



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 09:17 PM UTC

PDB ID : 9SAF / pdb_00009saf
EMDB ID : EMD-54690
Title : Ternary PROTAC-mediated complex of BRD4-BD1/CRBN/DDB1 and JQ1-AcQ bifunctional degrader
Authors : Peter, D.; Fischer, G.; Arce Solano, S.; Kessler, D.
Deposited on : 2025-08-07
Resolution : 2.55 Å(reported)

This is a wwPDB EM Validation Summary 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

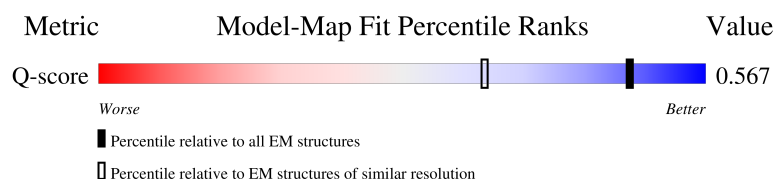
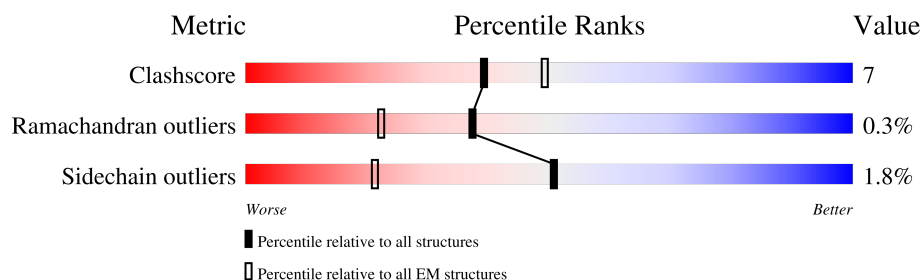
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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	7475 (2.05 - 3.05)

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	836	 5% 88% 11% •
2	B	442	 7% 73% 13% • 13%
3	C	127	 9% 43% 52% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1JM8	B	502	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10773 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	824	Total	C	N	O	S	0	0
			6470	4095	1091	1249	35		

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	TRP	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	TRP	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	TRP	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	GLY	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	GLN	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	ARG	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	HIS	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	PHE	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	LYS	deletion	UNP Q16531
A	?	-	GLU	deletion	UNP Q16531
A	?	-	VAL	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q16531
A	?	-	MET	deletion	UNP Q16531
A	?	-	CYS	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	TYR	deletion	UNP Q16531
A	?	-	PRO	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531
A	?	-	SER	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	ALA	deletion	UNP Q16531
A	?	-	ASN	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	LEU	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	THR	deletion	UNP Q16531
A	?	-	ILE	deletion	UNP Q16531
A	?	-	ASP	deletion	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	385	Total	C	N	O	S	0	0
			3106	1980	533	569	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			1056	684	173	192	7		

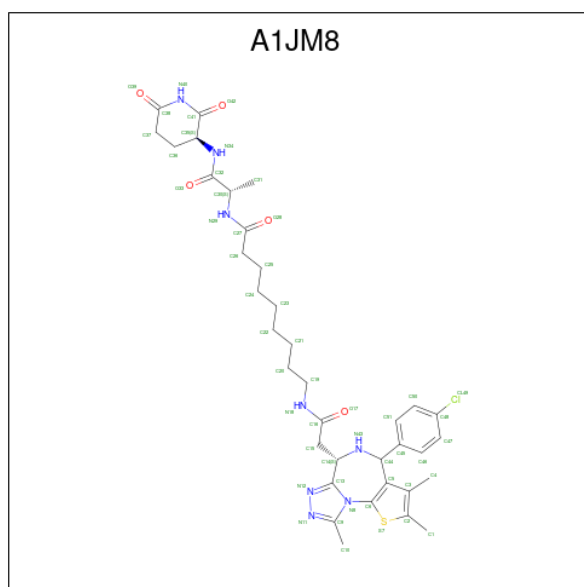
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	42	SER	-	expression tag	UNP O60885
C	43	MET	-	expression tag	UNP O60885

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is {N}-[(2 {S})-1-[[[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]amino]-1-oxidanylidene-propan-2-yl]-9-[2-[(9 {S})-7-(4-chlorophenyl)-4,5,13-trimethyl-3-thia-1,8,11,12-tetrazatricyclo[8.3.0.0[^]{2,6}]trideca-2(6),4,10,12-tetraen-9-yl]ethanoylamino]nonanamide (CCD ID: A1JM8) (formula: C₃₆H₄₇ClN₈O₅S).



Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	Cl	N	O	S	0
			51	36	1	8	5	1	

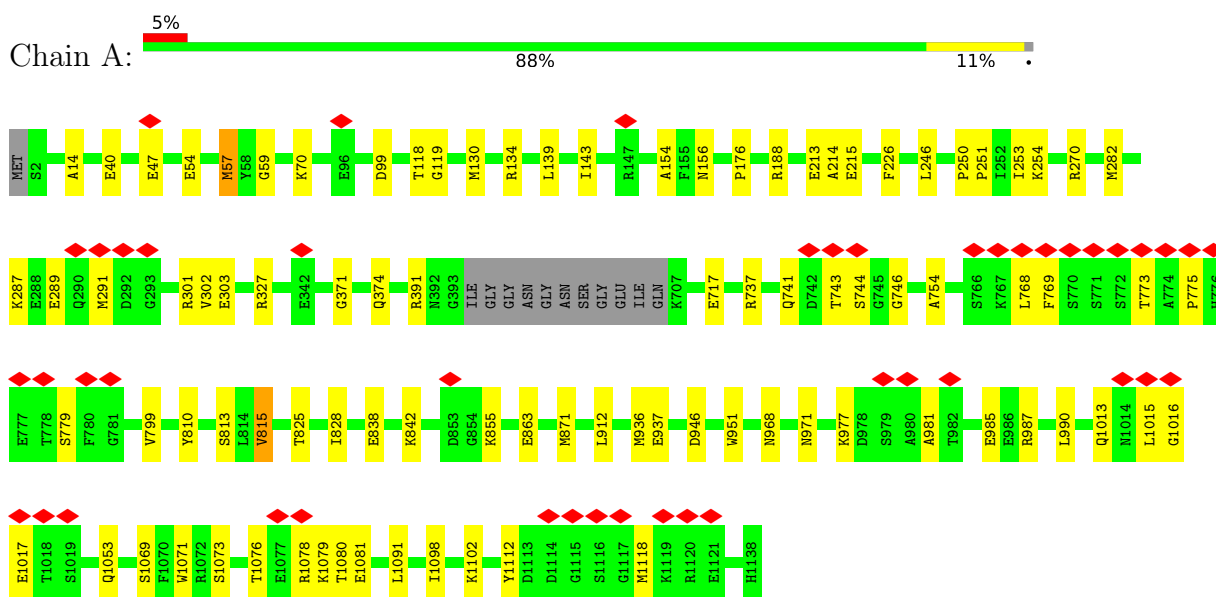
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	86	Total	O	0
			86	86	
6	B	3	Total	O	0
			3	3	

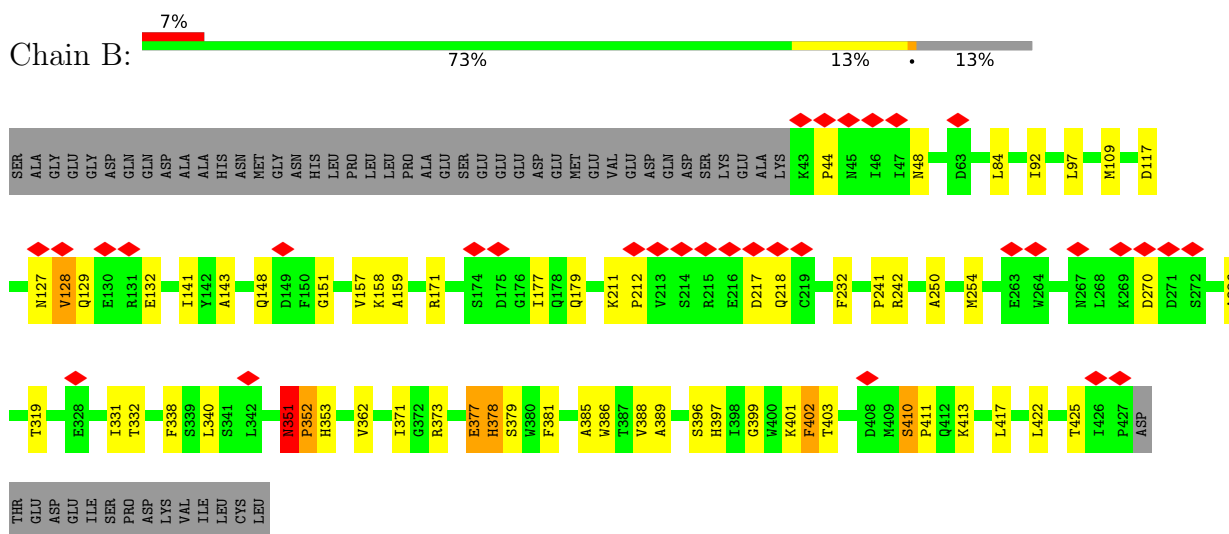
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

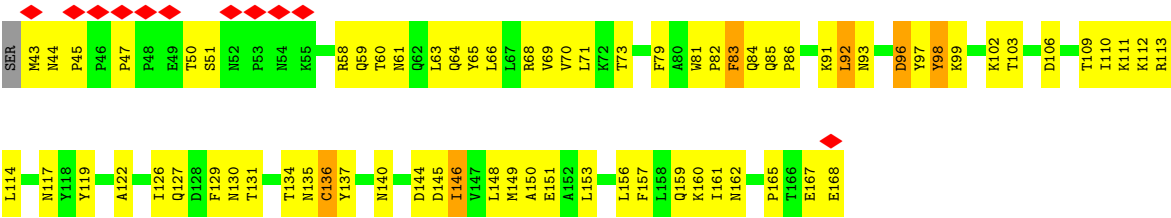
• Molecule 1: DNA damage-binding protein 1



• Molecule 2: Protein cereblon



• Molecule 3: Bromodomain-containing protein 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158212	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	48.590	Depositor
Minimum map value	-31.691	Depositor
Average map value	0.027	Depositor
Map value standard deviation	1.084	Depositor
Recommended contour level	8	Depositor
Map size (Å)	287.616, 287.616, 287.616	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.749, 0.749, 0.749	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: ZN, A1JM8

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	0.11	0/6587	0.28	0/8909
2	B	0.38	2/3181 (0.1%)	0.63	6/4316 (0.1%)
3	C	0.52	0/1086	0.94	7/1476 (0.5%)
All	All	0.28	2/10854 (0.0%)	0.50	13/14701 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	379	SER	CA-CB	-5.60	1.45	1.53
2	B	396	SER	CA-CB	-5.40	1.45	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	LYS	CB-CA-C	-14.98	86.61	110.74
2	B	351	ASN	CB-CA-C	-8.31	93.20	110.31
2	B	352	PRO	N-CA-CB	-7.35	95.84	103.19
2	B	402	PHE	CA-CB-CG	6.89	120.69	113.80
3	C	136	CYS	N-CA-C	-6.11	105.06	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	373	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	A	6470	0	6433	53	0
2	B	3106	0	3101	35	0
3	C	1056	0	1051	67	0
4	B	1	0	0	0	0
5	B	51	0	0	4	0
6	A	86	0	0	0	0
6	B	3	0	0	0	0
All	All	10773	0	10585	154	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.

The worst 5 of 154 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:C:44:ASN:H	3:C:98:TYR:HD2	1.33	0.75
3:C:61:ASN:ND2	3:C:168:GLU:OE1	2.21	0.74
3:C:129:PHE:HD2	3:C:157:PHE:HE2	1.37	0.72
3:C:43:MET:SD	3:C:98:TYR:HB2	2.30	0.72
1:A:985:GLU:N	1:A:985:GLU:OE2	2.24	0.71

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	820/836 (98%)	789 (96%)	31 (4%)	0	100	100
2	B	383/442 (87%)	358 (94%)	23 (6%)	2 (0%)	24	34
3	C	124/127 (98%)	105 (85%)	17 (14%)	2 (2%)	7	9
All	All	1327/1405 (94%)	1252 (94%)	71 (5%)	4 (0%)	37	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	44	PRO
3	C	96	ASP
3	C	144	ASP
2	B	128	VAL

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	719/727 (99%)	708 (98%)	11 (2%)	57	74
2	B	349/398 (88%)	342 (98%)	7 (2%)	48	67
3	C	119/120 (99%)	116 (98%)	3 (2%)	42	60
All	All	1187/1245 (95%)	1166 (98%)	21 (2%)	51	70

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	378	HIS
2	B	413	LYS
3	C	146	ILE
3	C	92	LEU
2	B	410	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18

such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
3	C	116	ASN
3	C	59	GLN
2	B	86	GLN
2	B	276	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 2 ligands modelled in this entry, 1 is 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$
5	A1JM8	B	502	-	51,55,55	1.74	2 (3%)	59,77,77	1.28	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1JM8	B	502	-	1/1/9/14	8/32/61/61	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	A1JM8	C44-C5	-11.62	1.37	1.50
5	B	502	A1JM8	C45-C44	-3.40	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	A1JM8	C5-C44-N43	8.48	125.20	112.45
5	B	502	A1JM8	C14-C15-C16	-2.37	106.59	113.72
5	B	502	A1JM8	C36-C37-C38	-2.21	109.31	113.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	502	A1JM8	C44

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	A1JM8	C20-C21-C22-C23
5	B	502	A1JM8	C22-C23-C24-C25
5	B	502	A1JM8	C24-C25-C26-C27
5	B	502	A1JM8	N18-C19-C20-C21
5	B	502	A1JM8	N43-C14-C15-C16

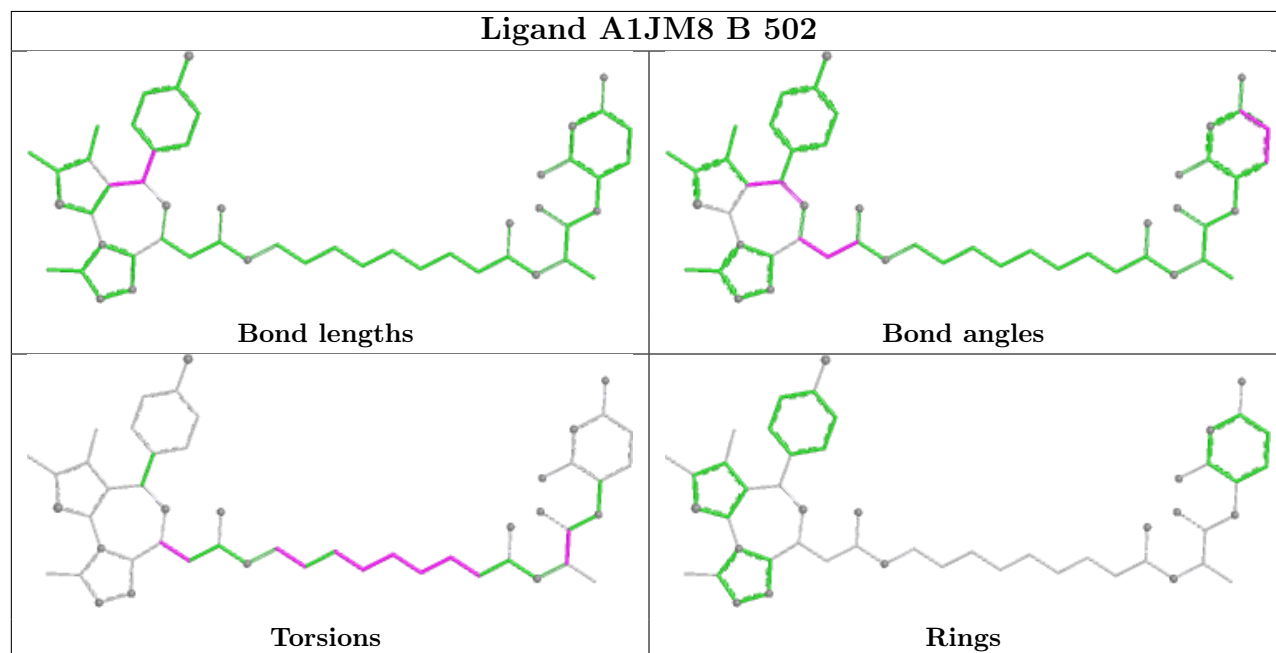
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	A1JM8	4	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.

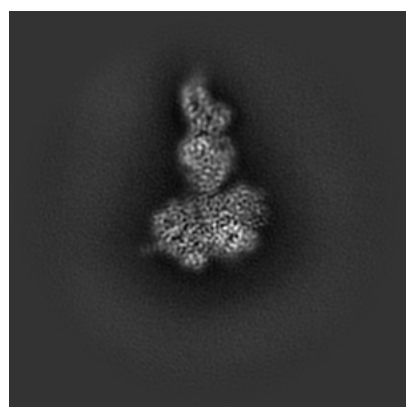
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54690. These allow visual inspection of the internal detail of the map and identification of artifacts.

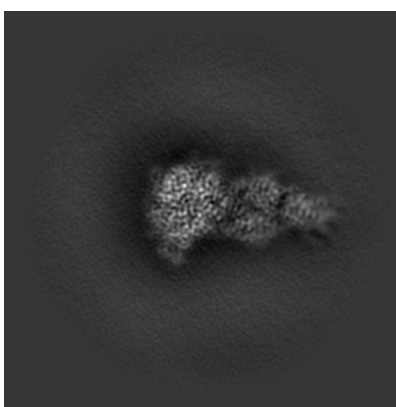
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

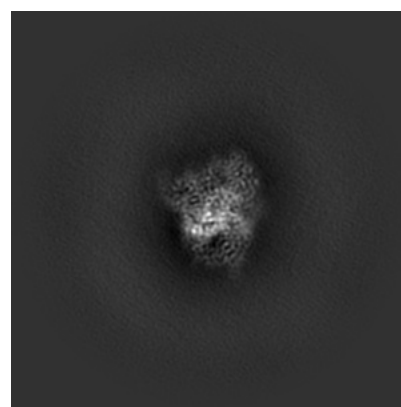
6.1.1 Primary map



X



Y

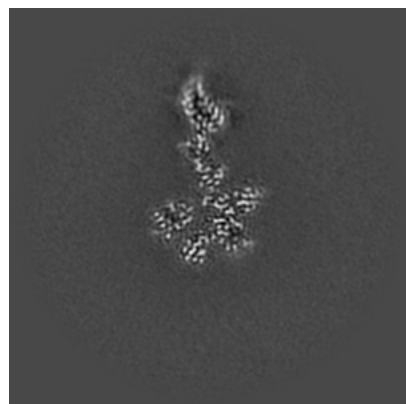


Z

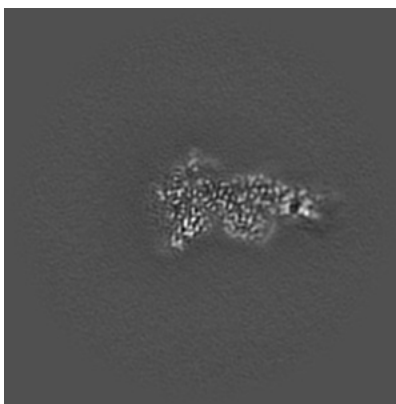
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

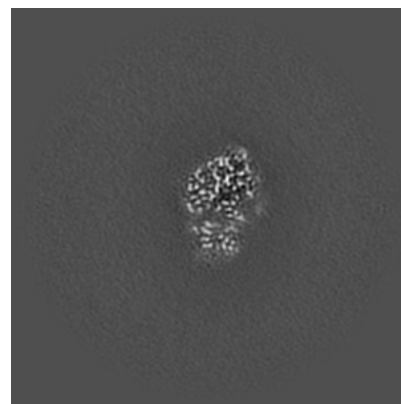
6.2.1 Primary map



X Index: 192



Y Index: 192

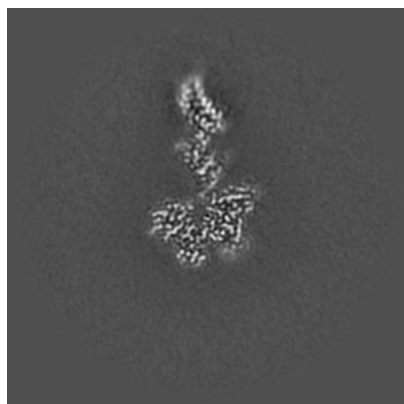


Z Index: 192

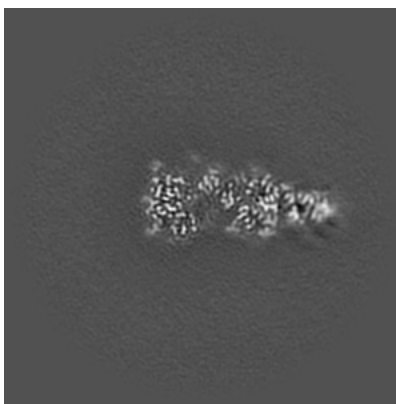
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

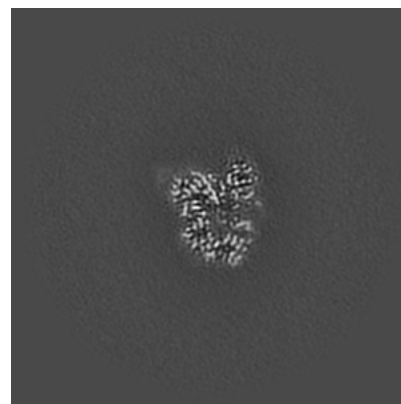
6.3.1 Primary map



X Index: 189



Y Index: 183

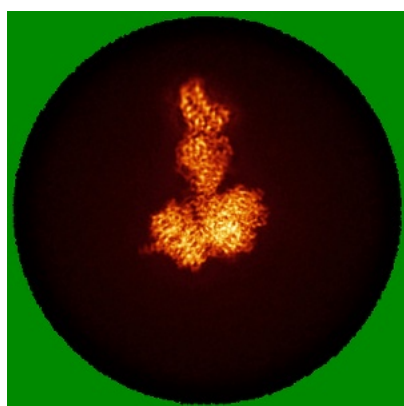


Z Index: 174

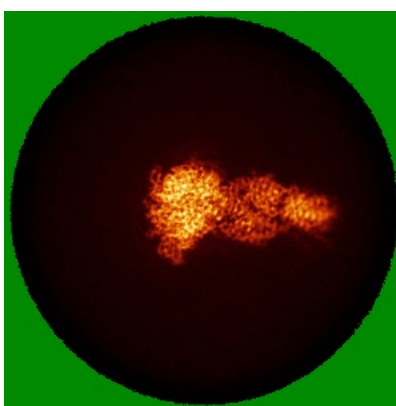
The images above show the largest variance slices of the map in three orthogonal directions.

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

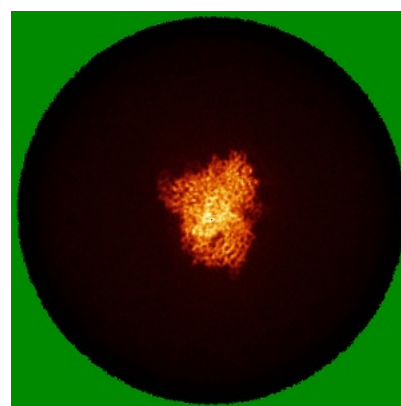
6.4.1 Primary map



X



Y

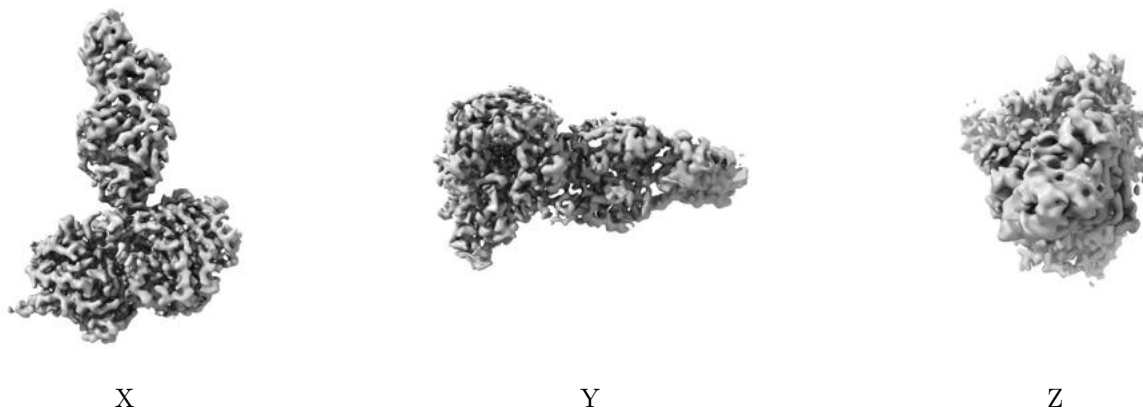


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

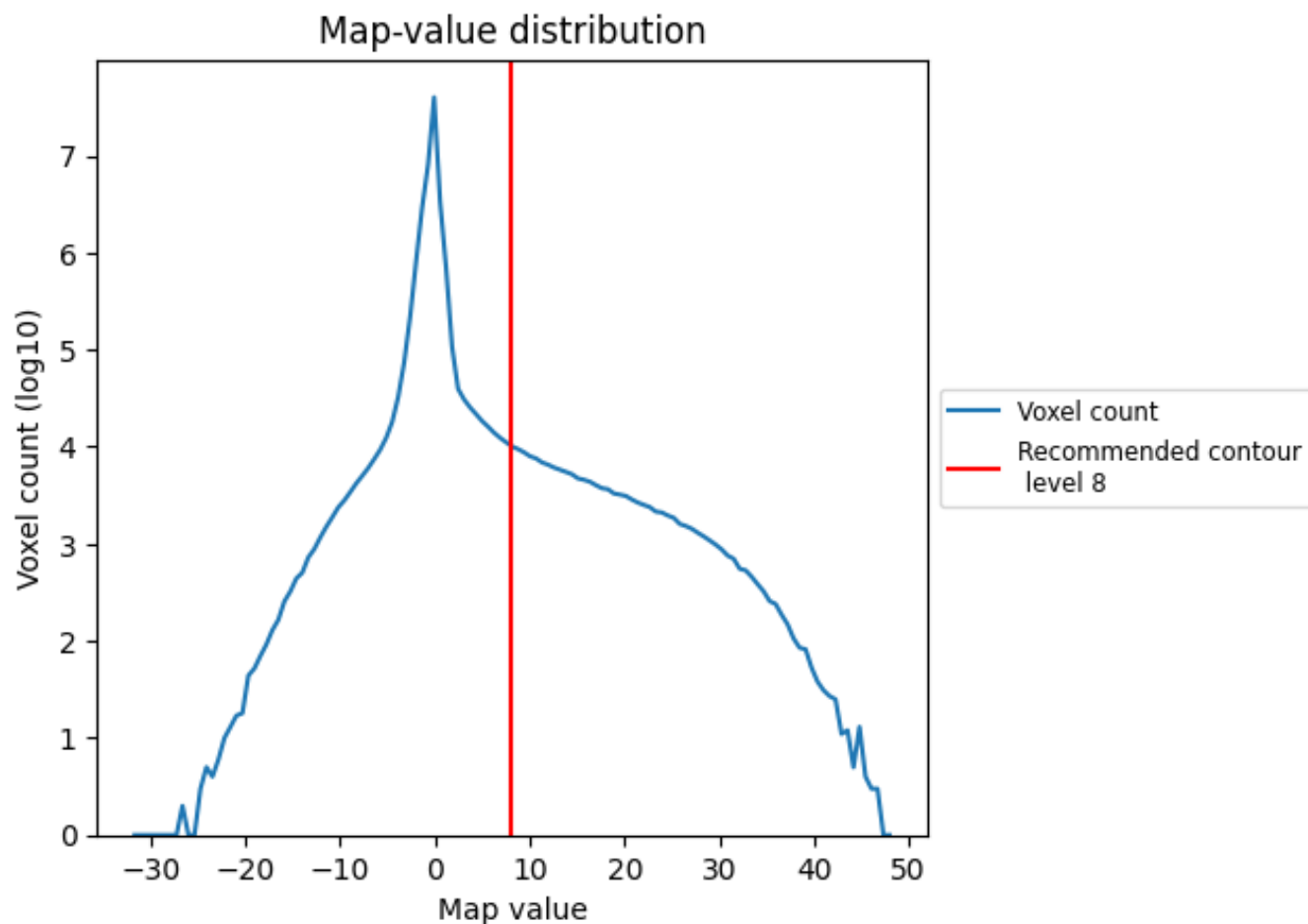
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

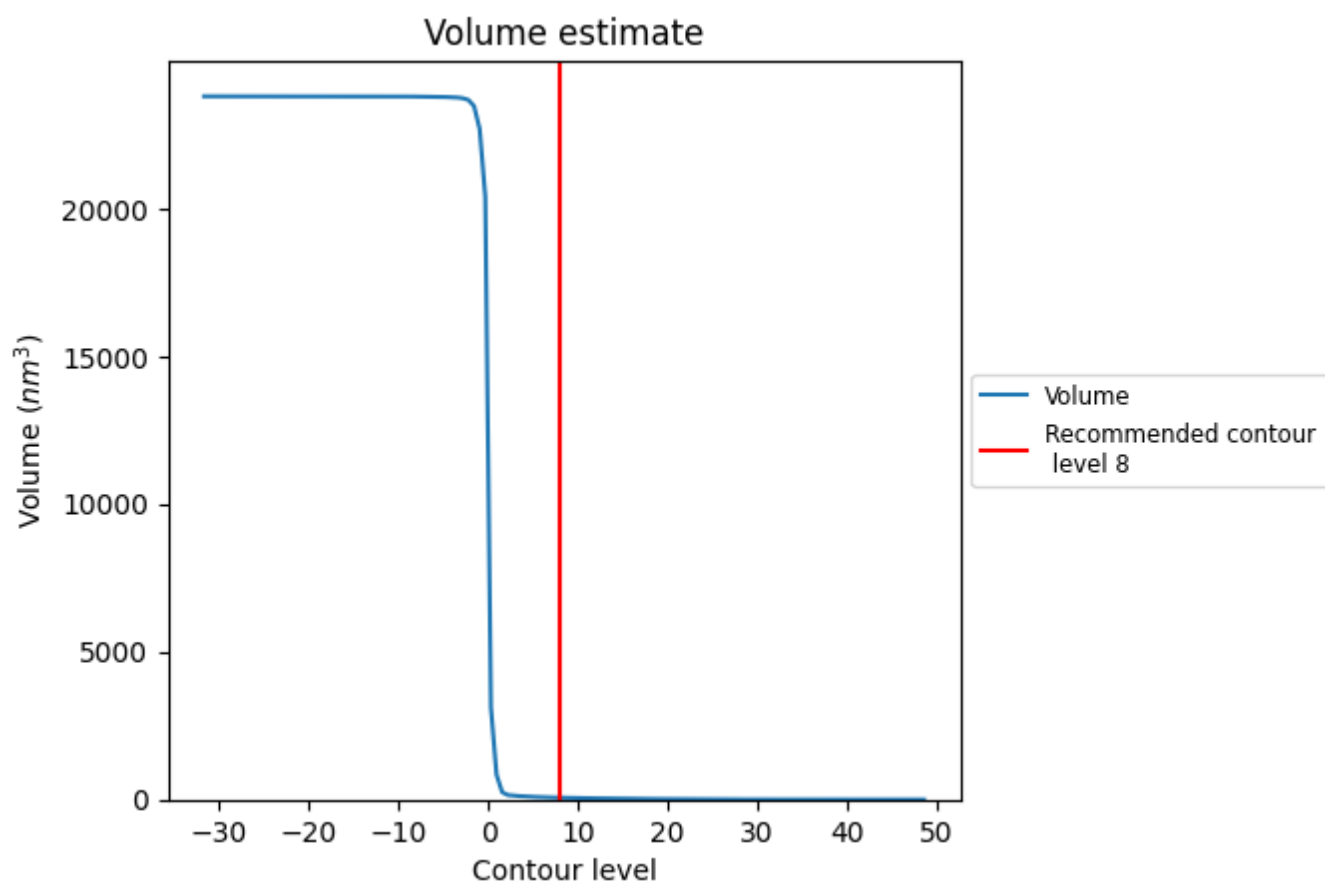
This section contains the results of statistical analysis of the map.

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.

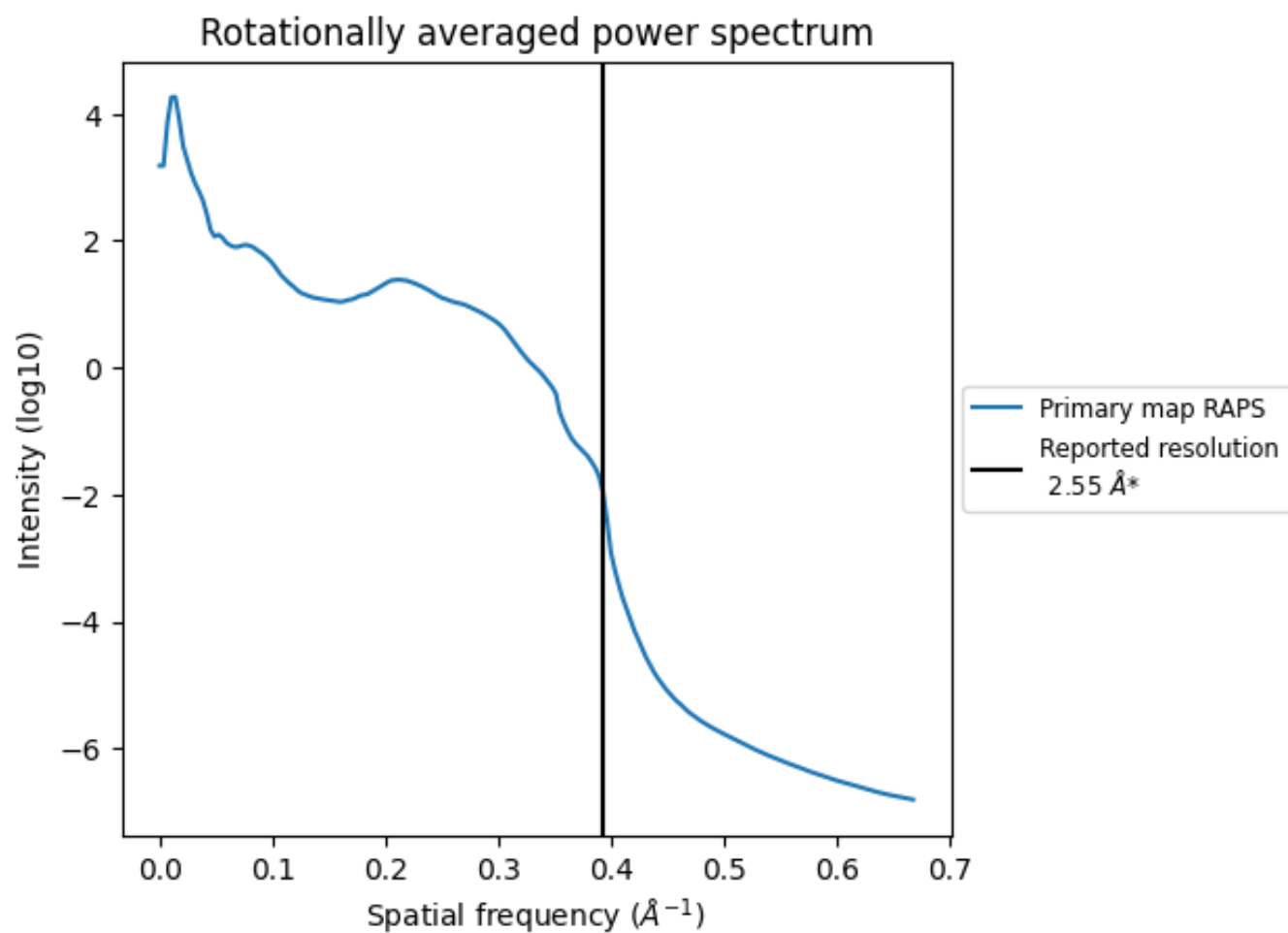
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm³; this corresponds to an approximate mass of 57 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 0.392 Å⁻¹

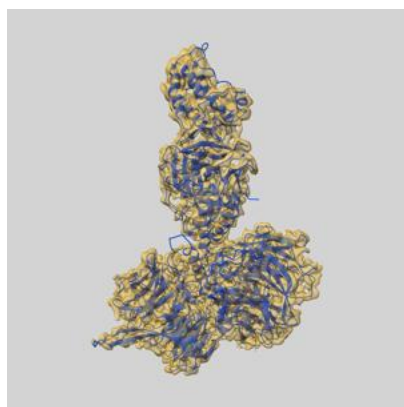
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

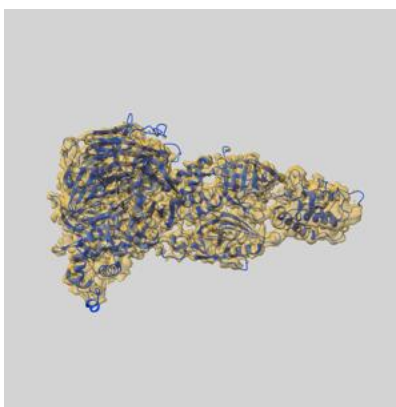
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54690 and PDB model 9SAF. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

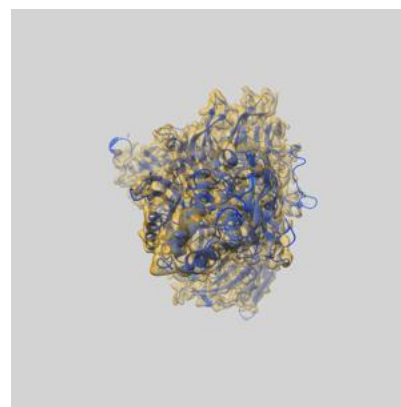
9.1 Map-model overlay [i](#)



X



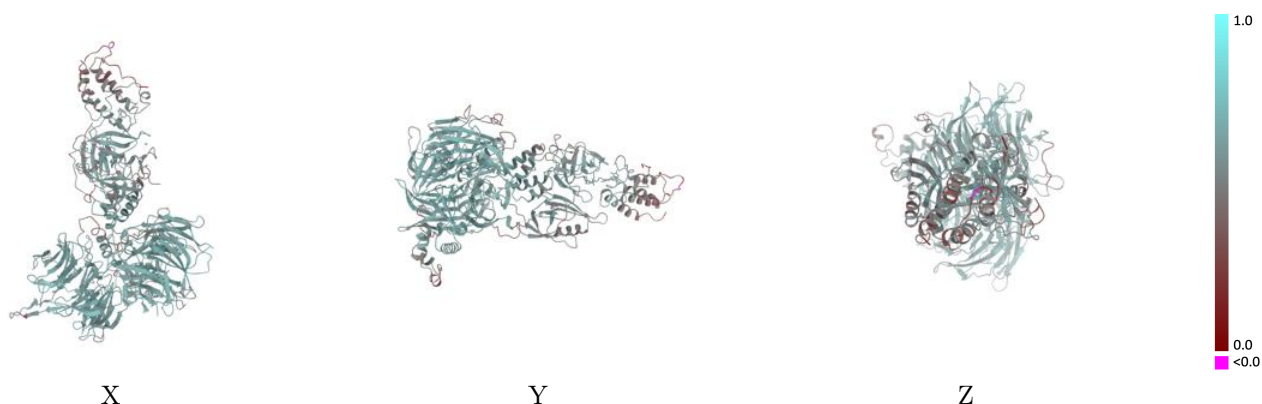
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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](#)



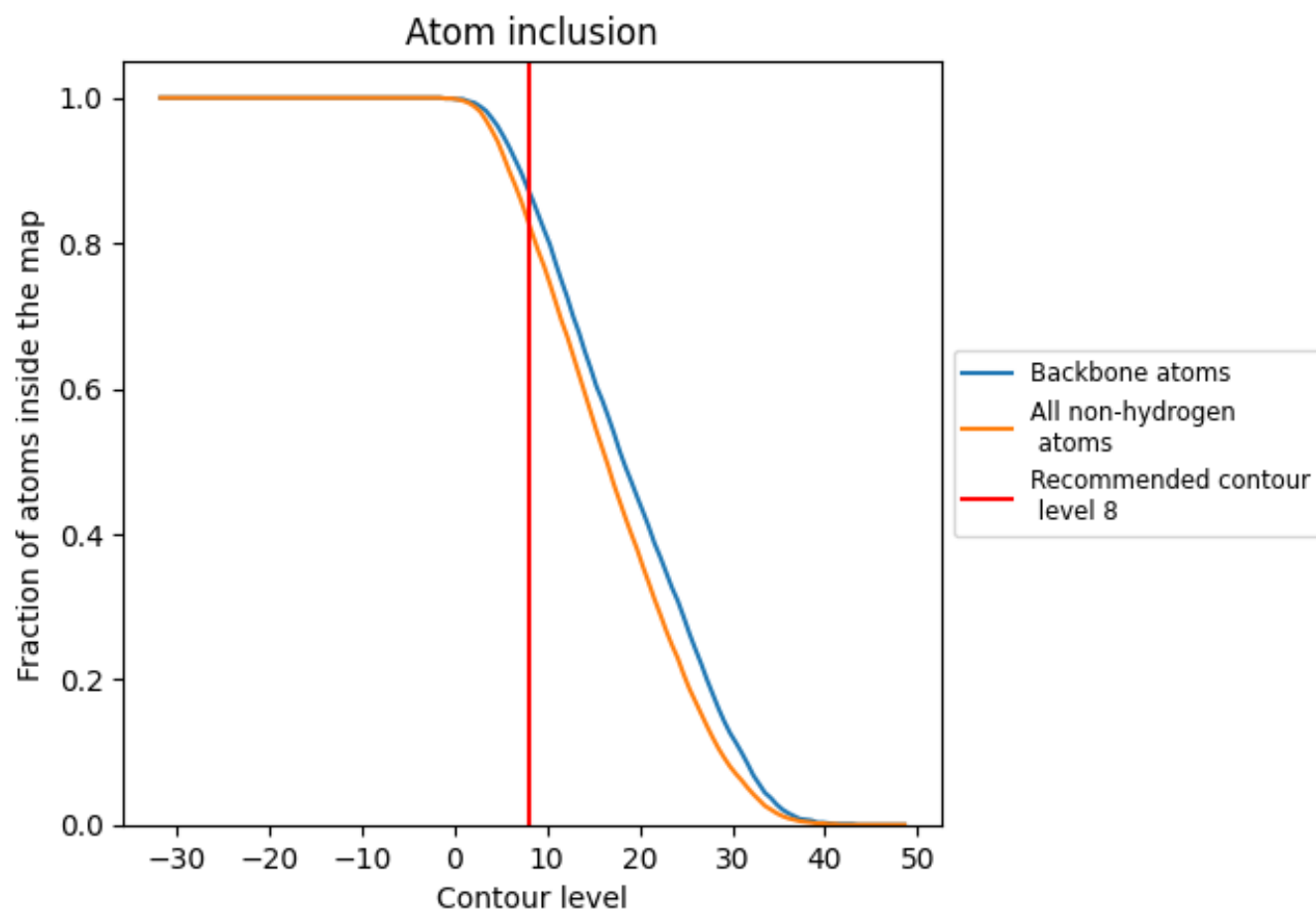
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.5670
A	0.8670	0.6020
B	0.7690	0.5400
C	0.7980	0.4330

