



## wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 08:41 PM EDT

PDB ID : 7M7F / pdb\_00007m7f  
EMDB ID : EMD-23711  
Title : 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1  
Authors : Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.  
Deposited on : 2021-03-28  
Resolution : 3.20 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

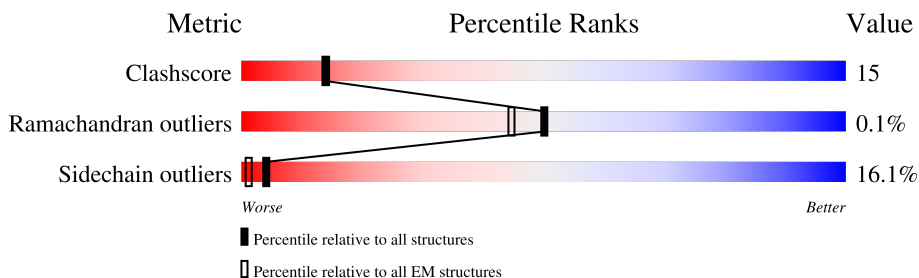
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1784	
1	B	1784	
2	C	249	
2	E	249	
3	D	236	
3	F	236	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23971 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	999	Total	C	N	O	S	0	0
			7417	4613	1363	1414	27		
1	A	1390	Total	C	N	O	S	0	0
			10319	6413	1899	1972	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133

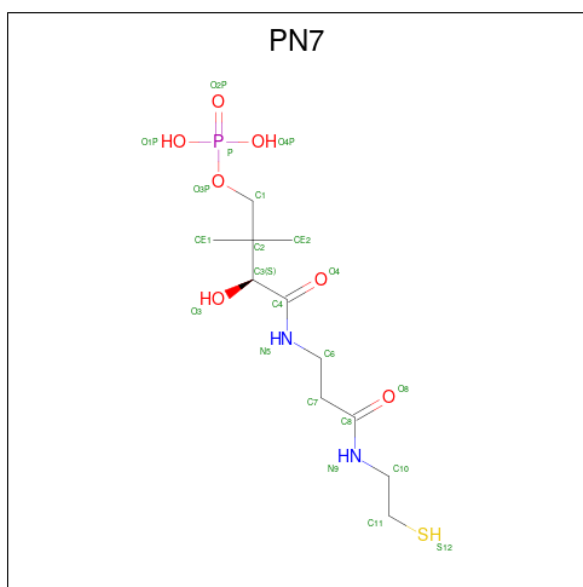
- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylet hyl)-beta-alaninamide (CCD ID: PN7) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).

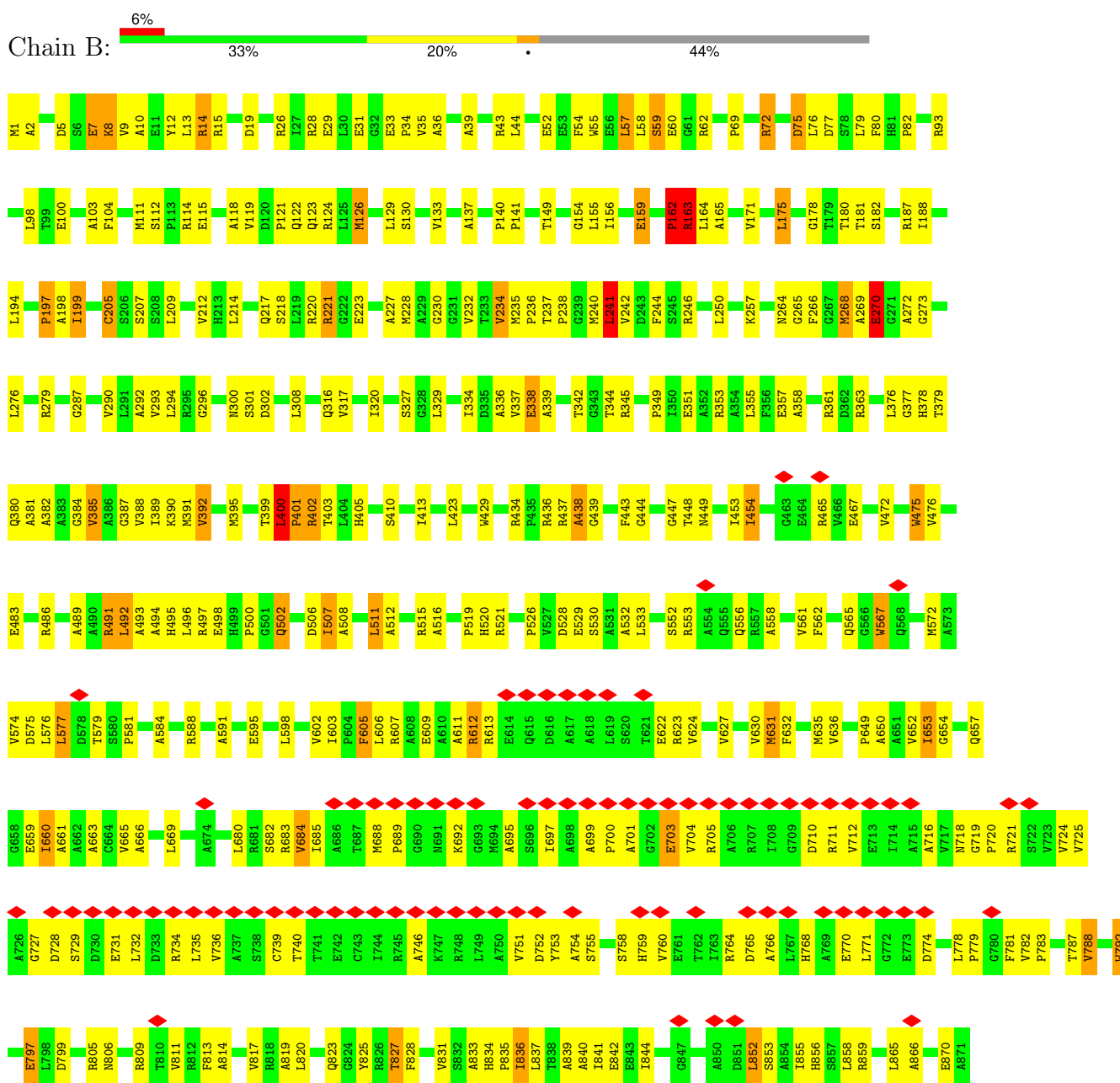


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	S
			21	11	2	6	1	1
								0

### 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: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

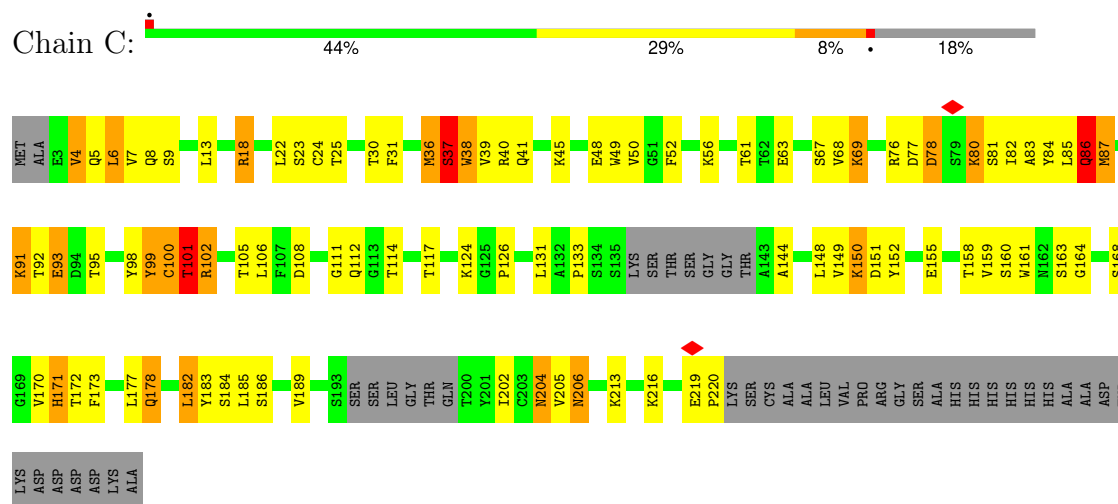




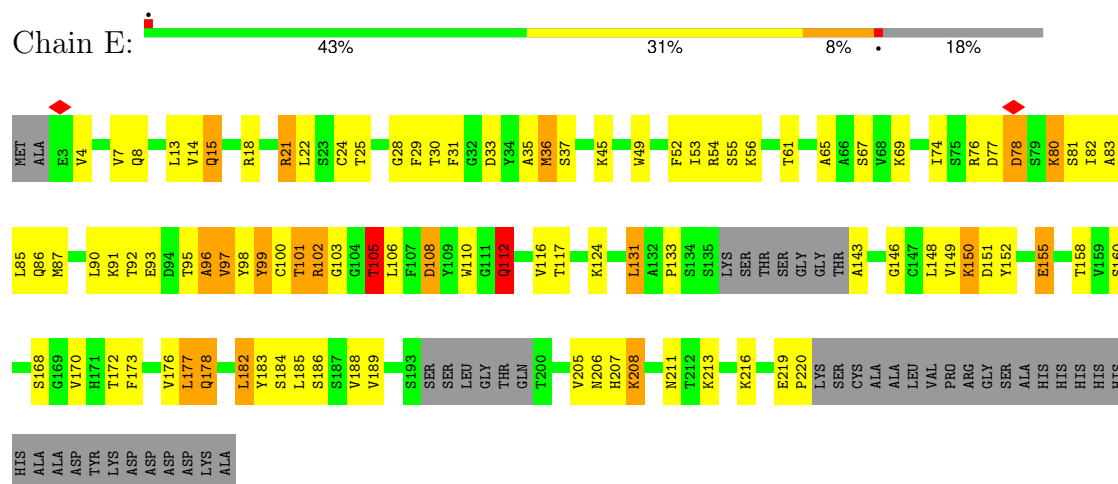


ASN	GLY	PRO	PRO	GLN	SER	ARG	SER
SER	LEU	ARG	GLY	GLN	ASP	LEU	LEU
SER	PRO	GLY	PRO	PRO	PHE	PRO	PRO
SER	THR	VAL	VAL	GLY	ARG	THR	THR
VAL	LEU	VAL	TYR	TYR	GLU	THR	GLU
ASP	LEU	LEU	GLU	GLU	HIS	THR	GLU
LYS	VAL	VAL	GLU	GLU	PHE	VAL	ARG
LEU	SER	ASP	GLY	GLY	ASP	PHE	GLU
ALA	ALA	VAL	VAL	GLU	GLY	ASP	GLU
ALA	GLY	TYR	PRO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

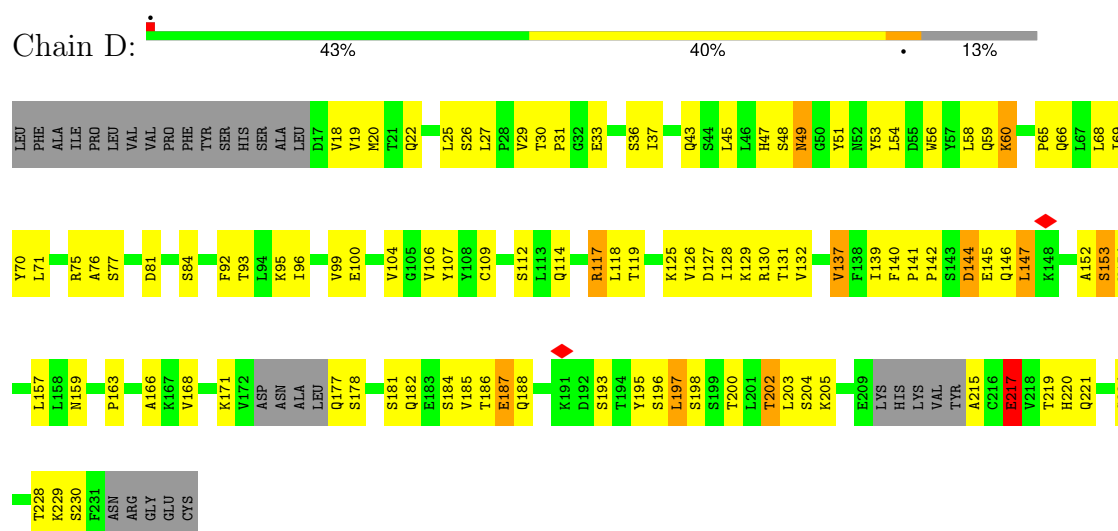
- Molecule 2: 1B2 (heavy chain)



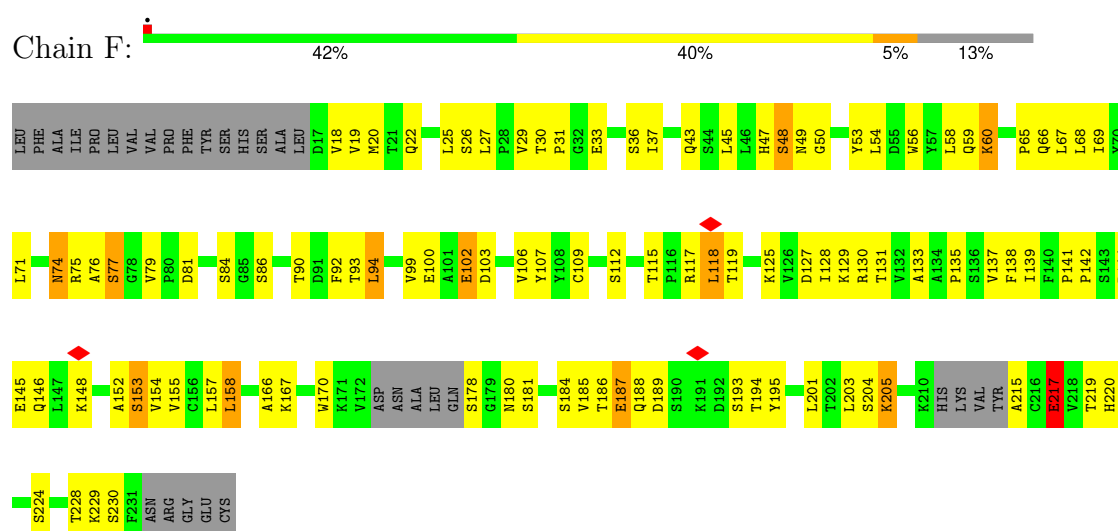
- Molecule 2: 1B2 (heavy chain)



- Molecule 3: 1B2 (light chain)



- Molecule 3: 1B2 (light chain)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.734	Depositor
Minimum map value	-4.602	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PN7

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	0.94	64/10522 (0.6%)	1.20	101/14323 (0.7%)
1	B	0.93	50/7566 (0.7%)	1.18	84/10293 (0.8%)
2	C	0.86	9/1575 (0.6%)	1.12	12/2141 (0.6%)
2	E	0.81	5/1575 (0.3%)	1.18	10/2141 (0.5%)
3	D	0.58	0/1601	0.97	7/2175 (0.3%)
3	F	0.70	5/1601 (0.3%)	1.05	12/2174 (0.6%)
All	All	0.89	133/24440 (0.5%)	1.17	226/33247 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
2	E	0	3
3	F	0	1
All	All	0	6

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	SER	CA-CB	-14.41	1.30	1.53
1	A	43	ARG	C-O	-14.33	1.07	1.24
1	A	207	SER	CA-CB	-14.15	1.28	1.53
1	B	197	PRO	C-O	-13.30	1.06	1.24
1	B	908	VAL	C-O	-12.62	1.08	1.23

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	PRO	N-CA-CB	-23.65	83.45	103.32
1	A	159	GLU	CB-CA-C	-19.80	78.12	110.19
1	B	883	ASP	CB-CA-C	-18.93	78.51	109.75
1	B	266	PHE	CA-CB-CG	17.75	131.55	113.80
1	A	43	ARG	CB-CA-C	-17.11	83.20	110.74

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLN	Mainchain
2	C	155	GLU	Peptide
2	E	155	GLU	Peptide
2	E	21	ARG	Sidechain
2	E	96	ALA	Mainchain

## 5.2 Too-close contacts

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	10319	0	10164	317	0
1	B	7417	0	7306	220	0
2	C	1539	0	1511	61	0
2	E	1539	0	1511	62	0
3	D	1568	0	1528	55	0
3	F	1568	0	1533	62	0
4	B	21	0	22	2	0
All	All	23971	0	23575	736	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 15.

The worst 5 of 736 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:777:PRO:HB3	1:A:796:ASP:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87
2:E:108:ASP:CG	3:F:67:LEU:CD2	2.60	0.75
2:E:108:ASP:CG	3:F:67:LEU:HD23	2.11	0.75
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.68	0.74

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	1388/1784 (78%)	1264 (91%)	123 (9%)	1 (0%)	48	80
1	B	995/1784 (56%)	915 (92%)	78 (8%)	2 (0%)	44	75
2	C	199/249 (80%)	179 (90%)	20 (10%)	0	100	100
2	E	199/249 (80%)	176 (88%)	23 (12%)	0	100	100
3	D	200/236 (85%)	184 (92%)	16 (8%)	0	100	100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
All	All	3181/4538 (70%)	2905 (91%)	273 (9%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1449	SER
1	B	720	PRO
1	A	779	PRO

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1028/1325 (78%)	873 (85%)	155 (15%)	2	12
1	B	746/1325 (56%)	651 (87%)	95 (13%)	3	17
2	C	170/203 (84%)	133 (78%)	37 (22%)	1	4
2	E	170/203 (84%)	135 (79%)	35 (21%)	1	5
3	D	182/208 (88%)	143 (79%)	39 (21%)	1	5
3	F	182/208 (88%)	145 (80%)	37 (20%)	1	5
All	All	2478/3472 (71%)	2080 (84%)	398 (16%)	4	9

5 of 398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1307	LEU
2	C	219	GLU
1	A	1357	VAL
2	C	69	LYS
3	D	96	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	52	ASN
3	F	52	ASN
3	D	111	GLN
3	D	188	GLN
3	F	111	GLN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	PN7	B	1801	1	14,20,21	2.13	4 (28%)	18,26,29	1.42	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PN7	B	1801	1	-	12/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	PN7	C8-N9	4.99	1.45	1.33
4	B	1801	PN7	C4-N5	4.97	1.45	1.33
4	B	1801	PN7	O4-C4	-2.36	1.18	1.23
4	B	1801	PN7	O8-C8	-2.15	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1801	PN7	C6-C7-C8	2.43	116.44	112.39
4	B	1801	PN7	C6-N5-C4	-2.25	118.50	122.55
4	B	1801	PN7	CE2-C2-C3	2.20	112.52	108.77
4	B	1801	PN7	C11-C10-N9	-2.04	107.68	112.31
4	B	1801	PN7	C3-C4-N5	2.03	120.34	116.48

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

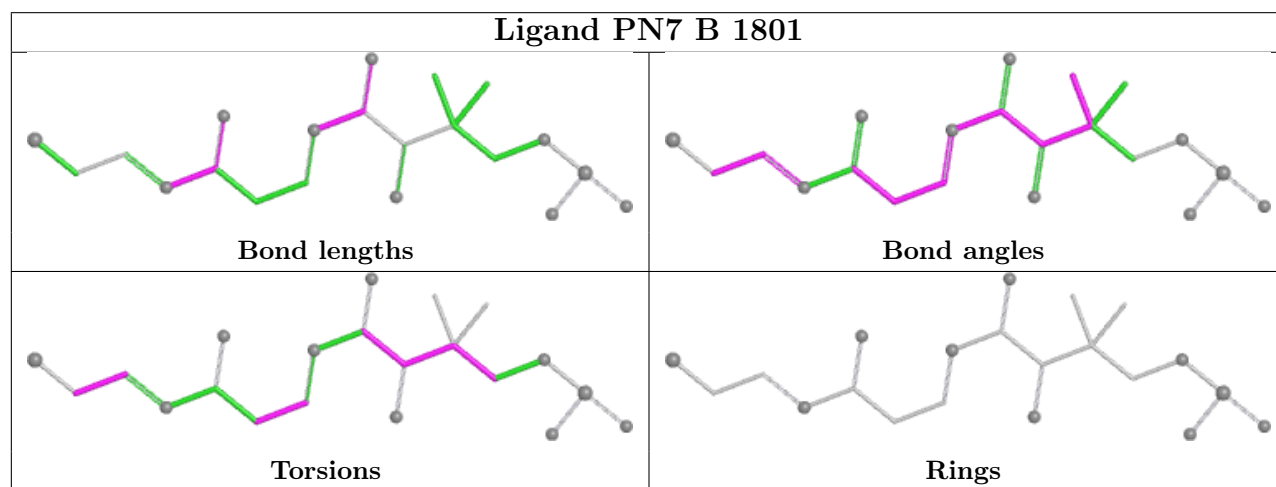
Mol	Chain	Res	Type	Atoms
4	B	1801	PN7	C1-C2-C3-O3
4	B	1801	PN7	C1-C2-C3-C4
4	B	1801	PN7	CE1-C2-C3-O3
4	B	1801	PN7	CE1-C2-C3-C4
4	B	1801	PN7	CE2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	PN7	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 [i](#)

There are no chain breaks in this entry.

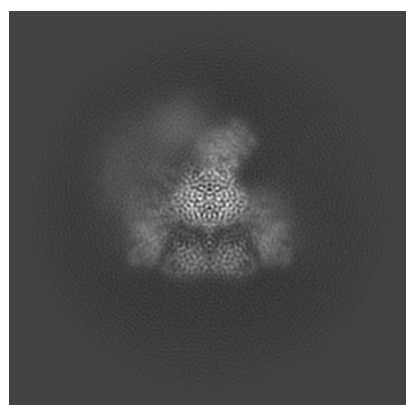
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23711. These allow visual inspection of the internal detail of the map and identification of artifacts.

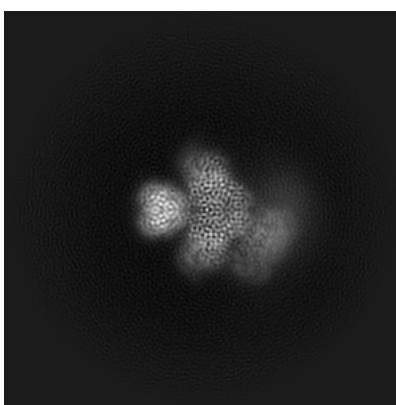
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

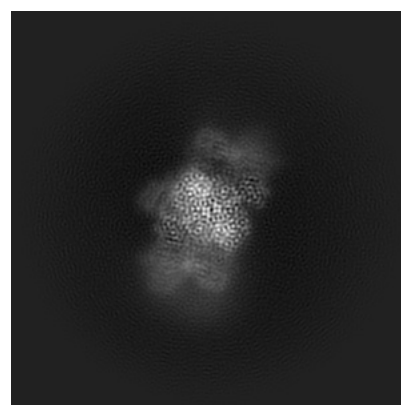
#### 6.1.1 Primary map



X



Y

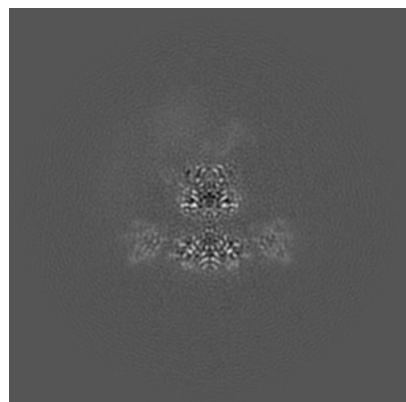


Z

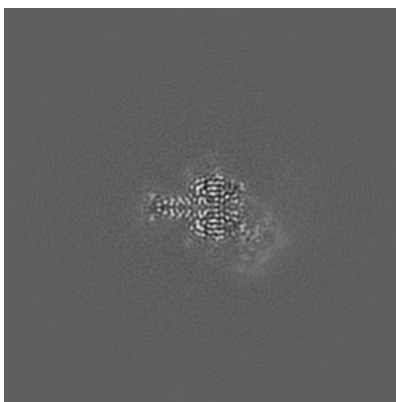
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

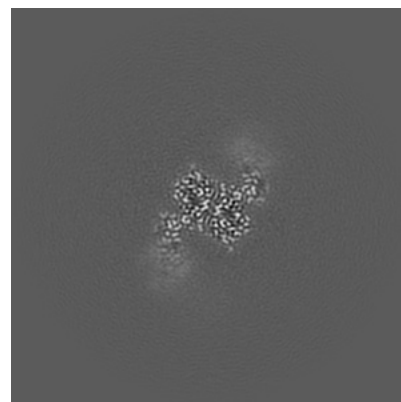
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

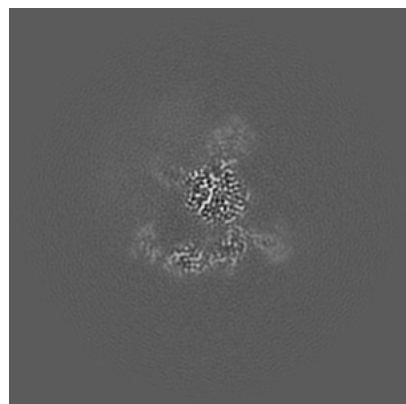


Z Index: 168

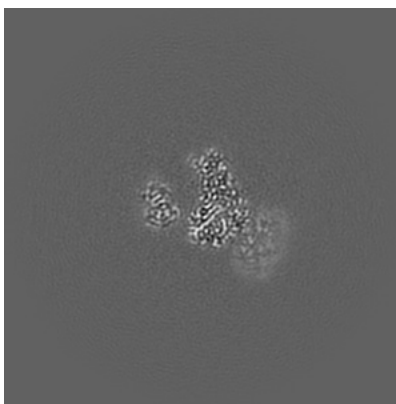
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

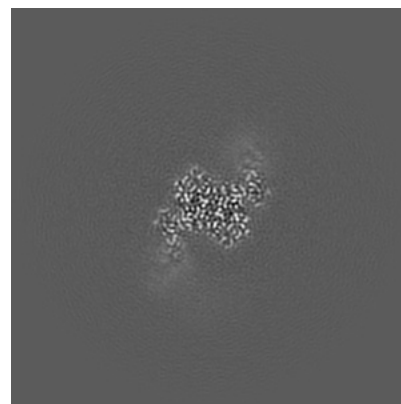
### 6.3.1 Primary map



X Index: 157



Y Index: 181

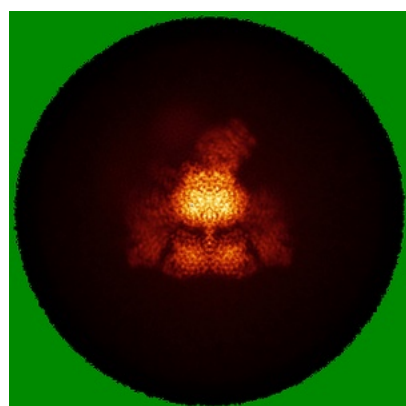


Z Index: 173

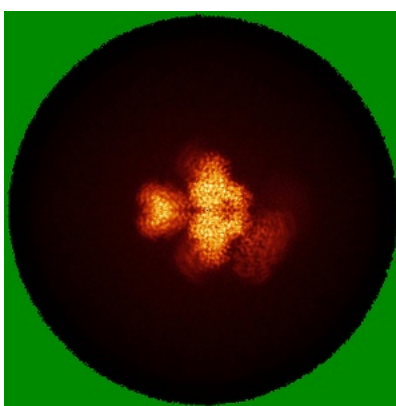
The images above show the largest variance slices of the map in three orthogonal directions.

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

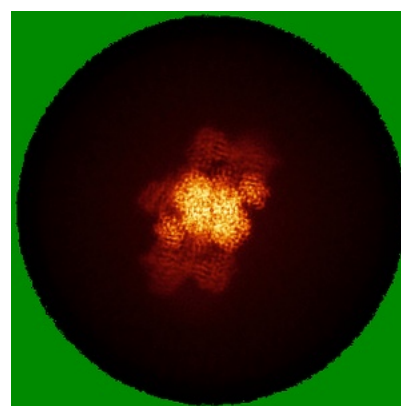
### 6.4.1 Primary map



X



Y

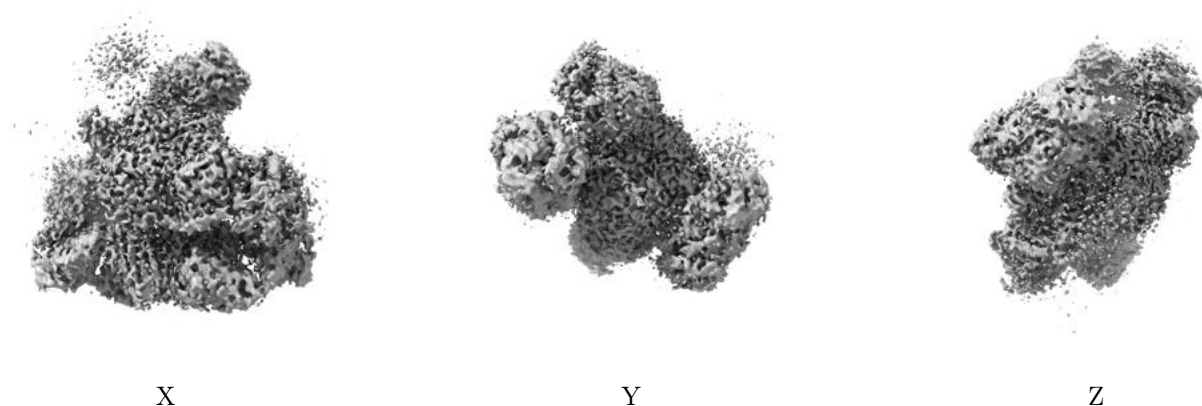


Z

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 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

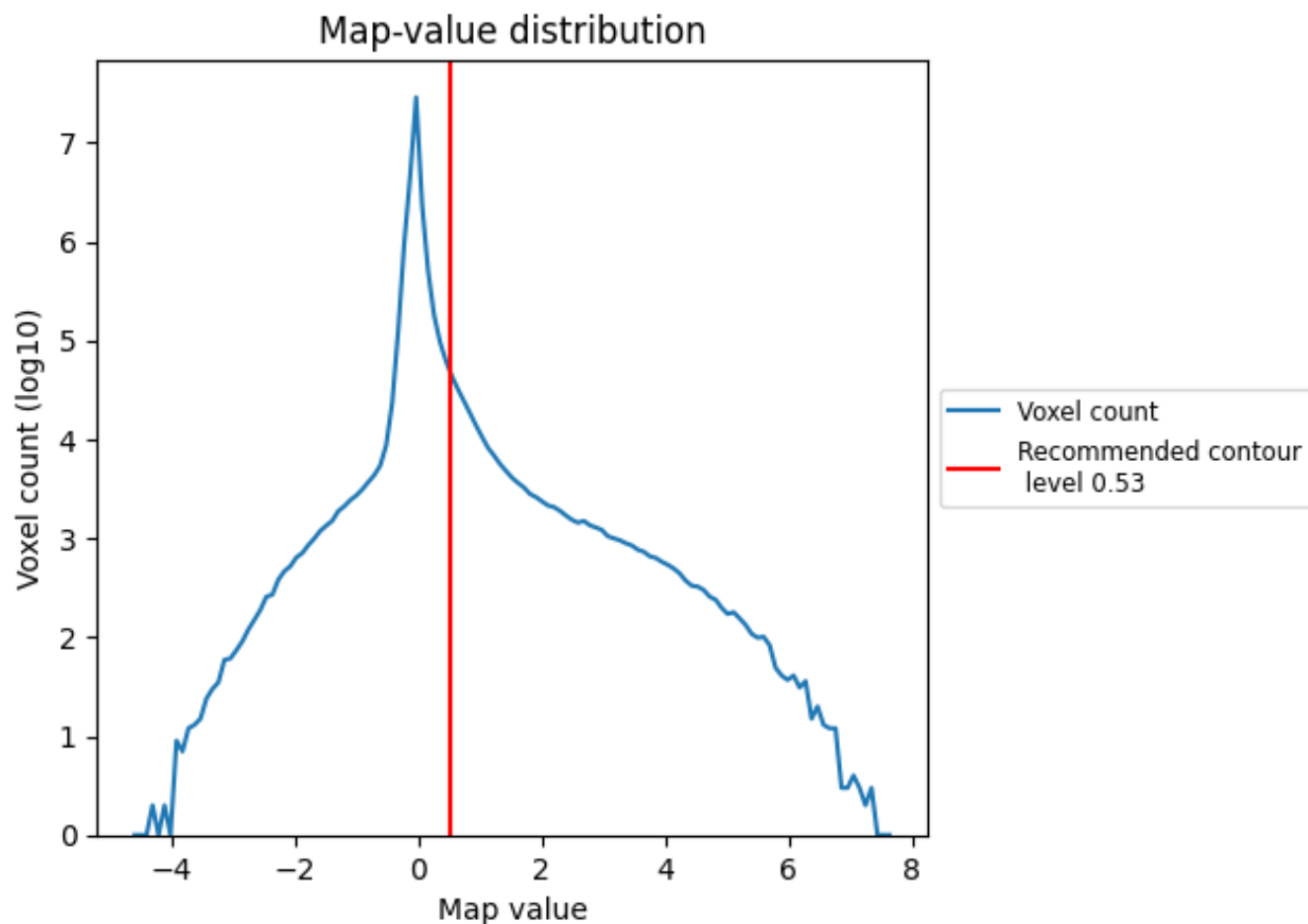
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

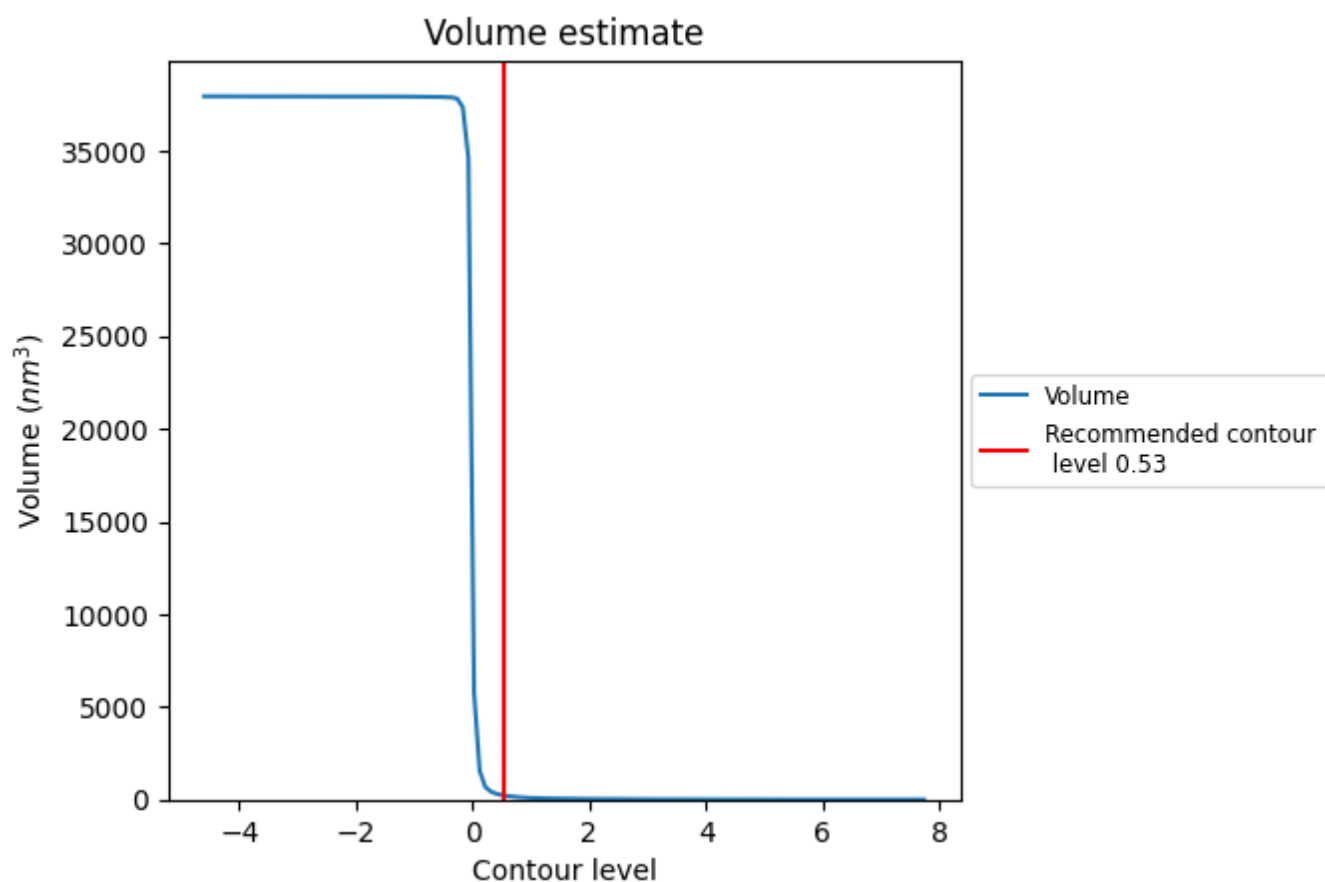
This section contains the results of statistical analysis of the map.

### 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.

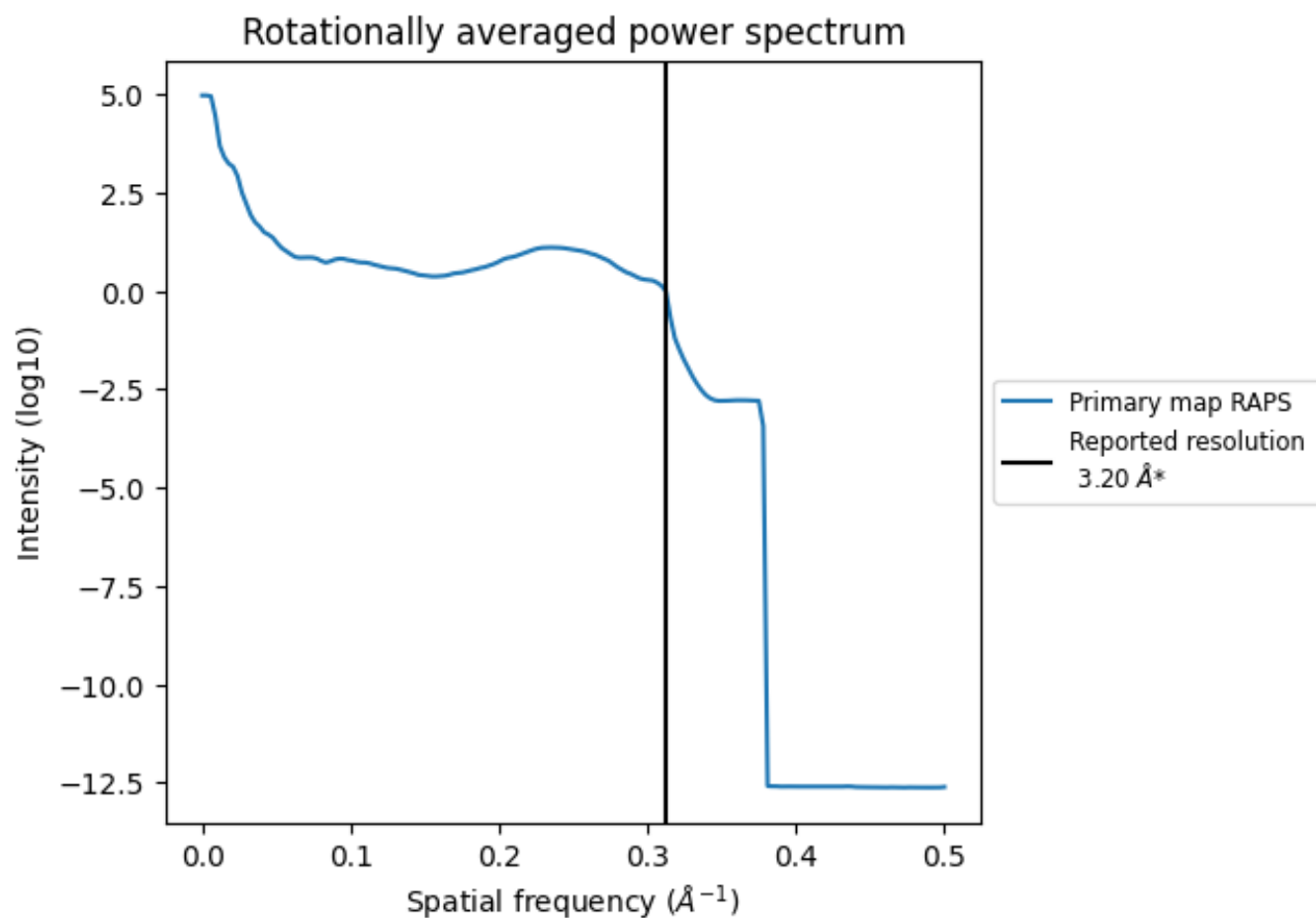
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm<sup>3</sup>; this corresponds to an approximate mass of 204 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<sup>-1</sup>

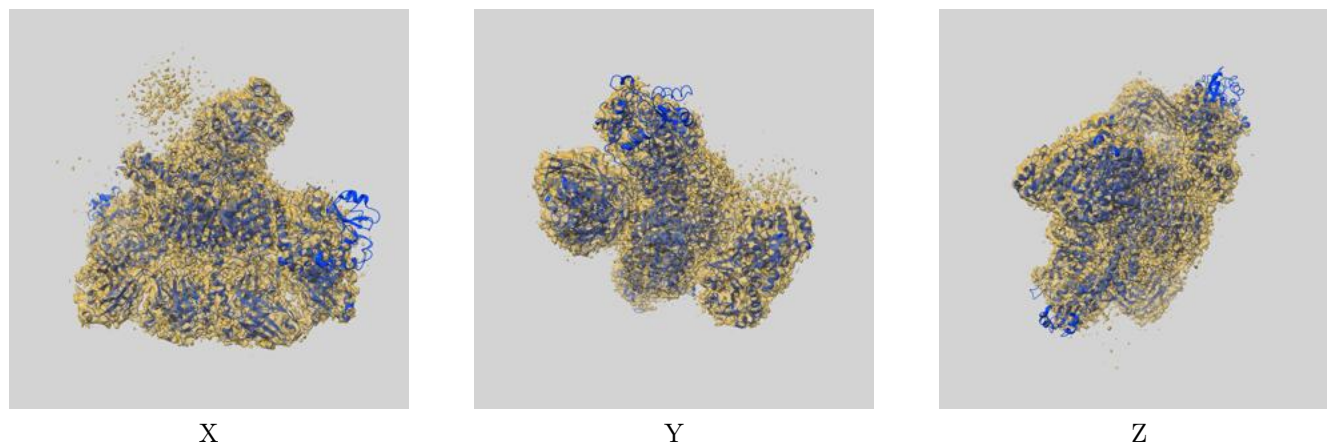
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

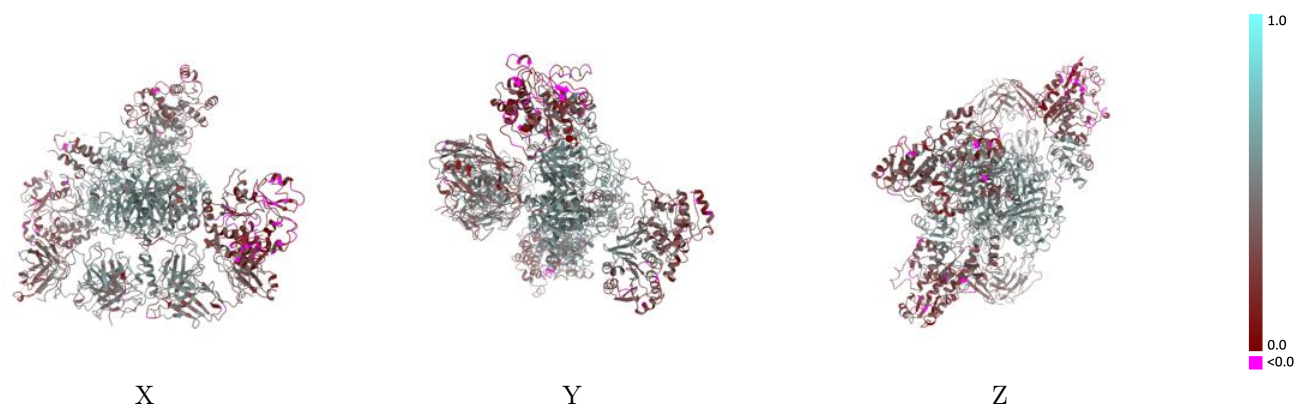
This section contains information regarding the fit between EMDB map EMD-23711 and PDB model 7M7F. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



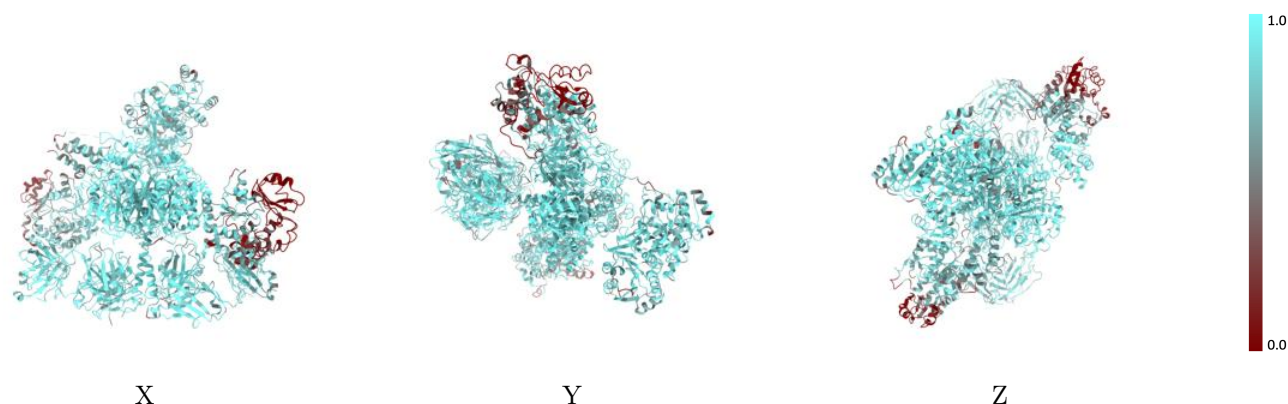
The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



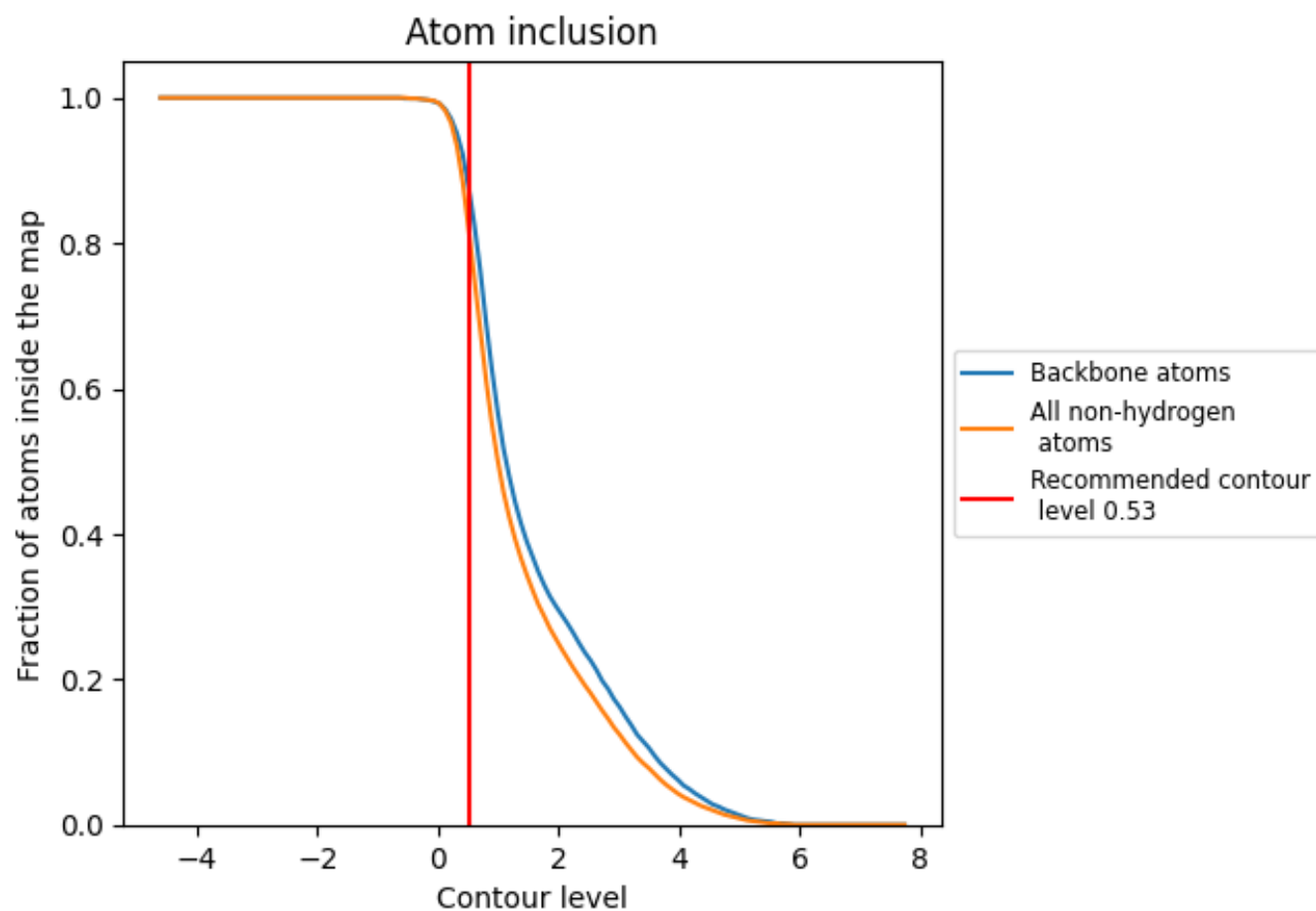
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.53).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8030</div>	<div><div></div>0.4030</div>
A	<div><div></div>0.7710</div>	<div><div></div>0.3800</div>
B	<div><div></div>0.8070</div>	<div><div></div>0.4320</div>
C	<div><div></div>0.8310</div>	<div><div></div>0.3850</div>
D	<div><div></div>0.8630</div>	<div><div></div>0.4110</div>
E	<div><div></div>0.8640</div>	<div><div></div>0.4200</div>
F	<div><div></div>0.8520</div>	<div><div></div>0.4070</div>

1.0

0.0

<0.0