



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 11:17 AM UTC

PDB ID : 9RGB / pdb_00009rgb
EMDB ID : EMD-53947
Title : M.tuberculosis MmpS5L5-acpM complex
Authors : Fountain, A.J.; Luisi, B.F.; Ramakrishnan, L.
Deposited on : 2025-06-06
Resolution : 3.20 Å(reported)
Based on initial model : .

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:

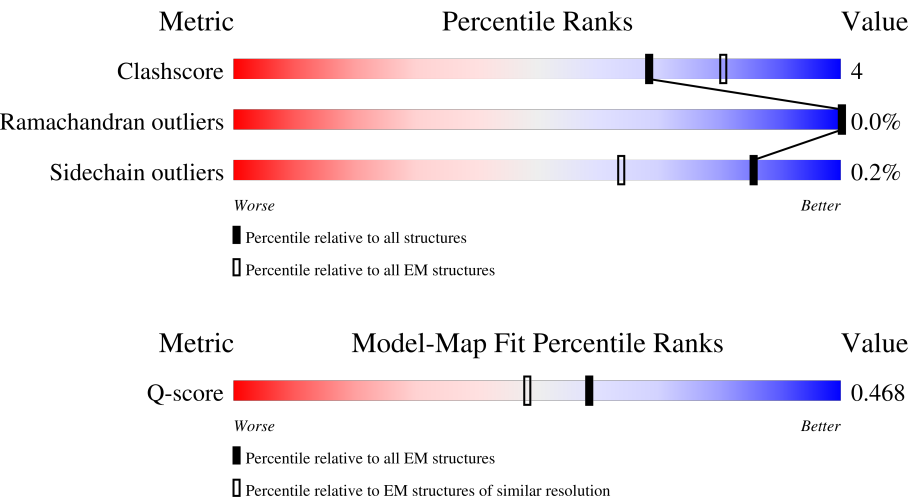
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.20 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.



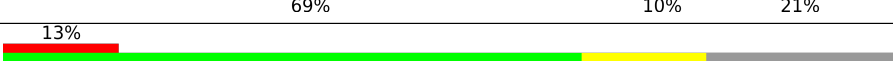
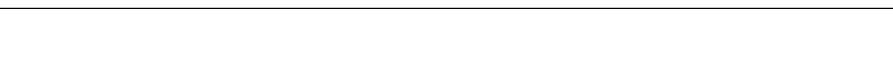
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	143	22%78%
1	B	143	20%78%
1	C	143	20%78%
2	D	1028	5%64%8%28%

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Mol	Chain	Length	Quality of chain
2	E	1028	
2	F	1028	
3	G	99	
3	H	99	
3	I	99	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19410 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 Siderophore export accessory protein MmpS5.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	31	Total	C	N	O	0	0
			244	165	43	36		
1	B	31	Total	C	N	O	0	0
			244	165	43	36		
1	C	31	Total	C	N	O	0	0
			244	165	43	36		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P9WJS7
A	1	SER	-	expression tag	UNP P9WJS7
B	0	MET	-	initiating methionine	UNP P9WJS7
B	1	SER	-	expression tag	UNP P9WJS7
C	0	MET	-	initiating methionine	UNP P9WJS7
C	1	SER	-	expression tag	UNP P9WJS7

- Molecule 2 is a protein called Siderophore exporter MmpL5, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	739	Total	C	N	O	S	0	0
			5569	3604	943	994	28		
2	E	739	Total	C	N	O	S	0	0
			5569	3604	943	994	28		
2	F	739	Total	C	N	O	S	0	0
			5569	3604	943	994	28		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	965	ALA	-	linker	UNP P9WJV1
D	966	LEU	-	linker	UNP P9WJV1
D	967	GLU	-	linker	UNP P9WJV1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	968	VAL	-	linker	UNP P9WJV1
D	969	LEU	-	linker	UNP P9WJV1
D	970	PHE	-	linker	UNP P9WJV1
D	971	GLN	-	linker	UNP P9WJV1
D	972	GLY	-	linker	UNP P9WJV1
D	973	PRO	-	linker	UNP P9WJV1
D	974	GLN	-	linker	UNP P9WJV1
D	975	PHE	-	linker	UNP P9WJV1
D	1038	LEU	PHE	conflict	UNP P42212
D	1039	THR	SER	conflict	UNP P42212
D	1054	ARG	GLN	conflict	UNP P42212
D	1073	SER	PHE	conflict	UNP P42212
D	1127	THR	MET	conflict	UNP P42212
D	1137	ALA	VAL	conflict	UNP P42212
D	1213	THR	-	expression tag	UNP P42212
D	1214	SER	-	expression tag	UNP P42212
D	1215	ASP	-	expression tag	UNP P42212
D	1216	TYR	-	expression tag	UNP P42212
D	1217	LYS	-	expression tag	UNP P42212
D	1218	ASP	-	expression tag	UNP P42212
D	1219	ASP	-	expression tag	UNP P42212
D	1220	ASP	-	expression tag	UNP P42212
D	1221	ASP	-	expression tag	UNP P42212
D	1222	LYS	-	expression tag	UNP P42212
E	965	ALA	-	linker	UNP P9WJV1
E	966	LEU	-	linker	UNP P9WJV1
E	967	GLU	-	linker	UNP P9WJV1
E	968	VAL	-	linker	UNP P9WJV1
E	969	LEU	-	linker	UNP P9WJV1
E	970	PHE	-	linker	UNP P9WJV1
E	971	GLN	-	linker	UNP P9WJV1
E	972	GLY	-	linker	UNP P9WJV1
E	973	PRO	-	linker	UNP P9WJV1
E	974	GLN	-	linker	UNP P9WJV1
E	975	PHE	-	linker	UNP P9WJV1
E	1038	LEU	PHE	conflict	UNP P42212
E	1039	THR	SER	conflict	UNP P42212
E	1054	ARG	GLN	conflict	UNP P42212
E	1073	SER	PHE	conflict	UNP P42212
E	1127	THR	MET	conflict	UNP P42212
E	1137	ALA	VAL	conflict	UNP P42212
E	1213	THR	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1214	SER	-	expression tag	UNP P42212
E	1215	ASP	-	expression tag	UNP P42212
E	1216	TYR	-	expression tag	UNP P42212
E	1217	LYS	-	expression tag	UNP P42212
E	1218	ASP	-	expression tag	UNP P42212
E	1219	ASP	-	expression tag	UNP P42212
E	1220	ASP	-	expression tag	UNP P42212
E	1221	ASP	-	expression tag	UNP P42212
E	1222	LYS	-	expression tag	UNP P42212
F	965	ALA	-	linker	UNP P9WJV1
F	966	LEU	-	linker	UNP P9WJV1
F	967	GLU	-	linker	UNP P9WJV1
F	968	VAL	-	linker	UNP P9WJV1
F	969	LEU	-	linker	UNP P9WJV1
F	970	PHE	-	linker	UNP P9WJV1
F	971	GLN	-	linker	UNP P9WJV1
F	972	GLY	-	linker	UNP P9WJV1
F	973	PRO	-	linker	UNP P9WJV1
F	974	GLN	-	linker	UNP P9WJV1
F	975	PHE	-	linker	UNP P9WJV1
F	1038	LEU	PHE	conflict	UNP P42212
F	1039	THR	SER	conflict	UNP P42212
F	1054	ARG	GLN	conflict	UNP P42212
F	1073	SER	PHE	conflict	UNP P42212
F	1127	THR	MET	conflict	UNP P42212
F	1137	ALA	VAL	conflict	UNP P42212
F	1213	THR	-	expression tag	UNP P42212
F	1214	SER	-	expression tag	UNP P42212
F	1215	ASP	-	expression tag	UNP P42212
F	1216	TYR	-	expression tag	UNP P42212
F	1217	LYS	-	expression tag	UNP P42212
F	1218	ASP	-	expression tag	UNP P42212
F	1219	ASP	-	expression tag	UNP P42212
F	1220	ASP	-	expression tag	UNP P42212
F	1221	ASP	-	expression tag	UNP P42212
F	1222	LYS	-	expression tag	UNP P42212

- Molecule 3 is a protein called Meromycolate extension acyl carrier protein.

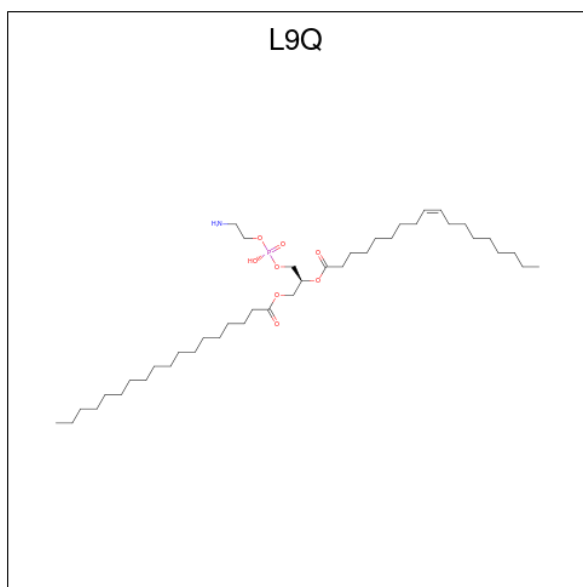
Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	77	Total	C	N	O	P	S	0	0
			609	382	89	135	1	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	78	Total	C	N	O	P	S	0	0
			614	385	90	136	1	2		
3	I	78	Total	C	N	O	P	S	0	0
			614	385	90	136	1	2		

- Molecule 4 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).

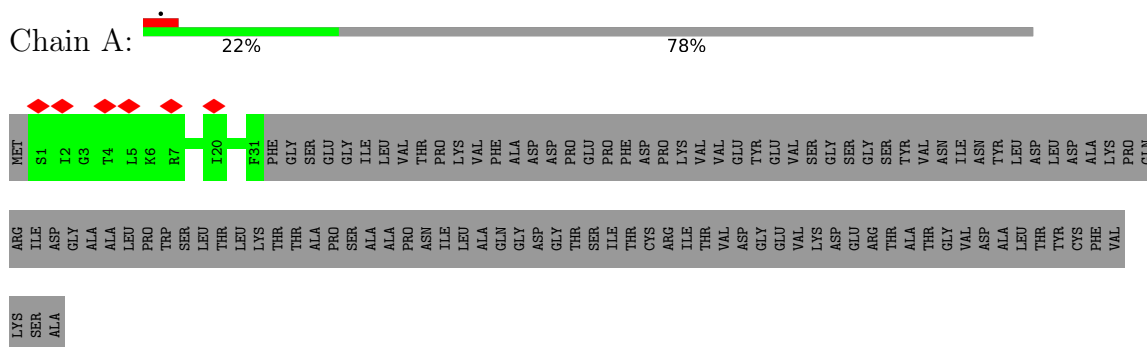


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

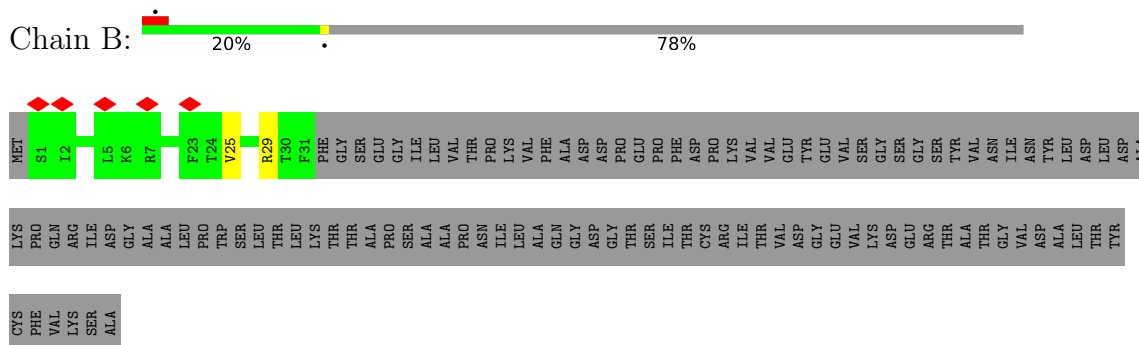
3 Residue-property plots

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.

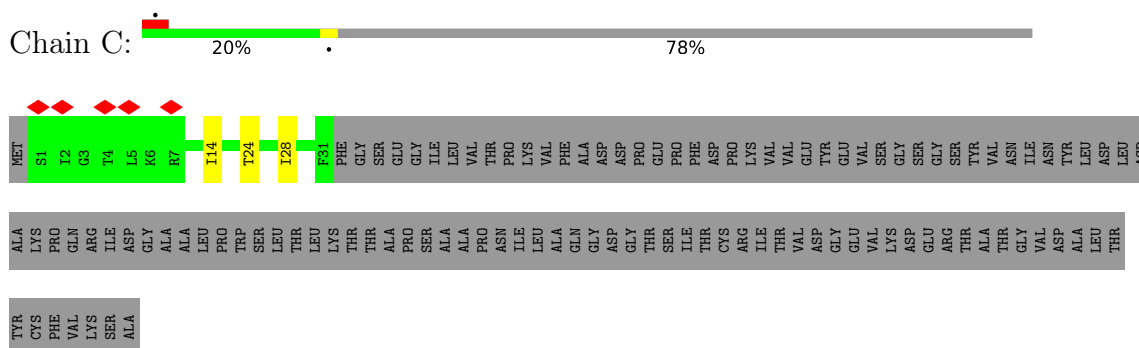
- Molecule 1: Siderophore export accessory protein MmpS5

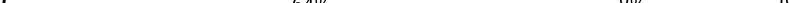


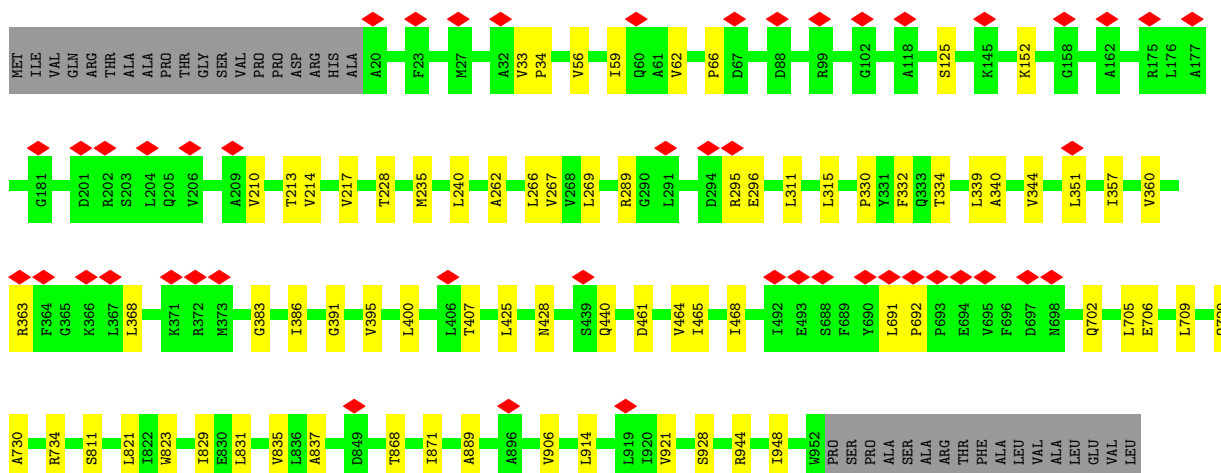
- Molecule 1: Siderophore export accessory protein MmpS5



- Molecule 1: Siderophore export accessory protein MmpS5



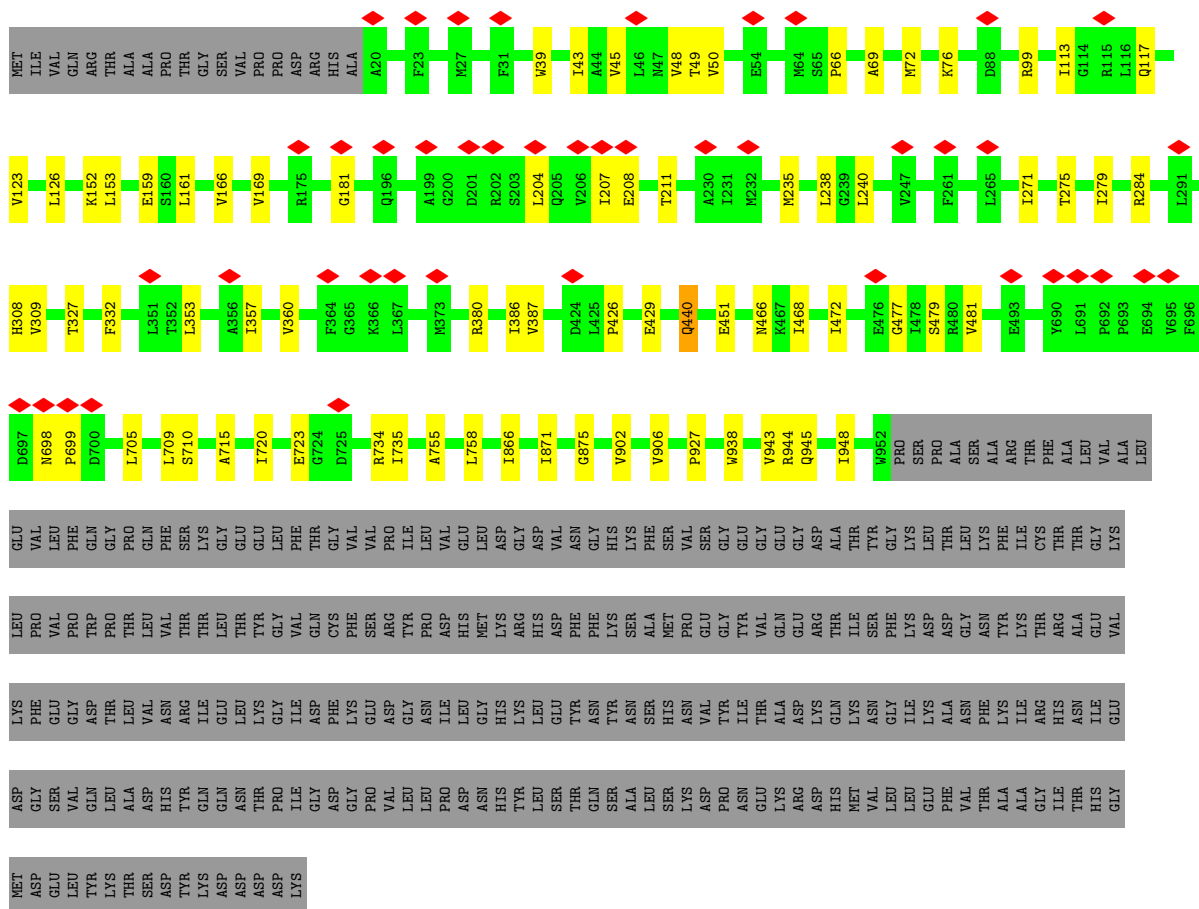
- Chain D:  5% 64% 8% 28%



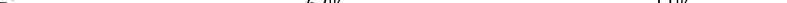
LEU	TYR	VAL	GLY	PRO	PHE
	LYS	GLN	ASP	TRP	GLN
	THR	LEU	THR	THR	GLY
	SER	ALA	LEU	PRO	GLN
	ASP	ASP	VAL	LEU	PHE
	TYR	HIS	ASN	VAL	SER
	LYS	GLN	ILE	THR	LYS
	ASP	GLN	LEU	LEU	GLY
	ASP	ASN	LEU	THR	GLU
	LYS	THR	LYS	TYR	GLU
ASP	ASP	PRO	GLY	GLY	LEU
	LYS	ILE	ILE	VAL	PHE
	GLY	GLY	ASP	GLN	THR
	ASP	PHE	PHE	CYS	GLY
	GLY	LYS	PHE	VAL	VAL
	PRO	GLU	SER	VAL	PRO
	VAL	ASP	ARG	THR	ILE
	LEU	GLY	TYR	PRO	LEU
	LEU	ASN	ASP	HIS	GLU
	ASP	LEU	LEU	MET	LEU
THR	ASN	GLY	HIS	LYS	ASP
	HIS	HIS	GLY	ARG	GLY
	TYR	LYS	LYS	ARG	LYS
	LEU	LEU	GLU	ASP	VAL
	SER	GLU	ASP	ASN	ASN
	THR	THR	THR	PHE	GLY
	GLN	ASN	PHE	GLY	LYS
	SER	TYR	LYS	LYS	HIS
	ALA	ASN	SER	ALA	LYS
	LEU	SER	HIS	MET	PHE
GLY	SER	LYS	ASN	PRO	VAL
	ASP	VAL	THR	GLU	SER
	PRO	ASN	TYR	GLY	GLY
	ASN	ILE	ILE	TYR	GLU
	LYS	ALA	GLN	VAL	GLU
	ARG	ASP	GLU	GLU	GLY
	ASP	LYS	ARG	THR	ASP
	HIS	GLN	THR	ALA	ALA
	MET	LYS	ILE	THR	TYR
	VAL	ASN	PHE	LYS	LYS
PHE	LEU	LEU	ILE	LYS	LEU
	GLU	PHE	ALA	ASP	THR
	VAL	VAL	ASN	GLY	LEU
	THR	PHE	PHE	GLY	LYS
	ALA	ALA	ILE	LYS	ILE
	GLY	ILE	ARG	THR	CYS
	ILE	HIS	ARG	THR	THR
	THR	ASN	ILE	ALA	THR
	HIS	ILE	GLU	VAL	LYS
	GLY	ASP	LYS	LYS	LEU

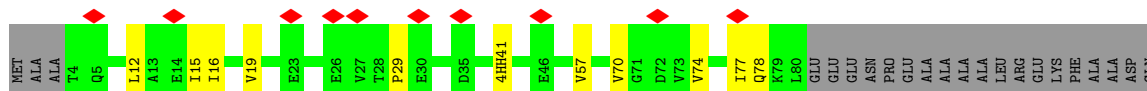
- Molecule 2: Siderophore exporter MmpL5, Green fluorescent protein

Chain F: 64% 7% 28%

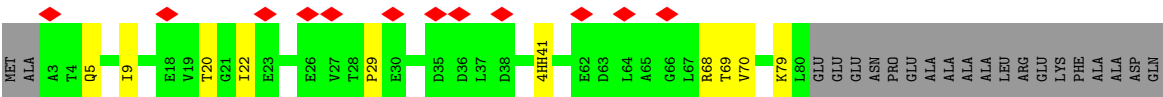


- Molecule 3: Meromycolate extension acyl carrier protein

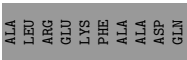
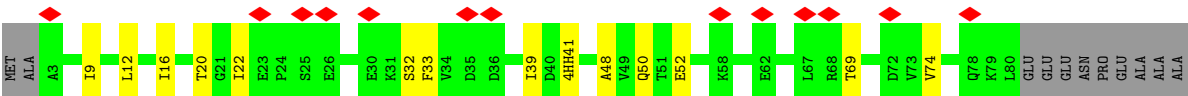
Chain G: 



● Molecule 3: Meromycolate extension acyl carrier protein



● Molecule 3: Meromycolate extension acyl carrier protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33185	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.190	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	382.0, 382.0, 382.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	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: 4HH, L9Q

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	0.20	0/248	0.37	0/337
1	B	0.21	0/248	0.48	0/337
1	C	0.24	0/248	0.45	0/337
2	D	0.22	0/5683	0.48	0/7738
2	E	0.22	0/5683	0.47	0/7738
2	F	0.23	0/5683	0.50	0/7738
3	G	0.22	0/586	0.52	0/795
3	H	0.20	0/591	0.48	0/802
3	I	0.24	0/591	0.54	0/802
All	All	0.22	0/19561	0.49	0/26624

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	244	0	279	0	0
1	B	244	0	279	1	0
1	C	244	0	279	1	0
2	D	5569	0	5752	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5569	0	5752	39	0
2	F	5569	0	5752	41	0
3	G	609	0	604	6	0
3	H	614	0	609	5	0
3	I	614	0	609	7	0
4	A	46	0	66	3	0
4	B	45	0	64	0	0
4	C	43	0	60	1	0
All	All	19410	0	20105	145	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 4.

The worst 5 of 145 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:D:327:THR:HG21	2:D:332:PHE:HB2	1.73	0.69
2:F:99:ARG:HH12	2:F:181:GLY:HA3	1.57	0.68
2:E:235:MET:HG2	2:E:357:ILE:HD11	1.77	0.66
2:D:89:SER:HA	2:D:157:GLN:HE22	1.62	0.64
2:F:72:MET:HG3	2:F:76:LYS:HE3	1.79	0.64

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	29/143 (20%)	29 (100%)	0	0	100	100
1	B	29/143 (20%)	28 (97%)	1 (3%)	0	100	100
1	C	29/143 (20%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	737/1028 (72%)	728 (99%)	8 (1%)	1 (0%)	48	79
2	E	737/1028 (72%)	728 (99%)	9 (1%)	0	100	100
2	F	737/1028 (72%)	722 (98%)	15 (2%)	0	100	100
3	G	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
3	H	75/99 (76%)	70 (93%)	5 (7%)	0	100	100
3	I	75/99 (76%)	69 (92%)	6 (8%)	0	100	100
All	All	2522/3810 (66%)	2473 (98%)	48 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	372	ARG

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	26/118 (22%)	26 (100%)	0	100	100
1	B	26/118 (22%)	26 (100%)	0	100	100
1	C	26/118 (22%)	25 (96%)	1 (4%)	29	62
2	D	581/830 (70%)	581 (100%)	0	100	100
2	E	581/830 (70%)	579 (100%)	2 (0%)	86	88
2	F	581/830 (70%)	580 (100%)	1 (0%)	87	89
3	G	66/80 (82%)	66 (100%)	0	100	100
3	H	66/80 (82%)	66 (100%)	0	100	100
3	I	66/80 (82%)	66 (100%)	0	100	100
All	All	2019/3084 (66%)	2015 (100%)	4 (0%)	85	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	14	ILE
2	E	440	GLN
2	E	729	GLN
2	F	440	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	437	HIS
2	F	772	ASN
2	F	111	GLN
3	H	50	GLN
2	F	698	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	4HH	H	41	3	22,26,27	1.85	5 (22%)	27,35,37	1.41	3 (11%)
3	4HH	I	41	3	22,26,27	1.87	5 (22%)	27,35,37	1.61	4 (14%)
3	4HH	G	41	3	22,26,27	1.86	5 (22%)	27,35,37	1.14	2 (7%)

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	4HH	H	41	3	-	4/33/35/37	-
3	4HH	I	41	3	-	6/33/35/37	-
3	4HH	G	41	3	-	11/33/35/37	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	41	4HH	CL3-NN	5.13	1.45	1.33
3	G	41	4HH	CQ-NR	5.12	1.45	1.33
3	I	41	4HH	CQ-NR	5.08	1.45	1.33
3	H	41	4HH	CQ-NR	5.06	1.45	1.33
3	G	41	4HH	CL3-NN	4.98	1.45	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	41	4HH	OG-CB-CA	4.39	112.42	108.14
3	I	41	4HH	P-OG-CB	-4.30	96.69	121.35
3	H	41	4HH	P-OG-CB	3.82	143.23	121.35
3	G	41	4HH	OG-CB-CA	3.51	111.56	108.14
3	H	41	4HH	OG-CB-CA	2.79	110.86	108.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	41	4HH	CB-OG-P-O1P
3	G	41	4HH	CB-OG-P-O2P
3	G	41	4HH	CB-OG-P-O3P
3	G	41	4HH	O3P-CJ-CK-CL1
3	G	41	4HH	O3P-CJ-CK-CL2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	L9Q	C	201	-	42,42,50	0.52	0	45,47,55	0.53	0
4	L9Q	A	201	-	45,45,50	0.50	0	48,50,55	0.52	0
4	L9Q	B	201	-	44,44,50	0.50	0	47,49,55	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L9Q	C	201	-	-	18/46/46/54	-
4	L9Q	A	201	-	-	24/49/49/54	-
4	L9Q	B	201	-	-	17/48/48/54	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

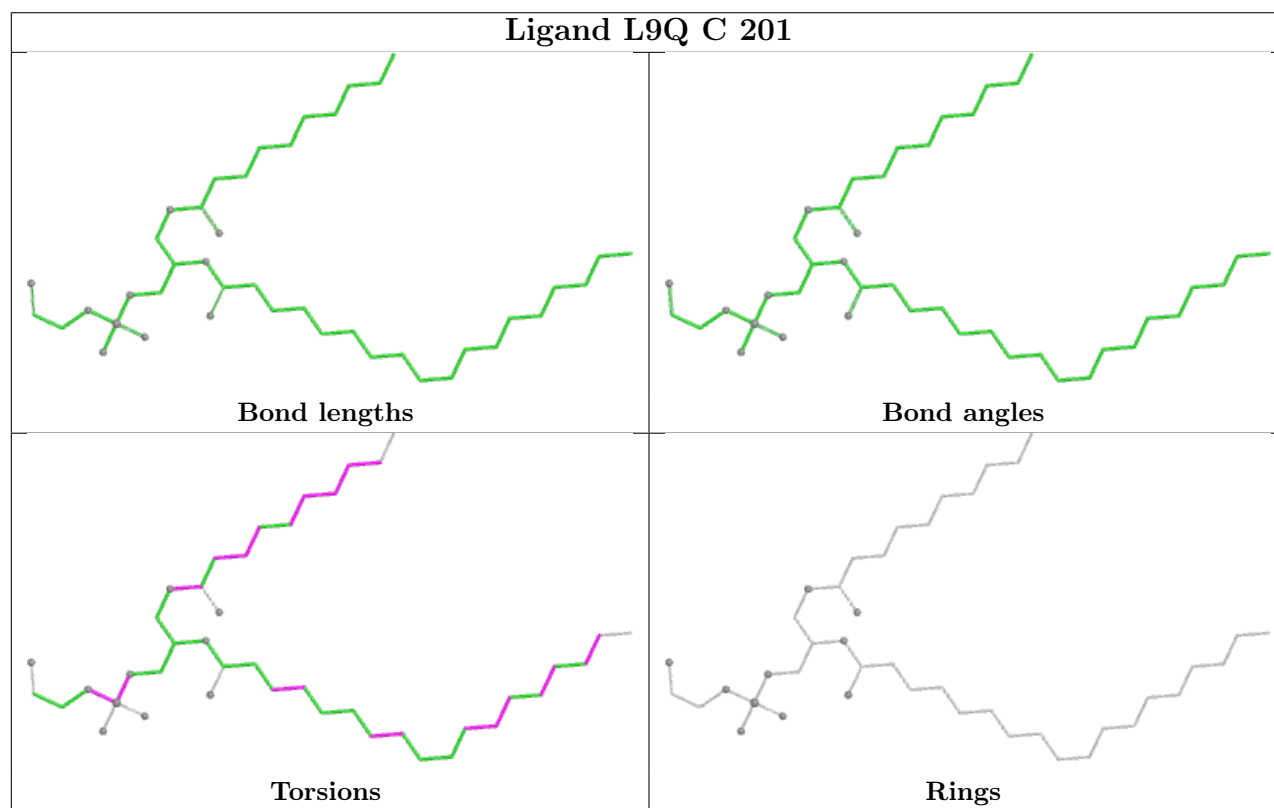
Mol	Chain	Res	Type	Atoms
4	A	201	L9Q	C1-O3P-P-O2P
4	A	201	L9Q	C1-O3P-P-O4P
4	A	201	L9Q	C32-C31-O2-C2
4	B	201	L9Q	C1-O3P-P-O1P
4	B	201	L9Q	C4-O4P-P-O2P

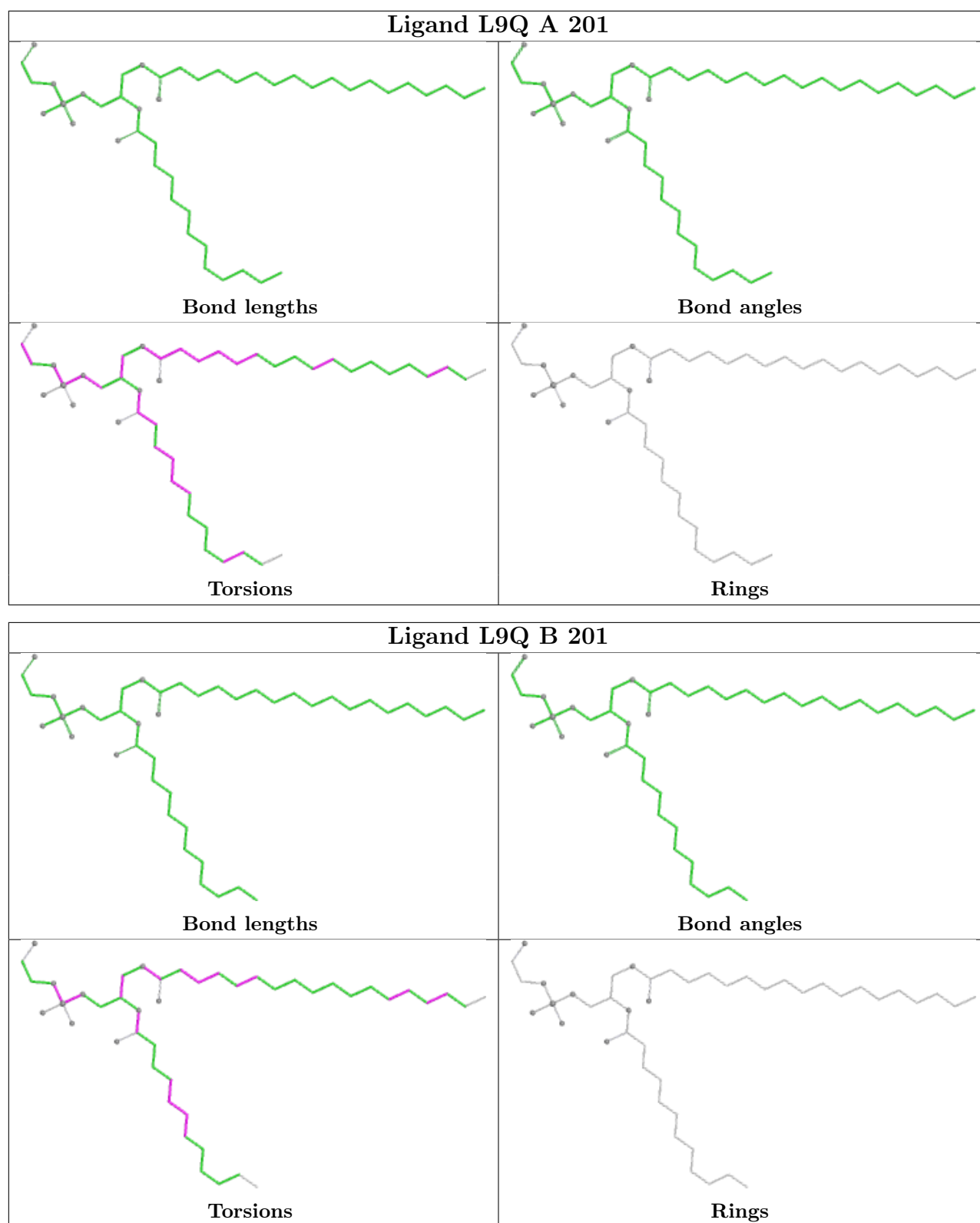
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	L9Q	1	0
4	A	201	L9Q	3	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 ⓘ

There are no chain breaks in this entry.

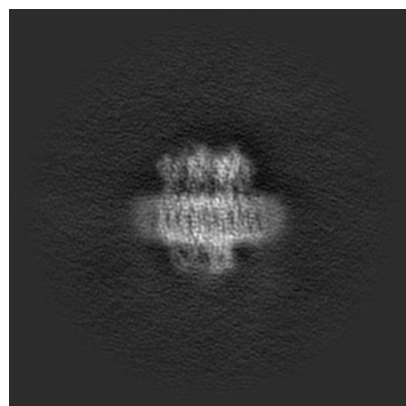
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53947. These allow visual inspection of the internal detail of the map and identification of artifacts.

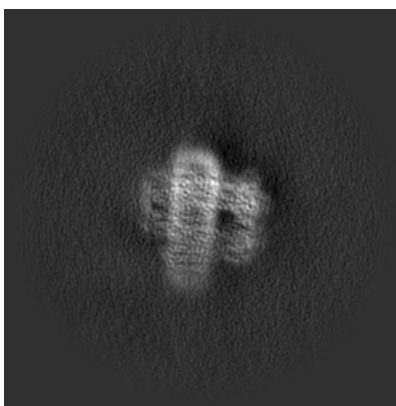
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

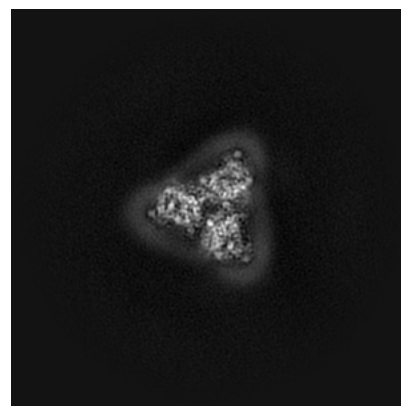
6.1.1 Primary map



X

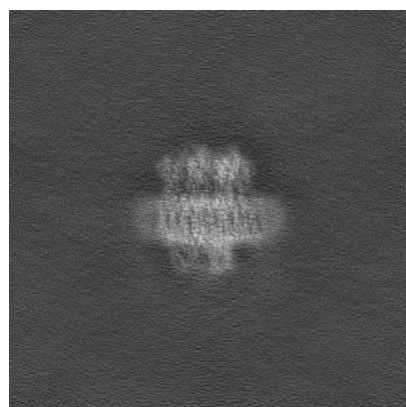


Y

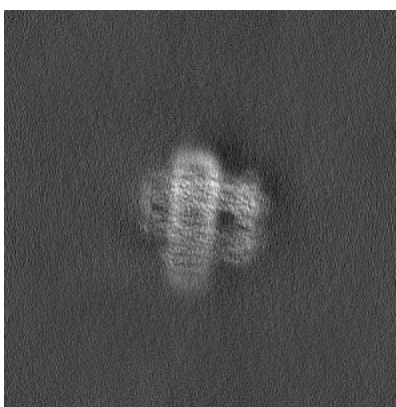


Z

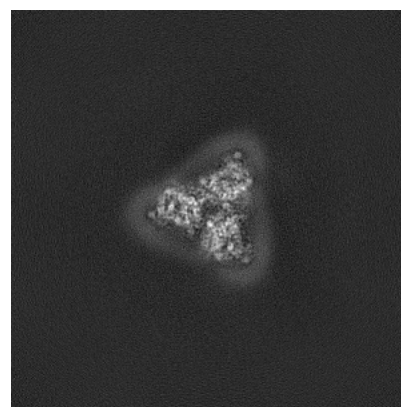
6.1.2 Raw map



X



Y

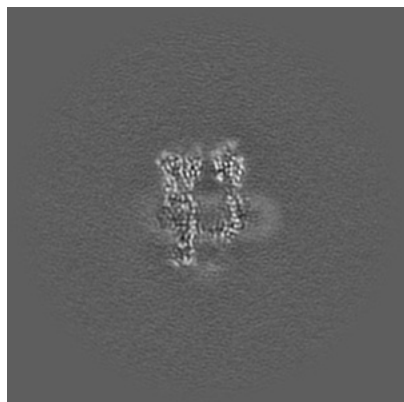


Z

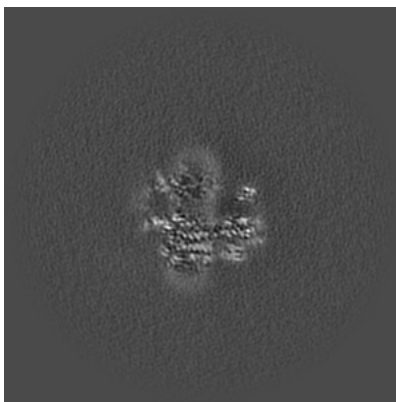
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

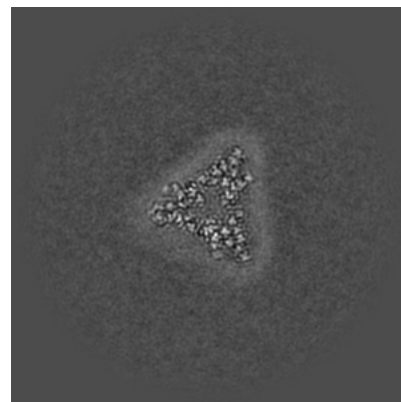
6.2.1 Primary map



X Index: 200

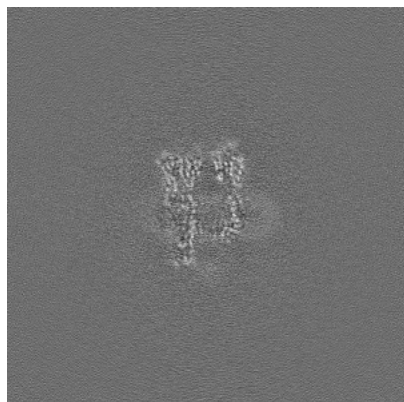


Y Index: 200

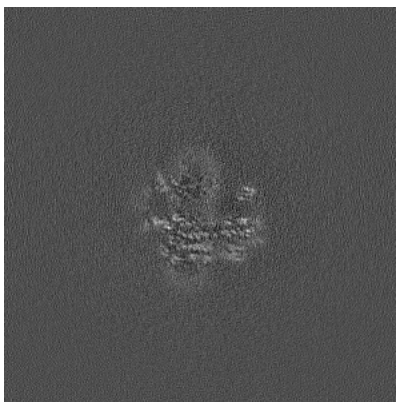


Z Index: 200

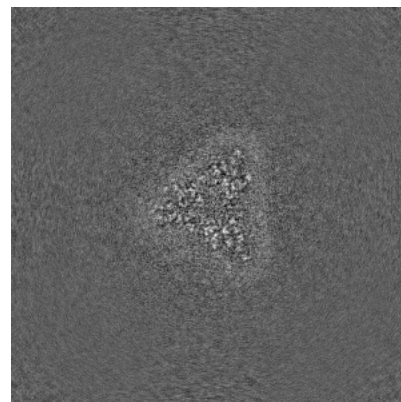
6.2.2 Raw map



X Index: 200



Y Index: 200

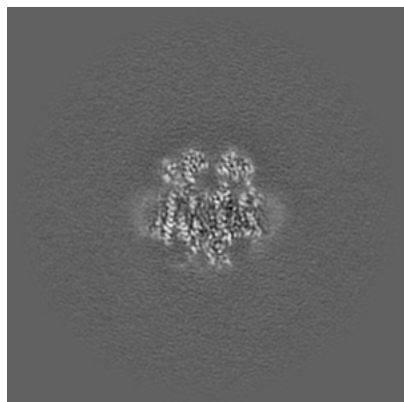


Z Index: 200

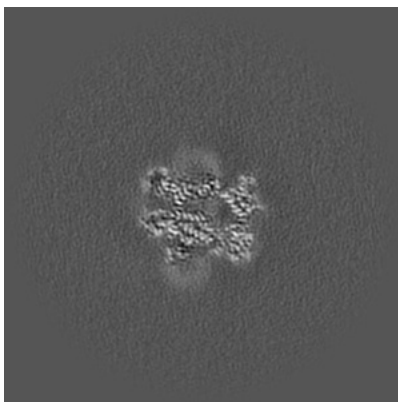
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

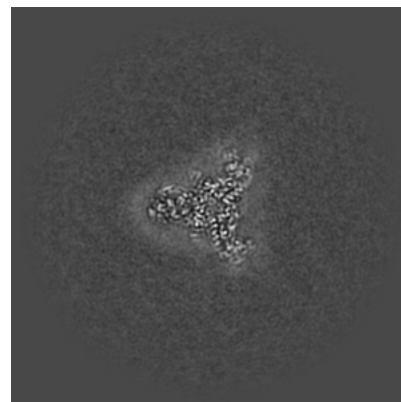
6.3.1 Primary map



X Index: 219

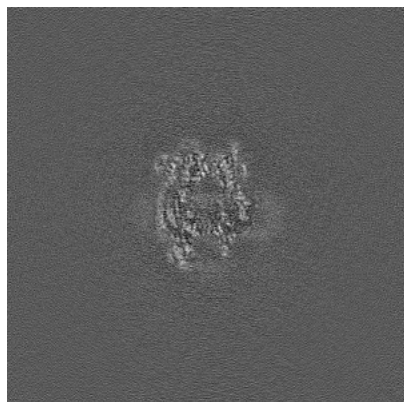


Y Index: 211

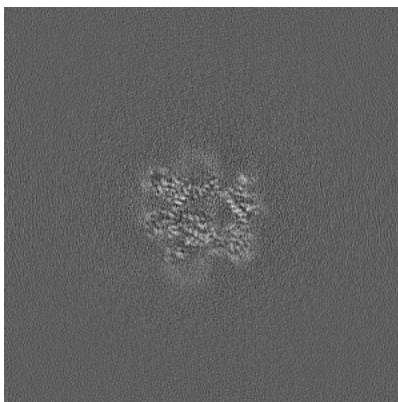


Z Index: 172

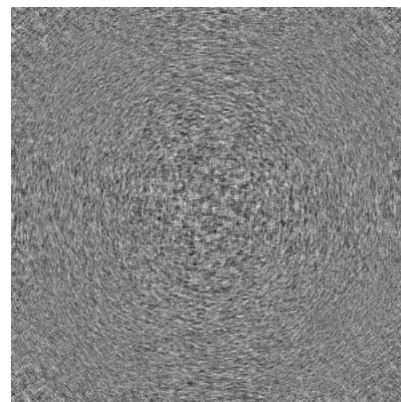
6.3.2 Raw map



X Index: 208



Y Index: 212

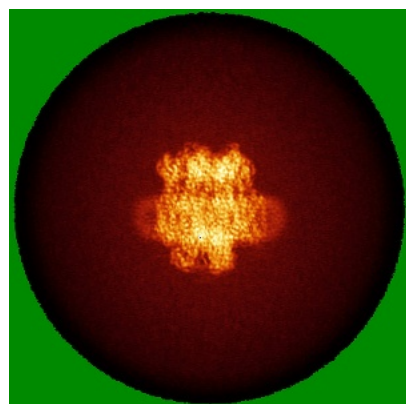


Z Index: 0

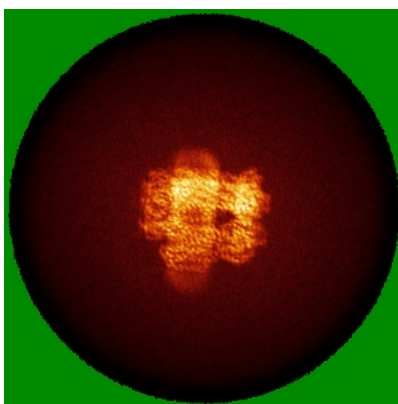
The images above show the largest variance slices of the map in three orthogonal directions.

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

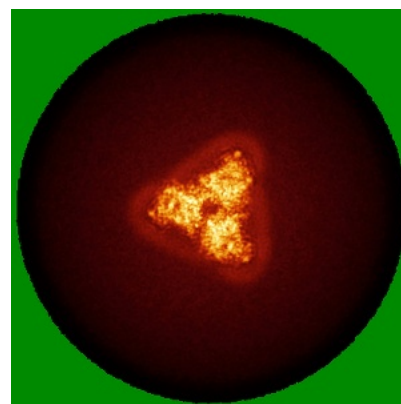
6.4.1 Primary map



X

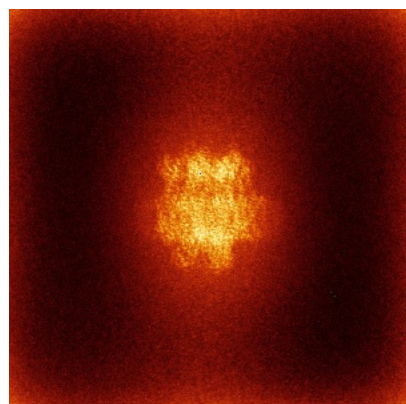


Y

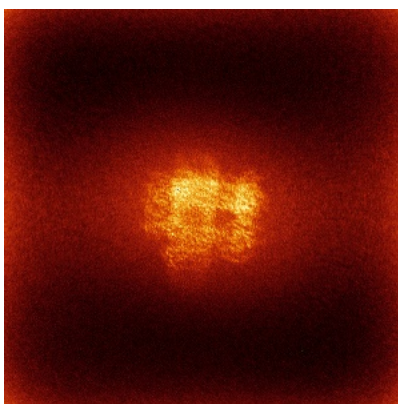


Z

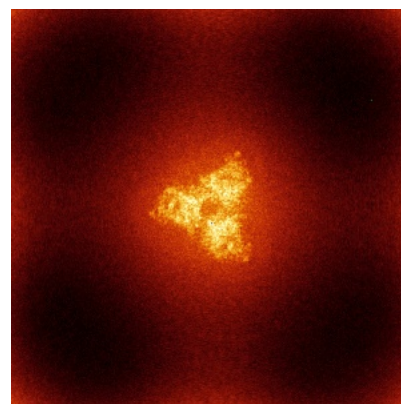
6.4.2 Raw map



X



Y

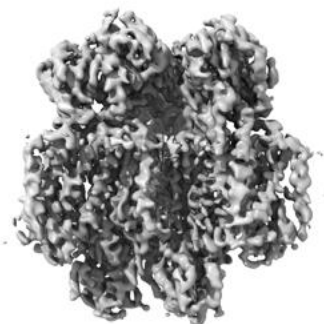


Z

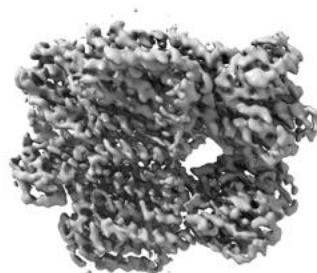
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

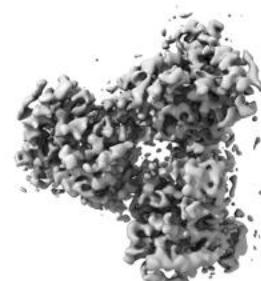
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. 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



X



Y



Z

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.

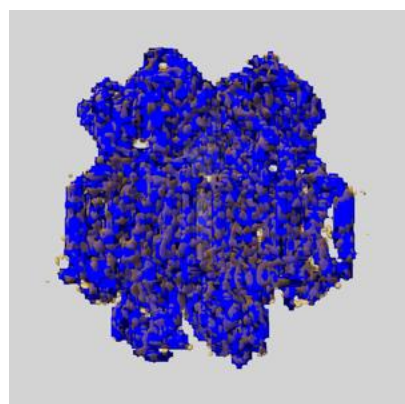
6.6 Mask visualisation [i](#)

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

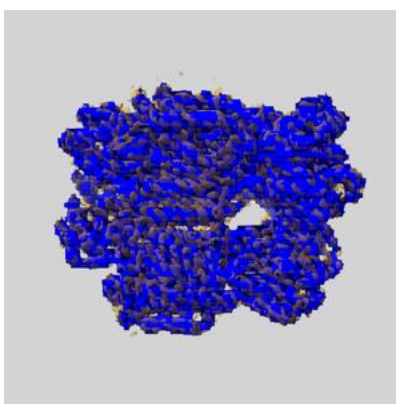
A mask typically either:

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

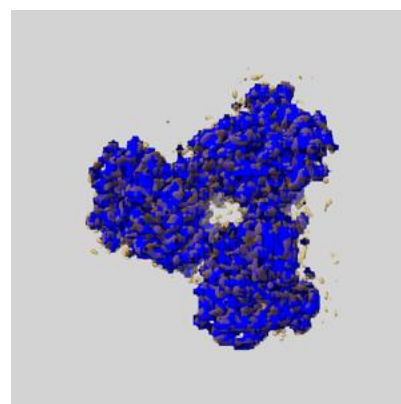
6.6.1 emd_53947_msk_1.map [i](#)



X



Y

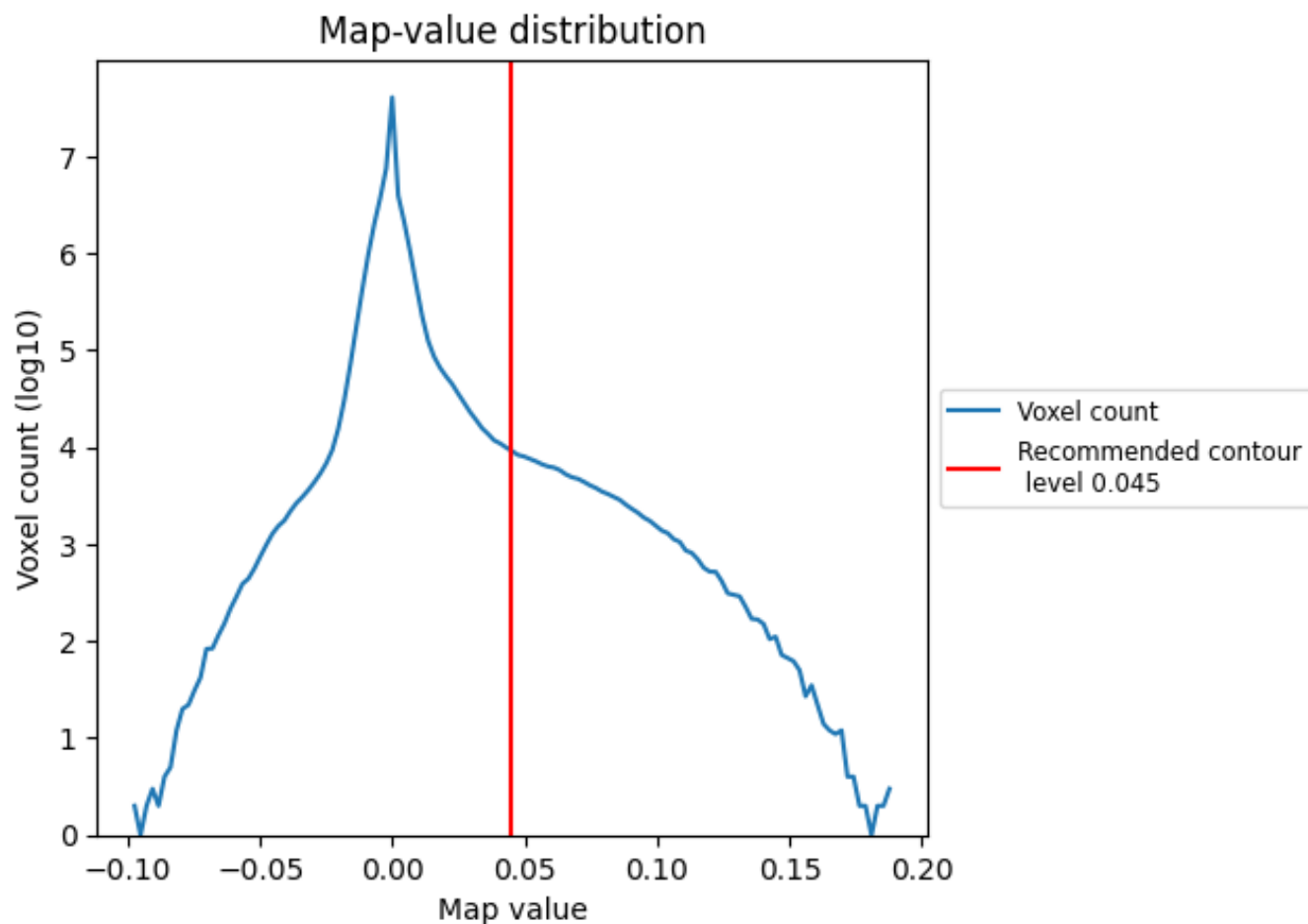


Z

7 Map analysis [i](#)

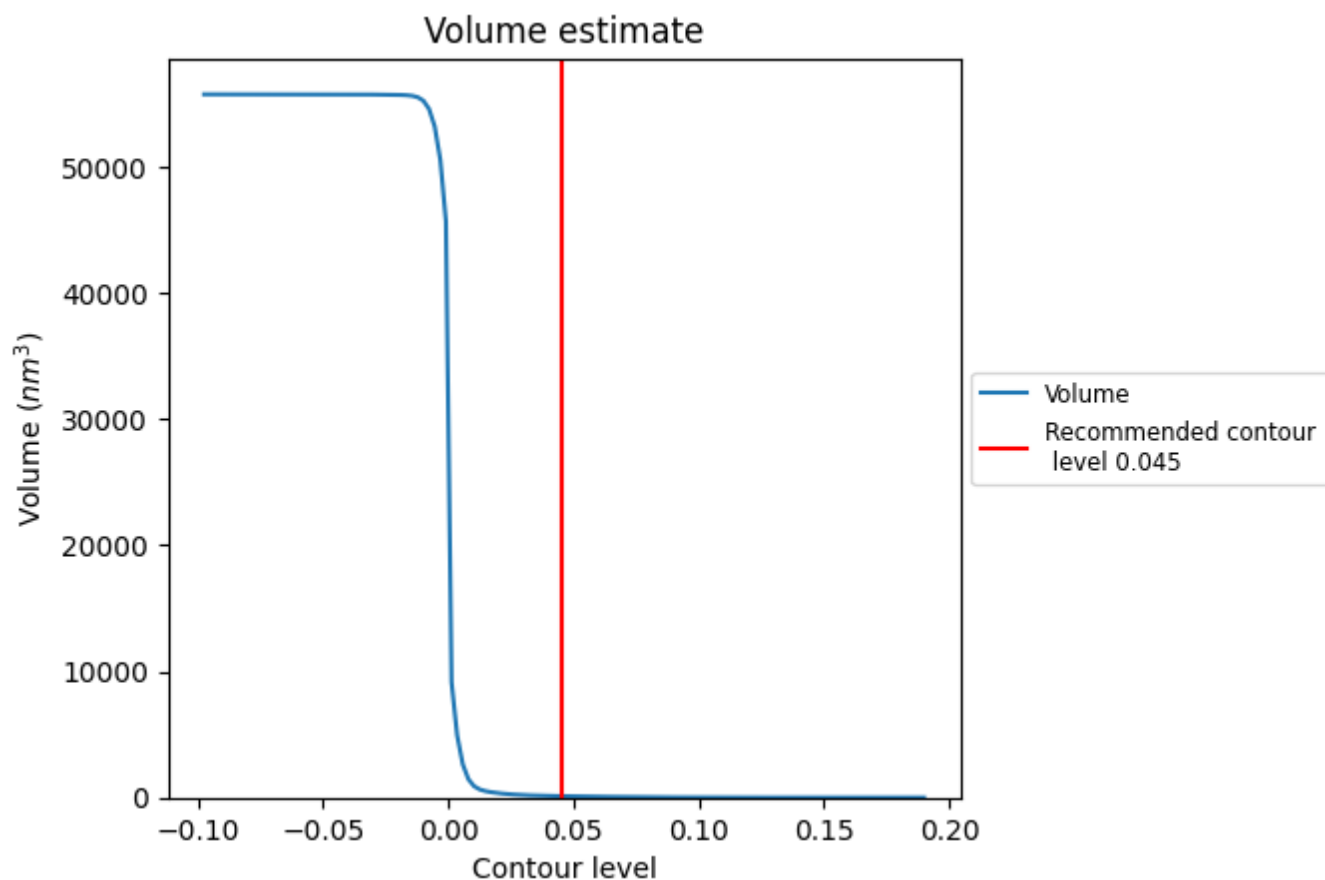
This section contains the results of statistical analysis of the map.

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.

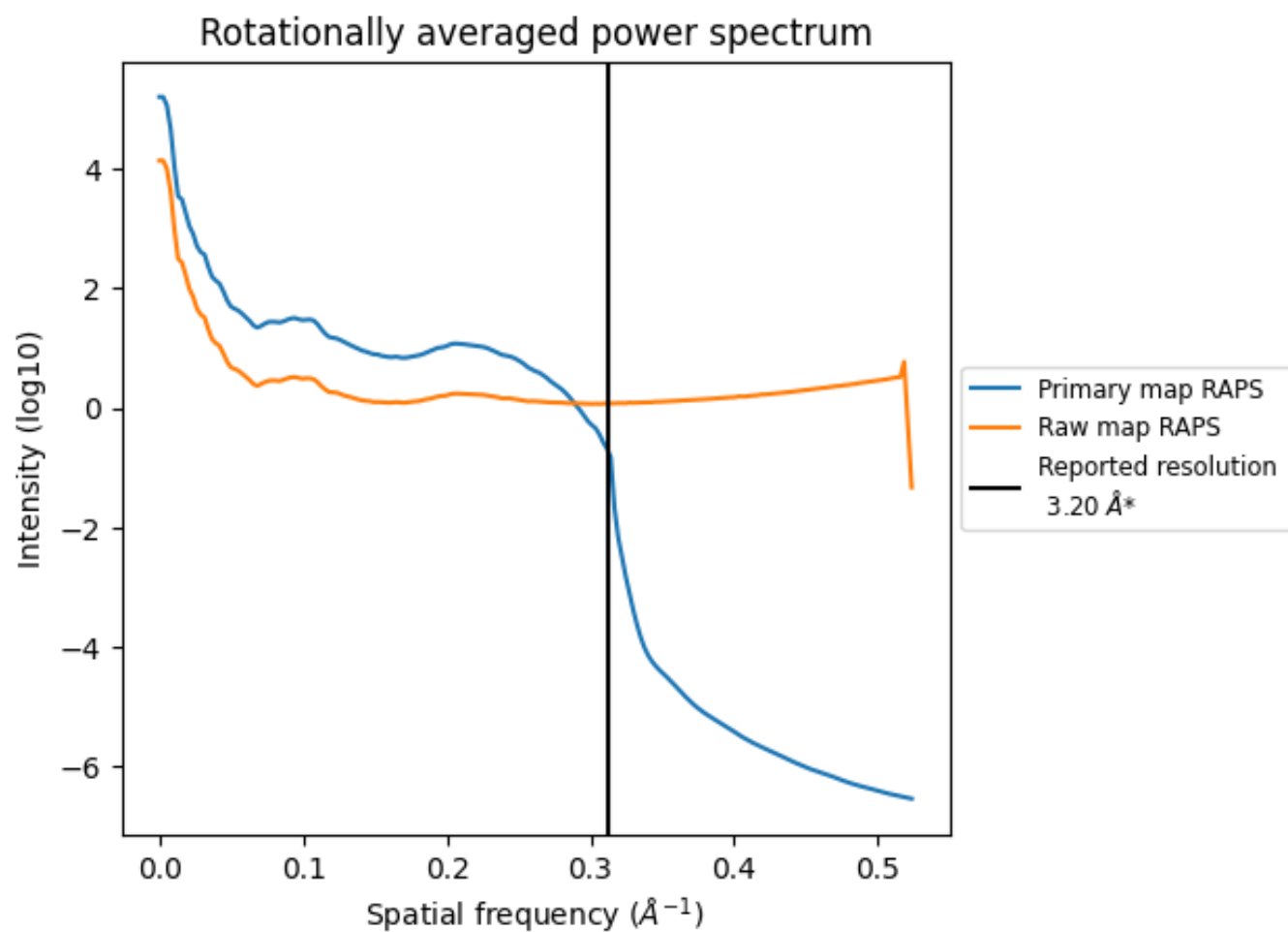
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 102 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 ⓘ

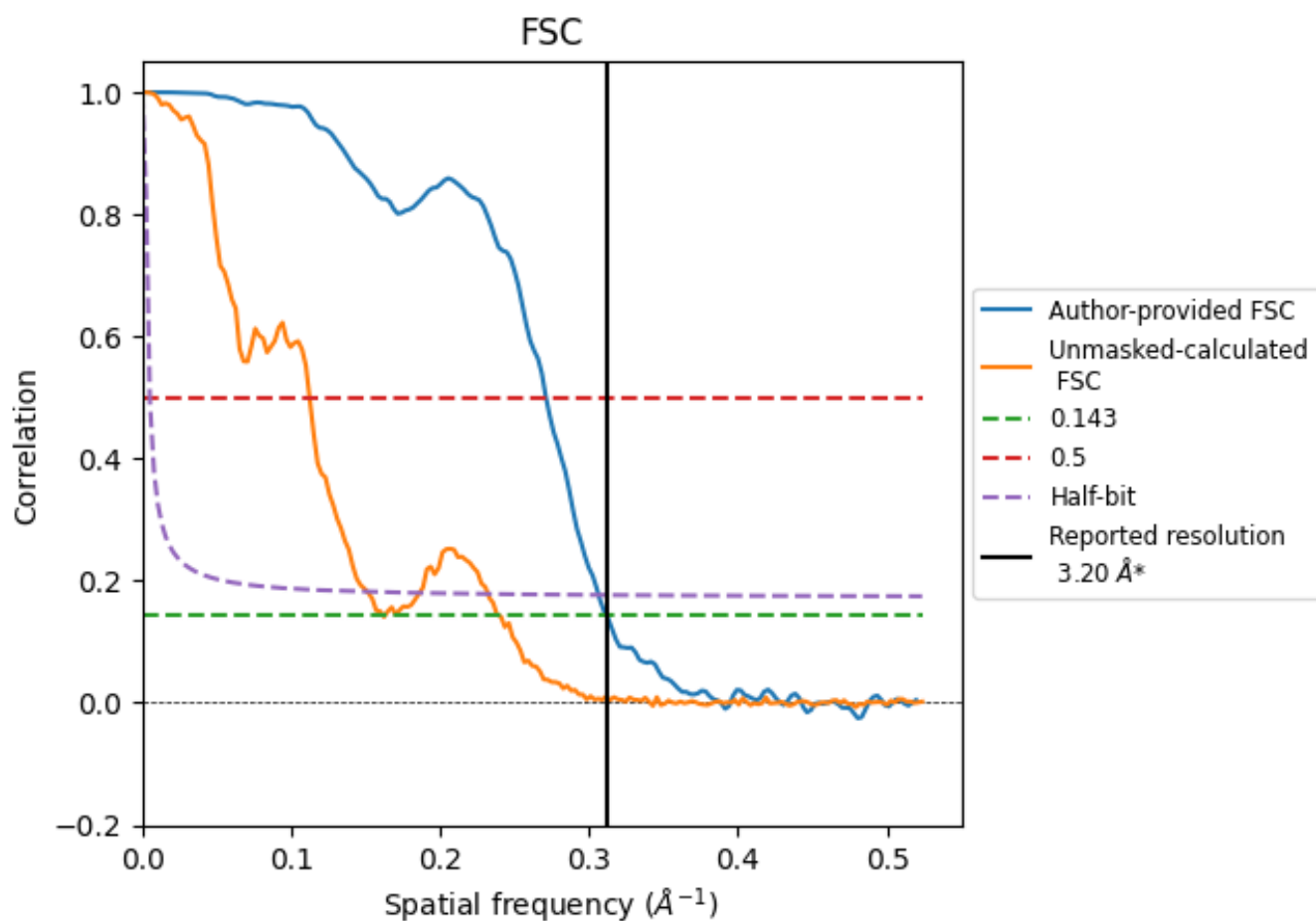


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

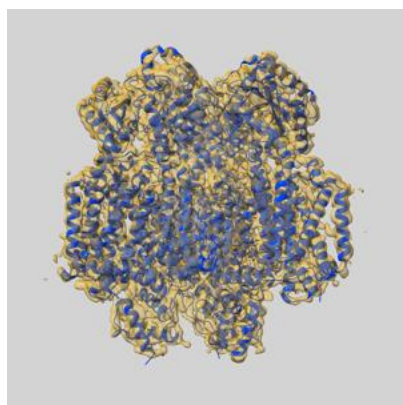
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.69	3.26
Unmasked-calculated*	6.18	8.90	6.61

*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 6.18 differs from the reported value 3.2 by more than 10 %

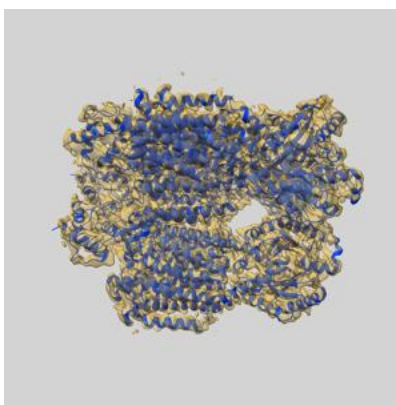
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53947 and PDB model 9RGB. Per-residue inclusion information can be found in section [3](#) on page [8](#).

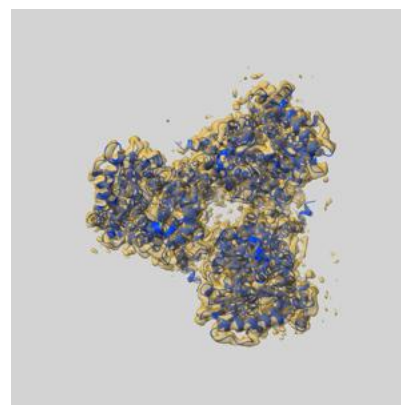
9.1 Map-model overlay [i](#)



X



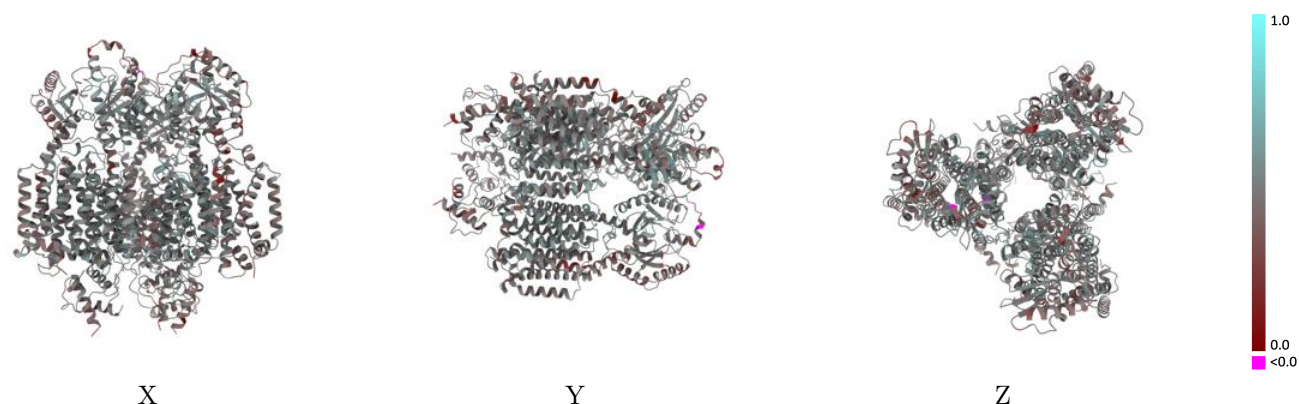
Y



Z

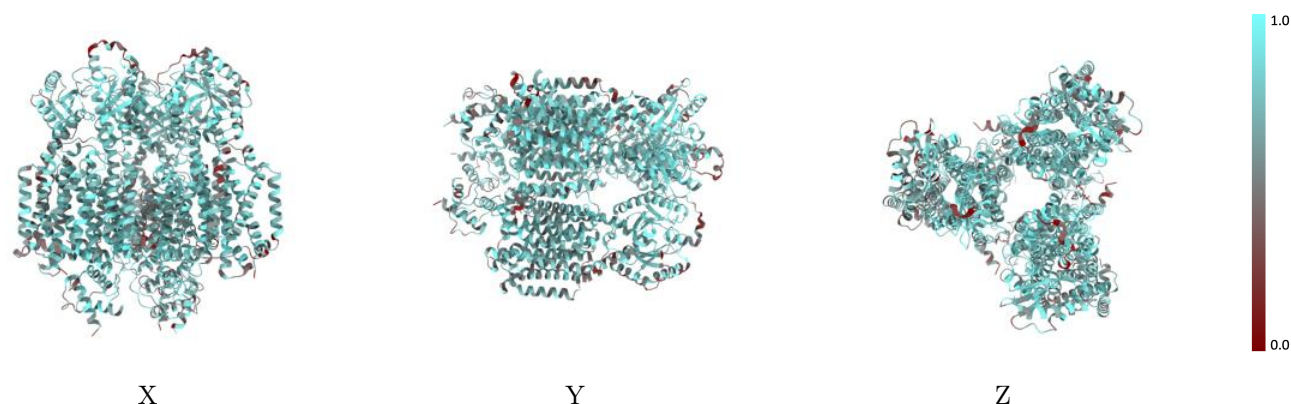
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



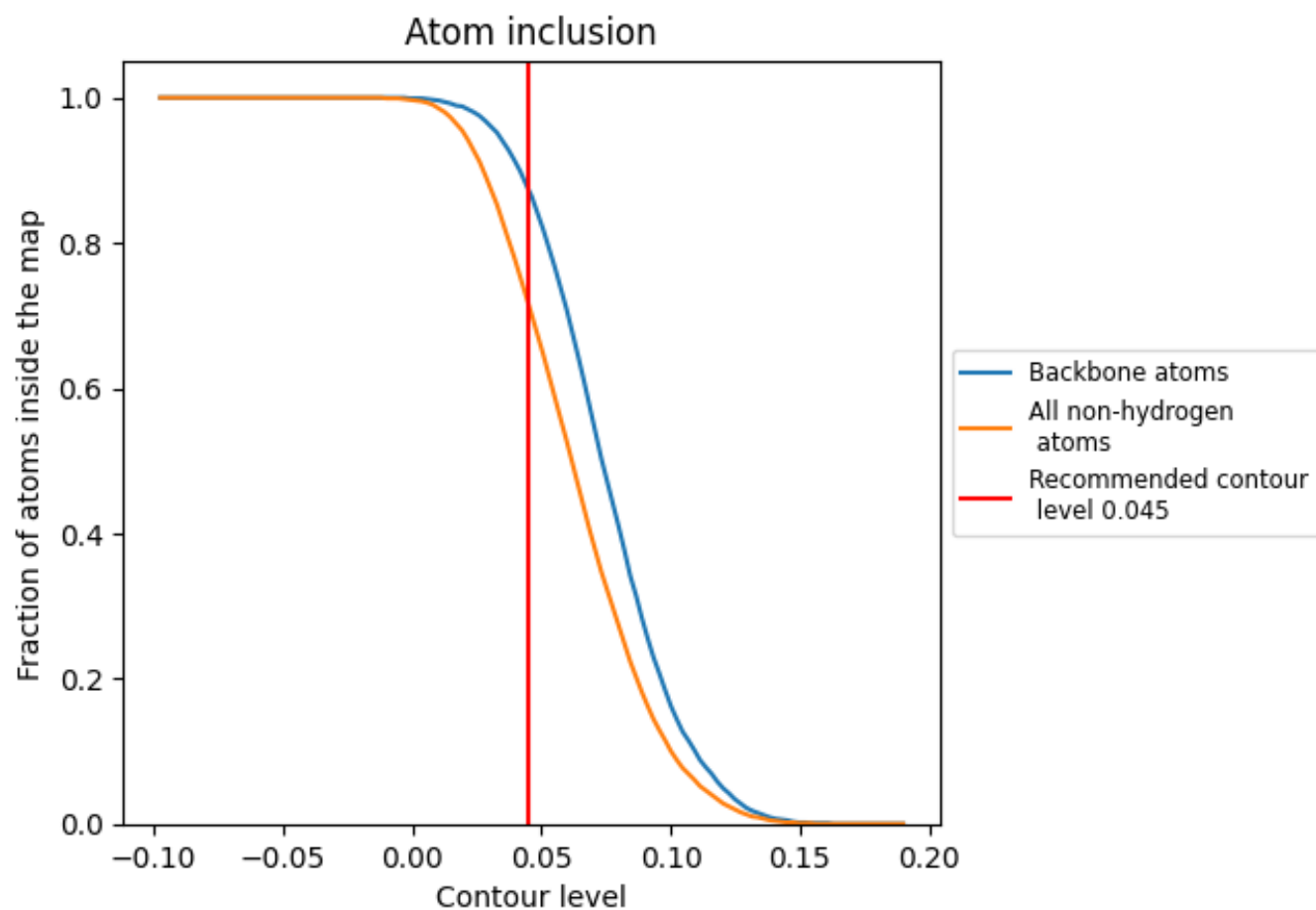
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.4680
A	0.5800	0.4780
B	0.5920	0.4820
C	0.5430	0.4230
D	0.7210	0.4710
E	0.7340	0.4720
F	0.7380	0.4730
G	0.6460	0.4390
H	0.6690	0.4440
I	0.6180	0.4180

1.0

0.0

<0.0