



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:05 PM UTC

PDB ID : 7CCS / pdb_00007ccs
EMDB ID : EMD-30341
Title : Consensus mutated xCT-CD98hc complex
Authors : Oda, K.; Lee, Y.; Takemoto, M.; Yamashita, K.; Nishizawa, T.; Nureki, O.
Deposited on : 2020-06-17
Resolution : 6.20 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

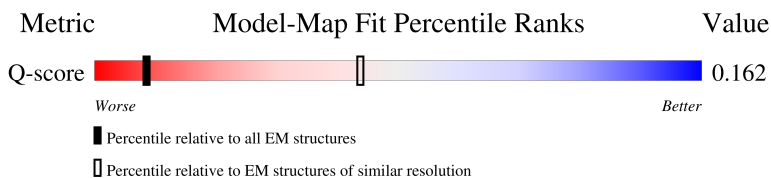
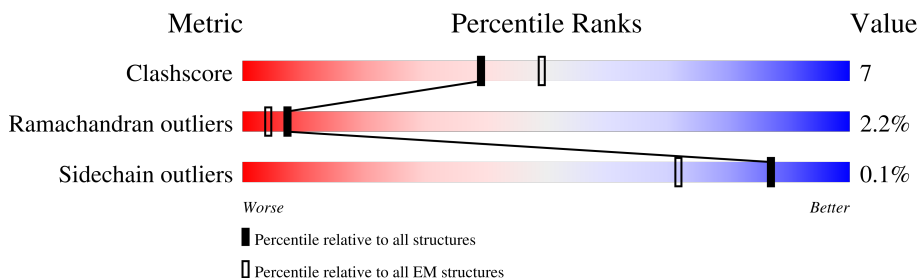
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	537 (5.70 - 6.70)

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	631	 5% 59% 13% • 26%
2	B	509	 9% 71% 12% 5% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7177 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 4F2 cell-surface antigen heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	469	Total	C	N	O	S	0	0
			3651	2333	626	685	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P08195
A	2	SER	-	expression tag	UNP P08195

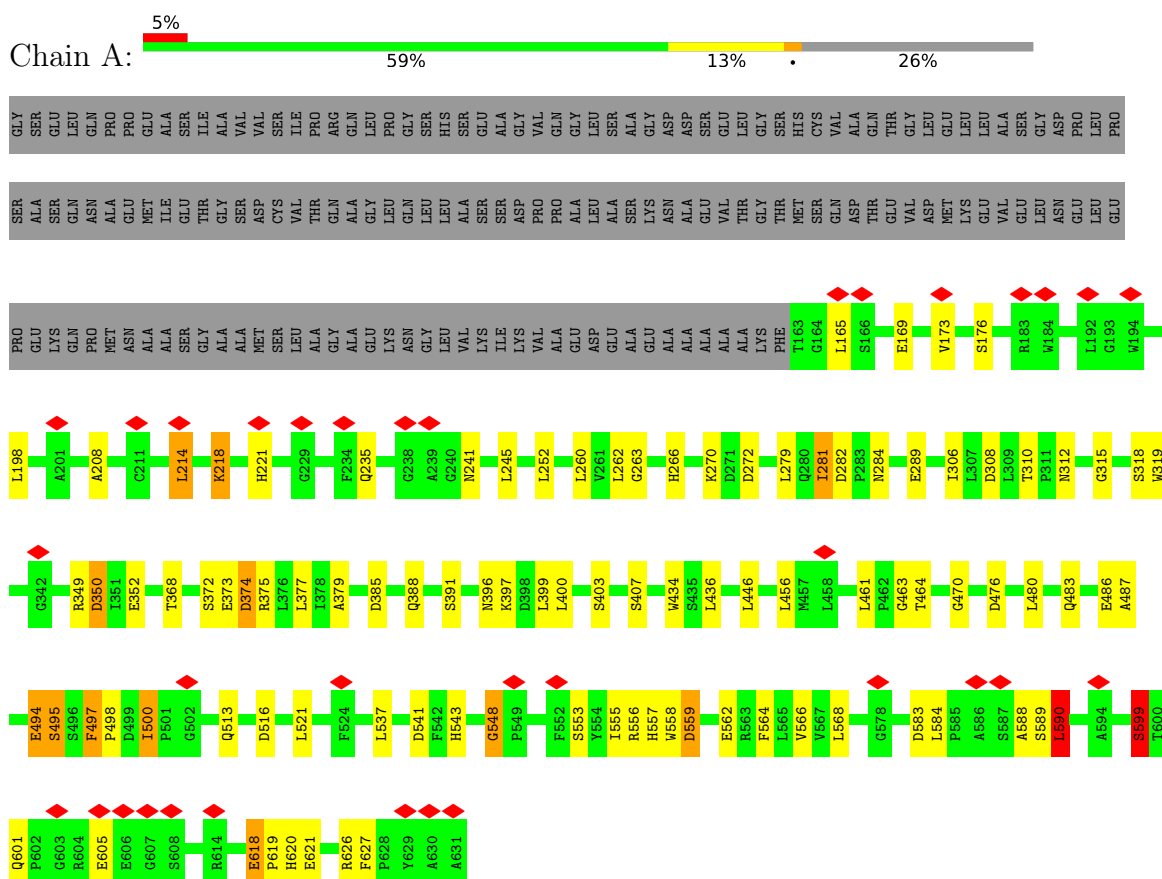
- Molecule 2 is a protein called Consensus mutated Anionic Amino Acid Transporter Light Chain, Xc- System.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	454	Total	C	N	O	S	0	0
			3526	2371	548	596	11		

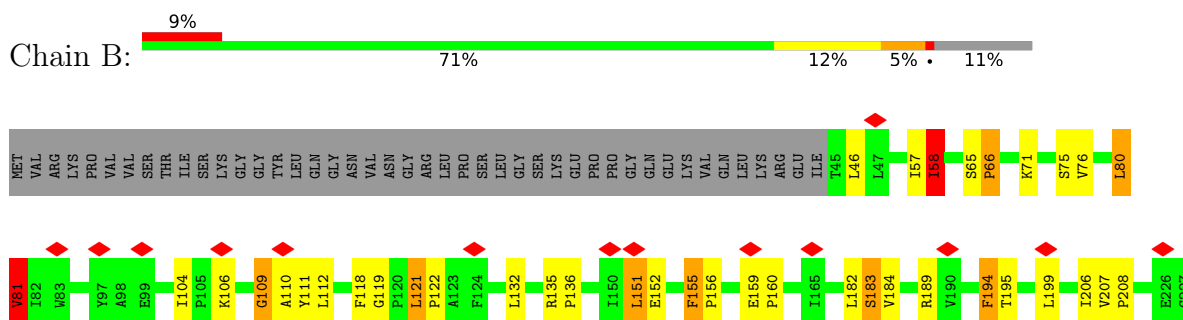
3 Residue-property plots [i](#)

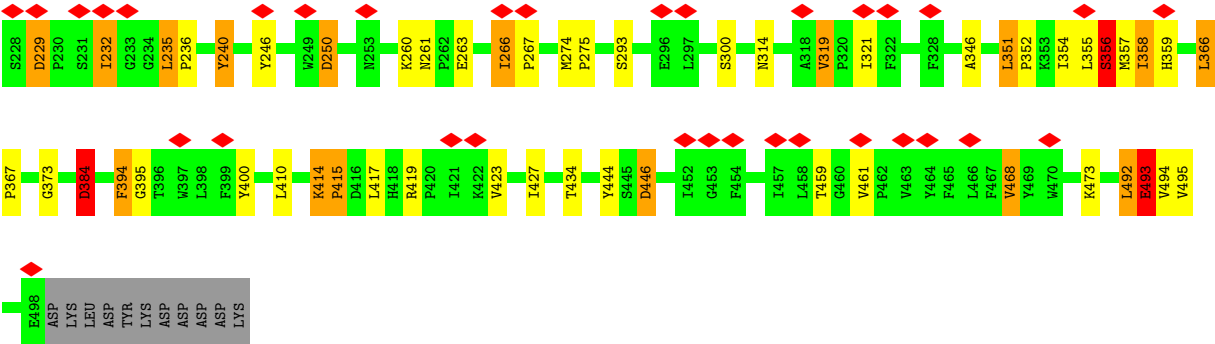
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 4F2 cell-surface antigen heavy chain



- Molecule 2: Consensus mutated Anionic Amino Acid Transporter Light Chain, Xc- System





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86395	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 ($e^-/\text{\AA}^2$)	49.76	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	265.6008, 265.6008, 265.6008	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.47556, 1.47556, 1.47556	Depositor

5 Model quality

5.1 Standard geometry

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	0.88	0/3734	1.53	59/5065 (1.2%)
2	B	0.78	0/3624	1.45	72/4953 (1.5%)
All	All	0.83	0/7358	1.49	131/10018 (1.3%)

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
1	A	0	9
2	B	0	22
All	All	0	31

There are no bond length outliers.

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ASP	CA-C-N	22.38	151.12	120.46
1	A	350	ASP	C-N-CA	22.38	151.12	120.46
1	A	218	LYS	CA-C-N	17.82	152.34	121.14
1	A	218	LYS	C-N-CA	17.82	152.34	121.14
2	B	118	PHE	CA-C-N	17.56	149.44	121.87
2	B	118	PHE	C-N-CA	17.56	149.44	121.87
2	B	58	ILE	CA-C-N	15.45	149.86	120.66
2	B	58	ILE	C-N-CA	15.45	149.86	120.66
1	A	373	GLU	CA-C-N	11.28	142.00	121.70
1	A	373	GLU	C-N-CA	11.28	142.00	121.70
2	B	119	GLY	CA-C-N	10.91	130.59	119.24
2	B	119	GLY	C-N-CA	10.91	130.59	119.24
1	A	494	GLU	N-CA-C	10.48	123.97	111.82
2	B	159	GLU	CA-C-N	10.14	126.96	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	159	GLU	C-N-CA	10.14	126.96	119.66
1	A	494	GLU	CA-C-N	10.04	139.77	121.70
1	A	494	GLU	C-N-CA	10.04	139.77	121.70
1	A	173	VAL	N-CA-C	9.61	119.56	110.53
1	A	310	THR	CA-C-N	9.47	129.22	119.56
1	A	310	THR	C-N-CA	9.47	129.22	119.56
1	A	590	LEU	CA-C-N	9.43	129.37	120.03
1	A	590	LEU	C-N-CA	9.43	129.37	120.03
1	A	446	LEU	CA-C-N	9.27	129.22	119.85
1	A	446	LEU	C-N-CA	9.27	129.22	119.85
1	A	282	ASP	CA-C-N	9.10	128.74	119.82
1	A	282	ASP	C-N-CA	9.10	128.74	119.82
2	B	235	LEU	CA-C-N	8.98	129.56	119.32
2	B	235	LEU	C-N-CA	8.98	129.56	119.32
2	B	414	LYS	CA-C-N	8.90	130.96	119.84
2	B	414	LYS	C-N-CA	8.90	130.96	119.84
2	B	160	PRO	CA-C-N	8.72	129.16	120.52
2	B	160	PRO	C-N-CA	8.72	129.16	120.52
1	A	173	VAL	CA-C-N	8.68	137.33	121.70
1	A	173	VAL	C-N-CA	8.68	137.33	121.70
2	B	395	GLY	N-CA-C	-8.66	102.01	112.49
1	A	487	ALA	CA-C-N	8.58	129.01	120.52
1	A	487	ALA	C-N-CA	8.58	129.01	120.52
2	B	423	VAL	CA-C-N	8.57	129.01	120.52
2	B	423	VAL	C-N-CA	8.57	129.01	120.52
1	A	176	SER	CA-C-N	8.47	129.30	119.47
1	A	176	SER	C-N-CA	8.47	129.30	119.47
2	B	373	GLY	CA-C-N	8.38	128.88	119.32
2	B	373	GLY	C-N-CA	8.38	128.88	119.32
2	B	446	ASP	CA-C-N	8.27	127.92	119.82
2	B	446	ASP	C-N-CA	8.27	127.92	119.82
2	B	495	VAL	CA-C-N	8.22	128.17	120.03
2	B	495	VAL	C-N-CA	8.22	128.17	120.03
1	A	584	LEU	CA-C-N	8.18	128.61	120.52
1	A	584	LEU	C-N-CA	8.18	128.61	120.52
1	A	601	GLN	CA-C-N	8.17	130.05	119.84
1	A	601	GLN	C-N-CA	8.17	130.05	119.84
2	B	319	VAL	CA-C-N	8.08	129.94	119.84
2	B	319	VAL	C-N-CA	8.08	129.94	119.84
2	B	492	LEU	N-CA-C	7.72	119.33	111.07
2	B	229	ASP	CA-C-N	7.70	128.41	119.47
2	B	229	ASP	C-N-CA	7.70	128.41	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	419	ARG	CA-C-N	7.64	127.28	119.56
2	B	419	ARG	C-N-CA	7.64	127.28	119.56
1	A	208	ALA	CA-C-N	7.63	128.66	120.11
1	A	208	ALA	C-N-CA	7.63	128.66	120.11
1	A	516	ASP	CA-C-N	7.57	127.21	119.56
1	A	516	ASP	C-N-CA	7.57	127.21	119.56
1	A	483	GLN	CA-C-N	7.55	127.71	120.31
1	A	483	GLN	C-N-CA	7.55	127.71	120.31
2	B	473	LYS	CA-C-N	7.37	127.36	119.76
2	B	473	LYS	C-N-CA	7.37	127.36	119.76
1	A	500	ILE	CA-C-N	7.30	128.97	119.84
1	A	500	ILE	C-N-CA	7.30	128.97	119.84
2	B	394	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	403	SER	N-CA-C	7.21	119.49	108.52
2	B	293	SER	CA-C-N	7.13	127.45	119.32
2	B	293	SER	C-N-CA	7.13	127.45	119.32
1	A	548	GLY	CA-C-N	7.08	128.69	119.84
1	A	548	GLY	C-N-CA	7.08	128.69	119.84
2	B	194	PHE	CA-C-O	-6.92	113.22	120.55
1	A	470	GLY	N-CA-C	-6.78	106.32	113.58
2	B	494	VAL	N-CA-C	6.76	120.12	108.90
1	A	374	ASP	N-CA-CB	6.67	121.85	110.50
1	A	464	THR	CA-C-N	6.64	126.87	119.90
1	A	464	THR	C-N-CA	6.64	126.87	119.90
1	A	627	PHE	CA-C-N	6.61	126.58	120.03
1	A	627	PHE	C-N-CA	6.61	126.58	120.03
2	B	155	PHE	CA-C-N	6.57	128.05	119.84
2	B	155	PHE	C-N-CA	6.57	128.05	119.84
2	B	81	VAL	CA-C-O	-6.50	113.96	120.85
2	B	394	PHE	CA-C-O	-6.41	113.63	120.42
2	B	261	ASN	CA-C-N	6.34	126.68	119.83
2	B	261	ASN	C-N-CA	6.34	126.68	119.83
1	A	480	LEU	CA-C-N	6.28	126.64	119.93
1	A	480	LEU	C-N-CA	6.28	126.64	119.93
2	B	121	LEU	CA-C-N	6.20	127.59	119.84
2	B	121	LEU	C-N-CA	6.20	127.59	119.84
1	A	214	LEU	CA-C-N	6.17	127.55	119.84
1	A	214	LEU	C-N-CA	6.17	127.55	119.84
2	B	461	VAL	CA-C-N	6.06	125.95	119.28
2	B	461	VAL	C-N-CA	6.06	125.95	119.28
1	A	599	SER	CA-C-O	-6.06	114.20	120.99
1	A	281	ILE	N-CA-C	6.04	116.87	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	LEU	CA-C-N	5.96	126.31	119.93
2	B	351	LEU	C-N-CA	5.96	126.31	119.93
1	A	263	GLY	CA-C-N	5.93	127.25	119.84
1	A	263	GLY	C-N-CA	5.93	127.25	119.84
2	B	493	GLU	CA-C-N	-5.92	114.28	122.69
2	B	493	GLU	C-N-CA	-5.92	114.28	122.69
2	B	366	LEU	CA-C-N	5.92	126.06	119.32
2	B	366	LEU	C-N-CA	5.92	126.06	119.32
2	B	80	LEU	N-CA-C	-5.91	104.42	111.69
2	B	104	ILE	CA-C-N	5.84	125.53	119.64
2	B	104	ILE	C-N-CA	5.84	125.53	119.64
2	B	468	VAL	CA-C-O	-5.81	113.52	120.78
2	B	266	ILE	CA-C-N	5.77	125.62	119.28
2	B	266	ILE	C-N-CA	5.77	125.62	119.28
1	A	537	LEU	N-CA-C	-5.75	105.09	111.36
1	A	618	GLU	CA-C-N	5.72	126.99	119.84
1	A	618	GLU	C-N-CA	5.72	126.99	119.84
2	B	427	ILE	CA-C-N	5.67	125.20	119.19
2	B	427	ILE	C-N-CA	5.67	125.20	119.19
2	B	240	TYR	CA-C-O	-5.63	114.45	120.42
2	B	206	ILE	N-CA-C	5.58	115.78	110.42
2	B	151	LEU	CA-C-O	-5.55	114.67	120.55
2	B	358	ILE	CA-C-N	5.52	131.63	121.70
2	B	358	ILE	C-N-CA	5.52	131.63	121.70
2	B	152	GLU	CA-C-N	5.48	126.69	119.84
2	B	152	GLU	C-N-CA	5.48	126.69	119.84
2	B	250	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	461	LEU	CA-C-N	5.32	126.49	119.84
1	A	461	LEU	C-N-CA	5.32	126.49	119.84
2	B	356	SER	CA-C-O	-5.24	113.02	120.51
1	A	434	TRP	N-CA-C	5.13	117.78	108.69
2	B	384	ASP	CA-C-O	-5.09	114.85	120.70
2	B	195	THR	N-CA-C	-5.04	105.49	111.69

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	ASN	Peptide,Mainchain
1	A	349	ARG	Peptide,Mainchain
1	A	397	LYS	Peptide,Mainchain
1	A	588	ALA	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	A	599	SER	Mainchain
2	B	110	ALA	Peptide,Mainchain
2	B	132	LEU	Mainchain
2	B	151	LEU	Mainchain
2	B	194	PHE	Mainchain
2	B	199	LEU	Peptide,Mainchain
2	B	240	TYR	Peptide,Mainchain
2	B	355	LEU	Peptide,Mainchain
2	B	356	SER	Peptide,Mainchain
2	B	384	ASP	Mainchain
2	B	394	PHE	Mainchain
2	B	434	THR	Mainchain
2	B	459	THR	Peptide,Mainchain
2	B	468	VAL	Mainchain
2	B	493	GLU	Peptide,Mainchain
2	B	81	VAL	Mainchain

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	3651	0	3640	60	0
2	B	3526	0	3690	45	0
All	All	7177	0	7330	105	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 7.

All (105) 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:620:HIS:O	1:A:620:HIS:CD2	2.33	0.82
2:B:81:VAL:HG12	2:B:81:VAL:O	1.83	0.77
1:A:252:LEU:C	1:A:252:LEU:HD23	2.18	0.69
1:A:626:ARG:HD3	1:A:626:ARG:C	2.18	0.69
2:B:81:VAL:O	2:B:81:VAL:CG1	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LYS:NZ	2:B:300:SER:OG	2.28	0.66
1:A:260:LEU:C	1:A:260:LEU:HD12	2.20	0.66
2:B:493:GLU:O	2:B:493:GLU:HG2	1.98	0.63
1:A:350:ASP:C	1:A:350:ASP:OD1	2.42	0.62
1:A:500:ILE:HG23	1:A:500:ILE:O	2.02	0.60
2:B:263:GLU:OE1	2:B:263:GLU:N	2.29	0.58
2:B:232:ILE:O	2:B:232:ILE:HG22	2.04	0.57
2:B:446:ASP:OD1	2:B:446:ASP:O	2.22	0.57
1:A:245:LEU:C	1:A:245:LEU:HD23	2.29	0.57
1:A:352:GLU:OE1	1:A:352:GLU:N	2.38	0.56
1:A:318:SER:HG	1:A:319:TRP:CD1	2.24	0.56
1:A:260:LEU:HD12	1:A:260:LEU:O	2.06	0.56
1:A:621:GLU:HA	1:A:621:GLU:OE1	2.05	0.56
2:B:266:ILE:N	2:B:267:PRO:CD	2.70	0.54
2:B:121:LEU:HB3	2:B:122:PRO:HD3	1.89	0.54
1:A:289:GLU:H	1:A:289:GLU:CD	2.16	0.54
1:A:252:LEU:HD23	1:A:252:LEU:O	2.06	0.53
2:B:111:TYR:CD1	2:B:111:TYR:C	2.86	0.53
2:B:135:ARG:HB2	2:B:136:PRO:HD3	1.91	0.52
1:A:272:ASP:OD1	1:A:272:ASP:C	2.51	0.52
1:A:368:THR:HB	1:A:375:ARG:HB2	1.92	0.52
2:B:414:LYS:N	2:B:415:PRO:CD	2.73	0.51
2:B:446:ASP:OD1	2:B:446:ASP:C	2.53	0.51
2:B:492:LEU:O	2:B:493:GLU:HB3	2.11	0.50
1:A:372:SER:OG	1:A:375:ARG:HG3	2.11	0.50
2:B:182:LEU:O	2:B:183:SER:C	2.54	0.50
1:A:396:ASN:OD1	1:A:396:ASN:C	2.54	0.50
1:A:620:HIS:O	1:A:620:HIS:CG	2.56	0.50
2:B:274:MET:C	2:B:274:MET:SD	2.95	0.50
2:B:57:ILE:O	2:B:58:ILE:HB	2.12	0.49
1:A:289:GLU:OE1	1:A:289:GLU:N	2.32	0.49
2:B:400:TYR:CD1	2:B:400:TYR:N	2.80	0.49
2:B:189:ARG:NE	2:B:189:ARG:HA	2.27	0.49
1:A:235:GLN:NE2	1:A:241:ASN:O	2.45	0.49
2:B:446:ASP:O	2:B:446:ASP:CG	2.56	0.48
2:B:358:ILE:HA	2:B:359:HIS:HB3	1.95	0.48
1:A:456:LEU:C	1:A:456:LEU:HD23	2.39	0.48
1:A:241:ASN:OD1	1:A:241:ASN:C	2.56	0.47
1:A:214:LEU:HD23	1:A:214:LEU:C	2.39	0.47
1:A:308:ASP:OD1	1:A:308:ASP:C	2.57	0.47
2:B:354:ILE:HA	2:B:357:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:TYR:N	2:B:400:TYR:HD1	2.12	0.47
1:A:568:LEU:C	1:A:568:LEU:HD23	2.39	0.47
2:B:109:GLY:HA2	2:B:112:LEU:HB2	1.96	0.47
2:B:366:LEU:HB3	2:B:367:PRO:HD3	1.97	0.46
1:A:252:LEU:C	1:A:252:LEU:CD2	2.88	0.46
1:A:541:ASP:C	1:A:541:ASP:OD1	2.57	0.46
2:B:356:SER:OG	2:B:357:MET:N	2.44	0.46
2:B:493:GLU:O	2:B:493:GLU:CG	2.60	0.46
1:A:221:HIS:HA	1:A:463:GLY:HA2	1.98	0.46
2:B:155:PHE:N	2:B:156:PRO:HD3	2.31	0.46
1:A:621:GLU:OE1	1:A:621:GLU:CA	2.64	0.46
2:B:246:TYR:HD2	2:B:246:TYR:O	1.99	0.46
1:A:494:GLU:N	1:A:495:SER:HB3	2.31	0.45
2:B:314:ASN:OD1	2:B:314:ASN:C	2.56	0.45
1:A:385:ASP:C	1:A:385:ASP:OD1	2.59	0.45
1:A:476:ASP:OD1	1:A:476:ASP:C	2.58	0.45
2:B:207:VAL:HB	2:B:208:PRO:HD3	1.99	0.45
1:A:583:ASP:OD1	1:A:583:ASP:C	2.59	0.45
1:A:169:GLU:OE1	1:A:169:GLU:N	2.39	0.45
2:B:384:ASP:C	2:B:384:ASP:OD1	2.59	0.45
1:A:589:SER:O	1:A:590:LEU:HB3	2.17	0.44
1:A:379:ALA:N	1:A:400:LEU:O	2.51	0.44
1:A:486:GLU:OE1	1:A:486:GLU:N	2.37	0.44
2:B:75:SER:HB3	2:B:76:VAL:HA	2.00	0.44
1:A:279:LEU:N	1:A:279:LEU:HD12	2.33	0.44
2:B:351:LEU:HA	2:B:352:PRO:HD3	1.93	0.44
1:A:618:GLU:HB3	1:A:619:PRO:HD2	2.00	0.43
2:B:235:LEU:HA	2:B:236:PRO:HD3	1.86	0.43
1:A:198:LEU:C	1:A:198:LEU:HD23	2.43	0.43
1:A:407:SER:HB3	1:A:436:LEU:O	2.18	0.43
2:B:410:LEU:HB3	2:B:417:LEU:HD21	2.00	0.43
1:A:559:ASP:OD1	1:A:559:ASP:C	2.59	0.43
2:B:155:PHE:N	2:B:156:PRO:CD	2.82	0.43
1:A:266:HIS:HA	1:A:281:ILE:HA	2.00	0.43
2:B:274:MET:N	2:B:275:PRO:HD2	2.33	0.43
1:A:262:LEU:N	1:A:306:ILE:O	2.52	0.43
1:A:562:GLU:HA	1:A:562:GLU:OE1	2.17	0.42
2:B:65:SER:N	2:B:66:PRO:CD	2.82	0.42
1:A:599:SER:O	1:A:599:SER:OG	2.32	0.42
2:B:319:VAL:O	2:B:319:VAL:HG12	2.20	0.42
1:A:556:ARG:HB3	1:A:564:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:HB3	1:A:318:SER:HA	2.02	0.42
1:A:557:HIS:O	1:A:558:TRP:C	2.62	0.42
1:A:260:LEU:C	1:A:260:LEU:CD1	2.89	0.41
1:A:543:HIS:HB3	1:A:555:ILE:HB	2.02	0.41
1:A:497:PHE:N	1:A:498:PRO:HD3	2.36	0.41
1:A:289:GLU:CD	1:A:289:GLU:N	2.79	0.41
1:A:388:GLN:NE2	1:A:391:SER:OG	2.54	0.41
2:B:444:TYR:CD2	2:B:444:TYR:N	2.86	0.41
1:A:513:GLN:HB3	1:A:521:LEU:HB3	2.03	0.41
1:A:553:SER:HA	1:A:566:VAL:O	2.21	0.41
1:A:165:LEU:HD23	1:A:165:LEU:C	2.46	0.41
1:A:270:LYS:HD2	1:A:315:GLY:HA2	2.03	0.41
1:A:377:LEU:HB2	1:A:399:LEU:HD22	2.03	0.41
1:A:396:ASN:OD1	1:A:396:ASN:O	2.39	0.41
2:B:80:LEU:HD12	2:B:80:LEU:N	2.36	0.41
2:B:229:ASP:OD1	2:B:229:ASP:C	2.62	0.41
2:B:346:ALA:HA	2:B:351:LEU:O	2.21	0.40
2:B:246:TYR:CD2	2:B:246:TYR:C	2.99	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	465/631 (74%)	419 (90%)	38 (8%)	8 (2%)	7	36
2	B	452/509 (89%)	411 (91%)	29 (6%)	12 (3%)	4	25
All	All	917/1140 (80%)	830 (90%)	67 (7%)	20 (2%)	7	29

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASP
1	A	605	GLU
2	B	58	ILE
2	B	106	LYS
2	B	109	GLY
2	B	260	LYS
1	A	218	LYS
2	B	183	SER
2	B	184	VAL
1	A	495	SER
2	B	415	PRO
1	A	590	LEU
1	A	559	ASP
2	B	66	PRO
2	B	321	ILE
1	A	497	PHE
2	B	250	ASP
2	B	493	GLU
1	A	548	GLY
2	B	232	ILE

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	392/514 (76%)	392 (100%)	0	100	100
2	B	385/434 (89%)	384 (100%)	1 (0%)	86	85
All	All	777/948 (82%)	776 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	388	GLN
1	A	543	HIS
2	B	449	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	213:GLU	C	214:LEU	N	3.35

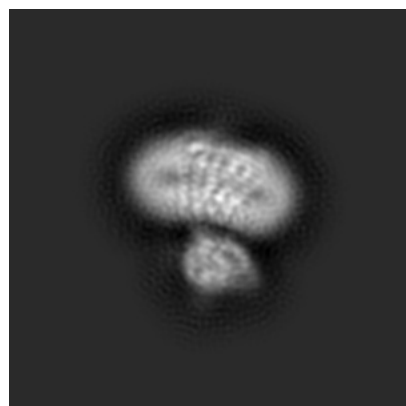
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30341. These allow visual inspection of the internal detail of the map and identification of artifacts.

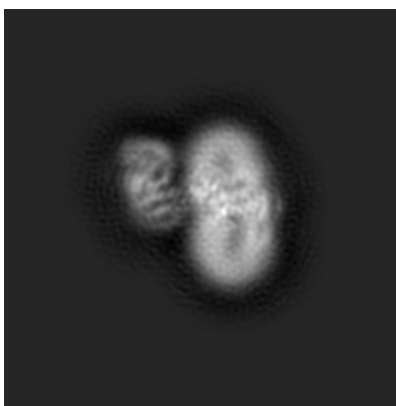
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

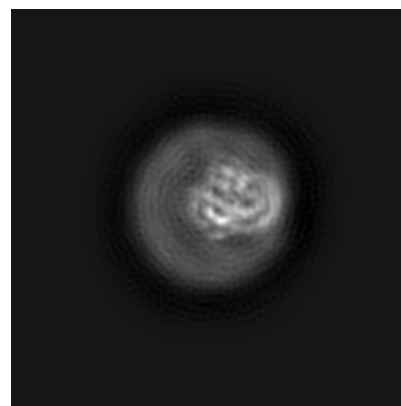
6.1.1 Primary map



X

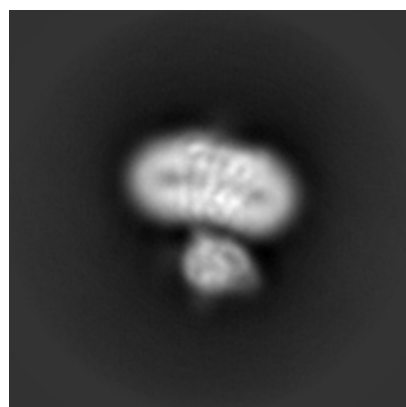


Y

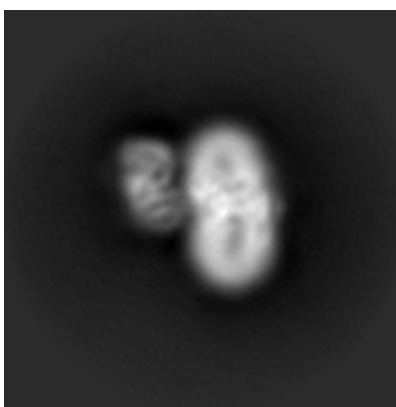


Z

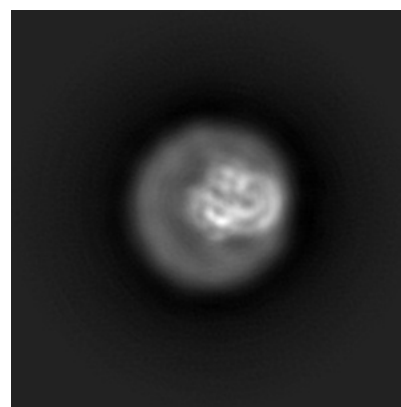
6.1.2 Raw map



X



Y

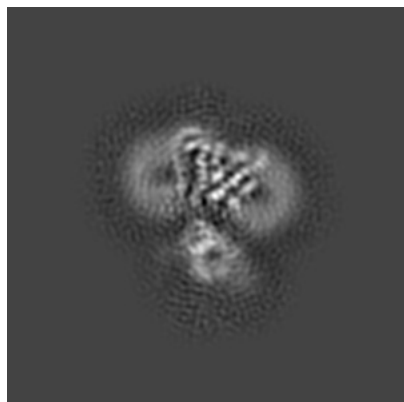


Z

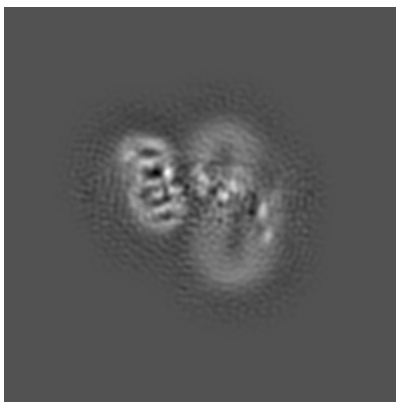
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

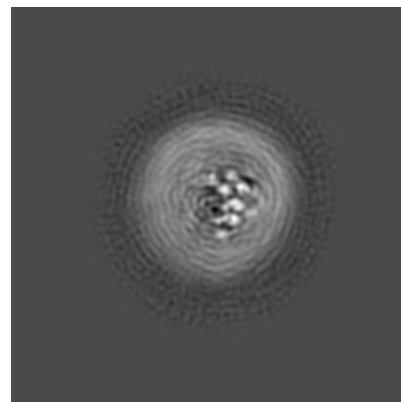
6.2.1 Primary map



X Index: 90

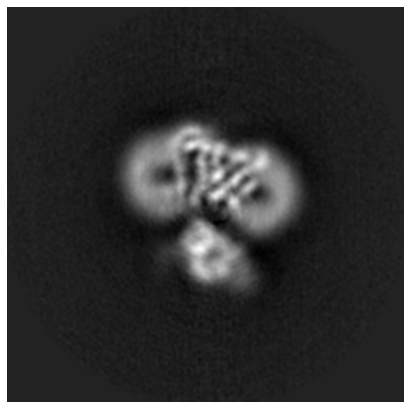


Y Index: 90

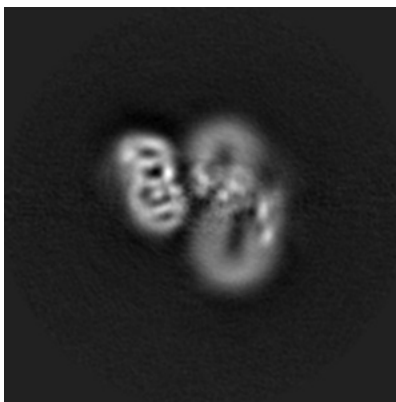


Z Index: 90

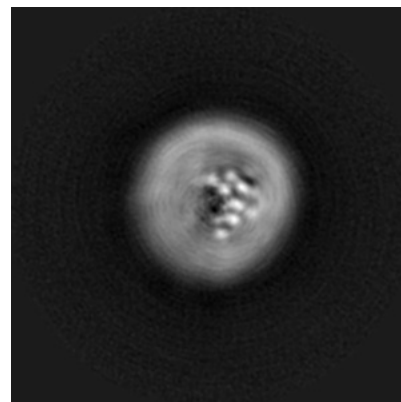
6.2.2 Raw map



X Index: 90



Y Index: 90

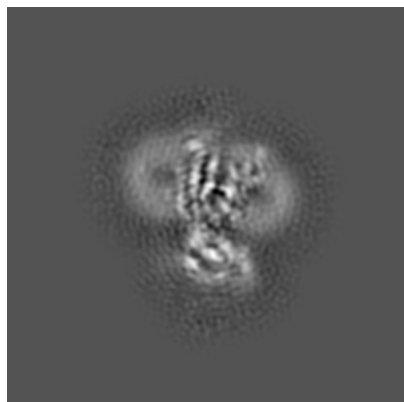


Z Index: 90

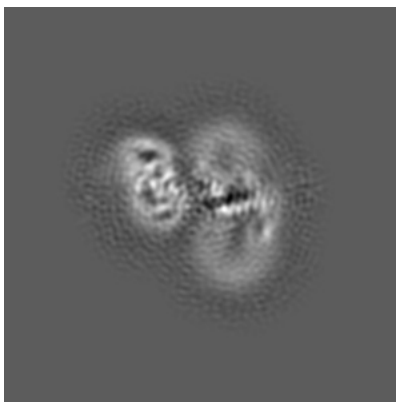
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

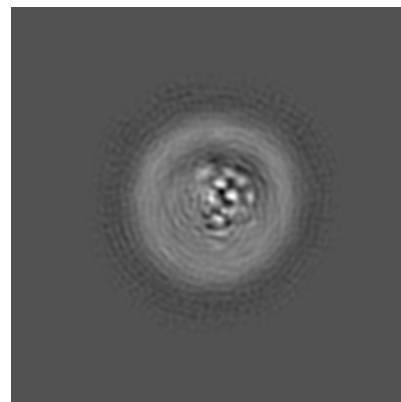
6.3.1 Primary map



X Index: 95

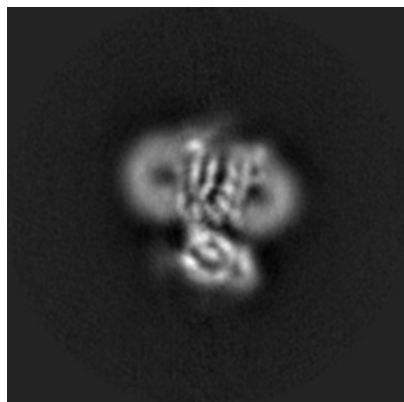


Y Index: 88

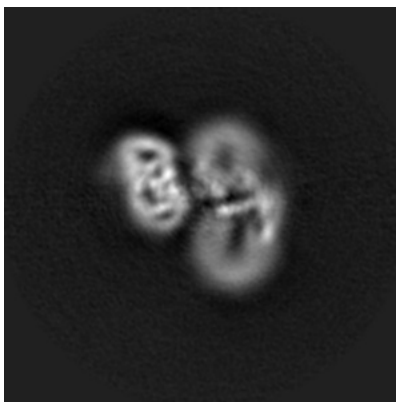


Z Index: 95

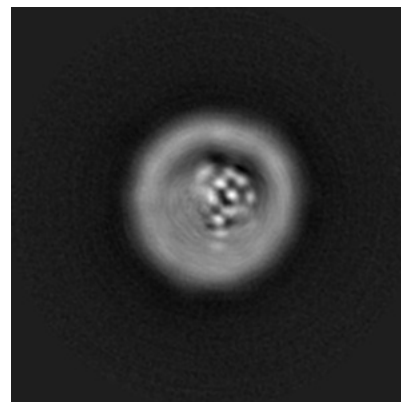
6.3.2 Raw map



X Index: 96



Y Index: 88



Z Index: 95

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

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

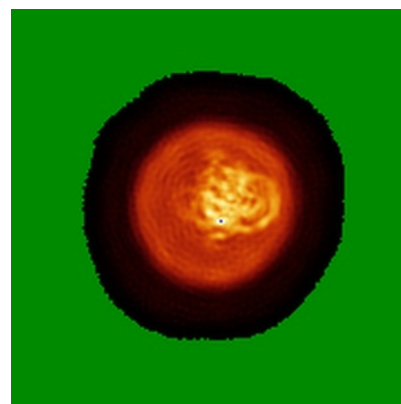
6.4.1 Primary map



X

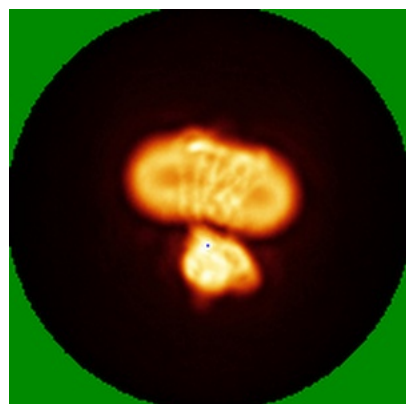


Y



Z

6.4.2 Raw map



X



Y

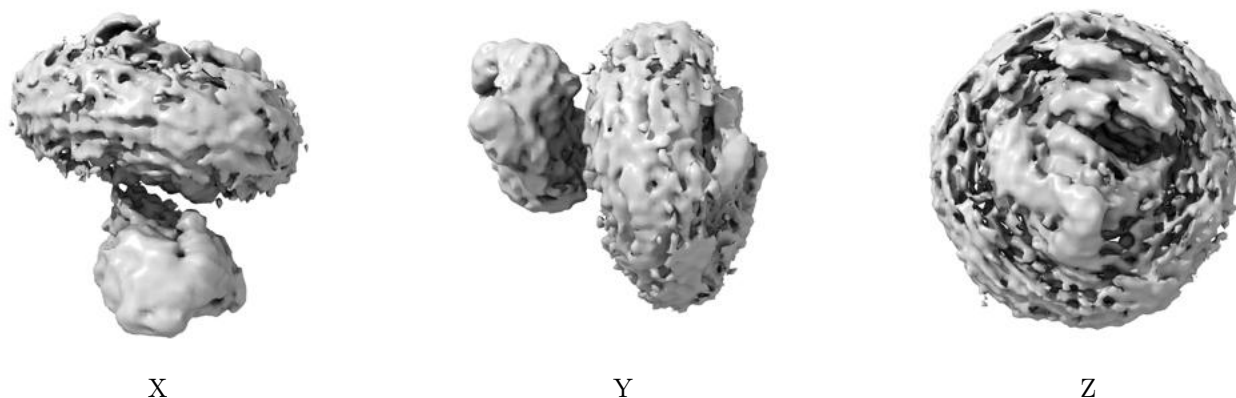


Z

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.

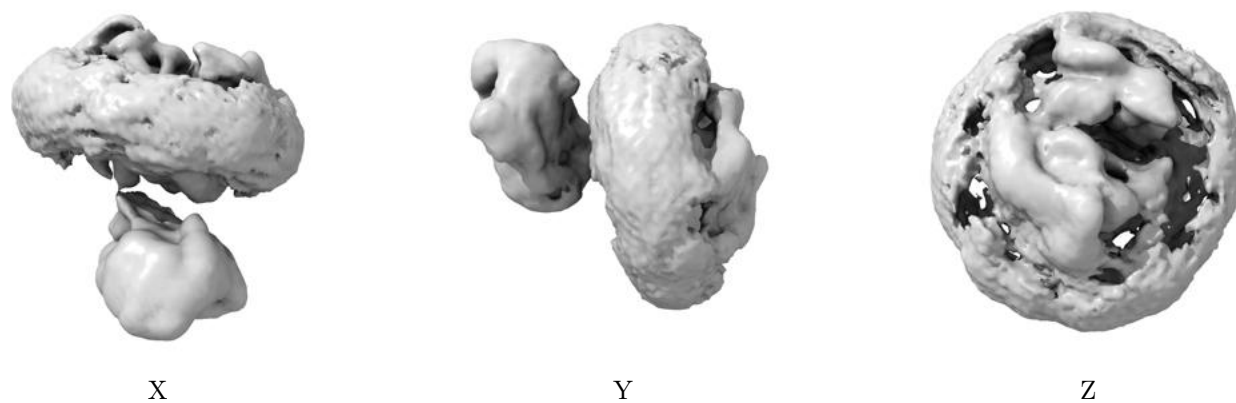
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

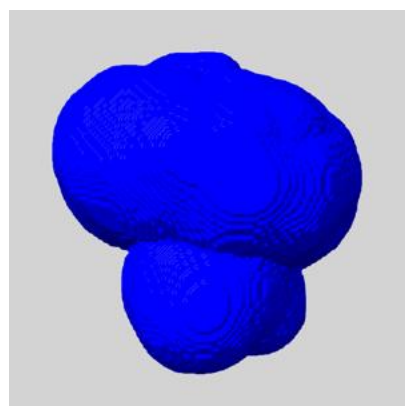
6.6 Mask visualisation [i](#)

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

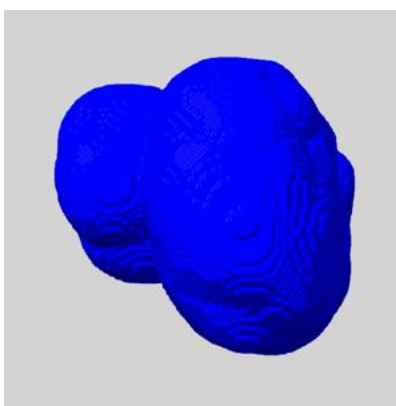
A mask typically either:

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

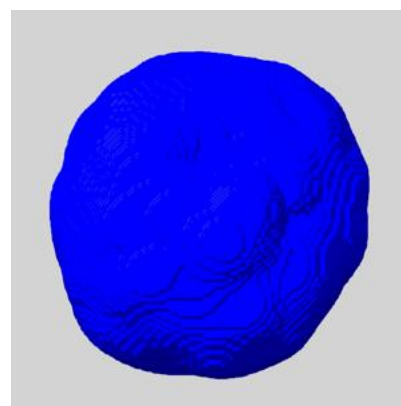
6.6.1 emd_30341_msk_1.map [i](#)



X



Y

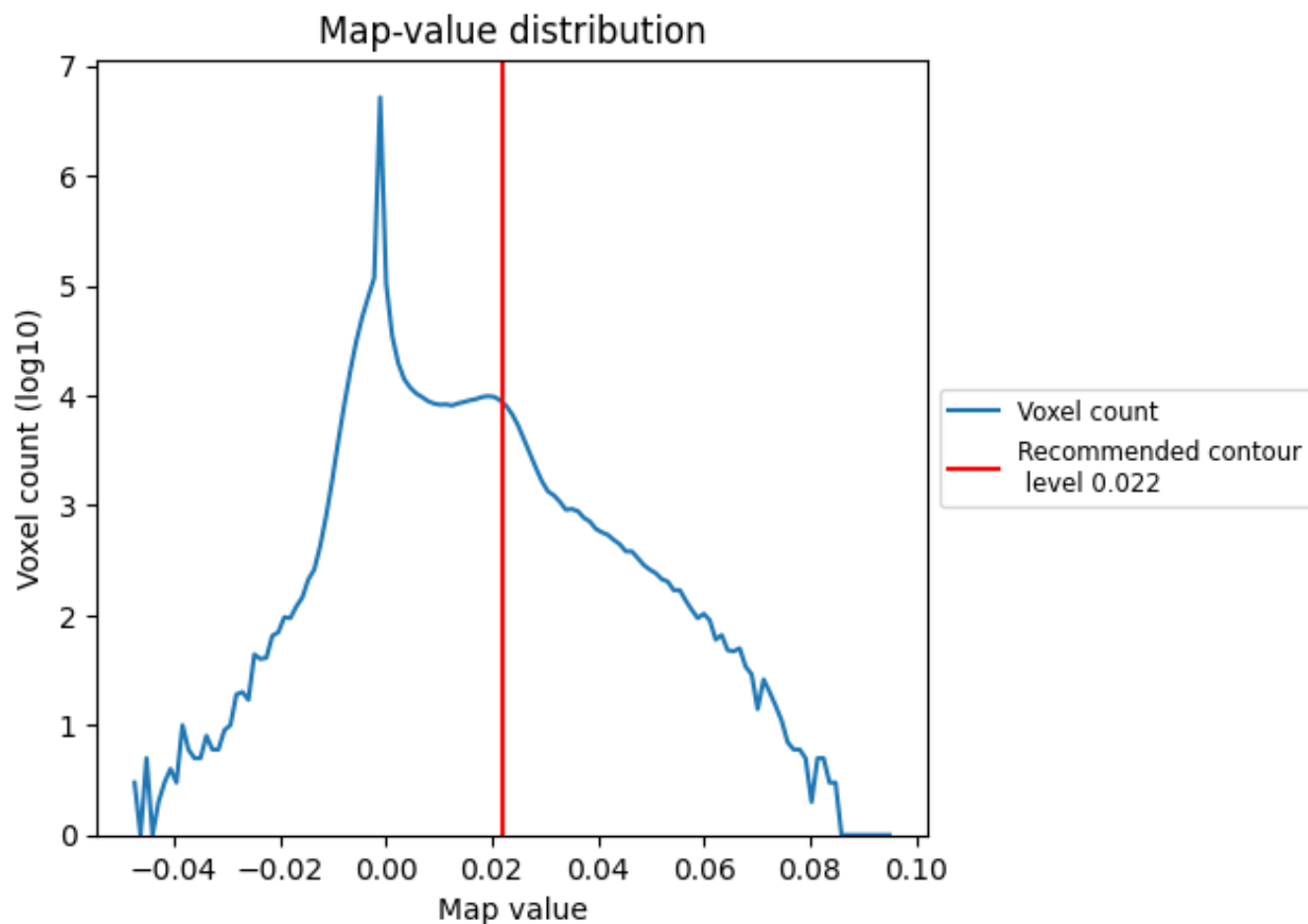


Z

7 Map analysis [i](#)

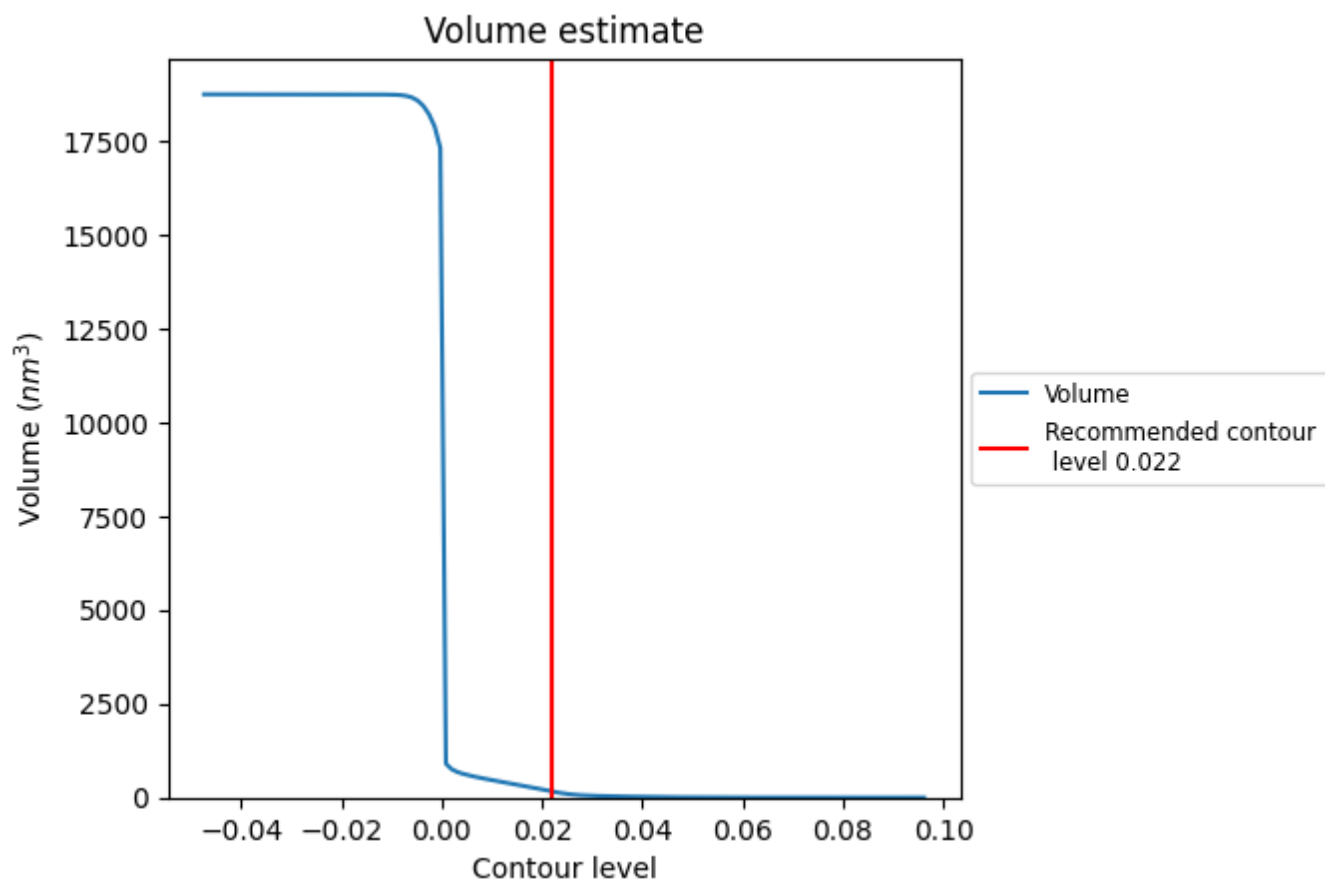
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

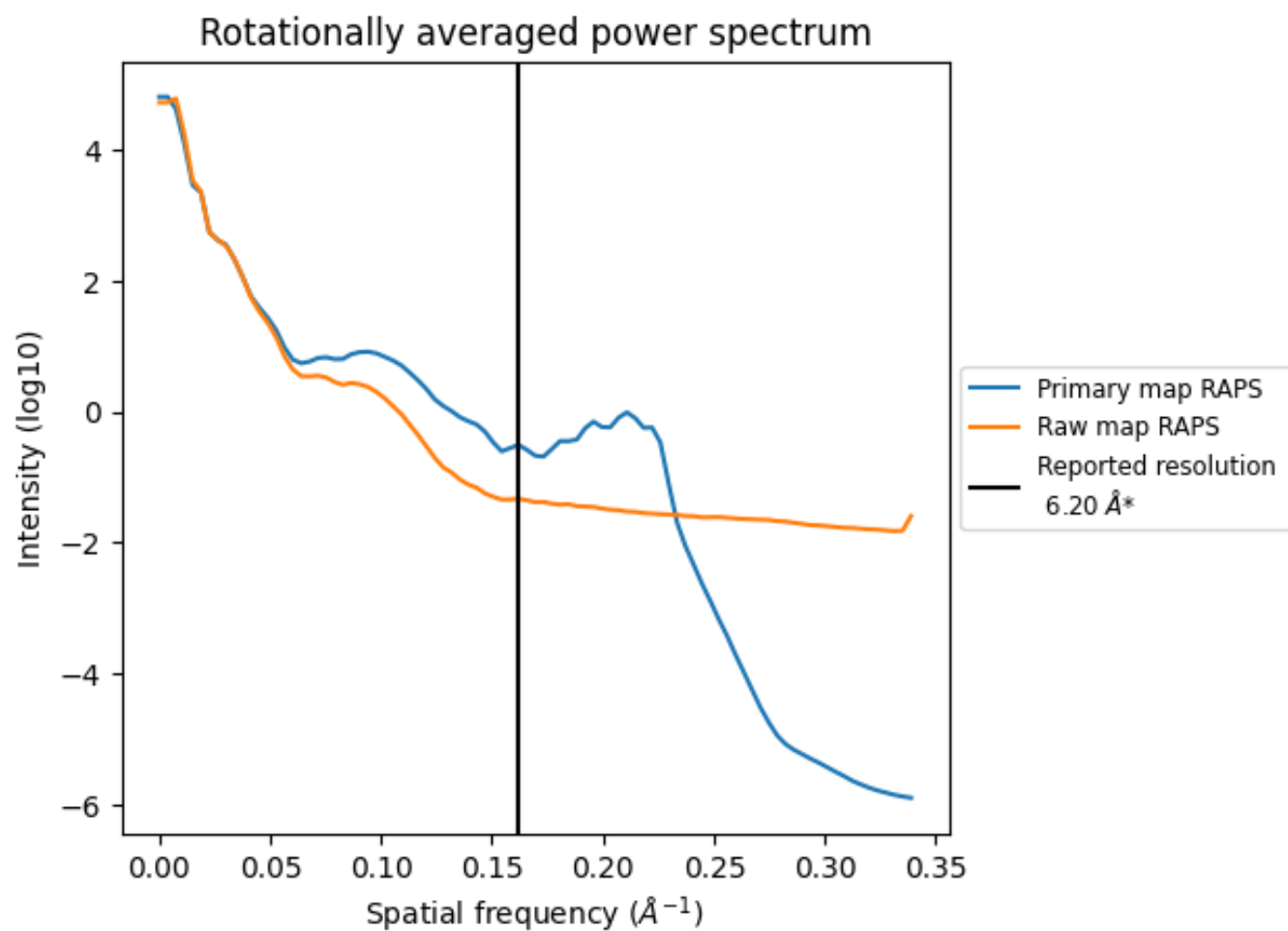
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 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 ⓘ

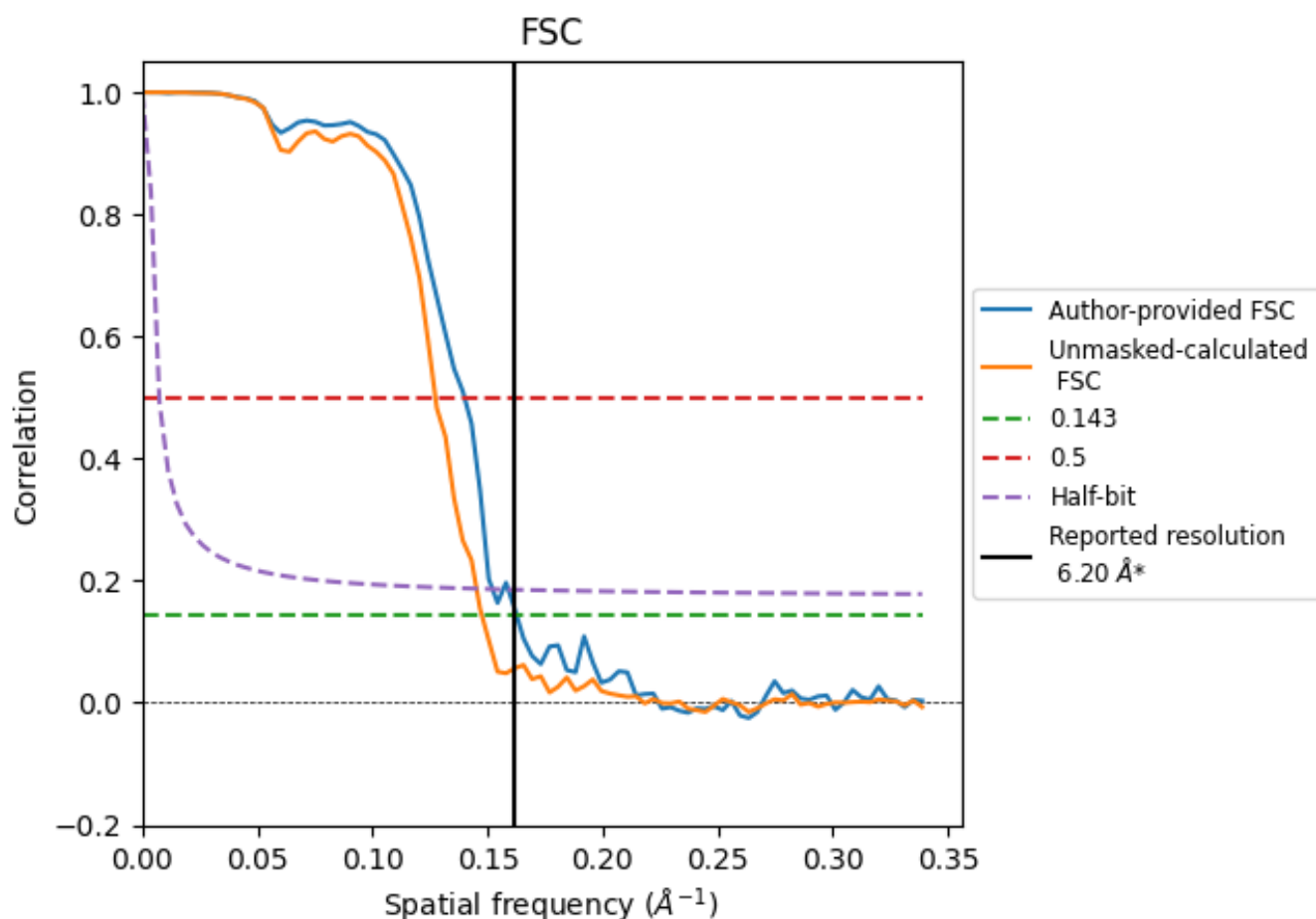


*Reported resolution corresponds to spatial frequency of 0.161 $\text{\AA}^{-1}$

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 $0.161 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

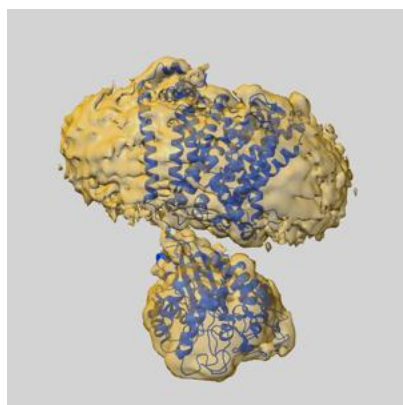
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.15	7.14	6.57
Unmasked-calculated*	6.78	7.85	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

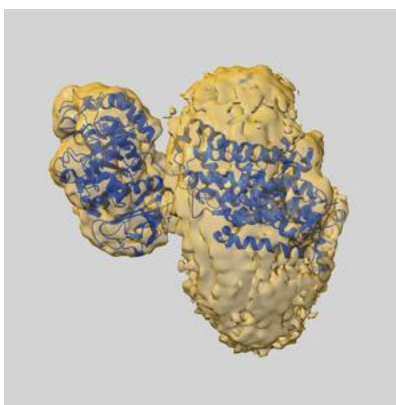
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30341 and PDB model 7CCS. Per-residue inclusion information can be found in section [3](#) on page [4](#).

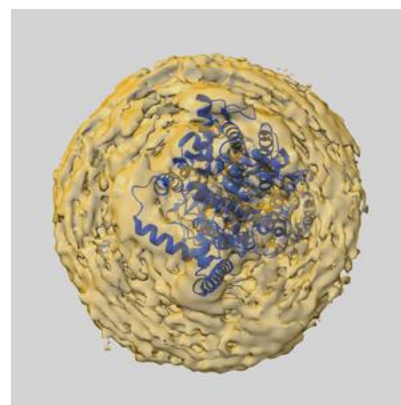
9.1 Map-model overlay [i](#)



X



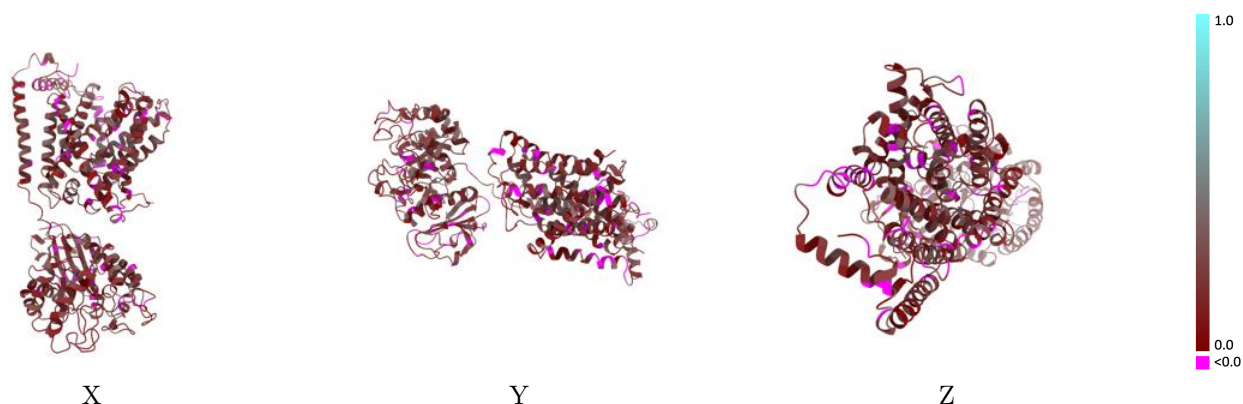
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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](#)

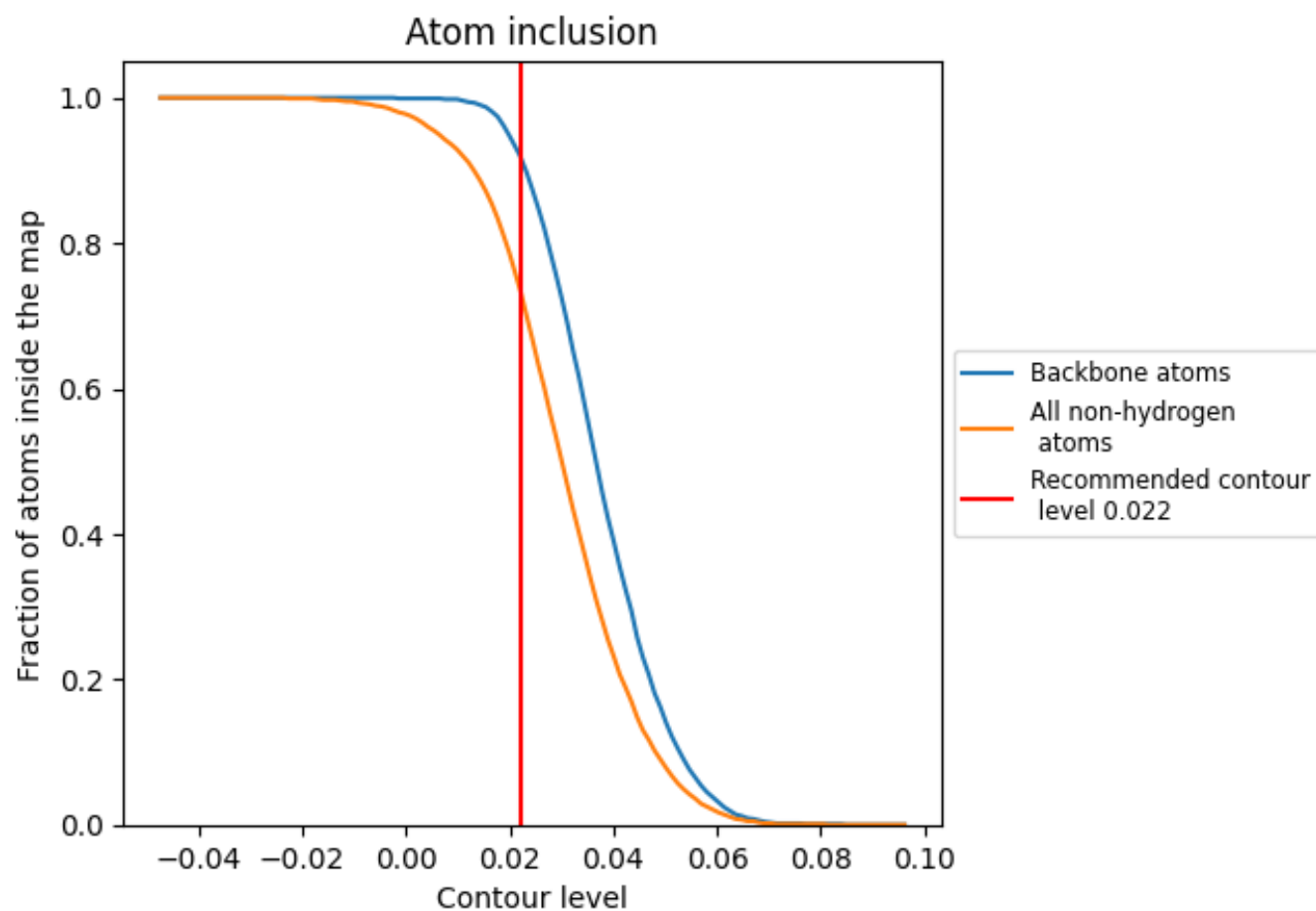


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.1620
A	0.7790	0.1630
B	0.6920	0.1610

