



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:27 PM UTC

PDB ID : 8ZL8 / pdb_00008zl8
EMDB ID : EMD-60222
Title : Structure of Polycystin-1/Polycystin-2 complex with 7b,27-DHC
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-05-17
Resolution : 3.38 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
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

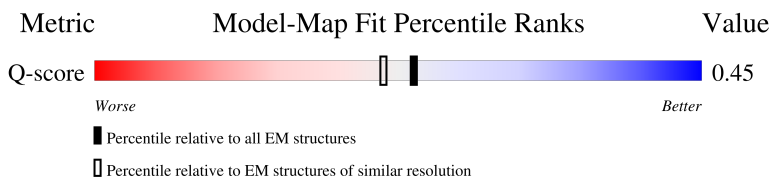
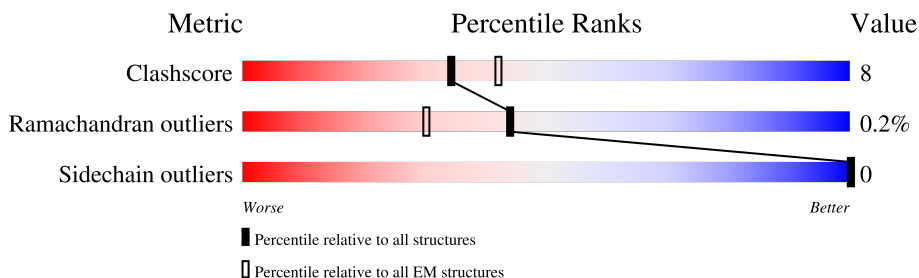
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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	14261 (2.88 - 3.88)

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	1261	12% 48% 12% 40%
2	B	1007	41% 7% 53%
2	C	1007	38% 8% 54%
2	D	1007	10% 41% 6% 53%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16728 atoms, of which 46 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 Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	759	5636	3636	1029	953	18	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	476	3938	2601	622	694	21	0	0
2	C	467	3858	2549	608	682	19	0	0
2	D	474	3136	2030	528	565	13	0	0

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

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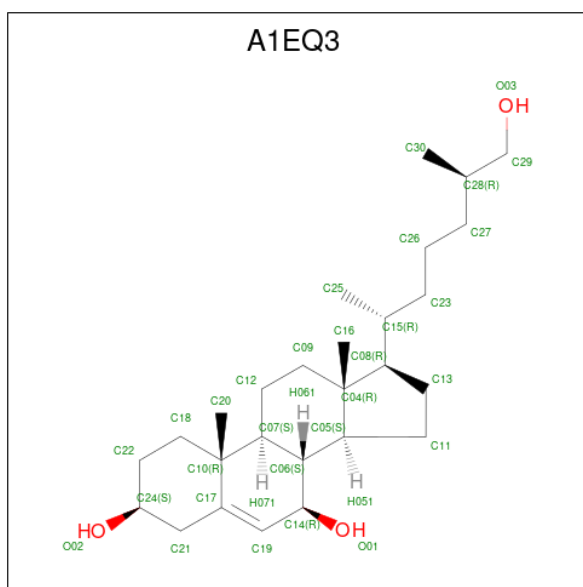
Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

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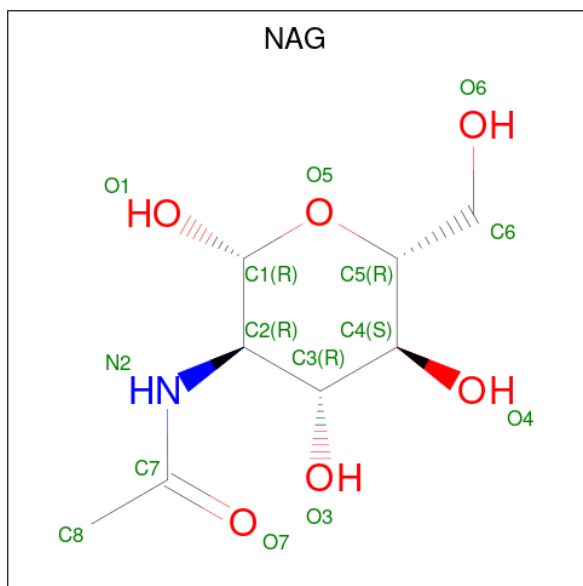
Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 is (3 {S},7 {R},8 {S},9 {S},10 {R},13 {R},14 {S},17 {R})-10,13-dimethyl-17-[(2 {R},6 {R})-6-methyl-7-oxidanyl-heptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1 {H}-cyclopenta[a]phenanthrene-3,7-diol (CCD ID: A1EQ3) (formula: C₂₇H₄₆O₃).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			76	27	46	3	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

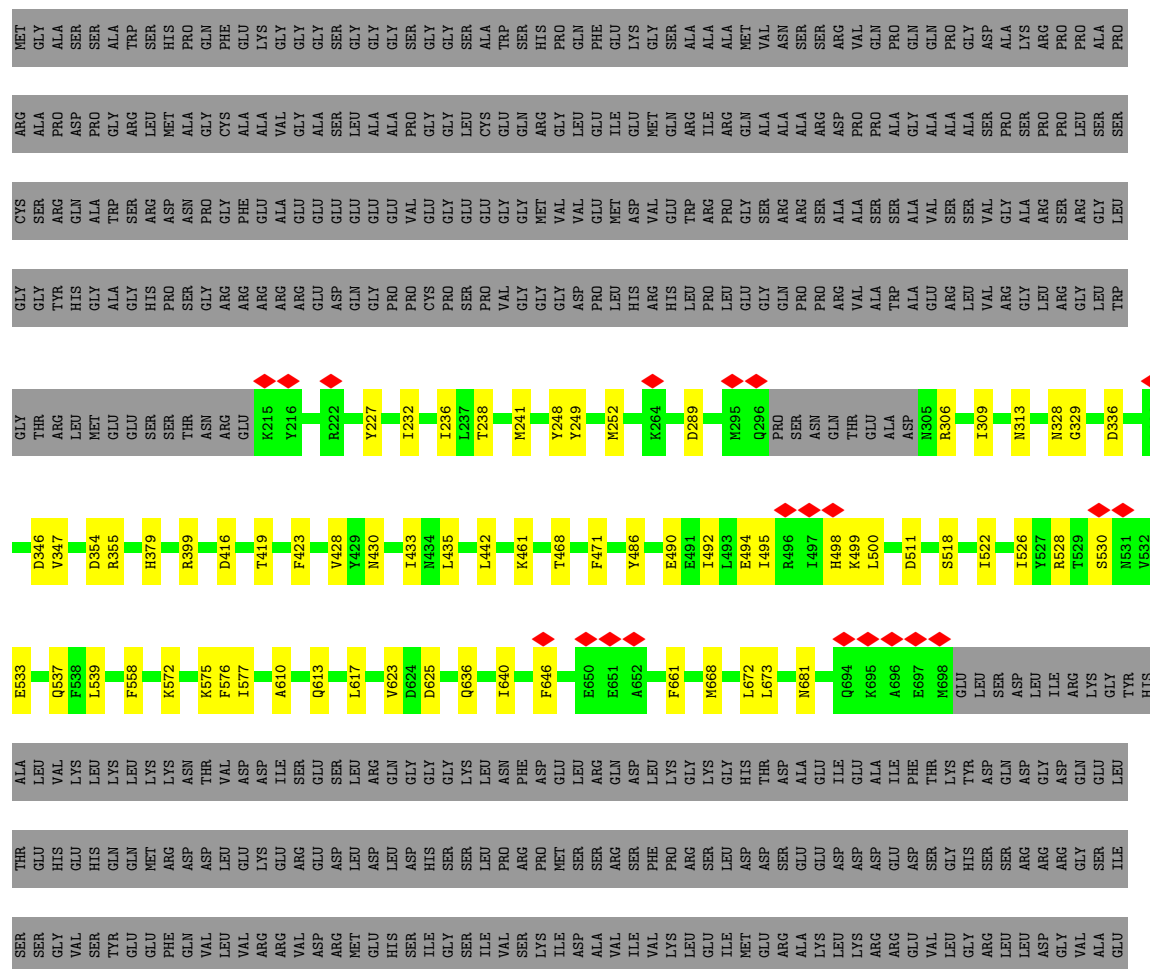


Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

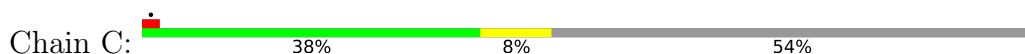
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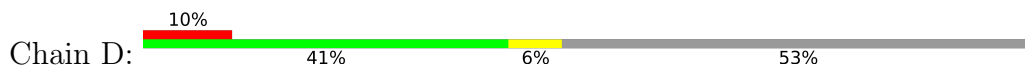
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	



- Molecule 2: Polycystin-2

[illegible]

- Molecule 2: Polycystin-2



MET	GLY	ALA	SER	TRP	SER	HIS	GLN	PHE	GLU	LYS	GLY	GLY	SER	GLY	GLY	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	SER	VAL	ASN	SER	SER	ARG	VAL	GLN	PRO	GLN	PRO	ASP	ALA	LYS	ARG	PRO	PRO	ALA	PRO
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ASP	ALA	ASP	GLU	HIS	LEU	GLU	Y660	L510	R397	GLN	GLY	CYS	ARG	ALA	ARG
ALA	ALA	ALA	LEU	GLY	LEU	LEU	Y670	V513	T398	THR	THR	SER	PRO	PRO	ALA
GLN	GLN	VAL	GLN	ASP	GLN	GLN	I671	A521	T402	ALA	ASP	GLN	ASP	ASP	GLN
ILE	ILE	VAL	LEU	PHE	LEU	LYS	I674	I522	A403	N305	GLU	ALA	TRP	GLY	ARG
SER	SER	LYS	LYS	PRO	ARG	GLY	N674	G523	A407	R306	GLU	GLY	SER	GLY	GLY
HIS	HIS	LEU	GLY	ARG	ARG	GLY	N681	I524			SER	HIS	ARG	LEU	LEU
GLY	GLY	GLU	LYS	SER	LEU	GLY	N688	N531			THR	PRO	ASP	MET	ASP
LEU	LEU	ILE	LEU	LEU	LEU	GLY	K688	V532	K411	F308	SER	ASN	ASN	ASN	GLY
THR	THR	MET	ASP	ASP	ASP	THR	S688	E533	M412	F310	THR	GLY	SER	PRO	GLY
GLU	GLU	GLU	ASP	SER	ASP	ASP	D690	V534	V413		GLU	ARG	ARG	PHE	GLY
ALA	ALA	ALA	ALA	GLU	ALA	ALA		V534	D416	R325	LYS	ALA	ARG	ALA	ALA
LYS	LYS	LYS	GLU	GLU	GLU	GLU	Q694	L535	R417			ARG	ALA	VAL	VAL
LEU	LEU	LYS	ASP	ASP	GLU	GLU	K695	L536	R417			ARG	GLU	GLY	GLY
ASN	ASN	ARG	GLU	ASP	ASP	GLU	A696	Q337	G418	G529		ASP	GLU	GLU	ALA
GLN	GLN	ARG	ILE	GLU	ILE	ILE	F697	F338	T419			GLN	LEU	SER	SER
PRO	PRO	GLU	PHE	ASP	PRO	THR	MET	L539	S427	S332		GLY	LEU	ALA	ALA
ARG	ARG	VAL	SER	SER	THR	THR		E540		I333		PRO	VAL	PRO	PRO
LEU	LEU	GLY	LYS	HIS	TYR	TYR	D541	D541	M432	P334		CYS	GLY	GLY	GLY
THR	THR	GLY	ASP	SER	ASP	ASP	Q542	Q542		Q335		PRO	GLY	GLY	GLY
GLY	GLY	LEU	SER	ARG	GLN	GLN	N543	N543	C437	D336		SER	LEU	LEU	LEU
ARG	ARG	LEU	ARG	SER	ASP	ASP	T544	T544	F445	L337		PRO	GLU	GLY	CYS
PRO	PRO	ASP	GLY	ARG	ASP	GLY	F545	F545	P446	R338		VAL	GLY	GLY	GLN
SER	SER	VAL	GLY	ARG	GLN	GLN	P546	P546	A447	D339		GLY	GLY	GLY	GLN
SER	SER	ALA	GLY	ILE	GLU	GLU	N547	N547	T448	E340		MET	ARG	ARG	ARG
GLN	GLN	GLU	ILE	LEU	LEU	LEU	F548	F548	G449			ASP	VAL	VAL	VAL
SER	SER	ASP	THR	SER	THR	THR	LYS	LYS	G450	K342		PRO	GLU	GLY	GLY
THR	THR	GLU	SER	SER	GLY	HIS	E549	E549	G451	E343		LEU	MET	LEU	ILE
GLU	GLU	ARG	GLY	GLY	VAL	GLU	Y553	Y553	I452	C344		HIS	ASP	GLU	GLU
GLY	GLY	LEU	VAL	LYS	GLU	GLU	W554	W554	P453	Y345		ARG	VAL	GLU	MET
MET	MET	GLY	ARG	LEU	LEU	LEU	Q555	Q555		Y345		HIS	GLU	GLU	GLN
GLU	GLU	ASP	GLN	LEU	GLN	GLN	I556	I556	S454	D346		TRP	TRP	GLY	GLY
ALA	ALA	SER	LYS	LEU	LYS	LYS	N559	N559	G455	V347		PRO	PRO	GLY	GLY
GLY	GLY	GLU	LEU	PHE	LEU	ARG				Y348		GLY	SER	ALA	ALA
GLY	GLY	ILE	LYS	GLN	ASP	ASP	N560	N560	K461			SER	ALA	ALA	ALA
ASN	ASN	HIS	VAL	ASP	ASN	ASP	T565	T565	L462	R355		GLN	ARG	ARG	ARG
GLY	GLY	ARG	LEU	LEU	THR	THR	V566	V566	I463	A356		PRO	ARG	ALA	ALA
SER	SER	GLU	VAL	VAL	VAL	LYS	F567	F567	I463	P357		PRO	SER	ALA	ALA
SER	SER	GLN	ARG	ARG	ARG	LYS	F667	F667	R464	F358		ARG	ALA	ASP	ASP
ASN	ASN	MET	ARG	ARG	GLU	GLU	F568	F568	Y465	G359		VAL	ALA	PRO	PRO
VAL	VAL	GLU	VAL	VAL	ARG	ARG	V569	V569		G359		ALA	SER	SER	ALA
HIS	HIS	ARG	ARG	ASP	ASP	GLU	M570	M570	D470	P360		ALA	SER	ALA	ALA
VAL	VAL	LEU	LEU	ASP	GLU	GLU	K571	K571	F480	R361		GLY	VAL	VAL	ALA
		ARG	GLU	ASP	SER	ASP	K572	K572		G361		ARG	SER	SER	ALA
		GLU	LEU	LEU	LEU	LEU	K575	K575	I484	N375		LEU	SER	ALA	ALA
		GLU	GLN	ASP	GLN	GLN	G520	G520	F485	G376		VAL	VAL	VAL	SER
		LEU	GLY	HIS	GLY	HIS			V488	S377		ARG	GLY	GLY	PRO
		GLY	SER	ILE	GLY	GLY	V623	V623		S378		ALA	ALA	ALA	SER
		TRP	SER	SER	GLY	SER	D824	D824	I492	H379		ARG	ARG	ARG	PRO
		GLU	LEU	ILE	LEU	LEU	D625	D625	L493	W380		GLY	SER	GLY	PRO
		GLU	VAL	VAL	PRO	PRO	F626	F626	E494	G381		LEU	ARG	LEU	LEU
		ASP	ARG	SER	ASN	ASN			H498	G382		GLY	SER	SER	SER
		ASP	PHE	SER	PHE	PHE	Q636	Q636	K499	I382		LEU	GLY	GLY	LEU
		ASP	ASP	LYS	ASP	ASP	E648	E648	L500	I383		TRP	LEU	LEU	SER
										G387					
										G388					
										A389					
										G390					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, A1EQ3

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	0.15	0/5771	0.42	1/7869 (0.0%)
2	B	0.14	0/4042	0.37	0/5481
2	C	0.16	0/3960	0.48	5/5373 (0.1%)
2	D	0.15	0/3188	0.46	1/4365 (0.0%)
All	All	0.15	0/16961	0.43	7/23088 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	375	ASN	CA-C-N	-10.21	113.38	122.47
2	C	375	ASN	C-N-CA	-10.21	113.38	122.47
2	C	532	VAL	N-CA-C	-6.08	107.93	113.71
1	A	3320	VAL	N-CA-C	-5.39	108.59	113.71
2	C	623	VAL	CA-C-N	5.21	135.03	126.86
2	C	623	VAL	C-N-CA	5.21	135.03	126.86
2	D	522	ILE	N-CA-C	-5.02	107.84	111.90

There are no chirality outliers.

There are no planarity outliers.

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	A	5636	0	5449	121	0
2	B	3938	0	3897	45	0
2	C	3858	0	3818	53	0
2	D	3136	0	2473	43	0
3	A	30	46	0	13	0
4	B	42	0	39	1	0
4	C	42	0	39	0	0
All	All	16682	46	15715	262	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 8.

All (262) 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:A:4401:A1EQ3:C14	3:A:4401:A1EQ3:C06	1.78	1.60
3:A:4401:A1EQ3:C07	3:A:4401:A1EQ3:C10	1.79	1.56
3:A:4401:A1EQ3:C13	3:A:4401:A1EQ3:C11	1.75	1.43
1:A:3753:ARG:O	1:A:3754:LEU:HG	1.18	1.35
1:A:3753:ARG:O	1:A:3754:LEU:CG	1.87	1.22
1:A:3306:ALA:O	1:A:3308:SER:N	1.73	1.22
1:A:3754:LEU:HD12	1:A:3756:GLU:H	0.91	1.08
1:A:3754:LEU:HD21	1:A:3846:ARG:HB3	1.08	1.06
1:A:3754:LEU:HD11	1:A:3846:ARG:HG2	1.39	1.00
1:A:3754:LEU:HD12	1:A:3756:GLU:N	1.76	0.99
1:A:3754:LEU:CD2	1:A:3846:ARG:HB3	1.94	0.97
1:A:3297:VAL:O	1:A:3301:ALA:HB3	1.68	0.92
1:A:3854:LEU:HD12	1:A:3855:THR:N	1.88	0.87
1:A:3854:LEU:HD12	1:A:3855:THR:H	1.41	0.84
1:A:3753:ARG:O	1:A:3754:LEU:CD2	2.26	0.84
1:A:3754:LEU:CD1	1:A:3756:GLU:H	1.84	0.83
3:A:4401:A1EQ3:C06	3:A:4401:A1EQ3:C10	2.58	0.80
3:A:4401:A1EQ3:C14	3:A:4401:A1EQ3:C07	2.56	0.79
2:C:585:GLN:HE22	2:C:688:LYS:HE3	1.47	0.78
1:A:3306:ALA:C	1:A:3308:SER:H	1.90	0.78
1:A:4107:ARG:HH22	2:D:681:ASN:HD21	1.32	0.78
3:A:4401:A1EQ3:C07	3:A:4401:A1EQ3:C18	2.62	0.77
2:C:345:TYR:O	2:C:420:ARG:NH2	2.18	0.76
2:C:375:ASN:HB2	2:C:547:ASN:ND2	2.00	0.76
1:A:3306:ALA:C	1:A:3308:SER:N	2.45	0.75
2:D:227:TYR:OH	2:D:572:LYS:O	2.05	0.74
2:D:325:ARG:HA	2:D:419:THR:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:623:VAL:HG12	2:B:625:ASP:H	1.52	0.73
1:A:3753:ARG:C	1:A:3754:LEU:HG	2.13	0.73
1:A:4022:ALA:HB2	1:A:4109:ARG:HG3	1.71	0.71
2:B:238:THR:HA	2:B:241:MET:HE3	1.74	0.70
1:A:3755:GLN:HB2	1:A:3777:SER:HB2	1.73	0.70
2:B:433:ILE:HD12	2:B:435:LEU:HD12	1.74	0.69
2:B:511:ASP:OD1	2:B:572:LYS:NZ	2.24	0.69
1:A:3290:LEU:HB3	1:A:3333:VAL:HG21	1.76	0.68
2:C:320:ARG:NH1	2:C:374:LEU:HD11	2.09	0.68
1:A:3269:ARG:HH11	1:A:3277:ARG:HB2	1.58	0.67
1:A:3343:LEU:HD22	1:A:3558:ALA:HB2	1.77	0.67
2:C:533:GLU:HA	2:C:536:LEU:HD23	1.76	0.66
3:A:4401:A1EQ3:C07	3:A:4401:A1EQ3:C20	2.72	0.66
2:D:670:PHE:O	2:D:674:ASN:ND2	2.29	0.66
1:A:3306:ALA:O	1:A:3307:TYR:C	2.39	0.66
2:D:681:ASN:C	2:D:681:ASN:HD22	2.05	0.64
2:C:323:GLN:HE21	2:C:419:THR:HG22	1.64	0.63
2:D:636:GLN:NE2	2:D:660:TYR:OH	2.31	0.63
3:A:4401:A1EQ3:C14	3:A:4401:A1EQ3:C05	2.73	0.61
2:C:225:VAL:O	2:C:229:LEU:HG	2.00	0.61
1:A:3255:ARG:HD3	1:A:3624:PRO:HB2	1.82	0.60
2:C:396:SER:H	2:C:402:THR:HG22	1.66	0.60
3:A:4401:A1EQ3:C10	3:A:4401:A1EQ3:C12	2.77	0.60
1:A:3755:GLN:HA	1:A:3846:ARG:HH21	1.65	0.60
2:C:291:LEU:HD11	2:C:315:LEU:HD13	1.84	0.60
2:C:593:CYS:HB3	2:C:683:THR:HG21	1.83	0.59
3:A:4401:A1EQ3:C07	3:A:4401:A1EQ3:C17	2.71	0.59
2:C:227:TYR:OH	2:C:569:VAL:O	2.21	0.59
1:A:4091:TRP:CG	1:A:4092:ALA:H	2.20	0.59
2:B:313:ASN:OD1	2:B:430:ASN:ND2	2.29	0.58
2:B:499:LYS:NZ	2:B:500:LEU:O	2.28	0.58
2:C:375:ASN:HB2	2:C:547:ASN:HD21	1.67	0.58
2:C:597:LEU:HD13	2:D:671:ILE:HD12	1.85	0.58
2:D:292:TYR:HA	2:D:306:ARG:H	1.69	0.58
2:C:500:LEU:HD12	2:C:501:HIS:H	1.66	0.58
1:A:3867:VAL:HG22	1:A:3885:VAL:HG22	1.86	0.58
2:C:681:ASN:HD22	2:C:681:ASN:C	2.08	0.57
2:B:526:ILE:O	2:B:530:SER:OG	2.19	0.57
1:A:3066:PHE:HD1	1:A:3575:TRP:HH2	1.52	0.57
2:C:234:LEU:HD23	2:C:569:VAL:HG11	1.85	0.57
1:A:3846:ARG:HD3	1:A:3846:ARG:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4401:A1EQ3:C06	3:A:4401:A1EQ3:C19	2.76	0.57
2:C:374:LEU:O	2:C:376:GLY:N	2.38	0.57
1:A:3749:LEU:HB2	1:A:3821:GLN:HB2	1.86	0.56
1:A:3655:PHE:N	1:A:3658:LYS:HZ2	2.04	0.56
1:A:3297:VAL:O	1:A:3301:ALA:CB	2.50	0.56
1:A:3993:SER:O	1:A:3996:PHE:HB3	2.05	0.56
4:B:1003:NAG:H83	4:B:1003:NAG:H3	1.88	0.56
2:C:328:ASN:OD1	2:C:329:GLY:N	2.38	0.56
2:D:228:LEU:O	2:D:232:ILE:HD12	2.06	0.56
2:C:371:GLU:O	2:C:374:LEU:O	2.23	0.56
1:A:4108:TRP:CH2	2:D:688:LYS:HE2	2.41	0.56
2:B:328:ASN:OD1	2:B:329:GLY:N	2.39	0.56
1:A:3753:ARG:O	1:A:3754:LEU:HD23	2.04	0.56
2:B:249:TYR:HE1	2:B:313:ASN:HD21	1.54	0.56
1:A:3750:ARG:NH1	1:A:3815:ASP:O	2.40	0.55
1:A:3966:PHE:HA	1:A:3975:THR:HG21	1.87	0.55
1:A:3798:SER:OG	1:A:3818:GLY:O	2.25	0.54
1:A:3854:LEU:CD1	1:A:3855:THR:H	2.16	0.54
1:A:3724:TRP:HZ2	1:A:3843:LEU:HB3	1.71	0.54
2:B:528:ARG:NH2	2:B:558:PHE:CD2	2.76	0.54
1:A:3770:CYS:HB3	1:A:3874:PRO:HB3	1.90	0.54
2:C:537:GLN:O	2:C:542:GLN:NE2	2.40	0.54
2:D:566:VAL:HA	2:D:569:VAL:HG12	1.89	0.54
1:A:3753:ARG:C	1:A:3754:LEU:CG	2.74	0.53
1:A:3751:GLN:HE22	1:A:3847:SER:HA	1.74	0.53
2:D:553:TYR:HA	2:D:556:ILE:HD12	1.90	0.53
1:A:3754:LEU:HD11	1:A:3846:ARG:CG	2.27	0.53
2:C:608:PHE:HE2	2:C:633:ILE:HG23	1.74	0.53
2:D:559:ASN:OD1	2:D:560:ASN:ND2	2.39	0.53
1:A:3736:HIS:NE2	1:A:3825:LEU:O	2.31	0.52
1:A:3766:ARG:HD2	1:A:3769:THR:HA	1.91	0.52
2:C:324:LEU:HB2	2:C:421:ALA:HB3	1.91	0.52
1:A:3841:ASN:OD1	1:A:3844:ASP:HB2	2.08	0.52
2:B:681:ASN:C	2:B:681:ASN:HD22	2.14	0.52
2:B:577:ILE:HG13	2:B:577:ILE:O	2.09	0.52
1:A:3562:SER:O	1:A:3566:VAL:HG22	2.10	0.52
1:A:4108:TRP:CH2	2:D:688:LYS:CE	2.93	0.52
2:C:320:ARG:NH1	2:C:374:LEU:CD1	2.73	0.52
1:A:3757:ALA:HA	1:A:3846:ARG:CG	2.40	0.52
2:C:346:ASP:OD1	2:C:347:VAL:N	2.43	0.52
1:A:3754:LEU:HA	1:A:3776:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:TYR:O	2:B:252:MET:HG2	2.10	0.52
1:A:3856:ARG:HB3	1:A:3865:ALA:HB3	1.93	0.51
1:A:4038:VAL:HG23	2:D:239:TYR:HD1	1.76	0.51
2:D:521:ALA:HA	2:D:524:ILE:HB	1.92	0.51
1:A:3725:PRO:O	1:A:3729:HIS:ND1	2.43	0.51
1:A:4025:GLU:OE2	3:A:4401:A1EQ3:C25	2.57	0.51
2:B:539:LEU:HD13	2:C:336:ASP:HB3	1.93	0.51
1:A:3347:SER:HA	1:A:3551:PRO:HB2	1.92	0.51
1:A:3753:ARG:O	1:A:3754:LEU:CB	2.58	0.50
2:D:231:LEU:HD23	2:D:572:LYS:NZ	2.27	0.50
1:A:3754:LEU:O	1:A:3775:GLY:O	2.30	0.50
2:C:398:THR:OG1	2:C:401:GLU:OE1	2.28	0.50
2:B:518:SER:O	2:B:522:ILE:HG13	2.12	0.50
2:D:224:LEU:O	2:D:228:LEU:HG	2.12	0.50
2:D:623:VAL:HG12	2:D:625:ASP:H	1.76	0.50
1:A:3811:CYS:SG	1:A:3848:ARG:NH2	2.84	0.49
1:A:3724:TRP:HB2	1:A:3725:PRO:HD3	1.93	0.49
2:C:246:VAL:O	2:C:250:THR:HG23	2.13	0.49
2:C:313:ASN:HD22	2:C:428:VAL:HG21	1.76	0.49
2:D:227:TYR:CE1	2:D:575:LYS:HD3	2.48	0.49
2:B:346:ASP:OD1	2:B:347:VAL:N	2.46	0.48
2:D:500:LEU:HD23	2:D:500:LEU:H	1.78	0.48
1:A:3334:TYR:CZ	1:A:3338:LEU:HD11	2.47	0.48
2:D:492:ILE:HG13	2:D:493:LEU:HD12	1.96	0.48
2:D:620:GLY:HA2	2:D:626:PHE:O	2.13	0.48
1:A:3325:VAL:HA	1:A:3328:VAL:HG22	1.95	0.48
1:A:3123:LEU:HA	1:A:3167:ILE:HA	1.95	0.48
1:A:3827:LEU:HD11	1:A:3831:ARG:HH21	1.79	0.47
2:C:375:ASN:CB	2:C:547:ASN:ND2	2.73	0.47
2:B:435:LEU:HD23	2:B:461:LYS:HB2	1.97	0.47
1:A:4101:LEU:O	1:A:4104:VAL:HG22	2.14	0.47
2:D:231:LEU:HD23	2:D:572:LYS:HZ3	1.79	0.47
1:A:4033:LEU:HB2	1:A:4096:TRP:CZ2	2.49	0.47
2:D:559:ASN:OD1	2:D:560:ASN:N	2.47	0.47
1:A:3726:TRP:O	1:A:3730:VAL:HG12	2.14	0.47
2:C:470:ASP:HA	2:C:473:LEU:HB2	1.96	0.47
2:D:445:PHE:HA	2:D:451:VAL:HA	1.97	0.47
1:A:3063:ARG:HD3	1:A:3305:SER:HB3	1.96	0.47
2:B:492:ILE:HA	2:B:495:ILE:HG22	1.98	0.46
1:A:3605:PRO:HA	1:A:3608:VAL:HG22	1.97	0.46
1:A:4107:ARG:HH22	2:D:681:ASN:ND2	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3275:PHE:CE2	1:A:3280:ARG:HG2	2.51	0.46
2:D:568:PHE:HA	2:D:571:ILE:HB	1.97	0.46
1:A:3872:GLU:O	1:A:3879:ALA:HA	2.15	0.46
2:B:430:ASN:HD21	2:C:448:THR:HA	1.79	0.46
2:D:494:GLU:O	2:D:498:HIS:HB3	2.16	0.46
1:A:3699:TYR:O	1:A:3702:GLN:HG3	2.16	0.46
2:C:423:PHE:CE1	2:C:442:LEU:HD13	2.51	0.46
2:B:468:THR:HA	2:B:471:PHE:HD2	1.80	0.46
2:C:592:ARG:HH21	2:C:687:VAL:HG23	1.81	0.46
2:D:232:ILE:O	2:D:236:ILE:HG13	2.16	0.46
1:A:3747:PRO:HG2	1:A:3823:LEU:HB3	1.98	0.46
2:B:227:TYR:CE1	2:B:572:LYS:HD3	2.50	0.46
2:B:289:ASP:OD1	2:B:399:ARG:NH1	2.49	0.46
2:D:510:LEU:HA	2:D:513:VAL:HG12	1.97	0.46
2:B:423:PHE:CE2	2:B:442:LEU:HD13	2.51	0.46
1:A:4091:TRP:CG	1:A:4092:ALA:N	2.83	0.46
2:C:313:ASN:HA	2:C:430:ASN:HA	1.98	0.45
2:B:528:ARG:NH2	2:B:558:PHE:CE2	2.84	0.45
1:A:3814:TYR:CD2	1:A:3851:PHE:HZ	2.33	0.45
1:A:3572:VAL:O	1:A:3576:VAL:HG12	2.16	0.45
1:A:3854:LEU:O	1:A:3855:THR:HB	2.17	0.45
2:B:668:MET:HA	2:B:672:LEU:HB2	1.99	0.45
2:C:337:LEU:H	2:C:337:LEU:HD23	1.81	0.45
2:B:309:ILE:HD12	2:B:428:VAL:HG11	1.99	0.45
1:A:4107:ARG:NH2	2:D:681:ASN:HD21	2.09	0.44
1:A:3249:LEU:HD11	1:A:3613:LEU:HD13	1.99	0.44
2:B:533:GLU:O	2:B:537:GLN:HG3	2.18	0.44
2:C:312:GLU:OE1	2:C:312:GLU:N	2.49	0.44
2:D:498:HIS:CE1	2:D:499:LYS:HG2	2.52	0.44
1:A:3873:PHE:HE1	1:A:3879:ALA:HB2	1.82	0.44
2:B:232:ILE:O	2:B:236:ILE:HG12	2.18	0.44
2:C:681:ASN:C	2:C:681:ASN:ND2	2.74	0.44
1:A:3253:LEU:O	1:A:3257:PHE:HB2	2.17	0.44
2:B:617:LEU:HD23	2:B:617:LEU:HA	1.81	0.44
2:B:494:GLU:O	2:B:498:HIS:HB2	2.17	0.44
1:A:3569:ALA:O	1:A:3572:VAL:HG12	2.18	0.43
1:A:3275:PHE:O	1:A:3276:THR:OG1	2.34	0.43
2:B:486:TYR:O	2:B:490:GLU:HG2	2.18	0.43
1:A:3245:PHE:O	1:A:3249:LEU:HD23	2.18	0.43
2:C:415:LEU:HD13	2:C:419:THR:HG21	2.00	0.43
2:C:491:GLU:OE1	2:C:491:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3091:MET:HG3	1:A:3671:LEU:HD11	2.01	0.43
1:A:3922:TRP:CZ3	1:A:3929:ARG:HB3	2.54	0.43
1:A:3552:ALA:HB3	1:A:3553:TRP:HE3	1.83	0.43
2:D:465:TYR:HA	2:D:470:ASP:OD2	2.18	0.43
2:D:485:PHE:HA	2:D:488:VAL:HG12	2.00	0.43
1:A:3854:LEU:HD12	1:A:3855:THR:O	2.19	0.43
1:A:3951:VAL:HG12	1:A:3987:ALA:HB2	1.99	0.43
1:A:4021:ARG:HG3	1:A:4109:ARG:HH11	1.83	0.43
2:B:610:ALA:O	2:B:613:GLN:HG3	2.19	0.43
2:C:476:CYS:HA	2:C:479:ILE:HG22	2.01	0.43
1:A:3260:LYS:HB2	1:A:3608:VAL:HG12	2.01	0.42
1:A:3269:ARG:H	1:A:3277:ARG:NH1	2.18	0.42
1:A:3333:VAL:O	1:A:3336:VAL:HG12	2.19	0.42
2:B:416:ASP:O	2:B:419:THR:HG22	2.18	0.42
1:A:3559:HIS:O	1:A:3562:SER:OG	2.28	0.42
1:A:3684:THR:HG21	1:A:3998:LEU:HD22	2.01	0.42
1:A:3755:GLN:O	1:A:3755:GLN:HG2	2.19	0.42
2:B:672:LEU:HD23	2:B:672:LEU:HA	1.92	0.42
1:A:3315:LEU:HD11	1:A:3897:LEU:H	1.84	0.42
2:B:575:LYS:HD2	2:B:576:PHE:HE1	1.85	0.42
2:D:565:THR:HG23	2:D:566:VAL:HG13	2.01	0.42
1:A:4001:LYS:HE3	1:A:4001:LYS:HB2	1.66	0.42
2:C:675:MET:O	2:C:679:ILE:HG13	2.20	0.42
1:A:3723:LEU:HD22	1:A:3871:LEU:HD12	2.02	0.42
1:A:3751:GLN:NE2	1:A:3752:VAL:O	2.53	0.42
2:B:249:TYR:HE1	2:B:313:ASN:ND2	2.17	0.42
2:B:306:ARG:NH1	2:C:340:GLU:OE1	2.38	0.42
2:C:562:ALA:HA	2:C:565:THR:HG22	2.01	0.42
1:A:4091:TRP:O	1:A:4093:LEU:N	2.53	0.41
2:D:480:PHE:O	2:D:484:ILE:HG12	2.20	0.41
1:A:3748:ARG:NH2	1:A:3750:ARG:HD3	2.35	0.41
1:A:3761:ASP:HB2	1:A:3762:PRO:HD2	2.02	0.41
3:A:4401:A1EQ3:C06	3:A:4401:A1EQ3:O01	2.50	0.41
2:C:500:LEU:CD1	2:C:501:HIS:H	2.33	0.41
2:C:519:VAL:O	2:C:522:ILE:HG22	2.20	0.41
1:A:3801:ASP:OD1	1:A:3802:LEU:HD23	2.21	0.41
1:A:4109:ARG:HA	1:A:4109:ARG:HD3	1.84	0.41
1:A:3931:LEU:O	2:D:222:ARG:NH2	2.54	0.41
2:B:379:HIS:CE1	2:B:442:LEU:HD22	2.55	0.41
1:A:4042:GLN:HE21	1:A:4043:LEU:HD12	1.85	0.41
2:B:336:ASP:OD1	2:B:336:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:ASP:OD1	2:B:355:ARG:N	2.53	0.41
2:B:673:LEU:HD12	2:B:673:LEU:HA	1.90	0.41
2:C:510:LEU:O	2:C:514:ILE:HG13	2.20	0.41
2:C:493:LEU:O	2:C:497:ILE:HG12	2.21	0.41
1:A:3873:PHE:CE1	1:A:3879:ALA:HB2	2.55	0.41
1:A:3287:LEU:HD21	1:A:3337:TYR:CG	2.56	0.41
1:A:3996:PHE:HD1	2:B:610:ALA:HB1	1.86	0.41
1:A:3276:THR:O	1:A:3278:ILE:HG22	2.21	0.41
1:A:3930:VAL:O	1:A:3931:LEU:HB2	2.20	0.41
2:C:600:PHE:CE1	2:C:675:MET:HG2	2.56	0.41
1:A:3260:LYS:HB3	1:A:3260:LYS:HE3	1.95	0.41
2:B:636:GLN:O	2:B:640:ILE:HG12	2.20	0.41
2:C:397:ARG:HH12	2:C:541:ASP:HB3	1.85	0.40
1:A:3261:HIS:CE1	1:A:3263:TRP:HB2	2.55	0.40
2:B:646:PHE:HB3	2:B:661:PHE:CD2	2.57	0.40
2:B:673:LEU:HD11	2:C:670:PHE:CE1	2.56	0.40
1:A:3855:THR:OG1	1:A:3856:ARG:N	2.55	0.40
2:C:224:LEU:O	2:C:228:LEU:HD23	2.22	0.40
2:D:229:LEU:O	2:D:233:VAL:HG23	2.22	0.40
2:D:531:ASN:C	2:D:554:TRP:HE1	2.28	0.40
1:A:3722:GLU:C	1:A:3725:PRO:HD2	2.47	0.40
1:A:3781:TYR:HD2	1:A:3786:GLU:HB2	1.87	0.40
2:D:480:PHE:HE2	2:D:522:ILE:HD11	1.86	0.40
1:A:3287:LEU:HD21	1:A:3337:TYR:CD1	2.56	0.40
1:A:3899:LEU:N	1:A:3900:PRO:HD2	2.37	0.40
1:A:4023:LEU:HB3	1:A:4024:PRO:HD3	2.03	0.40
2:C:489:VAL:O	2:C:492:ILE:HG22	2.21	0.40
2:C:623:VAL:O	2:C:624:ASP:OD1	2.39	0.40
2:D:427:SER:HA	2:D:437:CYS:O	2.21	0.40
2:D:648:GLU:HA	2:D:651:GLU:HB3	2.03	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	747/1261 (59%)	676 (90%)	68 (9%)	3 (0%)	30	58
2	B	472/1007 (47%)	439 (93%)	33 (7%)	0	100	100
2	C	463/1007 (46%)	439 (95%)	23 (5%)	1 (0%)	43	70
2	D	470/1007 (47%)	428 (91%)	42 (9%)	0	100	100
All	All	2152/4282 (50%)	1982 (92%)	166 (8%)	4 (0%)	44	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3307	TYR
2	C	375	ASN
1	A	3754	LEU
1	A	4092	ALA

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	521/1041 (50%)	521 (100%)	0	100	100
2	B	431/860 (50%)	431 (100%)	0	100	100
2	C	422/860 (49%)	422 (100%)	0	100	100
2	D	212/860 (25%)	212 (100%)	0	100	100
All	All	1586/3621 (44%)	1586 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3751	GLN
1	A	3789	HIS

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Mol	Chain	Res	Type
2	B	547	ASN
2	B	636	GLN
2	B	681	ASN
2	C	313	ASN
2	C	323	GLN
2	C	501	HIS
2	C	547	ASN
2	C	585	GLN
2	C	622	GLN
2	C	681	ASN
2	D	636	GLN
2	D	674	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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1002	2	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	B	1003	2	14,14,15	0.48	0	17,19,21	1.35	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1003	2	14,14,15	0.94	1 (7%)	17,19,21	1.24	1 (5%)
3	A1EQ3	A	4401	-	33,33,33	7.37	18 (54%)	49,51,51	2.37	16 (32%)
4	NAG	B	1002	2	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	B	1001	2	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	C	1001	-	14,14,15	0.30	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1003	2	-	6/6/23/26	0/1/1/1
4	NAG	C	1003	2	-	4/6/23/26	0/1/1/1
3	A1EQ3	A	4401	-	-	3/12/73/73	0/4/4/4
4	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1001	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1001	-	-	4/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4401	A1EQ3	C06-C14	22.70	1.78	1.53
3	A	4401	A1EQ3	C19-C17	17.71	1.61	1.33
3	A	4401	A1EQ3	C09-C04	-15.47	1.27	1.54
3	A	4401	A1EQ3	C10-C07	14.79	1.79	1.56
3	A	4401	A1EQ3	C06-C07	-12.79	1.29	1.53
3	A	4401	A1EQ3	O01-C14	-8.11	1.28	1.43
3	A	4401	A1EQ3	C11-C13	7.70	1.75	1.54
3	A	4401	A1EQ3	C04-C08	6.90	1.67	1.55
3	A	4401	A1EQ3	C15-C08	-6.89	1.42	1.54
3	A	4401	A1EQ3	C11-C05	5.50	1.65	1.54
3	A	4401	A1EQ3	C09-C12	4.36	1.62	1.53
3	A	4401	A1EQ3	C12-C07	4.16	1.60	1.53
3	A	4401	A1EQ3	C10-C17	-3.33	1.46	1.52
3	A	4401	A1EQ3	C21-C24	-3.31	1.46	1.52
4	C	1003	NAG	O5-C1	3.18	1.49	1.43
3	A	4401	A1EQ3	C21-C17	2.74	1.57	1.51
3	A	4401	A1EQ3	C06-C05	2.42	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4401	A1EQ3	C23-C15	2.25	1.59	1.54
3	A	4401	A1EQ3	C14-C19	2.12	1.53	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4401	A1EQ3	C14-C19-C17	-7.26	118.58	125.18
3	A	4401	A1EQ3	C21-C17-C19	6.13	125.26	120.70
3	A	4401	A1EQ3	C04-C08-C15	-4.84	112.02	119.50
4	C	1003	NAG	C1-O5-C5	4.66	118.43	112.19
4	B	1003	NAG	C2-N2-C7	4.53	128.97	122.90
3	A	4401	A1EQ3	C08-C04-C05	3.85	104.52	100.10
3	A	4401	A1EQ3	C09-C04-C05	3.78	112.90	107.25
3	A	4401	A1EQ3	C16-C04-C09	-3.77	105.05	110.61
3	A	4401	A1EQ3	C21-C17-C10	-3.68	111.71	116.42
3	A	4401	A1EQ3	C09-C04-C08	3.50	121.75	116.60
3	A	4401	A1EQ3	C16-C04-C05	-3.47	105.39	111.68
3	A	4401	A1EQ3	C18-C10-C07	-3.32	104.34	108.74
3	A	4401	A1EQ3	C12-C07-C10	-3.26	109.06	113.08
3	A	4401	A1EQ3	C16-C04-C08	-3.13	105.99	111.68
3	A	4401	A1EQ3	C11-C05-C06	2.98	122.45	118.36
4	B	1003	NAG	C1-C2-N2	2.21	113.92	110.43
3	A	4401	A1EQ3	C25-C15-C08	-2.18	109.62	112.88
3	A	4401	A1EQ3	C07-C10-C17	2.15	112.80	109.65
3	A	4401	A1EQ3	C20-C10-C07	-2.09	109.31	111.66

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1001	NAG	O7-C7-N2-C2
4	C	1001	NAG	C8-C7-N2-C2
4	B	1001	NAG	C4-C5-C6-O6
4	B	1002	NAG	O5-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	C	1002	NAG	O5-C5-C6-O6
4	B	1002	NAG	C4-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6
4	B	1003	NAG	C4-C5-C6-O6
4	B	1003	NAG	C8-C7-N2-C2
4	B	1003	NAG	O7-C7-N2-C2
4	C	1003	NAG	O5-C5-C6-O6

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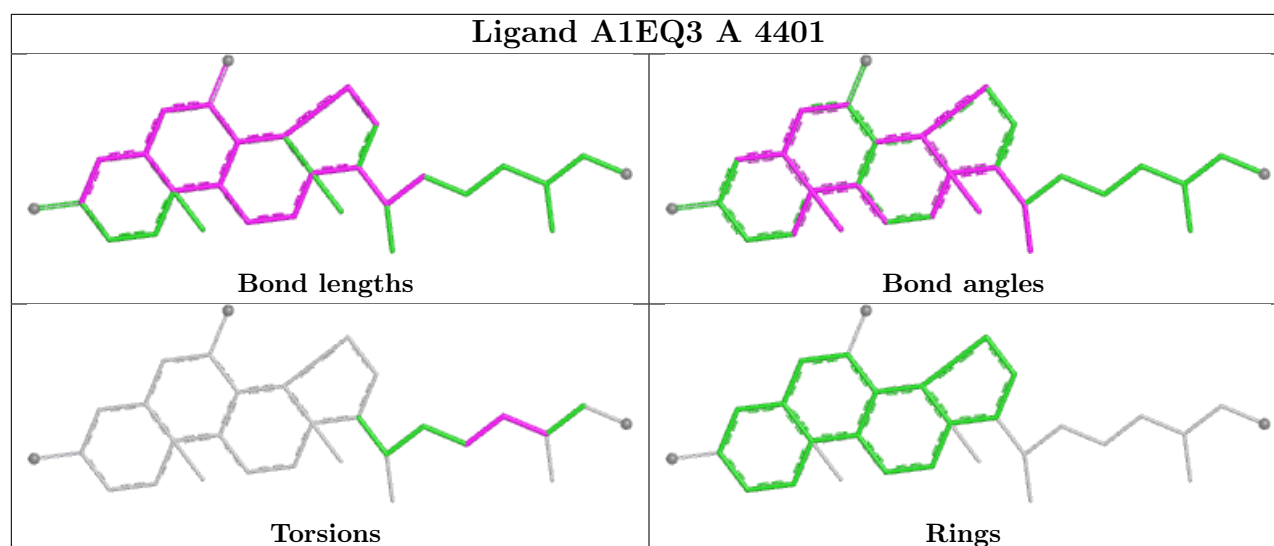
Mol	Chain	Res	Type	Atoms
4	C	1001	NAG	O5-C5-C6-O6
4	C	1002	NAG	C4-C5-C6-O6
3	A	4401	A1EQ3	C26-C27-C28-C30
3	A	4401	A1EQ3	C23-C26-C27-C28
4	C	1003	NAG	C4-C5-C6-O6
4	C	1003	NAG	C1-C2-N2-C7
4	B	1001	NAG	C3-C2-N2-C7
4	C	1003	NAG	C3-C2-N2-C7
3	A	4401	A1EQ3	C26-C27-C28-C29
4	B	1001	NAG	C1-C2-N2-C7
4	B	1003	NAG	C1-C2-N2-C7
4	B	1003	NAG	C3-C2-N2-C7
4	C	1001	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	NAG	1	0
3	A	4401	A1EQ3	13	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.

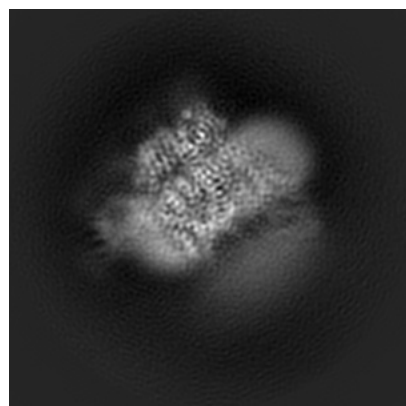
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60222. These allow visual inspection of the internal detail of the map and identification of artifacts.

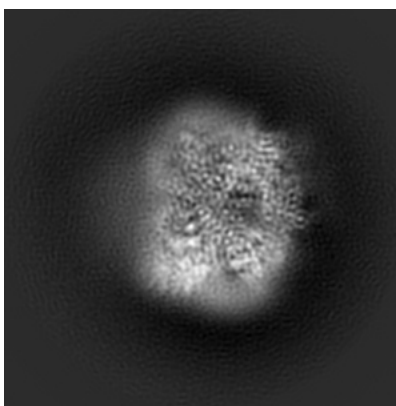
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

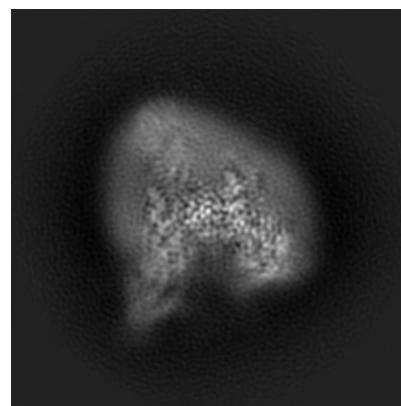
6.1.1 Primary map



X

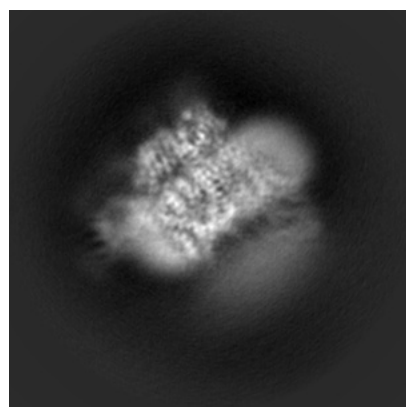


Y

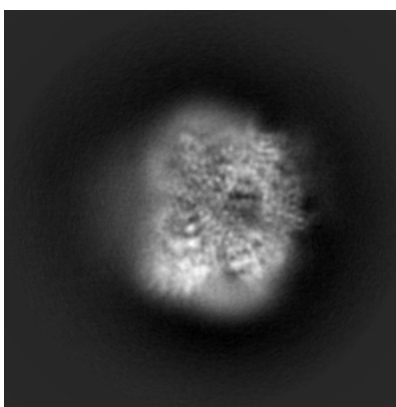


Z

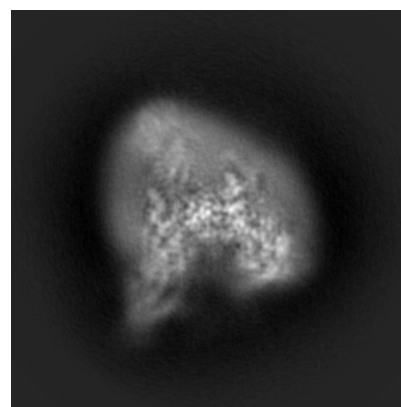
6.1.2 Raw map



X



Y

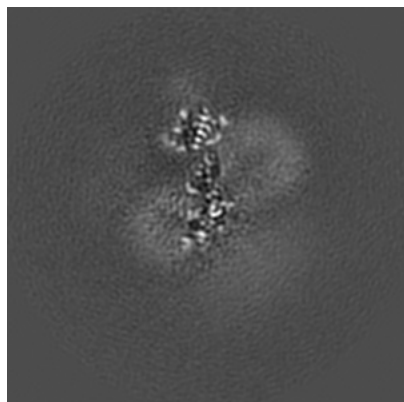


Z

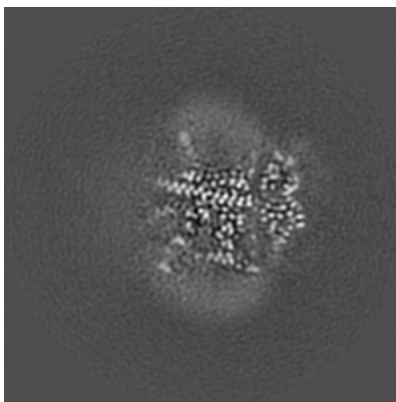
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

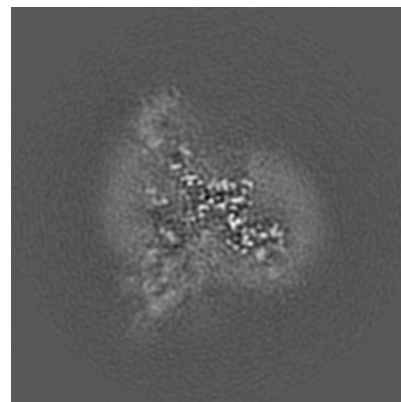
6.2.1 Primary map



X Index: 120

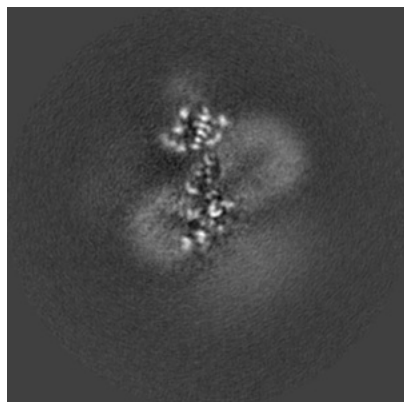


Y Index: 120

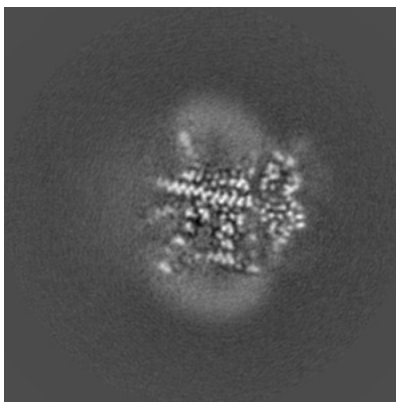


Z Index: 120

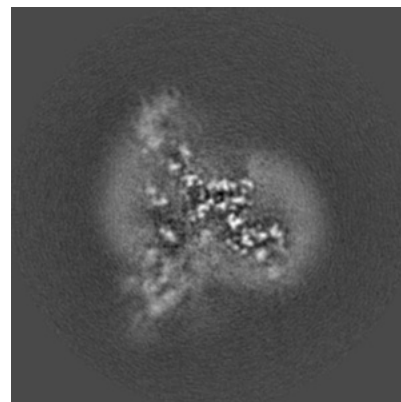
6.2.2 Raw map



X Index: 120



Y Index: 120

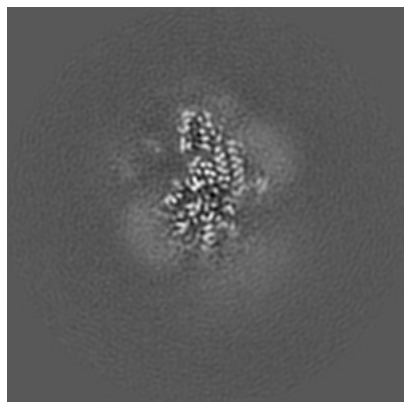


Z Index: 120

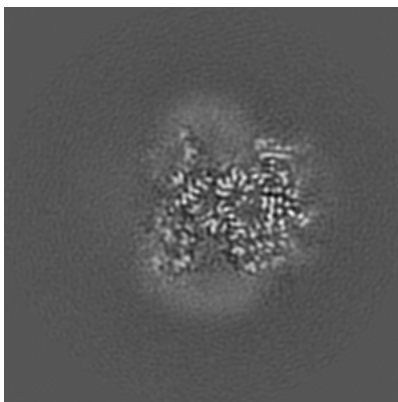
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

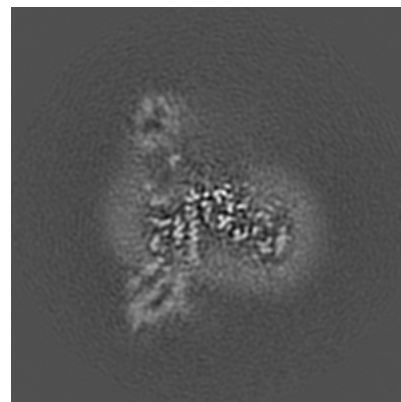
6.3.1 Primary map



X Index: 132

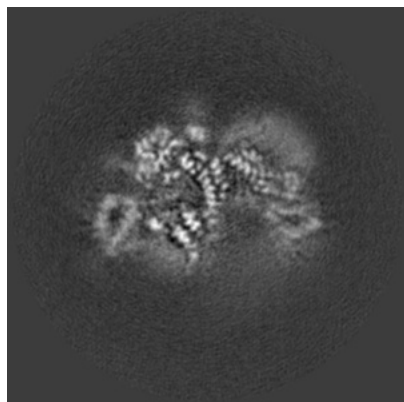


Y Index: 113

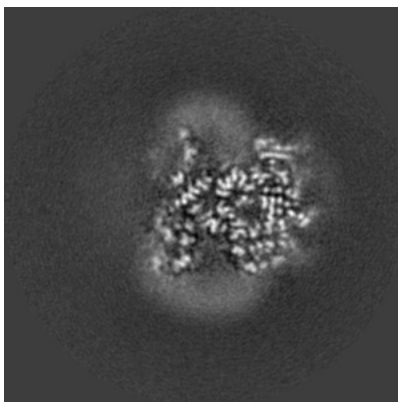


Z Index: 112

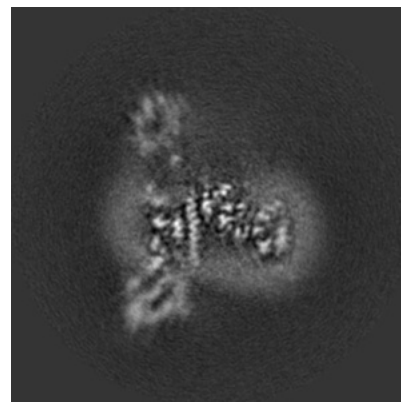
6.3.2 Raw map



X Index: 89



Y Index: 113

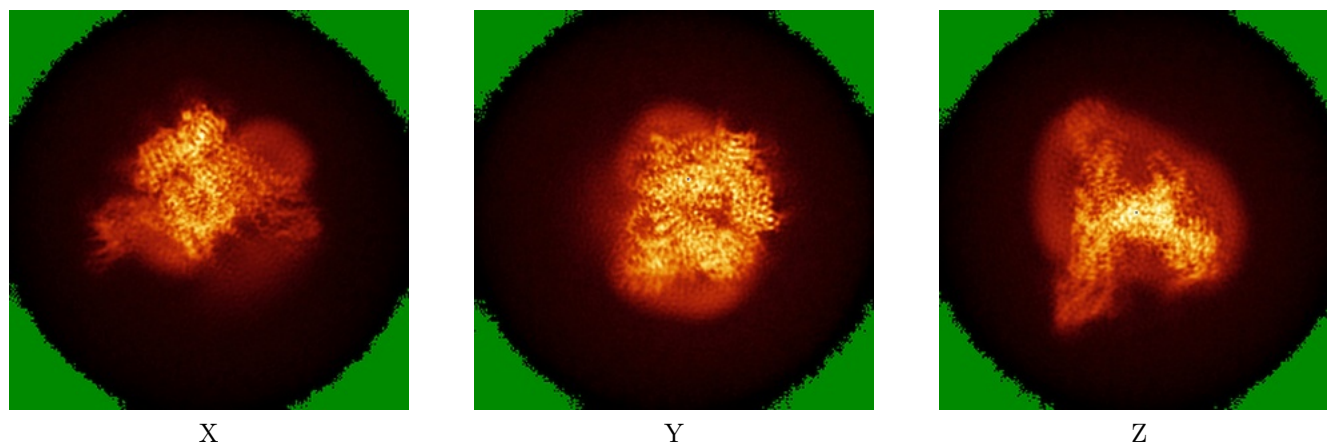


Z Index: 111

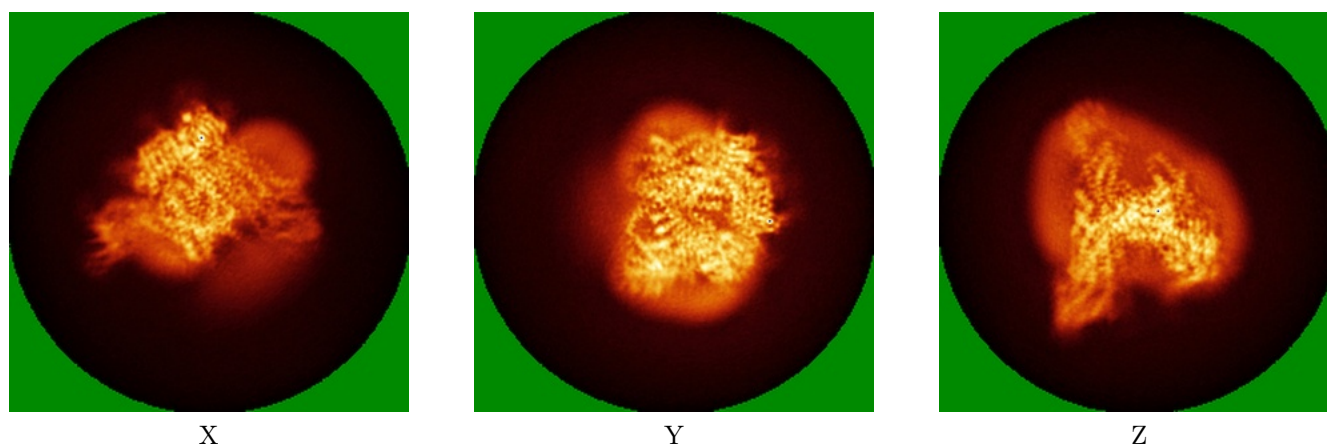
The images above show the largest variance slices of the map in three orthogonal directions.

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.

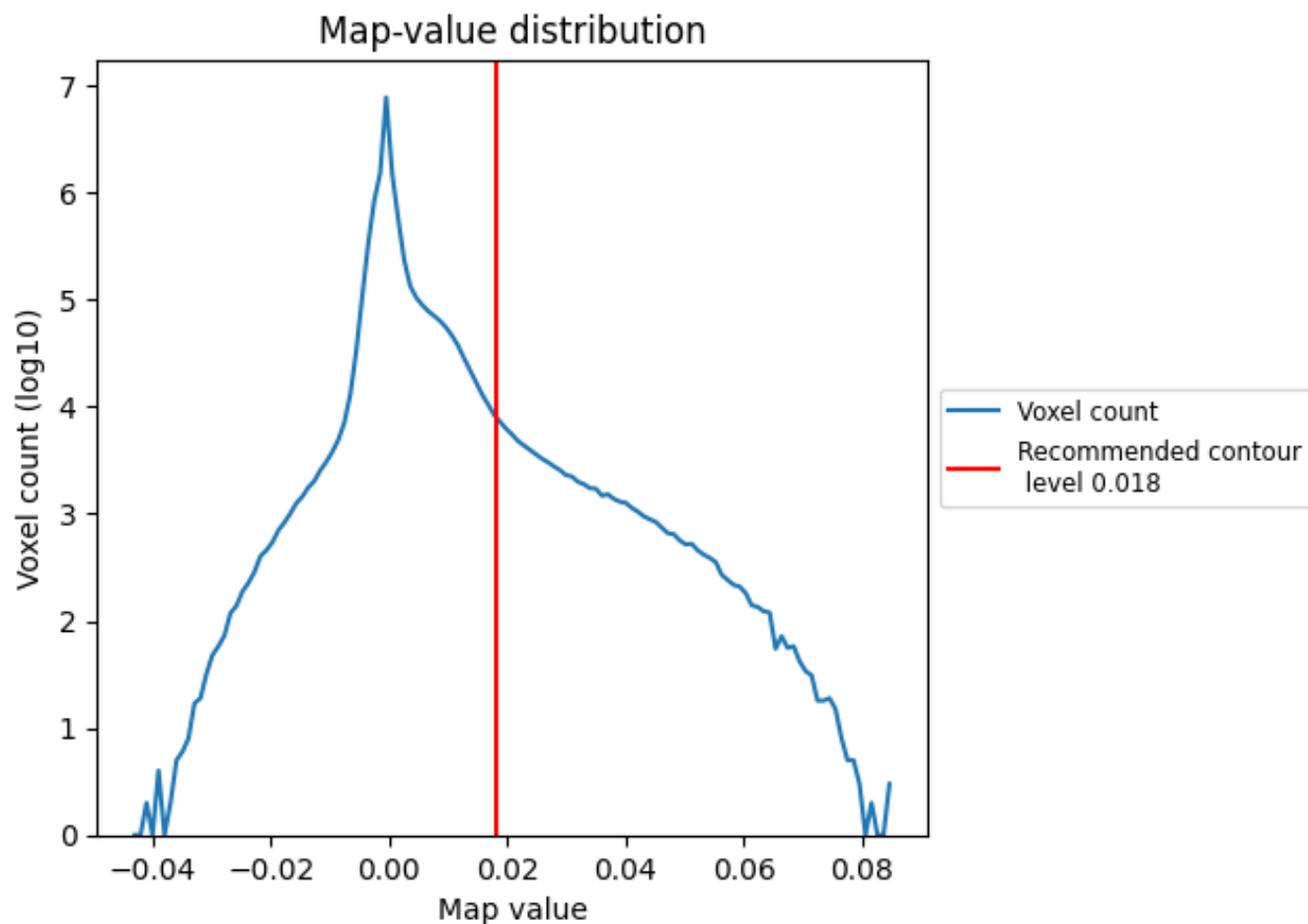
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

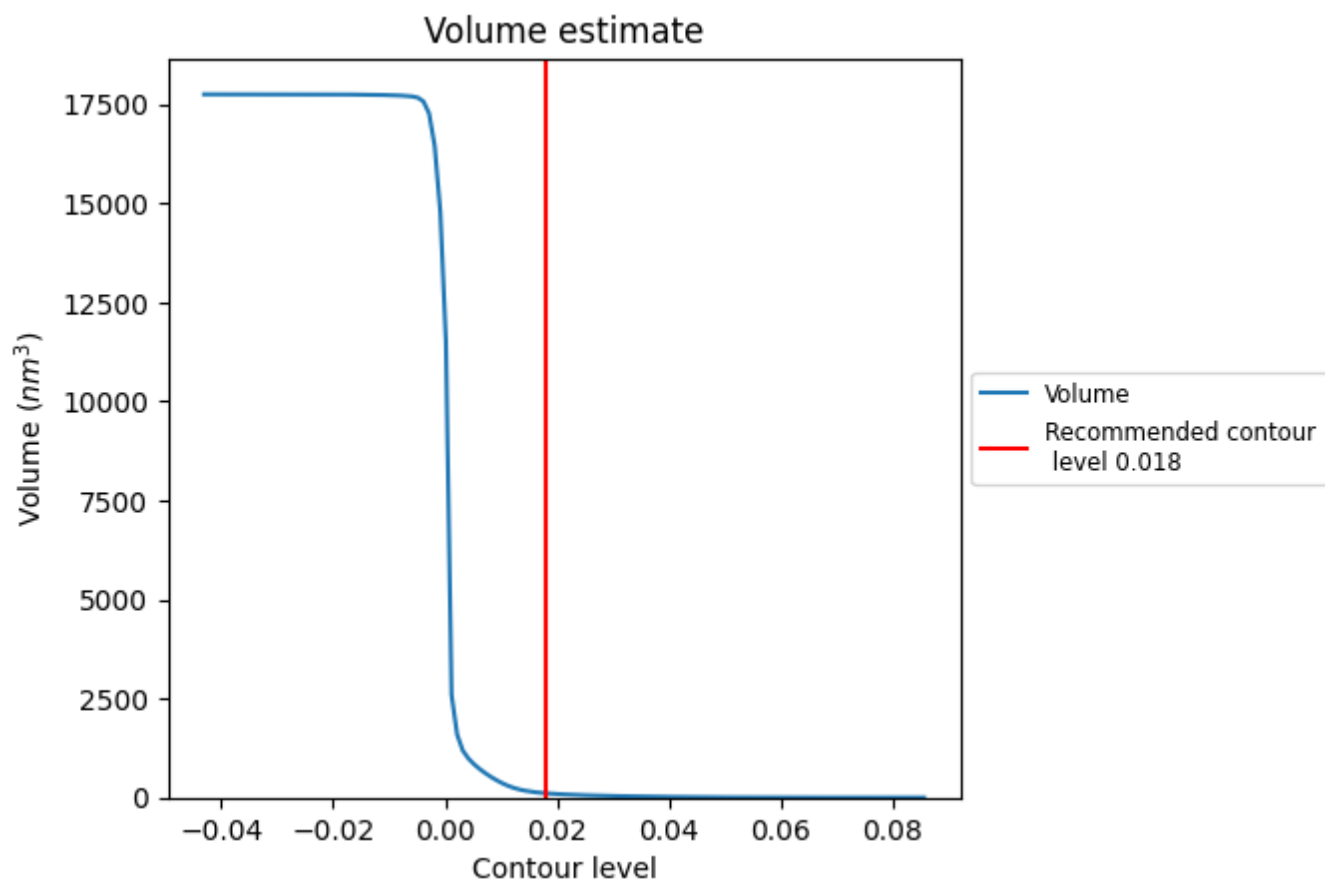
This section contains the results of statistical analysis of the map.

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.

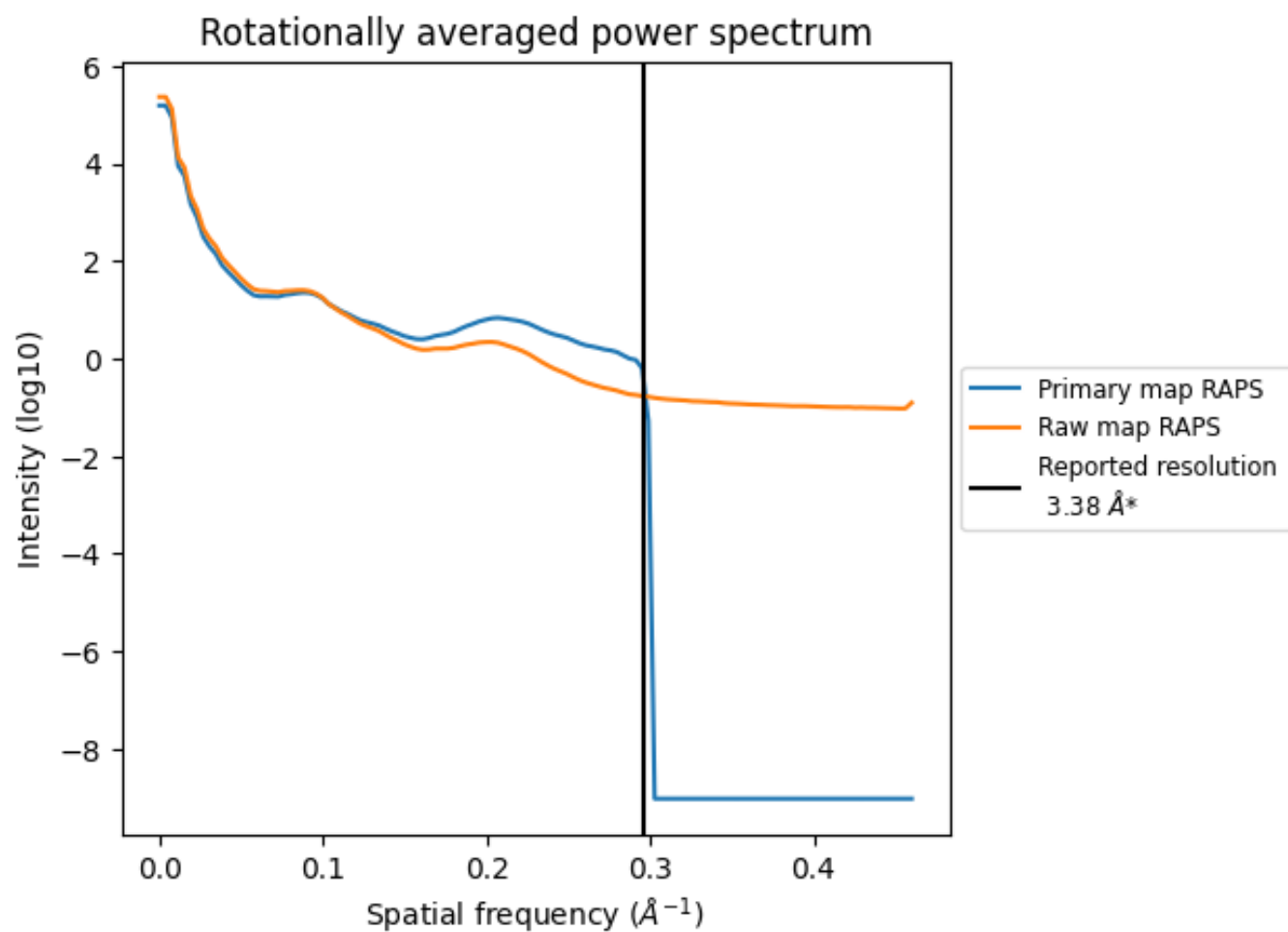
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ

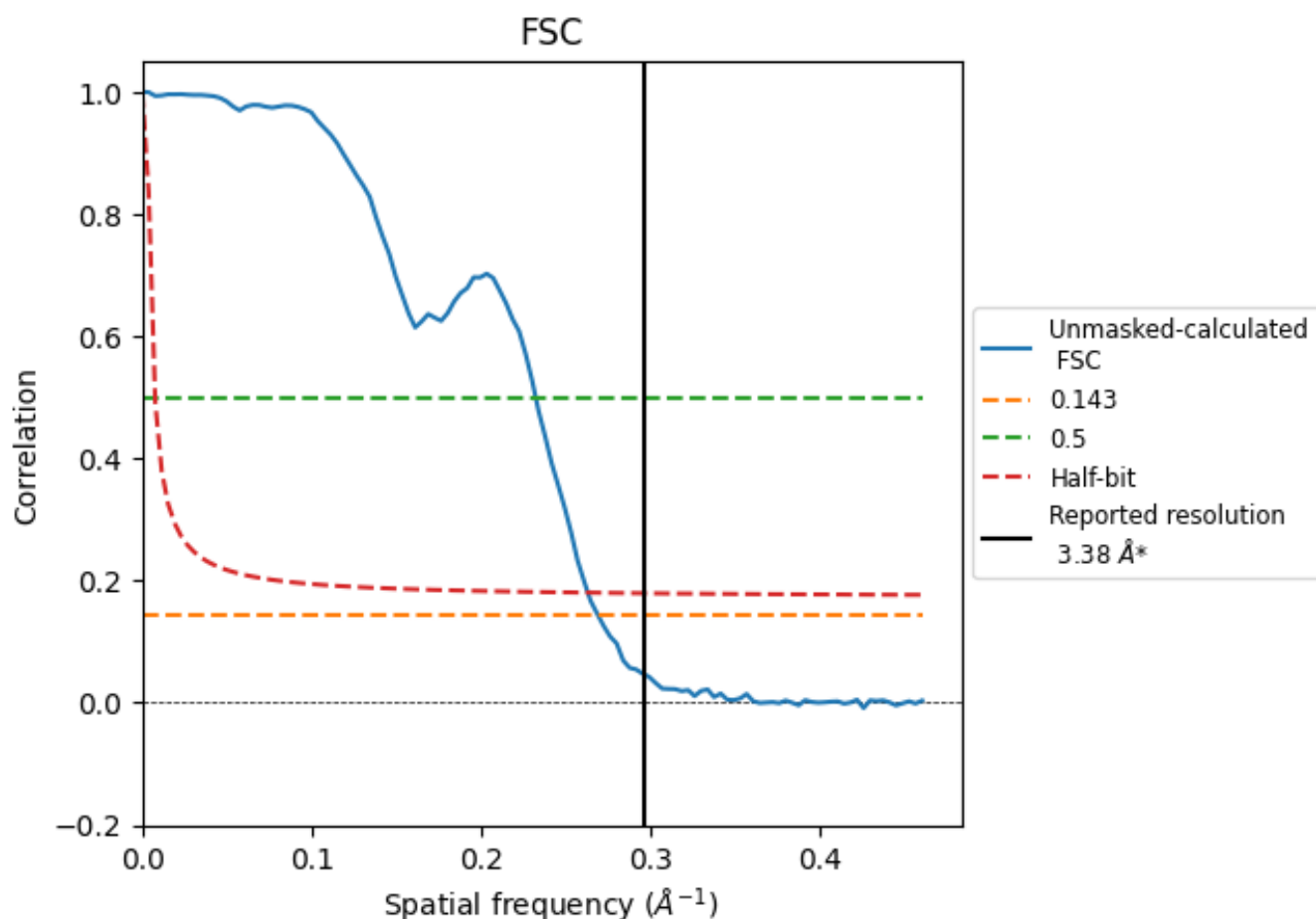


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

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 0.296 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

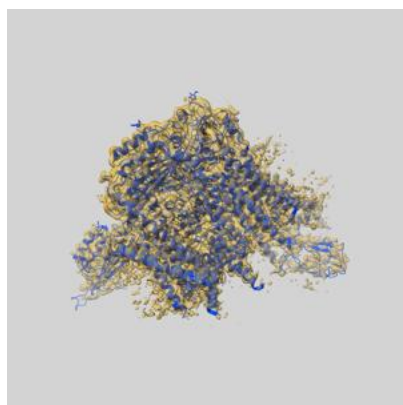
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.31	3.81

*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 3.72 differs from the reported value 3.38 by more than 10 %

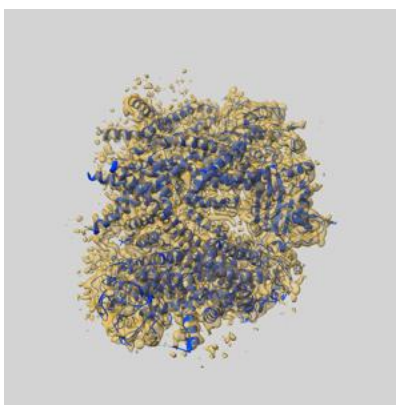
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60222 and PDB model 8ZL8. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

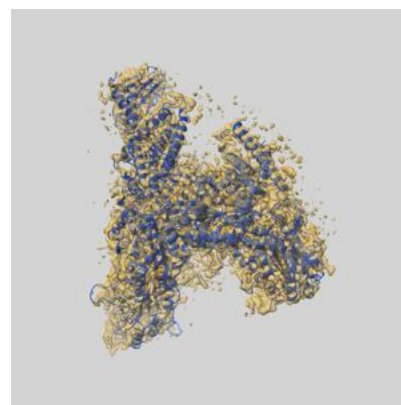
9.1 Map-model overlay [i](#)



X



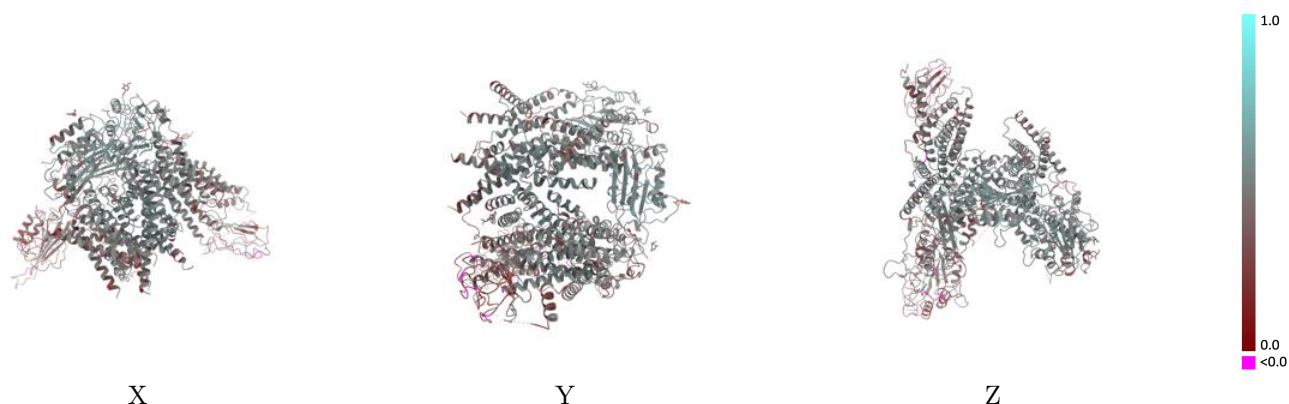
Y



Z

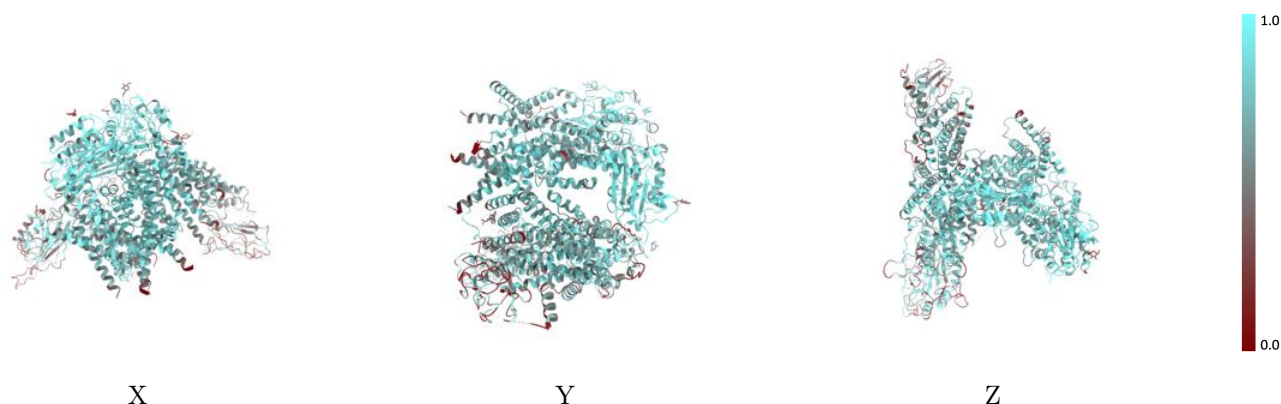
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



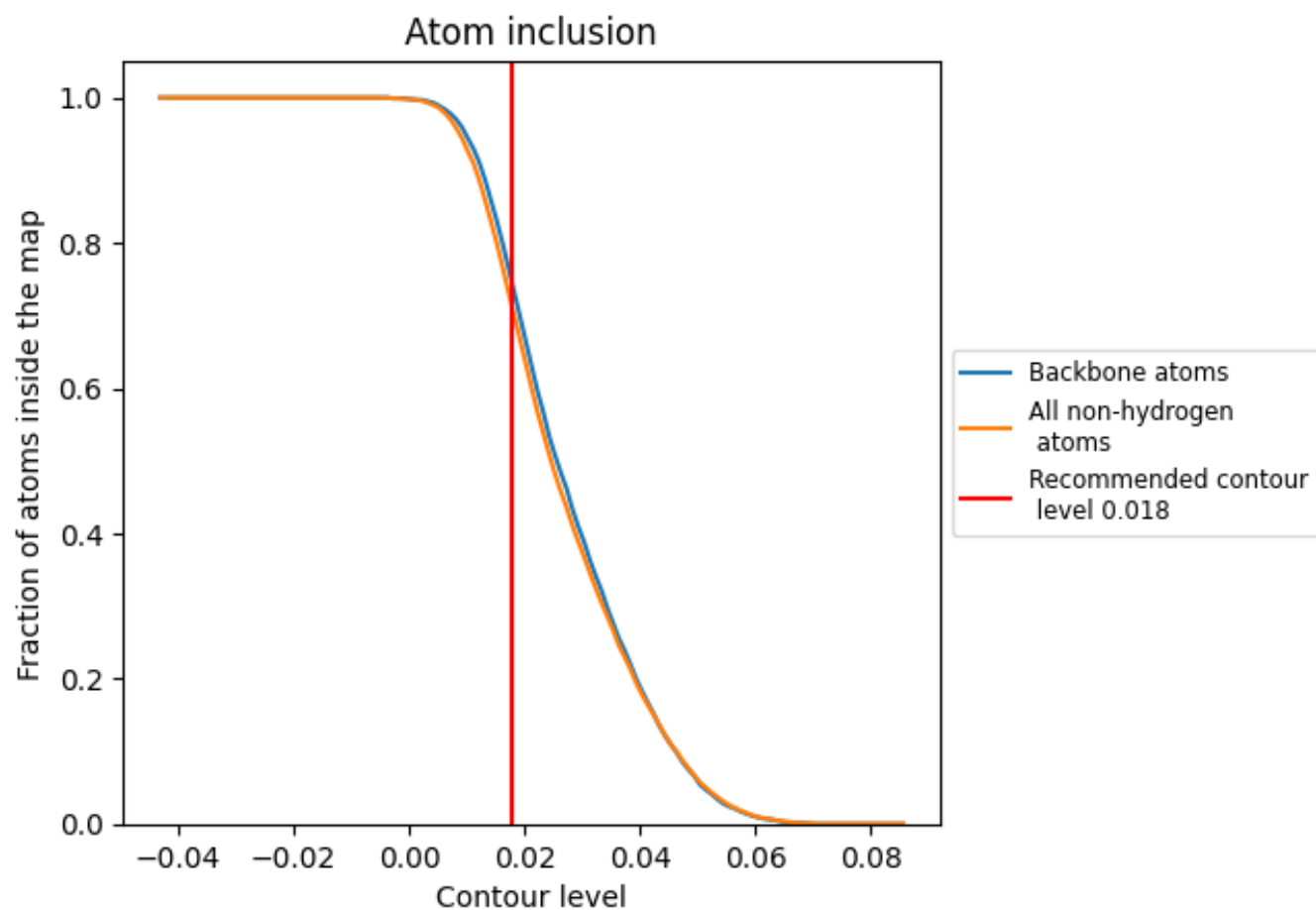
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4500
A	0.6390	0.4310
B	0.7870	0.4970
C	0.7700	0.4780
D	0.6690	0.3910

