



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:23 PM UTC

PDB ID : 8DSA / pdb_00008dsa
EMDB ID : EMD-27687
Title : LRRC8A:C in MSP1E3D1 nanodisc
Authors : Kern, D.M.; Brohawn, S.G.
Deposited on : 2022-07-21
Resolution : 3.48 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

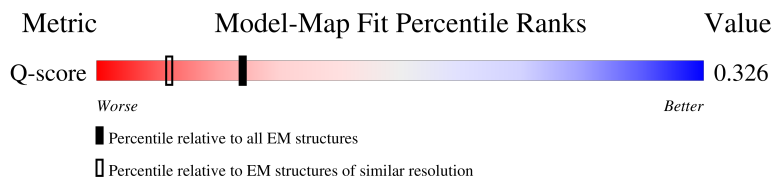
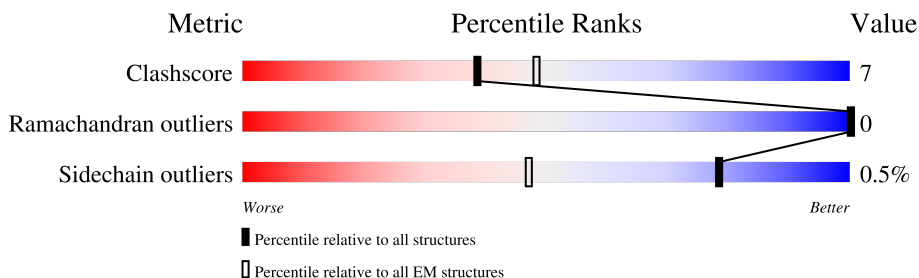
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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	13672 (2.98 - 3.98)

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	911	
1	B	911	
1	C	911	
1	D	911	

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Mol	Chain	Length	Quality of chain
1	E	911	 10% 17% 5% 78%
2	F	813	 12% 19% 5% 77%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12039 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 Volume-regulated anion channel subunit LRRC8A, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		
1	B	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		
1	C	320	Total	C	N	O	S	0	0
			2685	1771	431	466	17		
1	D	316	Total	C	N	O	S	0	0
			2646	1747	424	458	17		
1	E	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68D	TRP	-	linker	UNP Q80WG5
A	68E	ALA	-	linker	UNP Q80WG5
A	68F	ALA	-	linker	UNP Q80WG5
A	68G	SER	-	linker	UNP Q80WG5
A	68H	SER	-	linker	UNP Q80WG5
A	68O	TRP	MET	conflict	UNP P0ABE7
A	72F	ILE	HIS	conflict	UNP P0ABE7
A	72J	LEU	-	linker	UNP P0ABE7
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	68D	TRP	-	linker	UNP Q80WG5
B	68E	ALA	-	linker	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68F	ALA	-	linker	UNP Q80WG5
B	68G	SER	-	linker	UNP Q80WG5
B	68H	SER	-	linker	UNP Q80WG5
B	68O	TRP	MET	conflict	UNP P0ABE7
B	72F	ILE	HIS	conflict	UNP P0ABE7
B	72J	LEU	-	linker	UNP P0ABE7
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5
C	68D	TRP	-	linker	UNP Q80WG5
C	68E	ALA	-	linker	UNP Q80WG5
C	68F	ALA	-	linker	UNP Q80WG5
C	68G	SER	-	linker	UNP Q80WG5
C	68H	SER	-	linker	UNP Q80WG5
C	68O	TRP	MET	conflict	UNP P0ABE7
C	72F	ILE	HIS	conflict	UNP P0ABE7
C	72J	LEU	-	linker	UNP P0ABE7
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
D	68D	TRP	-	linker	UNP Q80WG5
D	68E	ALA	-	linker	UNP Q80WG5
D	68F	ALA	-	linker	UNP Q80WG5
D	68G	SER	-	linker	UNP Q80WG5
D	68H	SER	-	linker	UNP Q80WG5
D	68O	TRP	MET	conflict	UNP P0ABE7
D	72F	ILE	HIS	conflict	UNP P0ABE7
D	72J	LEU	-	linker	UNP P0ABE7
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
E	68D	TRP	-	linker	UNP Q80WG5
E	68E	ALA	-	linker	UNP Q80WG5
E	68F	ALA	-	linker	UNP Q80WG5
E	68G	SER	-	linker	UNP Q80WG5
E	68H	SER	-	linker	UNP Q80WG5
E	68O	TRP	MET	conflict	UNP P0ABE7
E	72F	ILE	HIS	conflict	UNP P0ABE7
E	72J	LEU	-	linker	UNP P0ABE7
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	191	Total	C	N	O	S	0	0
			1599	1071	246	264	18		

There are 10 discrepancies between the modelled and reference sequences:

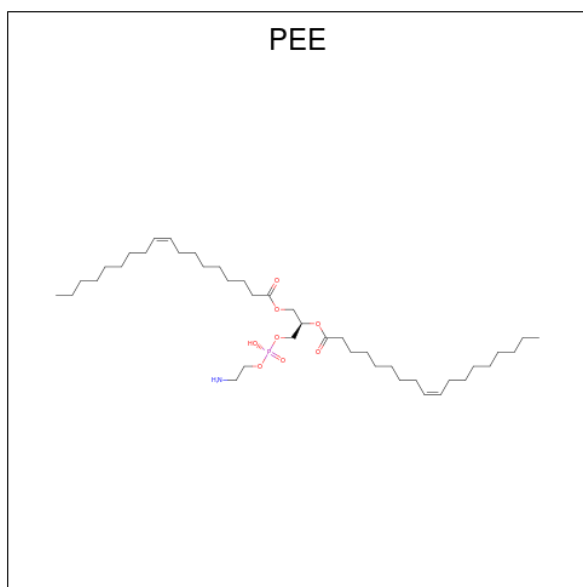
Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502

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Chain	Residue	Modelled	Actual	Comment	Reference
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	O			0
			10	8	2			
3	C	1	Total	C	O			0
			12	10	2			
3	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	O	0
			1	1	
4	B	1	Total	O	0
			1	1	
4	C	1	Total	O	0
			1	1	
4	D	1	Total	O	0
			1	1	

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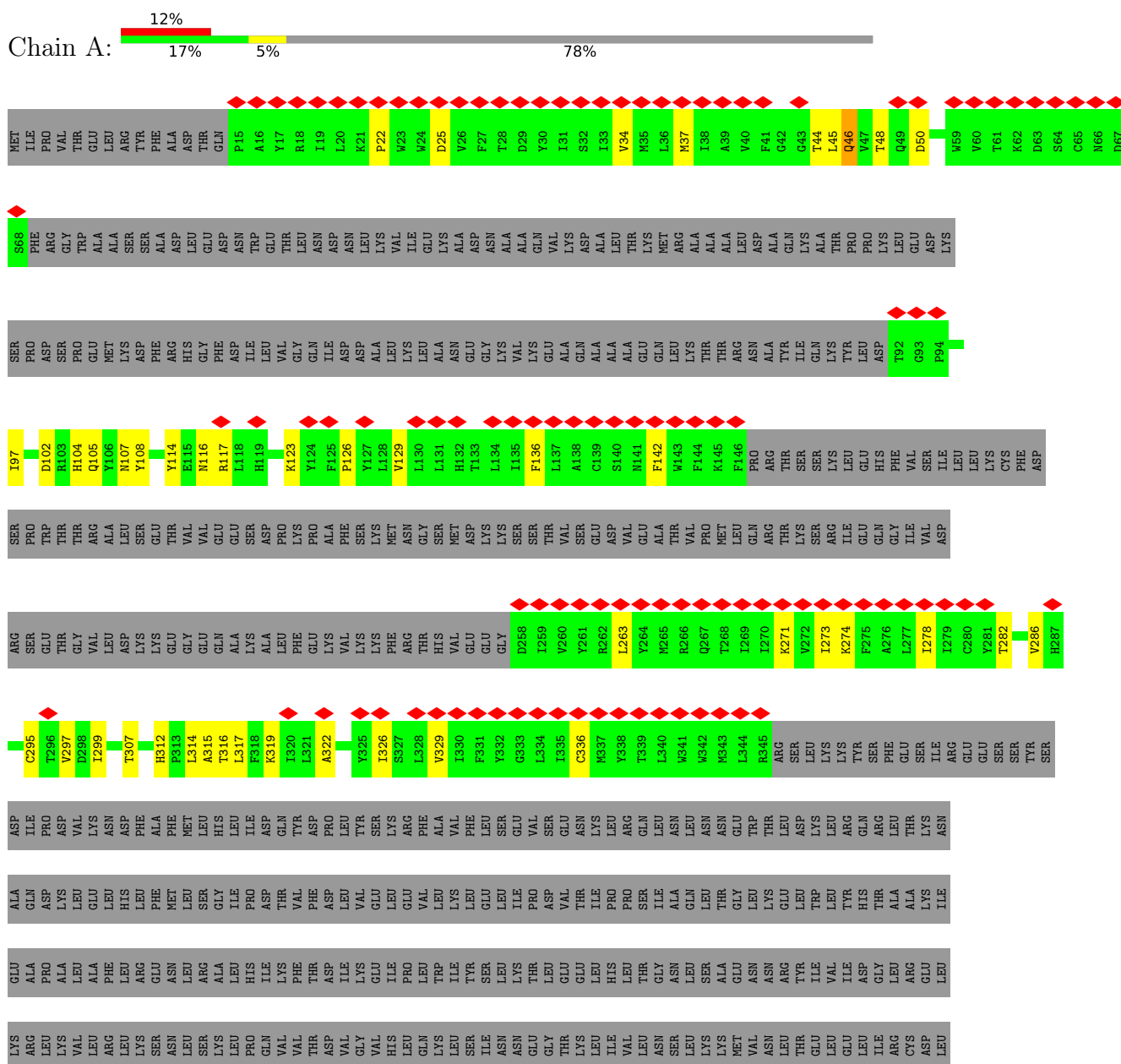
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Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	O	0
			1	1	
4	F	1	Total	O	0
			1	1	

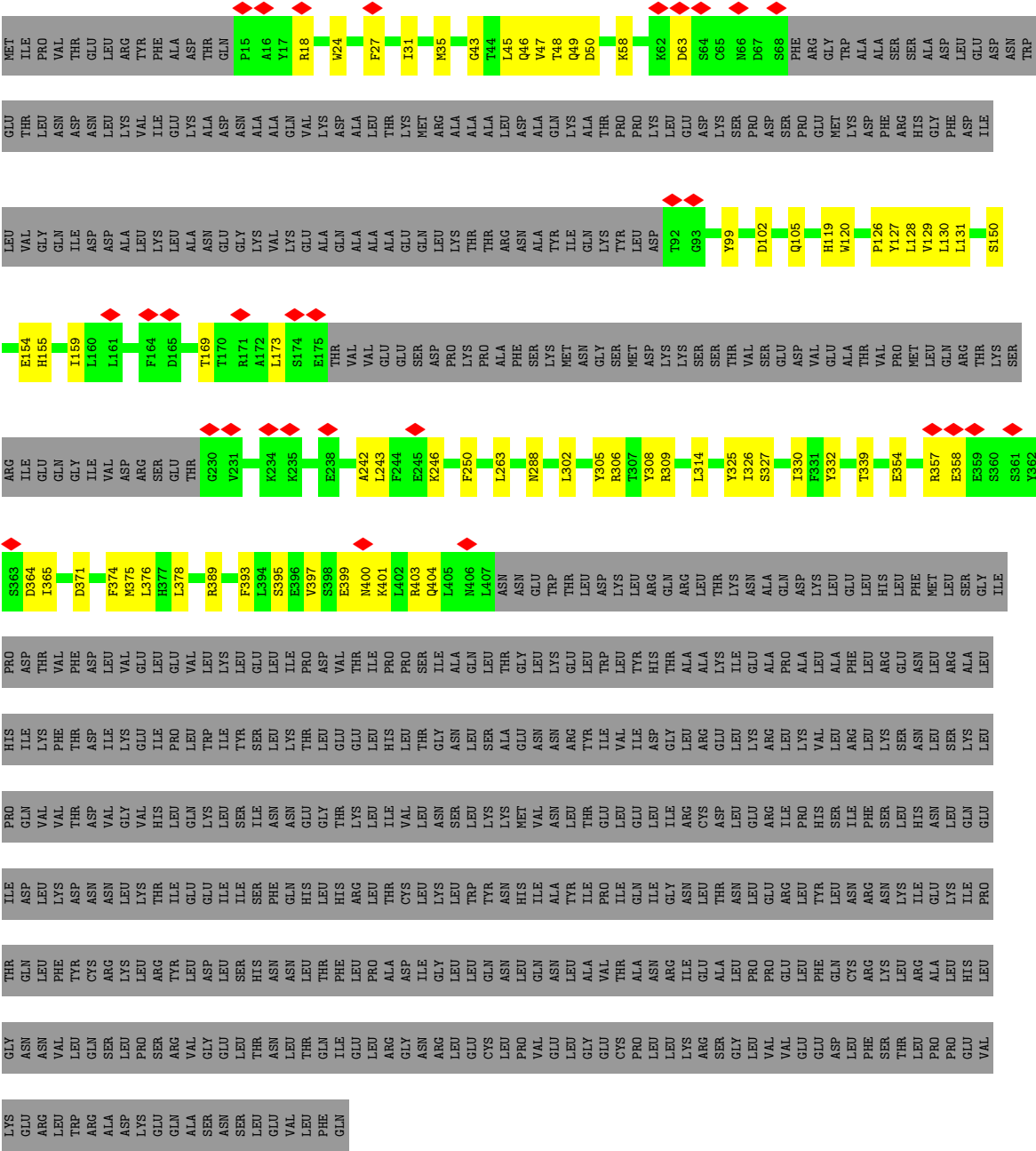
3 Residue-property plots

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.

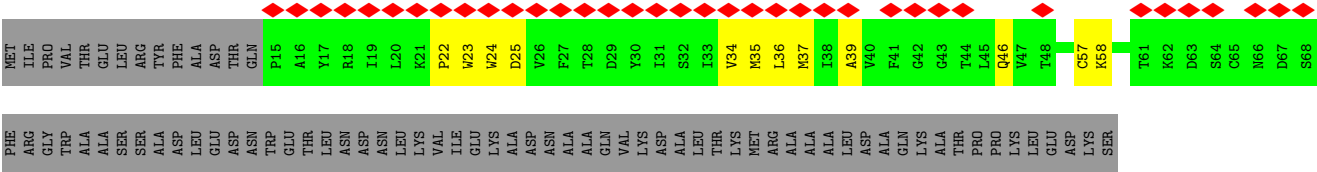
- Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

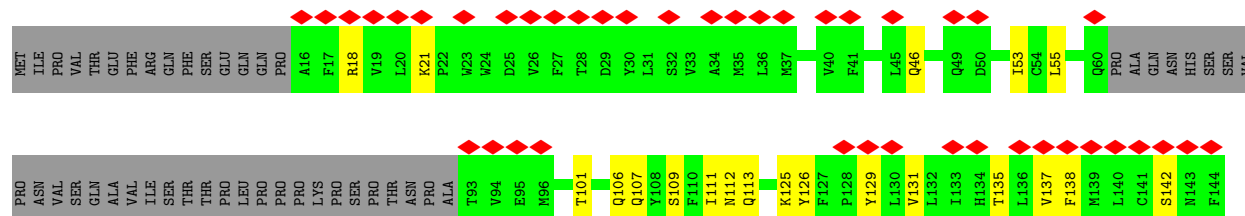
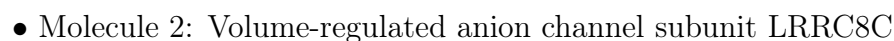






● Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562





HIS	VAL	GLY	LYS	ASN	GLY	ILE	LEU	LEU	ASN	LEU	Y343	Q285	GLY	W145
PHE	LEU	VAL	LEU	ASN	SER	ALA	ASN	ASN	ASN	GLU	R344	T266	ASN	F146
GLU	LEU	LEU	TRP	LEU	LEU	GLN	LEU	LEU	LEU	THR	R345	T267	LEU	K147
VAL	LEU	GLN	TYR	LYS	HIS	HIS	ASP	ASP	ASN	GLU	L268	L268	ARG	F148
LEU	SER	SER	ASN	LYS	ASP	ASP	ASN	ASN	ASN	GLU	ARG	K269	SER	PRO
PRO	LEU	LEU	SER	MET	ILE	ILE	THR	THR	GLU	THR	GLU	V270	GLN	GLY
PRO	PRO	GLN	ILE	THR	ASN	GLN	LEU	LEU	PRO	TYR	TYR	I271	SER	SER
GLU	GLU	PHE	ALA	ASN	SER	GLN	LEU	LEU	LEU	PHE	ASP	K272	LEU	SER
LEU	LEU	SER	ILE	THR	ASN	GLU	VAL	LEU	LEU	GLY	TYR	F273	SER	SER
ASP	ASP	ILE	PRO	GLU	VAL	CYS	LEU	THR	LEU	THR	ILE	I274	ILE	LYS
CYS	THR	THR	GLU	LEU	THR	LEU	HIS	ARG	ARG	VAL	ARG	I275	PRO	ILE
ARG	ARG	CYS	HIS	GLU	LEU	GLU	GLN	GLN	GLN	ARG	ARG	I276	GLU	GLU
ALA	ASN	ASN	ILE	LEU	GLU	CYS	VAL	GLN	GLN	GLN	GLN	I277	LYS	PHE
LEU	LEU	VAL	LYS	VAL	LEU	THR	LEU	LEU	LEU	THR	THR	A278	PHE	ILE
LYS	ARG	ARG	LEU	CYS	ARG	VAL	VAL	VAL	VAL	GLY	ILE	Y279	VAL	SER
ALA	ALA	SER	THR	ASP	ASP	LYS	THR	THR	ASN	ILE	ASP	N280	VAL	ILE
GLY	LEU	LEU	SER	LEU	LEU	ILE	ASN	ASN	ALA	ASP	ASP	S281	GLY	LEU
LEU	PRO	PRO	LEU	GLU	LYS	HIS	ALA	ALA	HIS	ASP	ASP	A282	LYS	GLY
VAL	VAL	ASP	GLU	ARG	LEU	LEU	SER	SER	ASN	ILE	ILE	L283	ALA	CYS
THR	THR	TYR	PHE	PRO	LYS	ALA	ARG	ARG	PRO	PRO	PRO	V284	ALA	PHE
ASP	ASP	TYR	PHE	HIS	ILE	ILE	LEU	LEU	ASP	ASP	ASP	S285	GLY	ASP
ALA	ALA	PHE	PHE	ALA	LEU	SER	PHE	PHE	VAL	VAL	VAL	K286	ALA	SER
LEU	LEU	CYS	SER	VAL	SER	LEU	THR	THR	GLU	GLU	LYS		LEU	PRO
PHE	LEU	LYS	HIS	PHE	ILE	LEU	LEU	LEU	PRO	ASN	ASN		ASP	TRP
GLU	GLU	LYS	ASN	SER	LYS	LYS	LEU	LEU	LEU	ASP	ASP	F289	LYS	THR
THR	THR	LEU	LYS	LEU	SER	GLU	ILE	ILE	ILE	PHE	PHE	D296	GLY	ARG
PRO	PRO	THR	GLU	SER	VAL	ASN	LEU	LEU	MET	ALA	ALA		GLY	ALA
LEU	LEU	LEU	VAL	LEU	SER	LYS	SER	GLY	SER	LEU	MET		GLY	LEU
ASP	ASP	LYS	LEU	GLN	LYS	ILE	LYS	VAL	GLY	LEU	HIS	M300	GLN	SER
VAL	VAL	ILE	PRO	GLU	ILE	LEU	LEU	LEU	LEU	LEU	MET	T301	ALA	GLU
ARG	ARG	GLY	SER	LEU	PRO	GLN	PRO	PRO	PRO	MET	GLY	G302	ALA	VAL
GLU	GLU	ASN	LEU	ASP	GLN	VAL	VAL	VAL	ASP	ILE	ILE	Y303	LYS	SER
GLN	GLN	MET	PHE	LYS	VAL	PHE	THR	THR	THR	ASP	ASP		LEU	GLY
LYS	LYS	LYS	LEU	GLU	VAL	VAL	VAL	VAL	GLN	GLN	GLN	N309	PHE	GLY
ALA	ALA	LEU	CYS	ASN	ASN	ASP	ASP	ASP	GLU	ASP	ASP		GLY	ASP
ASP	ASP	VAL	VAL	ASN	VAL	MET	ASP	ASP	ILE	PRO	PRO	H314	LYS	SER
SER	SER	LEU	LYS	LEU	SER	ARG	SER	GLU	THR	LEU	LEU	K318	VAL	GLU
ASN	ASN	SER	ILE	LYS	LEU	GLU	GLU	GLU	TYR	TYR	TYR	L319	LYS	GLU
SER	SER	PRO	ARG	SER	HIS	GLU	LEU	LEU	SER	SER	SER	S320	PHE	ASP
GLU	GLU	LYS	TYR	ILE	LEU	PRO	GLN	GLN	ARG	ARG	ARG		LEU	ASN
ASN	ASN	ILE	LEU	GLU	GLN	TRP	PRO	SER	THR	PHE	PHE	Y323	LEU	ARG
LEU	LEU	GLY	ASP	GLU	LYS	LYS	ILE	ILE	LEU	ALA	ALA	L324	HIS	LYS
TYR	TYR	ASN	LEU	ILE	MET	MET	THR	LEU	LEU	VAL	VAL	C325	VAL	ASN
THR	PHE	LEU	SER	VAL	CYS	TYR	GLY	GLU	PHE	VAL	VAL	F326	GLU	ASN
GLY	SER	LEU	LEU	PHE	HIS	HIS	LEU	LEU	ILE	LEU	LEU	V327	GLY	GLY
ASN	ASN	THR	ASP	GLN	ASN	ARG	ASN	ILE	SER	SER	SER	S328	GLY	ASP
LEU	LEU	TYR	ILE	THR	GLY	THR	GLY	LYS	GLU	VAL	VAL	I329	GLU	ARG
LEU	LEU	ASP	ILE	HIS	ASP	GLY	LEU	ASN	ASN	VAL	VAL	Y330	GLU	SER
LEU	LEU	ARG	THR	LEU	GLY	LEU	LEU	LYS	SER	SER	SER	G331	ASN	GLY
LEU	LEU	SER	ILE	LEU	THR	VAL	VAL	THR	PRO	LYS	LYS	L332	LEU	GLN
LEU	LEU	TYR	ARG	LEU	THR	GLY	GLY	ASN	VAL	VAL	VAL	T333	LEU	SER
LEU	LEU	ASP	PHE	ARG	ARG	LEU	LEU	LEU	GLU	GLU	GLU	C334	GLY	PRO
LEU	LEU	ASP	ILE	HIS	GLY	THR	GLY	GLY	ASN	VAL	VAL	L335	GLY	GLY
LEU	LEU	THR	THR	LEU	GLY	LEU	LEU	LEU	ASN	VAL	VAL	Y336	GLY	PRO
LEU	LEU	ASP	PHE	LEU	THR	GLY	GLY	GLY	VAL	VAL	VAL	T337	GLY	GLY
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	L338	GLY	GLY
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	Y339	GLY	GLY
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	W340	GLY	PRO
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	L341	GLY	PRO
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	R264	GLY	GLY
LEU	LEU	ASP	ILE	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	F342	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176166	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)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.703	Depositor
Minimum map value	-2.113	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	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: PEE

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	0.21	0/1715	0.43	0/2333
1	B	0.18	0/1715	0.40	0/2333
1	C	0.21	0/2762	0.44	0/3741
1	D	0.24	0/2721	0.47	0/3684
1	E	0.23	0/1715	0.51	0/2333
2	F	0.17	0/1644	0.39	0/2226
All	All	0.21	0/12272	0.45	0/16650

There are no bond length outliers.

There are no bond angle outliers.

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	1662	0	1657	30	0
1	B	1662	0	1657	21	0
1	C	2685	0	2670	34	0
1	D	2646	0	2642	46	0
1	E	1662	0	1657	32	0
2	F	1599	0	1605	29	0
3	C	22	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	95	0	147	6	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	12039	0	12063	175	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 175 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HD3	1:C:302:LEU:HD11	1.63	0.80
1:E:291:PHE:HE2	1:E:316:THR:H	1.33	0.76
1:D:46:GLN:HA	1:D:50:ASP:HB2	1.68	0.74
2:F:258:LEU:HA	2:F:261:MET:HE2	1.70	0.72
1:B:39:ALA:HB1	1:B:130:LEU:HD22	1.71	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	191/911 (21%)	183 (96%)	8 (4%)	0	100	100
1	B	191/911 (21%)	186 (97%)	5 (3%)	0	100	100
1	C	314/911 (34%)	308 (98%)	6 (2%)	0	100	100
1	D	310/911 (34%)	303 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	191/911 (21%)	183 (96%)	8 (4%)	0	100	100
2	F	185/813 (23%)	183 (99%)	2 (1%)	0	100	100
All	All	1382/5368 (26%)	1346 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/830 (22%)	179 (98%)	3 (2%)	55	70
1	B	182/830 (22%)	181 (100%)	1 (0%)	81	80
1	C	297/830 (36%)	295 (99%)	2 (1%)	76	77
1	D	293/830 (35%)	293 (100%)	0	100	100
1	E	182/830 (22%)	181 (100%)	1 (0%)	81	80
2	F	178/756 (24%)	178 (100%)	0	100	100
All	All	1314/4906 (27%)	1307 (100%)	7 (0%)	78	80

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	TRP
1	C	253	HIS
1	E	314	LEU
1	C	263	LEU
1	A	329	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	119	HIS
1	D	288	ASN

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Mol	Chain	Res	Type
2	F	288	GLN
1	A	267	GLN
1	B	49	GLN

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](#)

4 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	$\# Z > 2$
3	PEE	D	902	-	50,50,50	1.31	4 (8%)	53,55,55	0.97	1 (1%)
3	PEE	C	902	-	11,11,50	1.93	3 (27%)	11,11,55	1.59	2 (18%)
3	PEE	C	901	-	9,9,50	1.70	2 (22%)	9,9,55	1.63	2 (22%)
3	PEE	D	901	-	43,43,50	1.36	4 (9%)	46,48,55	1.05	2 (4%)

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
3	PEE	D	902	-	-	30/54/54/54	-
3	PEE	C	902	-	-	5/9/9/54	-
3	PEE	C	901	-	-	4/7/7/54	-
3	PEE	D	901	-	-	20/47/47/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	PEE	P-O4P	4.78	1.78	1.59
3	D	901	PEE	P-O4P	4.77	1.78	1.59
3	C	902	PEE	O4-C10	4.29	1.36	1.22
3	C	901	PEE	O4-C10	4.29	1.36	1.22
3	D	902	PEE	C39-C38	3.99	1.54	1.31

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	PEE	O2P-P-O1P	4.48	133.28	112.44
3	D	901	PEE	O2P-P-O1P	4.46	133.19	112.44
3	C	901	PEE	O2-C10-C11	3.38	124.69	114.00
3	C	902	PEE	O2-C10-C11	3.38	124.67	114.00
3	C	901	PEE	O4-C10-C11	-2.69	114.56	123.09

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

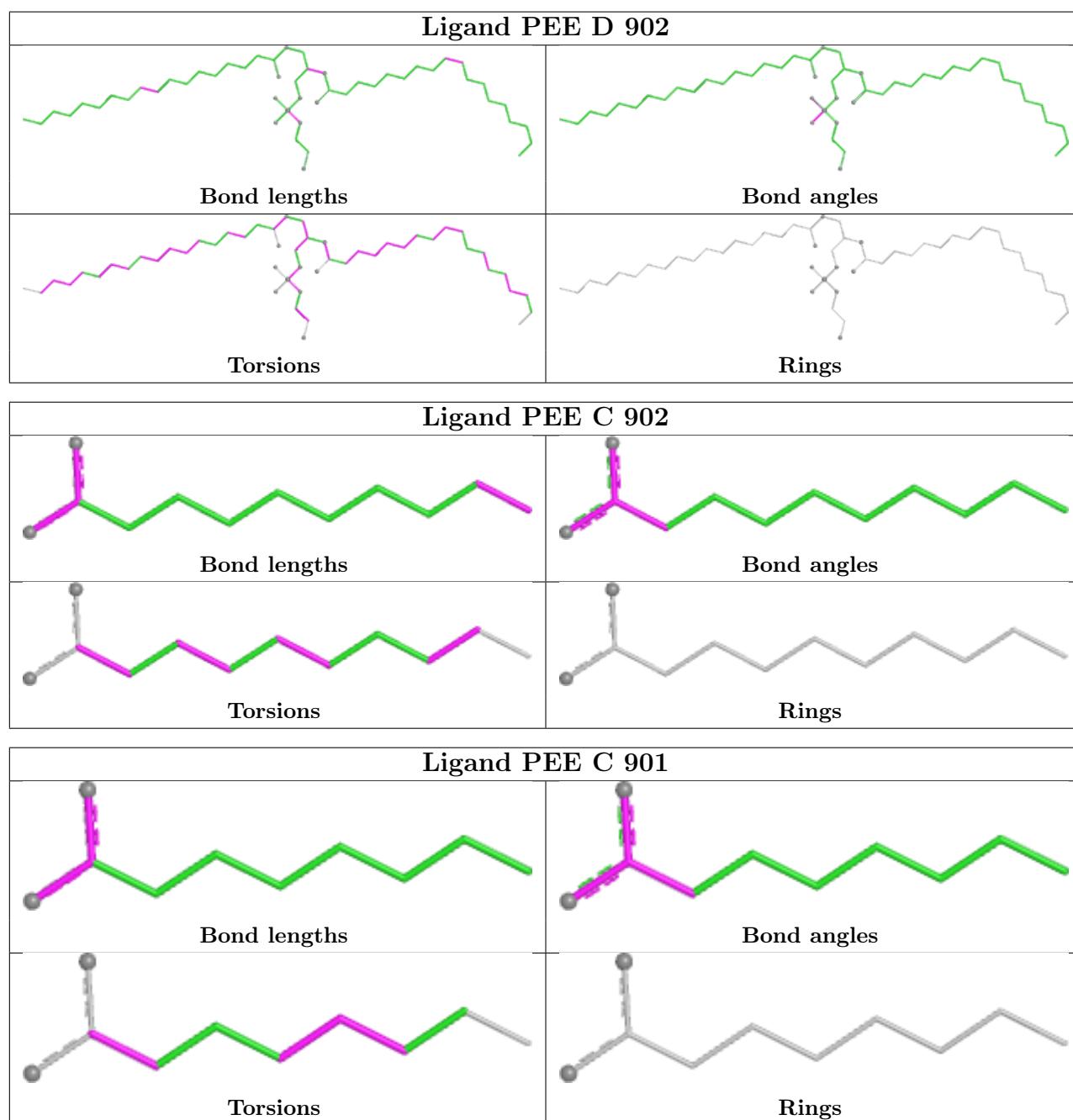
Mol	Chain	Res	Type	Atoms
3	D	901	PEE	C1-O3P-P-O1P
3	D	901	PEE	C1-O3P-P-O4P
3	D	901	PEE	C4-O4P-P-O3P
3	D	901	PEE	C37-C38-C39-C40
3	D	902	PEE	O4-C10-O2-C2

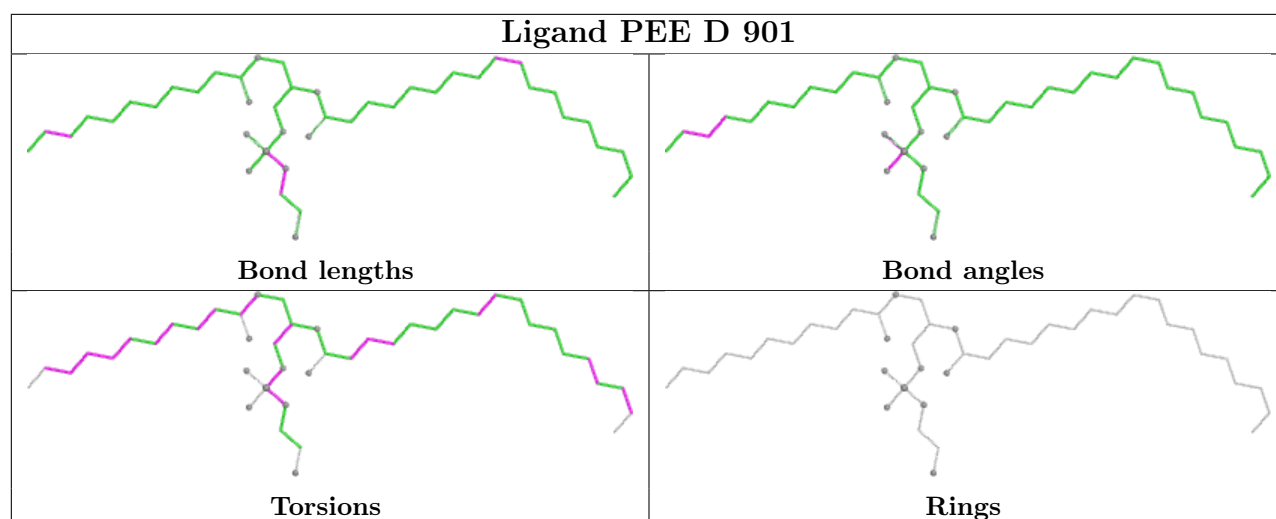
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	PEE	5	0
3	C	902	PEE	1	0
3	D	901	PEE	1	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.

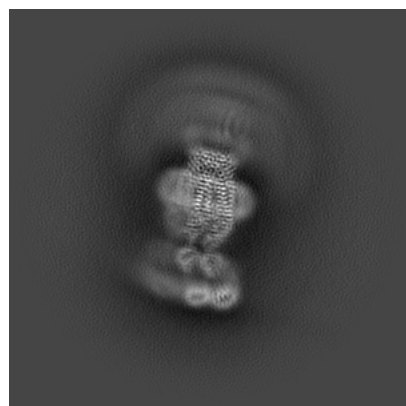
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27687. These allow visual inspection of the internal detail of the map and identification of artifacts.

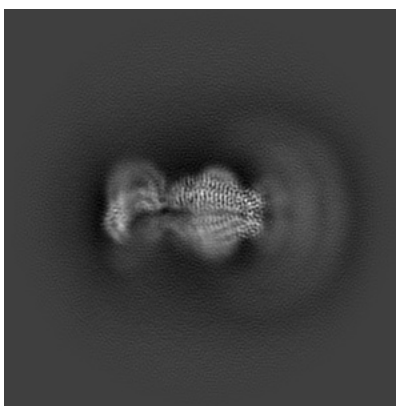
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

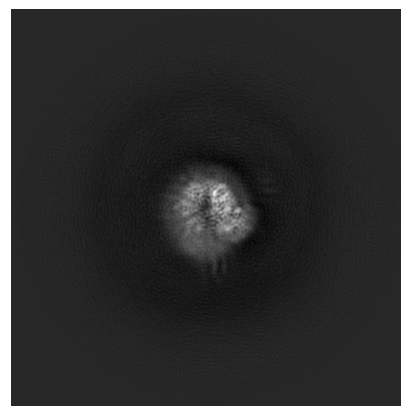
6.1.1 Primary map



X

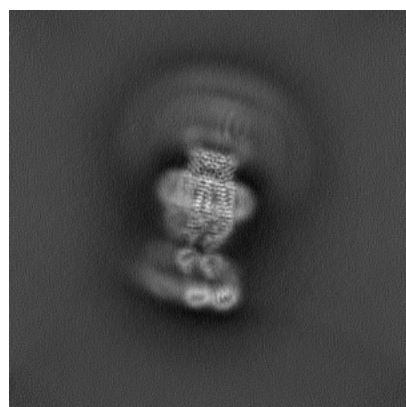


Y

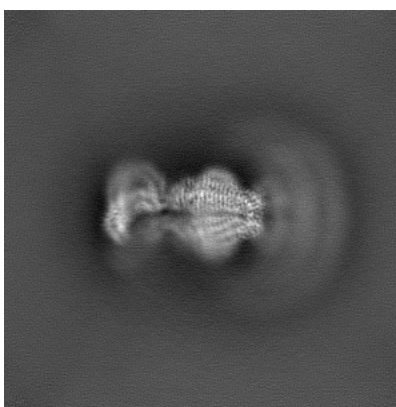


Z

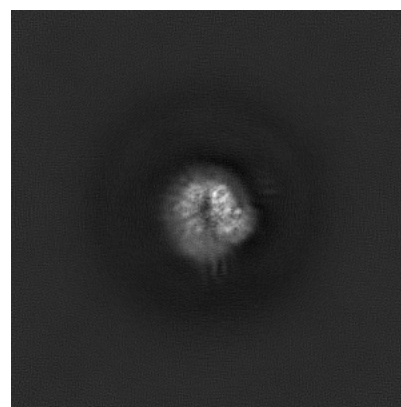
6.1.2 Raw map



X



Y

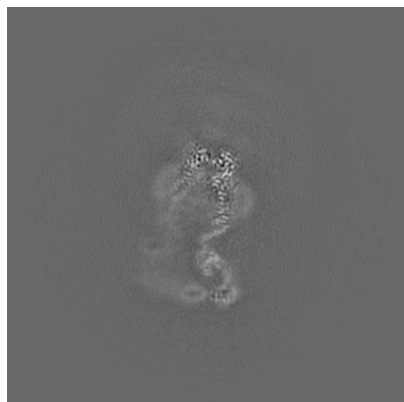


Z

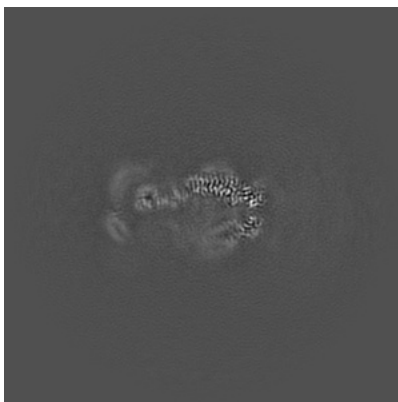
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

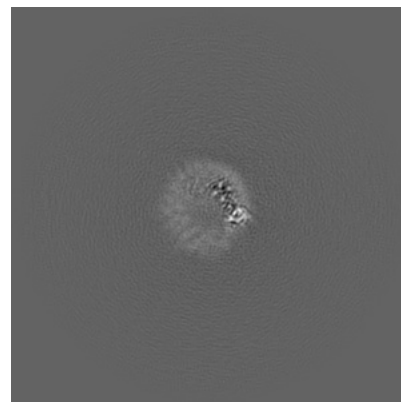
6.2.1 Primary map



X Index: 208

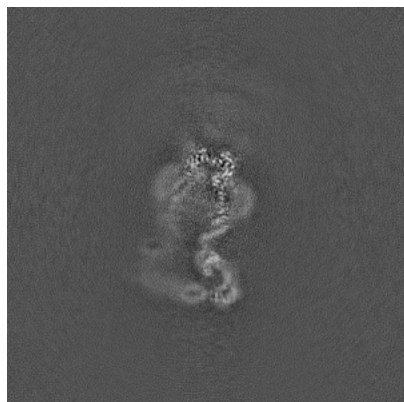


Y Index: 208

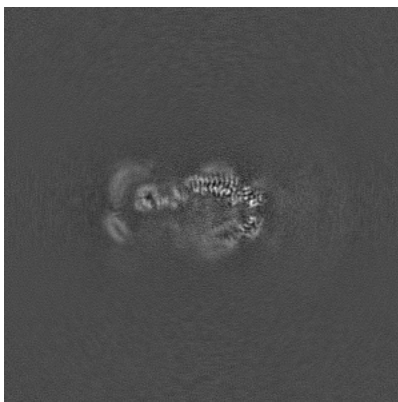


Z Index: 208

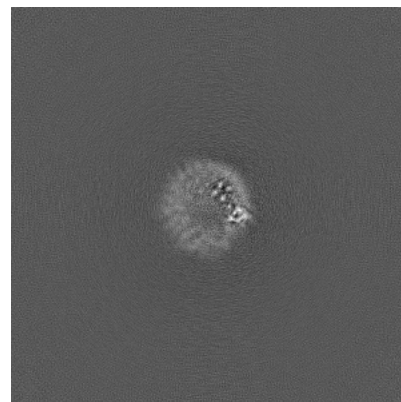
6.2.2 Raw map



X Index: 208



Y Index: 208

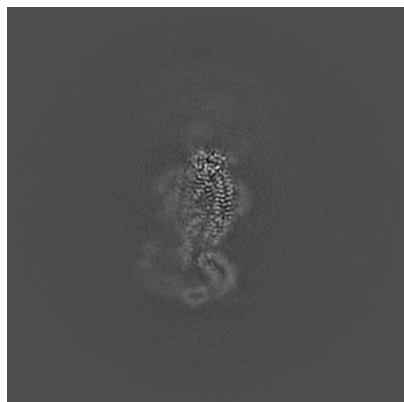


Z Index: 208

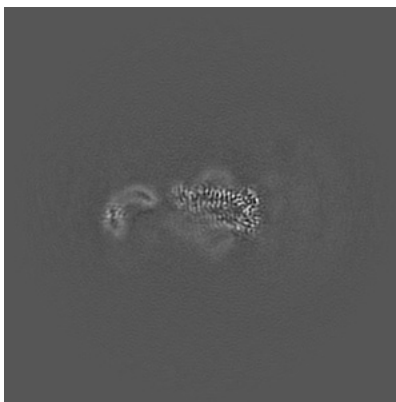
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

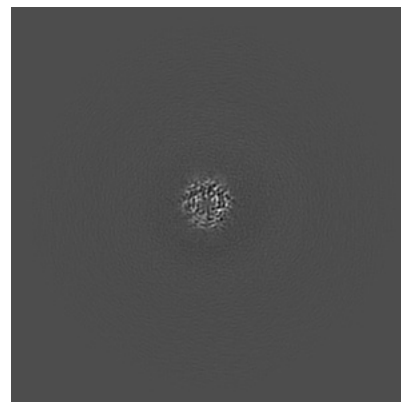
6.3.1 Primary map



X Index: 221

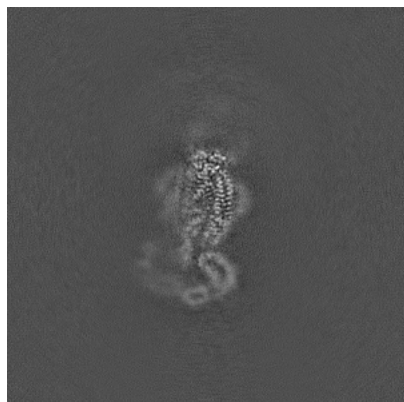


Y Index: 222

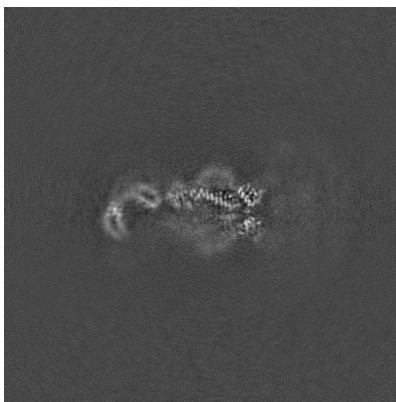


Z Index: 255

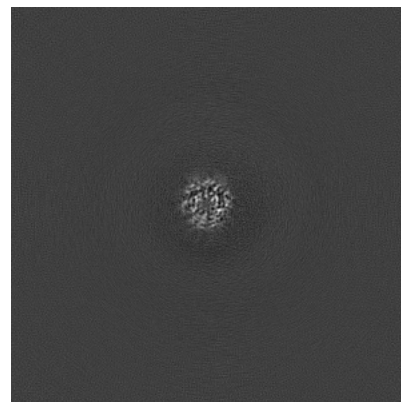
6.3.2 Raw map



X Index: 221



Y Index: 217

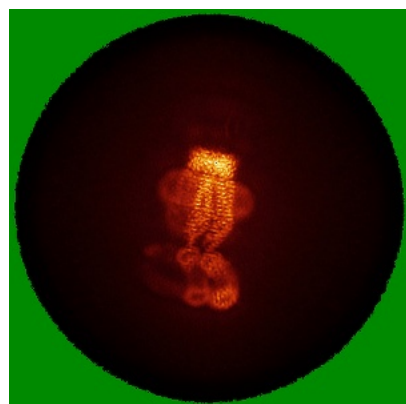


Z Index: 255

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

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

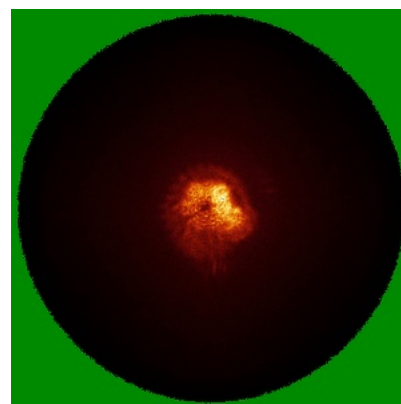
6.4.1 Primary map



X

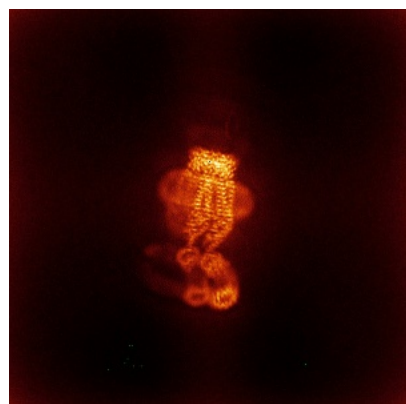


Y

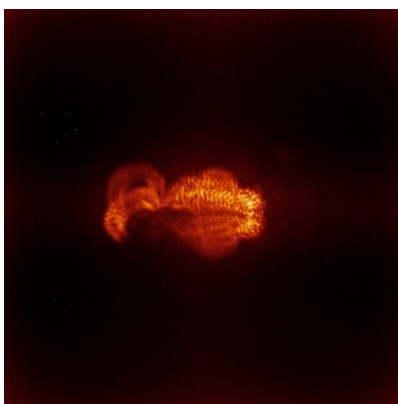


Z

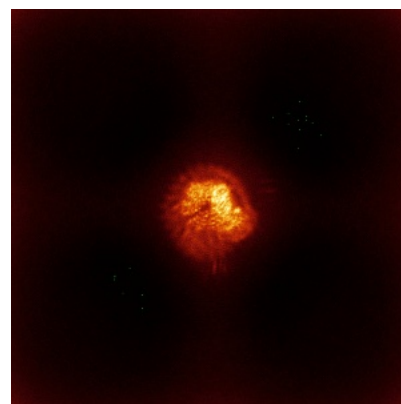
6.4.2 Raw map



X



Y

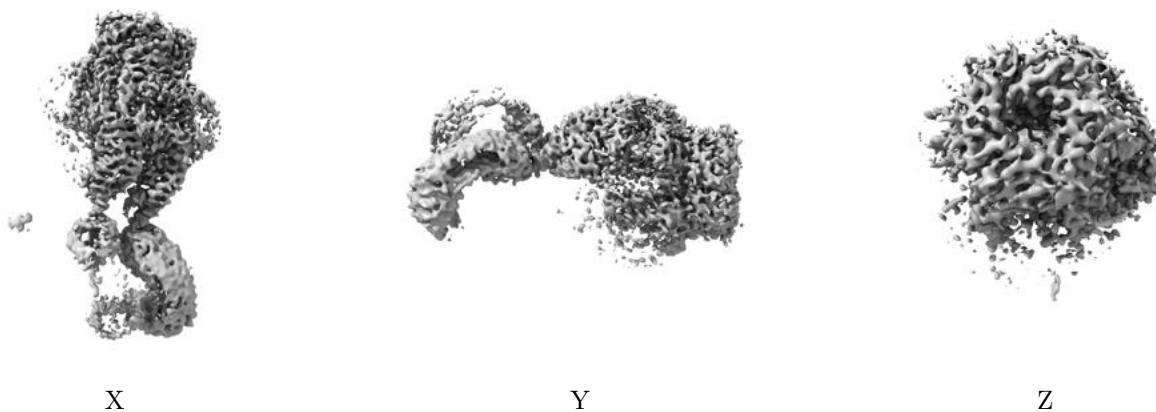


Z

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.

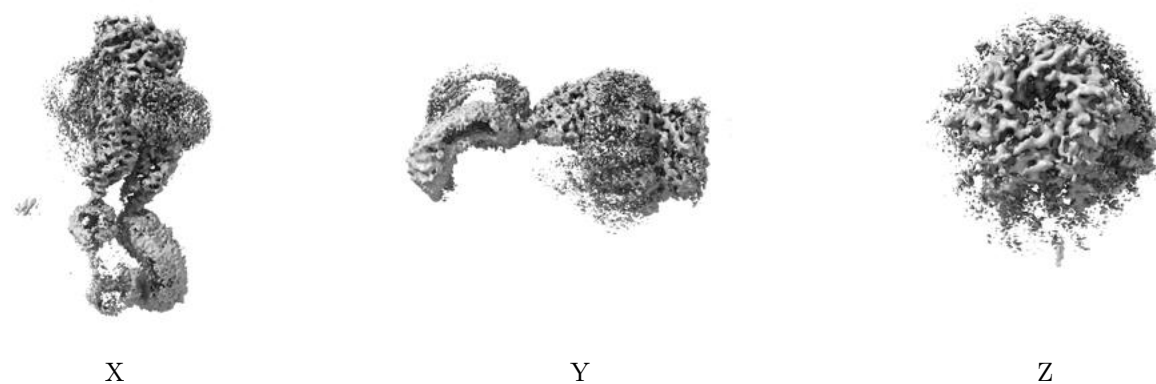
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

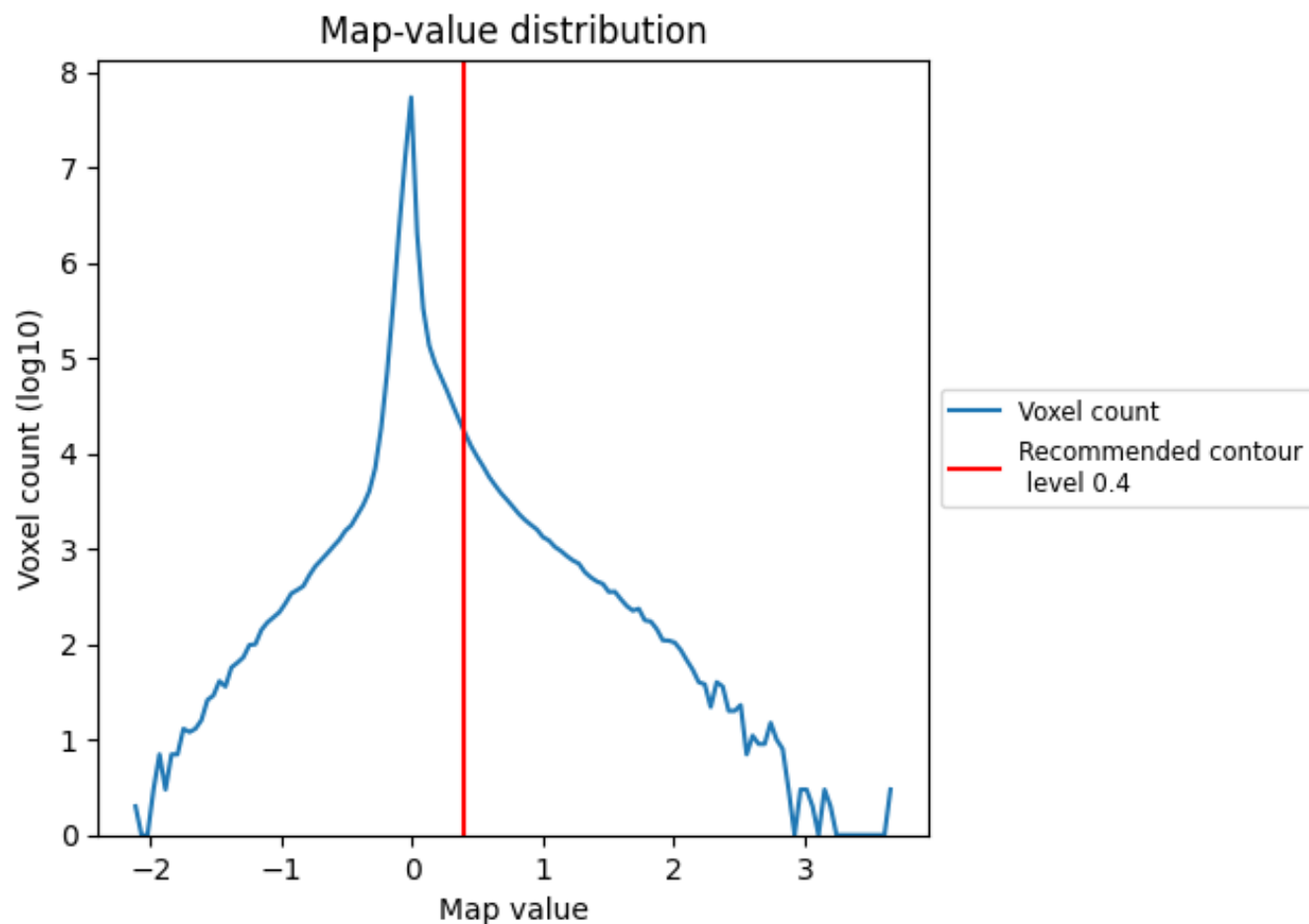
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

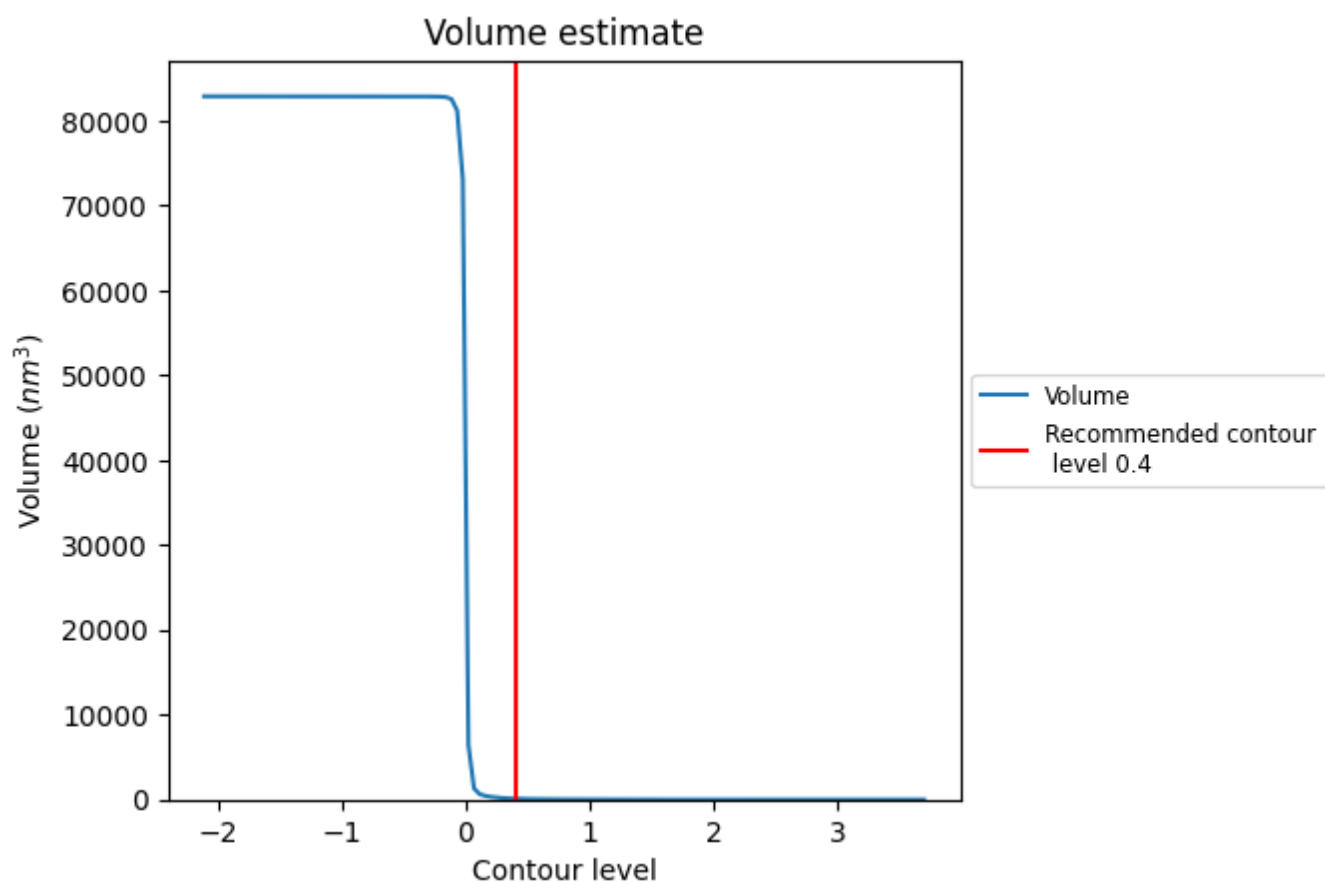
This section contains the results of statistical analysis of the map.

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.

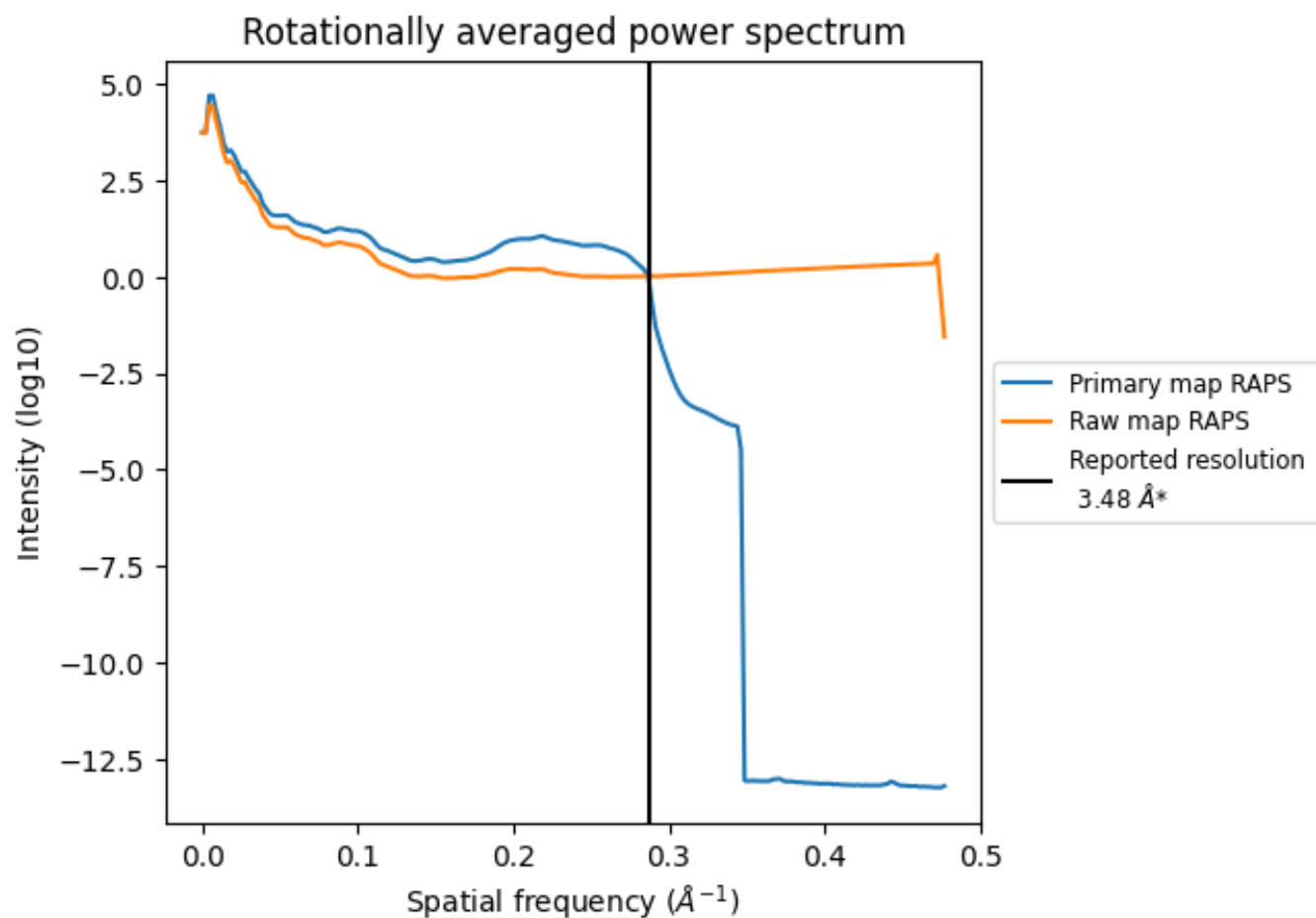
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 91 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 ⓘ

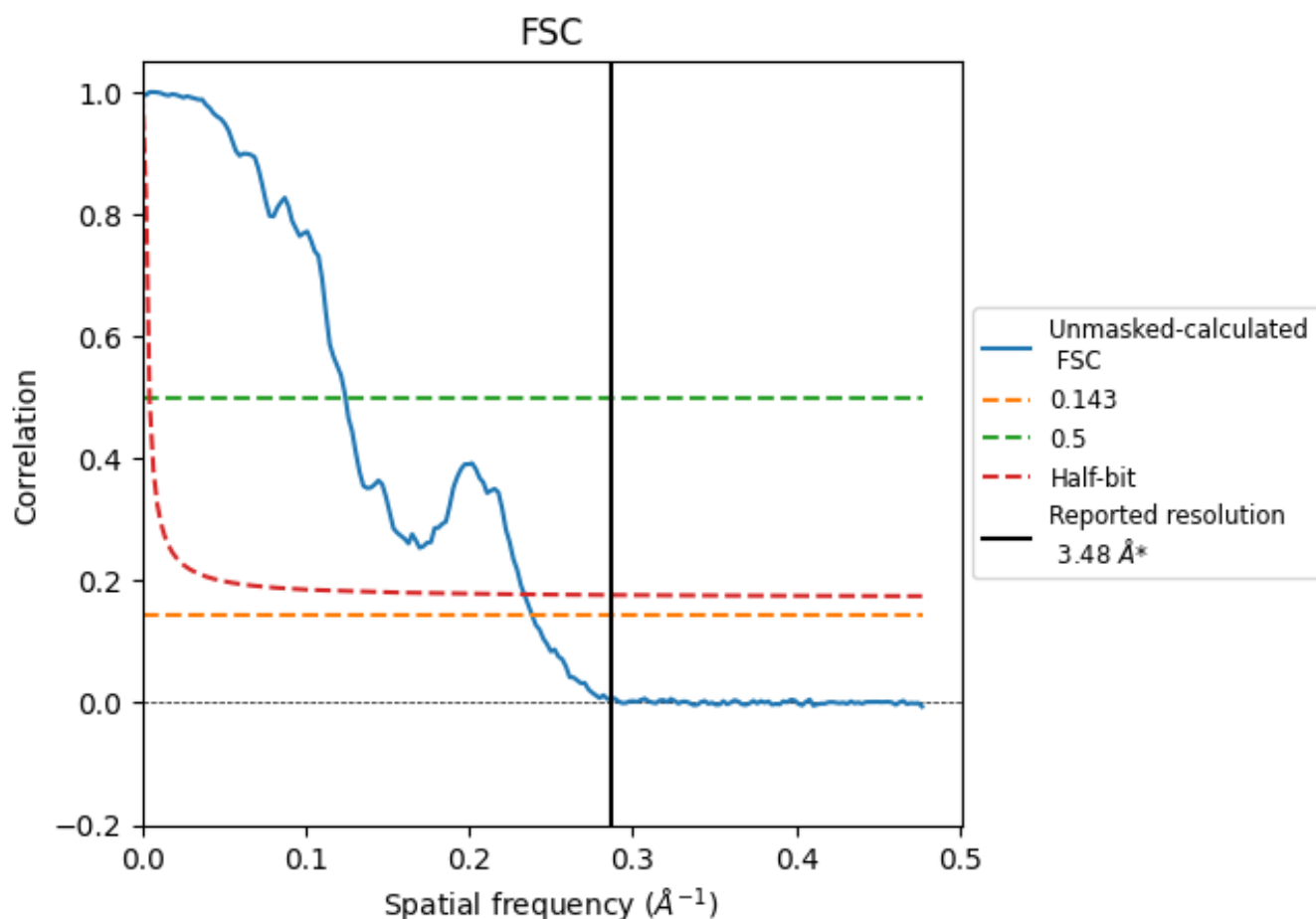


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

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 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

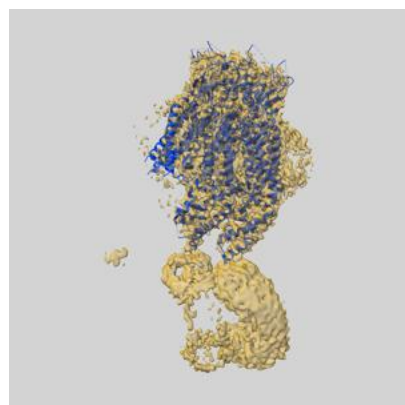
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.19	8.05	4.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.48 by more than 10 %

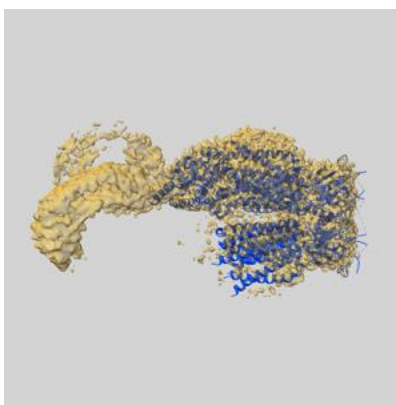
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27687 and PDB model 8DSA. Per-residue inclusion information can be found in section 3 on page 9.

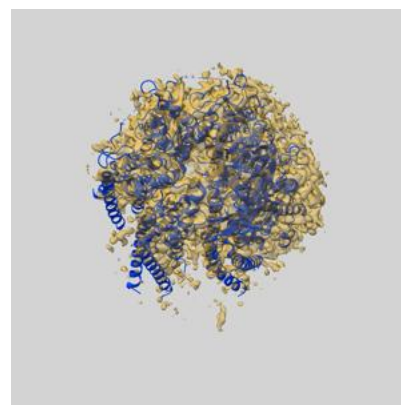
9.1 Map-model overlay [i](#)



X



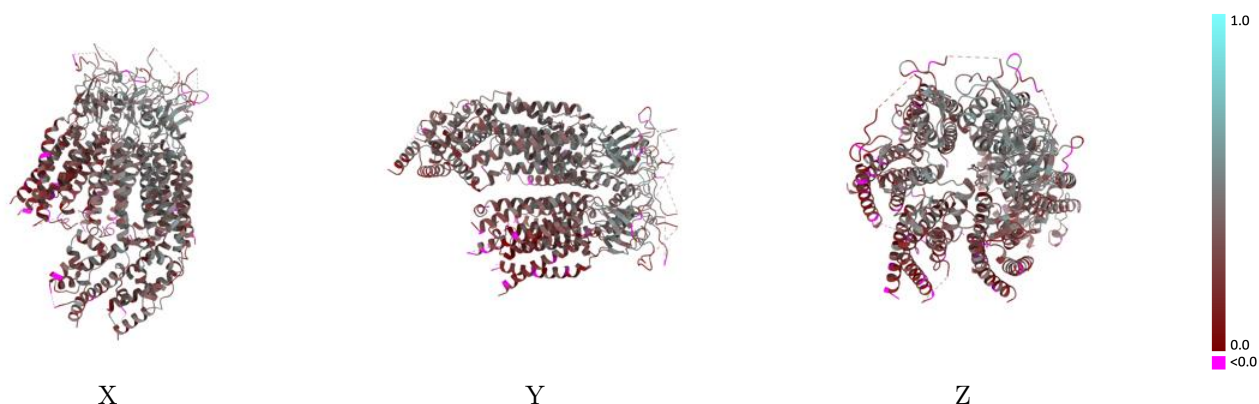
Y



Z

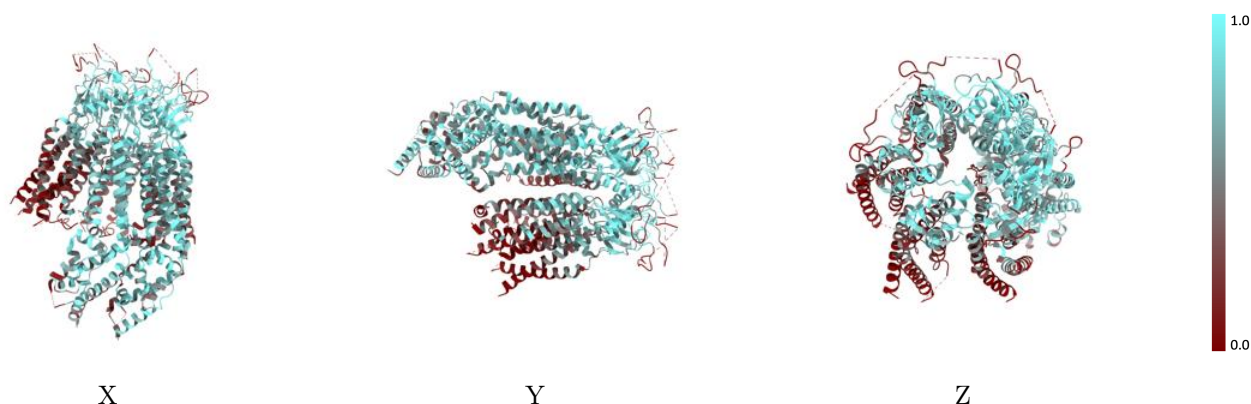
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



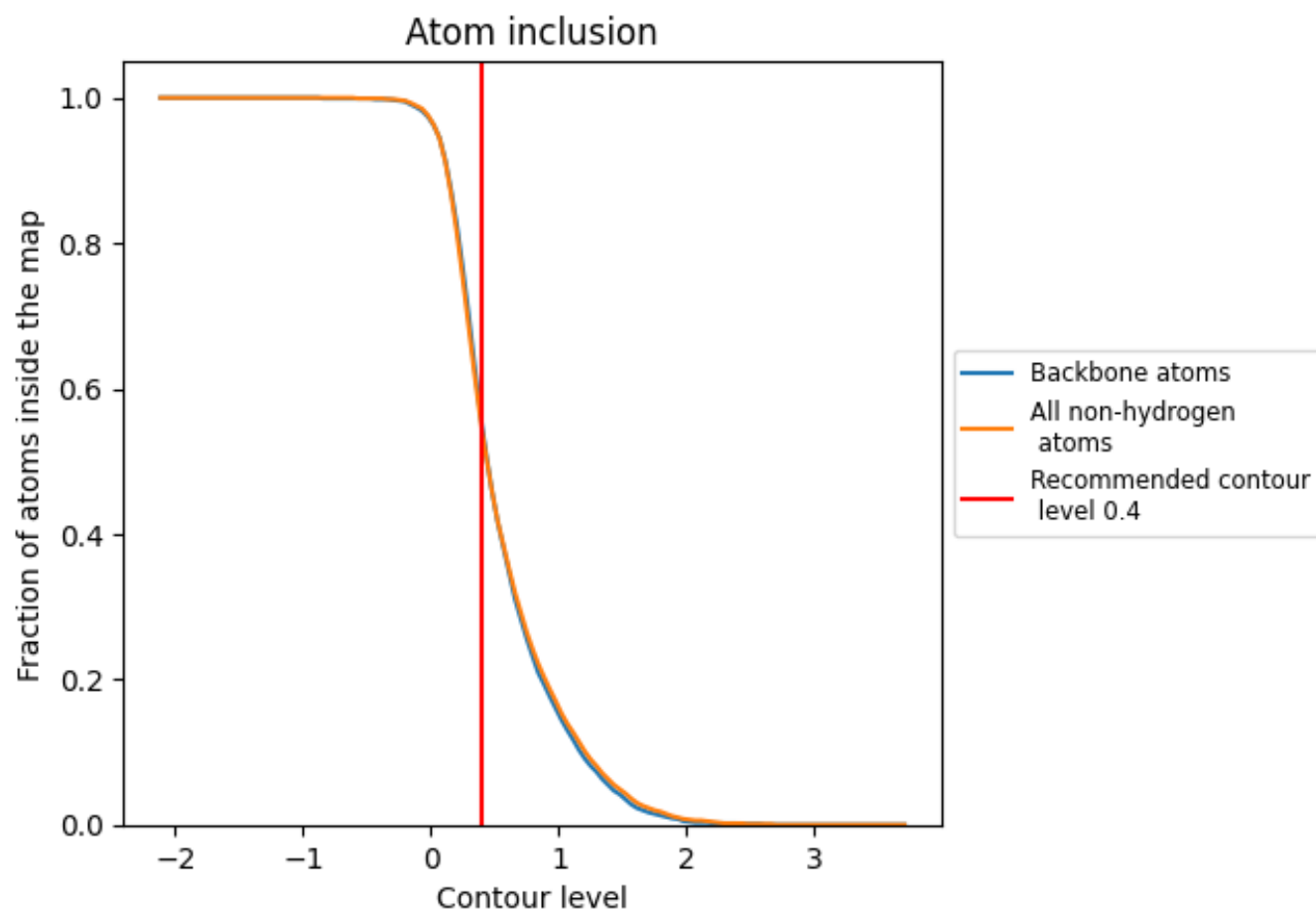
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 54% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5420	<div></div> 0.3260
A	<div></div> 0.3550	<div></div> 0.2530
B	<div></div> 0.5000	<div></div> 0.3220
C	<div></div> 0.7120	<div></div> 0.3920
D	<div></div> 0.6980	<div></div> 0.3770
E	<div></div> 0.4370	<div></div> 0.2910
F	<div></div> 0.4020	<div></div> 0.2450

1.0
0.0
<0.0