



Full wwPDB EM Validation Report ⓘ

May 17, 2026 – 02:52 PM JST

PDB ID : 9VUL / pdb_00009vul
EMDB ID : EMD-65367
Title : Cryo-EM structure of the human measles virus RNA-dependent RNA polymerase bound to allosteric inhibitor ERDRP-0519
Authors : Du, T.; Wang, J.; Wu, S.; Ru, H.
Deposited on : 2025-07-13
Resolution : 3.13 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:

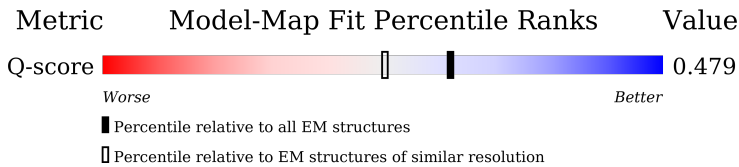
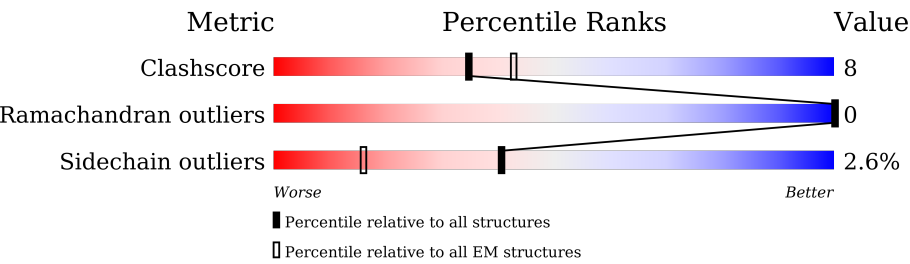
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	602	<div><div>18%</div><div>78%</div></div>
1	B	602	<div><div>95%</div></div>
1	C	602	<div><div>8%</div><div>90%</div></div>
1	D	602	<div><div>5%</div><div>93%</div></div>

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Mol	Chain	Length	Quality of chain
2	L	2630	<div><div><div></div><div></div><div></div></div><div>38%10%52%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12206 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 Maltose/maltodextrin-binding periplasmic protein, Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1034	655	187	186	6		
1	B	32	Total	C	N	O	S	0	0
			249	156	44	48	1		
1	C	59	Total	C	N	O	S	0	0
			443	279	75	88	1		
1	D	42	Total	C	N	O	S	0	0
			317	199	56	61	1		

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-94	MET	-	initiating methionine	UNP P0AEX9
A	-93	GLY	-	expression tag	UNP P0AEX9
A	-92	SER	-	expression tag	UNP P0AEX9
A	-91	SER	-	expression tag	UNP P0AEX9
A	-90	HIS	-	expression tag	UNP P0AEX9
A	-89	HIS	-	expression tag	UNP P0AEX9
A	-88	HIS	-	expression tag	UNP P0AEX9
A	-87	HIS	-	expression tag	UNP P0AEX9
A	-86	HIS	-	expression tag	UNP P0AEX9
A	-85	HIS	-	expression tag	UNP P0AEX9
A	-84	GLY	-	expression tag	UNP P0AEX9
A	-83	THR	-	expression tag	UNP P0AEX9
A	-82	LYS	-	expression tag	UNP P0AEX9
A	-81	THR	-	expression tag	UNP P0AEX9
A	284	GLY	-	linker	UNP P0AEX9
A	285	THR	-	linker	UNP P0AEX9
A	286	ASP	-	linker	UNP P0AEX9
A	287	TYR	-	linker	UNP P0AEX9
A	288	ASP	-	linker	UNP P0AEX9
A	289	ILE	-	linker	UNP P0AEX9
A	290	PRO	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	291	THR	-	linker	UNP P0AEX9
A	292	THR	-	linker	UNP P0AEX9
A	293	LEU	-	linker	UNP P0AEX9
A	294	GLU	-	linker	UNP P0AEX9
A	295	VAL	-	linker	UNP P0AEX9
A	296	LEU	-	linker	UNP P0AEX9
A	297	PHE	-	linker	UNP P0AEX9
A	298	GLN	-	linker	UNP P0AEX9
A	299	GLY	-	linker	UNP P0AEX9
A	300	PRO	-	linker	UNP P0AEX9
A	301	LEU	-	linker	UNP P0AEX9
A	302	GLY	-	linker	UNP P0AEX9
A	303	SER	-	linker	UNP P0AEX9
B	-94	MET	-	initiating methionine	UNP P0AEX9
B	-93	GLY	-	expression tag	UNP P0AEX9
B	-92	SER	-	expression tag	UNP P0AEX9
B	-91	SER	-	expression tag	UNP P0AEX9
B	-90	HIS	-	expression tag	UNP P0AEX9
B	-89	HIS	-	expression tag	UNP P0AEX9
B	-88	HIS	-	expression tag	UNP P0AEX9
B	-87	HIS	-	expression tag	UNP P0AEX9
B	-86	HIS	-	expression tag	UNP P0AEX9
B	-85	HIS	-	expression tag	UNP P0AEX9
B	-84	GLY	-	expression tag	UNP P0AEX9
B	-83	THR	-	expression tag	UNP P0AEX9
B	-82	LYS	-	expression tag	UNP P0AEX9
B	-81	THR	-	expression tag	UNP P0AEX9
B	284	GLY	-	linker	UNP P0AEX9
B	285	THR	-	linker	UNP P0AEX9
B	286	ASP	-	linker	UNP P0AEX9
B	287	TYR	-	linker	UNP P0AEX9
B	288	ASP	-	linker	UNP P0AEX9
B	289	ILE	-	linker	UNP P0AEX9
B	290	PRO	-	linker	UNP P0AEX9
B	291	THR	-	linker	UNP P0AEX9
B	292	THR	-	linker	UNP P0AEX9
B	293	LEU	-	linker	UNP P0AEX9
B	294	GLU	-	linker	UNP P0AEX9
B	295	VAL	-	linker	UNP P0AEX9
B	296	LEU	-	linker	UNP P0AEX9
B	297	PHE	-	linker	UNP P0AEX9
B	298	GLN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	GLY	-	linker	UNP P0AEX9
B	300	PRO	-	linker	UNP P0AEX9
B	301	LEU	-	linker	UNP P0AEX9
B	302	GLY	-	linker	UNP P0AEX9
B	303	SER	-	linker	UNP P0AEX9
C	-94	MET	-	initiating methionine	UNP P0AEX9
C	-93	GLY	-	expression tag	UNP P0AEX9
C	-92	SER	-	expression tag	UNP P0AEX9
C	-91	SER	-	expression tag	UNP P0AEX9
C	-90	HIS	-	expression tag	UNP P0AEX9
C	-89	HIS	-	expression tag	UNP P0AEX9
C	-88	HIS	-	expression tag	UNP P0AEX9
C	-87	HIS	-	expression tag	UNP P0AEX9
C	-86	HIS	-	expression tag	UNP P0AEX9
C	-85	HIS	-	expression tag	UNP P0AEX9
C	-84	GLY	-	expression tag	UNP P0AEX9
C	-83	THR	-	expression tag	UNP P0AEX9
C	-82	LYS	-	expression tag	UNP P0AEX9
C	-81	THR	-	expression tag	UNP P0AEX9
C	284	GLY	-	linker	UNP P0AEX9
C	285	THR	-	linker	UNP P0AEX9
C	286	ASP	-	linker	UNP P0AEX9
C	287	TYR	-	linker	UNP P0AEX9
C	288	ASP	-	linker	UNP P0AEX9
C	289	ILE	-	linker	UNP P0AEX9
C	290	PRO	-	linker	UNP P0AEX9
C	291	THR	-	linker	UNP P0AEX9
C	292	THR	-	linker	UNP P0AEX9
C	293	LEU	-	linker	UNP P0AEX9
C	294	GLU	-	linker	UNP P0AEX9
C	295	VAL	-	linker	UNP P0AEX9
C	296	LEU	-	linker	UNP P0AEX9
C	297	PHE	-	linker	UNP P0AEX9
C	298	GLN	-	linker	UNP P0AEX9
C	299	GLY	-	linker	UNP P0AEX9
C	300	PRO	-	linker	UNP P0AEX9
C	301	LEU	-	linker	UNP P0AEX9
C	302	GLY	-	linker	UNP P0AEX9
C	303	SER	-	linker	UNP P0AEX9
D	-94	MET	-	initiating methionine	UNP P0AEX9
D	-93	GLY	-	expression tag	UNP P0AEX9
D	-92	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-91	SER	-	expression tag	UNP P0AEX9
D	-90	HIS	-	expression tag	UNP P0AEX9
D	-89	HIS	-	expression tag	UNP P0AEX9
D	-88	HIS	-	expression tag	UNP P0AEX9
D	-87	HIS	-	expression tag	UNP P0AEX9
D	-86	HIS	-	expression tag	UNP P0AEX9
D	-85	HIS	-	expression tag	UNP P0AEX9
D	-84	GLY	-	expression tag	UNP P0AEX9
D	-83	THR	-	expression tag	UNP P0AEX9
D	-82	LYS	-	expression tag	UNP P0AEX9
D	-81	THR	-	expression tag	UNP P0AEX9
D	284	GLY	-	linker	UNP P0AEX9
D	285	THR	-	linker	UNP P0AEX9
D	286	ASP	-	linker	UNP P0AEX9
D	287	TYR	-	linker	UNP P0AEX9
D	288	ASP	-	linker	UNP P0AEX9
D	289	ILE	-	linker	UNP P0AEX9
D	290	PRO	-	linker	UNP P0AEX9
D	291	THR	-	linker	UNP P0AEX9
D	292	THR	-	linker	UNP P0AEX9
D	293	LEU	-	linker	UNP P0AEX9
D	294	GLU	-	linker	UNP P0AEX9
D	295	VAL	-	linker	UNP P0AEX9
D	296	LEU	-	linker	UNP P0AEX9
D	297	PHE	-	linker	UNP P0AEX9
D	298	GLN	-	linker	UNP P0AEX9
D	299	GLY	-	linker	UNP P0AEX9
D	300	PRO	-	linker	UNP P0AEX9
D	301	LEU	-	linker	UNP P0AEX9
D	302	GLY	-	linker	UNP P0AEX9
D	303	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,RNA-directed RNA polymerase L,Strep II and FLAG tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	1262	Total	C	N	O	S	0	0
			10125	6474	1740	1855	56		

There are 34 discrepancies between the modelled and reference sequences:

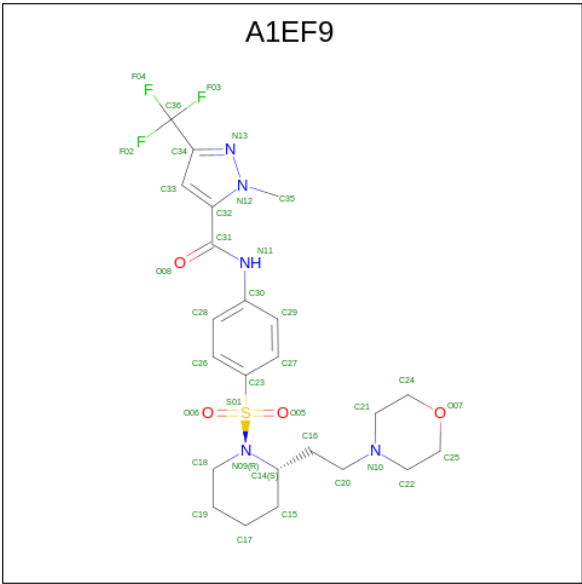
Chain	Residue	Modelled	Actual	Comment	Reference
L	-397	MET	-	initiating methionine	UNP P0AEX9
L	-396	GLY	-	expression tag	UNP P0AEX9
L	-395	SER	-	expression tag	UNP P0AEX9
L	-394	SER	-	expression tag	UNP P0AEX9
L	-393	HIS	-	expression tag	UNP P0AEX9
L	-392	HIS	-	expression tag	UNP P0AEX9
L	-391	HIS	-	expression tag	UNP P0AEX9
L	-390	HIS	-	expression tag	UNP P0AEX9
L	-389	HIS	-	expression tag	UNP P0AEX9
L	-388	HIS	-	expression tag	UNP P0AEX9
L	-387	GLY	-	expression tag	UNP P0AEX9
L	-386	THR	-	expression tag	UNP P0AEX9
L	-385	LYS	-	expression tag	UNP P0AEX9
L	-384	THR	-	expression tag	UNP P0AEX9
L	-19	GLY	-	linker	UNP P0AEX9
L	-18	THR	-	linker	UNP P0AEX9
L	-17	ASP	-	linker	UNP P0AEX9
L	-16	TYR	-	linker	UNP P0AEX9
L	-15	ASP	-	linker	UNP P0AEX9
L	-14	ILE	-	linker	UNP P0AEX9
L	-13	PRO	-	linker	UNP P0AEX9
L	-12	THR	-	linker	UNP P0AEX9
L	-11	THR	-	linker	UNP P0AEX9
L	-10	LEU	-	linker	UNP P0AEX9
L	-9	GLU	-	linker	UNP P0AEX9
L	-8	VAL	-	linker	UNP P0AEX9
L	-7	LEU	-	linker	UNP P0AEX9
L	-6	PHE	-	linker	UNP P0AEX9
L	-5	GLN	-	linker	UNP P0AEX9
L	-4	GLY	-	linker	UNP P0AEX9
L	-3	PRO	-	linker	UNP P0AEX9
L	-2	LEU	-	linker	UNP P0AEX9
L	-1	GLY	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	L	2	Total Zn 2 2	0

- Molecule 4 is 2-methyl- {N}-[4-[(2 {S})-2-(2-morpholin-4-ylethyl)piperidin-1-yl]sul

fonylphenyl]-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EF9) (formula: C₂₃H₃₀F₃N₅O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	L	1	36	23	3	5	4	1	0

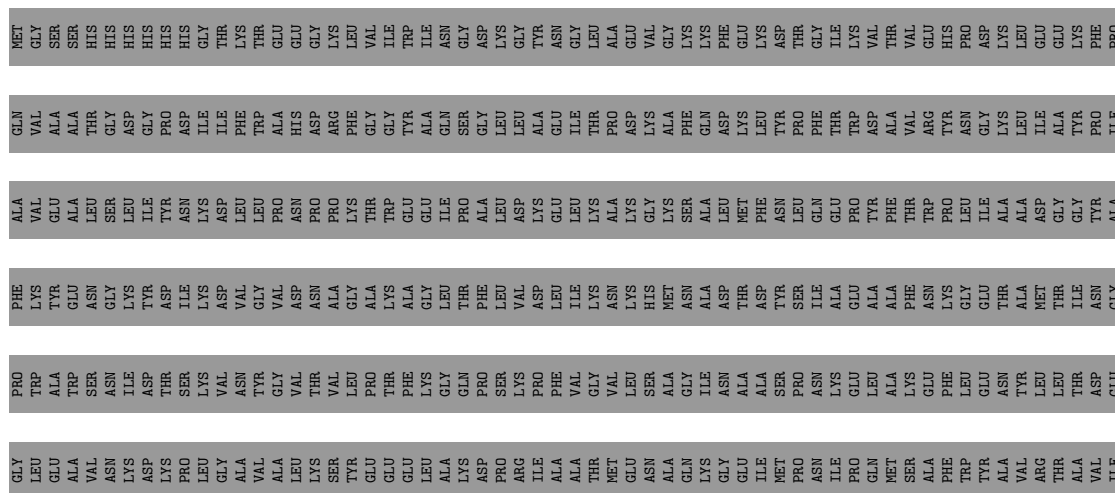
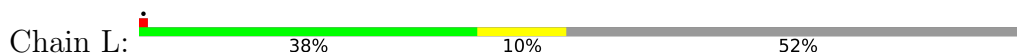
ASP	THR	ASP	LYS	HIS	ASN	GLY	PRO	PHE	ALA
THR	GLY	GLU	PRO	GLU	ALA	LEU	TRP	THR	VAL
GLY	ASP	ASN	ILE	ASN	ALA	GLU	ALA	TYR	GLU
PRO	ILE	ASN	GLY	GLN	SER	VAL	TRP	GLU	ALA
ALA	SER	LYS	ARG	LYS	ARG	ASN	ASN	GLY	SER
SER	ARG	ILE	ASP	ILE	GLN	LYS	ILE	LYS	LEU
ARG	SER	SER	ASP	ILE	THR	ASP	ASP	TYR	ILE
VAL	VAL	SER	GLY	SER	VAL	LYS	THR	ASP	LEU
ILE	ARG	LYS	ARG	LYS	ASP	PRO	SER	ILE	ASN
ARG	ALA	LEU	ALA	GLU	GLU	GLY	VAL	LYS	LYS
SER	LEU	SER	ALA	GLU	ALA	GLY	VAL	ASP	ASP
ILE	ALA	SER	ALA	SER	LEU	ALA	ASN	VAL	LEU
ILE	GLU	LEU	VAL	LEU	LEU	VAL	TYR	GLY	PRO
LYS	VAL	LEU	LYS	LEU	ASP	ALA	GLY	VAL	ASN
SER	LEU	LEU	LEU	LEU	ASN	LEU	THR	ASN	PRO
SER	LYS	LEU	LYS	GLN	GLN	LYS	VAL	ALA	PRO
ARG	PRO	PRO	PRO	GLY	THR	TYR	LEU	GLY	LYS
LEU	VAL	VAL	VAL	K343	THR	GLU	PRO	ALA	THR
GLU	ALA	G344	THR	E345	ASP	GLU	ALA	LYS	TRP
GLU	SER	E346	THR	Y346	TYR	GLU	PHE	ALA	GLU
ASP	ARG	E347	ARG	E348	ASP	LEU	GLY	GLY	ALA
ARG	LYS	E349	GLN	E349	ILE	ALA	GLY	LEU	ILE
LYS	LEU	E350	LEU	E350	PRO	LYS	GLN	THR	PRO
ARG	TYR	E351	GLN	K351	THR	ASP	PRO	PHE	ALA
TYR	GLY	E352	GLY	E352	THR	PRO	SER	LEU	ALA
LEU	MET	E353	MET	E353	LEU	ARG	LYS	VAL	ASP
MET	THR	E354	THR	E354	GLU	ILE	PRO	ASP	LYS
THR	LEU	E355	ASN	E355	VAL	ALA	PHE	LEU	ASP
LEU	GLY	E356	GLY	E356	LEU	THR	VAL	ILE	GLU
ASP	ARG	E357	ARG	E357	PHE	THR	GLY	LYS	LYS
ASP	THR	E358	THR	E358	GLN	MET	VAL	ASN	ALA
ILE	ILE	E359	SER	E359	GLY	GLU	LEU	LYS	GLY
LYS	SER	E360	SER	E360	PRO	ASN	SER	HIS	GLY
GLY	ARG	E361	ARG	E361	LEU	ALA	MET	ASN	LYS
ALA	GLY	E362	GLY	E362	GLY	GLN	GLY	MET	SER
ASN	GLN	E363	GLN	E363	SER	LYS	ILE	ALA	ALA
ASP	LEU	E364	LEU	E364	GLY	GLY	ASN	ASP	LEU
LEU	LEU	E365	LEU	E365	GLU	GLU	ALA	THR	PHE
ALA	ALA	E366	LYS	E366	TYR	ILE	ALA	ASP	ASN
LYS	GLU	E367	GLU	E367	TYR	MET	SER	TYR	ASN
PHE	PHE	E368	PHE	E368	ILE	PRO	PRO	SER	ASN
HIS	GLN	E369	GLN	E369	ASP	ASN	ASN	ILE	GLN
GLN	PRO	E370	PRO	E370	GLY	ILE	GLU	GLU	ASN
MET	LYS	E371	LYS	E371	LEU	PRO	GLU	GLU	TRP
LEU	PRO	E372	PRO	E372	PHE	GLN	LEU	ALA	ALA
MET	MET	E373	ILE	E373	SER	MET	ALA	ALA	PHE
LYS	LYS	E374	LYS	E374	ASP	SER	ALA	ALA	THR
		E375	SER	E375	THR	ILE	ALA	ASN	THR
		E376	THR	E376	LYS	VAL	VAL	TYR	ALA
		E377	VAL	E377	ALA	ARG	LEU	ALA	ASP
		E378	VAL	E378	THR	THR	THR	GLY	MET
		E379	VAL	E379	GLY	GLU	THR	THR	GLY
		E380	VAL	E380	ILE	ALA	THR	ILE	ILE
		E381	VAL	E381	ILE	VAL	THR	GLY	ALA
		E382	VAL	E382	ILE	VAL	THR	THR	ALA
		E383	VAL	E383	ILE	VAL	THR	THR	ALA
		E384	VAL	E384	ILE	VAL	THR	THR	ALA
		E385	VAL	E385	ILE	VAL	THR	THR	ALA
		E386	VAL	E386	ILE	VAL	THR	THR	ALA
		E387	VAL	E387	ILE	VAL	THR	THR	ALA
		E388	VAL	E388	ILE	VAL	THR	THR	ALA
		E389	VAL	E389	ILE	VAL	THR	THR	ALA
		E390	VAL	E390	ILE	VAL	THR	THR	ALA
		E391	VAL	E391	ILE	VAL	THR	THR	ALA
		E392	VAL	E392	ILE	VAL	THR	THR	ALA
		E393	VAL	E393	ILE	VAL	THR	THR	ALA
		E394	VAL	E394	ILE	VAL	THR	THR	ALA
		E395	VAL	E395	ILE	VAL	THR	THR	ALA
		E396	VAL	E396	ILE	VAL	THR	THR	ALA
		E397	VAL	E397	ILE	VAL	THR	THR	ALA
		E398	VAL	E398	ILE	VAL	THR	THR	ALA
		E399	VAL	E399	ILE	VAL	THR	THR	ALA
		E400	VAL	E400	ILE	VAL	THR	THR	ALA
		E401	VAL	E401	ILE	VAL	THR	THR	ALA
		E402	VAL	E402	ILE	VAL	THR	THR	ALA
		E403	VAL	E403	ILE	VAL	THR	THR	ALA
		E404	VAL	E404	ILE	VAL	THR	THR	ALA
		E405	VAL	E405	ILE	VAL	THR	THR	ALA
		E406	VAL	E406	ILE	VAL	THR	THR	ALA
		E407	VAL	E407	ILE	VAL	THR	THR	ALA
		E408	VAL	E408	ILE	VAL	THR	THR	ALA
		E409	VAL	E409	ILE	VAL	THR	THR	ALA
		E410	VAL	E410	ILE	VAL	THR	THR	ALA
		E411	VAL	E411	ILE	VAL	THR	THR	ALA
		E412	VAL	E412	ILE	VAL	THR	THR	ALA
		E413	VAL	E413	ILE	VAL	THR	THR	ALA
		E414	VAL	E414	ILE	VAL	THR	THR	ALA
		E415	VAL	E415	ILE	VAL	THR	THR	ALA
		E416	VAL	E416	ILE	VAL	THR	THR	ALA
		E417	VAL	E417	ILE	VAL	THR	THR	ALA
		E418	VAL	E418	ILE	VAL	THR	THR	ALA
		E419	VAL	E419	ILE	VAL	THR	THR	ALA
		E420	VAL	E420	ILE	VAL	THR	THR	ALA
		E421	VAL	E421	ILE	VAL	THR	THR	ALA
		E422	VAL	E422	ILE	VAL	THR	THR	ALA
		E423	VAL	E423	ILE	VAL	THR	THR	ALA
		E424	VAL	E424	ILE	VAL	THR	THR	ALA
		E425	VAL	E425	ILE	VAL	THR	THR	ALA
		E426	VAL	E426	ILE	VAL	THR	THR	ALA
		E427	VAL	E427	ILE	VAL	THR	THR	ALA
		E428	VAL	E428	ILE	VAL	THR	THR	ALA
		E429	VAL	E429	ILE	VAL	THR	THR	ALA
		E430	VAL	E430	ILE	VAL	THR	THR	ALA
		E431	VAL	E431	ILE	VAL	THR	THR	ALA
		E432	VAL	E432	ILE	VAL	THR	THR	ALA
		E433	VAL	E433	ILE	VAL	THR	THR	ALA
		E434	VAL	E434	ILE	VAL	THR	THR	ALA
		E435	VAL	E435	ILE	VAL	THR	THR	ALA
		E436	VAL	E436	ILE	VAL	THR	THR	ALA
		E437	VAL	E437	ILE	VAL	THR	THR	ALA
		E438	VAL	E438	ILE	VAL	THR	THR	ALA
		E439	VAL	E439	ILE	VAL	THR	THR	ALA
		E440	VAL	E440	ILE	VAL	THR	THR	ALA
		E441	VAL	E441	ILE	VAL	THR	THR	ALA
		E442	VAL	E442	ILE	VAL	THR	THR	ALA
		E443	VAL	E443	ILE	VAL	THR	THR	ALA
		E444	VAL	E444	ILE	VAL	THR	THR	ALA
		E445	VAL	E445	ILE	VAL	THR	THR	ALA
		E446	VAL	E446	ILE	VAL	THR	THR	ALA
		E447	VAL	E447	ILE	VAL	THR	THR	ALA
		E448	VAL	E448	ILE	VAL	THR	THR	ALA
		E449	VAL	E449	ILE	VAL	THR	THR	ALA
		E450	VAL	E450	ILE	VAL	THR	THR	ALA
		E451	VAL	E451	ILE	VAL	THR	THR	ALA
		E452	VAL	E452	ILE	VAL	THR	THR	ALA
		E453	VAL	E453	ILE	VAL	THR	THR	ALA
		E454	VAL	E454	ILE	VAL	THR	THR	ALA
		E455	VAL	E455	ILE	VAL	THR	THR	ALA
		E456	VAL	E456	ILE	VAL	THR	THR	ALA
		E457	VAL	E457	ILE	VAL	THR	THR	ALA
		E458	VAL	E458	ILE	VAL	THR	THR	ALA
		E459	VAL	E459	ILE	VAL	THR	THR	ALA
		E460	VAL	E460	ILE	VAL	THR	THR	ALA
		E461	VAL	E461	ILE	VAL	THR	THR	ALA
		E462	VAL	E462	ILE	VAL	THR	THR	ALA
		E463	VAL	E463	ILE	VAL	THR	THR	ALA
		E464	VAL	E464	ILE	VAL	THR	THR	ALA
		E465	VAL	E465	ILE	VAL	THR	THR	ALA
		E466	VAL	E466	ILE	VAL	THR	THR	ALA
		E467	VAL	E467	ILE	VAL	THR	THR	ALA
		E468	VAL	E468	ILE	VAL	THR	THR	ALA
		E469	VAL	E469	ILE	VAL	THR	THR	ALA
		E470	VAL	E470	ILE	VAL	THR	THR	ALA
		E471	VAL	E471	ILE	VAL	THR	THR	ALA
		E472	VAL	E472	ILE	VAL	THR	THR	ALA
		E473	VAL	E473	ILE	VAL	THR	THR	ALA
		E474	VAL	E474	ILE	VAL	THR	THR	ALA
		E475	VAL	E475	ILE	VAL	THR	THR	ALA
		E476	VAL	E476	ILE	VAL	THR	THR	ALA
		E477	VAL	E477	ILE	VAL	THR	THR	ALA
		E478	VAL	E478	ILE	VAL	THR	THR	ALA
		E479	VAL	E479	ILE	VAL	THR	THR	ALA
		E480	VAL	E480	ILE	VAL	THR	THR	ALA
		E481	VAL	E481	ILE	VAL	THR	THR	ALA
		E482	VAL	E482	ILE	VAL	THR	THR	ALA
		E483	VAL	E483	ILE	VAL	THR	THR	ALA
		E484	VAL	E484	ILE	VAL	THR	THR	ALA
		E485	VAL	E485	ILE	VAL	THR	THR	ALA
		E486	VAL	E486	ILE	VAL	THR	THR	ALA
		E487	VAL	E487	ILE	VAL	THR	THR	ALA
		E488	VAL	E488	ILE	VAL	THR	THR	ALA
		E489	VAL	E489	ILE	VAL	THR	THR	ALA
		E490	VAL	E490	ILE	VAL	THR	THR	ALA
		E491	VAL	E491	ILE	VAL	THR	THR	ALA
		E492	VAL	E492	ILE	VAL	THR	THR	ALA
		E493	VAL	E493	ILE	VAL	THR	THR	ALA
		E494	VAL	E494	ILE	VAL	THR	THR	ALA
		E495	VAL	E495	ILE	VAL	THR	THR	ALA
		E496	VAL	E496	ILE	VAL	THR	THR	ALA
		E497	VAL	E497	ILE	VAL	THR	THR	ALA
		E498	VAL	E498	ILE	VAL	THR	THR	ALA
		E499	VAL	E499	ILE	VAL	THR	THR	ALA
		E500	VAL	E500	ILE	VAL	THR	THR	ALA
		E501	VAL	E501	ILE	VAL	THR	THR	ALA
		E502	VAL	E502	ILE	VAL	THR	THR	ALA
		E503	VAL	E503	ILE	VAL	THR	THR	ALA
		E504	VAL	E504	ILE	VAL	THR	THR	ALA
		E505	VAL	E505	ILE	VAL	THR	THR	ALA
		E506	VAL	E506	ILE	VAL	THR	THR	ALA
		E507	VAL	E507	ILE	VAL	THR	THR	ALA
		E508	VAL	E508	ILE	VAL	THR	THR	ALA
		E509	VAL	E509	ILE	VAL	THR	THR	ALA
		E510	VAL	E510	ILE	VAL	THR	THR	ALA
		E511	VAL	E511	ILE	VAL	THR	THR	ALA
		E512	VAL	E512	ILE	VAL	THR	THR	ALA
		E513	VAL	E513	ILE	VAL	THR	THR	ALA
		E514	VAL	E514	ILE	VAL	THR	THR	ALA
		E515	VAL	E515	ILE	VAL	THR	THR	ALA
		E516	VAL	E516	ILE	VAL	THR	THR	ALA

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Phosphoprotein

Chain C: 

SER	LYS	HIS	ASN	GLY	PRO	PHE	ALA	GLN	MET
	ARG	GLU	ALA	LEU	TRP	LYS	VAL	VAL	GLY
LEU	PRO	ASP	ALA	GLU	ALA	TRP	GLU	ALA	SER
GLU	VAL	ASN	SER	VAL	SER	ASN	LEU	THR	HIS
ASP	SER	LYS	ARG	ASN	ILE	GLN	SER	GLY	HIS
ARG	ARG	ILE	GLN	ASP	LYS	LYS	LEU	ASP	HIS
LYS	GLN	ILE	THR	LYS	ASP	TRP	TRP	GLY	LYS
ARG	LEU	SER	VAL	LYS	THR	ASN	TYR	PRO	HIS
TYR	GLN	LYS	ASP	PRO	SER	ILE	ASN	ASP	HIS
LEU	GLY	LEU	GLU	LEU	LYS	LYS	LYS	ILE	GLY
MET	MET	GLU	ALA	GLY	VAL	ASP	ASP	ILE	THR
THR	THR	SER	LEU	ALA	ASN	VAL	LEU	PHE	LYS
LEU	ASN	SER	LYS	VAL	TYR	GLY	LEU	THR	LYS
LEU	GLY	LEU	ASP	VAL	GLY	VAL	PRO	ALA	GLU
ASP	ARG	L341	ALA	LEU	VAL	ASN	ASN	HIS	GLY
ASP	THR	L342	THR	SER	THR	ALA	PRO	ARG	LYS
ILE	SER	K343	GLY	TYR	VAL	ALA	PRO	ARG	LYS
GLY	ARG	G344	THR	GLU	GLY	ALA	THR	PHE	VAL
ASN	GLY	E345	ASP	GLU	THR	LYS	TRP	GLY	TRP
ASN	GLN	V346	TYR	GLU	PHE	ALA	GLU	TYR	ILE
ASP	LEU	E347	ASP	LEU	LYS	GLY	GLU	ALA	ILE
LEU	LEU	S348	ILE	ALA	GLY	LEU	PRO	GLN	ASN
ALA	LYS	I349	PRO	LYS	GLN	THR	ILE	ILE	GLY
LYS	GLU	K350	THR	ASP	PRO	PHE	ALA	GLY	ASP
PHE	PHE	K351	THR	PRO	SER	LEU	LEU	LEU	LYS
GLN	GLN	Q356	LEU	ARG	LYS	VAL	ASP	ASP	GLY
PRO	PRO	L367	GLU	ILE	PRO	ASP	LYS	ALA	TYR
LYS	PRO	L367	VAL	ALA	PHE	LEU	GLU	GLU	ASN
ILE	GLY	I370	GLN	MET	VAL	ASN	LYS	PRO	ALA
LYS	LYS	M371	GLY	GLU	LEU	LYS	LYS	ASP	GLY
ILE	LYS		PRO	ASN	SER	HIS	GLY	LYS	VAL
MET	MET	G378	LEU	GLN	ALA	MET	GLY	ALA	GLY
LYS	SER	K379	SER	GLN	GLY	ASN	SER	PHE	LYS
ALA	ALA	D380	GLY	GLY	ILE	ALA	ALA	GLN	LYS
VAL	VAL	P381	ASP	GLY	ASN	ASP	LEU	ASP	PHE
GLY	GLY	N382	TYR	ILE	ALA	THR	MET	LYS	GLY
PHE	PHE		TYR	GLU	ALA	ASP	PHE	LEU	ASP
VAL	VAL	V388	ASP	MET	SER	TRP	ASN	TYR	THR
PRO	PRO	N391	ASP	PRO	PRO	ILE	GLN	PRO	ILE
ASP	ASP		GLU	ILE	LYS	ALA	GLU	THR	ILE
THR	THR	L394	PHE	PRO	GLU	ALA	PRO	ASP	VAL
PRO	PRO		SER	GLN	LEU	ALA	TYR	THR	LYS
ALA	ALA	I397	ASP	MET	LYS	PHE	THR	VAL	VAL
SER	SER	I398	VAL	ALA	GLU	ASN	TRP	ARG	GLU
ARG	ARG	G399	GLN	PHE	PHE	LYS	PRO	TYR	HIS
SER	SER	ARG	ASP	TRP	LEU	GLY	LEU	ASN	PRO
VAL	VAL		ILE	TYR	GLU	GLU	ILE	GLY	ASP
ILE	ILE	ASP	LYS	ALA	ASN	THR	ALA	LYS	LYS
ARG	ARG	SER	THR	VAL	LEU	ALA	TYR	LEU	ARG
SER	SER	GLY	ALA	ARG	LEU	MET	ASP	ILE	GLU
ILE	ILE	ARG	LEU	THR	LEU	THR	GLY	ALA	GLY
LYS	LYS	ALA	ALA	ALA	THR	ILE	GLY	TYR	LYS
LEU	LEU	LEU	LYS	VAL	ASP	ASN	ASN	PRO	PHE
SER	SER	GLU	ILE	ILE	GLU	GLY	ALA	ILE	PRO

- Chain D:  5% 93%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177478	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 ($e^-/\text{\AA}^2$)	52.52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.280	Depositor
Minimum map value	-0.866	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	306.36002, 306.36002, 306.36002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8510001, 0.8510001, 0.8510001	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: A1EF9, 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	0.13	0/1043	0.36	0/1388
1	B	0.10	0/249	0.21	0/331
1	C	0.15	0/448	0.34	0/606
1	D	0.12	0/319	0.31	0/427
2	L	0.16	0/10352	0.37	1/14034 (0.0%)
All	All	0.16	0/12411	0.36	1/16786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	864	THR	N-CA-C	6.77	118.66	111.28

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	1034	0	1123	15	0
1	B	249	0	270	7	0
1	C	443	0	466	12	0
1	D	317	0	340	6	0
2	L	10125	0	10132	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2	0	0	0	0
4	L	36	0	0	0	0
All	All	12206	0	12331	195	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 (195) 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)
2:L:1180:CYS:SG	2:L:1364:HIS:HE1	1.92	0.91
2:L:284:GLU:HG3	2:L:285:PRO:HD3	1.59	0.81
2:L:1052:ARG:HD2	2:L:1380:ILE:HG22	1.64	0.80
2:L:464:LEU:HD12	2:L:1078:MET:HE3	1.66	0.76
2:L:1057:PRO:HG2	2:L:1157:LEU:HD11	1.71	0.72
2:L:1192:VAL:HG22	2:L:1311:THR:HG22	1.71	0.72
2:L:858:GLU:H	2:L:858:GLU:CD	1.98	0.72
2:L:1161:ASP:HB3	2:L:1164:GLU:HG2	1.72	0.72
2:L:1189:TRP:HB3	2:L:1314:SER:HB3	1.72	0.72
1:B:356:GLN:NE2	1:C:356:GLN:OE1	2.22	0.71
1:A:479:ARG:NH2	1:A:482:MET:SD	2.64	0.71
2:L:1166:MET:HE3	2:L:1363:LEU:HG	1.75	0.69
2:L:15:HIS:NE2	2:L:856:TRP:O	2.28	0.67
2:L:662:THR:HG22	2:L:823:THR:HG23	1.77	0.66
2:L:193:PRO:HB2	2:L:204:LEU:HD11	1.77	0.65
2:L:856:TRP:CZ3	2:L:899:GLN:NE2	2.64	0.65
2:L:554:ARG:O	2:L:558:VAL:HG23	1.97	0.65
2:L:845:GLN:N	2:L:845:GLN:OE1	2.29	0.65
2:L:856:TRP:HH2	2:L:903:SER:OG	1.80	0.64
2:L:841:LEU:HG	2:L:1309:ARG:HH12	1.63	0.63
2:L:11:TYR:CD1	2:L:861:VAL:HG13	2.34	0.62
2:L:343:ILE:HD12	2:L:343:ILE:H	1.63	0.62
2:L:1107:ASP:HA	2:L:1110:GLN:HE21	1.64	0.62
2:L:27:ALA:HB2	2:L:45:LEU:HD21	1.82	0.62
2:L:226:GLU:H	2:L:226:GLU:CD	2.08	0.62
2:L:123:LYS:HB2	2:L:972:LEU:HD13	1.83	0.61
2:L:555:ALA:O	2:L:559:ILE:HG12	2.01	0.61
2:L:549:MET:HE3	2:L:553:MET:HB3	1.83	0.60
2:L:1166:MET:SD	2:L:1365:VAL:HG22	2.42	0.60
2:L:1185:VAL:O	2:L:1317:ASN:ND2	2.34	0.60
2:L:1261:LEU:HD13	2:L:1386:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:68:VAL:HG11	2:L:209:LEU:HD21	1.83	0.59
2:L:965:LYS:NZ	2:L:1131:SER:O	2.35	0.59
2:L:214:SER:OG	2:L:216:GLU:OE2	2.22	0.58
2:L:856:TRP:HH2	2:L:903:SER:HG	1.48	0.57
2:L:856:TRP:CH2	2:L:899:GLN:NE2	2.73	0.57
2:L:865:ARG:NH1	2:L:939:GLY:O	2.37	0.57
2:L:860:ILE:CD1	2:L:1083:LYS:HG2	2.35	0.57
2:L:245:MET:HE1	2:L:258:VAL:HG11	1.87	0.57
2:L:538:GLU:OE1	2:L:544:ARG:NH2	2.38	0.56
2:L:1249:TYR:HD2	2:L:1380:ILE:HB	1.71	0.56
1:C:367:LEU:O	1:C:371:MET:HE3	2.05	0.56
1:A:363:LEU:HD13	1:B:364:GLU:HA	1.87	0.56
1:C:348:SER:HA	1:C:351:LYS:HD2	1.88	0.56
2:L:714:PRO:HB2	2:L:716:LEU:HD13	1.86	0.56
2:L:1012:LEU:O	2:L:1016:ILE:HG22	2.05	0.56
1:A:484:LEU:HB3	1:A:497:PHE:HE1	1.72	0.55
2:L:1401:ASN:OD1	2:L:1402:ALA:N	2.39	0.55
2:L:423:ASN:O	2:L:427:SER:OG	2.25	0.54
2:L:11:TYR:CE1	2:L:861:VAL:HG13	2.43	0.54
2:L:107:ARG:O	2:L:111:LYS:HG3	2.08	0.54
2:L:343:ILE:HD11	2:L:1200:ASP:HB2	1.90	0.54
1:D:352:GLN:HG3	1:D:355:ARG:HH21	1.73	0.54
2:L:1124:ASN:HB3	2:L:1127:ILE:HG12	1.90	0.53
2:L:461:THR:HG22	2:L:465:LYS:HZ3	1.73	0.53
2:L:371:ARG:HB2	2:L:732:ILE:HG12	1.90	0.53
2:L:170:THR:O	2:L:174:GLU:HG2	2.09	0.53
2:L:294:ARG:NH2	2:L:1200:ASP:OD2	2.42	0.53
2:L:368:GLU:OE2	2:L:371:ARG:NH1	2.42	0.53
2:L:863:GLU:HG3	2:L:866:ALA:HB3	1.91	0.53
2:L:1348:PHE:HZ	2:L:1359:THR:HG21	1.74	0.52
1:C:388:VAL:HG12	2:L:685:GLU:HG3	1.92	0.52
2:L:165:PHE:HZ	2:L:855:PHE:HE2	1.55	0.52
2:L:11:TYR:OH	2:L:909:ASN:ND2	2.43	0.52
2:L:865:ARG:HG3	2:L:1110:GLN:OE1	2.09	0.52
2:L:243:THR:O	2:L:247:ILE:HG13	2.09	0.51
2:L:875:MET:O	2:L:879:ILE:HG13	2.09	0.51
2:L:460:LEU:HD12	2:L:1029:MET:HG2	1.92	0.51
2:L:916:VAL:HG22	2:L:920:LEU:HD12	1.92	0.51
2:L:42:ASP:OD1	2:L:42:ASP:N	2.38	0.51
2:L:480:TYR:HB2	2:L:485:LEU:HD11	1.91	0.51
2:L:202:GLU:OE2	2:L:215:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:864:THR:OG1	2:L:1107:ASP:OD1	2.28	0.51
2:L:885:ARG:HG2	2:L:948:LEU:HB3	1.91	0.51
2:L:1008:SER:O	2:L:1012:LEU:HD12	2.11	0.51
2:L:142:ARG:HH12	2:L:249:ALA:HB3	1.76	0.51
1:A:502:MET:SD	2:L:298:VAL:HB	2.52	0.50
1:A:501:LEU:O	1:A:505:ILE:HG13	2.11	0.50
1:C:391:ASN:ND2	2:L:687:TYR:O	2.27	0.50
2:L:1166:MET:CE	2:L:1363:LEU:HG	2.40	0.50
2:L:122:ASP:OD1	2:L:122:ASP:N	2.43	0.49
2:L:1315:ASN:OD1	2:L:1337:MET:HE3	2.12	0.49
2:L:203:LEU:HD12	2:L:212:ILE:HG12	1.94	0.49
2:L:1107:ASP:HA	2:L:1110:GLN:HG2	1.94	0.49
2:L:1245:TYR:OH	2:L:1258:GLU:OE1	2.25	0.49
2:L:1265:GLN:HA	2:L:1392:LEU:HD11	1.95	0.49
2:L:1187:TYR:HB3	2:L:1364:HIS:ND1	2.28	0.49
2:L:988:ASP:OD1	2:L:988:ASP:N	2.44	0.49
2:L:108:GLU:HA	2:L:111:LYS:HE2	1.95	0.49
2:L:863:GLU:OE2	2:L:1008:SER:OG	2.30	0.49
2:L:467:LYS:HD3	2:L:554:ARG:HE	1.78	0.49
2:L:116:LEU:HA	2:L:119:LYS:HD3	1.94	0.48
2:L:343:ILE:HG22	2:L:843:VAL:HG11	1.94	0.48
2:L:656:VAL:HG22	2:L:796:ALA:HB2	1.94	0.48
1:C:346:VAL:O	1:C:349:ILE:HG22	2.13	0.48
2:L:933:LEU:HB3	2:L:939:GLY:HA3	1.94	0.48
2:L:832:TYR:CE2	2:L:834:LYS:HB3	2.48	0.48
2:L:1231:PRO:HG2	2:L:1236:ARG:HH12	1.78	0.48
2:L:48:ASN:OD1	2:L:486:ARG:HD2	2.14	0.48
1:A:350:LYS:HB2	1:D:349:ILE:HD11	1.96	0.48
2:L:1379:ARG:C	2:L:1380:ILE:HD13	2.39	0.48
2:L:536:GLU:CD	2:L:537:LYS:HG3	2.39	0.48
2:L:856:TRP:CH2	2:L:903:SER:OG	2.61	0.48
1:A:352:GLN:OE1	1:B:357:ASN:ND2	2.46	0.47
2:L:858:GLU:OE1	2:L:858:GLU:N	2.43	0.47
2:L:465:LYS:N	2:L:465:LYS:HD2	2.30	0.47
2:L:658:ALA:HB3	2:L:800:THR:OG1	2.14	0.47
2:L:1192:VAL:HB	2:L:1359:THR:OG1	2.13	0.47
2:L:654:GLU:N	2:L:654:GLU:OE2	2.48	0.47
2:L:1246:SER:HA	2:L:1250:GLY:HA3	1.96	0.47
2:L:1395:ASN:OD1	2:L:1396:PRO:HD2	2.15	0.47
2:L:10:LEU:HD13	2:L:860:ILE:HG23	1.95	0.47
2:L:1013:LEU:HD22	2:L:1086:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:GLU:HG2	1:D:346:VAL:HG12	1.97	0.47
2:L:798:ARG:HA	2:L:801:ARG:HH21	1.80	0.46
2:L:885:ARG:HH21	2:L:1346:THR:HG1	1.58	0.46
2:L:845:GLN:HG2	2:L:848:LYS:HD3	1.97	0.46
2:L:1048:PHE:O	2:L:1052:ARG:NH1	2.48	0.46
1:B:370:ILE:HD11	1:C:371:MET:HE2	1.97	0.46
2:L:343:ILE:O	2:L:346:THR:OG1	2.28	0.46
2:L:1184:SER:OG	2:L:1364:HIS:ND1	2.49	0.46
2:L:917:VAL:HG13	2:L:921:LEU:HD12	1.98	0.46
2:L:156:MET:HE3	2:L:239:LEU:HD21	1.99	0.45
2:L:728:ASP:OD1	2:L:729:GLN:N	2.50	0.45
2:L:999:TYR:OH	2:L:1058:ARG:NH1	2.49	0.45
2:L:1165:SER:HB2	2:L:1367:THR:HG22	1.98	0.45
1:C:394:LEU:HG	2:L:515:MET:HE1	1.98	0.45
2:L:24:LYS:NZ	2:L:226:GLU:OE2	2.33	0.45
2:L:984:GLN:HB3	2:L:1117:LEU:HD13	1.99	0.45
2:L:16:LEU:HD22	2:L:230:MET:HB2	1.99	0.45
1:B:367:LEU:HD23	1:B:367:LEU:HA	1.87	0.45
2:L:733:LYS:HE2	2:L:734:TYR:CE2	2.52	0.45
2:L:1009:ILE:HG22	2:L:1103:LEU:HD22	1.98	0.45
2:L:1087:ARG:HG2	2:L:1091:ARG:HH11	1.82	0.45
2:L:717:ASP:OD2	2:L:717:ASP:C	2.60	0.44
1:C:397:ILE:HG13	2:L:511:TYR:HB2	1.99	0.44
2:L:945:MET:HE3	2:L:945:MET:HB2	1.89	0.44
2:L:1261:LEU:HD22	2:L:1388:LEU:HD12	1.99	0.44
2:L:1042:ASP:OD1	2:L:1072:ARG:NH2	2.50	0.44
2:L:790:ASN:O	2:L:794:ARG:HG3	2.18	0.44
2:L:282:MET:HE2	2:L:282:MET:HB2	1.86	0.44
2:L:781:LYS:HD3	2:L:799:VAL:HG21	2.00	0.44
2:L:1307:VAL:O	2:L:1311:THR:HG23	2.18	0.44
2:L:121:SER:HB3	2:L:150:ILE:HA	1.99	0.43
2:L:1190:PHE:HB2	2:L:1361:LEU:HB3	2.00	0.43
1:C:370:ILE:HD13	1:C:370:ILE:HA	1.88	0.43
1:B:347:GLU:HG2	1:B:351:LYS:HE3	2.00	0.43
2:L:152:LEU:HD22	2:L:894:LEU:HD13	2.01	0.43
2:L:128:LEU:HD13	2:L:886:TYR:HB3	2.00	0.43
2:L:1046:ALA:O	2:L:1050:MET:HG3	2.18	0.43
2:L:860:ILE:HD12	2:L:1083:LYS:HG2	1.98	0.43
1:A:341:LEU:HG	1:A:342:LEU:H	1.83	0.43
1:A:434:LEU:HB2	1:A:437:PHE:HD2	1.83	0.43
2:L:1379:ARG:O	2:L:1380:ILE:HD13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:TYR:O	1:A:483:THR:OG1	2.34	0.43
2:L:224:THR:H	2:L:227:LEU:HD12	1.82	0.43
1:A:405:ALA:O	1:A:409:VAL:HG13	2.18	0.42
1:A:450:VAL:HG13	2:L:801:ARG:HD2	2.00	0.42
2:L:13:GLU:H	2:L:13:GLU:CD	2.27	0.42
2:L:877:LYS:HE3	2:L:877:LYS:HB2	1.60	0.42
2:L:200:SER:O	2:L:215:LYS:HG2	2.19	0.42
2:L:752:ILE:N	2:L:753:PRO:HD2	2.34	0.42
2:L:1162:VAL:HG22	2:L:1339:LEU:HD22	2.01	0.42
2:L:1029:MET:HE3	2:L:1029:MET:HB2	1.73	0.42
2:L:834:LYS:HE3	2:L:834:LYS:HB2	1.88	0.42
2:L:863:GLU:HG3	2:L:866:ALA:CB	2.49	0.42
2:L:247:ILE:HG13	2:L:247:ILE:H	1.72	0.42
2:L:247:ILE:HG22	2:L:887:LEU:HD13	2.01	0.42
2:L:536:GLU:OE1	2:L:537:LYS:HG3	2.19	0.42
2:L:1087:ARG:O	2:L:1091:ARG:HG3	2.19	0.42
1:C:397:ILE:HG13	2:L:511:TYR:CB	2.50	0.42
2:L:1007:GLN:HG3	2:L:1012:LEU:HD11	2.01	0.42
1:A:494:LEU:HD12	1:A:494:LEU:HA	1.85	0.42
2:L:768:SER:OG	2:L:775:GLN:NE2	2.48	0.42
2:L:788:PRO:O	2:L:792:LYS:HG3	2.20	0.42
2:L:918:ILE:HB	2:L:919:PRO:HD3	2.01	0.42
2:L:1086:ILE:O	2:L:1090:MET:HG3	2.20	0.42
2:L:30:GLU:OE1	2:L:36:HIS:NE2	2.50	0.41
2:L:49:ILE:HD13	2:L:49:ILE:HA	1.93	0.41
2:L:793:LYS:HA	2:L:793:LYS:HD3	1.88	0.41
2:L:1177:CYS:HB3	2:L:1180:CYS:HB2	2.01	0.41
2:L:503:LEU:O	2:L:1026:PRO:HD2	2.21	0.41
2:L:516:TYR:OH	2:L:525:ASP:OD2	2.27	0.41
1:D:359:SER:O	1:D:362:THR:HG22	2.21	0.41
1:D:379:LYS:HD2	2:L:734:TYR:CE1	2.56	0.41
1:A:363:LEU:HD11	1:B:367:LEU:HD12	2.03	0.41
2:L:1003:LEU:HD23	2:L:1144:MET:HE1	2.04	0.40
2:L:1013:LEU:HD21	2:L:1095:LEU:HD21	2.03	0.40
1:A:396:PRO:HG2	1:D:370:ILE:HG13	2.03	0.40
2:L:242:GLU:HA	2:L:245:MET:HE2	2.03	0.40
2:L:465:LYS:NZ	2:L:1078:MET:SD	2.94	0.40
2:L:789:TYR:HA	2:L:792:LYS:HE2	2.03	0.40
2:L:724:LYS:HE3	2:L:724:LYS:HB3	1.89	0.40
2:L:104:ARG:O	2:L:108:GLU:HG2	2.22	0.40
2:L:745:LYS:O	2:L:749:ILE:HG12	2.21	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	127/602 (21%)	123 (97%)	4 (3%)	0	100	100
1	B	30/602 (5%)	30 (100%)	0	0	100	100
1	C	57/602 (10%)	57 (100%)	0	0	100	100
1	D	40/602 (7%)	39 (98%)	1 (2%)	0	100	100
2	L	1250/2630 (48%)	1212 (97%)	38 (3%)	0	100	100
All	All	1504/5038 (30%)	1461 (97%)	43 (3%)	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	117/499 (23%)	115 (98%)	2 (2%)	53	70
1	B	30/499 (6%)	30 (100%)	0	100	100
1	C	52/499 (10%)	52 (100%)	0	100	100
1	D	37/499 (7%)	35 (95%)	2 (5%)	20	46
2	L	1121/2301 (49%)	1090 (97%)	31 (3%)	38	62
All	All	1357/4297 (32%)	1322 (97%)	35 (3%)	41	64

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	LEU
1	A	484	LEU
1	D	352	GLN
1	D	364	GLU
2	L	67	GLU
2	L	137	LEU
2	L	152	LEU
2	L	156	MET
2	L	160	GLN
2	L	179	ILE
2	L	216	GLU
2	L	258	VAL
2	L	293	LEU
2	L	381	VAL
2	L	427	SER
2	L	434	GLU
2	L	501	VAL
2	L	689	LEU
2	L	769	LEU
2	L	770	VAL
2	L	783	VAL
2	L	795	GLU
2	L	812	HIS
2	L	821	ASN
2	L	831	VAL
2	L	849	SER
2	L	859	THR
2	L	864	THR
2	L	904	LEU
2	L	928	ILE
2	L	1006	VAL
2	L	1078	MET
2	L	1246	SER
2	L	1386	LEU
2	L	1393	CYS

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	356	GLN
1	B	356	GLN

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Mol	Chain	Res	Type
2	L	23	ASN
2	L	89	ASN
2	L	319	ASN
2	L	344	HIS
2	L	711	HIS
2	L	812	HIS
2	L	909	ASN
2	L	1061	HIS
2	L	1105	ASN
2	L	1186	ASN
2	L	1268	ASN
2	L	1358	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 3 ligands modelled in this entry, 2 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	$\# Z > 2$
4	A1EF9	L	4003	-	39,39,39	2.79	15 (38%)	54,57,57	2.74	15 (27%)

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	A1EF9	L	4003	-	-	4/31/50/50	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	4003	A1EF9	C20-N10	-7.36	1.30	1.47
4	L	4003	A1EF9	S01-N09	6.67	1.73	1.63
4	L	4003	A1EF9	C31-N11	6.10	1.48	1.35
4	L	4003	A1EF9	C23-S01	5.82	1.84	1.76
4	L	4003	A1EF9	C30-N11	3.56	1.48	1.41
4	L	4003	A1EF9	O06-S01	3.49	1.47	1.43
4	L	4003	A1EF9	C36-C34	3.31	1.54	1.48
4	L	4003	A1EF9	C16-C20	3.28	1.59	1.52
4	L	4003	A1EF9	C18-N09	3.21	1.54	1.48
4	L	4003	A1EF9	O05-S01	3.20	1.47	1.43
4	L	4003	A1EF9	C22-N10	-3.13	1.38	1.46
4	L	4003	A1EF9	C21-N10	-3.09	1.38	1.46
4	L	4003	A1EF9	C32-C31	2.90	1.56	1.49
4	L	4003	A1EF9	C17-C15	-2.85	1.45	1.53
4	L	4003	A1EF9	O08-C31	-2.75	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4003	A1EF9	O06-S01-O05	-10.83	101.98	119.52
4	L	4003	A1EF9	C36-C34-N13	6.23	127.14	119.23
4	L	4003	A1EF9	C15-C14-N09	5.62	119.24	109.50
4	L	4003	A1EF9	C19-C18-N09	5.18	117.90	110.31
4	L	4003	A1EF9	O05-S01-C23	4.50	113.74	108.05
4	L	4003	A1EF9	C32-C33-C34	4.11	107.75	103.64
4	L	4003	A1EF9	C33-C34-N13	-3.88	107.24	111.92
4	L	4003	A1EF9	C35-N12-N13	3.84	124.76	119.35
4	L	4003	A1EF9	C16-C14-C15	-3.55	107.17	112.58
4	L	4003	A1EF9	C34-N13-N12	3.47	107.50	104.36
4	L	4003	A1EF9	C35-N12-C32	-3.33	125.28	129.51
4	L	4003	A1EF9	O06-S01-C23	3.03	111.87	108.05
4	L	4003	A1EF9	C33-C32-C31	-2.99	122.85	129.91
4	L	4003	A1EF9	O05-S01-N09	2.98	112.41	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4003	A1EF9	O06-S01-N09	2.81	112.08	106.97

There are no chirality outliers.

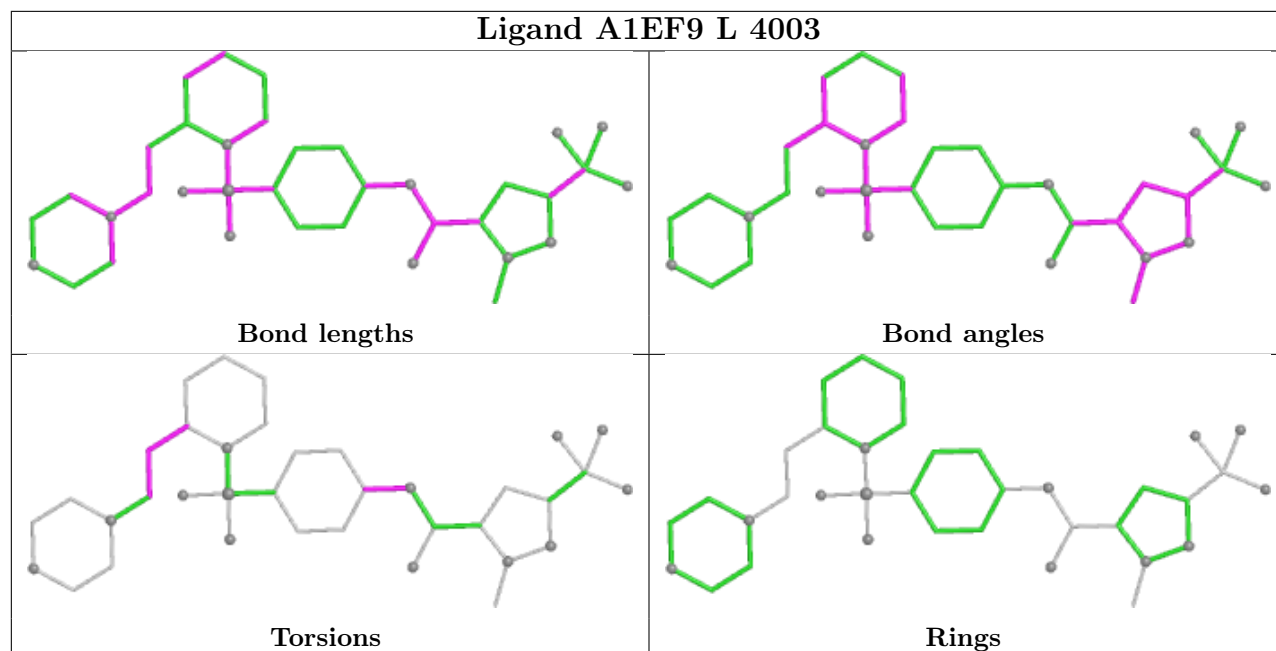
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	4003	A1EF9	C14-C16-C20-N10
4	L	4003	A1EF9	C28-C30-N11-C31
4	L	4003	A1EF9	C29-C30-N11-C31
4	L	4003	A1EF9	C15-C14-C16-C20

There are no ring outliers.

No monomer is involved in short contacts.

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.

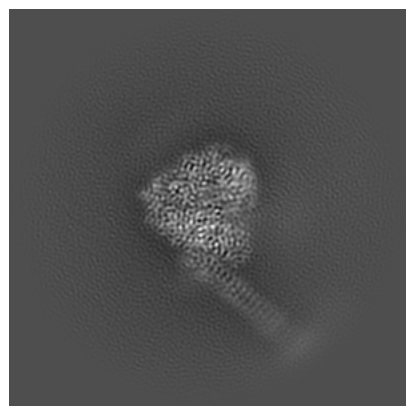
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65367. These allow visual inspection of the internal detail of the map and identification of artifacts.

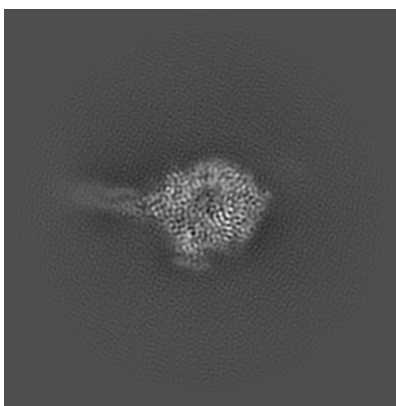
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

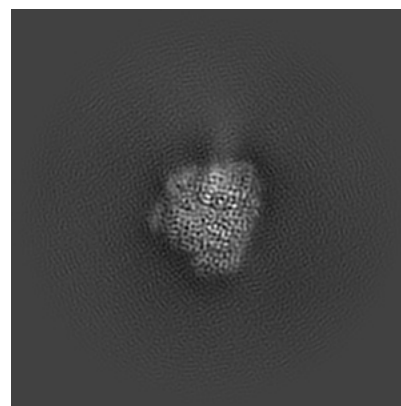
6.1.1 Primary map



X

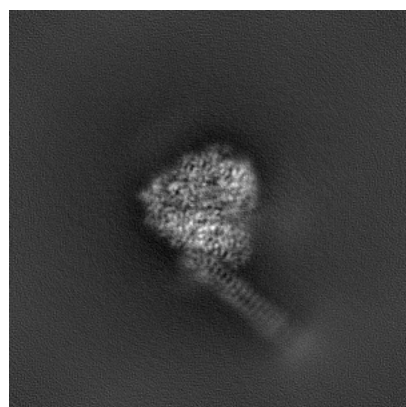


Y

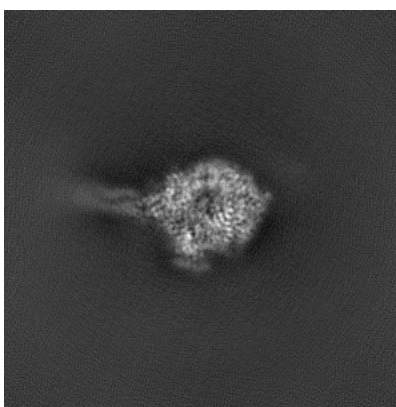


Z

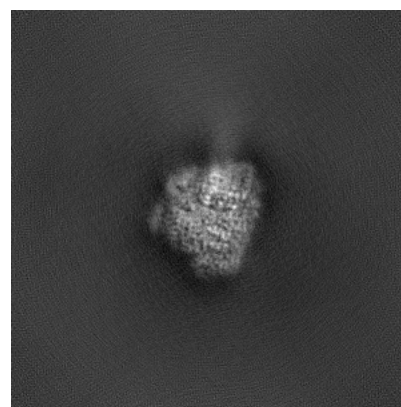
6.1.2 Raw map



X



Y

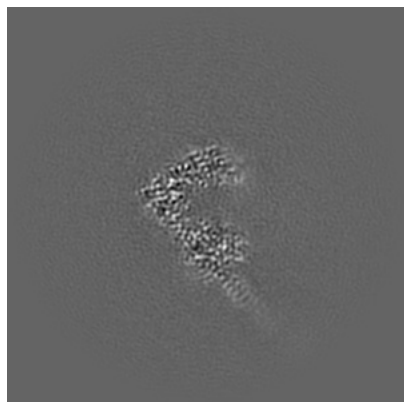


Z

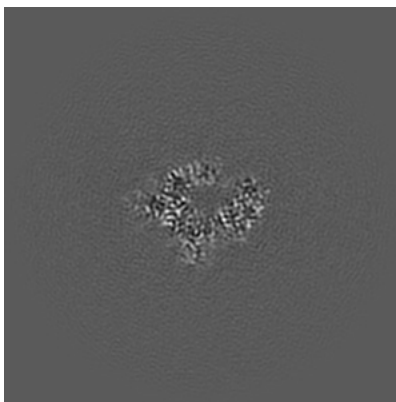
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

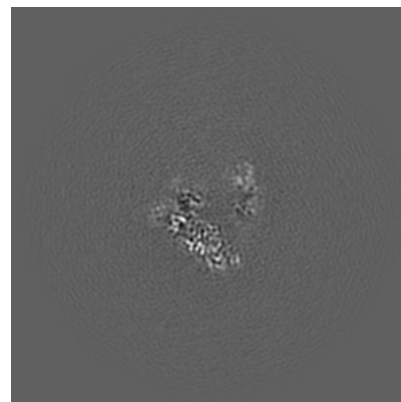
6.2.1 Primary map



X Index: 180

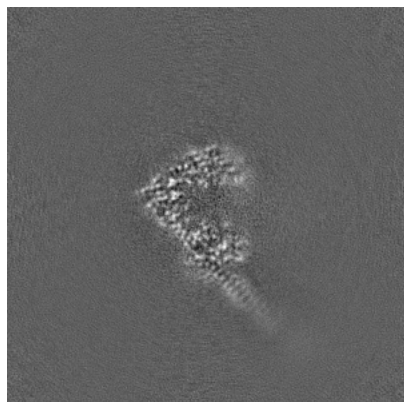


Y Index: 180

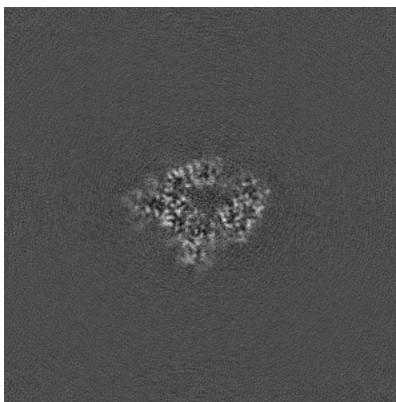


Z Index: 180

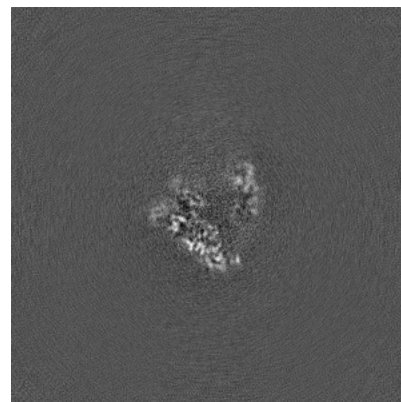
6.2.2 Raw map



X Index: 180



Y Index: 180

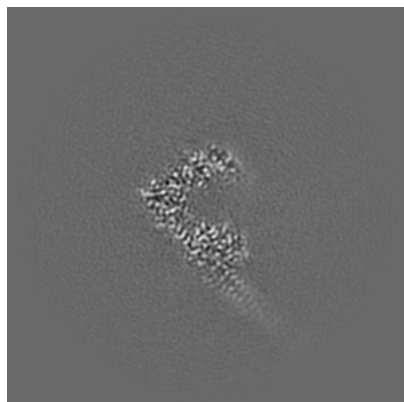


Z Index: 180

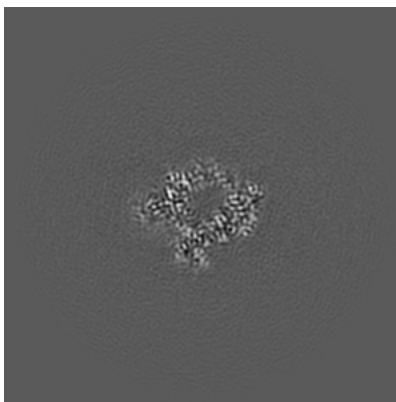
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

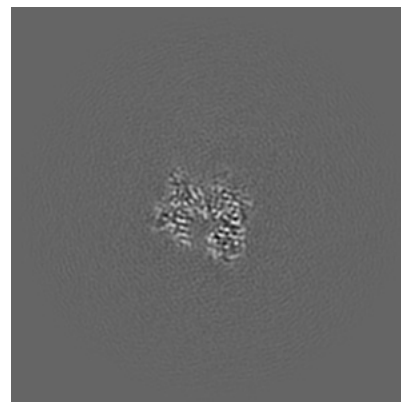
6.3.1 Primary map



X Index: 182

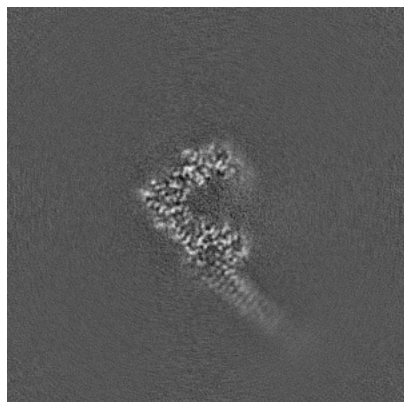


Y Index: 172

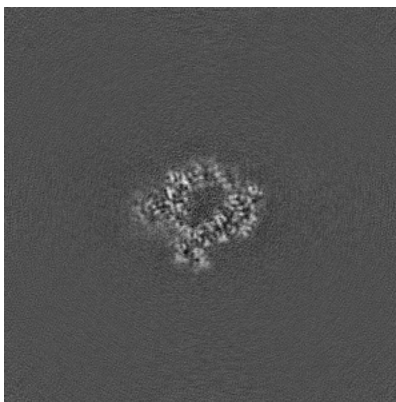


Z Index: 163

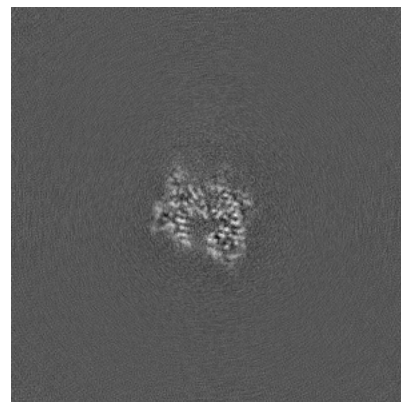
6.3.2 Raw map



X Index: 183



Y Index: 172

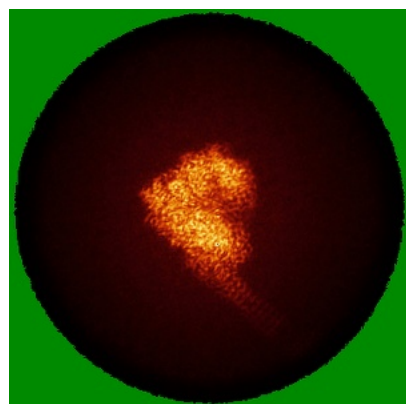


Z Index: 163

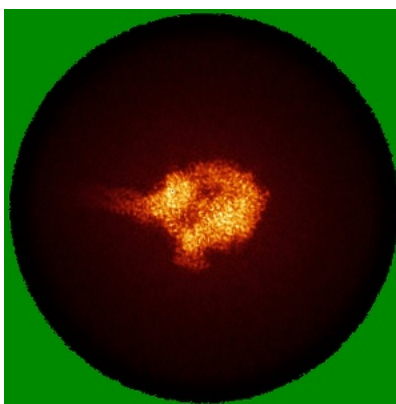
The images above show the largest variance slices of the map in three orthogonal directions.

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

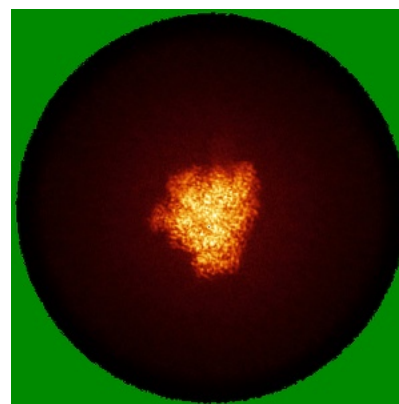
6.4.1 Primary map



X

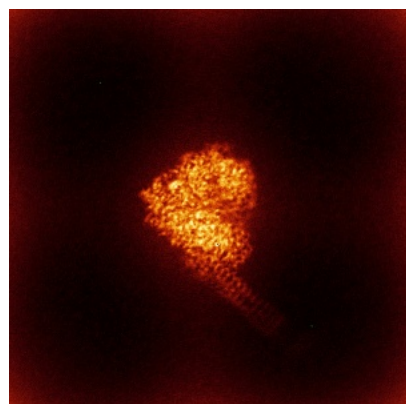


Y

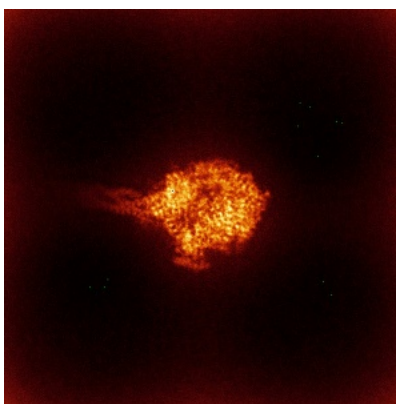


Z

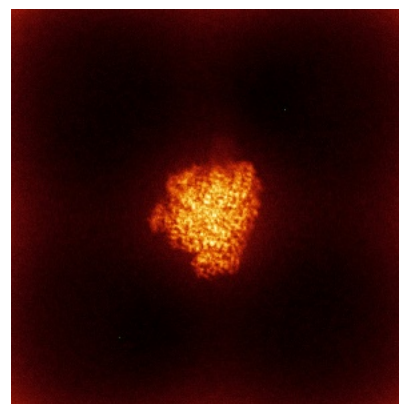
6.4.2 Raw map



X



Y

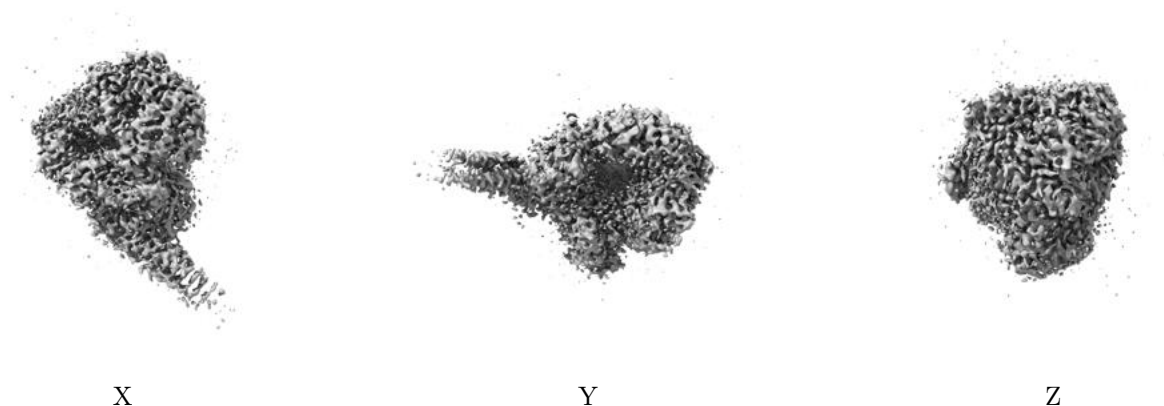


Z

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

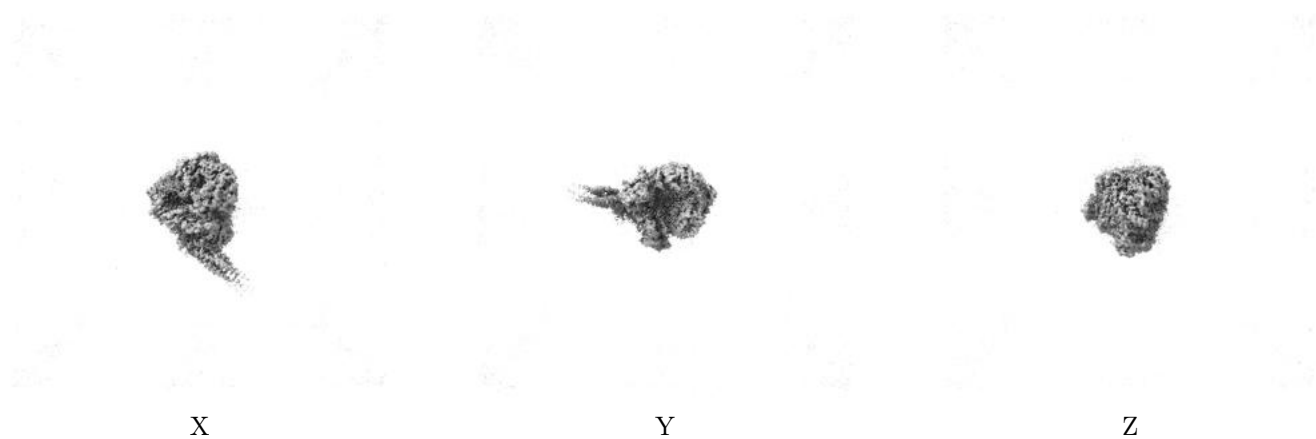
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

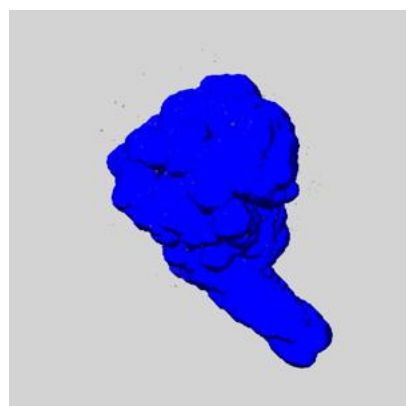
6.6 Mask visualisation [i](#)

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

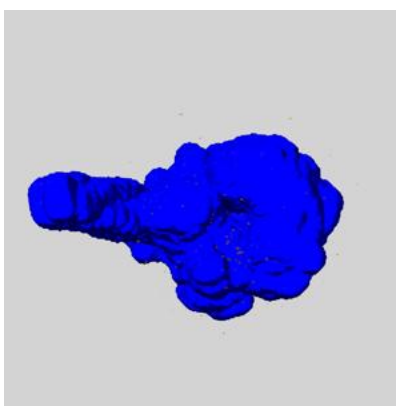
A mask typically either:

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

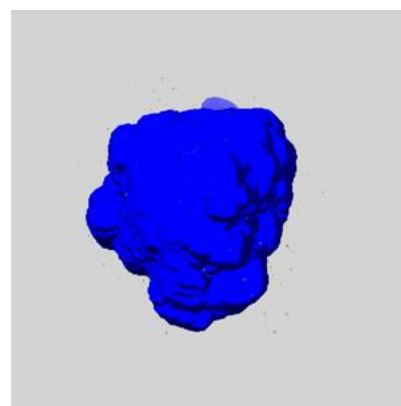
6.6.1 emd_65367_msk_1.map [i](#)



X



Y

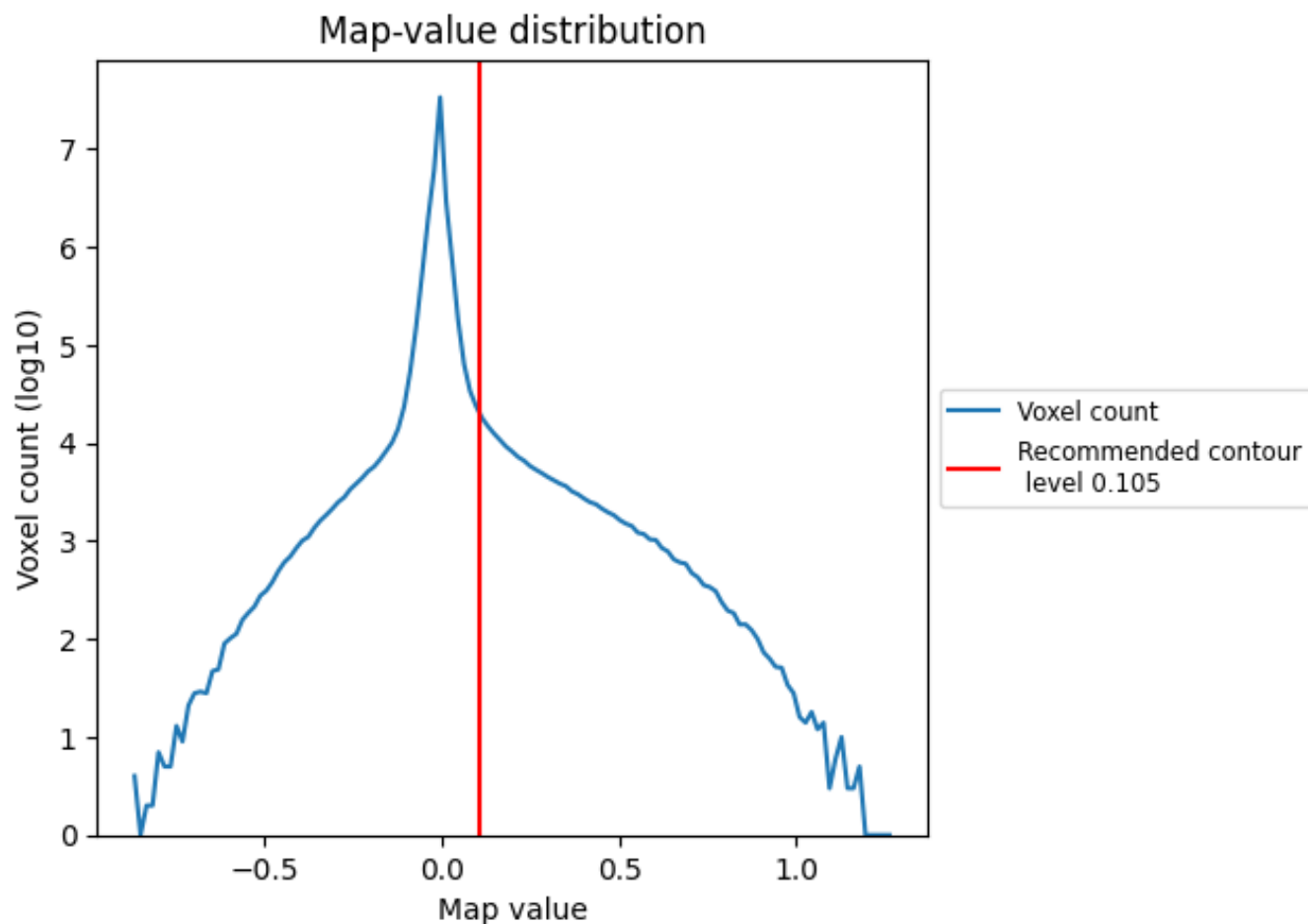


Z

7 Map analysis [i](#)

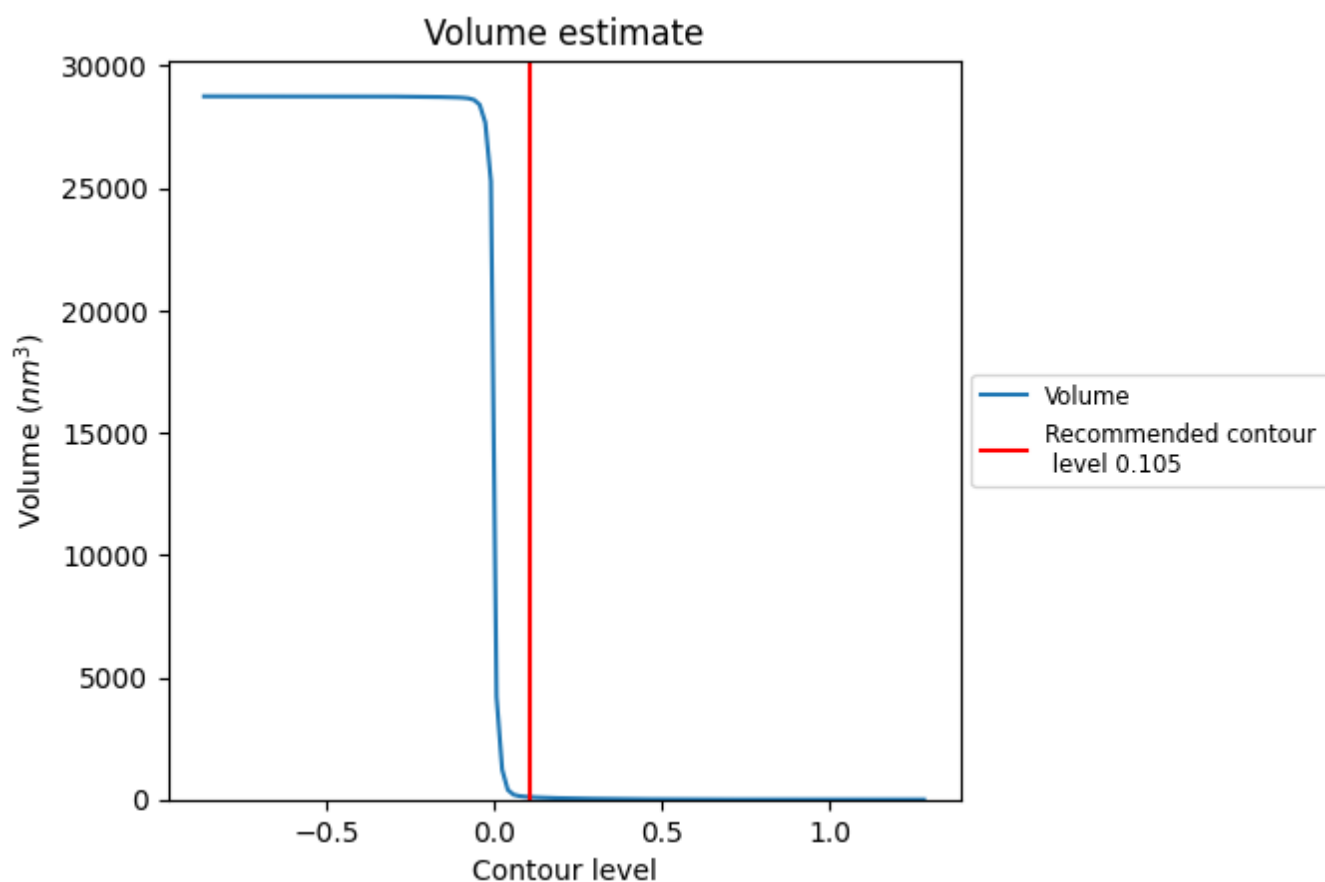
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

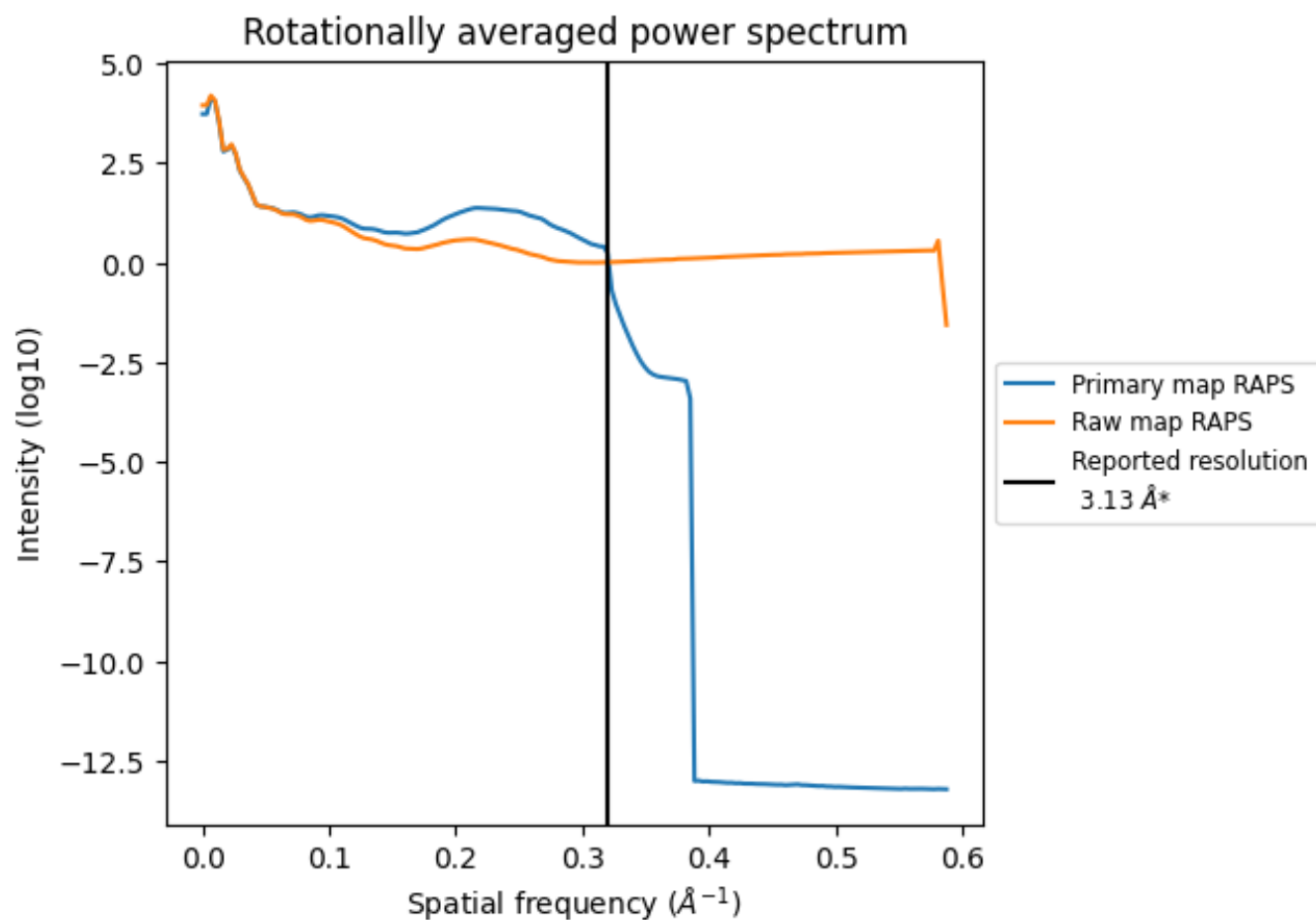
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

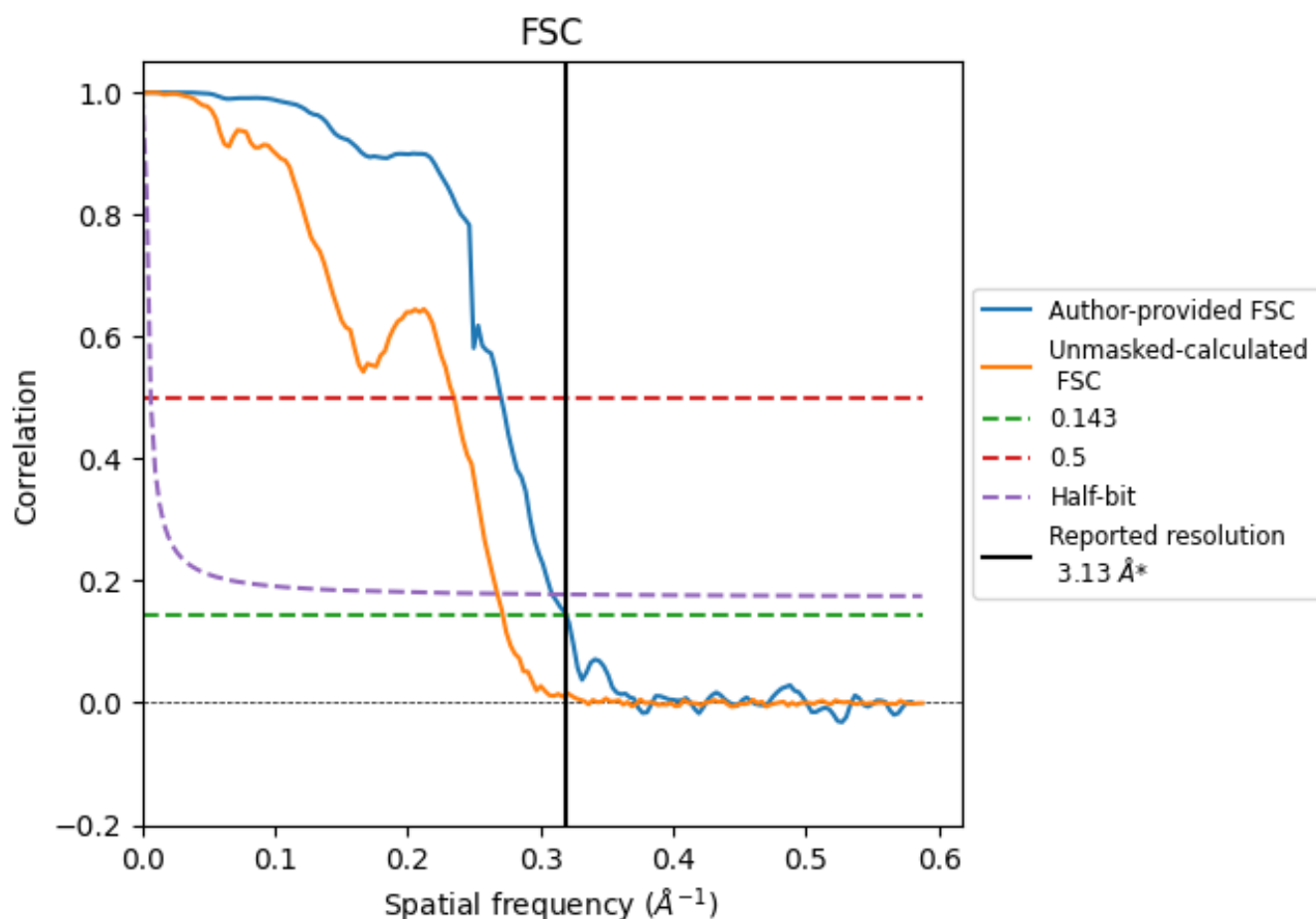


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

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 0.319 Å⁻¹

8.2 Resolution estimates [i](#)

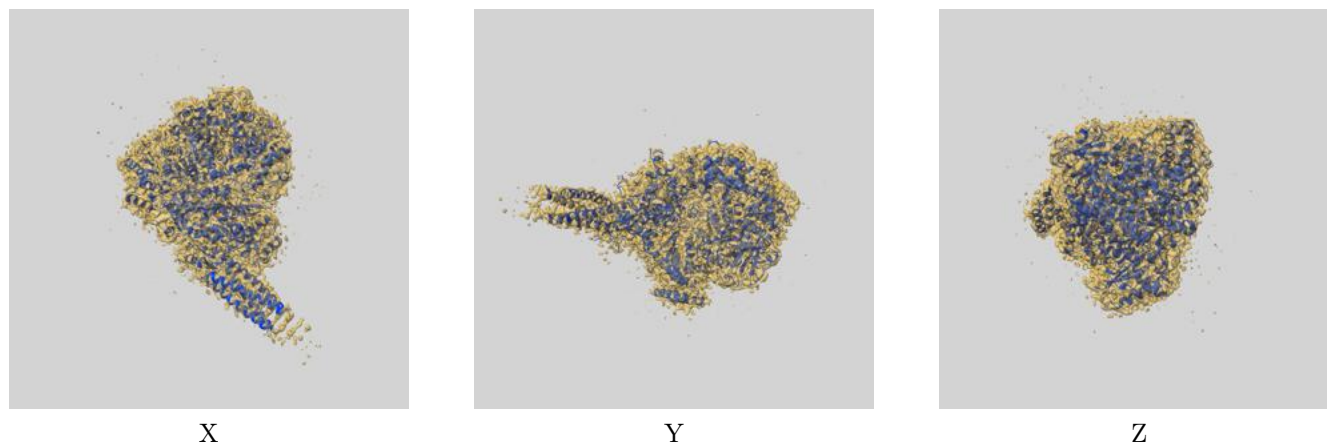
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.70	3.24
Unmasked-calculated*	3.68	4.26	3.74

*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 3.68 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

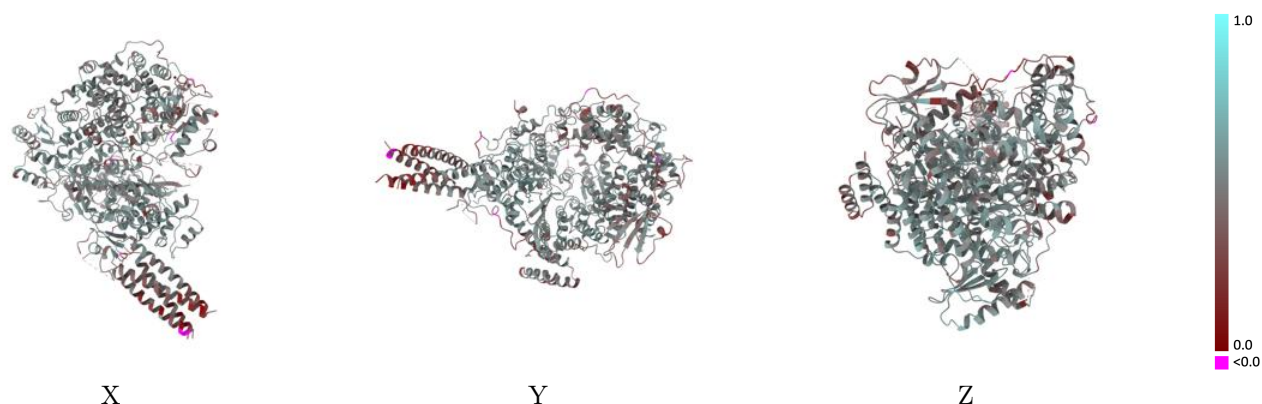
This section contains information regarding the fit between EMDB map EMD-65367 and PDB model 9VUL. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



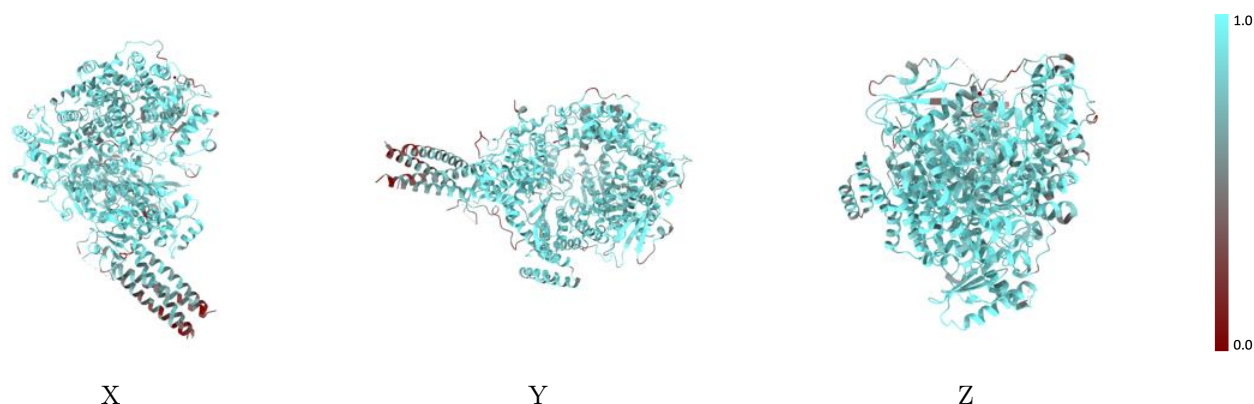
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



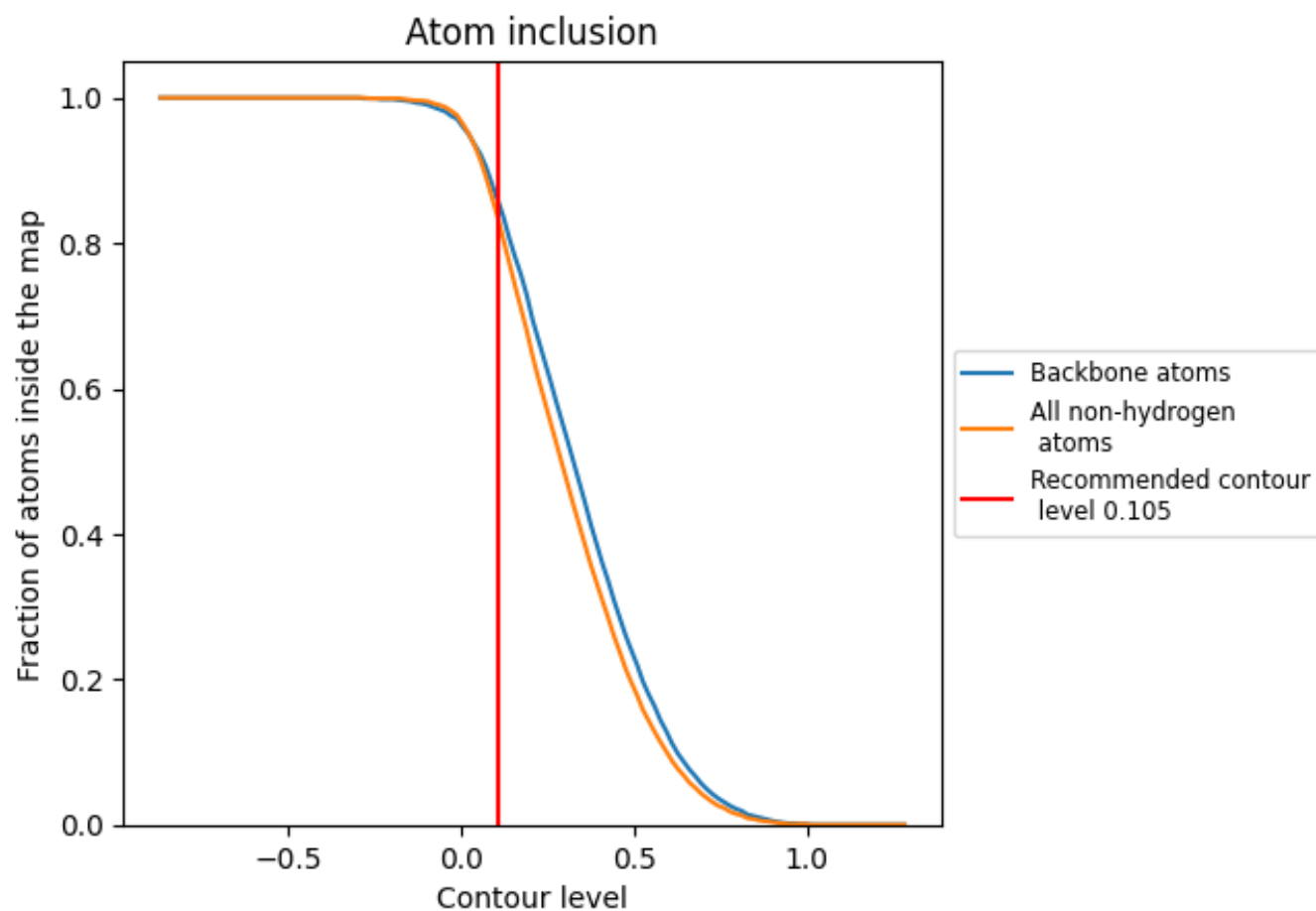
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8390	<div></div> 0.4790
A	<div></div> 0.6850	<div></div> 0.3990
B	<div></div> 0.5510	<div></div> 0.3410
C	<div></div> 0.6640	<div></div> 0.4040
D	<div></div> 0.6920	<div></div> 0.3840
L	<div></div> 0.8740	<div></div> 0.4970

