



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 06:17 AM UTC

PDB ID : 7S6C / pdb_00007s6c
EMDB ID : EMD-24868
Title : CryoEM structure of modular PKS holo-Lsd14 stalled at the condensation step and bound to antibody fragment 1B2, composite structure
Authors : Bagde, S.R.; Kim, C.-Y.; Fromme, J.C.
Deposited on : 2021-09-13
Resolution : 3.10 Å (reported)
Based on initial models : 6C9U, 7S6B

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

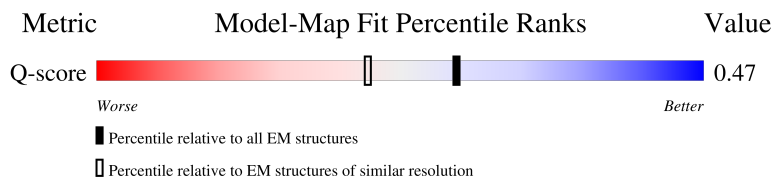
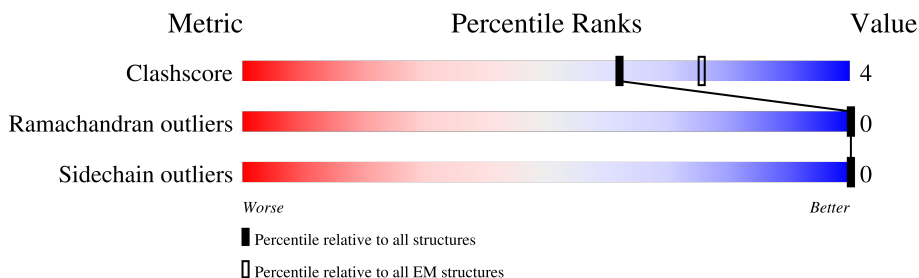
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1649	
1	B	1649	
1	C	1649	
1	D	1649	

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Mol	Chain	Length	Quality of chain
2	E	249	73%10%17%
2	H	249	78%18%
3	F	236	86%6%8%
3	G	236	6%78%13%9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47400 atoms, of which 23451 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 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4, Lsd14 Polyketide synthase fusion.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	895	Total	C	H	N	O	S	0	0
			13235	4176	6542	1220	1277	20		
1	B	891	Total	C	H	N	O	S	0	0
			13199	4162	6521	1218	1278	20		
1	C	480	Total	C	H	N	O	S	0	0
			6988	2208	3471	638	668	3		
1	D	82	Total	C	H	N	O	S	0	0
			1257	388	632	120	115	2		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP Q03132
A	8	VAL	-	expression tag	UNP Q03132
A	1648	LEU	-	expression tag	UNP B6ZK67
A	1649	GLU	-	expression tag	UNP B6ZK67
A	1650	HIS	-	expression tag	UNP B6ZK67
A	1651	HIS	-	expression tag	UNP B6ZK67
A	1652	HIS	-	expression tag	UNP B6ZK67
A	1653	HIS	-	expression tag	UNP B6ZK67
A	1654	HIS	-	expression tag	UNP B6ZK67
A	1655	HIS	-	expression tag	UNP B6ZK67
B	7	MET	-	initiating methionine	UNP Q03132
B	8	VAL	-	expression tag	UNP Q03132
B	1648	LEU	-	expression tag	UNP B6ZK67
B	1649	GLU	-	expression tag	UNP B6ZK67
B	1650	HIS	-	expression tag	UNP B6ZK67
B	1651	HIS	-	expression tag	UNP B6ZK67
B	1652	HIS	-	expression tag	UNP B6ZK67
B	1653	HIS	-	expression tag	UNP B6ZK67
B	1654	HIS	-	expression tag	UNP B6ZK67
B	1655	HIS	-	expression tag	UNP B6ZK67
C	7	MET	-	initiating methionine	UNP Q03132

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	VAL	-	expression tag	UNP Q03132
C	1648	LEU	-	expression tag	UNP B6ZK67
C	1649	GLU	-	expression tag	UNP B6ZK67
C	1650	HIS	-	expression tag	UNP B6ZK67
C	1651	HIS	-	expression tag	UNP B6ZK67
C	1652	HIS	-	expression tag	UNP B6ZK67
C	1653	HIS	-	expression tag	UNP B6ZK67
C	1654	HIS	-	expression tag	UNP B6ZK67
C	1655	HIS	-	expression tag	UNP B6ZK67
D	7	MET	-	initiating methionine	UNP Q03132
D	8	VAL	-	expression tag	UNP Q03132
D	1648	LEU	-	expression tag	UNP B6ZK67
D	1649	GLU	-	expression tag	UNP B6ZK67
D	1650	HIS	-	expression tag	UNP B6ZK67
D	1651	HIS	-	expression tag	UNP B6ZK67
D	1652	HIS	-	expression tag	UNP B6ZK67
D	1653	HIS	-	expression tag	UNP B6ZK67
D	1654	HIS	-	expression tag	UNP B6ZK67
D	1655	HIS	-	expression tag	UNP B6ZK67

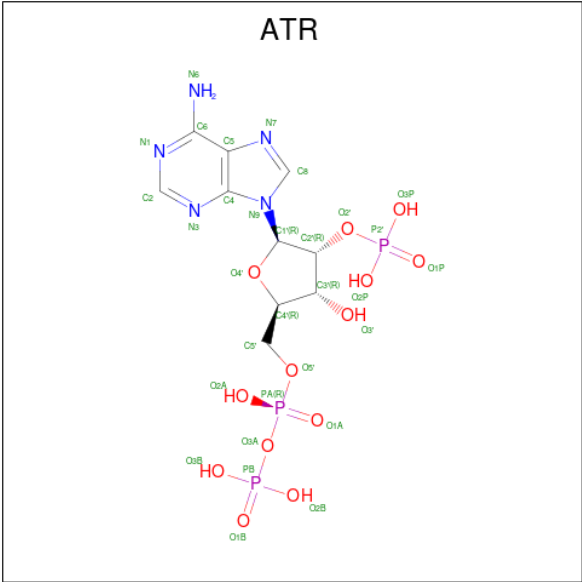
- Molecule 2 is a protein called Fab 1B2 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	207	Total	C	H	N	O	S	0	0
			3081	987	1526	260	302	6		
2	H	205	Total	C	H	N	O	S	0	0
			3053	979	1513	257	298	6		

- Molecule 3 is a protein called Fab 1B2 light chain.

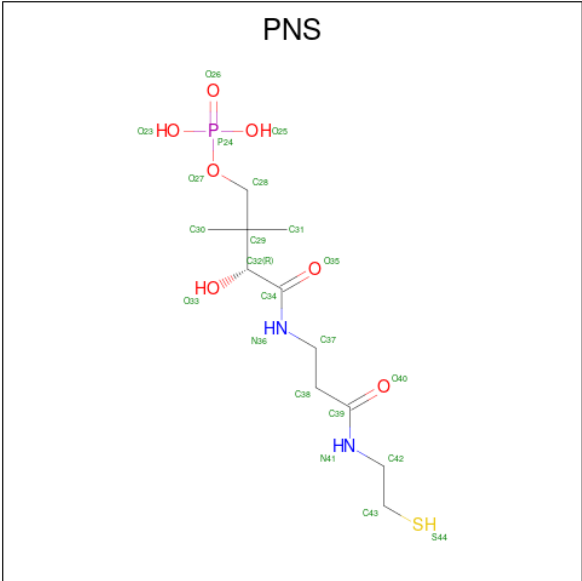
Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	216	Total	C	H	N	O	S	0	0
			3255	1033	1604	280	332	6		
3	G	214	Total	C	H	N	O	S	0	0
			3249	1029	1611	278	325	6		

- Molecule 4 is 2'-MONOPHOSPHADENOSINE-5'-DIPHOSPHATE (CCD ID: ATR) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 5 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).

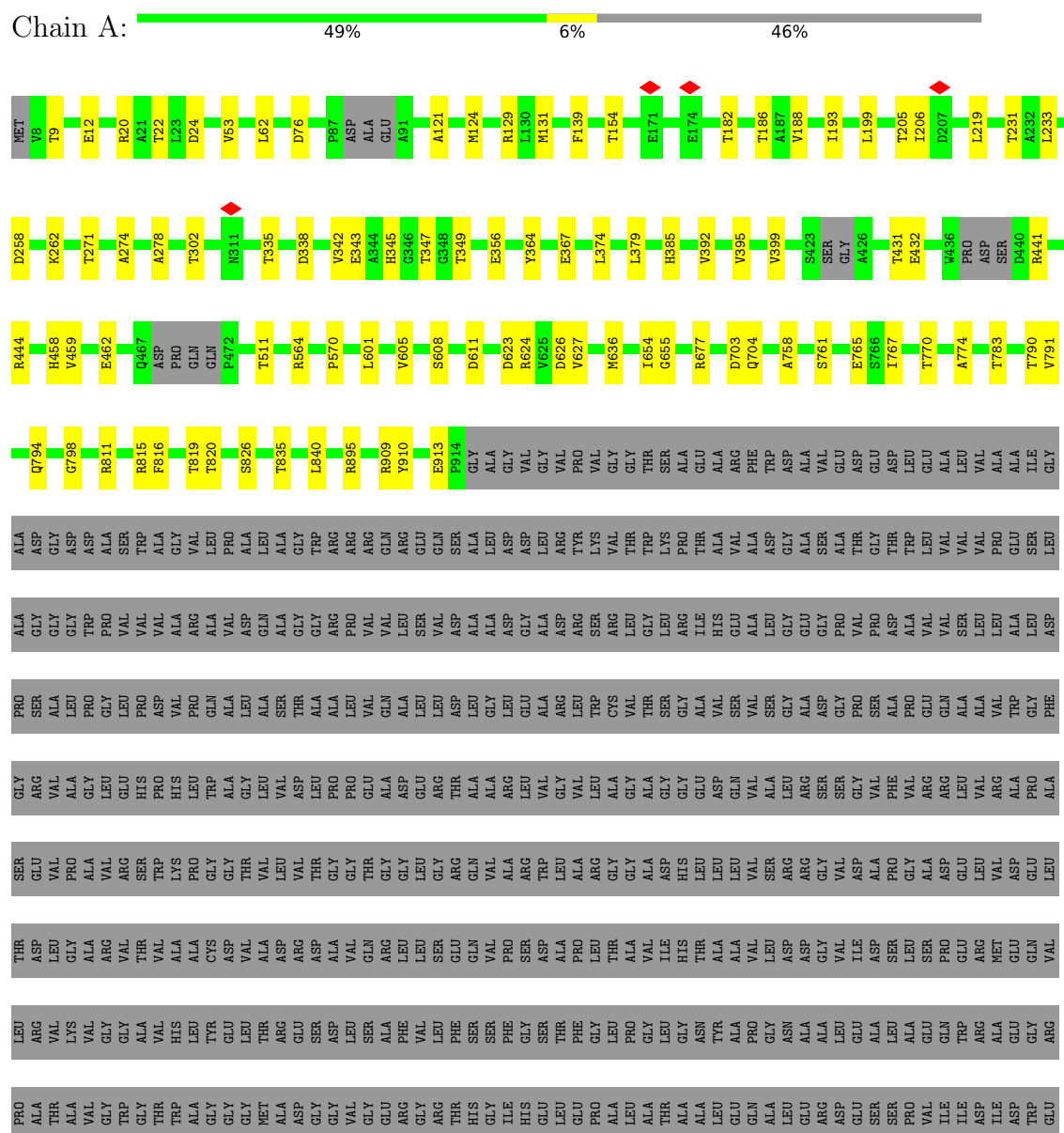


Mol	Chain	Residues	Atoms							AltConf
5	D	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	

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: 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4, Lsd14 Polyketide synthase fusion



- Molecule 1: 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4, Lsd14 Polyketide synthase fusion

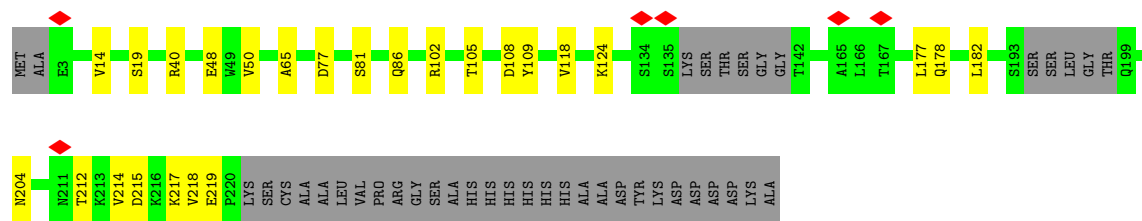
SER	PRO	PHE	ALA	SER	PRO	GLY	VAL	ALA	THR	ASP	THR	ASP	Q773	R821	L280	MET
LEU	ALA	VAL	PRO	LEU	ALA	GLU	ARG	GLU	TRP	LEU	TRP	LEU	L787	L530	E283	V8
ILE	ILE	TRP	GLN	PRO	ASP	ALA	ARG	GLN	VAL	ALA	VAL	GLN	V791	D534	E16	E16
ASP	ASP	ARG	ALA	LEU	LEU	VAL	VAL	ALA	VAL	VAL	PRO	VAL	T796	T837	R289	R20
ILE	ASP	ARG	VAL	ASP	VAL	TRP	ARG	TRP	ALA	ALA	ALA	ALA	D797	A541	N311	A21
GLU	GLU	ARG	PHE	ALA	ASP	GLU	PHE	ALA	SER	ILE	SER	ILE	G798	G312	T22	T22
ARG	PRO	SER	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	ALA	GLY	T799	D551	D24	D24
PHE	PHE	GLU	ARG	GLU	ASP	GLU	ARG	VAL	GLY	ASP	GLY	ASP	Y805	A552	S337	E38
ALA	VAL	VAL	VAL	VAL	ALA	VAL	VAL	VAL	GLY	GLY	GLY	GLY	R811	Q575	D340	A41
VAL	ALA	PRO	GLY	PRO	PRO	ALA	GLY	PRO	TRP	ASP	TRP	ASP	R811	Q575	D340	A41
ALA	ALA	VAL	GLY	VAL	GLY	PRO	VAL	GLY	PRO	ASP	PRO	ASP	R816	R581	E343	D68
THR	THR	SER	GLY	GLY	VAL	VAL	GLY	GLY	VAL	SER	VAL	SER	F815	A344	A344	E82
ALA	ALA	TRP	HIS	PRO	ASP	PRO	HIS	PRO	VAL	TRP	VAL	ALA	E817	E598	H345	E82
THR	VAL	VAL	PRO	ASP	ASP	ASP	THR	ALA	VAL	ALA	VAL	GLY	R821	T610	E356	D110
ARG	ARG	LYS	HIS	VAL	VAL	VAL	HIS	VAL	ALA	GLY	ALA	VAL	H830	R614	G365	R129
PRO	PRO	PRO	LEU	PRO	PRO	PRO	LEU	PRO	ARG	VAL	ARG	VAL	R614	R614	G365	R129
GLY	GLY	GLY	TRP	GLY	TRP	GLY	TRP	GLY	VAL	ALA	VAL	PRO	E846	R624	H366	L130
GLY	GLY	THR	GLY	ALA	ALA	LEU	GLY	LEU	VAL	LEU	ASP	ASP	E846	V625	E367	M131
THR	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLN	ALA	GLN	LEU	T860	D626	V376	L132
ARG	ASP	VAL	VAL	SER	THR	THR	VAL	SER	GLY	ALA	GLY	ALA	T860	V627	V376	E133
GLY	ASP	THR	LEU	LEU	LEU	LEU	LEU	LEU	GLY	TRP	GLY	TRP	H881	V628	K380	V166
ASP	ALA	GLY	PRO	ALA	ALA	ALA	PRO	ALA	ARG	ARG	ARG	ARG	Q906	L632	G384	SER
VAL	VAL	GLY	PRO	LEU	LEU	LEU	VAL	LEU	PRO	ARG	PRO	ARG	R907	L639	G384	PRO
ALA	ALA	GLY	GLY	VAL	VAL	VAL	GLY	GLN	VAL	ARG	VAL	GLN	Y910	L639	V395	ALA
ALA	ASP	GLY	ASP	ALA	ALA	ALA	ASP	ALA	VAL	GLN	LEU	GLN	Y910	L639	V395	ALA
LEU	LEU	GLY	GLY	LEU	LEU	LEU	LEU	LEU	SER	GLY	LEU	GLY	E913	I648	L429	VAL
GLY	ARG	GLY	ARG	THR	ARG	ASP	GLY	THR	VAL	GLN	VAL	GLN	E913	I648	L429	VAL
THR	THR	ARG	THR	ALA	ASP	ASP	THR	ALA	ASP	SER	ASP	SER	P914	E660	D435	GLY
ALA	ALA	GLN	ALA	ALA	ALA	LEU	GLN	ALA	ALA	ALA	ALA	ALA	P914	L686	V436	GLY
ALA	VAL	VAL	ALA	ALA	GLY	GLY	VAL	GLY	LEU	LEU	LEU	LEU	P914	L686	V436	GLY
ILE	PHE	ALA	ARG	ALA	ARG	LEU	ALA	ARG	ASP	ASP	ASP	ASP	GLY	D438	D437	ALA
GLY	HIS	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	D703	S439	GLY
GLY	THR	TRP	VAL	VAL	VAL	VAL	VAL	VAL	ALA	LEU	ALA	LEU	GLY	Q704	D440	G178
PRO	ALA	LEU	GLY	GLY	ARG	ALA	GLY	GLY	ASP	ARG	ASP	ARG	VAL	Q710	R441	I193
GLY	PRO	ALA	VAL	VAL	VAL	VAL	VAL	VAL	ARG	TYR	ARG	TYR	PRO	Q710	R4	

- Molecule 1: 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4, Lsd14 Polyketide synthase fusion

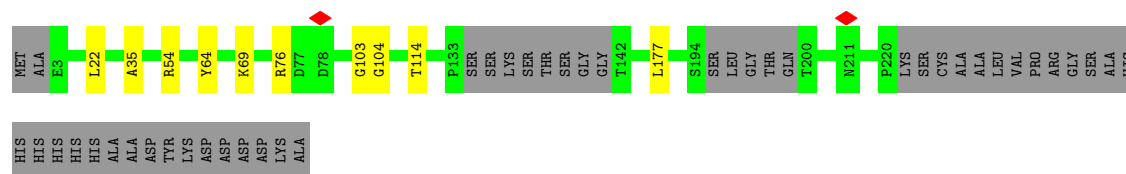
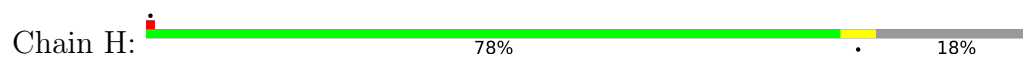


THR	ILE	GLU	ALA	THR	GLY	SER	ASP	ALA	ARG	VAL	THR	THR	THR	LEU	ARG	ARG	ASP	HIS	GLY	ASP	LEU	THR	GLN	LEU	LEU	HIS	THR	ALA	ALA	LEU	ALA	THR	ALA	THR	TRP	THR	HIS	GLY	ILE	ASP	VAL	ASP	THR	THR	THR	ALA	VAL	LEU	GLY	ASP	ARG	ARG	THR	PRO	PRO	PHE	GLU	LEU	LEU	THR	TYR	ALA	ALA	PHE
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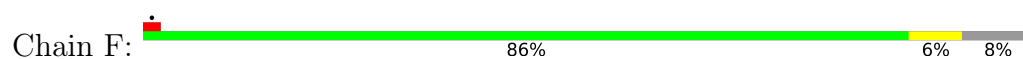




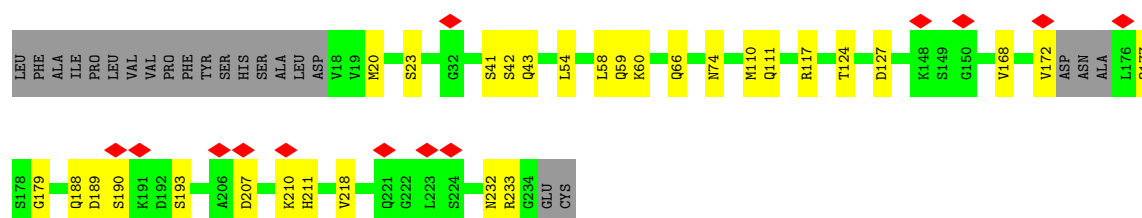
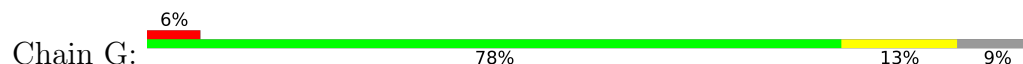
• Molecule 2: Fab 1B2 heavy chain



• Molecule 3: Fab 1B2 light chain



• Molecule 3: Fab 1B2 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	397539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	79000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	47.709	Depositor
Minimum map value	-21.716	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.126	Depositor
Recommended contour level	7	Depositor
Map size (Å)	379.652, 379.652, 379.652	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.043, 1.043, 1.043	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: PNS, ATR

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	0.14	0/6844	0.31	0/9349
1	B	0.14	0/6830	0.33	0/9332
1	C	0.15	0/3591	0.36	0/4914
1	D	0.15	0/633	0.34	0/857
2	E	0.15	0/1591	0.38	0/2163
2	H	0.13	0/1576	0.35	0/2143
3	F	0.12	0/1686	0.31	0/2289
3	G	0.15	0/1674	0.35	0/2273
All	All	0.14	0/24425	0.33	0/33320

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	6693	6542	6545	55	0
1	B	6678	6521	6524	61	0
1	C	3517	3471	3471	35	0
1	D	625	632	632	8	0
2	E	1555	1526	1526	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1540	1513	1513	6	0
3	F	1651	1604	1604	11	0
3	G	1638	1611	1611	17	0
4	C	31	11	11	2	0
5	D	21	20	21	0	0
All	All	23949	23451	23458	202	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 202 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:A:206:ILE:HD11	1:A:219:LEU:HD12	1.66	0.78
1:A:367:GLU:N	1:A:367:GLU:OE1	2.25	0.70
1:C:980:ARG:NH2	1:C:1417:GLU:OE1	2.25	0.70
1:B:38:GLU:O	1:B:225:ARG:NH1	2.25	0.69
1:C:977:ASP:OD2	1:C:1189:SER:OG	2.10	0.69

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	885/1649 (54%)	849 (96%)	36 (4%)	0	100	100
1	B	885/1649 (54%)	848 (96%)	37 (4%)	0	100	100
1	C	476/1649 (29%)	457 (96%)	19 (4%)	0	100	100
1	D	78/1649 (5%)	75 (96%)	3 (4%)	0	100	100
2	E	201/249 (81%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	199/249 (80%)	193 (97%)	6 (3%)	0	100	100
3	F	210/236 (89%)	203 (97%)	7 (3%)	0	100	100
3	G	210/236 (89%)	197 (94%)	13 (6%)	0	100	100
All	All	3144/7566 (42%)	3017 (96%)	127 (4%)	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	684/1242 (55%)	684 (100%)	0	100	100
1	B	685/1242 (55%)	685 (100%)	0	100	100
1	C	348/1242 (28%)	348 (100%)	0	100	100
1	D	64/1242 (5%)	64 (100%)	0	100	100
2	E	172/203 (85%)	172 (100%)	0	100	100
2	H	170/203 (84%)	170 (100%)	0	100	100
3	F	190/208 (91%)	190 (100%)	0	100	100
3	G	189/208 (91%)	189 (100%)	0	100	100
All	All	2502/5790 (43%)	2502 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1215	GLN
2	E	206	ASN
3	G	52	ASN
3	F	232	ASN
1	B	404	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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$
5	PNS	D	1701	1	14,20,21	2.24	4 (28%)	18,26,29	1.66	4 (22%)
4	ATR	C	1701	-	32,33,33	2.99	6 (18%)	50,52,52	1.71	14 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PNS	D	1701	1	-	11/24/26/27	-
4	ATR	C	1701	-	-	2/21/37/37	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1701	ATR	P2'-O2'	13.44	1.83	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1701	ATR	PB-O3B	5.73	1.76	1.54
5	D	1701	PNS	C39-N41	5.37	1.46	1.33
5	D	1701	PNS	C34-N36	5.06	1.45	1.33
4	C	1701	ATR	PA-O3A	4.47	1.64	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1701	ATR	P2'-O2'-C2'	-4.43	111.59	123.43
5	D	1701	PNS	C38-C39-N41	3.98	123.59	116.34
4	C	1701	ATR	O2'-P2'-O1P	-3.59	96.53	109.33
4	C	1701	ATR	O3A-PA-O1A	-3.47	100.26	110.70
4	C	1701	ATR	O2B-PB-O1B	3.27	123.59	110.83

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

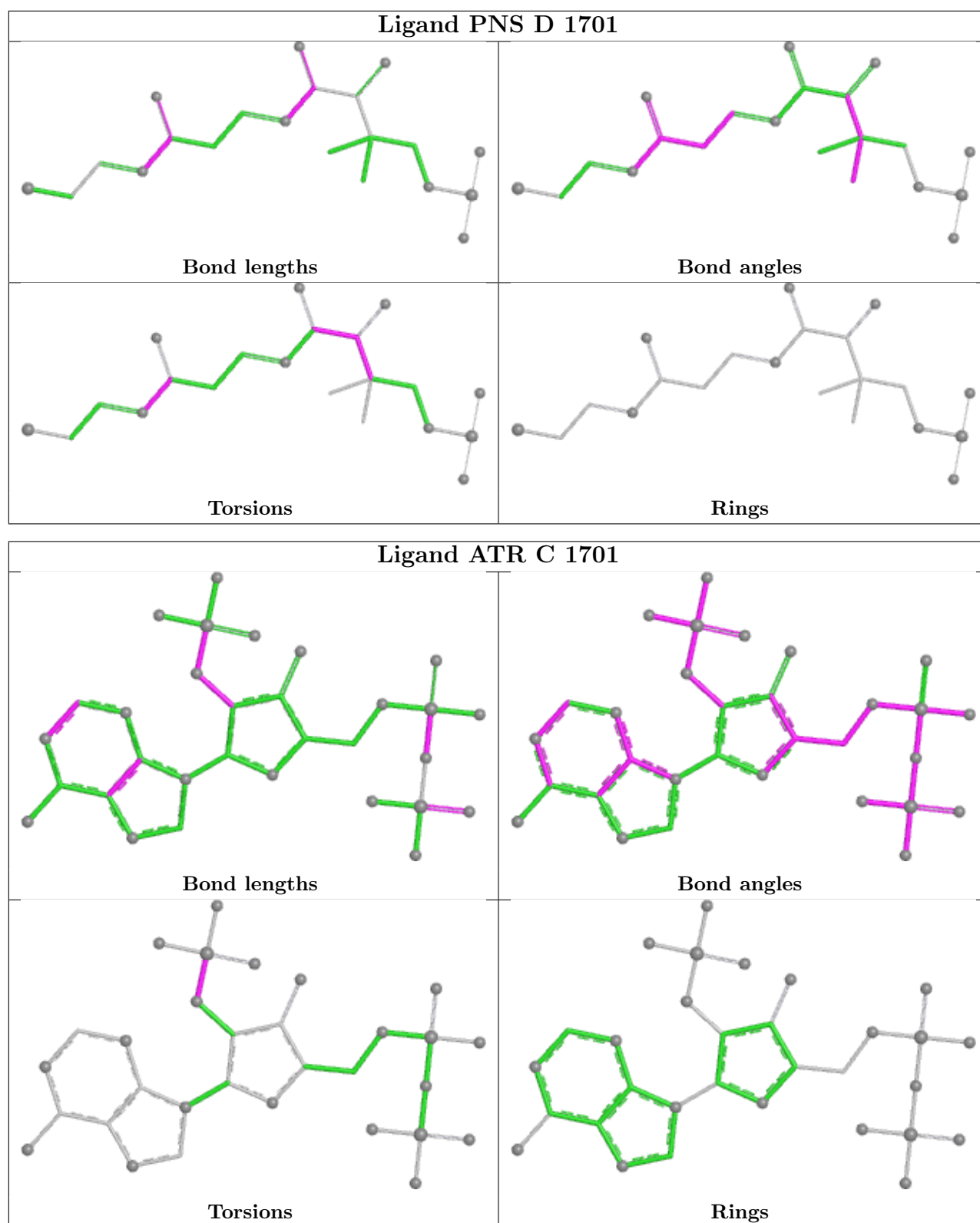
Mol	Chain	Res	Type	Atoms
5	D	1701	PNS	C28-C29-C32-C34
5	D	1701	PNS	C38-C39-N41-C42
5	D	1701	PNS	O40-C39-N41-C42
5	D	1701	PNS	C30-C29-C32-O33
5	D	1701	PNS	C29-C32-C34-N36

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1701	ATR	2	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.

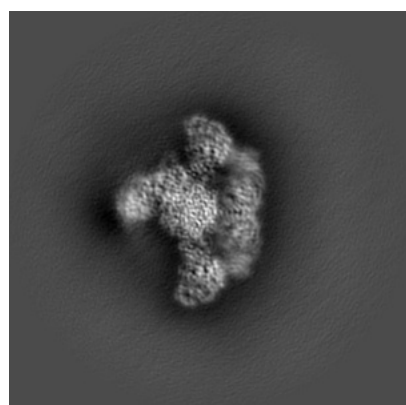
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24868. These allow visual inspection of the internal detail of the map and identification of artifacts.

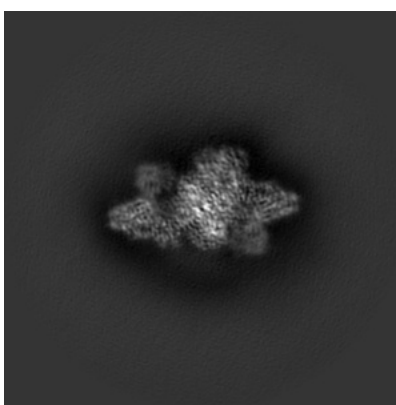
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

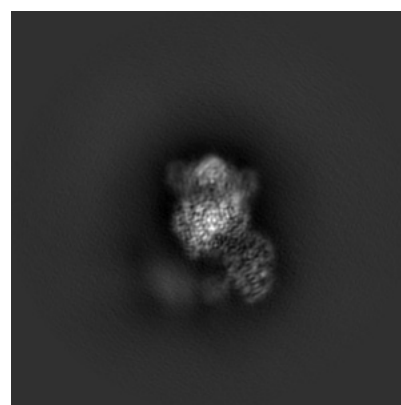
6.1.1 Primary map



X



Y

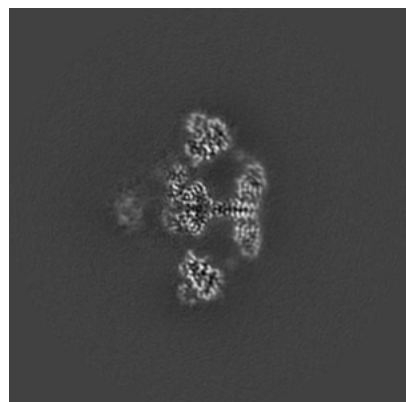


Z

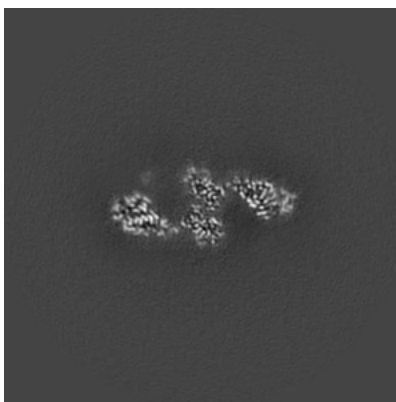
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

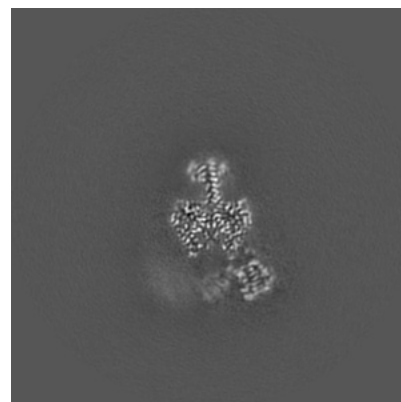
6.2.1 Primary map



X Index: 182



Y Index: 182

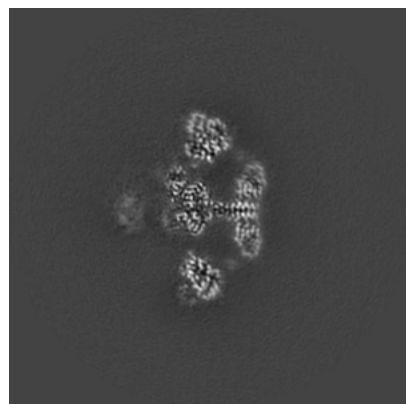


Z Index: 182

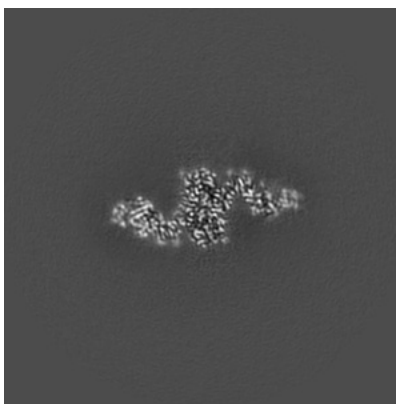
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

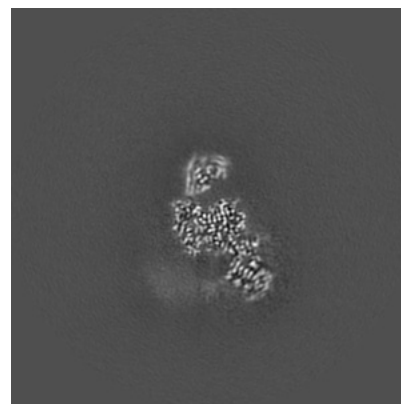
6.3.1 Primary map



X Index: 183



Y Index: 174

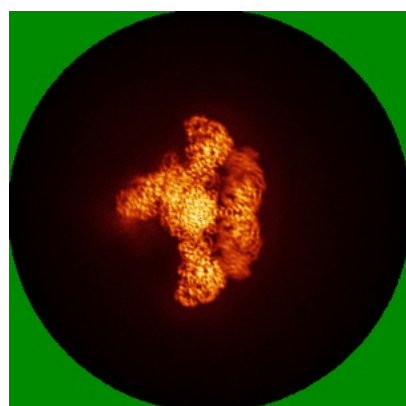


Z Index: 191

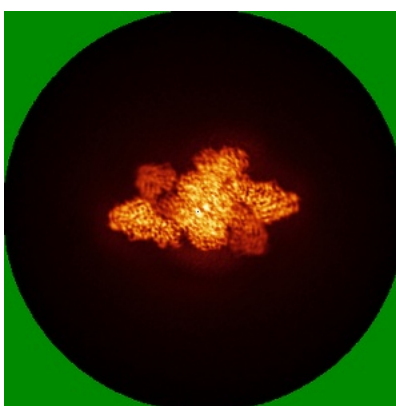
The images above show the largest variance slices of the map in three orthogonal directions.

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

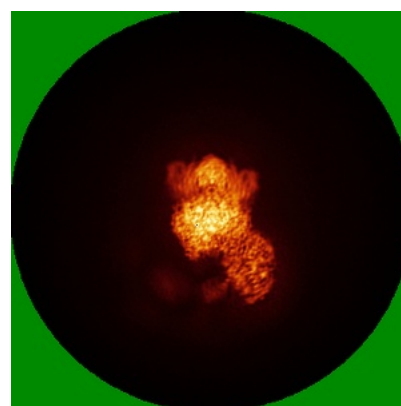
6.4.1 Primary map



X



Y

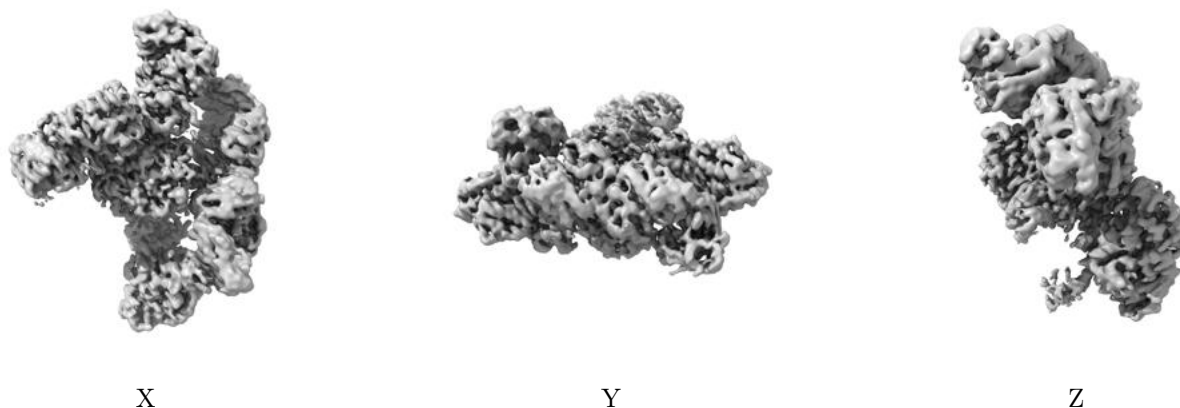


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

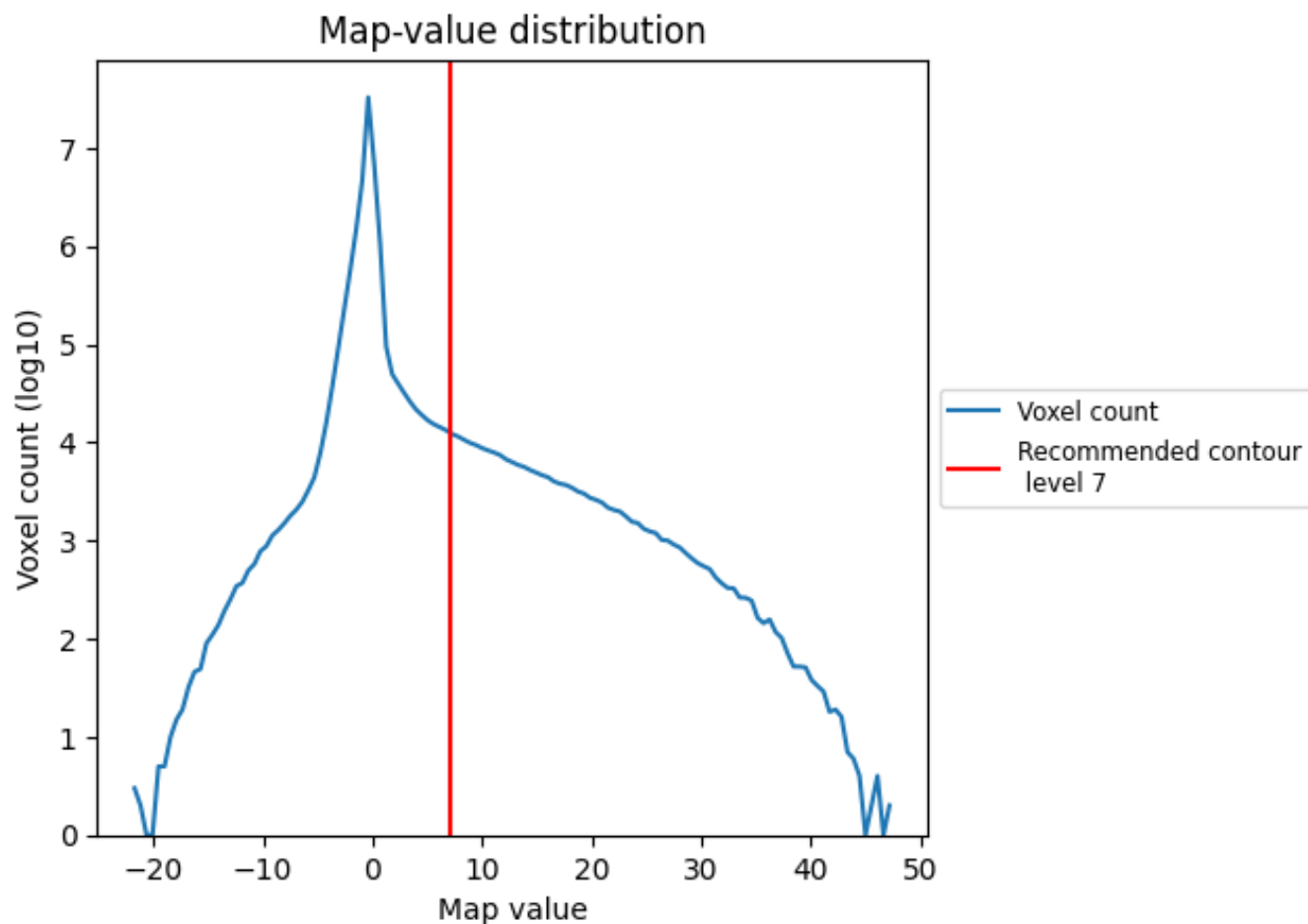
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

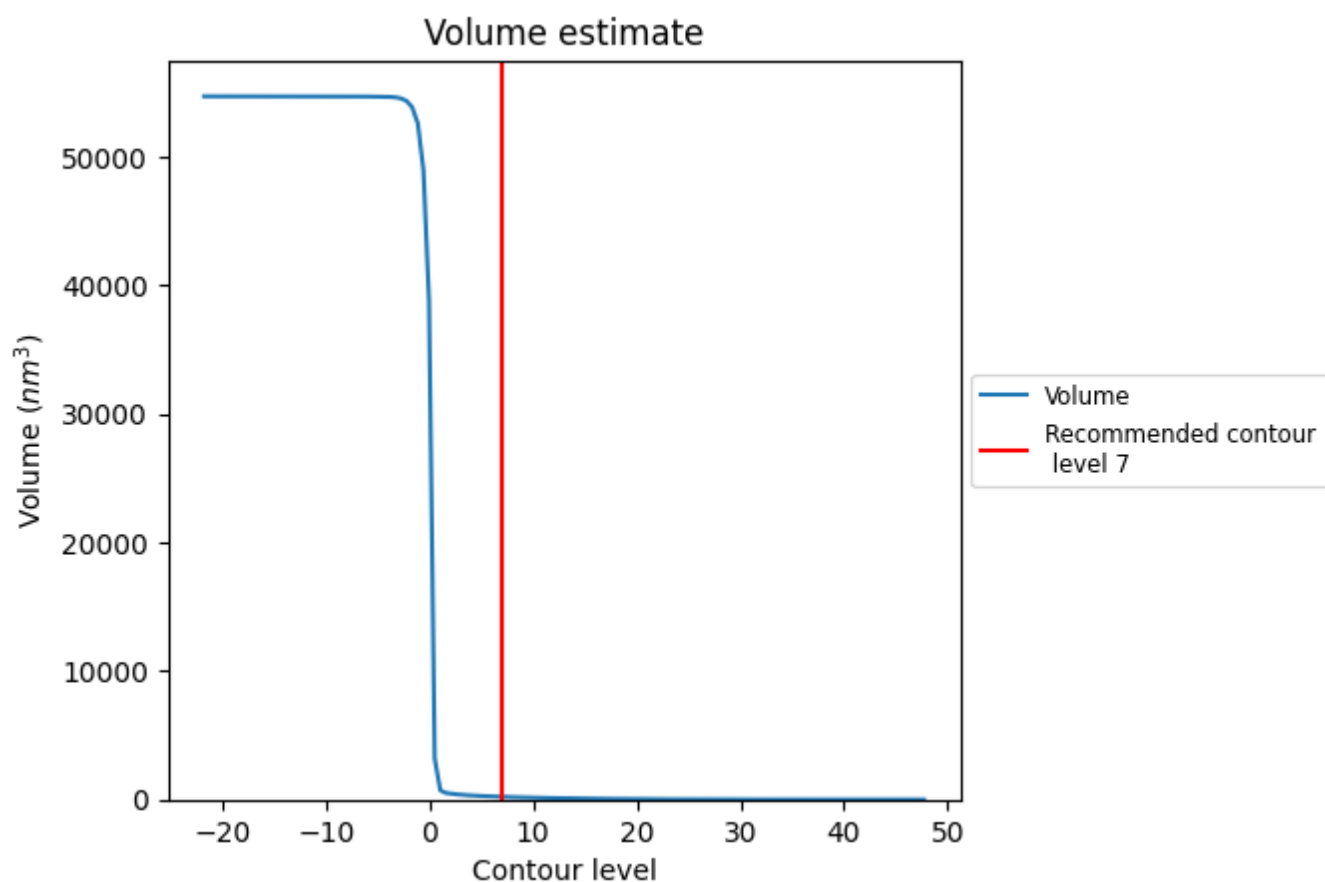
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

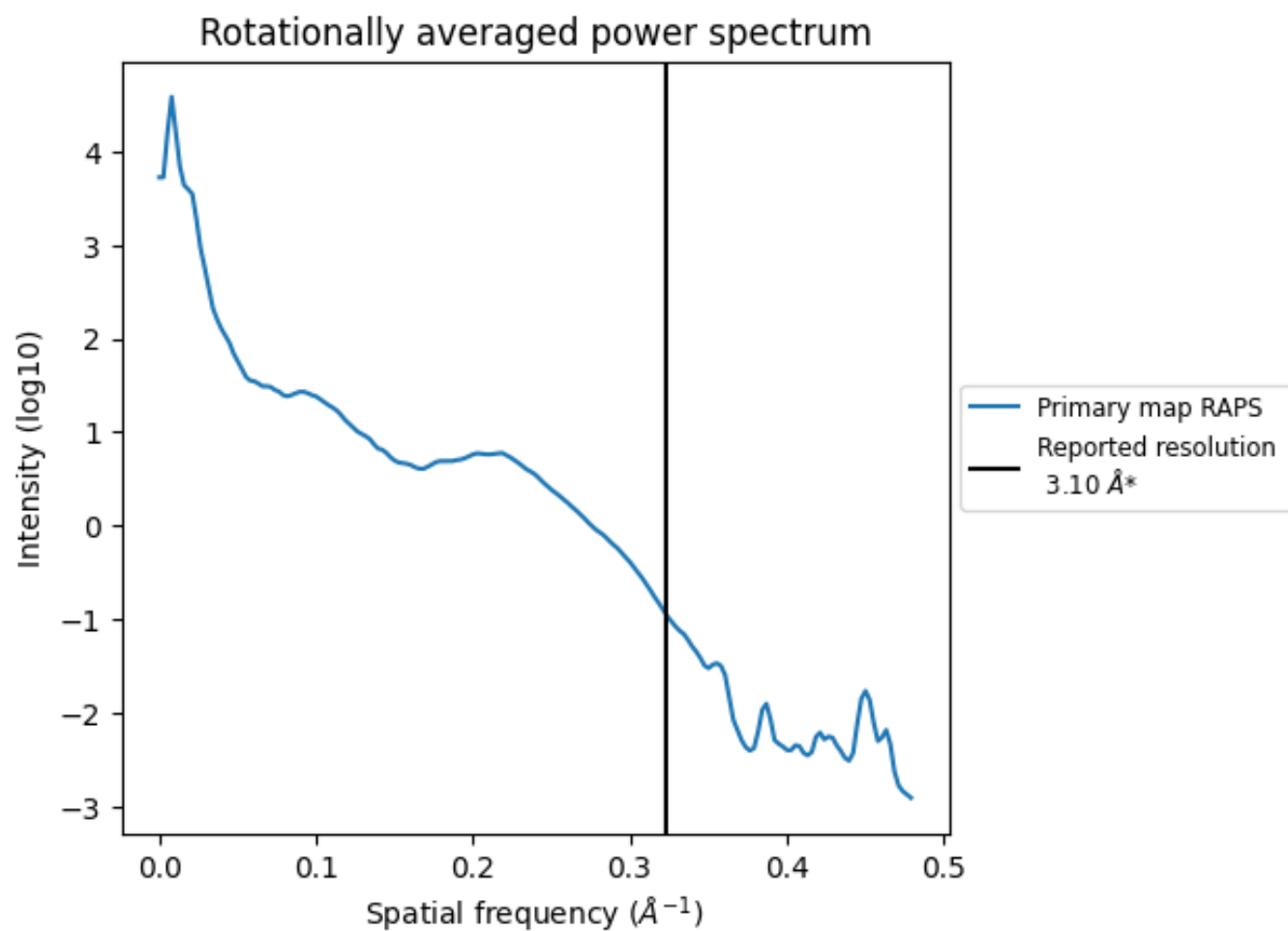
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm^3 ; this corresponds to an approximate mass of 194 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 0.323 Å⁻¹

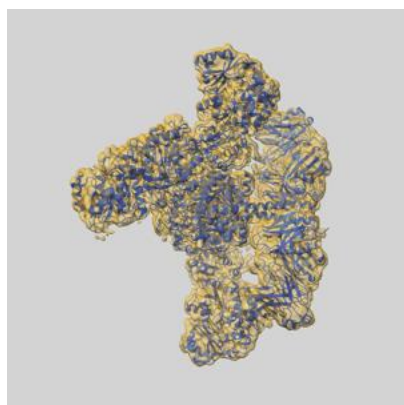
8 Fourier-Shell correlation

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

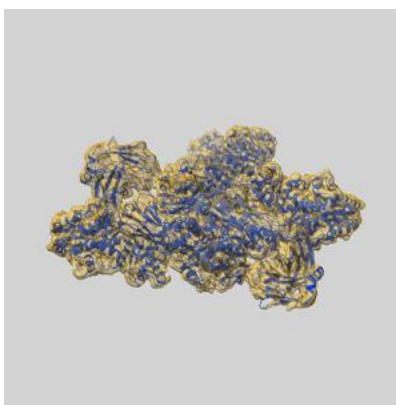
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24868 and PDB model 7S6C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

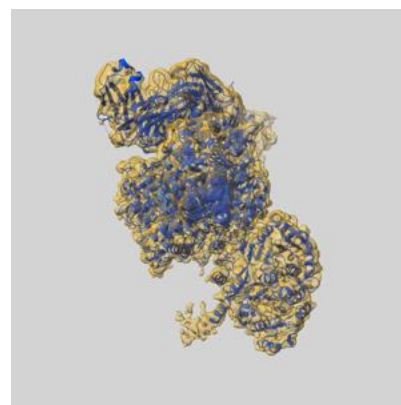
9.1 Map-model overlay [i](#)



X



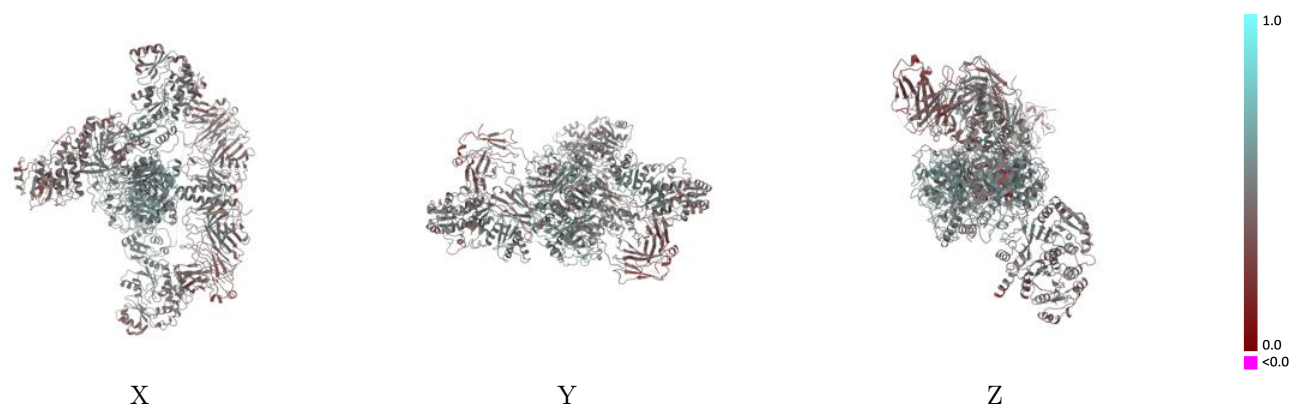
Y



Z

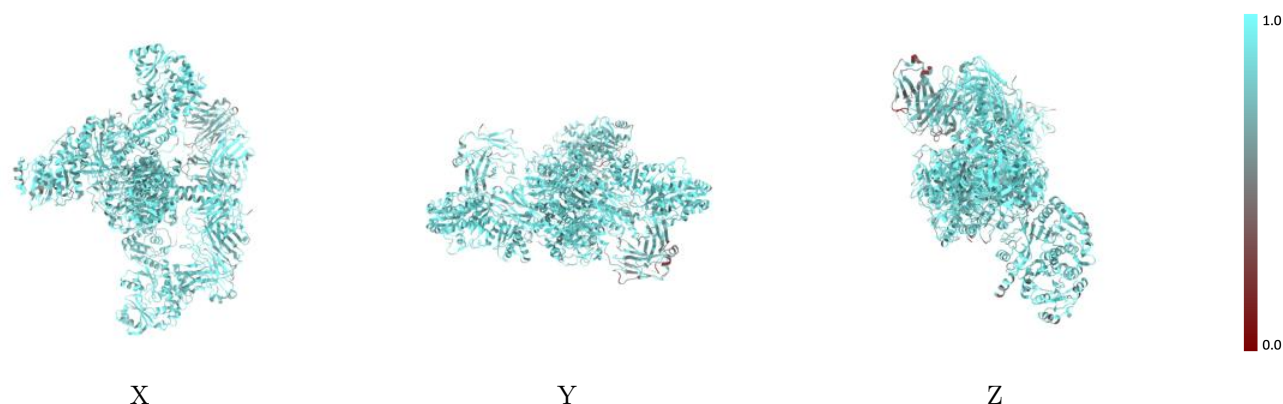
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



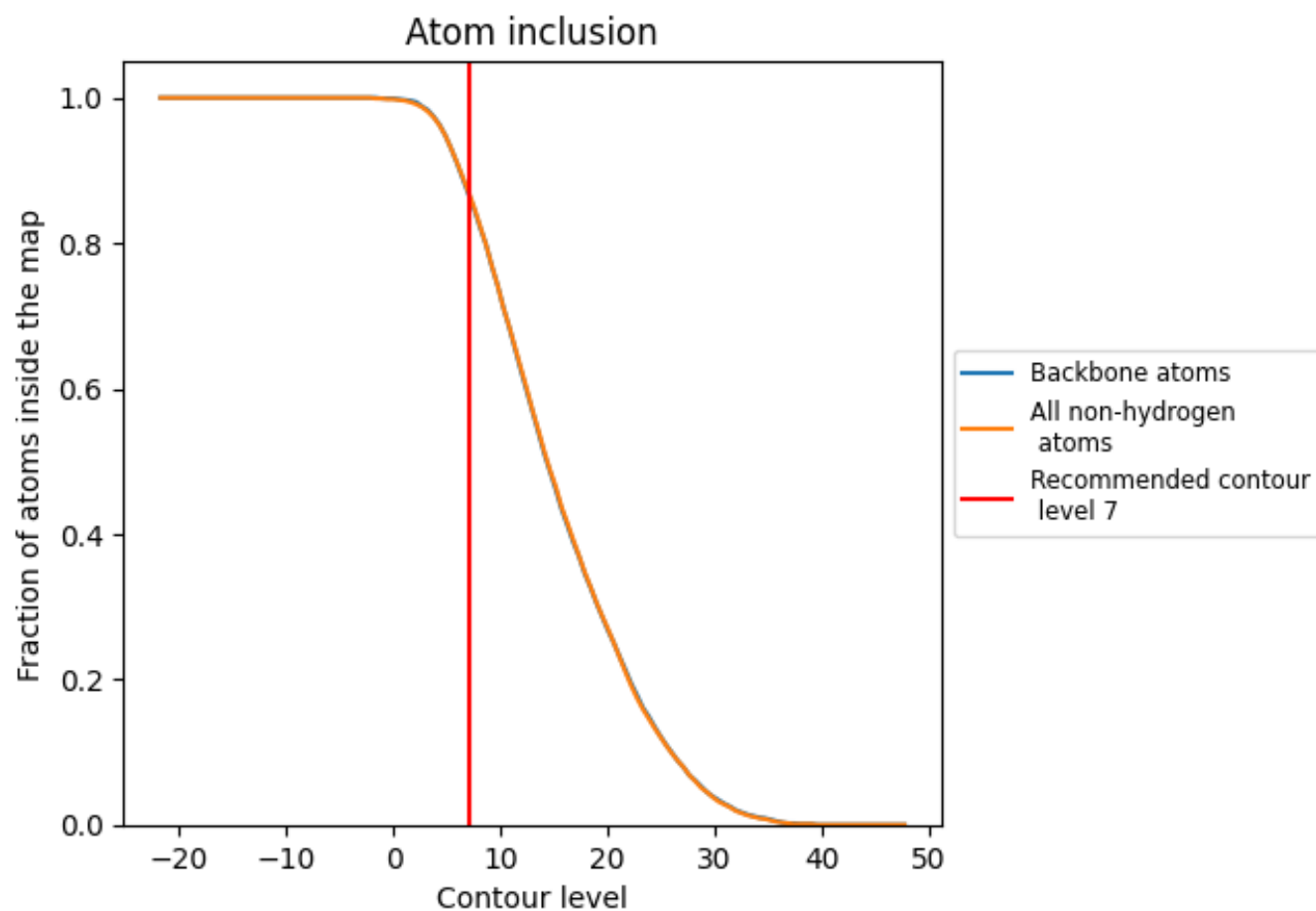
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.4700
A	0.9050	0.5070
B	0.9170	0.5100
C	0.8360	0.4370
D	0.8440	0.4860
E	0.8400	0.4100
F	0.8640	0.4070
G	0.7750	0.3890
H	0.8560	0.4270

1.0

0.0

<0.0