



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:52 AM UTC

PDB ID : 6PUW / pdb_00006puw
EMDB ID : EMD-20483
Title : Structure of HIV cleaved synaptic complex (CSC) intasome bound with magnesium and Bictegravir (BIC)
Authors : Lyumkis, D.; Jozwik, I.K.; Passos, D.
Deposited on : 2019-07-18
Resolution : 2.90 Å (reported)
Based on initial models : 1K6Y, 5U1C, 3L3U

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

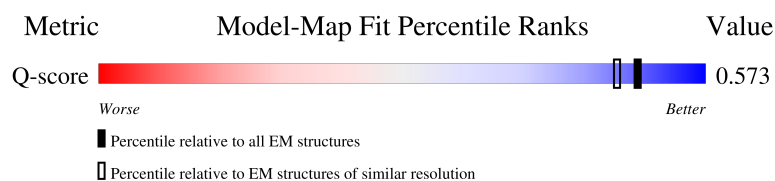
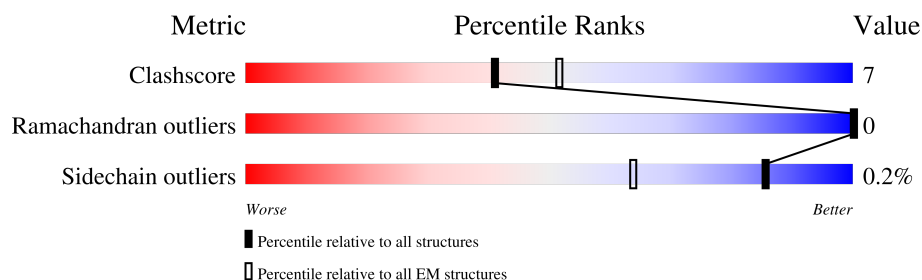
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	383	
1	B	383	
1	C	383	
1	D	383	

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Mol	Chain	Length	Quality of chain
2	E	27	48% 22% 30%
3	F	25	36% 32% 32%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5558 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 Chimeric Sso7d and HIV-1 integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	249	Total	C	N	O	S	0	0
			1935	1238	336	352	9		
1	B	224	Total	C	N	O	S	0	0
			1749	1115	304	323	7		
1	C	65	Total	C	N	O	S	0	0
			539	345	101	92	1		
1	D	47	Total	C	N	O		0	0
			388	251	73	64			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-94	MET	-	expression tag	UNP P39476
A	-93	GLY	-	expression tag	UNP P39476
A	-92	SER	-	expression tag	UNP P39476
A	-91	SER	-	expression tag	UNP P39476
A	-90	HIS	-	expression tag	UNP P39476
A	-89	HIS	-	expression tag	UNP P39476
A	-88	HIS	-	expression tag	UNP P39476
A	-87	HIS	-	expression tag	UNP P39476
A	-86	HIS	-	expression tag	UNP P39476
A	-85	HIS	-	expression tag	UNP P39476
A	-84	SER	-	expression tag	UNP P39476
A	-83	SER	-	expression tag	UNP P39476
A	-82	GLY	-	expression tag	UNP P39476
A	-81	LEU	-	expression tag	UNP P39476
A	-80	VAL	-	expression tag	UNP P39476
A	-79	PRO	-	expression tag	UNP P39476
A	-78	ARG	-	expression tag	UNP P39476
A	-77	GLY	-	expression tag	UNP P39476
A	-76	SER	-	expression tag	UNP P39476
A	-75	HIS	-	expression tag	UNP P39476
A	-10	GLY	-	linker	UNP P39476
A	-9	GLY	-	linker	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	linker	UNP P39476
A	-7	GLY	-	linker	UNP P39476
A	-6	GLY	-	linker	UNP P39476
A	-5	GLY	-	linker	UNP P39476
A	-4	GLY	-	linker	UNP P39476
A	-3	GLY	-	linker	UNP P39476
A	-2	GLY	-	linker	UNP P39476
A	-1	GLY	-	linker	UNP P39476
A	0	GLY	-	linker	UNP P39476
B	-94	MET	-	expression tag	UNP P39476
B	-93	GLY	-	expression tag	UNP P39476
B	-92	SER	-	expression tag	UNP P39476
B	-91	SER	-	expression tag	UNP P39476
B	-90	HIS	-	expression tag	UNP P39476
B	-89	HIS	-	expression tag	UNP P39476
B	-88	HIS	-	expression tag	UNP P39476
B	-87	HIS	-	expression tag	UNP P39476
B	-86	HIS	-	expression tag	UNP P39476
B	-85	HIS	-	expression tag	UNP P39476
B	-84	SER	-	expression tag	UNP P39476
B	-83	SER	-	expression tag	UNP P39476
B	-82	GLY	-	expression tag	UNP P39476
B	-81	LEU	-	expression tag	UNP P39476
B	-80	VAL	-	expression tag	UNP P39476
B	-79	PRO	-	expression tag	UNP P39476
B	-78	ARG	-	expression tag	UNP P39476
B	-77	GLY	-	expression tag	UNP P39476
B	-76	SER	-	expression tag	UNP P39476
B	-75	HIS	-	expression tag	UNP P39476
B	-10	GLY	-	linker	UNP P39476
B	-9	GLY	-	linker	UNP P39476
B	-8	GLY	-	linker	UNP P39476
B	-7	GLY	-	linker	UNP P39476
B	-6	GLY	-	linker	UNP P39476
B	-5	GLY	-	linker	UNP P39476
B	-4	GLY	-	linker	UNP P39476
B	-3	GLY	-	linker	UNP P39476
B	-2	GLY	-	linker	UNP P39476
B	-1	GLY	-	linker	UNP P39476
B	0	GLY	-	linker	UNP P39476
C	-94	MET	-	expression tag	UNP P39476
C	-93	GLY	-	expression tag	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-92	SER	-	expression tag	UNP P39476
C	-91	SER	-	expression tag	UNP P39476
C	-90	HIS	-	expression tag	UNP P39476
C	-89	HIS	-	expression tag	UNP P39476
C	-88	HIS	-	expression tag	UNP P39476
C	-87	HIS	-	expression tag	UNP P39476
C	-86	HIS	-	expression tag	UNP P39476
C	-85	HIS	-	expression tag	UNP P39476
C	-84	SER	-	expression tag	UNP P39476
C	-83	SER	-	expression tag	UNP P39476
C	-82	GLY	-	expression tag	UNP P39476
C	-81	LEU	-	expression tag	UNP P39476
C	-80	VAL	-	expression tag	UNP P39476
C	-79	PRO	-	expression tag	UNP P39476
C	-78	ARG	-	expression tag	UNP P39476
C	-77	GLY	-	expression tag	UNP P39476
C	-76	SER	-	expression tag	UNP P39476
C	-75	HIS	-	expression tag	UNP P39476
C	-10	GLY	-	linker	UNP P39476
C	-9	GLY	-	linker	UNP P39476
C	-8	GLY	-	linker	UNP P39476
C	-7	GLY	-	linker	UNP P39476
C	-6	GLY	-	linker	UNP P39476
C	-5	GLY	-	linker	UNP P39476
C	-4	GLY	-	linker	UNP P39476
C	-3	GLY	-	linker	UNP P39476
C	-2	GLY	-	linker	UNP P39476
C	-1	GLY	-	linker	UNP P39476
C	0	GLY	-	linker	UNP P39476
D	-94	MET	-	expression tag	UNP P39476
D	-93	GLY	-	expression tag	UNP P39476
D	-92	SER	-	expression tag	UNP P39476
D	-91	SER	-	expression tag	UNP P39476
D	-90	HIS	-	expression tag	UNP P39476
D	-89	HIS	-	expression tag	UNP P39476
D	-88	HIS	-	expression tag	UNP P39476
D	-87	HIS	-	expression tag	UNP P39476
D	-86	HIS	-	expression tag	UNP P39476
D	-85	HIS	-	expression tag	UNP P39476
D	-84	SER	-	expression tag	UNP P39476
D	-83	SER	-	expression tag	UNP P39476
D	-82	GLY	-	expression tag	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-81	LEU	-	expression tag	UNP P39476
D	-80	VAL	-	expression tag	UNP P39476
D	-79	PRO	-	expression tag	UNP P39476
D	-78	ARG	-	expression tag	UNP P39476
D	-77	GLY	-	expression tag	UNP P39476
D	-76	SER	-	expression tag	UNP P39476
D	-75	HIS	-	expression tag	UNP P39476
D	-10	GLY	-	linker	UNP P39476
D	-9	GLY	-	linker	UNP P39476
D	-8	GLY	-	linker	UNP P39476
D	-7	GLY	-	linker	UNP P39476
D	-6	GLY	-	linker	UNP P39476
D	-5	GLY	-	linker	UNP P39476
D	-4	GLY	-	linker	UNP P39476
D	-3	GLY	-	linker	UNP P39476
D	-2	GLY	-	linker	UNP P39476
D	-1	GLY	-	linker	UNP P39476
D	0	GLY	-	linker	UNP P39476

- Molecule 2 is a DNA chain called viral DNA non-transferred strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	19	Total	C	N	O	P	0	0
			384	185	67	114	18		

- Molecule 3 is a DNA chain called viral DNA transferred strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	17	Total	C	N	O	P	1	0
			371	176	73	104	18		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

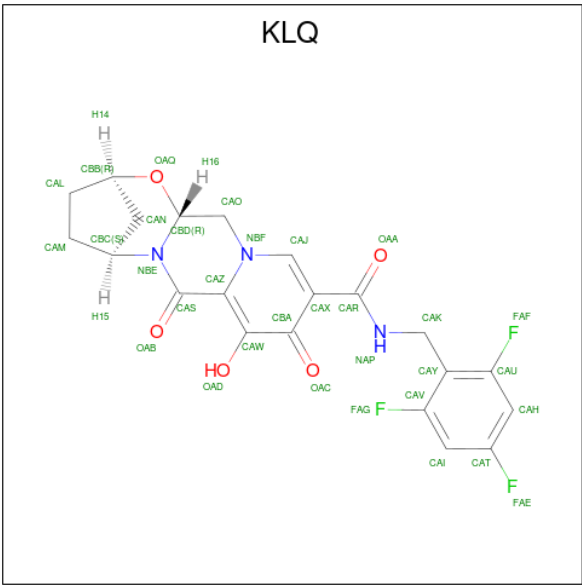
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	

- Molecule 6 is Bictegravir (CCD ID: KLQ) (formula: C₂₁H₁₈F₃N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	F	N	O	0
			32	21	3	3	5	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	92	Total	O	0
			92	92	
7	B	16	Total	O	0
			16	16	
7	C	9	Total	O	0
			9	9	
7	D	12	Total	O	0
			12	12	
7	E	15	Total	O	0
			15	15	
7	F	12	Total	O	0
			12	12	

THR	GLN	ALA	PHE	THR	MET
ASP	SER	GLU	ASN	GLY	GLY
ILE	GLN	VAL	LEU	ARG	SER
GLN	GLY	ILE	PRO	GLY	HIS
THR	VAL	PRO	PRO	ALA	SER
LYS	ILE	ALA	VAL	VAL	HIS
E212	GLU	THR	VAL	SER	HIS
L213	THR	THR	ALA	GLU	HIS
	MET	GLY	ALA	LYS	HIS
F223	ASN	GLN	GLU	ASP	HIS
	LYS	THR	ILE	ALA	SER
Y227	GLU	THR	VAL	PRO	SER
	LEU	ALA	ALA	LYS	GLY
W243	LYS	TYR	SER	GLU	GLY
	LYS	PHE	CYS	LEU	VAL
V250	ILE	LEU	ASP	LEU	PRO
	ILE	LEU	LYS	GLN	ARG
V260	GLY	LYS	CYS	MET	GLY
	GLN	LEU	GLN	LEU	SER
K264	VAL	ALA	LEU	GLU	HIS
A265	ARG	GLY	LYS	LYS	HIS
K266	ASP	ARG	GLY	GLN	ALA
	GLN	TRP	GLU	LYS	THR
R269	ALA	PRO	ALA	LYS	VAL
	GLU	VAL	MET	GLY	LYS
Q274	HIS	LYS	HIS	GLY	PHE
M275	LEU	THR	GLY	GLY	LYS
A276	LYS	VAL	GLN	TYR	LYS
	THR	HIS	VAL	GLY	GLY
GLY	THR	THR	ASP	GLY	GLY
ASP	ALA	THR	ASP	PHE	VAL
	VAL	ASN	ILE	GLY	VAL
CYS	GLN	ASN	GLN	LEU	ILE
VAL	MET	GLY	PRO	ASP	LYS
ALA	ALA	SER	GLY	GLY	GLY
SER	VAL	ASN	ILE	GLY	VAL
ARG	PHE	PHE	TRP	ASP	ASP
GLN	ILE	THR	GLN	LEU	ILE
ASP	HIS	THR	LEU	ASP	LYS
GLU	ASN	THR	ASP	GLY	LYS
	PHE	THR	CYS	ILE	ILE
ASP	LYS	VAL	THR	ASP	LYS
	ARG	LYS	HIS	LYS	LYS
	LYS	ALA	LEU	ALA	VAL
	GLY	ALA	GLU	GLN	TRP
	GLY	CYS	GLY	GLU	ARG
	ILE	TRP	LYS	GLU	VAL
	GLY	TRP	VAL	HIS	GLY
	GLY	ALA	ILE	GLU	LYS
	TYR	GLY	LEU	LYS	MET
	SER	ILE	VAL	TYR	ILE
	ALA	LYS	ALA	HIS	SER
	GLY	GLN	VAL	SER	PHE
	GLY	GLU	HIS	ASN	THR
	ARG	PHE	VAL	TRP	TYR
	ILE	ILE	ALA	ARG	ASP
	VAL	GLY	SER	ALA	GLY
	ASP	PRO	GLY	MET	GLY
	ILE	TYR	TYR	ALA	GLY
	ILE	ASN	GLN	SER	GLY
	ALA	THR	THR	ASP	LYS

Chain D: 10% 88%

THR	GLN	ALA	PHE	THR	MET
ASP	GLN	GLU	ASN	GLY	GLY
ILE	GLN	VAL	LEU	ARG	SER
GLN	GLY	ILE	PRO	GLY	SER
THR	VAL	PRO	PRO	ALA	HIS
LYS	ILE	ALA	VAL	VAL	HIS
GLU	GLU	GLU	VAL	SER	HIS
LEU	SER	THR	ALA	GLU	HIS
GLN	MET	GLY	LYS	LYS	HIS
GLN	ASN	GLN	GLU	ASP	HIS
ILE	LYS	THR	ILE	ALA	SER
ILE	GLU	THR	VAL	PRO	SER
THR	LEU	ALA	ALA	LYS	SER
LYS	LYS	TYR	SER	GLU	GLY
ILE	LYS	PHE	CYS	LEU	VAL
GLN	ILE	LEU	ASP	LEU	PRO
N222	ILE	LEU	LYS	GLN	ARG
	GLY	LYS	CYS	MET	GLY
V225	GLN	LEU	GLN	LEU	SER
	VAL	ALA	LEU	GLU	HIS
R228	ARG	ALA	LYS	GLY	MET
	ASP	ARG	GLY	GLN	ALA
V250	GLN	TRP	GLU	LYS	THR
I251	ALA	PRO	ALA	LYS	VAL
	GLU	VAL	MET	GLY	LYS
V259	HIS	LYS	HIS	GLY	LYS
V260	LEU	THR	GLY	GLY	PHE
P261	LYS	VAL	GLN	GLY	TYR
R262	THR	HIS	VAL	GLY	LYS
R263	ALA	THR	ASP	GLY	GLY
K264	VAL	ASN	CYS	GLY	GLU
	GLN	ASN	SER	GLY	LYS
I268	MET	GLY	PRO	GLY	LYS
ARG	ALA	SER	GLY	GLY	GLU
ASP	VAL	ASN	ILE	GLY	VAL
TYR	PHE	THR	TRP	PHE	ASP
GLY	ILE	THR	GLN	LEU	ILE
LYS	HIS	SER	LEU	ASP	LYS
GLN	ASN	THR	ASN	GLY	LYS
MET	PHE	THR	CYS	ILE	LYS
ALA	LYS	VAL	THR	ASP	LYS
GLY	ARG	LYS	HIS	LYS	LYS
ASP	LYS	ALA	LEU	ALA	VAL
ASP	GLY	ALA	GLU	GLN	TRP
CYS	GLY	CYS	GLY	GLU	ARG
VAL	ILE	TRP	LYS	GLU	VAL
ALA	GLY	TRP	VAL	HIS	GLY
SER	GLY	ALA	ILE	GLU	LYS
ARG	TYR	GLY	LEU	LYS	GLY
GLN	SER	ILE	VAL	TYR	ILE
ASP	ALA	LYS	ALA	HIS	SER
GLU	GLY	GLN	HIS	SER	PHE
ASP	ARG	PHE	VAL	ASN	THR
		GLY	VAL	TRP	TYR
		ILE	ALA	ARG	ASP
		ILE	SER	ALA	GLU
		PRO	GLY	MET	GLY
		TYR	TYR	ALA	GLY
		ASN	ILE	SER	GLY
		PRO	GLN	ASP	LYS

Chain E: 48% 22% 30%

A15	C16	T17	G18	C19	T20	A21	G22	A23		G33	DC	DC	DC	DA	DC	DG	DC	DT
-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	----	----	----	----	----	----	----	----

Chain F: 36% 32% 32%

DA	C5	T17	C20
DG	G6	A18	A21
DC	G7		
DG	G8		
DT			
DG			
DG			
DG			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	146022	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	63291	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.297	Depositor
Minimum map value	-18.487	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.693	Depositor
Recommended contour level	3	Depositor
Map size (Å)	303.36002, 303.36002, 303.36002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.79, 0.79, 0.79	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1972	0.41	1/2660 (0.0%)
1	B	0.15	0/1780	0.31	0/2400
1	C	0.19	0/549	0.35	0/736
1	D	0.20	0/397	0.40	0/535
2	E	0.25	0/429	0.36	0/660
3	F	0.35	0/416	0.39	0/637
All	All	0.23	0/5543	0.37	1/7628 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	123	SER	N-CA-C	5.50	117.17	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1935	0	1959	28	0
1	B	1749	0	1760	29	0
1	C	539	0	566	7	0
1	D	388	0	406	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	384	0	217	5	0
3	F	371	0	203	8	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	32	0	0	2	0
7	A	92	0	0	2	0
7	B	16	0	0	1	0
7	C	9	0	0	1	0
7	D	12	0	0	0	0
7	E	15	0	0	0	0
7	F	12	0	0	0	0
All	All	5558	0	5111	73	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 (73) 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:101:LEU:HD11	1:A:113:VAL:HG11	1.76	0.66
1:B:73:ILE:HG12	1:B:88:VAL:HG22	1.79	0.64
1:A:93:THR:HG22	1:A:95:GLN:H	1.64	0.63
1:A:152:GLU:O	1:A:155:ASN:HB2	1.99	0.62
1:B:62:GLN:HG2	1:B:151:ILE:HB	1.80	0.62
1:D:228:ARG:HH21	1:D:264:LYS:HG2	1.66	0.61
1:B:81:SER:HB3	1:B:203:ILE:HD12	1.83	0.59
1:A:141:ILE:HG21	1:D:261:PRO:HD3	1.84	0.59
1:A:177:GLN:OE1	1:B:107:ARG:NH1	2.36	0.59
1:A:81:SER:O	1:A:199:ARG:NH1	2.36	0.58
1:B:84:ILE:HD13	1:B:158:LEU:HD13	1.86	0.58
3:F:17:DT:H2''	3:F:18:DA:C8	2.39	0.58
1:B:117:ASN:O	1:B:117:ASN:OD1	2.23	0.57
1:B:30:PRO:HG2	1:C:274:GLN:HA	1.85	0.56
1:A:79:VAL:HG13	1:A:150:VAL:HG21	1.87	0.56
1:B:12:HIS:CE1	1:B:37:VAL:HG23	2.41	0.56
1:B:246:GLU:HG2	1:B:247:GLY:H	1.70	0.56
1:D:250:VAL:HG22	1:D:259:VAL:HG22	1.88	0.55
1:B:246:GLU:HG2	1:B:247:GLY:N	2.22	0.55
1:A:144:ASN:ND2	1:A:147:SER:OG	2.41	0.54
1:B:20:ARG:NH1	1:B:209:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:DG:H2''	3:F:7:DG:H5''	1.90	0.53
1:A:138:GLU:OE1	7:A:401:HOH:O	2.18	0.52
1:B:64:ASP:HB2	1:B:151:ILE:HG12	1.91	0.52
3:F:7:DG:H2''	3:F:8:DG:C8	2.45	0.51
3:F:5:DC:H2''	3:F:6:DG:C8	2.46	0.50
6:A:304:KLQ:CAR	3:F:21[B]:DA:H2'	2.41	0.50
1:A:184:ASN:HA	1:A:196:ALA:HB3	1.93	0.50
1:B:105:ALA:HB2	1:B:135:ILE:HD11	1.93	0.50
1:B:202:ASP:O	1:B:206:THR:HG23	2.10	0.50
1:B:63:LEU:HD13	1:B:113:VAL:HG13	1.96	0.48
1:B:157:GLU:O	1:B:161:ILE:HG13	2.14	0.48
1:A:103:LYS:O	1:A:107:ARG:HG2	2.13	0.48
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.70	0.47
1:D:225:VAL:HG11	1:D:251:ILE:HG21	1.96	0.47
1:A:144:ASN:OD1	1:D:263:ARG:NH2	2.48	0.47
1:B:186:LYS:HA	1:B:186:LYS:HD3	1.74	0.46
1:A:53:GLN:OE1	1:C:264:LYS:NZ	2.36	0.46
1:A:146:GLN:NE2	7:A:408:HOH:O	2.45	0.46
1:A:120:ASN:OD1	1:A:120:ASN:N	2.25	0.46
6:A:304:KLQ:CAR	3:F:21[B]:DA:C2'	2.94	0.46
1:C:227:TYR:HB2	1:C:260:VAL:HG11	1.97	0.45
1:A:77:VAL:HG21	1:A:154:MET:HG3	1.98	0.45
1:A:150:VAL:HG22	2:E:19:DC:H4'	1.98	0.45
1:B:174:THR:O	1:B:178:MET:HG3	2.17	0.45
1:A:141:ILE:HB	1:A:144:ASN:HB3	1.98	0.45
1:C:223:PHE:CD1	1:C:269:ARG:HB2	2.52	0.45
1:C:213:LEU:HD23	1:C:213:LEU:H	1.82	0.45
1:A:166:ARG:HA	1:A:166:ARG:HD2	1.71	0.44
1:B:187:ARG:HD3	1:B:187:ARG:HA	1.75	0.44
1:C:243:TRP:HE3	1:C:250:VAL:HG23	1.82	0.44
1:A:105:ALA:HB2	1:A:135:ILE:HD11	2.00	0.44
1:B:188:LYS:NZ	7:B:402:HOH:O	2.50	0.44
1:A:156:LYS:HD3	3:F:19:DG:N3	2.33	0.43
1:B:30:PRO:HB2	1:B:213:LEU:HD13	2.00	0.43
1:C:266:LYS:NZ	7:C:301:HOH:O	2.51	0.43
1:A:52:GLY:HA3	2:E:17:DT:H1'	1.99	0.43
1:B:12:HIS:HE1	1:B:43:CYS:SG	2.36	0.43
1:B:69:GLU:HB2	1:B:172:LEU:HD22	2.01	0.43
3:F:8:DG:C8	3:F:8:DG:H5'	2.55	0.42
1:A:141:ILE:HG12	2:E:17:DT:OP1	2.20	0.42
1:B:34:LYS:HG2	1:B:217:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:O	1:B:44:GLN:NE2	2.52	0.42
1:B:111:LYS:HD3	1:B:111:LYS:HA	1.81	0.42
2:E:22:DG:H2"	2:E:23:DA:C8	2.55	0.42
1:B:16:HIS:CE1	1:B:42:LYS:HB3	2.55	0.41
2:E:20:DT:H2"	2:E:21:DA:C8	2.54	0.41
1:A:73:ILE:HG12	1:A:88:VAL:HG22	2.02	0.41
1:A:225:VAL:HG22	1:A:267:ILE:HG12	2.01	0.41
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.87	0.41
1:B:35:GLU:OE1	1:B:252:GLN:NE2	2.54	0.41
1:A:33:ALA:O	1:A:37:VAL:HG23	2.20	0.40
1:A:186:LYS:HA	1:A:186:LYS:HD3	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/383 (63%)	238 (99%)	3 (1%)	0	100	100
1	B	216/383 (56%)	213 (99%)	3 (1%)	0	100	100
1	C	63/383 (16%)	60 (95%)	3 (5%)	0	100	100
1	D	45/383 (12%)	42 (93%)	3 (7%)	0	100	100
All	All	565/1532 (37%)	553 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/311 (66%)	204 (100%)	1 (0%)	81	93
1	B	186/311 (60%)	186 (100%)	0	100	100
1	C	57/311 (18%)	57 (100%)	0	100	100
1	D	41/311 (13%)	41 (100%)	0	100	100
All	All	489/1244 (39%)	488 (100%)	1 (0%)	85	96

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

Mol	Chain	Res	Type
1	A	120	ASN

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

Mol	Chain	Res	Type
1	A	114	HIS
1	A	222	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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	KLQ	A	304	4	33,36,36	5.50	16 (48%)	39,55,55	2.38	17 (43%)

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	KLQ	A	304	4	-	0/9/42/42	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	304	KLQ	OAQ-CBD	15.99	1.62	1.42
6	A	304	KLQ	CAZ-CAW	14.28	1.54	1.36
6	A	304	KLQ	CAN-CBB	-11.87	1.28	1.52
6	A	304	KLQ	CAN-CBC	-11.09	1.37	1.53
6	A	304	KLQ	CAS-NBE	7.40	1.43	1.36
6	A	304	KLQ	CAJ-NBF	6.98	1.50	1.37
6	A	304	KLQ	CAR-NAP	6.66	1.44	1.33
6	A	304	KLQ	CBC-NBE	-5.72	1.41	1.48
6	A	304	KLQ	CAJ-CAX	5.13	1.51	1.38
6	A	304	KLQ	CAO-NBF	4.60	1.50	1.46
6	A	304	KLQ	CAM-CBC	2.71	1.60	1.53
6	A	304	KLQ	CAM-CAL	2.70	1.61	1.54
6	A	304	KLQ	OAA-CAR	-2.63	1.18	1.23
6	A	304	KLQ	CAL-CBB	2.37	1.63	1.52
6	A	304	KLQ	OAB-CAS	-2.20	1.18	1.23
6	A	304	KLQ	OAC-CBA	-2.18	1.18	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	304	KLQ	CAH-CAU-CAY	-6.53	119.59	124.45
6	A	304	KLQ	CAI-CAV-CAY	-5.76	120.17	124.45
6	A	304	KLQ	CAV-CAY-CAU	4.50	120.61	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	304	KLQ	OAQ-CBB-CAN	3.63	113.03	109.50
6	A	304	KLQ	CBB-CAN-CBC	3.62	111.09	102.36
6	A	304	KLQ	CAK-NAP-CAR	-3.34	117.30	122.07
6	A	304	KLQ	OAQ-CBB-CAL	-3.23	106.89	113.25
6	A	304	KLQ	OAB-CAS-CAZ	-3.12	120.00	126.38
6	A	304	KLQ	CAU-CAH-CAT	2.65	119.49	116.67
6	A	304	KLQ	OAD-CAW-CBA	2.34	120.25	116.03
6	A	304	KLQ	CAZ-CAW-CBA	-2.33	119.53	121.76
6	A	304	KLQ	CAV-CAI-CAT	2.27	119.08	116.67
6	A	304	KLQ	CAL-CAM-CBC	-2.26	100.72	104.08
6	A	304	KLQ	CAX-CAR-NAP	2.11	121.17	116.67
6	A	304	KLQ	FAF-CAU-CAY	2.04	120.18	117.64
6	A	304	KLQ	OAA-CAR-NAP	-2.03	119.69	123.35
6	A	304	KLQ	CAI-CAT-CAH	-2.01	121.05	123.50

There are no chirality outliers.

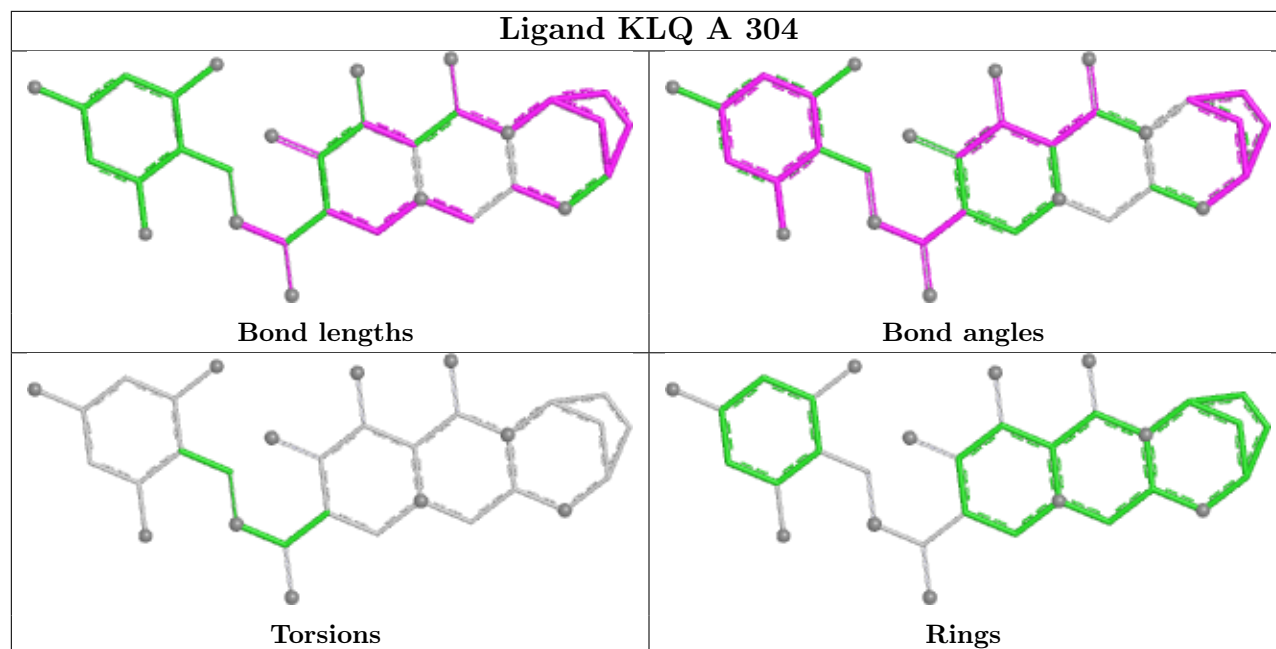
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	304	KLQ	2	0

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



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.

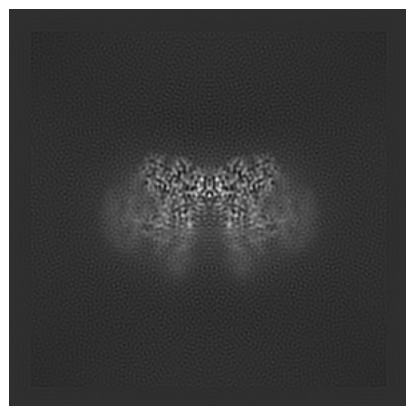
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20483. These allow visual inspection of the internal detail of the map and identification of artifacts.

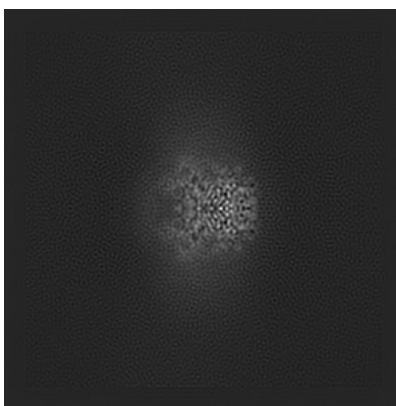
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

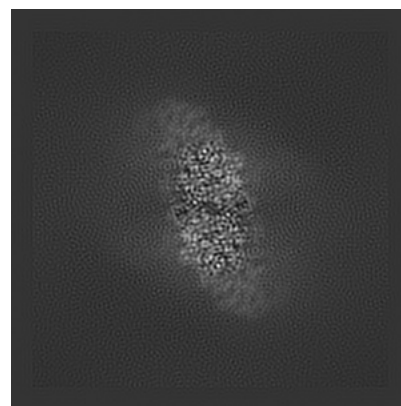
6.1.1 Primary map



X

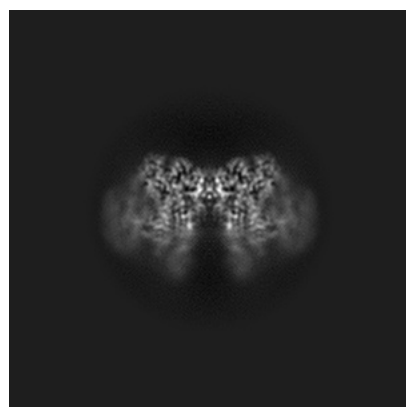


Y

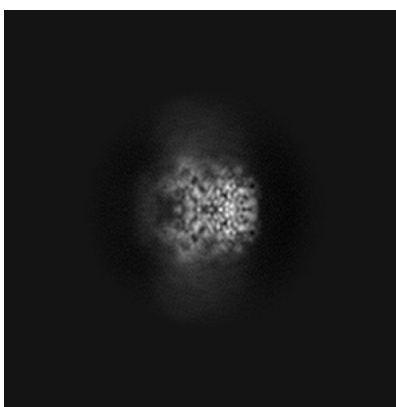


Z

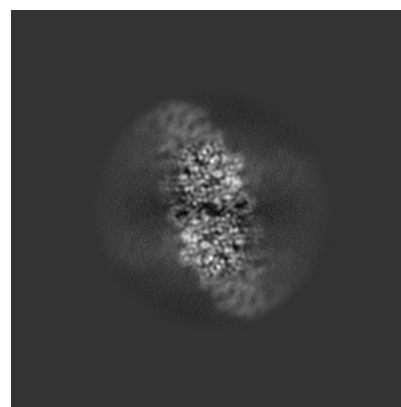
6.1.2 Raw map



X



Y

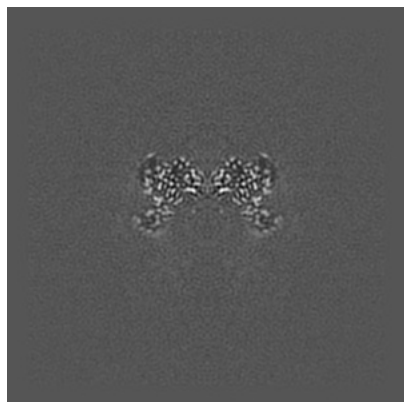


Z

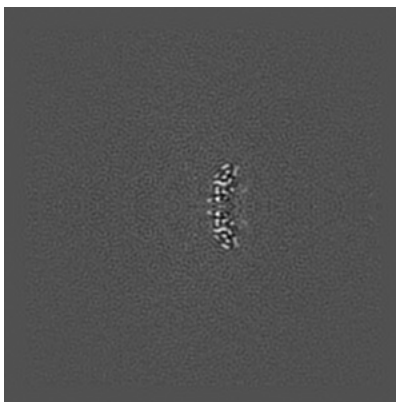
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

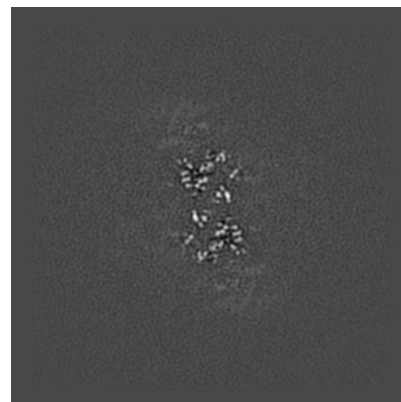
6.2.1 Primary map



X Index: 192

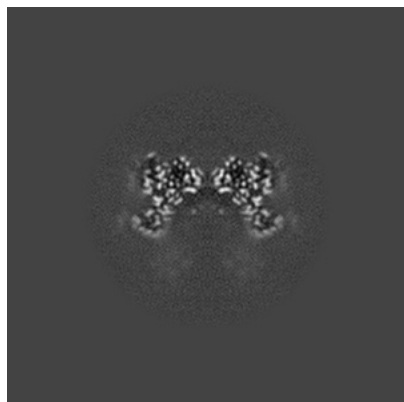


Y Index: 192

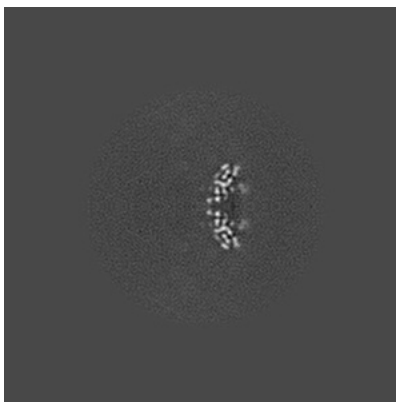


Z Index: 192

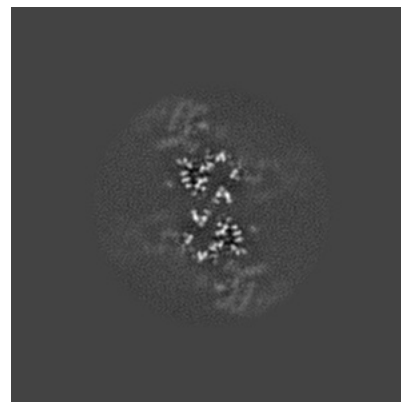
6.2.2 Raw map



X Index: 192



Y Index: 192

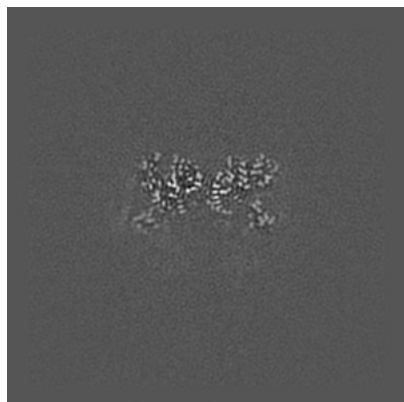


Z Index: 192

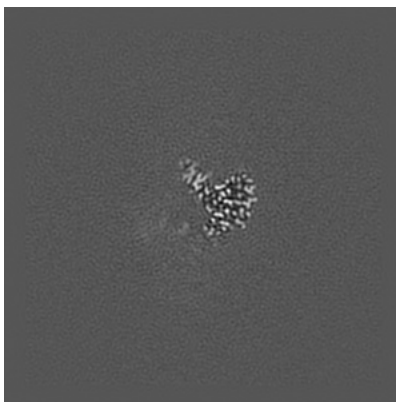
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

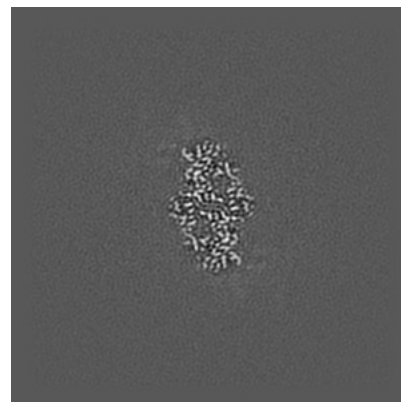
6.3.1 Primary map



X Index: 197

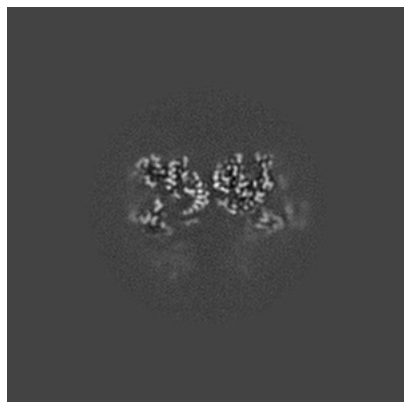


Y Index: 161

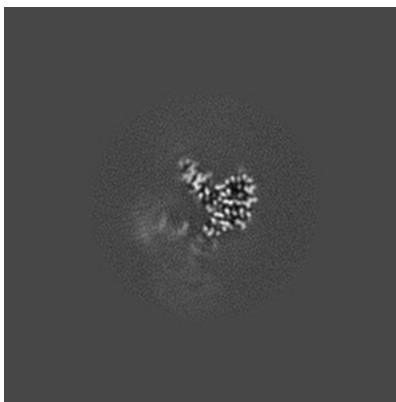


Z Index: 215

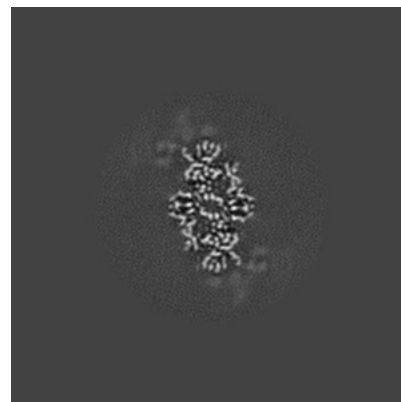
6.3.2 Raw map



X Index: 186



Y Index: 161

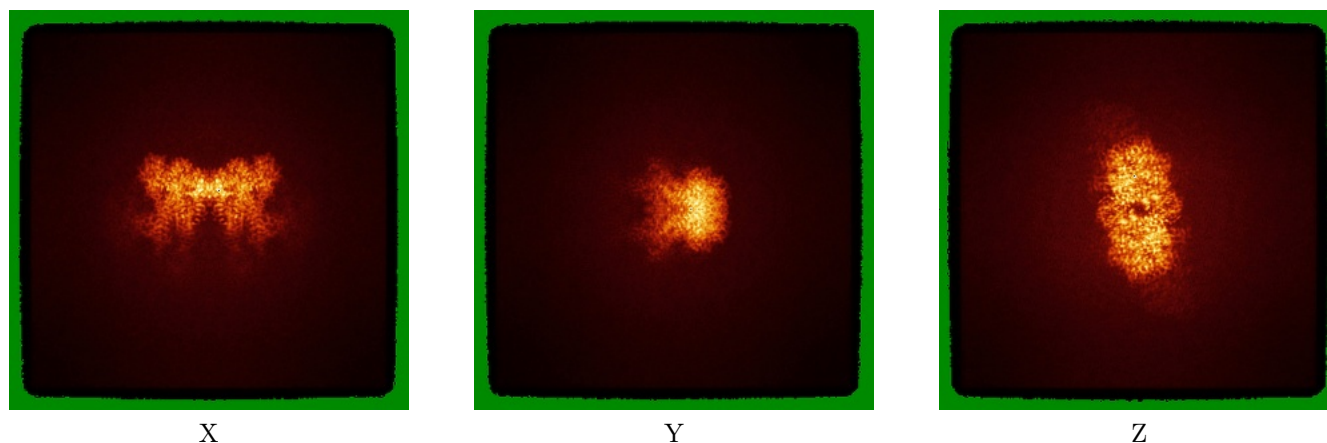


Z Index: 214

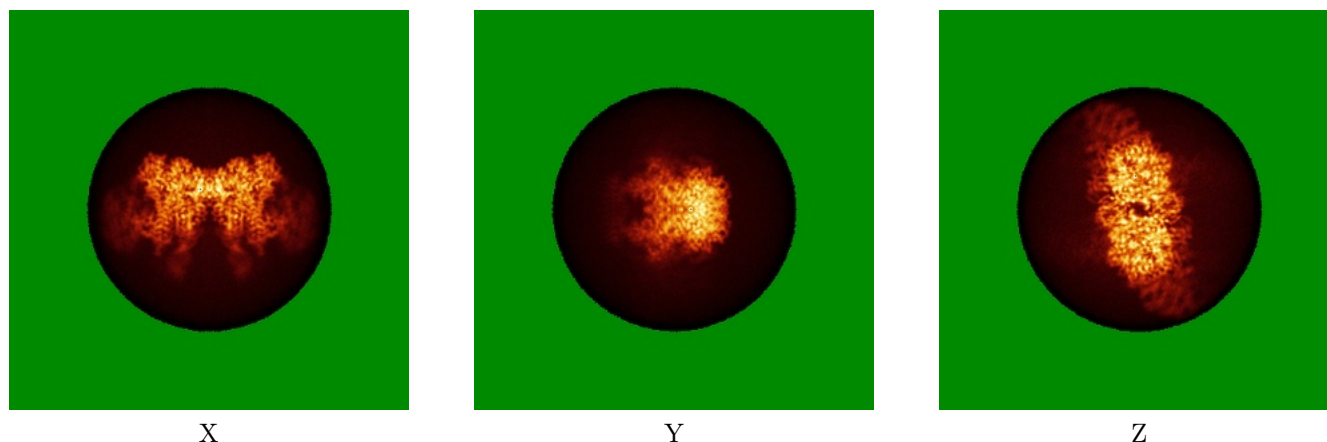
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

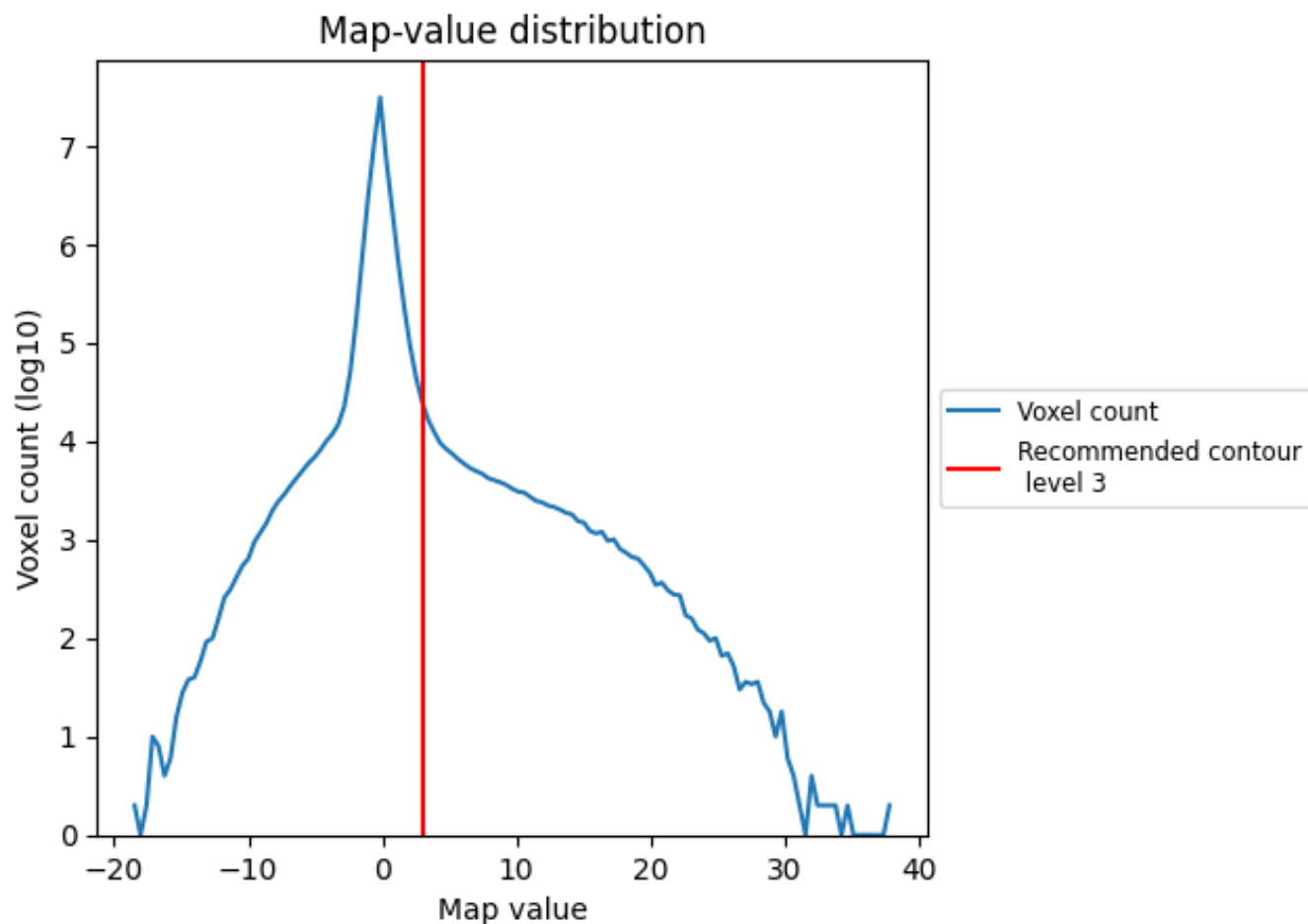
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

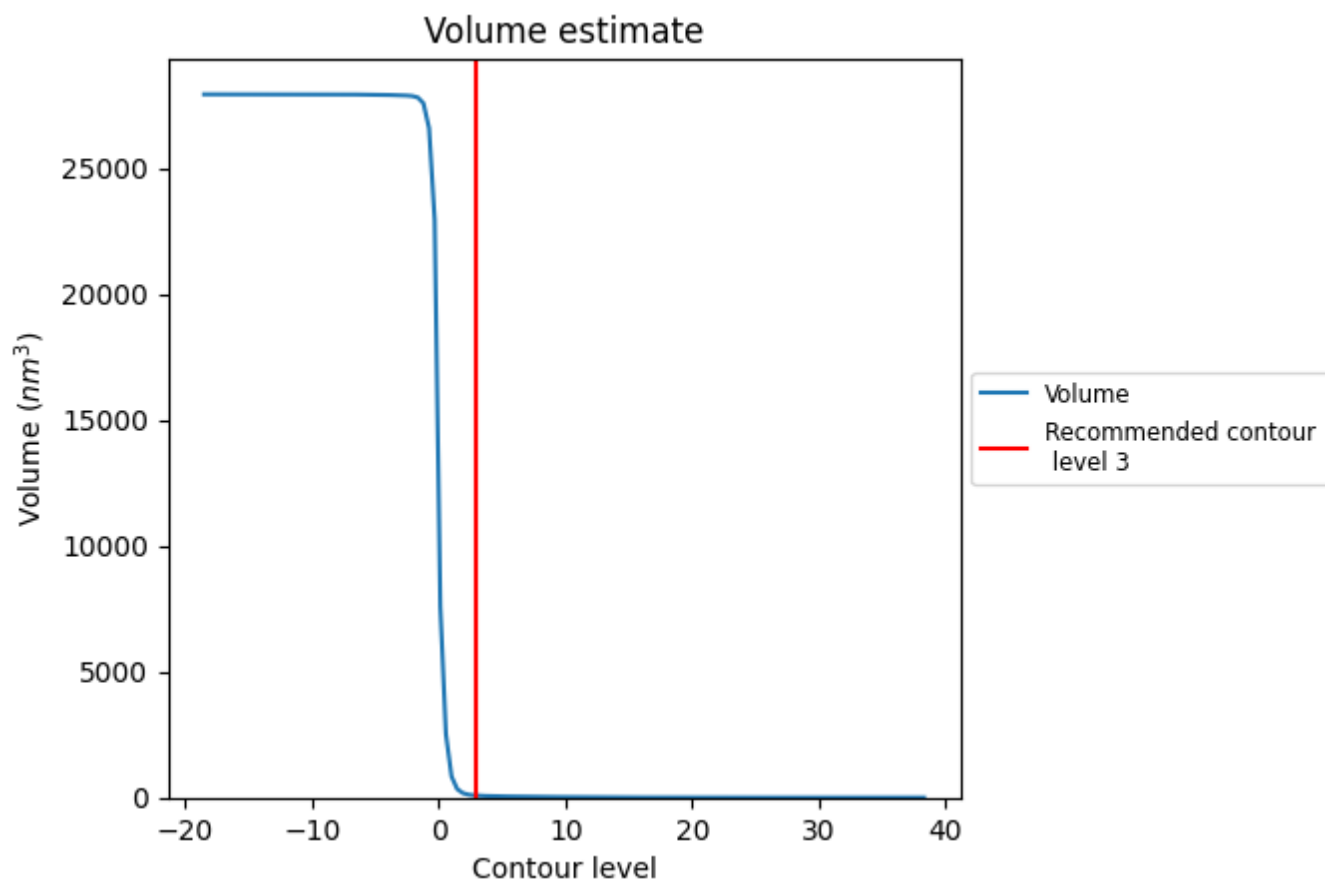
This section contains the results of statistical analysis of the map.

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.

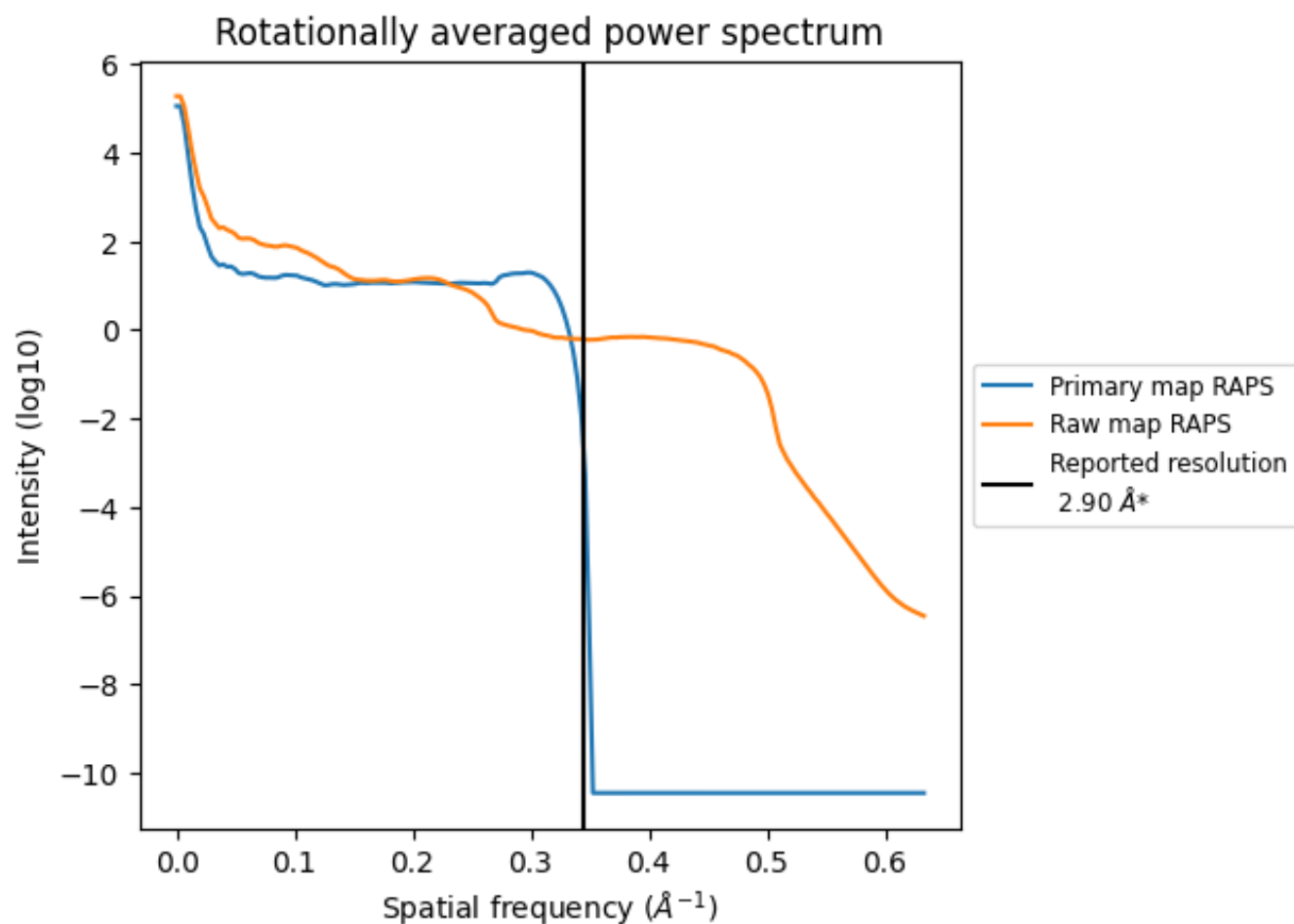
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm^3 ; this corresponds to an approximate mass of 73 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 ⓘ

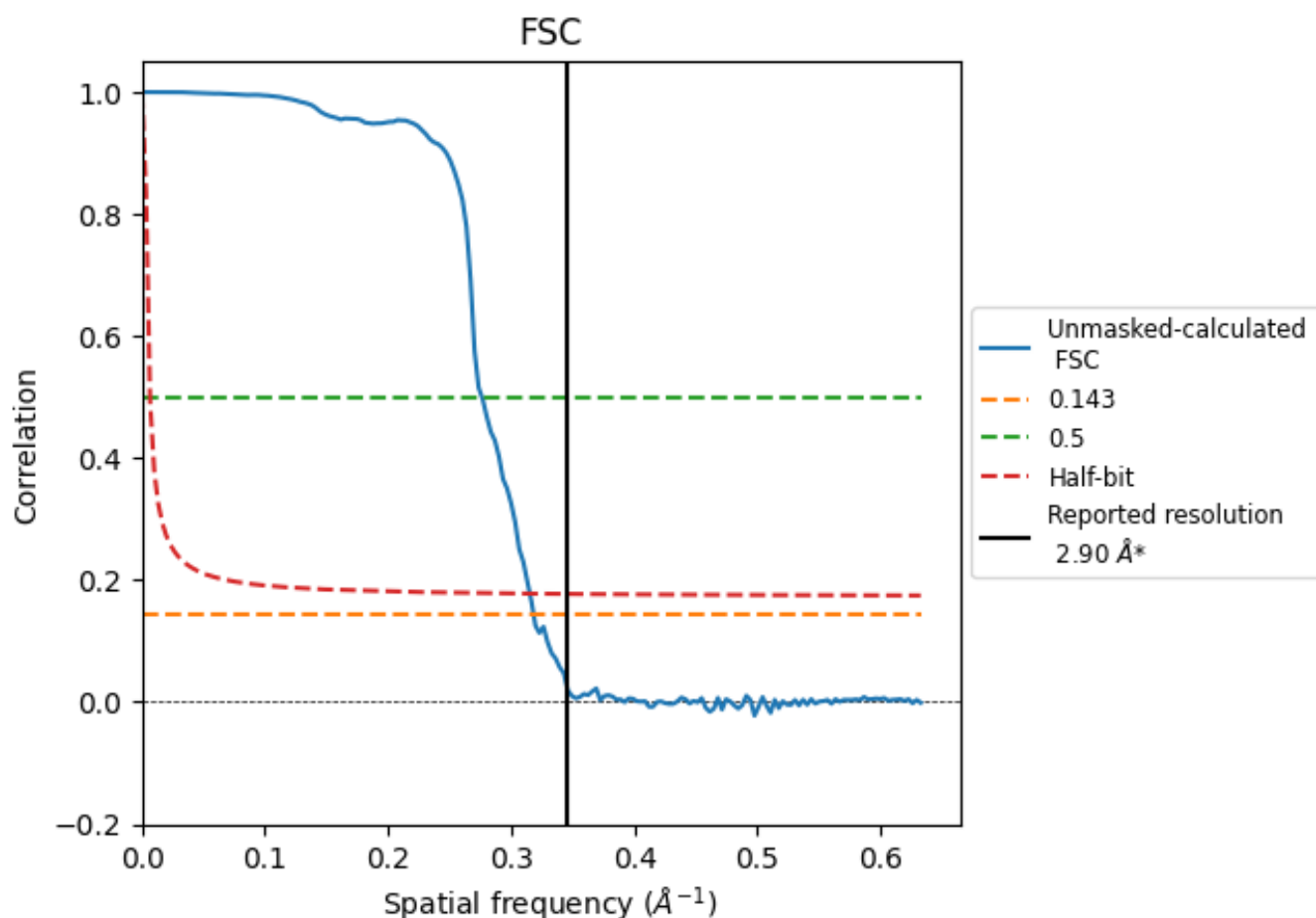


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.62	3.17

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

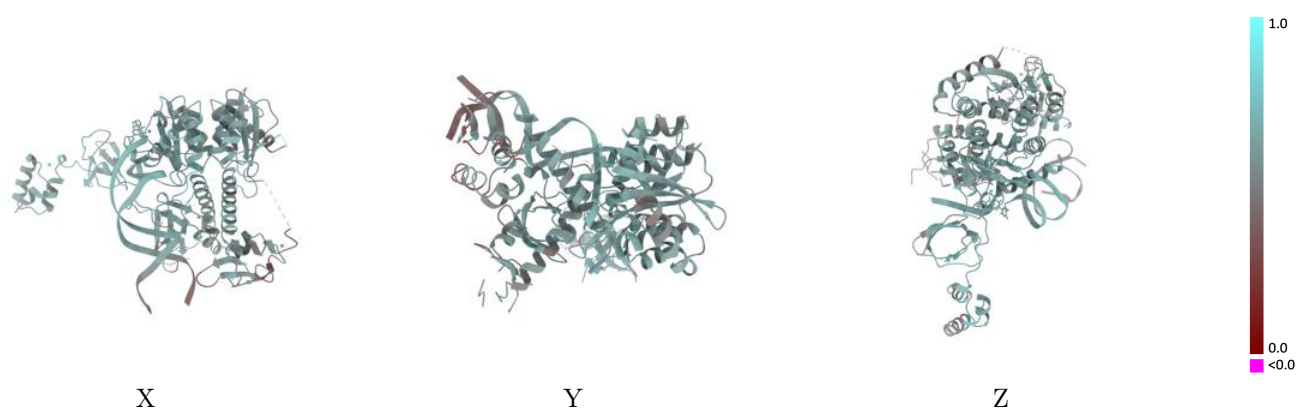
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20483 and PDB model 6PUW. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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



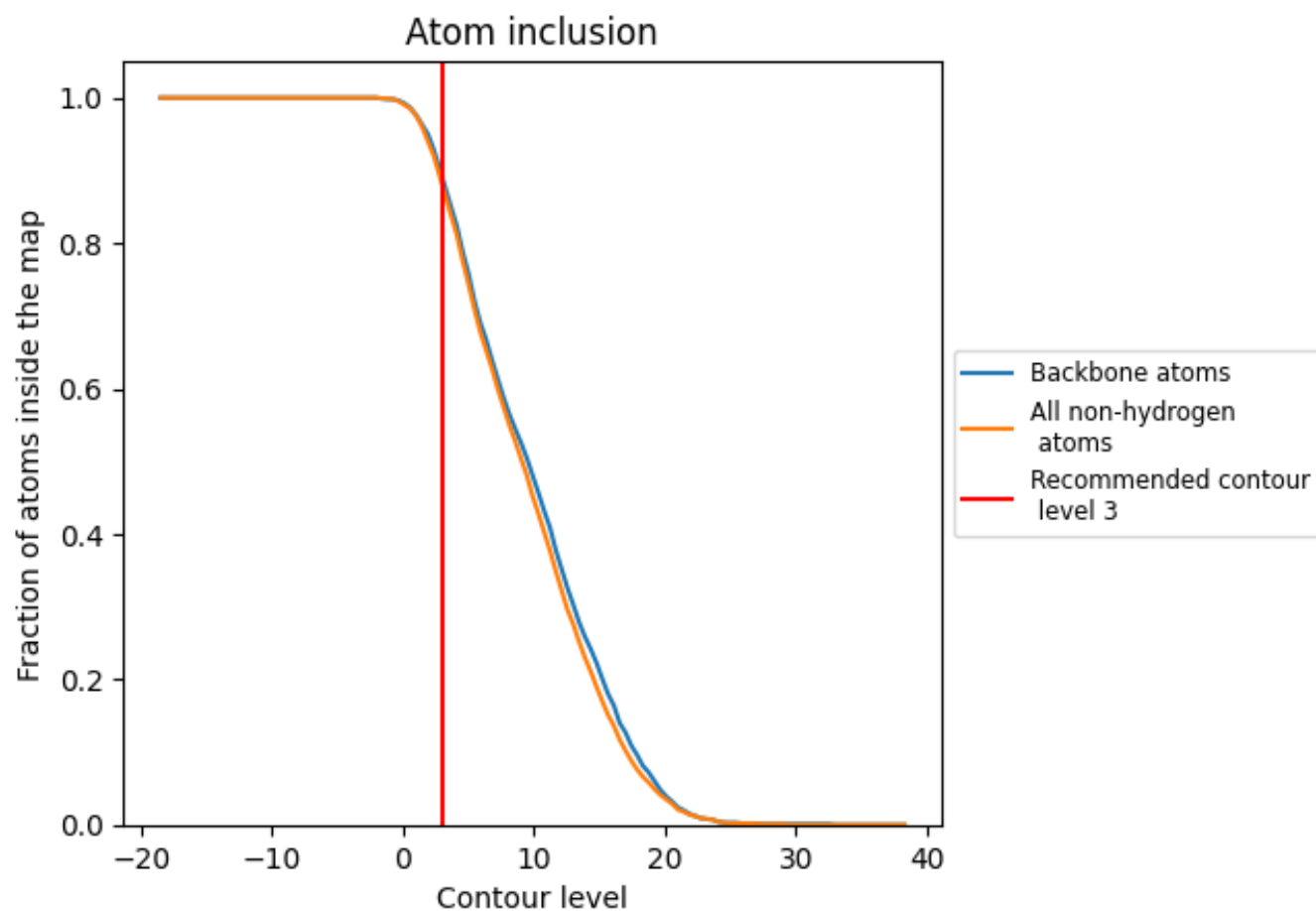
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.5730
A	0.9020	0.5870
B	0.8330	0.5480
C	0.8910	0.5850
D	0.9220	0.6020
E	0.9140	0.5750
F	0.9140	0.5670

1.0

0.0

<0.0