



Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 03:01 PM EDT

PDB ID : 9ORE / pdb_00009ore
EMDB ID : EMD-70773
Title : CryoEM structure of 4F11 Fab bound to stabilized MPV-2c HMPV preF
Authors : McGovern, M.R.; Pancera, M.
Deposited on : 2025-05-21
Resolution : 4.13 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

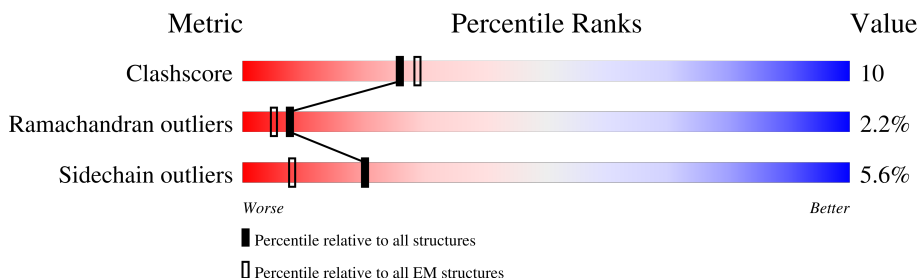
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





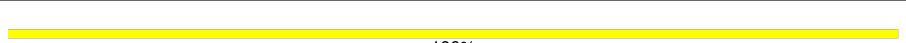

The reported resolution of this entry is 4.13 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	437	
2	B	438	
3	C	439	
4	H	123	
5	L	113	
6	D	3	
7	E	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23882 atoms, of which 11948 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	437	6679	2085	3351	572	650	21	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP C6F440
A	?	-	ARG	deletion	UNP C6F440
A	?	-	GLU	deletion	UNP C6F440
A	?	-	GLU	deletion	UNP C6F440
A	?	-	GLN	deletion	UNP C6F440
A	?	-	ILE	deletion	UNP C6F440
A	?	-	GLU	deletion	UNP C6F440
A	?	-	ASN	deletion	UNP C6F440
A	?	-	PRO	deletion	UNP C6F440
A	?	-	ARG	deletion	UNP C6F440
A	?	-	GLN	deletion	UNP C6F440
A	?	-	SER	deletion	UNP C6F440
A	112	ARG	VAL	conflict	UNP C6F440
A	209	GLU	ASP	conflict	UNP C6F440
A	231	ILE	VAL	conflict	UNP C6F440
A	368	ASN	HIS	conflict	UNP C6F440
A	453	PRO	GLU	conflict	UNP C6F440
A	468	ASN	-	expression tag	UNP C6F440

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	438	6696	2091	3360	573	651	21	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP Q8B9P3
B	?	-	ARG	deletion	UNP Q8B9P3
B	?	-	GLU	deletion	UNP Q8B9P3
B	?	-	GLU	deletion	UNP Q8B9P3
B	?	-	GLN	deletion	UNP Q8B9P3
B	?	-	ILE	deletion	UNP Q8B9P3
B	?	-	GLU	deletion	UNP Q8B9P3
B	?	-	ASN	deletion	UNP Q8B9P3
B	?	-	PRO	deletion	UNP Q8B9P3
B	?	-	ARG	deletion	UNP Q8B9P3
B	?	-	GLN	deletion	UNP Q8B9P3
B	?	-	SER	deletion	UNP Q8B9P3
B	112	ARG	VAL	conflict	UNP Q8B9P3
B	209	GLU	ASP	conflict	UNP Q8B9P3
B	231	ILE	VAL	conflict	UNP Q8B9P3
B	368	ASN	HIS	conflict	UNP Q8B9P3
B	453	PRO	GLU	conflict	UNP Q8B9P3
B	468	ASN	-	expression tag	UNP Q8B9P3

- Molecule 3 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	439	Total	C	H	N	O	S	0	0
			6721	2097	3374	577	652	21		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP Q8B9P3
C	?	-	ARG	deletion	UNP Q8B9P3
C	?	-	GLU	deletion	UNP Q8B9P3
C	?	-	GLU	deletion	UNP Q8B9P3
C	?	-	GLN	deletion	UNP Q8B9P3
C	?	-	ILE	deletion	UNP Q8B9P3
C	?	-	GLU	deletion	UNP Q8B9P3
C	?	-	ASN	deletion	UNP Q8B9P3
C	?	-	PRO	deletion	UNP Q8B9P3
C	?	-	ARG	deletion	UNP Q8B9P3
C	?	-	GLN	deletion	UNP Q8B9P3
C	90	ARG	SER	conflict	UNP Q8B9P3
C	112	ARG	VAL	conflict	UNP Q8B9P3
C	209	GLU	ASP	conflict	UNP Q8B9P3
C	231	ILE	VAL	conflict	UNP Q8B9P3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	368	ASN	HIS	conflict	UNP Q8B9P3
C	453	PRO	GLU	conflict	UNP Q8B9P3
C	468	ASN	-	expression tag	UNP Q8B9P3

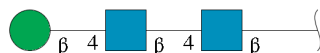
- Molecule 4 is a protein called 4F11 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	120	Total	C	H	N	O	0	0
			1847	609	902	151	179		

- Molecule 5 is a protein called 4F11 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	113	Total	C	H	N	O	0	0
			1724	547	855	145	172		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



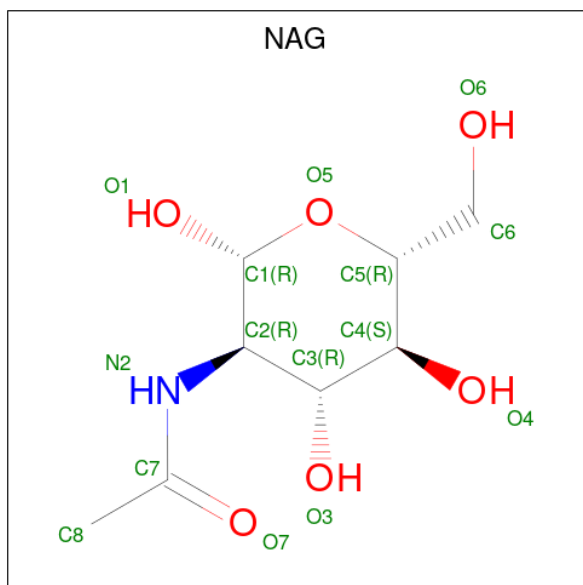
Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

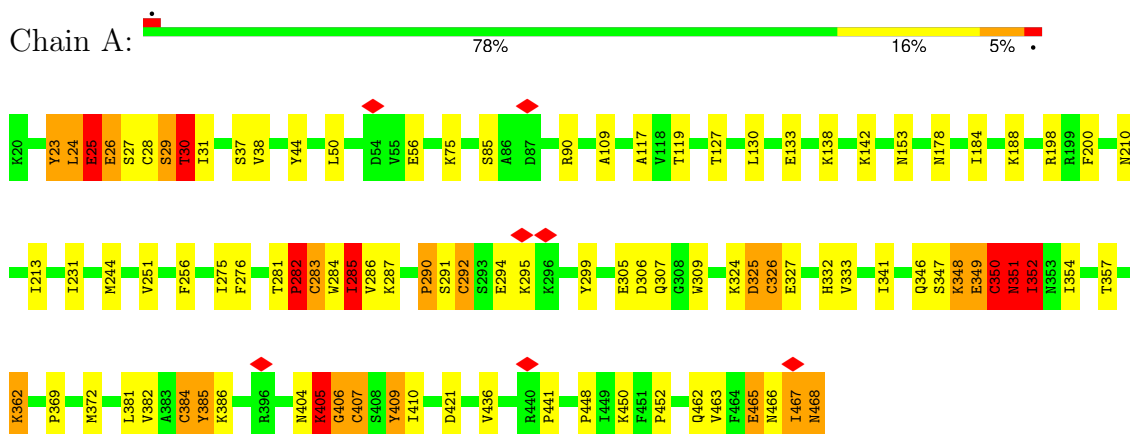


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

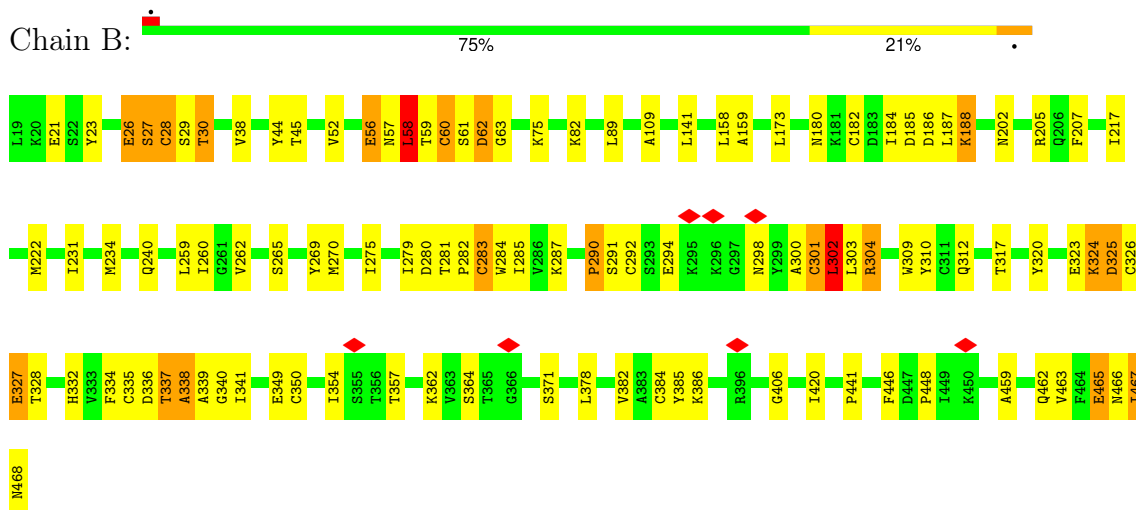
3 Residue-property plots

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: Fusion glycoprotein F0

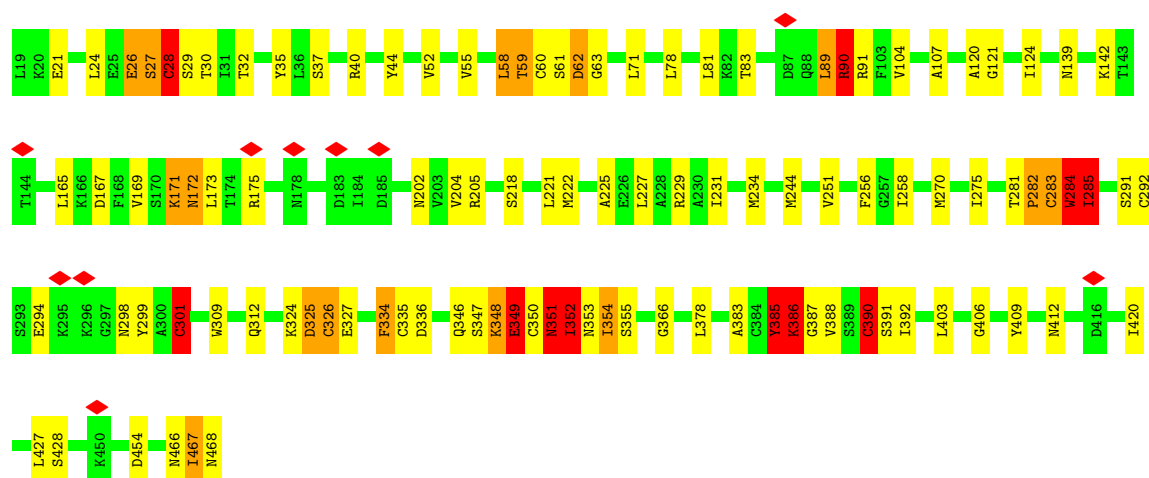


• Molecule 2: Fusion glycoprotein F0



• Molecule 3: Fusion glycoprotein F0





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.024	Depositor
Minimum map value	-2.361	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.812	Depositor
Map size (Å)	403.91998, 403.91998, 403.91998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	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: NAG, BMA

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	0.51	4/3375 (0.1%)	1.03	31/4572 (0.7%)
2	B	0.47	3/3383 (0.1%)	0.86	16/4583 (0.3%)
3	C	0.47	4/3394 (0.1%)	0.94	24/4597 (0.5%)
4	H	0.76	0/973	1.40	3/1321 (0.2%)
5	L	0.83	0/887	1.51	6/1199 (0.5%)
All	All	0.54	11/12012 (0.1%)	1.04	80/16272 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	2
4	H	0	2
5	L	0	3
All	All	0	8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TYR	CA-C	-8.06	1.42	1.52
2	B	188	LYS	C-O	-7.88	1.15	1.24
1	A	29	SER	CA-CB	-6.92	1.41	1.53
2	B	29	SER	CA-CB	-6.70	1.42	1.53
3	C	29	SER	CA-CB	-6.34	1.42	1.53
1	A	285	ILE	N-CA	6.18	1.53	1.46
3	C	285	ILE	N-CA	6.10	1.53	1.46
3	C	172	ASN	CA-C	5.79	1.56	1.52
3	C	27	SER	CA-CB	-5.17	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	291	SER	CA-CB	-5.07	1.45	1.53
1	A	30	THR	CA-C	-5.03	1.46	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	PRO	N-CA-CB	-17.41	84.97	103.25
1	A	25	GLU	CB-CA-C	-16.39	77.79	110.42
3	C	386	LYS	CB-CA-C	-16.16	78.27	110.42
1	A	351	ASN	N-CA-C	-12.74	99.47	112.97
3	C	172	ASN	CB-CA-C	12.60	129.79	111.65
1	A	384	CYS	CB-CA-C	-11.73	96.88	111.43
1	A	282	PRO	N-CA-C	10.41	133.93	112.47
3	C	334	PHE	N-CA-CB	-10.26	94.45	110.57
2	B	290	PRO	N-CA-CB	-10.22	92.52	103.25
4	H	98	PHE	CA-CB-CG	9.64	123.44	113.80
1	A	284	TRP	CA-C-O	-8.97	110.94	121.44
1	A	350	CYS	CB-CA-C	8.66	127.65	110.42
3	C	282	PRO	N-CD-CG	-8.49	90.47	103.20
1	A	385	TYR	N-CA-CB	-8.35	97.07	110.51
2	B	284	TRP	CA-C-O	-8.06	111.76	121.28
5	L	53	LYS	O-C-N	-8.04	113.43	122.75
2	B	301	CYS	N-CA-C	7.56	121.24	109.52
1	A	465	GLU	N-CA-C	-7.37	103.25	111.28
3	C	282	PRO	N-CA-CB	-7.35	95.53	103.25
3	C	283	CYS	CA-CB-SG	7.08	130.69	114.40
2	B	327	GLU	N-CA-CB	-6.95	100.39	111.43
1	A	324	LYS	O-C-N	6.91	130.31	122.22
2	B	282	PRO	N-CA-CB	-6.87	94.35	103.42
1	A	25	GLU	N-CA-CB	-6.87	98.89	110.49
3	C	385	TYR	N-CA-CB	6.87	122.22	110.68
1	A	352	ILE	CA-C-N	-6.76	112.92	123.13
1	A	352	ILE	C-N-CA	-6.76	112.92	123.13
3	C	390	CYS	CB-CA-C	-6.75	96.99	110.42
2	B	282	PRO	N-CD-CG	-6.73	93.11	103.20
1	A	29	SER	CA-C-N	-6.69	113.23	122.93
1	A	29	SER	C-N-CA	-6.69	113.23	122.93
4	H	97	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	350	CYS	CA-CB-SG	6.60	129.58	114.40
2	B	302	LEU	N-CA-CB	-6.57	99.81	110.71
1	A	348	LYS	N-CA-C	-6.57	104.12	111.28
3	C	385	TYR	CB-CA-C	-6.49	97.84	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	172	ASN	CA-C-O	-6.27	112.39	119.98
3	C	385	TYR	CA-C-O	-6.23	113.63	120.36
2	B	337	THR	CA-CB-OG1	-6.20	100.30	109.60
1	A	24	LEU	N-CA-CB	-6.16	101.81	111.23
2	B	282	PRO	CA-C-O	-6.13	113.67	122.31
1	A	384	CYS	CA-CB-SG	-6.03	100.53	114.40
3	C	334	PHE	CA-C-O	-5.87	113.98	120.38
2	B	301	CYS	CA-CB-SG	-5.83	101.00	114.40
3	C	301	CYS	CA-CB-SG	-5.72	101.23	114.40
3	C	298	ASN	CA-C-N	-5.71	112.84	123.01
3	C	298	ASN	C-N-CA	-5.71	112.84	123.01
1	A	325	ASP	CA-CB-CG	5.61	118.21	112.60
3	C	349	GLU	CA-C-N	-5.53	113.25	120.44
3	C	349	GLU	C-N-CA	-5.53	113.25	120.44
1	A	362	LYS	N-CA-CB	-5.47	101.49	110.52
3	C	59	THR	CA-CB-OG1	-5.46	101.41	109.60
3	C	283	CYS	CA-C-O	-5.42	114.78	120.58
1	A	23	TYR	CA-C-N	-5.39	115.80	123.03
1	A	23	TYR	C-N-CA	-5.39	115.80	123.03
5	L	49	TYR	N-CA-C	5.36	117.20	111.36
5	L	32	TYR	CA-CB-CG	5.35	123.53	113.90
5	L	61	ARG	NE-CZ-NH2	5.34	124.00	119.20
4	H	95	CYS	N-CA-C	5.32	118.61	110.36
2	B	465	GLU	N-CA-C	-5.32	105.56	111.36
1	A	290	PRO	N-CA-CB	-5.29	97.69	103.25
1	A	326	CYS	CB-CA-C	5.26	120.88	110.42
2	B	59	THR	CA-C-N	-5.24	111.00	123.16
2	B	59	THR	C-N-CA	-5.24	111.00	123.16
3	C	325	ASP	CA-C-N	-5.22	113.47	121.40
3	C	325	ASP	C-N-CA	-5.22	113.47	121.40
1	A	327	GLU	CB-CA-C	-5.19	101.22	111.60
3	C	90	ARG	CB-CA-C	5.18	116.17	109.80
2	B	58	LEU	CA-C-N	-5.17	114.56	122.62
2	B	58	LEU	C-N-CA	-5.17	114.56	122.62
1	A	381	LEU	CA-C-N	-5.14	115.85	122.99
1	A	381	LEU	C-N-CA	-5.14	115.85	122.99
1	A	290	PRO	N-CD-CG	-5.13	95.50	103.20
5	L	98	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	384	CYS	N-CA-C	5.06	115.81	107.20
2	B	60	CYS	CA-CB-SG	-5.05	102.80	114.40
3	C	28	CYS	CB-CA-C	5.05	120.46	110.42
5	L	27(C)	ARG	NE-CZ-NH2	5.04	123.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	CYS	N-CA-C	5.02	117.01	109.23
1	A	284	TRP	CA-CB-CG	5.01	123.12	113.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	26	GLU	Mainchain
3	C	90	ARG	Sidechain
3	C	91	ARG	Sidechain
4	H	91	TYR	Sidechain
4	H	98	PHE	Sidechain
5	L	32	TYR	Sidechain
5	L	36	TYR	Sidechain
5	L	54	ARG	Sidechain

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	A	3328	3351	3345	72	0
2	B	3336	3360	3356	72	0
3	C	3347	3374	3370	88	0
4	H	945	902	901	5	0
5	L	869	855	855	4	0
6	D	39	37	34	0	0
7	E	28	27	25	0	0
8	A	14	14	13	0	0
8	B	14	14	13	0	0
8	C	14	14	13	0	0
All	All	11934	11948	11925	235	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 10.

All (235) 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)
1:A:350:CYS:SG	1:A:354:ILE:HG13	1.64	1.37
3:C:350:CYS:SG	3:C:354:ILE:HG13	1.70	1.28
1:A:466:ASN:O	1:A:468:ASN:OD1	1.59	1.20
1:A:350:CYS:HB2	1:A:354:ILE:HA	1.43	1.01
2:B:60:CYS:SG	2:B:180:ASN:O	2.22	0.98
2:B:23:TYR:OH	2:B:28:CYS:SG	2.22	0.96
3:C:37:SER:HB3	3:C:283:CYS:SG	2.08	0.94
2:B:283:CYS:SG	2:B:310:TYR:O	2.26	0.93
1:A:292:CYS:SG	1:A:369:PRO:HB3	2.11	0.90
3:C:467:ILE:O	3:C:468:ASN:OXT	1.95	0.84
3:C:37:SER:CB	3:C:283:CYS:SG	2.67	0.83
3:C:350:CYS:SG	3:C:354:ILE:CG1	2.62	0.82
1:A:350:CYS:SG	1:A:354:ILE:CG1	2.60	0.81
1:A:450:LYS:HZ3	1:A:467:ILE:HA	1.47	0.80
1:A:292:CYS:SG	1:A:369:PRO:CB	2.69	0.80
2:B:82:LYS:HG2	2:B:262:VAL:HG21	1.67	0.76
2:B:56:GLU:HA	2:B:75:LYS:HE2	1.68	0.75
3:C:350:CYS:SG	3:C:354:ILE:HA	2.26	0.75
1:A:292:CYS:SG	1:A:369:PRO:HG3	2.27	0.74
2:B:371:SER:HB3	2:B:420:ILE:HD11	1.68	0.74
1:A:468:ASN:OD1	1:A:468:ASN:N	2.19	0.74
3:C:292:CYS:HB2	3:C:385:TYR:CE2	2.24	0.72
3:C:291:SER:O	3:C:301:CYS:SG	2.49	0.70
2:B:337:THR:O	2:B:340:GLY:N	2.19	0.69
3:C:27:SER:O	3:C:28:CYS:C	2.36	0.69
1:A:450:LYS:NZ	1:A:467:ILE:HA	2.07	0.69
3:C:347:SER:O	3:C:348:LYS:C	2.36	0.68
3:C:61:SER:C	3:C:63:GLY:H	2.01	0.68
2:B:27:SER:O	2:B:28:CYS:C	2.35	0.68
3:C:52:VAL:HA	3:C:165:LEU:HD23	1.75	0.67
1:A:326:CYS:SG	1:A:333:VAL:HG22	2.36	0.66
1:A:463:VAL:O	1:A:466:ASN:HB2	1.95	0.66
1:A:462:GLN:HA	1:A:465:GLU:CD	2.21	0.66
2:B:300:ALA:C	2:B:301:CYS:SG	2.79	0.66
2:B:30:THR:HG23	2:B:287:LYS:HB2	1.78	0.65
1:A:450:LYS:O	1:A:450:LYS:HD3	1.97	0.65
2:B:61:SER:O	2:B:63:GLY:N	2.30	0.64
1:A:119:THR:HG23	3:C:428:SER:HB3	1.80	0.64
3:C:386:LYS:O	3:C:388:VAL:N	2.26	0.64
3:C:52:VAL:HG11	3:C:78:LEU:HD11	1.79	0.63
3:C:58:LEU:HB3	3:C:71:LEU:HD11	1.80	0.63
2:B:463:VAL:O	2:B:466:ASN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:CYS:SG	1:A:369:PRO:CG	2.88	0.62
5:L:32:TYR:C	5:L:33:LEU:HD22	2.25	0.62
2:B:240:GLN:HG3	2:B:279:ILE:HD12	1.82	0.61
3:C:350:CYS:O	3:C:352:ILE:N	2.30	0.61
1:A:37:SER:HB3	1:A:283:CYS:SG	2.41	0.60
2:B:349:GLU:HG3	2:B:357:THR:HG21	1.84	0.60
2:B:350:CYS:HB2	2:B:354:ILE:HG13	1.83	0.60
3:C:353:ASN:O	3:C:355:SER:N	2.35	0.60
2:B:60:CYS:SG	2:B:61:SER:N	2.73	0.60
2:B:336:ASP:O	2:B:337:THR:C	2.45	0.60
3:C:292:CYS:HB2	3:C:385:TYR:CZ	2.37	0.60
1:A:56:GLU:HA	1:A:75:LYS:HE2	1.83	0.59
1:A:349:GLU:O	1:A:352:ILE:N	2.35	0.59
3:C:383:ALA:HB1	3:C:385:TYR:HE1	1.67	0.59
3:C:466:ASN:O	3:C:467:ILE:C	2.44	0.59
3:C:353:ASN:C	3:C:355:SER:H	2.10	0.59
3:C:139:ASN:HA	3:C:142:LYS:HD2	1.83	0.59
3:C:55:VAL:HA	3:C:58:LEU:HG	1.84	0.59
1:A:326:CYS:SG	1:A:333:VAL:CG2	2.91	0.58
1:A:348:LYS:O	1:A:349:GLU:C	2.46	0.58
3:C:234:MET:HE1	3:C:244:MET:HE1	1.86	0.58
3:C:30:THR:HG22	3:C:409:TYR:HE2	1.69	0.57
3:C:61:SER:O	3:C:63:GLY:N	2.34	0.57
3:C:32:THR:HB	3:C:285:ILE:HG22	1.86	0.57
3:C:346:GLN:O	3:C:349:GLU:HB2	2.05	0.57
2:B:466:ASN:O	2:B:467:ILE:C	2.48	0.56
1:A:349:GLU:O	1:A:351:ASN:N	2.38	0.56
1:A:350:CYS:C	1:A:352:ILE:H	2.12	0.56
2:B:463:VAL:O	2:B:467:ILE:HD12	2.04	0.56
3:C:385:TYR:CE2	3:C:406:GLY:HA2	2.40	0.56
1:A:27:SER:O	1:A:28:CYS:C	2.48	0.56
3:C:172:ASN:HD22	3:C:175:ARG:HH11	1.52	0.56
3:C:21:GLU:HB2	3:C:378:LEU:HD22	1.88	0.56
3:C:390:CYS:HB3	3:C:420:ILE:HD13	1.88	0.56
1:A:24:LEU:O	1:A:26:GLU:N	2.40	0.55
2:B:337:THR:O	2:B:339:ALA:N	2.39	0.55
2:B:234:MET:SD	2:B:275:ILE:HG22	2.46	0.55
3:C:383:ALA:HB1	3:C:385:TYR:CE1	2.41	0.55
3:C:32:THR:HB	3:C:285:ILE:CG2	2.37	0.55
2:B:61:SER:C	2:B:63:GLY:N	2.63	0.55
2:B:141:LEU:HD11	2:B:159:ALA:HB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:ASP:O	2:B:186:ASP:C	2.49	0.54
3:C:59:THR:O	3:C:60:CYS:SG	2.65	0.54
3:C:61:SER:C	3:C:63:GLY:N	2.65	0.54
1:A:292:CYS:HB2	1:A:385:TYR:CE2	2.42	0.54
2:B:231:ILE:HA	2:B:234:MET:HE2	1.91	0.53
2:B:26:GLU:HA	2:B:441:PRO:HA	1.90	0.53
3:C:52:VAL:HG21	3:C:78:LEU:HD21	1.89	0.53
3:C:222:MET:HE3	3:C:227:LEU:HB2	1.90	0.53
2:B:61:SER:O	2:B:62:ASP:C	2.50	0.53
2:B:109:ALA:HB2	2:B:341:ILE:HD11	1.90	0.53
3:C:349:GLU:O	3:C:352:ILE:HB	2.09	0.53
2:B:465:GLU:O	2:B:466:ASN:C	2.49	0.52
1:A:44:TYR:HB2	1:A:275:ILE:HD11	1.91	0.52
2:B:362:LYS:HA	2:B:459:ALA:HA	1.90	0.52
1:A:349:GLU:HB3	1:A:357:THR:HG21	1.90	0.52
1:A:26:GLU:O	1:A:441:PRO:HA	2.10	0.52
1:A:332:HIS:CD2	2:B:89:LEU:HD13	2.44	0.52
1:A:346:GLN:O	1:A:349:GLU:HB2	2.09	0.51
1:A:295:LYS:HB2	1:A:448:PRO:HG2	1.93	0.51
3:C:24:LEU:C	3:C:26:GLU:H	2.19	0.51
2:B:312:GLN:HG2	2:B:317:THR:HG22	1.92	0.51
2:B:332:HIS:CD2	3:C:89:LEU:HD13	2.46	0.51
1:A:23:TYR:HD2	1:A:436:VAL:HG23	1.76	0.51
1:A:290:PRO:HD3	1:A:372:MET:HE2	1.93	0.50
3:C:353:ASN:C	3:C:355:SER:N	2.64	0.50
3:C:412:ASN:HA	3:C:427:LEU:HD13	1.93	0.50
1:A:244:MET:CE	1:A:276:PHE:H	2.24	0.50
4:H:33:TRP:HB2	4:H:95:CYS:SG	2.52	0.50
1:A:406:GLY:O	1:A:407:CYS:C	2.55	0.50
2:B:323:GLU:C	2:B:325:ASP:H	2.19	0.50
1:A:409:TYR:O	1:A:410:ILE:HD13	2.12	0.49
2:B:217:ILE:HG21	2:B:222:MET:HE3	1.94	0.49
2:B:184:ILE:O	2:B:185:ASP:C	2.55	0.49
1:A:325:ASP:OD1	1:A:326:CYS:N	2.46	0.49
3:C:467:ILE:C	3:C:468:ASN:OXT	2.56	0.49
1:A:347:SER:O	1:A:348:LYS:C	2.56	0.48
2:B:298:ASN:HB3	2:B:448:PRO:HB2	1.93	0.48
3:C:285:ILE:HB	3:C:309:TRP:CZ3	2.48	0.48
3:C:40:ARG:NE	3:C:336:ASP:OD1	2.40	0.48
2:B:45:THR:HG23	2:B:270:MET:HE2	1.94	0.48
3:C:35:TYR:HB2	3:C:283:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:GLY:O	3:C:270:MET:HE1	2.14	0.48
2:B:349:GLU:CG	2:B:357:THR:HG21	2.44	0.48
3:C:466:ASN:C	3:C:468:ASN:N	2.67	0.47
1:A:127:THR:HG21	1:A:153:ASN:HB3	1.96	0.47
1:A:285:ILE:HG12	1:A:286:VAL:N	2.29	0.47
3:C:89:LEU:O	3:C:90:ARG:C	2.57	0.47
3:C:104:VAL:HG12	3:C:107:ALA:H	1.79	0.47
1:A:117:ALA:HB1	1:A:256:PHE:HE2	1.79	0.47
1:A:231:ILE:HD11	1:A:251:VAL:HG11	1.97	0.47
2:B:279:ILE:HG22	2:B:280:ASP:OD1	2.14	0.47
2:B:285:ILE:HB	2:B:309:TRP:CZ3	2.50	0.47
2:B:324:LYS:HE3	2:B:324:LYS:HB2	1.61	0.46
3:C:294:GLU:HG3	3:C:299:TYR:CD1	2.50	0.46
2:B:302:LEU:HA	2:B:364:SER:O	2.15	0.46
3:C:466:ASN:O	3:C:468:ASN:N	2.49	0.46
4:H:29:PHE:CD1	4:H:76:THR:HA	2.50	0.46
2:B:302:LEU:HD13	2:B:446:PHE:CE2	2.51	0.46
2:B:323:GLU:C	2:B:325:ASP:N	2.72	0.46
1:A:198:ARG:HB3	1:A:198:ARG:CZ	2.45	0.46
1:A:405:LYS:HB3	1:A:405:LYS:HE3	1.53	0.46
2:B:61:SER:C	2:B:63:GLY:H	2.22	0.46
2:B:465:GLU:O	2:B:468:ASN:ND2	2.49	0.46
1:A:85:SER:HB2	1:A:90:ARG:HE	1.80	0.45
2:B:303:LEU:O	2:B:304:ARG:C	2.59	0.45
2:B:52:VAL:HG22	2:B:265:SER:O	2.17	0.45
2:B:44:TYR:OH	2:B:158:LEU:HB2	2.17	0.45
1:A:24:LEU:C	1:A:26:GLU:N	2.75	0.45
2:B:202:ASN:HA	2:B:205:ARG:HG2	1.99	0.45
2:B:459:ALA:HB3	2:B:462:GLN:OE1	2.18	0.45
5:L:6:GLN:CD	5:L:6:GLN:H	2.25	0.45
3:C:282:PRO:HD2	3:C:312:GLN:HB2	1.98	0.44
3:C:351:ASN:OD1	3:C:351:ASN:N	2.48	0.44
1:A:244:MET:HE1	1:A:276:PHE:H	1.82	0.44
2:B:187:LEU:HD12	2:B:187:LEU:O	2.17	0.44
3:C:218:SER:H	3:C:221:LEU:HD12	1.83	0.44
3:C:227:LEU:O	3:C:231:ILE:HG12	2.17	0.44
3:C:348:LYS:O	3:C:349:GLU:C	2.60	0.44
1:A:294:GLU:HB2	1:A:299:TYR:CE2	2.53	0.44
2:B:61:SER:OG	2:B:62:ASP:N	2.50	0.44
5:L:35:TRP:CD1	5:L:52:SER:HB3	2.53	0.44
1:A:50:LEU:HD21	1:A:200:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:CD2	1:A:385:TYR:N	2.79	0.43
3:C:347:SER:OG	3:C:348:LYS:N	2.50	0.43
1:A:24:LEU:C	1:A:26:GLU:H	2.26	0.43
2:B:326:CYS:SG	2:B:334:PHE:O	2.76	0.43
3:C:44:TYR:HB2	3:C:275:ILE:HD11	1.99	0.43
3:C:349:GLU:O	3:C:350:CYS:C	2.61	0.43
3:C:120:ALA:O	3:C:124:ILE:HD12	2.18	0.43
3:C:386:LYS:HB2	3:C:388:VAL:HG23	2.00	0.43
3:C:229:ARG:HA	3:C:229:ARG:NH2	2.34	0.43
3:C:326:CYS:SG	3:C:334:PHE:O	2.76	0.43
1:A:23:TYR:CD2	1:A:436:VAL:HG23	2.53	0.43
1:A:30:THR:HG23	1:A:287:LYS:HB2	2.01	0.43
2:B:207:PHE:CD1	2:B:259:LEU:HB2	2.54	0.43
3:C:256:PHE:HE2	3:C:258:ILE:HD11	1.84	0.43
3:C:284:TRP:NE1	3:C:348:LYS:HG3	2.34	0.43
3:C:350:CYS:C	3:C:352:ILE:N	2.77	0.43
1:A:37:SER:OG	1:A:281:THR:HB	2.19	0.43
1:A:306:ASP:OD1	1:A:362:LYS:HB2	2.19	0.43
3:C:231:ILE:HD11	3:C:251:VAL:HG11	2.01	0.43
2:B:260:ILE:H	2:B:269:TYR:HA	1.84	0.42
3:C:366:GLY:HA2	3:C:454:ASP:OD1	2.19	0.42
3:C:169:VAL:HG22	3:C:173:LEU:HD23	2.00	0.42
3:C:78:LEU:HD23	3:C:78:LEU:HA	1.91	0.42
1:A:285:ILE:HB	1:A:309:TRP:CE3	2.54	0.42
3:C:55:VAL:O	3:C:58:LEU:HB2	2.19	0.42
1:A:109:ALA:HB2	1:A:341:ILE:HD11	2.02	0.42
1:A:285:ILE:HB	1:A:309:TRP:CZ3	2.55	0.42
2:B:21:GLU:OE1	2:B:378:LEU:HB2	2.20	0.42
1:A:210:ASN:HB3	1:A:213:ILE:O	2.20	0.42
1:A:138:LYS:HB3	1:A:142:LYS:NZ	2.34	0.42
2:B:337:THR:O	2:B:338:ALA:C	2.62	0.42
3:C:385:TYR:O	3:C:386:LYS:HB2	2.18	0.42
1:A:38:VAL:HG12	1:A:276:PHE:CD1	2.55	0.42
1:A:465:GLU:O	1:A:466:ASN:C	2.63	0.42
1:A:285:ILE:HG12	1:A:286:VAL:H	1.85	0.41
2:B:182:CYS:C	2:B:184:ILE:H	2.28	0.41
2:B:332:HIS:CD2	3:C:89:LEU:HD22	2.55	0.41
3:C:81:LEU:HD22	3:C:204:VAL:HG22	2.02	0.41
3:C:467:ILE:HD12	3:C:467:ILE:HA	1.93	0.41
3:C:350:CYS:C	3:C:352:ILE:H	2.22	0.41
3:C:353:ASN:O	3:C:354:ILE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HA	1:A:295:LYS:HD3	1.95	0.41
2:B:38:VAL:HB	2:B:334:PHE:CD1	2.56	0.41
2:B:58:LEU:HD11	2:B:173:LEU:HD21	2.03	0.41
3:C:24:LEU:C	3:C:26:GLU:N	2.78	0.41
3:C:225:ALA:O	3:C:229:ARG:HG2	2.20	0.41
1:A:188:LYS:HG3	2:B:187:LEU:HD22	2.02	0.41
2:B:186:ASP:C	2:B:188:LYS:H	2.28	0.41
1:A:127:THR:O	1:A:127:THR:HG22	2.21	0.41
3:C:386:LYS:C	3:C:388:VAL:N	2.79	0.41
4:H:52(A):PRO:HA	4:H:71:VAL:HG11	2.03	0.41
1:A:305:GLU:C	1:A:307:GLN:H	2.28	0.41
2:B:182:CYS:C	2:B:184:ILE:N	2.79	0.41
4:H:100(B):TYR:CE2	5:L:48:ILE:HD11	2.56	0.41
1:A:130:LEU:HB2	1:A:133:GLU:OE1	2.20	0.40
4:H:100(F):MET:HE3	4:H:103:TRP:CH2	2.55	0.40
1:A:31:ILE:HD12	1:A:351:ASN:OD1	2.21	0.40
2:B:385:TYR:CE2	2:B:406:GLY:HA2	2.56	0.40
3:C:83:THR:HA	3:C:90:ARG:HH22	1.87	0.40
3:C:167:ASP:O	3:C:171:LYS:HB2	2.22	0.40
3:C:202:ASN:HA	3:C:205:ARG:HG2	2.03	0.40
3:C:353:ASN:O	3:C:353:ASN:CG	2.64	0.40
1:A:452:PRO:HG2	1:A:463:VAL:HG13	2.04	0.40
2:B:275:ILE:O	2:B:275:ILE:HG13	2.22	0.40
2:B:300:ALA:O	2:B:301:CYS:SG	2.79	0.40
2:B:320:TYR:CE1	2:B:335:CYS:HB3	2.56	0.40
1:A:292:CYS:SG	1:A:369:PRO:CA	3.08	0.40
2:B:303:LEU:O	2:B:303:LEU:HG	2.20	0.40
2:B:320:TYR:CZ	2:B:335:CYS:HB3	2.57	0.40
3:C:392:ILE:HG23	3:C:403:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/437 (99%)	392 (90%)	30 (7%)	11 (2%)	4	29
2	B	434/438 (99%)	398 (92%)	32 (7%)	4 (1%)	14	50
3	C	435/439 (99%)	400 (92%)	26 (6%)	9 (2%)	5	32
4	H	118/123 (96%)	107 (91%)	9 (8%)	2 (2%)	7	37
5	L	111/113 (98%)	82 (74%)	21 (19%)	8 (7%)	1	13
All	All	1531/1550 (99%)	1379 (90%)	118 (8%)	34 (2%)	8	32

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	282	PRO
1	A	421	ASP
3	C	62	ASP
3	C	285	ILE
3	C	386	LYS
3	C	387	GLY
5	L	2	ILE
5	L	48	ILE
1	A	291	SER
1	A	406	GLY
2	B	62	ASP
2	B	338	ALA
3	C	28	CYS
3	C	284	TRP
3	C	354	ILE
5	L	83	VAL
1	A	178	ASN
1	A	405	LYS
2	B	386	LYS
3	C	351	ASN
4	H	100(A)	GLY
4	H	97	ASP
5	L	90	GLN
1	A	29	SER
1	A	349	GLU
1	A	350	CYS
1	A	352	ILE
5	L	9	LEU
5	L	52	SER
5	L	78	VAL

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Mol	Chain	Res	Type
2	B	304	ARG
3	C	352	ILE
5	L	43	SER

5.3.2 Protein sidechains ⓘ

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	371/371 (100%)	353 (95%)	18 (5%)	21	44
2	B	372/372 (100%)	353 (95%)	19 (5%)	20	43
3	C	373/373 (100%)	348 (93%)	25 (7%)	13	36
4	H	101/104 (97%)	97 (96%)	4 (4%)	27	49
5	L	98/98 (100%)	90 (92%)	8 (8%)	9	30
All	All	1315/1318 (100%)	1241 (94%)	74 (6%)	20	41

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	26	GLU
1	A	30	THR
1	A	184	ILE
1	A	282	PRO
1	A	283	CYS
1	A	285	ILE
1	A	292	CYS
1	A	350	CYS
1	A	351	ASN
1	A	382	VAL
1	A	384	CYS
1	A	386	LYS
1	A	404	ASN
1	A	405	LYS
1	A	407	CYS

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Mol	Chain	Res	Type
1	A	467	ILE
1	A	468	ASN
2	B	27	SER
2	B	28	CYS
2	B	30	THR
2	B	56	GLU
2	B	57	ASN
2	B	58	LEU
2	B	281	THR
2	B	283	CYS
2	B	290	PRO
2	B	292	CYS
2	B	294	GLU
2	B	302	LEU
2	B	324	LYS
2	B	325	ASP
2	B	327	GLU
2	B	328	THR
2	B	382	VAL
2	B	384	CYS
2	B	467	ILE
3	C	26	GLU
3	C	28	CYS
3	C	58	LEU
3	C	62	ASP
3	C	89	LEU
3	C	90	ARG
3	C	171	LYS
3	C	281	THR
3	C	284	TRP
3	C	285	ILE
3	C	301	CYS
3	C	324	LYS
3	C	325	ASP
3	C	326	CYS
3	C	327	GLU
3	C	335	CYS
3	C	348	LYS
3	C	349	GLU
3	C	351	ASN
3	C	352	ILE
3	C	385	TYR

Continued on next page...

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Mol	Chain	Res	Type
3	C	386	LYS
3	C	390	CYS
3	C	391	SER
3	C	467	ILE
4	H	31	THR
4	H	79	TYR
4	H	80	LEU
4	H	97	ASP
5	L	6	GLN
5	L	21	ILE
5	L	32	TYR
5	L	48	ILE
5	L	54	ARG
5	L	92	LEU
5	L	106	ILE
5	L	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	404	ASN
2	B	247	ASN
2	B	272	GLN
2	B	395	ASN
2	B	468	ASN
3	C	145	ASN
3	C	312	GLN
3	C	353	ASN
3	C	413	GLN
3	C	462	GLN

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

5 monosaccharides 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
6	NAG	D	1	1,6	14,14,15	1.28	2 (14%)	17,19,21	0.96	1 (5%)
6	NAG	D	2	6	14,14,15	1.36	2 (14%)	17,19,21	1.64	1 (5%)
6	BMA	D	3	6	11,11,12	1.10	1 (9%)	15,15,17	0.77	0
7	NAG	E	1	7,2	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
7	NAG	E	2	7	14,14,15	0.73	0	17,19,21	0.85	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
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	BMA	D	3	6	-	0/2/19/22	0/1/1/1
7	NAG	E	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	NAG	O5-C5	2.88	1.49	1.43
6	D	1	NAG	O5-C5	2.51	1.48	1.43
6	D	1	NAG	O4-C4	2.34	1.48	1.43
6	D	2	NAG	O4-C4	2.16	1.48	1.43
6	D	3	BMA	O5-C5	2.14	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	NAG	C2-N2-C7	5.40	130.14	122.90
6	D	1	NAG	C4-C3-C2	2.23	114.28	111.02
7	E	1	NAG	O5-C1-C2	-2.21	107.88	111.29

There are no chirality outliers.

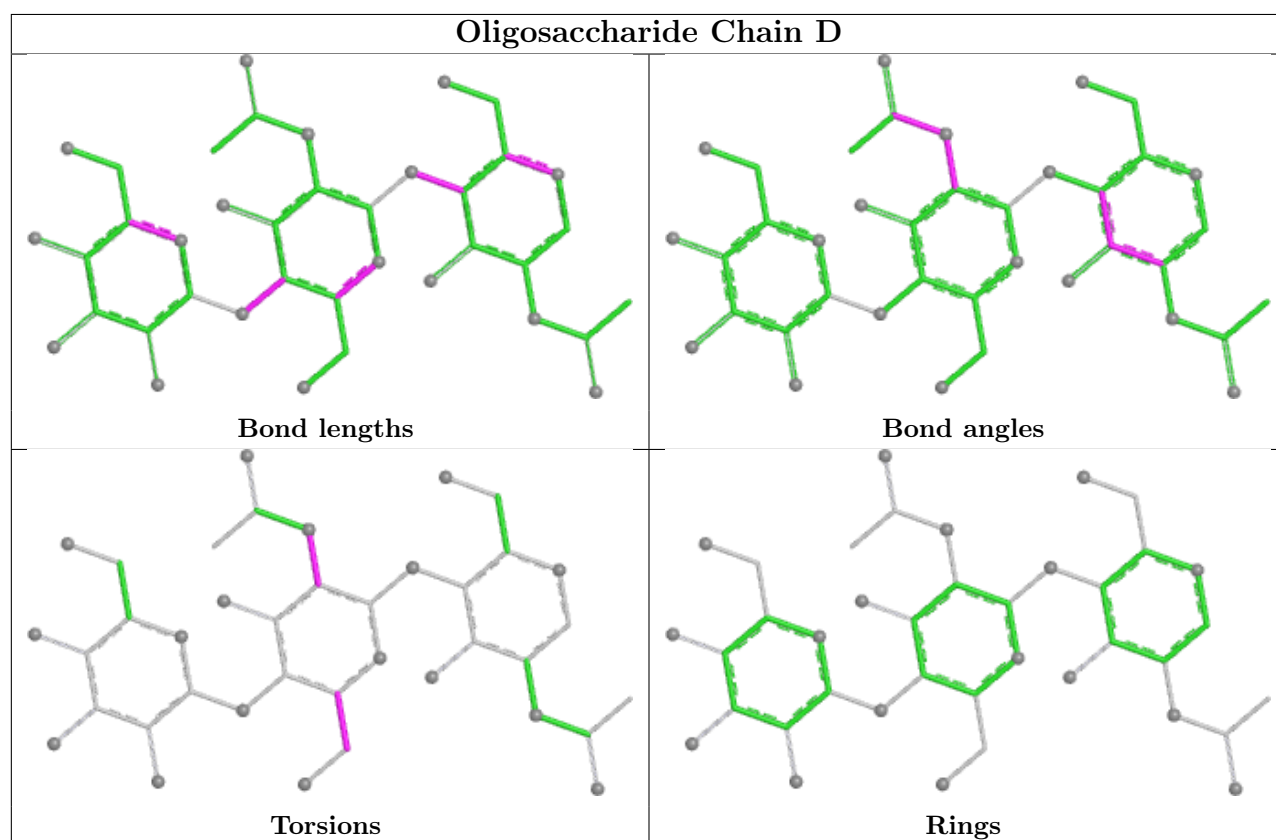
All (3) torsion outliers are listed below:

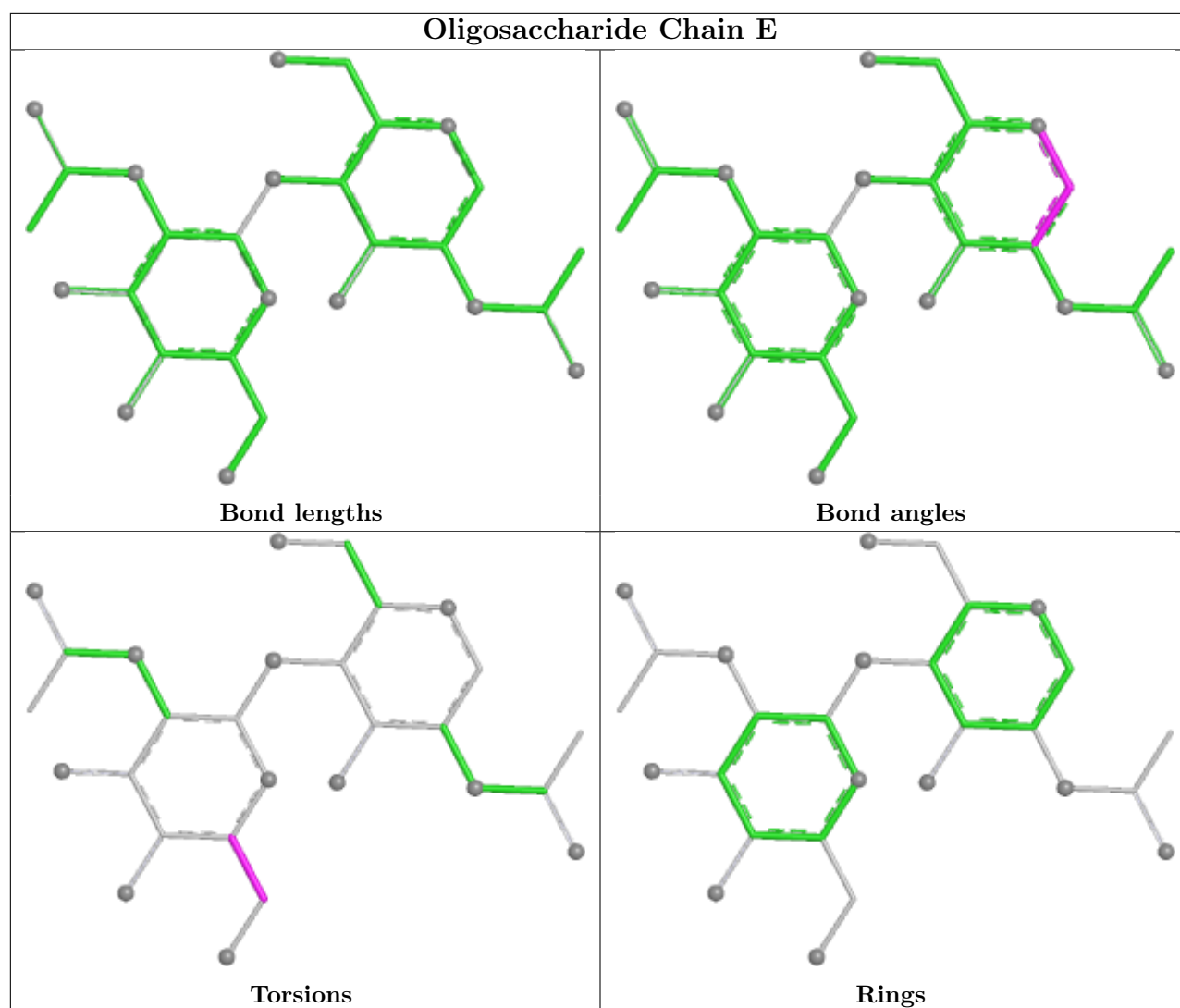
Mol	Chain	Res	Type	Atoms
6	D	2	NAG	C3-C2-N2-C7
7	E	2	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6

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 oligosaccharide.





5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
8	NAG	B	501	2	14,14,15	0.41	0	17,19,21	0.83	0
8	NAG	C	501	3	14,14,15	1.39	2 (14%)	17,19,21	0.85	1 (5%)
8	NAG	A	501	1	14,14,15	0.82	0	17,19,21	1.02	1 (5%)

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
8	NAG	B	501	2	-	2/6/23/26	0/1/1/1
8	NAG	C	501	3	-	0/6/23/26	0/1/1/1
8	NAG	A	501	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	NAG	C1-C2	3.22	1.56	1.52
8	C	501	NAG	O5-C5	2.68	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	NAG	C1-O5-C5	2.50	115.54	112.19
8	A	501	NAG	C2-N2-C7	2.35	126.06	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	NAG	C8-C7-N2-C2
8	B	501	NAG	O7-C7-N2-C2
8	A	501	NAG	O5-C5-C6-O6
8	A	501	NAG	C4-C5-C6-O6

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	91:ARG	C	103:PHE	N	44.68
1	B	90:ARG	C	103:PHE	N	43.61
1	A	90:ARG	C	103:PHE	N	42.85

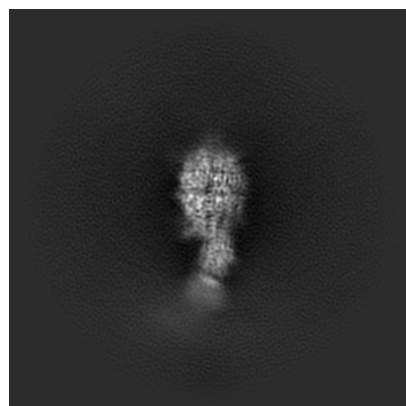
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70773. These allow visual inspection of the internal detail of the map and identification of artifacts.

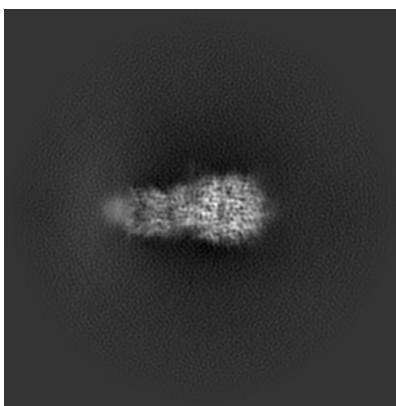
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

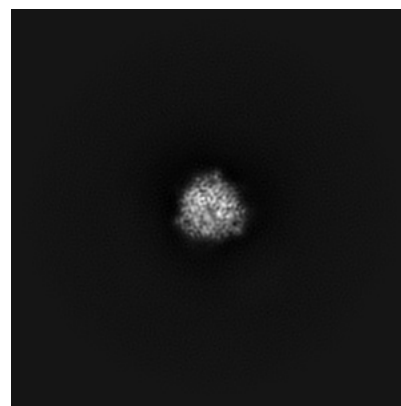
6.1.1 Primary map



X

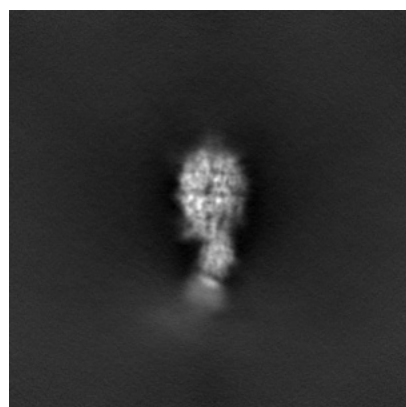


Y

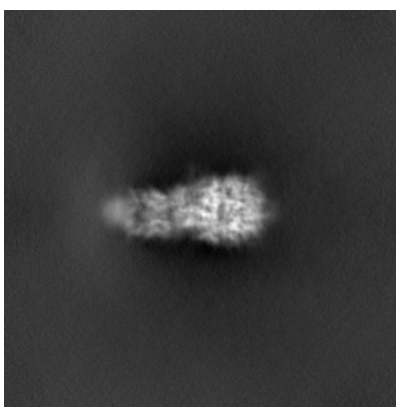


Z

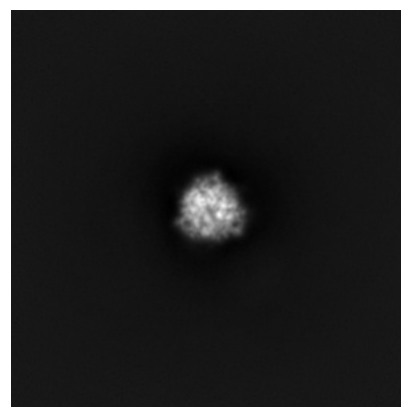
6.1.2 Raw map



X



Y

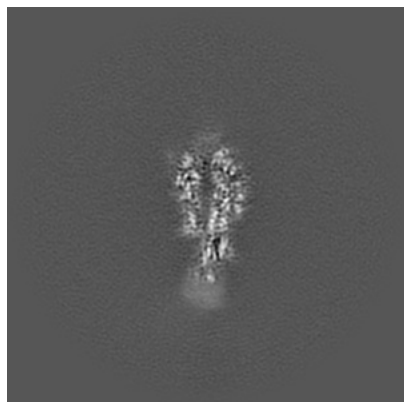


Z

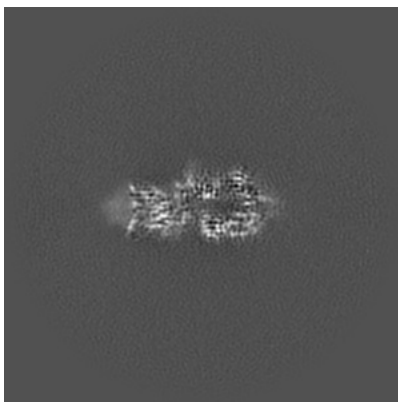
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

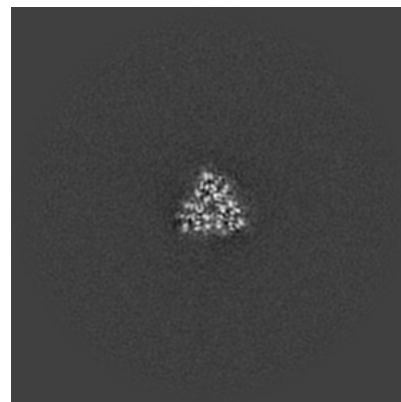
6.2.1 Primary map



X Index: 180

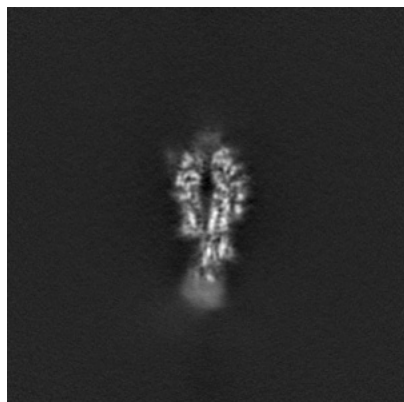


Y Index: 180

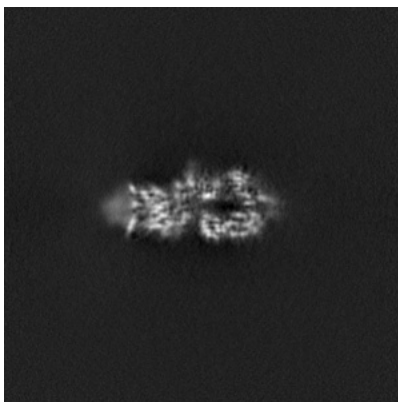


Z Index: 180

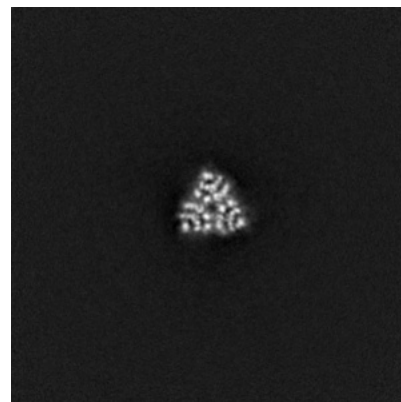
6.2.2 Raw map



X Index: 180



Y Index: 180

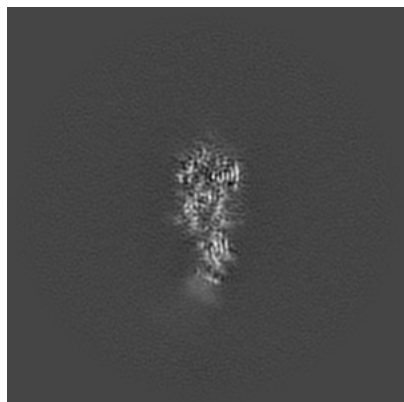


Z Index: 180

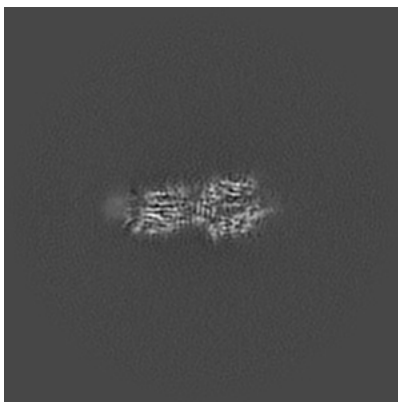
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

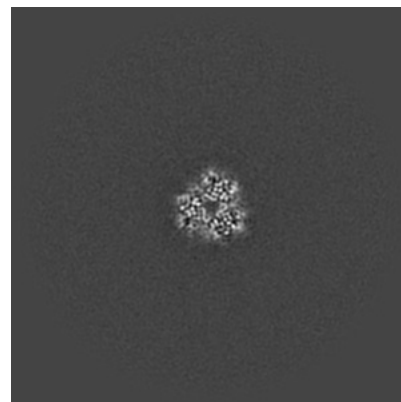
6.3.1 Primary map



X Index: 168

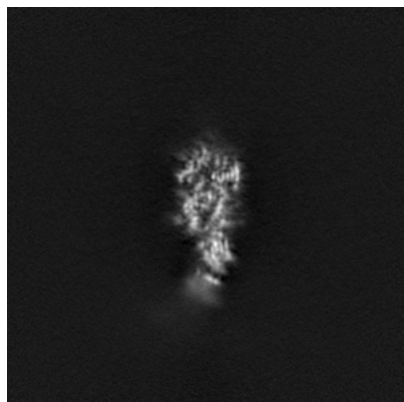


Y Index: 189

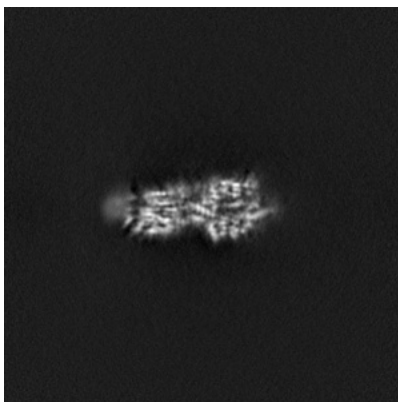


Z Index: 189

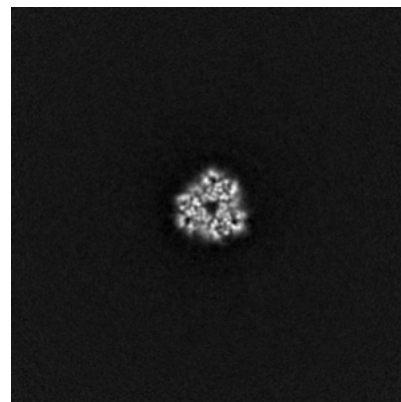
6.3.2 Raw map



X Index: 168



Y Index: 188



Z Index: 189

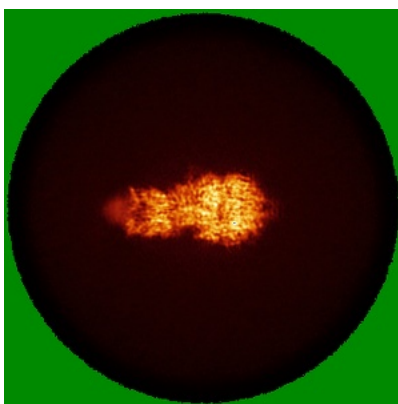
The images above show the largest variance slices of the map in three orthogonal directions.

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

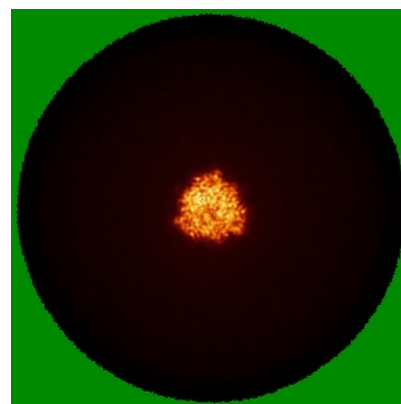
6.4.1 Primary map



X

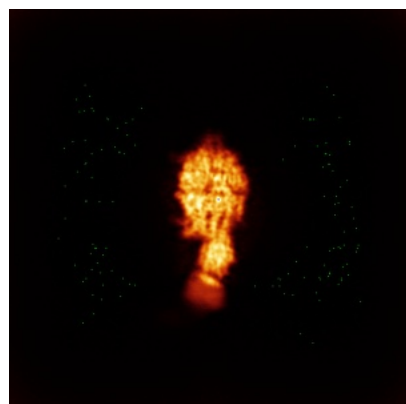


Y

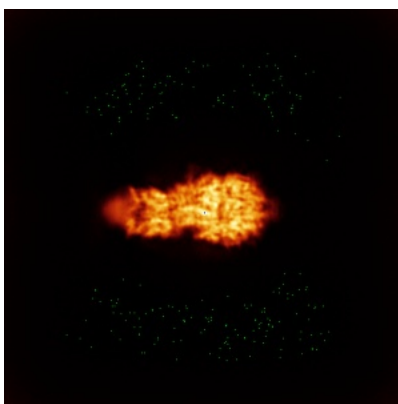


Z

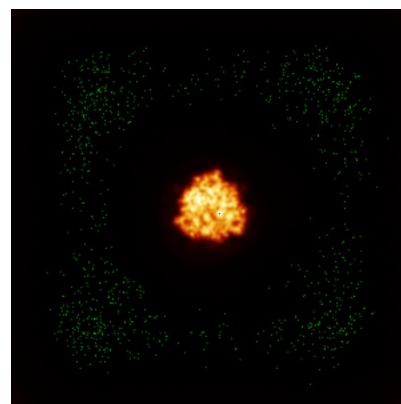
6.4.2 Raw map



X



Y

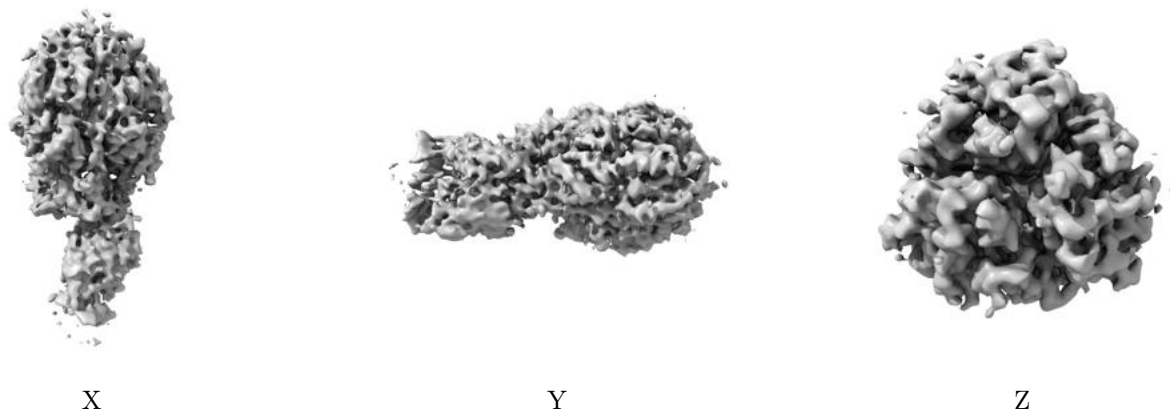


Z

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.

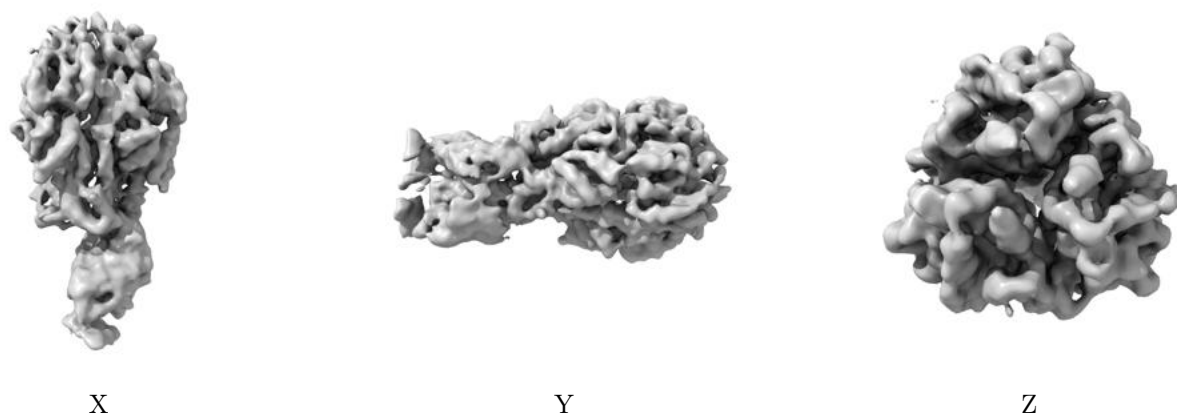
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.812. 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.

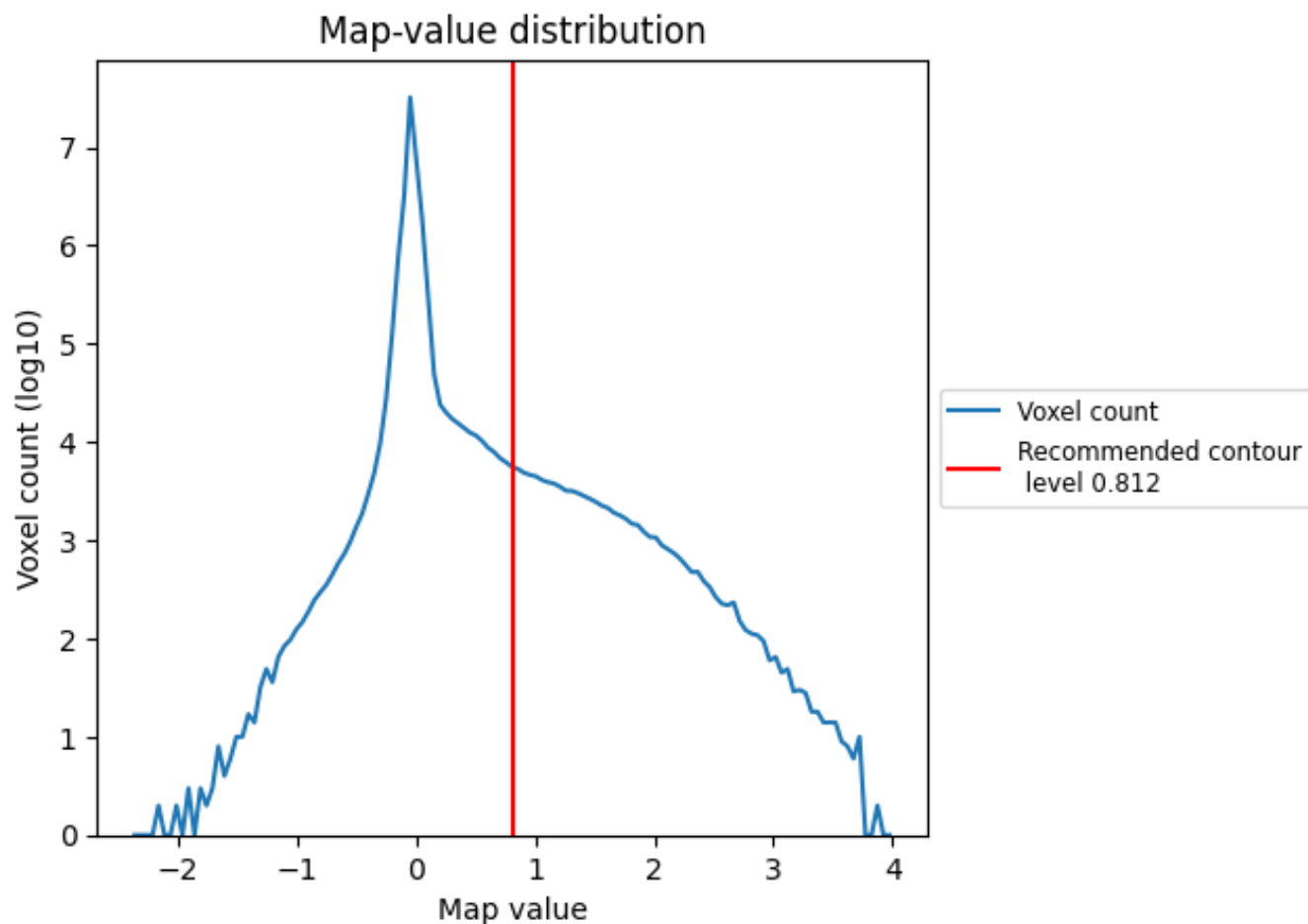
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

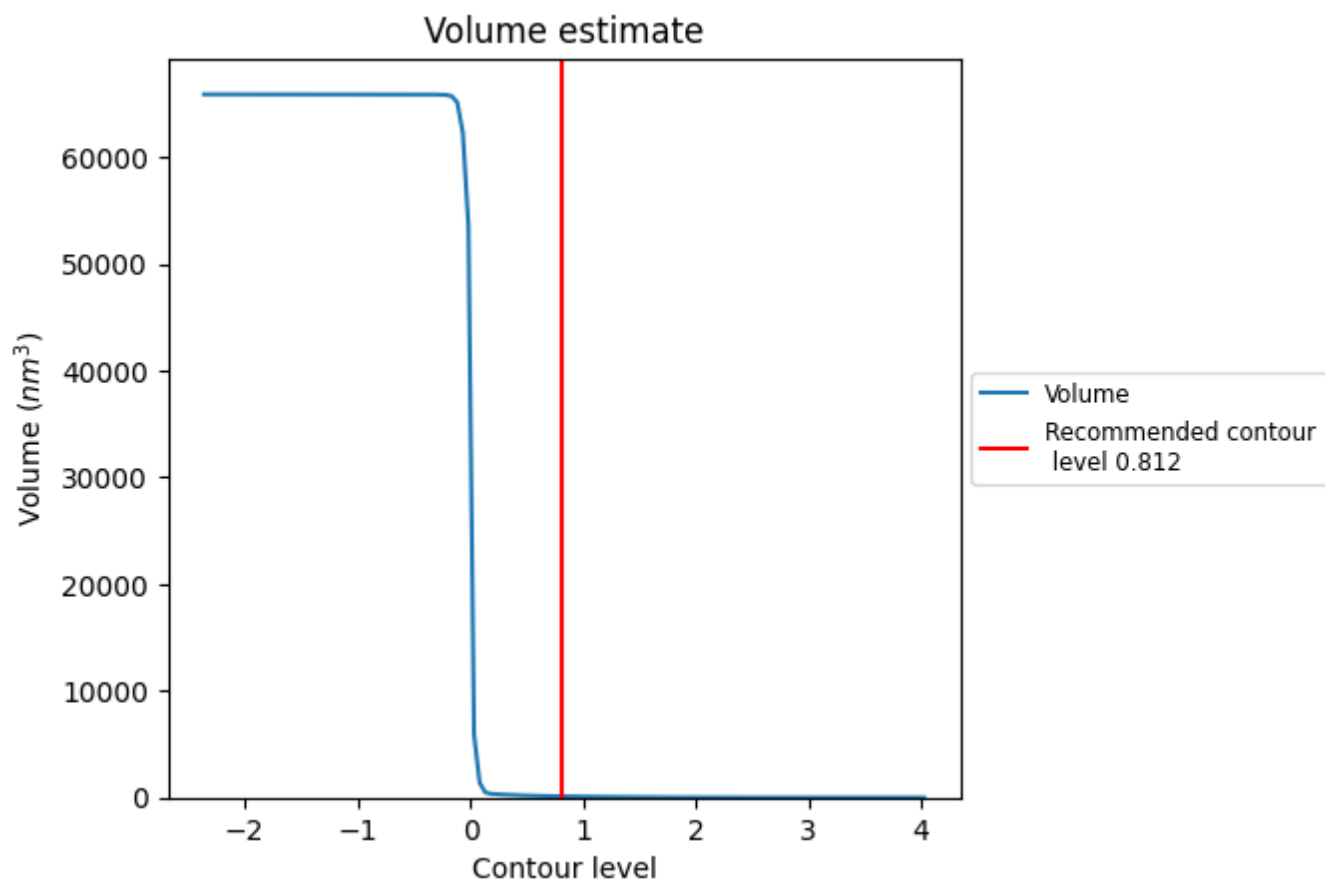
This section contains the results of statistical analysis of the map.

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.

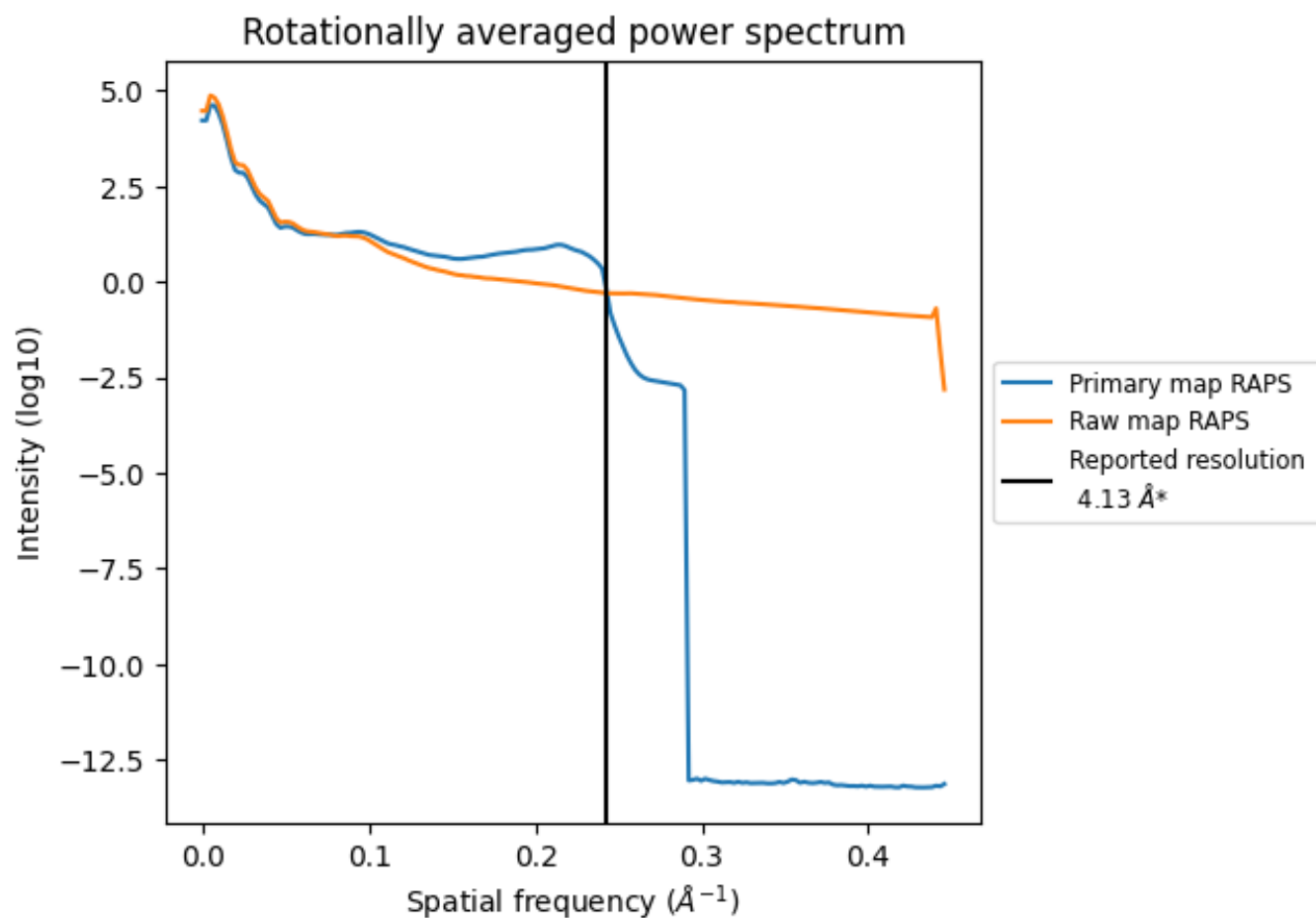
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 103 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 ⓘ

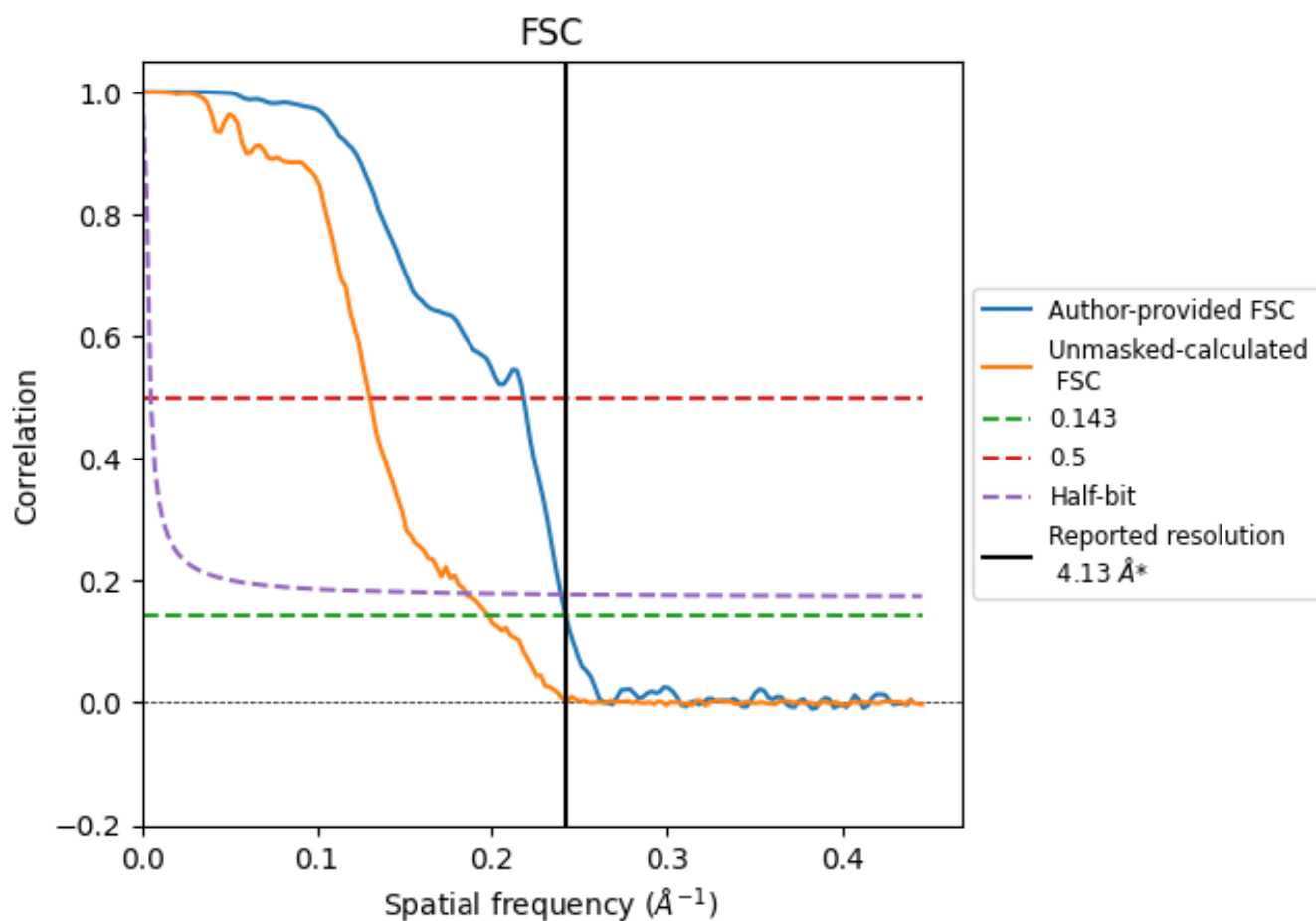


*Reported resolution corresponds to spatial frequency of 0.242 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.242 \AA^{-1}

8.2 Resolution estimates [i](#)

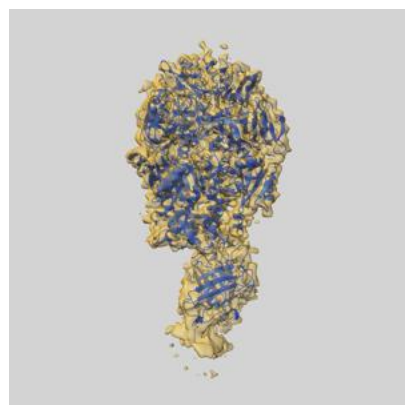
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.13	-	-
Author-provided FSC curve	4.13	4.59	4.18
Unmasked-calculated*	5.05	7.70	5.41

*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 5.05 differs from the reported value 4.13 by more than 10 %

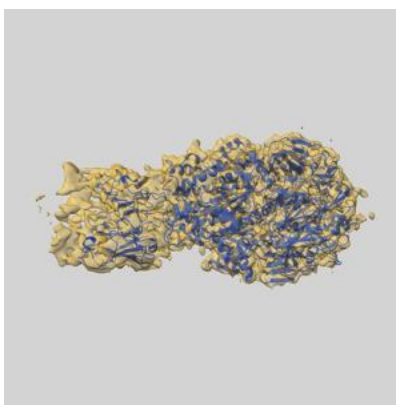
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70773 and PDB model 9ORE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

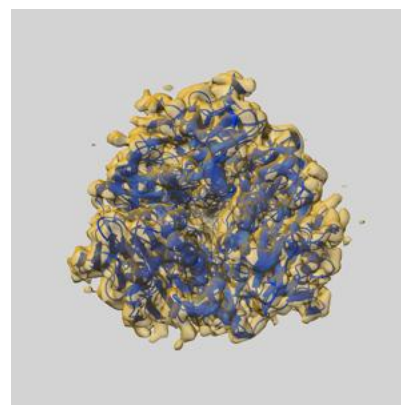
9.1 Map-model overlay [i](#)



X



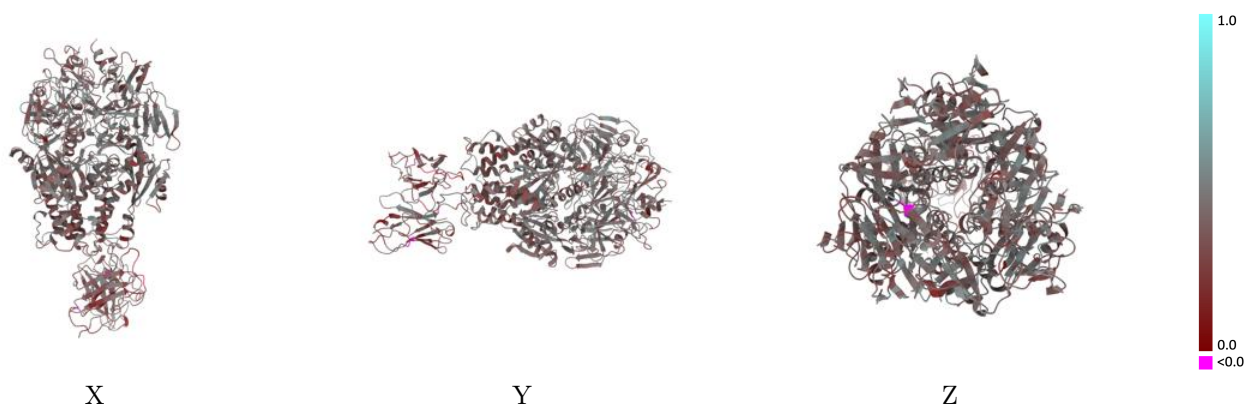
Y



Z

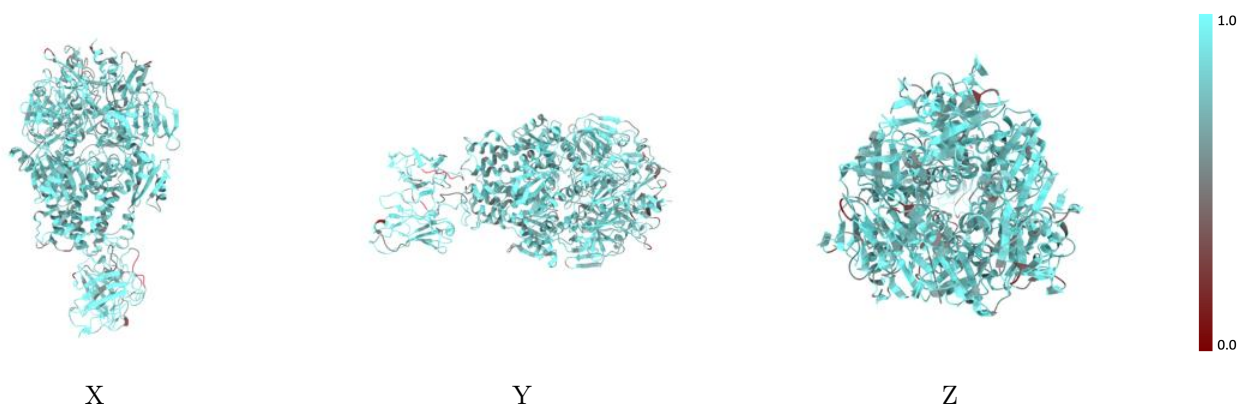
The images above show the 3D surface view of the map at the recommended contour level 0.812 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



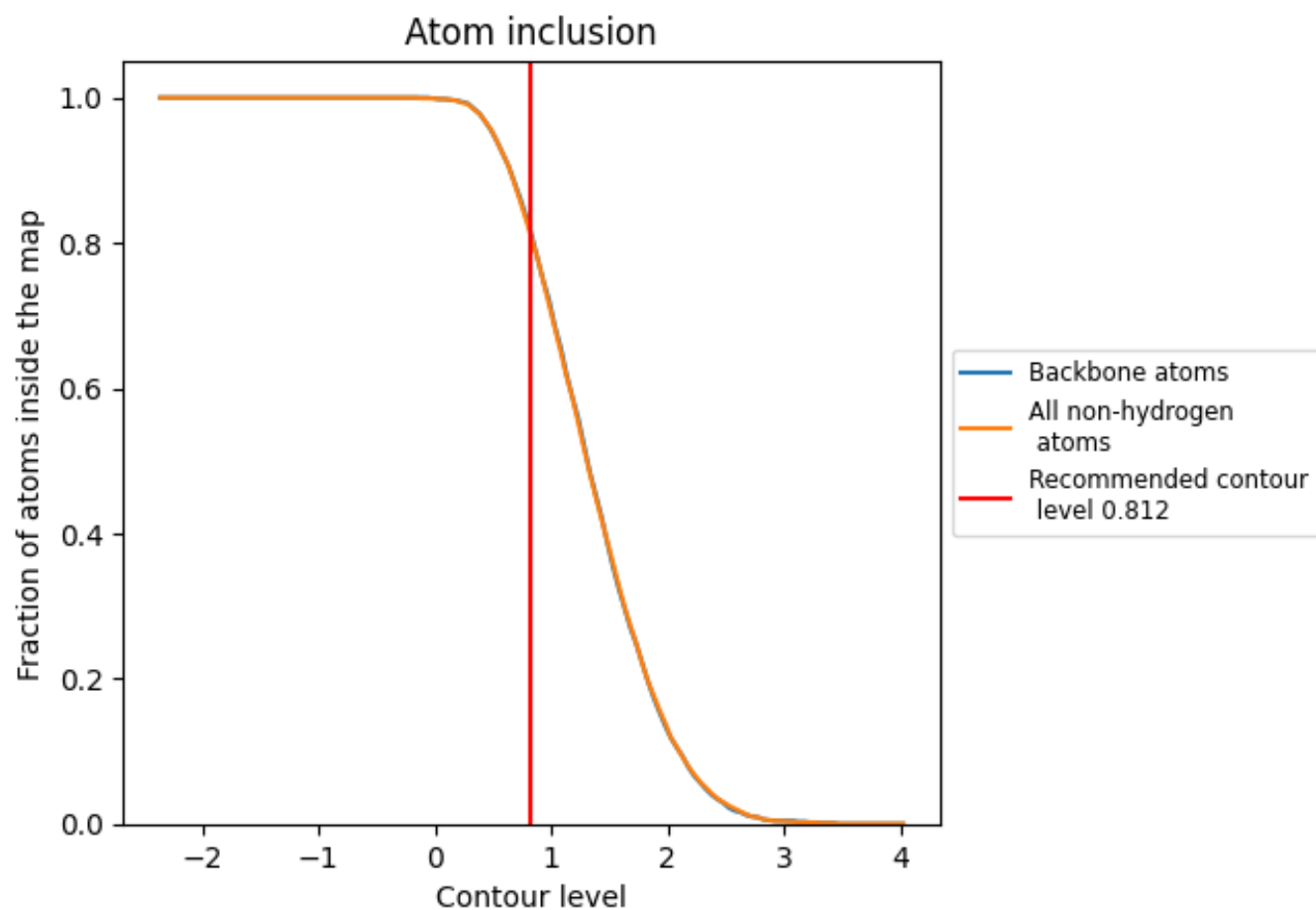
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.812).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.812) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8170	<div><div></div></div> 0.3910
A	<div><div></div></div> 0.8230	<div><div></div></div> 0.4040
B	<div><div></div></div> 0.8150	<div><div></div></div> 0.4010
C	<div><div></div></div> 0.8120	<div><div></div></div> 0.4010
D	<div><div></div></div> 0.8970	<div><div></div></div> 0.3900
E	<div><div></div></div> 0.5710	<div><div></div></div> 0.3390
H	<div><div></div></div> 0.8600	<div><div></div></div> 0.3320
L	<div><div></div></div> 0.8380	<div><div></div></div> 0.3290

1.0

0.0

<0.0