



Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 04:01 pm GMT

PDB ID : 8BBE
EMDB ID : EMD-15954
Title : Structure of the IFT-A complex; IFT-A2 module
Authors : Hesketh, S.J.; Mukhopadhyay, A.G.; Nakamura, D.; Toropova, K.; Roberts, A.J.
Deposited on : 2022-10-12
Resolution : 3.50 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

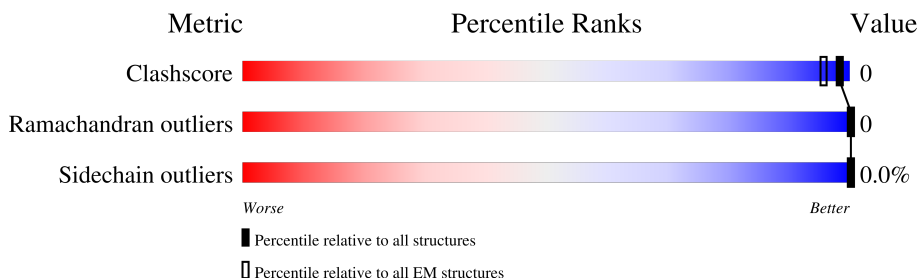
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	C	1241	
2	D	1500	
3	E	1184	
4	F	209	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20181 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 Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	702	Total	C	N	O	S	0	0
			5595	3569	951	1040	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	208	UNK	ASN	conflict	UNP Q9HBG6
C	209	UNK	ARG	conflict	UNP Q9HBG6
C	210	UNK	TYR	conflict	UNP Q9HBG6
C	211	UNK	ILE	conflict	UNP Q9HBG6
C	212	UNK	GLN	conflict	UNP Q9HBG6
C	213	UNK	GLU	conflict	UNP Q9HBG6

- Molecule 2 is a protein called SNAP-tag,Tetratricopeptide repeat protein 21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	648	Total	C	N	O	S	0	0
			5253	3318	916	978	41		

- Molecule 3 is a protein called WD repeat-containing protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1112	Total	C	N	O	S	0	0
			8863	5657	1497	1650	59		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PHE	-	expression tag	UNP Q9P2L0
E	-1	GLN	-	expression tag	UNP Q9P2L0
E	0	GLY	-	expression tag	UNP Q9P2L0

- Molecule 4 is a protein called Intraflagellar transport protein 43 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	57	Total	C	N	O	S	0	0
			470	296	74	98	2		

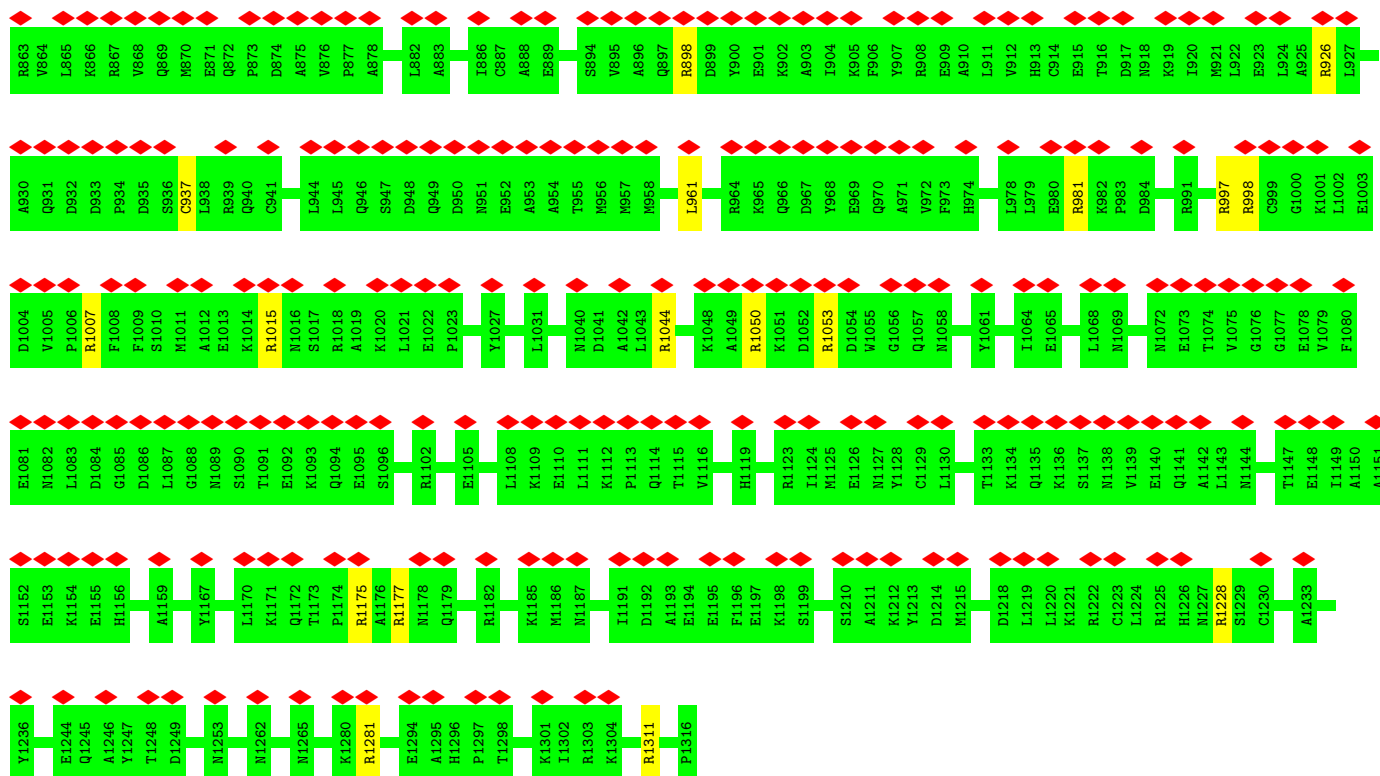
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP Q96FT9

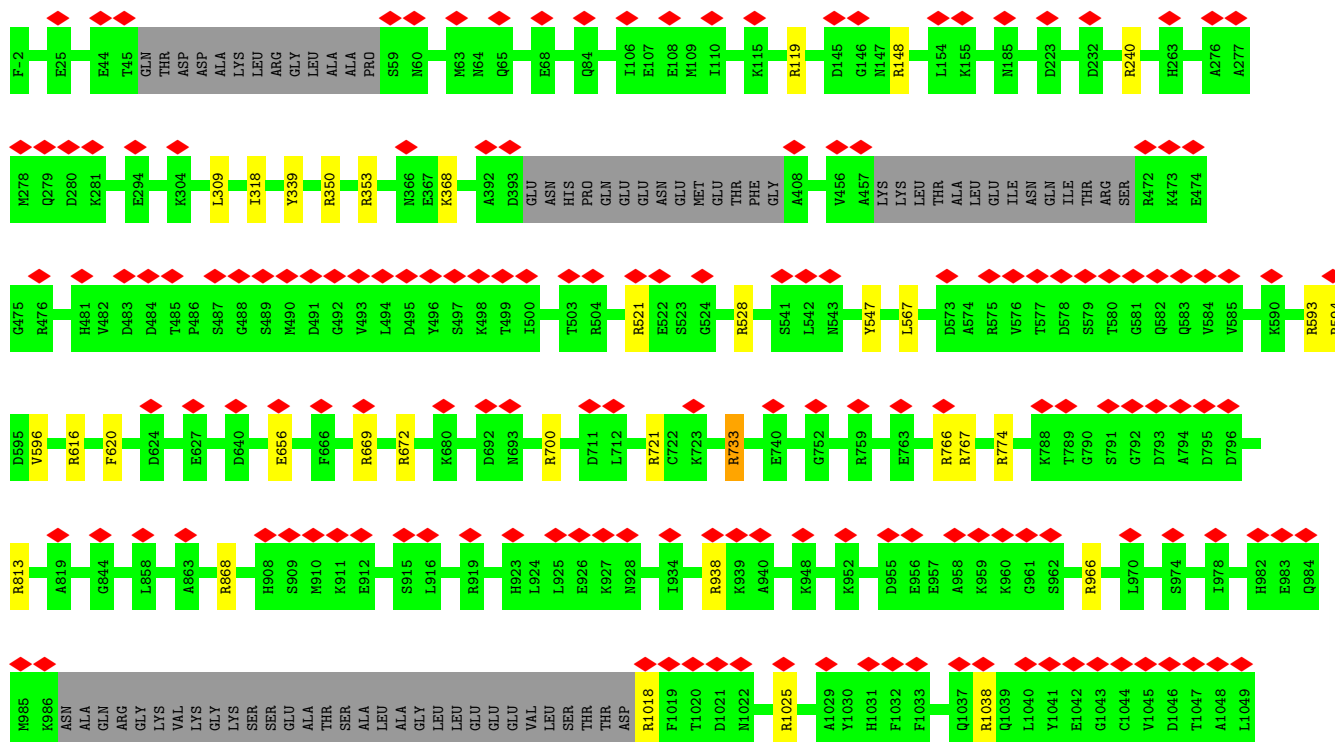
Chain D:

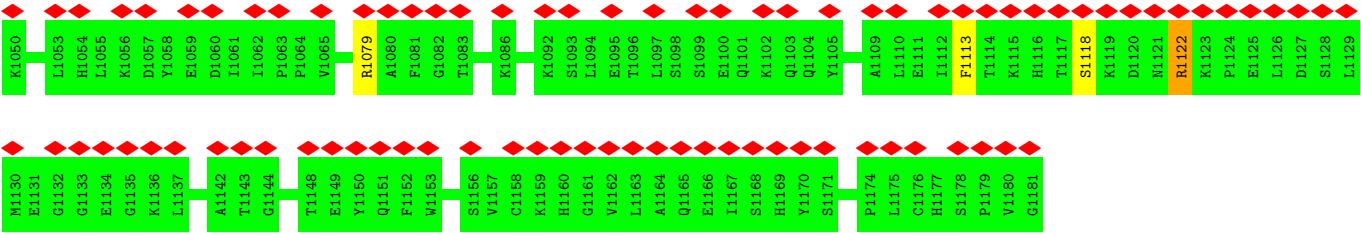


C792	P722	THR	ARG	LEU	CYS	ASN	SER	ARG	SER	ARG	THR	GLN	GLY	GLN	GLY	GLY	GLY
Y793	R723	ALA	ILE	LEU	ILE	LEU	VAL	THR	VAL	PHE	THR	ALA	ALA	ALA	ASN	THR	LYS
D794	S724	ASN	GLY	GLN	VAL	ASN	SER	CYS	SER	ALA	ALA	TRP	PRO	ALA	ASP	GLY	LYS
L795	F725	ALA	SER	GLU	LEU	ASP	LEU	ARG	GLY	ILE	ILE	ALA	MET	ALA	ASP	GLY	CYS
A796	L726	ASP	THR	VAL	GLU	VAL	VAL	SER	SER	GLY	GLY	LEU	ALA	LEU	ASP	GLY	GLY
E797	L727	LEU	LYS	LEU	THR	LEU	LEU	GLN	GLN	ARG	ARG	ILE	ILE	ALA	SER	LEU	MET
L798	L728	ALA	SER	LEU	VAL	ASP	PHE	LEU	LEU	LYS	LYS	ALA	ALA	LYS	GLN	ASN	GLY
K801	G729	LEU	LYS	CYS	ARG	HIS	THR	THR	ILE	ILE	HIS	ASN	ASN	GLU	GLN	ALA	ARG
L802	D730	ALA	ASP	SER	THR	GLN	ARG	GLN	GLN	CYS	ALA	GLN	GLN	LEU	LEU	THR	THR
K803	A731	GLY	LYS	GLN	VAL	SER	SER	LYS	LYS	LYS	GLY	GLY	GLY	THR	THR	GLN	THR
W804	Y732	D669	THR	LEU	PRO	LEU	LEU	ILE	GLN	ILE	GLN	MET	ILE	ALA	ILE	PRO	ASP
Y805	I735	1670	VAL	GLU	GLY	LEU	GLU	GLU	THR	ARG	THR	ARG	MET	ASN	ILE	GLU	ASP
L806	L736	5671	THR	CYS	LEU	GLN	GLY	GLY	LEU	GLN	GLN	GLN	ASN	TYR	TYR	ALA	PRO
D806	W807	R672	ASP	SER	THR	PRO	PRO	LEU	LEU	ALA	ASN	LEU	SER	CYS	GLY	ILE	GLY
K807	K807	R672	THR	LEU	THR	LEU	LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLY
A808	E739	S675	HIS	THR	VAL	LEU	GLY	ARG	ARG	ILE	GLY	ALA	GLY	ALA	ALA	PHE	LEU
E809	E740	ARG	ARG	ASP	PHE	GLY	GLY	ASP	ASP	ALA	GLY	LYS	LYS	ALA	ALA	PRO	GLU
K810	Y745	1679	LEU	PHE	ILE	ILE	ILE	ALA	ALA	PHE	VAL	ILE	ILE	ILE	PRO	VAL	LEU
Q813	E746	V680	SER	LYS	LEU	GLN	GLN	THR	ILE	SER	GLU	THR	CYS	TYR	ARG	VAL	SER
H814	Q747	T681	ILE	VAL	ALA	TYR	PHE	LEU	GLU	ASN	THR	GLY	GLY	ILE	ALA	ALA	GLY
A815	L748	A682	LEU	ARG	VAL	GLY	GLY	LEU	GLY	PRO	VAL	SER	HIS	GLY	PRO	LEU	CYS
L816	L749	E683	LEU	THR	LYS	LYS	LYS	THR	ILE	ASN	GLN	GLN	GLN	GLN	HIS	HIS	GLN
A817	W750	Q684	LEU	PRO	TYR	ASN	TYR	LEU	GLU	ASP	VAL	GLN	GLN	GLY	GLY	PRO	GLY
H818	Q751	P685	VAL	HIS	GLY	ASP	PHE	ILE	ILE	ILE	ALA	ALA	VAL	ASN	GLN	GLN	ILE
E819	K754	Y686	ARG	LEU	ILE	LEU	LEU	GLN	THR	THR	THR	THR	THR	ASP	GLY	GLY	ILE
P820	D755	F687	LEU	LYS	GLU	LEU	LEU	GLU	GLU	LEU	LEU	GLU	LEU	ARG	GLY	LEU	PHE
W821	G756	T688	ASN	ASN	ALA	GLU	GLU	ASN	LEU	LEU	THR	THR	THR	ASP	ILE	ASP	LEU
K822	T757	E689	GLY	GLN	ALA	VAL	ILE	ILE	ILE	PHE	PHE	LEU	LEU	ALA	GLY	THR	GLY
L827	K761	A690	GLN	LYS	ASN	MET	LYS	GLN	GLN	PRO	PRO	ILE	THR	GLY	TYR	VAL	THR
D830	M762	R691	HIS	LYS	ASN	GLY	SER	MET	ILE	ALA	PHE	ARG	ARG	GLY	GLY	LEU	SER
R832	A765	E692	ALA	GLY	LEU	LEU	LEU	ALA	LEU	THR	VAL	GLY	GLY	LYS	ASP	TRP	ALA
Q834	L766	K693	LYS	MET	HIS	SER	PHE	LEU	GLN	LEU	VAL	LYS	LEU	LYS	PRO	LYS	ALA
A838	T769	D696	LEU	ALA	GLU	PRO	THR	VAL	VAL	LYS	THR	THR	VAL	VAL	ARG	LYS	VAL
K839	H770	V698	GLY	ALA	ASN	GLN	HIS	MET	GLY	GLY	GLY	GLY	VAL	VAL	PHE	VAL	VAL
W840	Y771	L699	ILE	ILE	PRO	PRO	VAL	VAL	GLY	GLN	ALA	ALA	ASN	ASN	HIS	VAL	PRO
H841	Y772	K700	HIS	THR	TYR	SER	ALA	ALA	LYS	LYS	LYS	LEU	ASN	LYS	TYR	GLY	ALA
Y841	S773	H701	GLY	THR	ALA	PRO	PRO	MET	TRP	TRP	GLN	GLN	GLN	GLY	GLY	GLY	PRO
M844	M774	R702	PHE	HIS	ASP	GLY	GLY	LYS	TYR	LYS	ASP	ASP	GLY	ALA	THR	VAL	ALA
E845	A775	K703	SER	MET	ALA	GLN	GLN	LYS	THR	THR	THR	PHE	THR	GLY	GLY	ILE	ALA
K846	T776	D704	THR	GLY	HIS	PRO	PRO	ASN	THR	LYS	ASP	GLY	GLY	ASN	GLY	SER	LEU
L847	T777	K705	SER	MET	LEU	LEU	LEU	LYS	ALA	ALA	GLN	GLN	GLN	ASN	GLY	TYR	GLY
Q848	Y778	1709	GLU	LEU	LEU	PRO	PRO	GLN	THR	THR	VAL	LEU	THR	GLY	GLY	HIS	PRO
D849	E779	T710	GLY	PRO	ALA	LEU	LEU	GLU	LEU	LEU	GLU	GLU	GLU	GLY	THR	LEU	LEU
W850	Y780	C711	VAL	GLY	GLN	LEU	LEU	VAL	ASP	ASP	THR	ALA	ALA	GLY	GLY	ALA	PRO
L851	A781	F712	ARG	MET	VAL	ARG	ARG	THR	GLU	GLU	GLY	GLY	GLY	GLY	ALA	ALA	LEU
T852	E782	R713	VAL	ARG	TYR	THR	VAL	THR	THR	THR	ASN	PHE	THR	GLY	ILE	ALA	LEU
A853	L783	E714	THR	THR	LYS	LEU	LYS	ALA	THR	GLY	GLY	GLY	GLY	ARG	SER	ALA	LEU
L854	K784	1715	GLY	THR	ARG	CYS	ARG	MET	THR	GLY	THR	GLY	GLY	GLY	HIS	GLY	PRO
Q855	T785	A716	LYS	LEU	ALA	PRO	GLN	THR	LEU	LEU	VAL	GLN	GLN	HIS	GLY	LEU	LEU
Q856	G786	E717	GLY	LEU	ALA	LEU	GLU	THR	LEU	LEU	ALA	GLU	GLU	GLY	GLY	GLY	PRO
A857	Q787	R718	ARG	GLY	GLN	LEU	GLN	ASP	GLU	THR	THR	GLY	GLY	ALA	GLY	ALA	LEU
R858	E788	W719	VAL	THR	VAL	ARG	ARG	PHE	THR	ALA	GLN	GLY	GLY	GLY	ALA	ALA	MET
E859	W789	A720	LYS	LYS	TYR	THR	THR	SER	THR	GLN	GLN	LEU	LEU	LEU	LEU	LEU	LEU
L862	Y790	W721	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

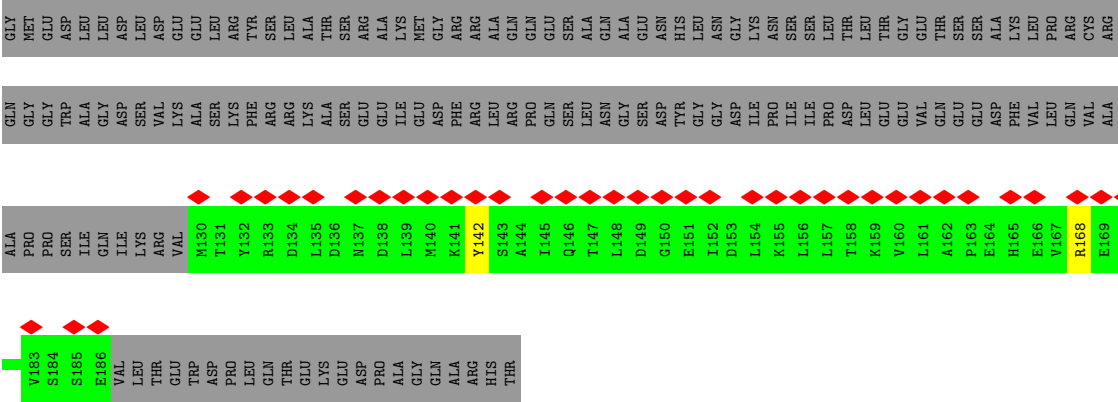


• Molecule 3: WD repeat-containing protein 35





● Molecule 4: Intraflagellar transport protein 43 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242645	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.701	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	546.304, 546.304, 546.304	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	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	C	0.65	0/5679	1.04	19/7662 (0.2%)
2	D	0.67	0/5347	0.98	21/7203 (0.3%)
3	E	0.65	0/9049	1.00	31/12229 (0.3%)
4	F	0.67	0/479	1.04	2/650 (0.3%)
All	All	0.66	0/20554	1.01	73/27744 (0.3%)

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	C	0	6
2	D	0	1
3	E	0	3
All	All	0	10

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	TYR	CB-CG-CD2	-10.31	114.81	121.00
3	E	669	ARG	NE-CZ-NH2	9.34	124.97	120.30
3	E	938	ARG	NE-CZ-NH2	8.64	124.62	120.30
2	D	997	ARG	NE-CZ-NH2	8.57	124.58	120.30
3	E	1122	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	C	189	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	D	1044	ARG	NE-CZ-NH2	7.98	124.29	120.30
2	D	672	ARG	NE-CZ-NH2	7.79	124.19	120.30
2	D	1007	ARG	NE-CZ-NH2	7.70	124.15	120.30
3	E	521	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	C	250	ARG	NE-CZ-NH2	7.55	124.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	168	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	684	ARG	NE-CZ-NH2	7.27	123.94	120.30
2	D	981	ARG	NE-CZ-NH2	7.22	123.91	120.30
3	E	593	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	C	159	ARG	NE-CZ-NH2	7.13	123.86	120.30
3	E	1038	ARG	NE-CZ-NH2	7.03	123.82	120.30
2	D	1228	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	C	647	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	C	453	ARG	NE-CZ-NH2	6.91	123.76	120.30
2	D	1175	ARG	NE-CZ-NH2	6.83	123.72	120.30
3	E	1079	ARG	NE-CZ-NH2	6.79	123.70	120.30
3	E	669	ARG	NE-CZ-NH1	-6.78	116.91	120.30
3	E	353	ARG	NE-CZ-NH2	6.60	123.60	120.30
2	D	1050	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	C	587	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	D	832	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	C	171	ARG	NE-CZ-NH2	6.41	123.51	120.30
3	E	721	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	384	ARG	NE-CZ-NH2	6.33	123.47	120.30
3	E	700	ARG	NE-CZ-NH2	6.13	123.36	120.30
3	E	350	ARG	NE-CZ-NH2	6.12	123.36	120.30
3	E	868	ARG	NE-CZ-NH2	6.11	123.35	120.30
3	E	240	ARG	NE-CZ-NH2	6.07	123.34	120.30
3	E	672	ARG	NE-CZ-NH2	6.05	123.33	120.30
2	D	1015	ARG	NE-CZ-NH2	5.84	123.22	120.30
3	E	119	ARG	NE-CZ-NH2	5.84	123.22	120.30
2	D	691	ARG	NE-CZ-NH2	5.83	123.22	120.30
2	D	723	ARG	NE-CZ-NH2	5.75	123.17	120.30
3	E	1025	ARG	NE-CZ-NH2	5.74	123.17	120.30
3	E	594	ARG	NE-CZ-NH2	5.71	123.16	120.30
2	D	898	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	C	474	ARG	NE-CZ-NH2	5.69	123.14	120.30
3	E	966	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	D	1281	ARG	NE-CZ-NH2	5.60	123.10	120.30
3	E	774	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	518	ARG	NE-CZ-NH2	5.59	123.10	120.30
3	E	528	ARG	NE-CZ-NH2	5.58	123.09	120.30
3	E	766	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	C	197	ARG	NE-CZ-NH2	5.48	123.04	120.30
3	E	813	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	C	465	ARG	NE-CZ-NH2	5.43	123.02	120.30
4	F	142	TYR	CB-CG-CD2	-5.42	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	ARG	NE-CZ-NH2	5.37	122.98	120.30
2	D	858	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	D	1053	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	C	673	ARG	NE-CZ-NH2	5.27	122.93	120.30
3	E	148	ARG	NE-CZ-NH2	5.26	122.93	120.30
3	E	620	PHE	CB-CG-CD2	-5.23	117.14	120.80
2	D	718	ARG	NE-CZ-NH2	5.19	122.90	120.30
3	E	1018	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	C	526	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	C	61	TYR	CA-CB-CG	5.15	123.19	113.40
2	D	1311	ARG	NE-CZ-NH2	5.14	122.87	120.30
3	E	767	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	C	362	ARG	NE-CZ-NH2	5.09	122.85	120.30
3	E	547	TYR	CB-CG-CD2	-5.07	117.96	121.00
3	E	1038	ARG	NE-CZ-NH1	-5.06	117.77	120.30
2	D	1177	ARG	NE-CZ-NH2	5.06	122.83	120.30
3	E	733	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	D	926	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	E	616	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	D	998	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	288	TYR	Sidechain
1	C	453	ARG	Sidechain
1	C	465	ARG	Sidechain
1	C	61	TYR	Sidechain
1	C	726	TYR	Sidechain
1	C	90	TYR	Sidechain
2	D	732	TYR	Sidechain
3	E	1122	ARG	Sidechain
3	E	339	TYR	Sidechain
3	E	733	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5595	0	5567	2	0
2	D	5253	0	5275	1	0
3	E	8863	0	8810	4	0
4	F	470	0	441	0	0
All	All	20181	0	20093	7	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 0.

All (7) 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)
3:E:567:LEU:HB2	3:E:596:VAL:HG21	1.93	0.49
3:E:309:LEU:HD11	3:E:318:ILE:HD11	1.97	0.46
3:E:1113:PHE:CG	3:E:1118:SER:HB3	2.53	0.44
1:C:169:ILE:HD13	1:C:266:TYR:CD1	2.53	0.42
2:D:937:CYS:SG	2:D:961:LEU:HD11	2.59	0.42
1:C:576:LEU:C	1:C:577:ASN:HD22	2.23	0.41
3:E:368:LYS:HZ1	3:E:656:GLU:CD	2.23	0.41

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	C	692/1241 (56%)	659 (95%)	33 (5%)	0	100	100
2	D	646/1500 (43%)	623 (96%)	23 (4%)	0	100	100
3	E	1102/1184 (93%)	1053 (96%)	49 (4%)	0	100	100
4	F	55/209 (26%)	55 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2495/4134 (60%)	2390 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	C	610/1085 (56%)	609 (100%)	1 (0%)	93	98
2	D	556/1279 (44%)	556 (100%)	0	100	100
3	E	961/1020 (94%)	961 (100%)	0	100	100
4	F	53/181 (29%)	53 (100%)	0	100	100
All	All	2180/3565 (61%)	2179 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	C	597	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	1116	HIS

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 [i](#)

There are no monosaccharides 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](#)

There are no chain breaks in this entry.

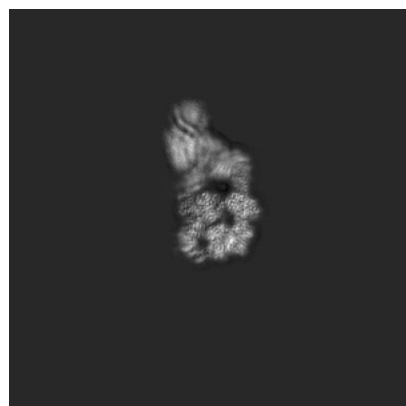
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15954. These allow visual inspection of the internal detail of the map and identification of artifacts.

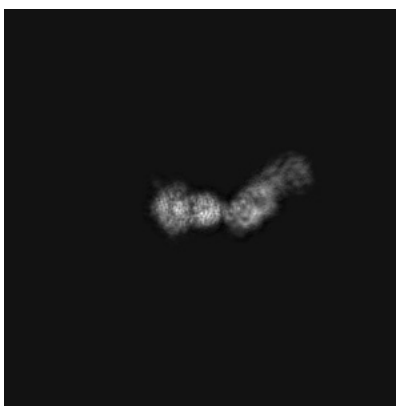
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

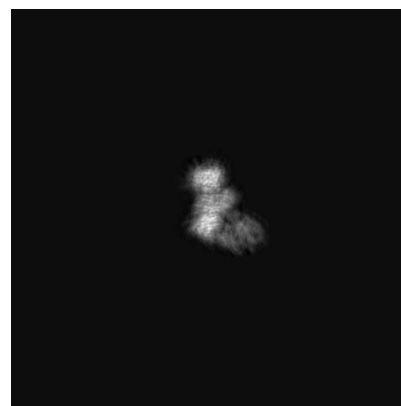
6.1.1 Primary map



X

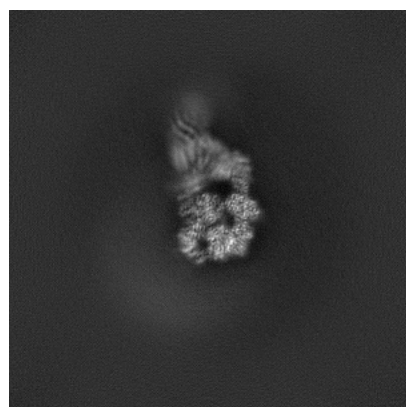


Y

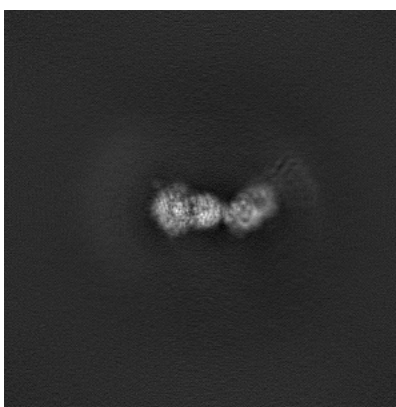


Z

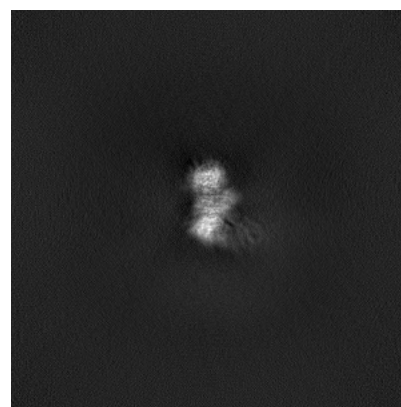
6.1.2 Raw map



X



Y



Z

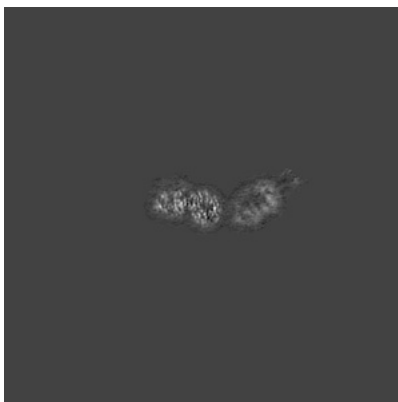
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

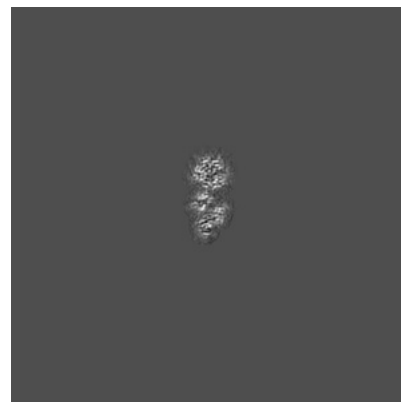
6.2.1 Primary map



X Index: 256

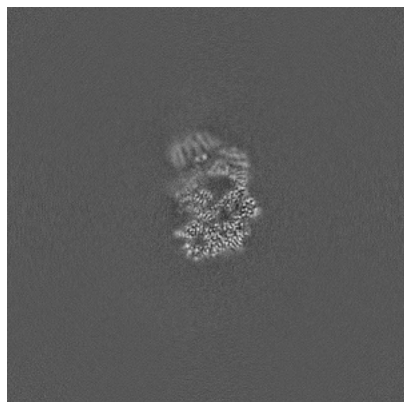


Y Index: 256

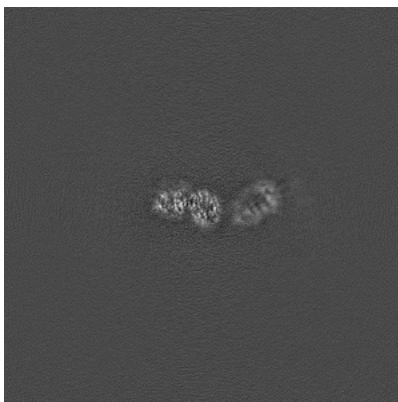


Z Index: 256

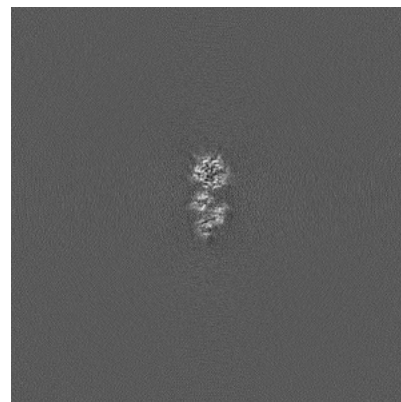
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

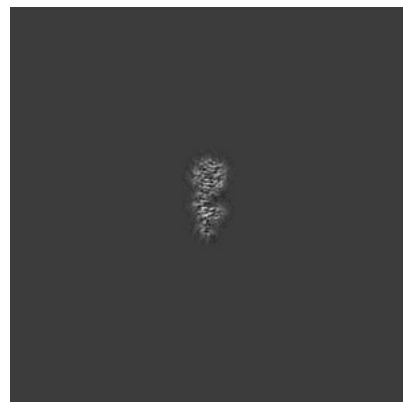
6.3.1 Primary map



X Index: 254

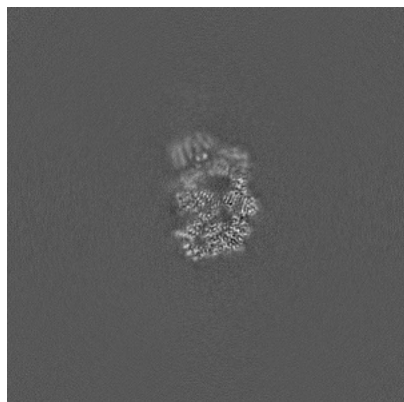


Y Index: 235

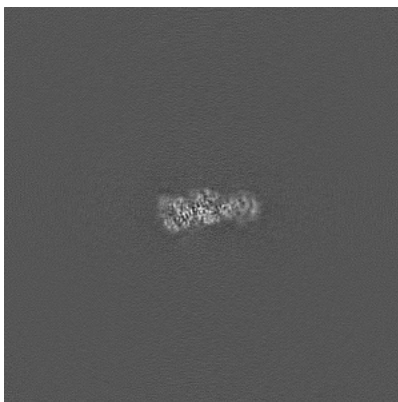


Z Index: 262

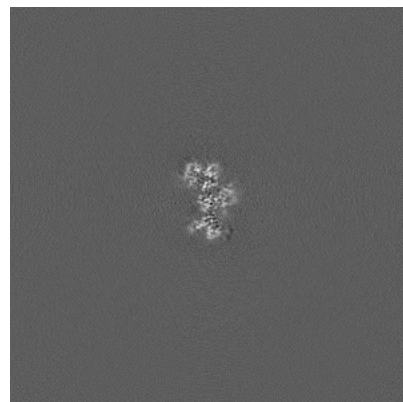
6.3.2 Raw map



X Index: 254



Y Index: 301



Z Index: 221

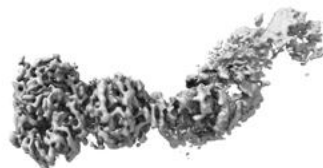
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

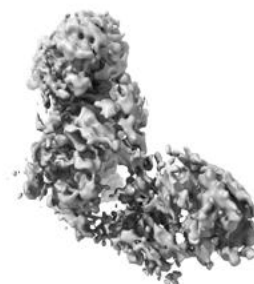
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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

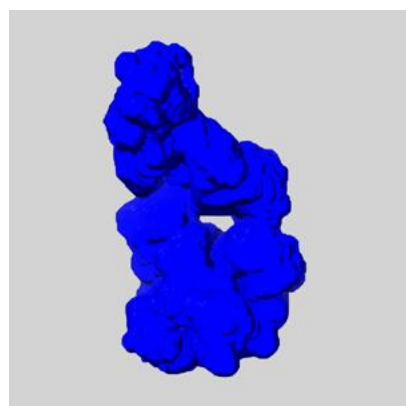
6.5 Mask visualisation [i](#)

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

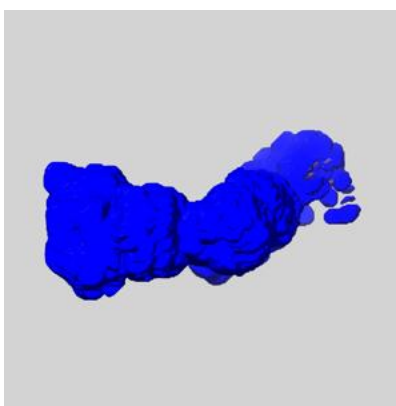
A mask typically either:

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

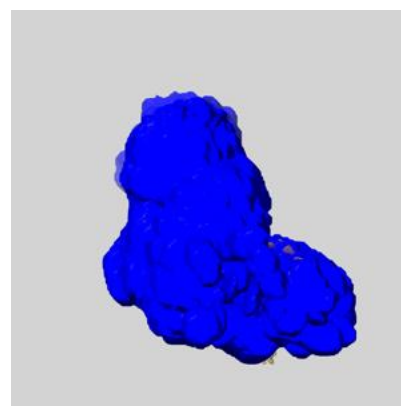
6.5.1 emd_15954_msk_1.map [i](#)



X



Y

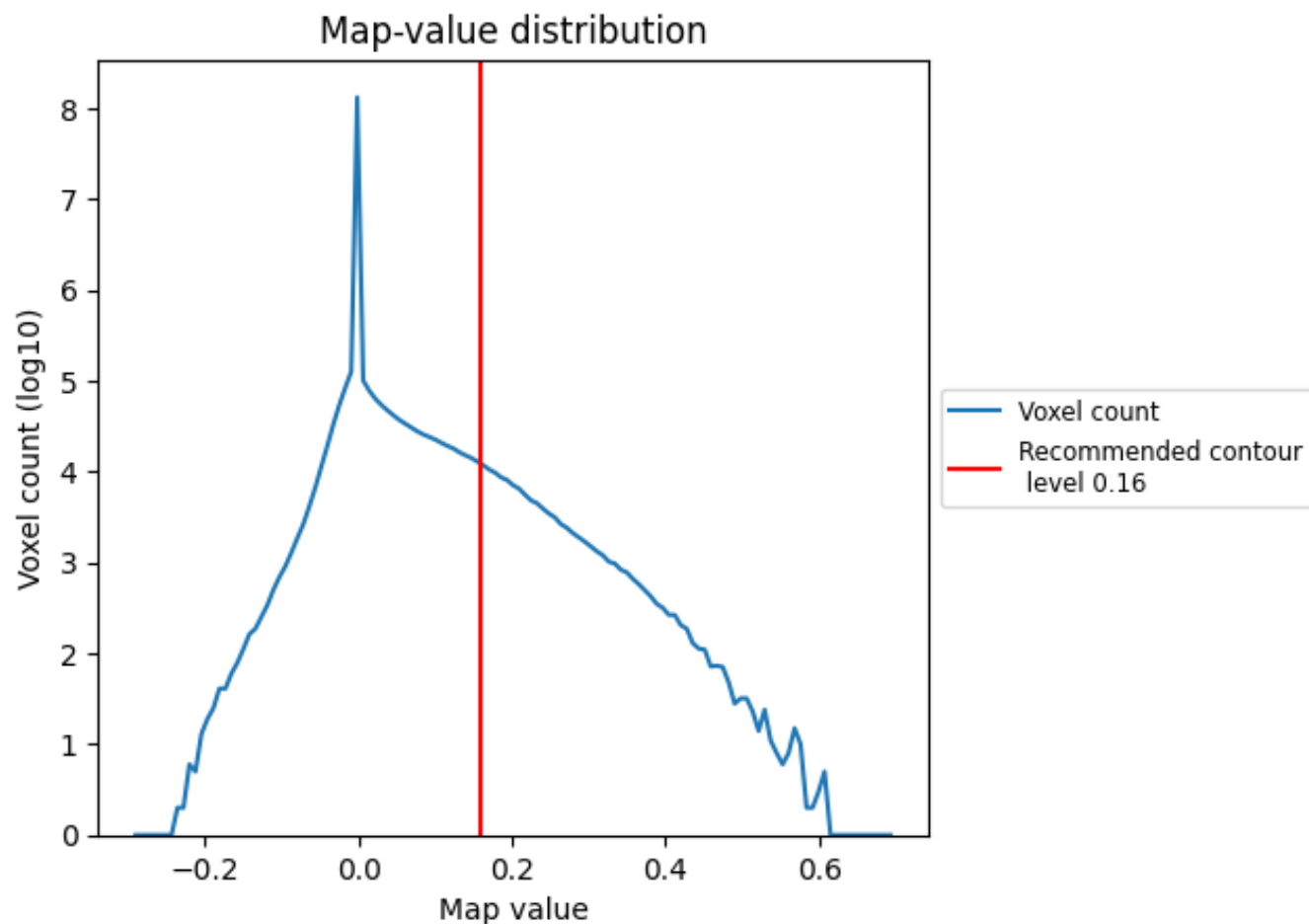


Z

7 Map analysis [i](#)

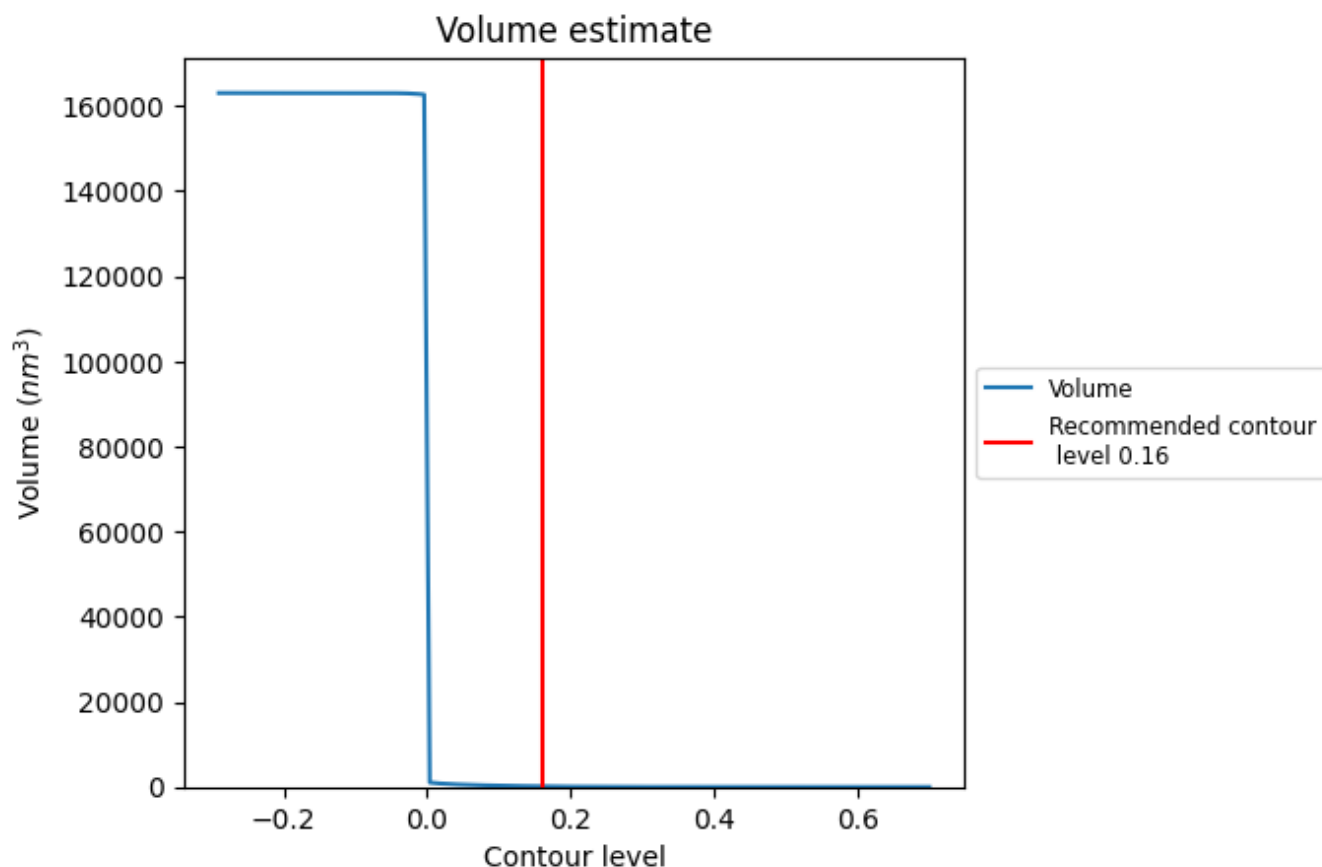
This section contains the results of statistical analysis of the map.

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.

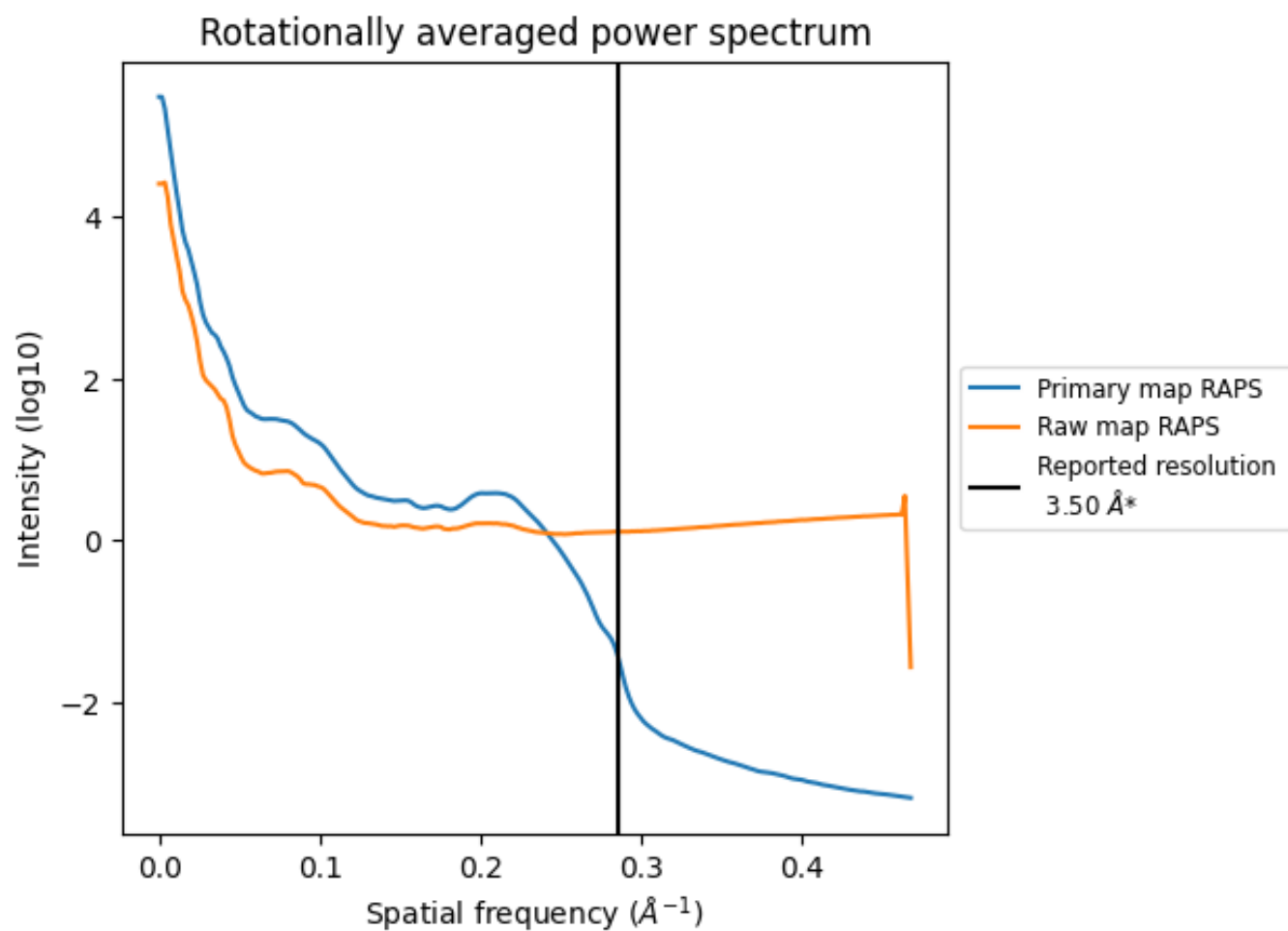
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm^3 ; this corresponds to an approximate mass of 126 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 ⓘ

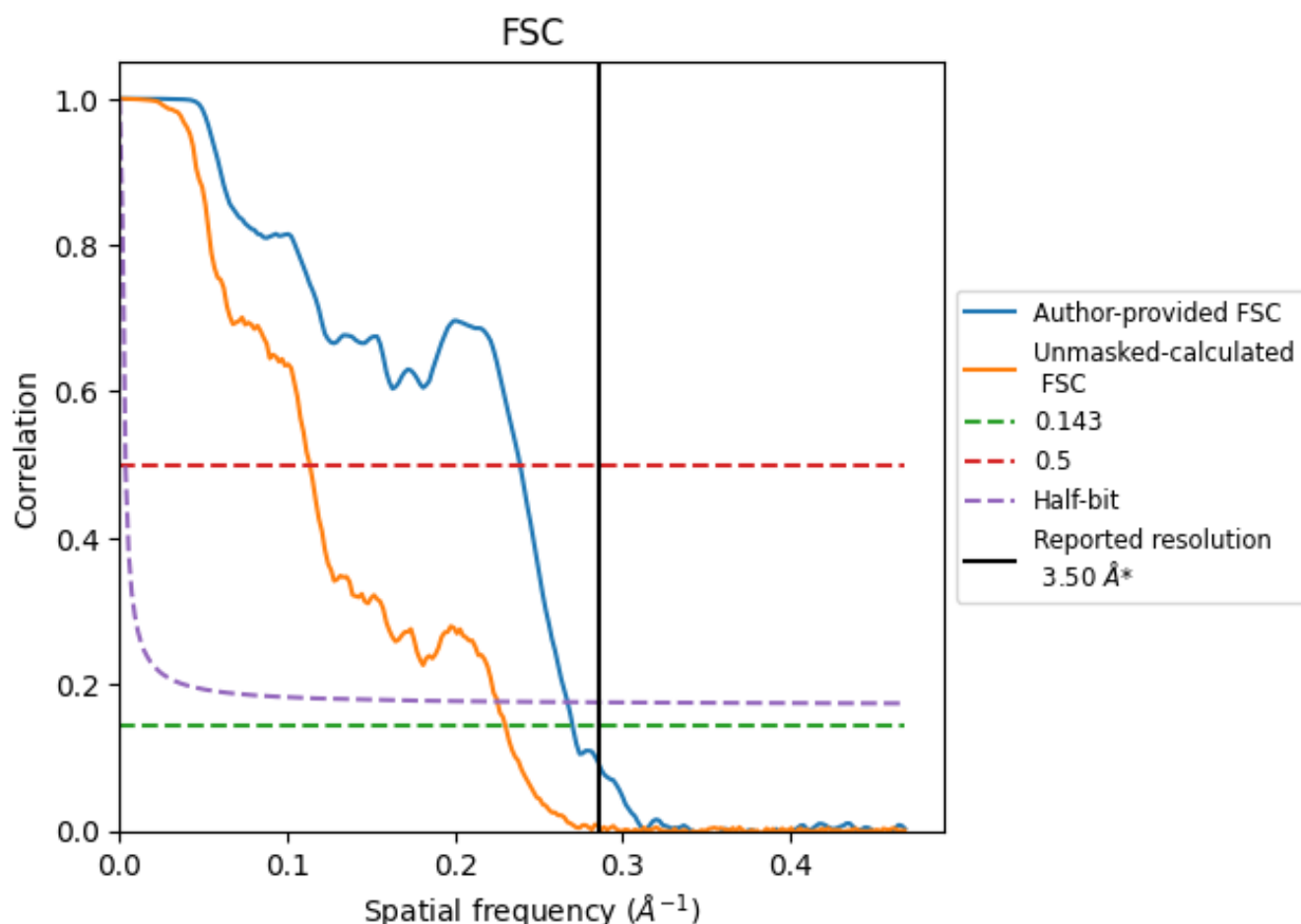


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

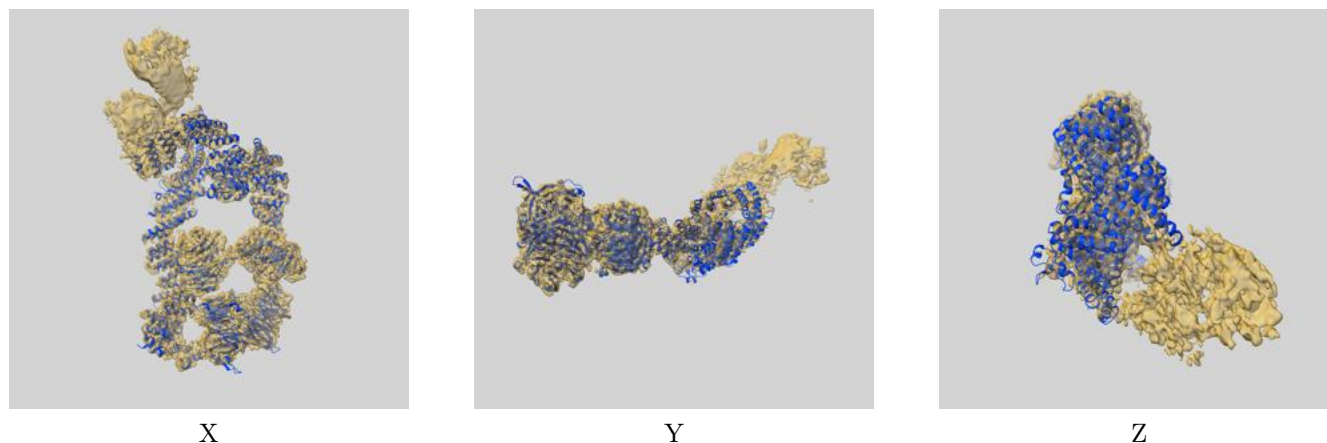
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.70	4.18	3.74
Unmasked-calculated*	4.34	8.80	4.43

*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 4.34 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

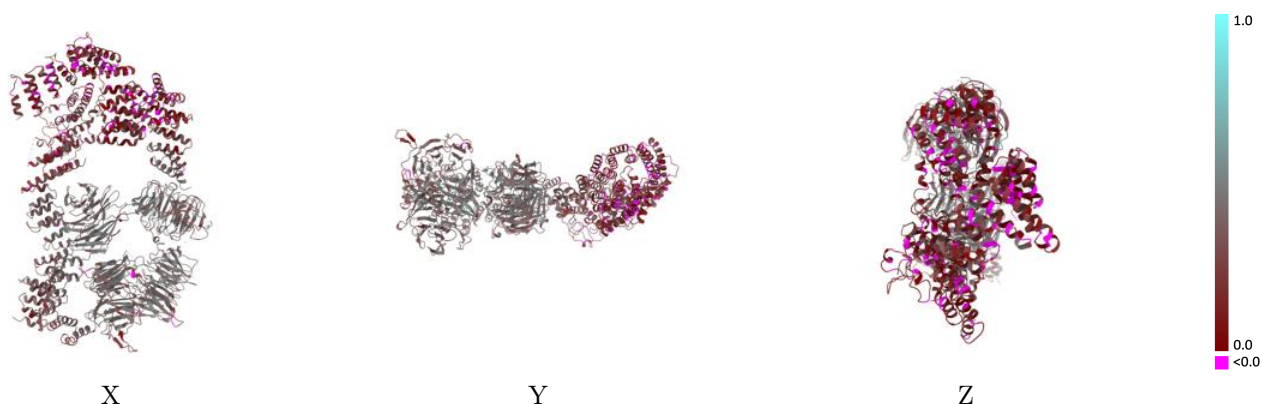
This section contains information regarding the fit between EMDB map EMD-15954 and PDB model 8BBE. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



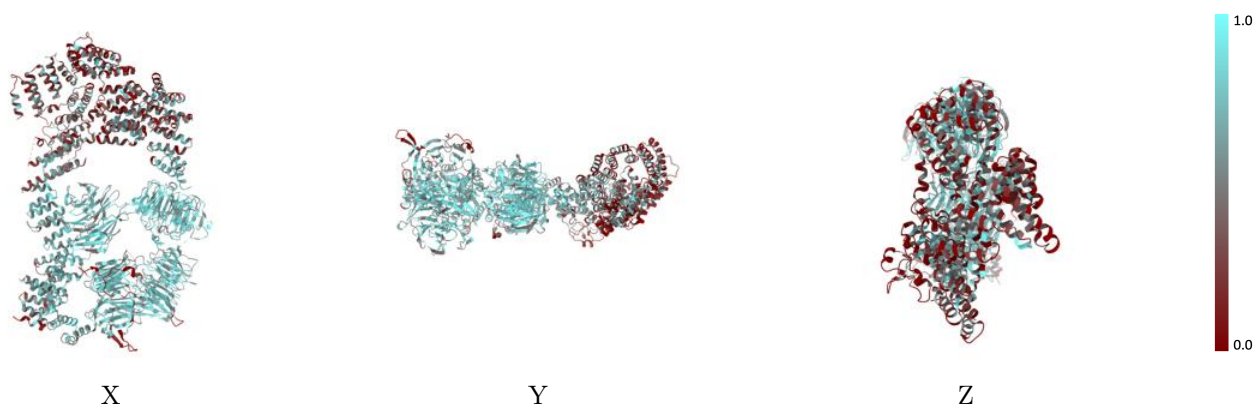
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



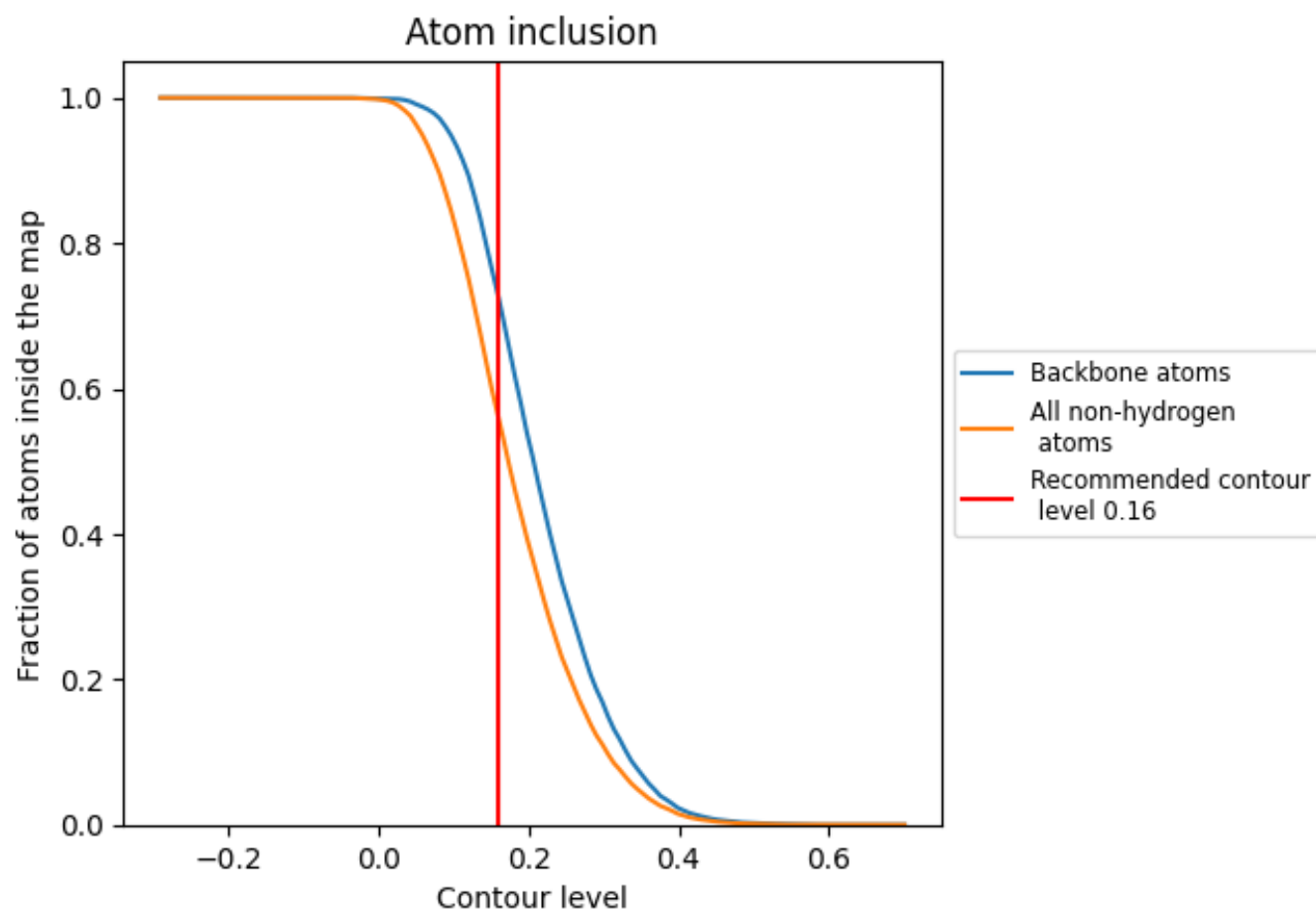
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 56% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5591	<div></div> 0.3060
C	<div></div> 0.7012	<div></div> 0.4050
D	<div></div> 0.3672	<div></div> 0.1580
E	<div></div> 0.6000	<div></div> 0.3390
F	<div></div> 0.2338	<div></div> 0.1710

