
2:A:76:GLN:NE2	2:A:79:LEU:HD12	2.01	0.74
2:A:393:ARG:O	2:A:394:ASN:OD1	2.05	0.74
1:B:336:CYS:SG	1:B:363:ALA:HA	2.30	0.72
2:A:381:TYR:CD2	2:A:385:TYR:CE2	2.76	0.72
1:B:455:LEU:HD21	2:A:34:TYR:CE2	2.23	0.71
2:A:526:GLN:NE2	2:A:542:CYS:SG	2.64	0.71
2:A:394:ASN:HB3	2:A:562:LYS:HE3	1.68	0.70
2:A:478:TRP:CD2	2:A:489:GLU:HG3	2.26	0.70
2:A:597:GLU:HG2	2:A:600:ARG:HH22	1.55	0.70
2:A:381:TYR:CD2	2:A:385:TYR:HE2	2.05	0.69
1:B:336:CYS:HB3	1:B:361:CYS:SG	2.31	0.69
1:B:424:LYS:HD3	1:B:463:PRO:HA	1.72	0.69
2:A:197:GLU:HB2	2:A:201:ASP:OD2	1.92	0.68
2:A:414:THR:HB	2:A:415:PRO:HD2	1.76	0.67
2:A:489:GLU:H	2:A:489:GLU:CD	2.03	0.66
1:B:336:CYS:SG	1:B:363:ALA:CA	2.84	0.65
2:A:485:VAL:O	2:A:485:VAL:CG1	2.45	0.64
1:B:391:CYS:SG	1:B:525:CYS:HB3	2.36	0.64
2:A:599:ASN:OD1	2:A:599:ASN:C	2.41	0.63
1:B:375:PHE:HE1	1:B:508:TYR:CE2	2.10	0.63
1:B:468:ILE:O	1:B:468:ILE:CG2	2.48	0.62
2:A:120:LEU:HD21	2:A:183:TYR:CE1	2.35	0.62
2:A:239:HIS:ND1	2:A:599:ASN:ND2	2.47	0.62
2:A:381:TYR:CD2	2:A:401:HIS:NE2	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:GLU:O	2:A:79:LEU:HG	1.99	0.61
2:A:21:THR:HG22	2:A:25:VAL:HG23	1.82	0.61
2:A:76:GLN:HE21	2:A:79:LEU:CD1	2.10	0.60
2:A:455:MET:HE1	2:A:481:LYS:CA	2.33	0.58
2:A:50:TYR:HB3	2:A:62:MET:CE	2.34	0.58
2:A:465:LYS:HD2	2:A:467:GLU:HG3	1.86	0.58
1:B:466:ARG:HD3	1:B:468:ILE:HD11	1.85	0.57
2:A:131:LYS:CG	2:A:143:LEU:CD2	2.80	0.56
1:B:477:ASN:OD1	1:B:478:LYS:N	2.38	0.56
1:B:375:PHE:HZ	1:B:508:TYR:CD2	1.95	0.56
1:B:489:TYR:CD1	2:A:31:LYS:HE2	2.42	0.55
2:A:445:THR:HG23	2:A:446:ILE:HG13	1.88	0.54
2:A:50:TYR:HB3	2:A:62:MET:HE1	1.90	0.54
2:A:131:LYS:CG	2:A:143:LEU:HD23	2.28	0.54
2:A:511:SER:OG	2:A:514:ARG:NH2	2.41	0.54
2:A:555:LEU:HG	2:A:559:LYS:HE3	1.89	0.53
2:A:455:MET:CE	2:A:481:LYS:N	2.69	0.53
2:A:131:LYS:HG2	2:A:143:LEU:HD21	1.89	0.53
1:B:353:TRP:HE1	1:B:466:ARG:HB2	1.73	0.53
1:B:396:TYR:HB2	1:B:514:SER:HG	1.74	0.52
2:A:394:ASN:HD22	2:A:562:LYS:HZ2	1.58	0.52
1:B:376:ALA:HB1	1:B:378:LYS:HG2	1.91	0.52
2:A:394:ASN:HB2	2:A:562:LYS:NZ	2.22	0.52
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.75	0.51
1:B:375:PHE:CZ	1:B:508:TYR:HE2	2.20	0.51
2:A:475:LYS:HG2	2:A:479:GLU:OE2	2.11	0.50
1:B:489:TYR:HD1	2:A:31:LYS:HE2	1.77	0.49
2:A:478:TRP:CE3	2:A:489:GLU:HG3	2.46	0.49
2:A:442:GLN:O	2:A:445:THR:CG2	2.57	0.49
2:A:455:MET:HE3	2:A:480:MET:HB2	1.93	0.49
1:B:334:ASN:O	1:B:362:VAL:N	2.41	0.49
1:B:379:CYS:CB	1:B:432:CYS:SG	3.00	0.49
2:A:381:TYR:CE2	2:A:385:TYR:CD2	2.98	0.49
1:B:336:CYS:SG	1:B:338:PHE:CD1	3.02	0.48
1:B:421:TYR:C	1:B:461:LEU:HD11	2.38	0.48
2:A:53:ASN:CB	2:A:340:ARG:HD2	2.43	0.48
2:A:487:VAL:HG12	2:A:488:VAL:N	2.27	0.48
1:B:383:SER:H	1:B:387:LEU:HD22	1.78	0.48
2:A:381:TYR:HH	2:A:395:GLY:CA	2.19	0.48
2:A:381:TYR:HD1	2:A:558:LEU:HD22	1.78	0.48
2:A:394:ASN:CB	2:A:562:LYS:NZ	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:394:ASN:HD22	2:A:562:LYS:NZ	2.11	0.47
2:A:153:GLU:CD	2:A:154:ASN:OD1	2.57	0.47
2:A:264:ALA:HB2	2:A:487:VAL:CG1	2.44	0.47
2:A:342:VAL:HG13	2:A:359:LYS:CE	2.45	0.47
1:B:438:SER:OG	1:B:509:ARG:HG3	2.15	0.47
2:A:53:ASN:CG	2:A:340:ARG:HD2	2.40	0.47
1:B:421:TYR:HB3	1:B:457:ARG:HE	1.78	0.47
1:B:377:PHE:HE1	1:B:434:ILE:HD11	1.79	0.47
2:A:445:THR:HG23	2:A:446:ILE:N	2.28	0.46
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.98	0.46
2:A:76:GLN:NE2	2:A:79:LEU:CD1	2.73	0.46
1:B:462:LYS:HA	1:B:462:LYS:HD2	1.41	0.45
2:A:381:TYR:HE2	2:A:385:TYR:CE2	2.02	0.45
1:B:422:ASN:N	1:B:461:LEU:HD11	2.31	0.45
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.98	0.45
1:B:379:CYS:HB2	1:B:432:CYS:SG	2.57	0.45
2:A:284:PRO:HD3	2:A:440:LEU:HD23	1.98	0.45
2:A:596:LYS:HZ2	2:A:596:LYS:HG2	1.64	0.45
2:A:394:ASN:O	2:A:562:LYS:HG3	2.16	0.45
2:A:418:LEU:HB2	2:A:424:LEU:CD1	2.47	0.45
1:B:480:CYS:CB	1:B:488:CYS:HG	2.29	0.44
2:A:455:MET:SD	2:A:481:LYS:HG2	2.57	0.44
2:A:122:SER:O	2:A:125:THR:OG1	2.35	0.44
1:B:377:PHE:O	1:B:378:LYS:C	2.59	0.44
2:A:53:ASN:CG	2:A:340:ARG:CD	2.91	0.44
2:A:482:ARG:NH1	2:A:489:GLU:OE2	2.52	0.43
1:B:360:ASN:H	1:B:524:VAL:HG22	1.84	0.43
2:A:251:THR:HG21	2:A:281:LEU:HD22	2.00	0.43
2:A:395:GLY:O	2:A:562:LYS:HE2	2.19	0.43
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.54	0.43
2:A:131:LYS:CG	2:A:143:LEU:HD21	2.48	0.42
2:A:201:ASP:OD1	2:A:204:ARG:NH2	2.52	0.42
2:A:455:MET:CE	2:A:481:LYS:CG	2.73	0.42
2:A:120:LEU:HD21	2:A:183:TYR:HE1	1.81	0.42
1:B:403:ARG:HG2	1:B:404:GLY:N	2.35	0.42
2:A:376:MET:HE2	2:A:376:MET:HB3	1.73	0.42
2:A:474:MET:HE1	2:A:499:ASP:CG	2.45	0.42
2:A:381:TYR:OH	2:A:395:GLY:CA	2.39	0.41
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.03	0.41
2:A:335:GLU:HB2	2:A:361:CYS:HB3	2.02	0.41
2:A:53:ASN:HB2	2:A:340:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:O	1:B:387:LEU:HB2	2.20	0.41
2:A:21:THR:O	2:A:22:GLU:C	2.61	0.41
1:B:439:ASN:HA	1:B:507:PRO:HG2	2.03	0.41
2:A:50:TYR:HB3	2:A:62:MET:HE3	2.01	0.41
2:A:183:TYR:CE1	2:A:187:LYS:HE3	2.56	0.41
2:A:74:GLU:HG2	2:A:78:LYS:HE3	2.03	0.41
2:A:360:MET:HE3	2:A:360:MET:HB2	1.93	0.41
1:B:336:CYS:CB	1:B:361:CYS:SG	3.05	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	B	193/247 (78%)	181 (94%)	12 (6%)	0	100	100
2	A	594/613 (97%)	581 (98%)	12 (2%)	1 (0%)	43	74
All	All	787/860 (92%)	762 (97%)	24 (3%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	105	SER

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	B	167/216 (77%)	157 (94%)	10 (6%)	17	44
2	A	530/542 (98%)	503 (95%)	27 (5%)	21	48
All	All	697/758 (92%)	660 (95%)	37 (5%)	22	47

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	358	ILE
1	B	455	LEU
1	B	456	PHE
1	B	460	ASN
1	B	462	LYS
1	B	483	VAL
1	B	486	VAL
1	B	492	LEU
1	B	493	GLN
1	B	500	THR
2	A	38	GLU
2	A	94	LYS
2	A	126	ILE
2	A	181	GLU
2	A	227	GLU
2	A	232	GLN
2	A	233	ILE
2	A	248	LEU
2	A	291	ILE
2	A	303	ASP
2	A	309	LYS
2	A	323	MET
2	A	351	LEU
2	A	358	ILE
2	A	402	GLU
2	A	431	ASP
2	A	471	ASP
2	A	479	GLU
2	A	489	GLU
2	A	491	VAL
2	A	520	ILE
2	A	541	LYS
2	A	545	SER
2	A	553	LYS
2	A	572	ILE

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Mol	Chain	Res	Type
2	A	596	LYS
2	A	607	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	370	ASN
1	B	414	GLN
1	B	417	ASN
1	B	437	ASN
1	B	474	GLN
2	A	26	ASN
2	A	60	GLN
2	A	76	GLN
2	A	238	GLN
2	A	241	HIS
2	A	394	ASN
2	A	437	ASN
2	A	508	ASN
2	A	526	GLN
2	A	599	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

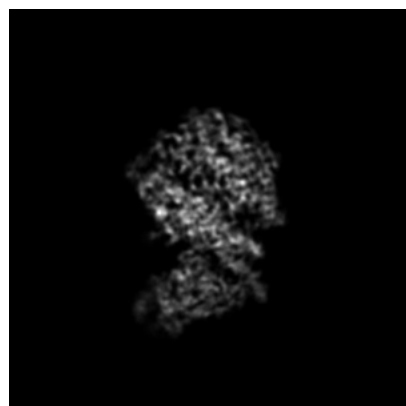
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38793. These allow visual inspection of the internal detail of the map and identification of artifacts.

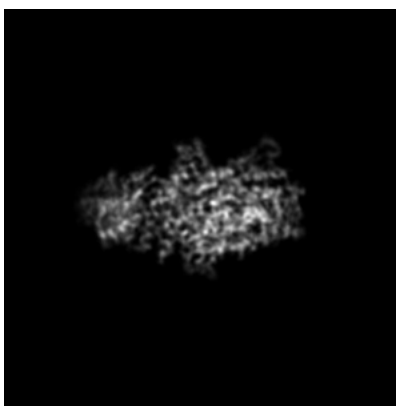
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

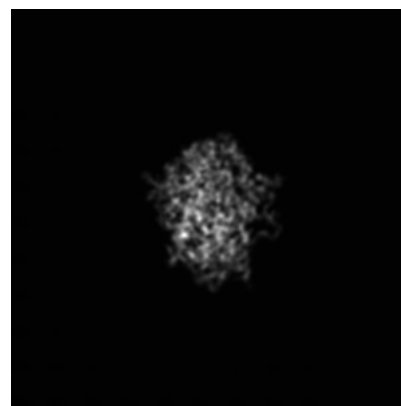
6.1.1 Primary map



X

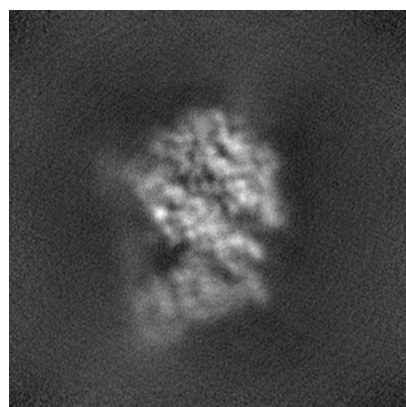


Y

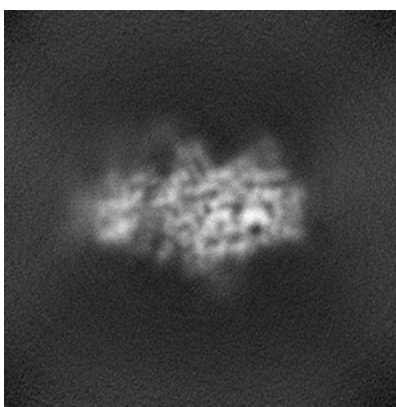


Z

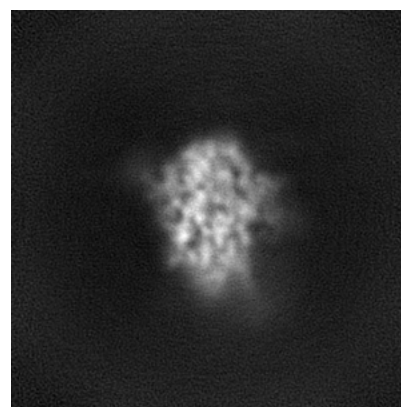
6.1.2 Raw map



X



Y

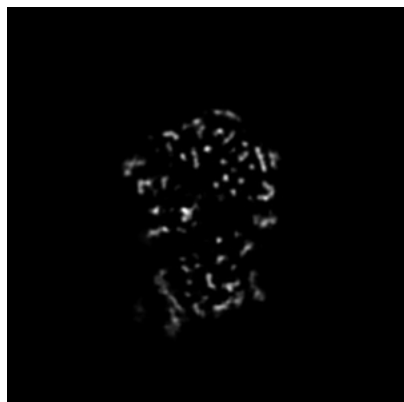


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

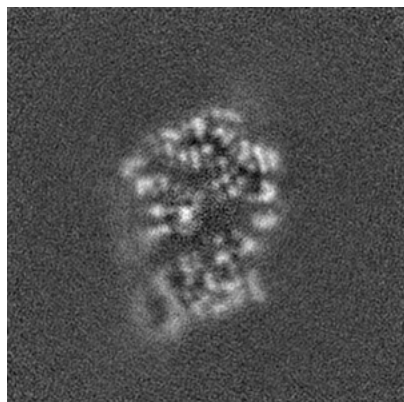


Y Index: 128

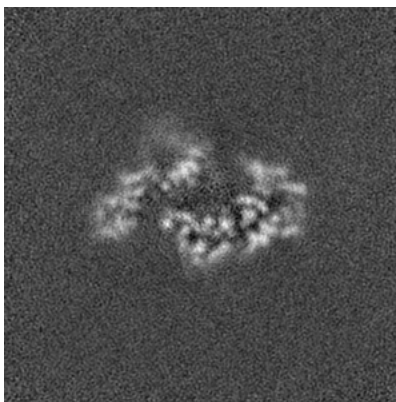


Z Index: 128

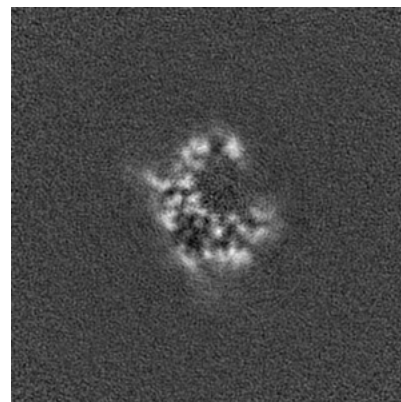
6.2.2 Raw map



X Index: 128



Y Index: 128

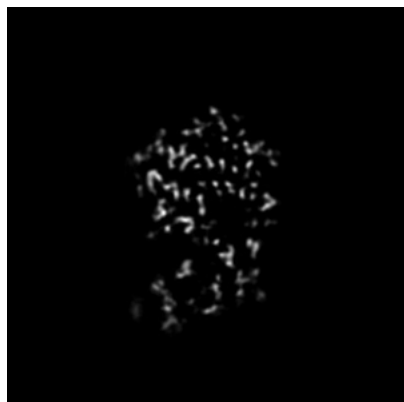


Z Index: 128

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

6.3 Largest variance slices [i](#)

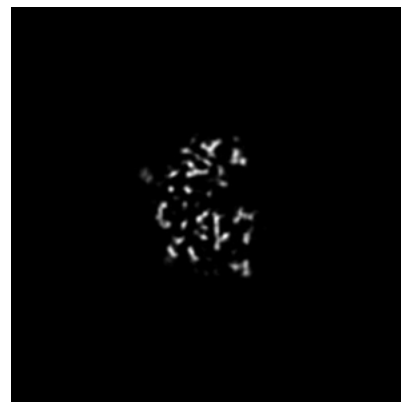
6.3.1 Primary map



X Index: 124

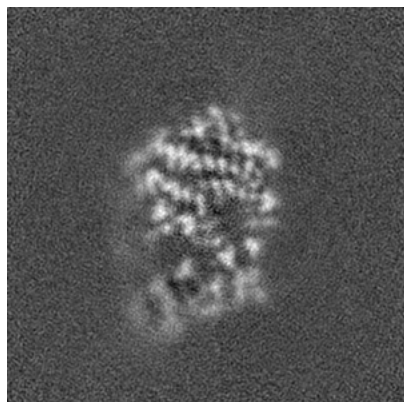


Y Index: 124

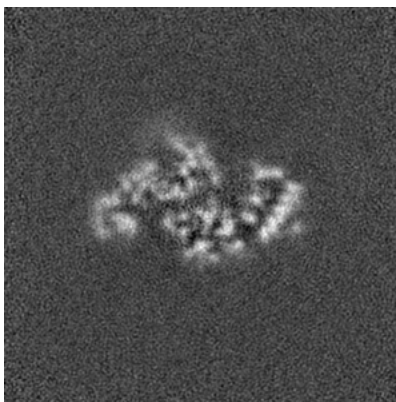


Z Index: 134

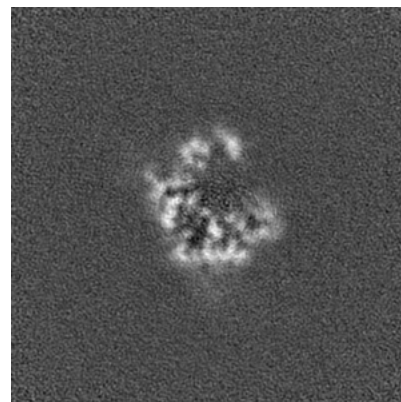
6.3.2 Raw map



X Index: 124



Y Index: 124

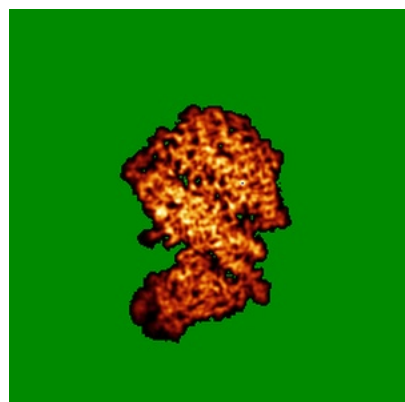


Z Index: 126

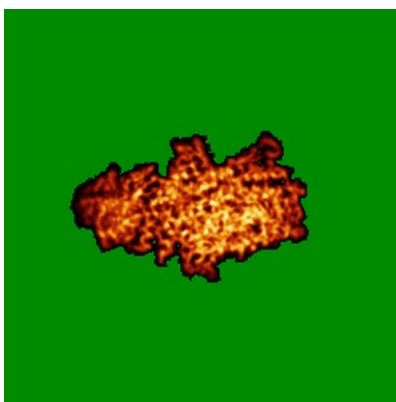
The images above show the largest variance slices of the map in three orthogonal directions.

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

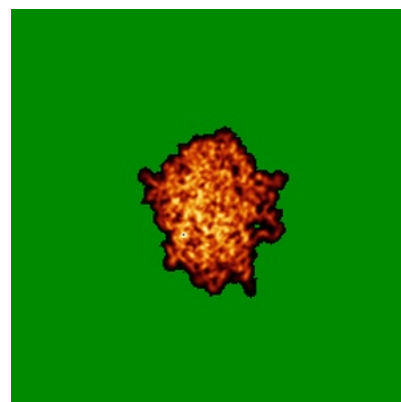
6.4.1 Primary map



X

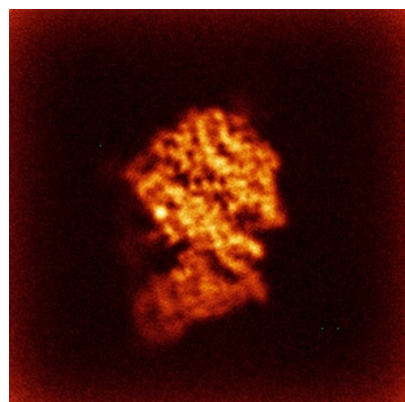


Y

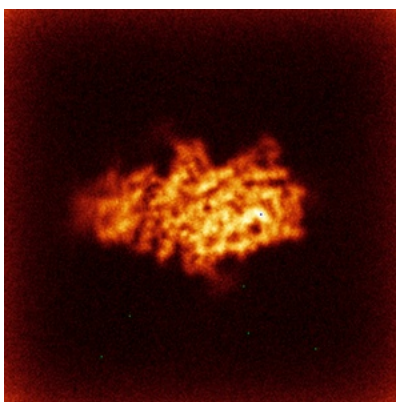


Z

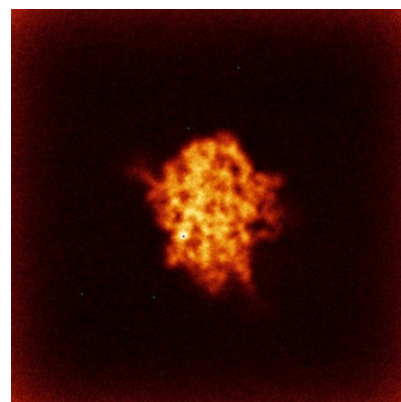
6.4.2 Raw map



X



Y

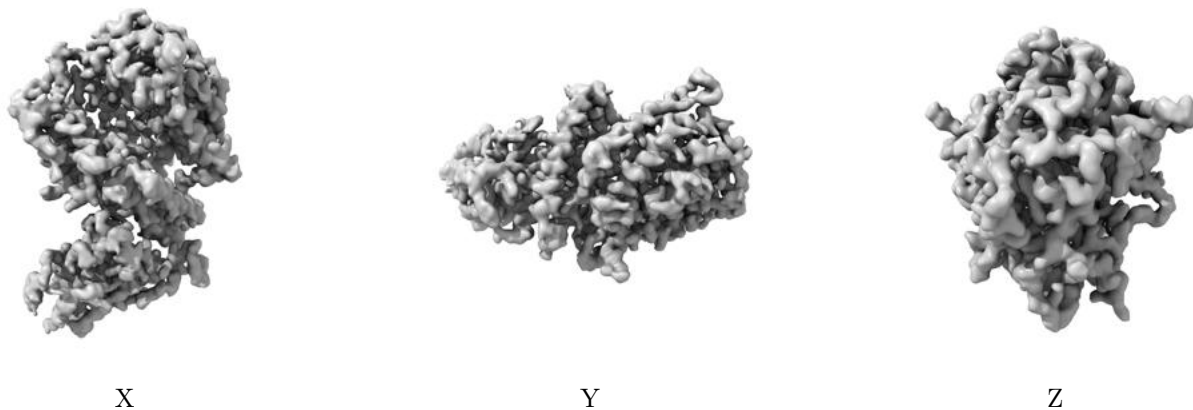


Z

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

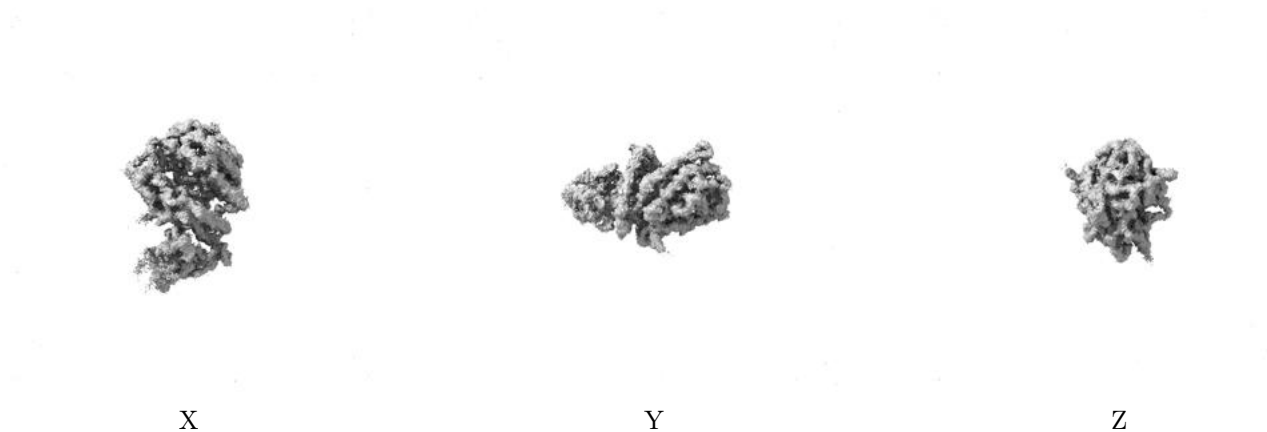
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.123. 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.

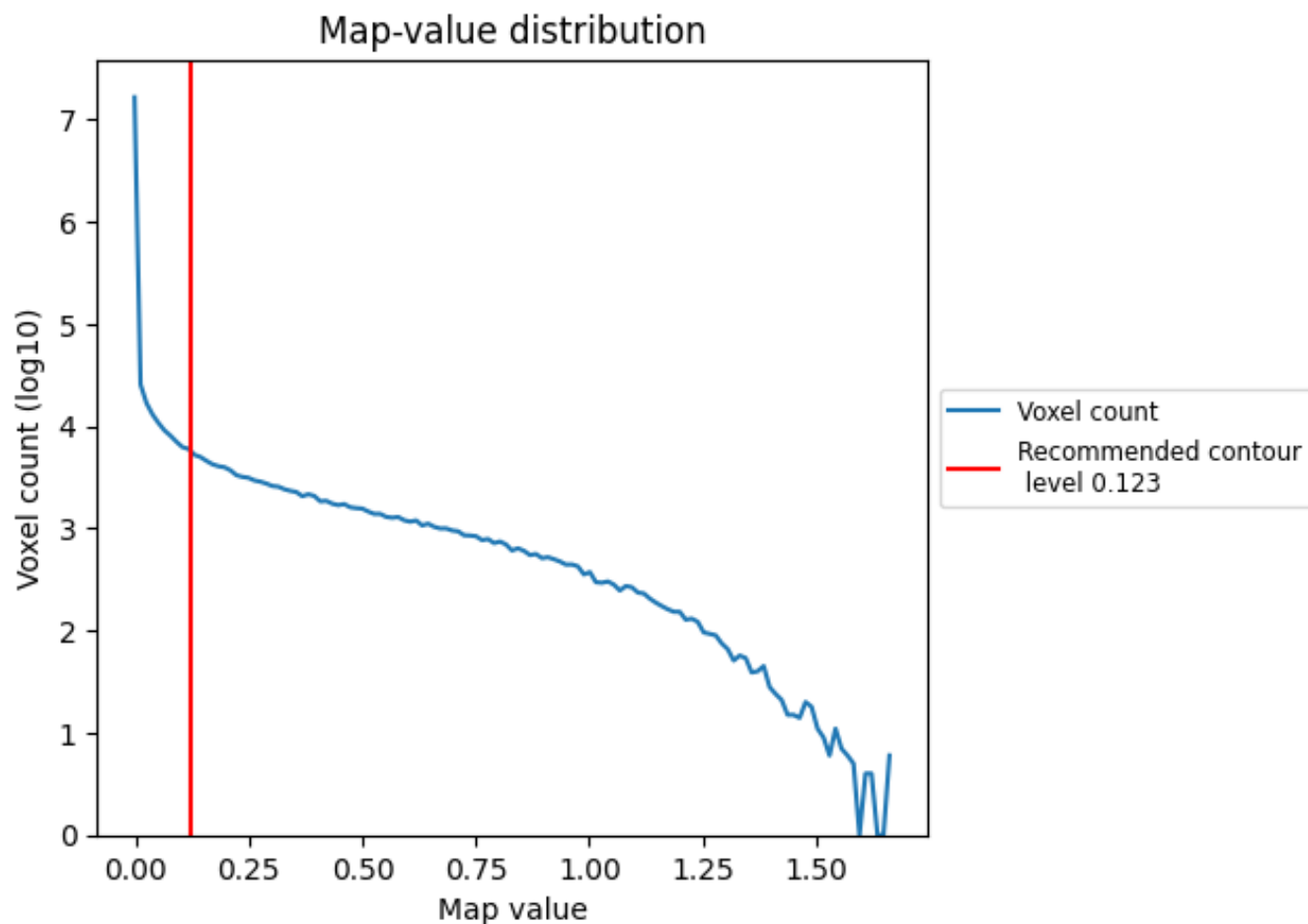
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

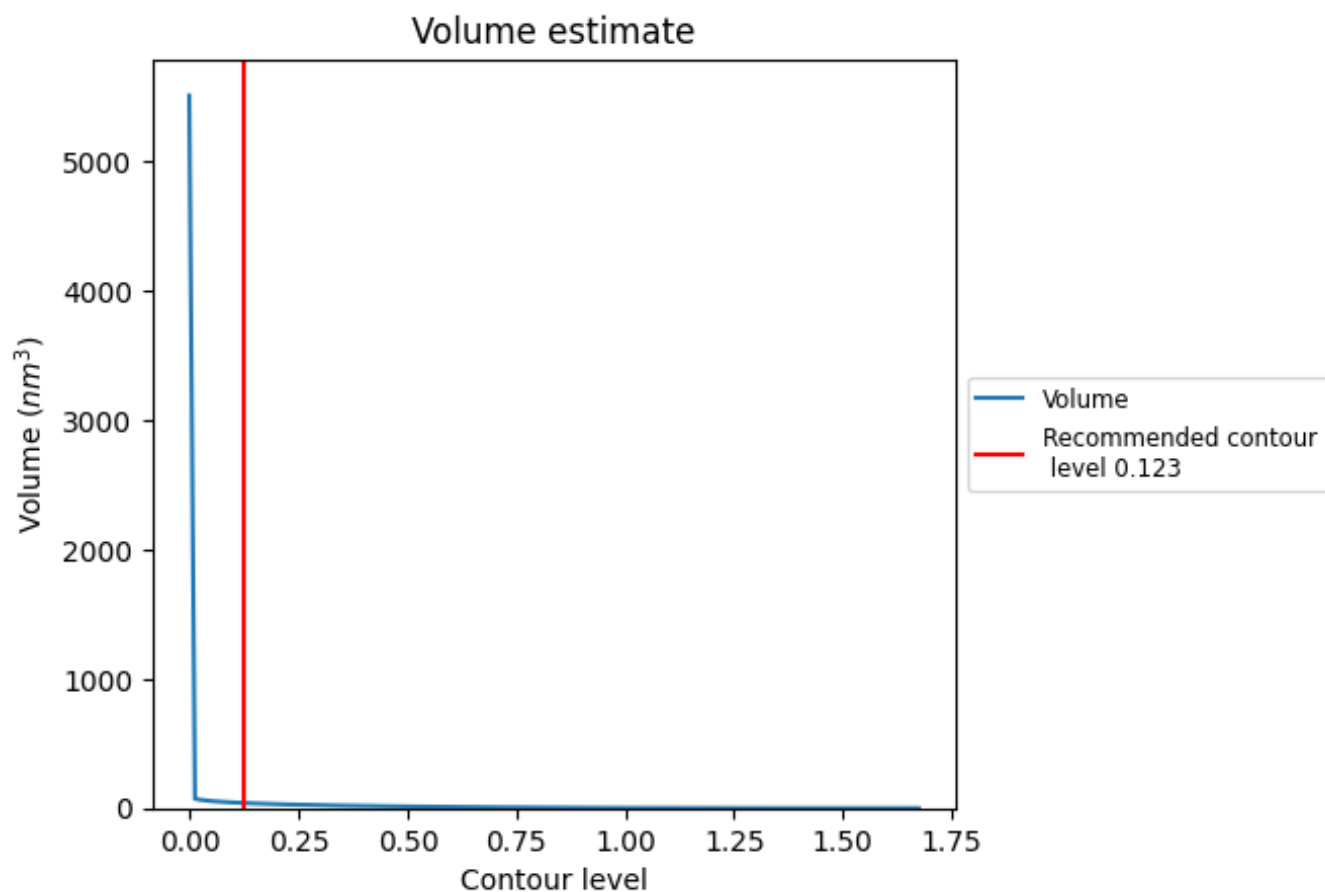
This section contains the results of statistical analysis of the map.

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.

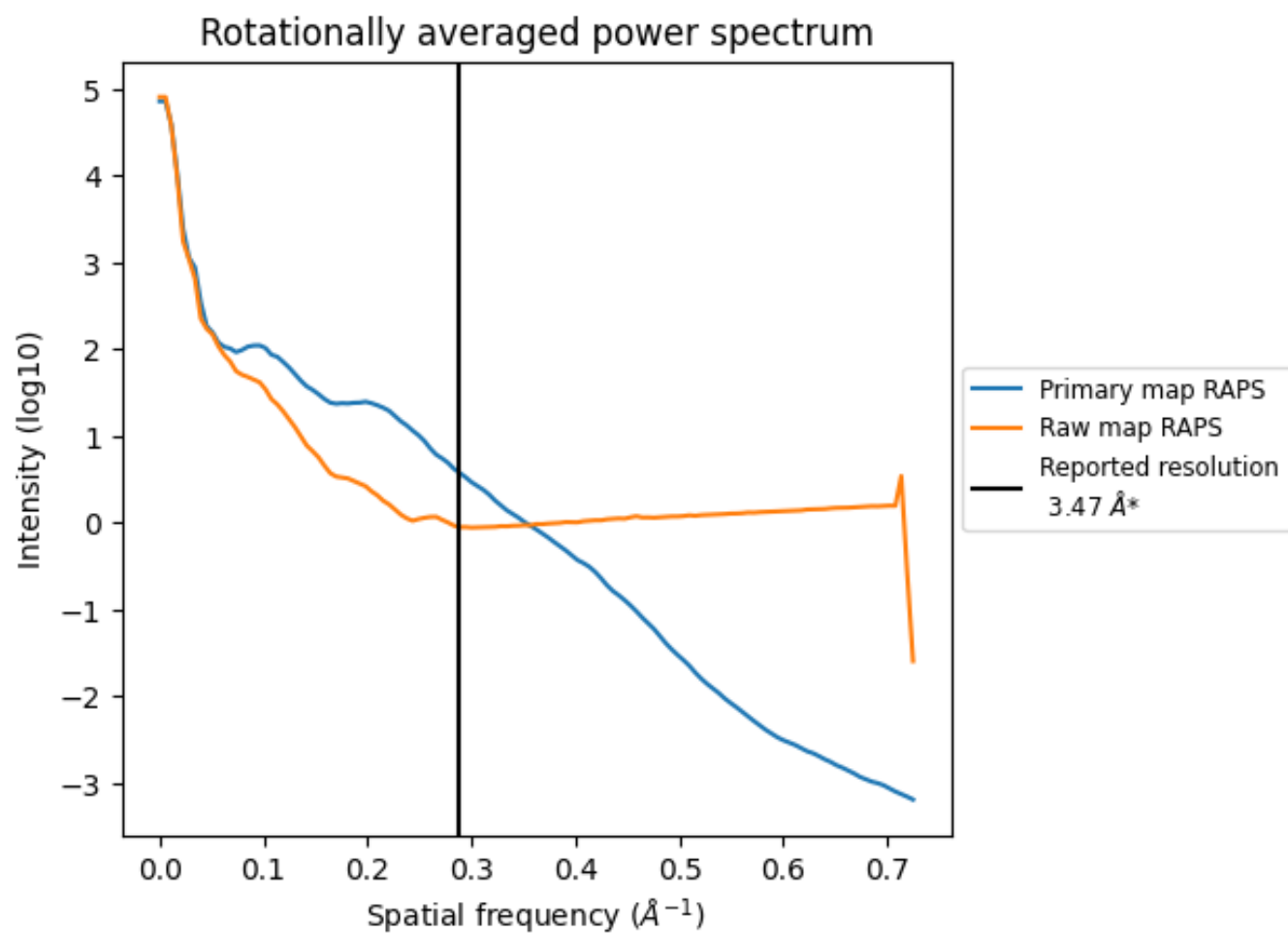
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm^3 ; this corresponds to an approximate mass of 36 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 ⓘ

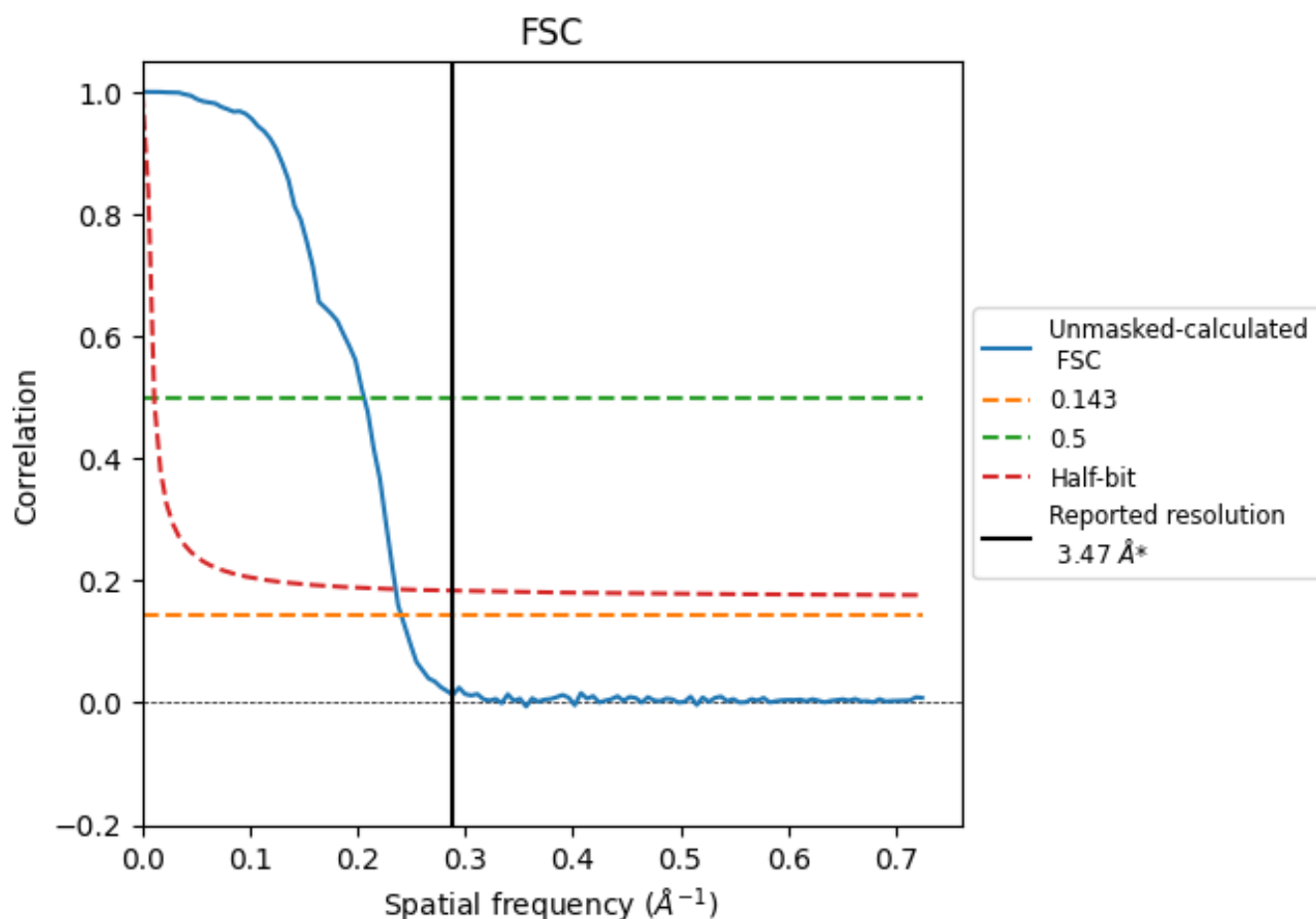


*Reported resolution corresponds to spatial frequency of 0.288 $\text{\AA}^{-1}$

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

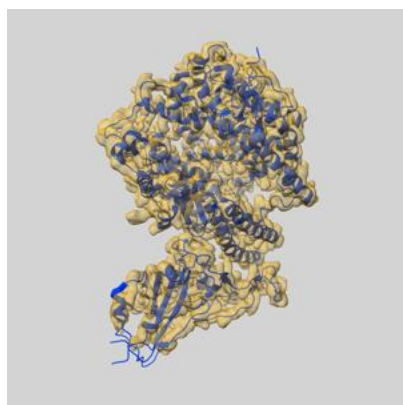
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	4.85	4.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.47 by more than 10 %

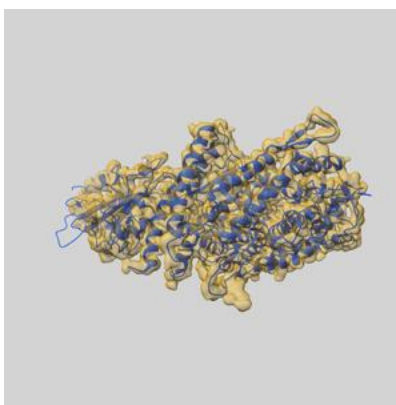
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38793 and PDB model 8XZD. Per-residue inclusion information can be found in section 3 on page 5.

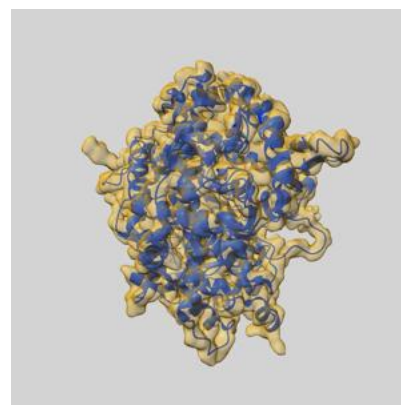
9.1 Map-model overlay [i](#)



X



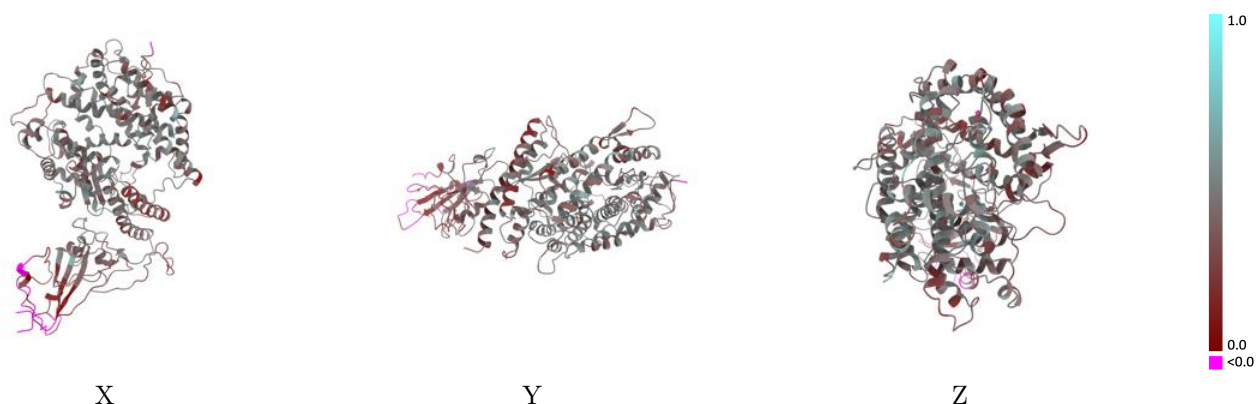
Y



Z

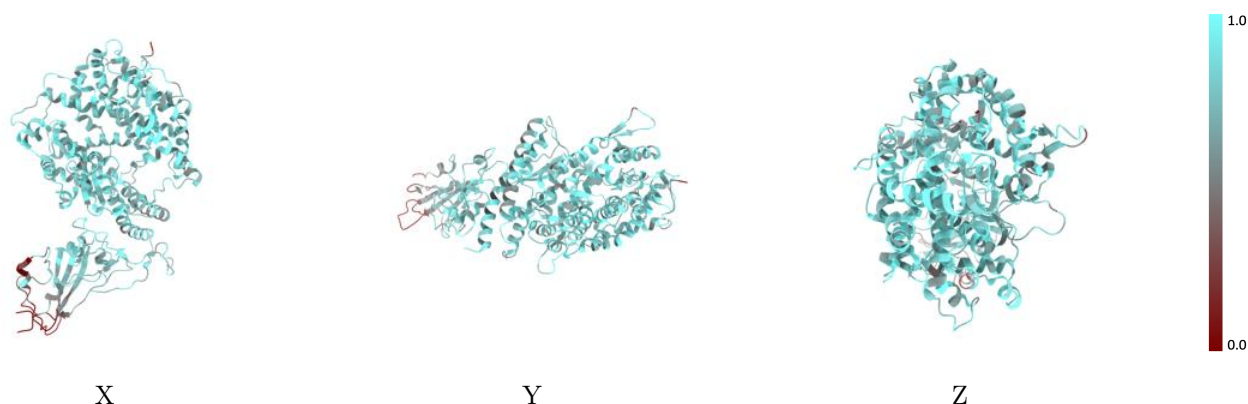
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



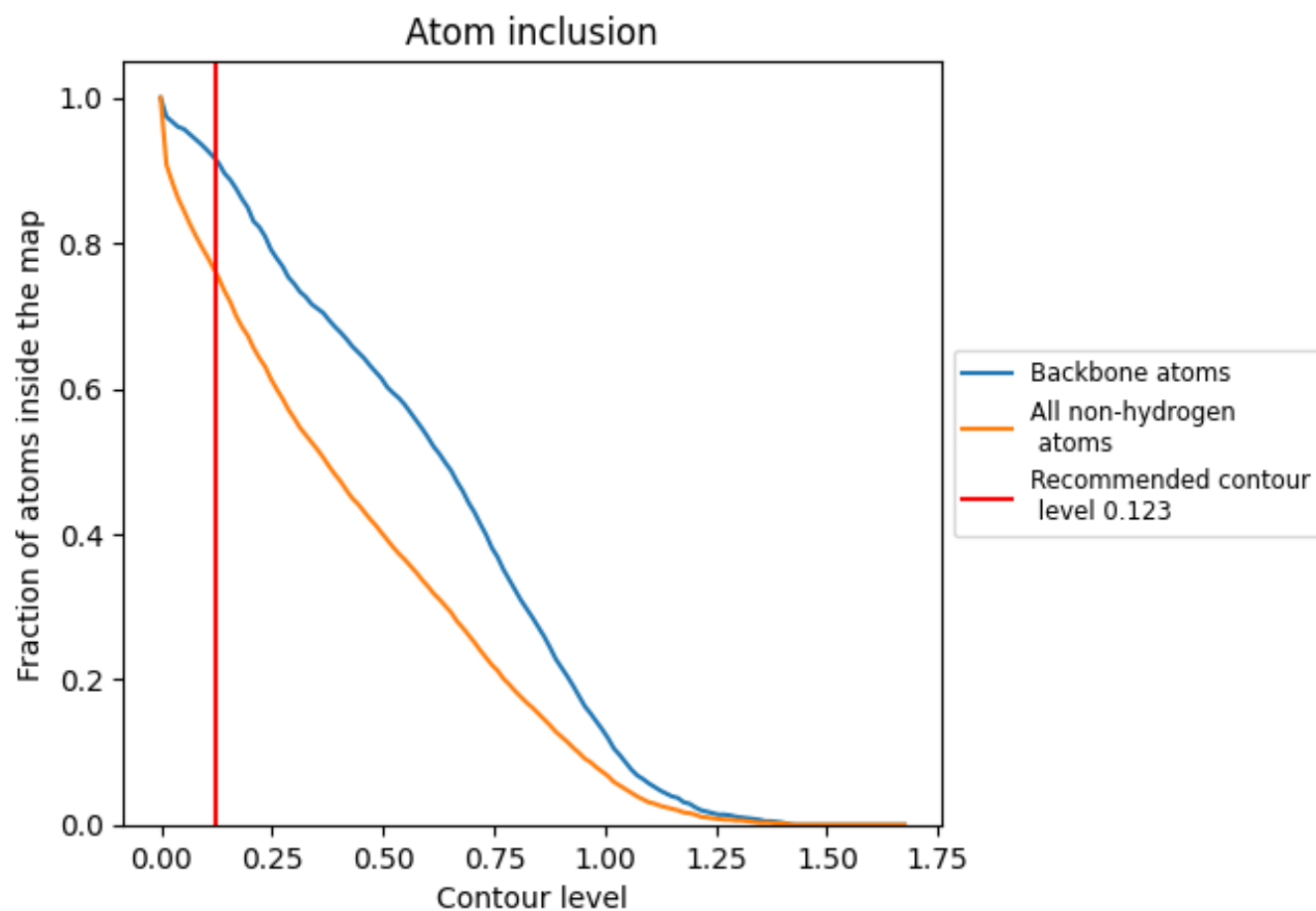
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.3870
A	0.8070	0.4270
B	0.6070	0.2640

