



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:07 PM UTC

PDB ID : 9OPU / pdb_00009opu
EMDB ID : EMD-70724
Title : Structure of a constitutively open human TRPC3 mutant
Authors : Bell, B.; Baker, M.L.; Cordero-Morales, J.F.
Deposited on : 2025-05-20
Resolution : 3.30 Å(reported)
Based on initial model : 7DXD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

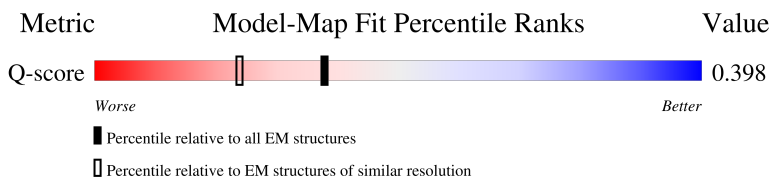
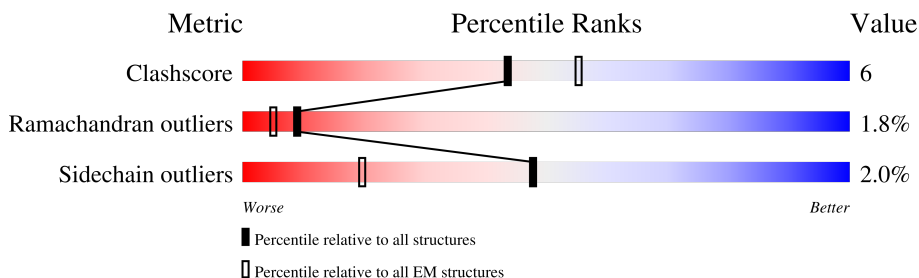
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

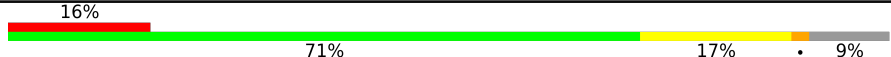

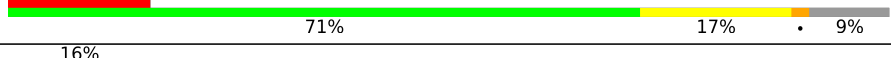

The reported resolution of this entry is 3.30 Å.

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	15087 (2.80 - 3.80)

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	820	
1	B	820	
1	C	820	
1	D	820	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNL	B	902	-	-	X	-
2	UNL	C	902	-	-	X	-
2	UNL	D	902	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 24480 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 Short transient receptor potential channel 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	745	Total 5990	C 3890	N 970	O 1097	S 33	0	0
1	B	745	Total 5990	C 3890	N 970	O 1097	S 33	0	0
1	C	745	Total 5990	C 3890	N 970	O 1097	S 33	0	0
1	D	745	Total 5990	C 3890	N 970	O 1097	S 33	0	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	ALA	THR	engineered mutation	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	THR	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ARG	deletion	UNP Q13507
A	?	-	VAL	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	GLU	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	HIS	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ILE	deletion	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	?	-	PRO	deletion	UNP Q13507
A	?	-	THR	deletion	UNP Q13507
A	?	-	ARG	deletion	UNP Q13507
A	?	-	TYR	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	839	ILE	-	expression tag	UNP Q13507
A	840	SER	-	expression tag	UNP Q13507
A	841	SER	-	expression tag	UNP Q13507
A	842	LEU	-	expression tag	UNP Q13507
A	843	ARG	-	expression tag	UNP Q13507
A	844	TYR	-	expression tag	UNP Q13507
A	845	GLU	-	expression tag	UNP Q13507
A	846	LEU	-	expression tag	UNP Q13507
A	847	LEU	-	expression tag	UNP Q13507
A	848	GLU	-	expression tag	UNP Q13507
B	573	ALA	THR	engineered mutation	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	THR	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ARG	deletion	UNP Q13507
B	?	-	VAL	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	GLU	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	HIS	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ILE	deletion	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	?	-	PRO	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q13507
B	?	-	ARG	deletion	UNP Q13507
B	?	-	TYR	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	839	ILE	-	expression tag	UNP Q13507
B	840	SER	-	expression tag	UNP Q13507
B	841	SER	-	expression tag	UNP Q13507
B	842	LEU	-	expression tag	UNP Q13507
B	843	ARG	-	expression tag	UNP Q13507
B	844	TYR	-	expression tag	UNP Q13507
B	845	GLU	-	expression tag	UNP Q13507
B	846	LEU	-	expression tag	UNP Q13507
B	847	LEU	-	expression tag	UNP Q13507
B	848	GLU	-	expression tag	UNP Q13507
C	573	ALA	THR	engineered mutation	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	THR	deletion	UNP Q13507
C	?	-	GLN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ARG	deletion	UNP Q13507
C	?	-	VAL	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	GLU	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	HIS	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ILE	deletion	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	GLN	deletion	UNP Q13507
C	?	-	PRO	deletion	UNP Q13507
C	?	-	THR	deletion	UNP Q13507
C	?	-	ARG	deletion	UNP Q13507
C	?	-	TYR	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLN	deletion	UNP Q13507
C	839	ILE	-	expression tag	UNP Q13507
C	840	SER	-	expression tag	UNP Q13507
C	841	SER	-	expression tag	UNP Q13507
C	842	LEU	-	expression tag	UNP Q13507
C	843	ARG	-	expression tag	UNP Q13507
C	844	TYR	-	expression tag	UNP Q13507
C	845	GLU	-	expression tag	UNP Q13507
C	846	LEU	-	expression tag	UNP Q13507
C	847	LEU	-	expression tag	UNP Q13507
C	848	GLU	-	expression tag	UNP Q13507
D	573	ALA	THR	engineered mutation	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	THR	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ARG	deletion	UNP Q13507
D	?	-	VAL	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	GLU	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	HIS	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ILE	deletion	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	?	-	PRO	deletion	UNP Q13507
D	?	-	THR	deletion	UNP Q13507
D	?	-	ARG	deletion	UNP Q13507
D	?	-	TYR	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	839	ILE	-	expression tag	UNP Q13507
D	840	SER	-	expression tag	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
D	841	SER	-	expression tag	UNP Q13507
D	842	LEU	-	expression tag	UNP Q13507
D	843	ARG	-	expression tag	UNP Q13507
D	844	TYR	-	expression tag	UNP Q13507
D	845	GLU	-	expression tag	UNP Q13507
D	846	LEU	-	expression tag	UNP Q13507
D	847	LEU	-	expression tag	UNP Q13507
D	848	GLU	-	expression tag	UNP Q13507

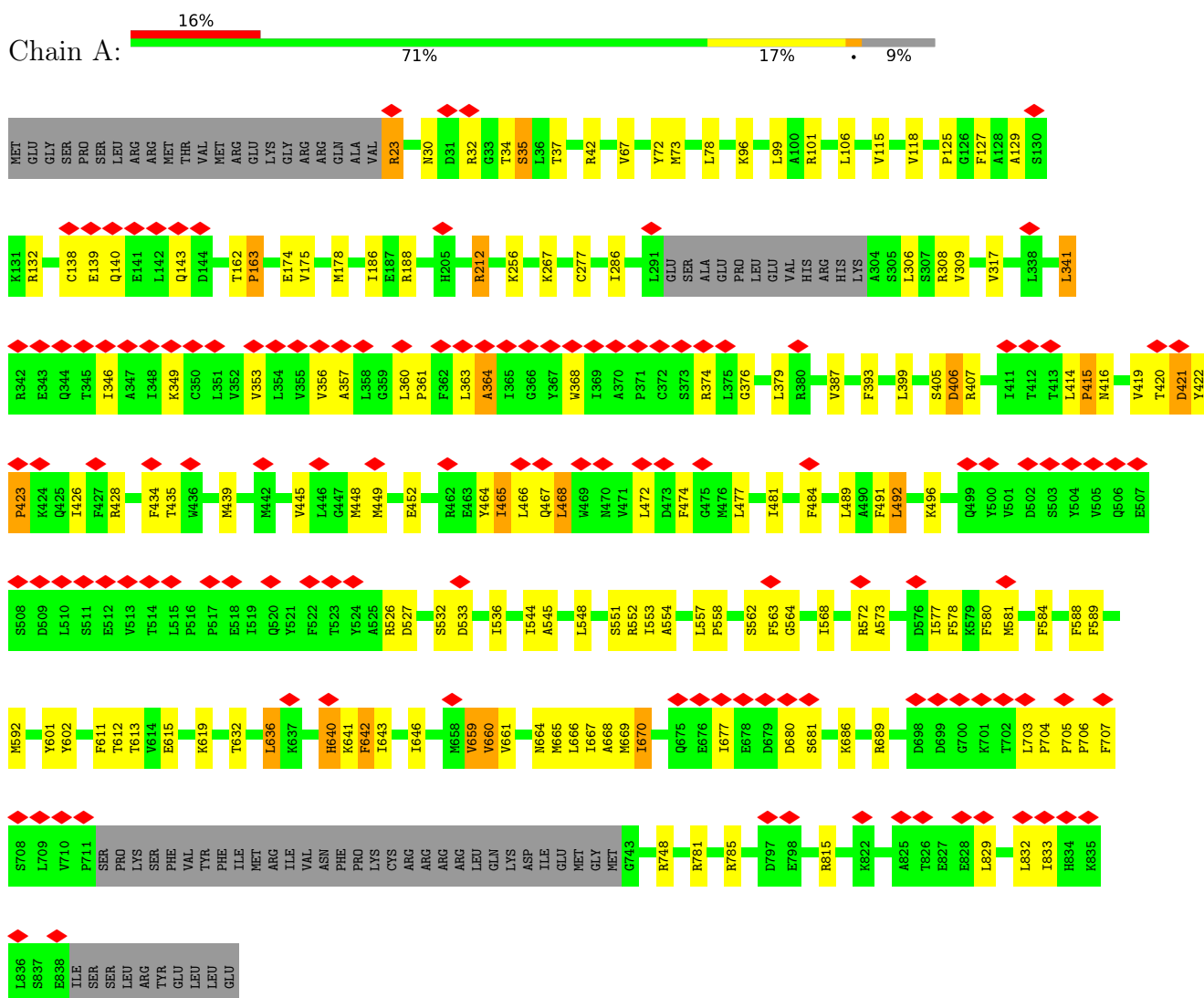
- Molecule 2 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms					AltConf
2	A	4	Total	C	N	O	P	0
			171	131	4	32	4	
2	B	3	Total	C	N	O	P	0
			130	100	3	24	3	
2	C	3	Total	C	N	O	P	0
			130	100	3	24	3	
2	D	2	Total	C	N	O	P	0
			89	69	2	16	2	

3 Residue-property plots

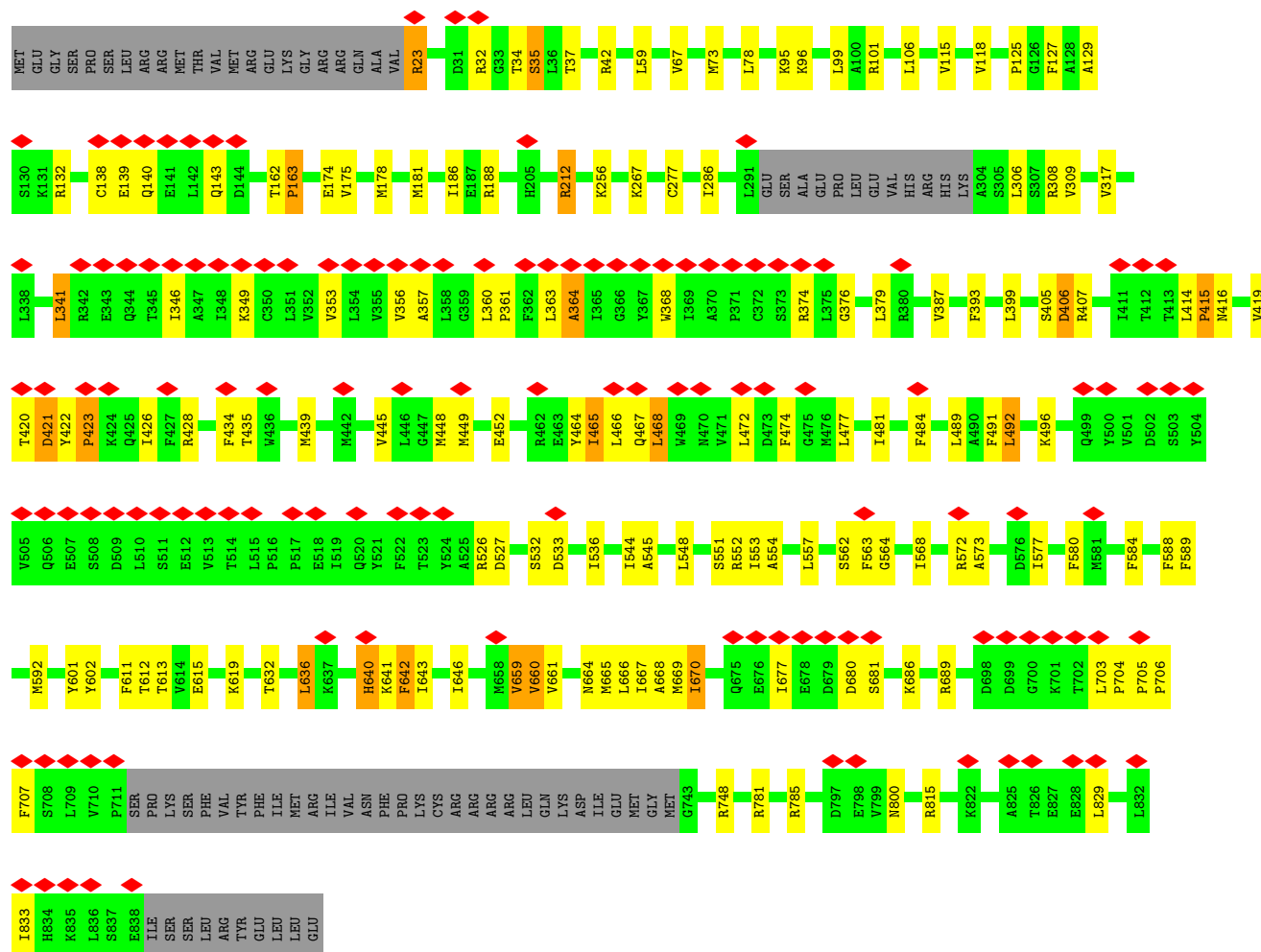
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Short transient receptor potential channel 3

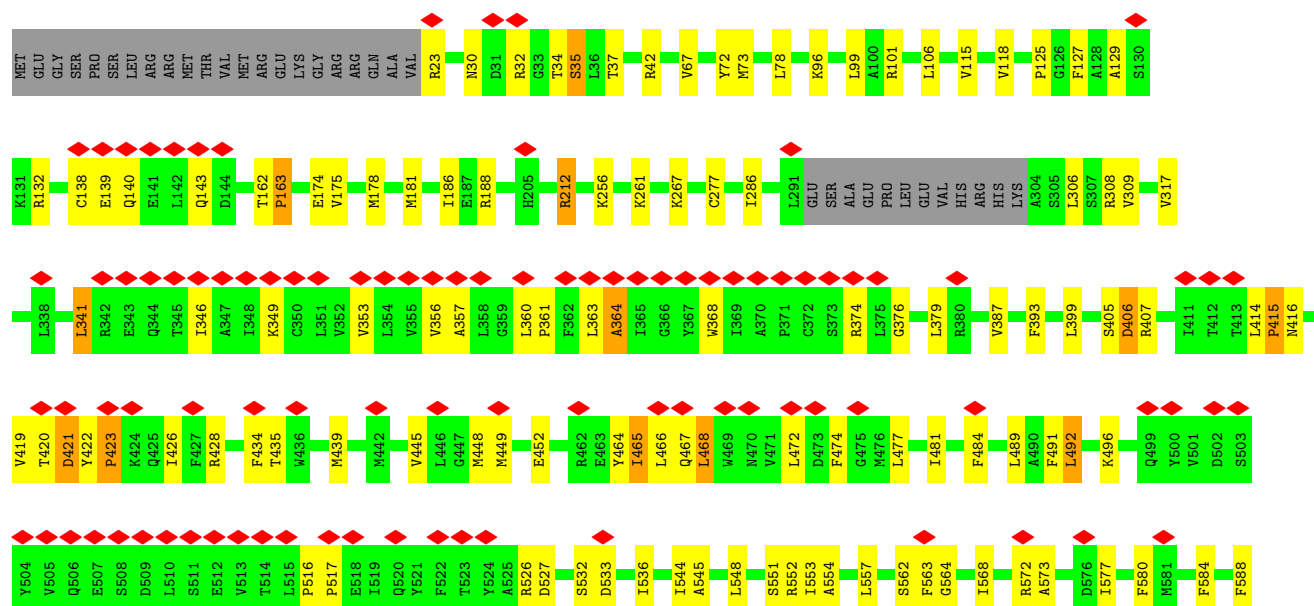


- Molecule 1: Short transient receptor potential channel 3

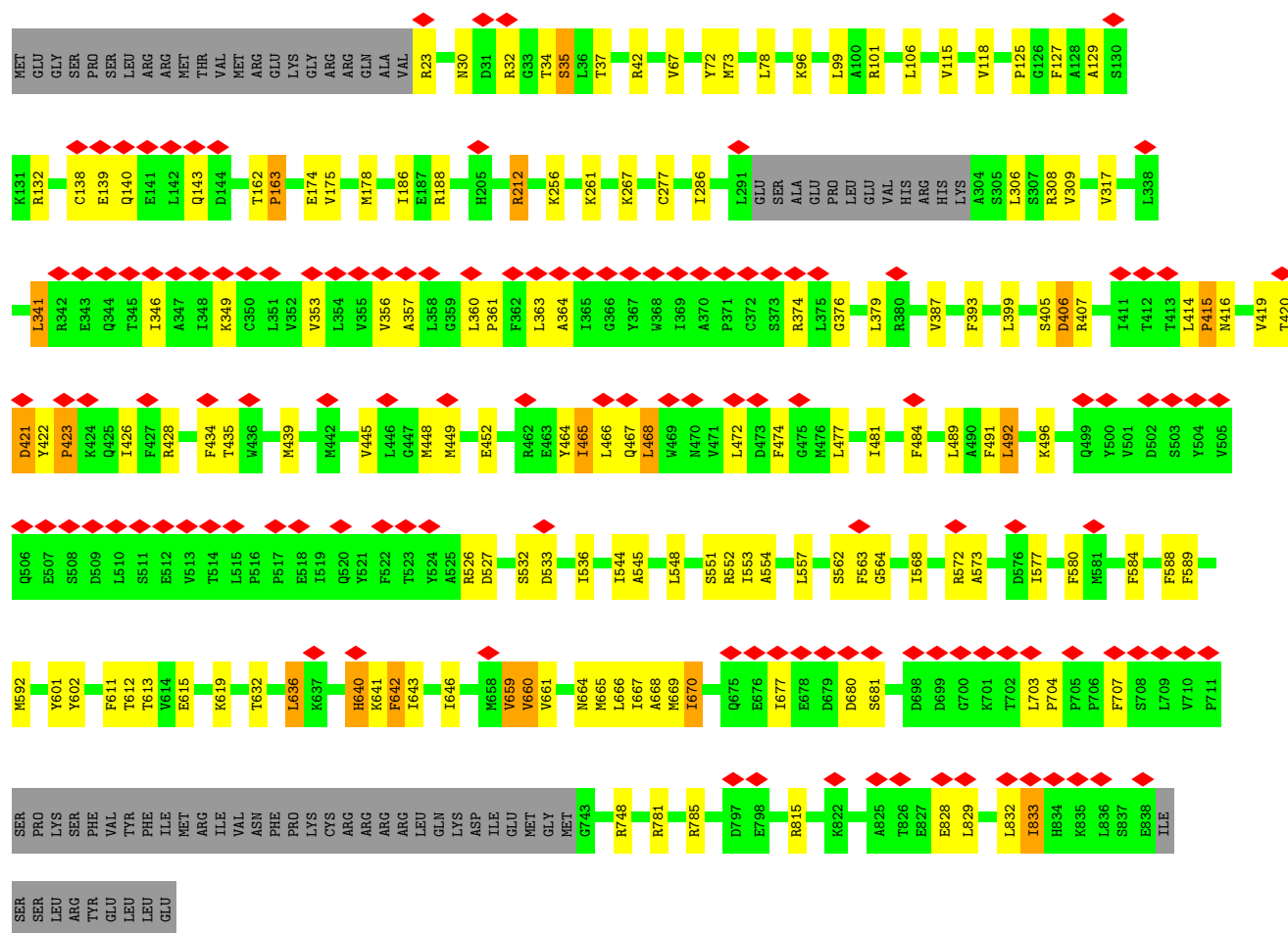
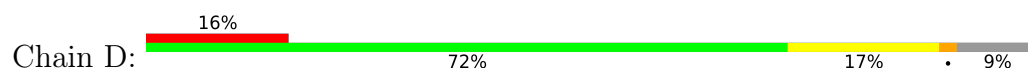




• Molecule 1: Short transient receptor potential channel 3



- Molecule 1: Short transient receptor potential channel 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	22373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.463	Depositor
Minimum map value	-0.275	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.057	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.85	7/6121 (0.1%)	1.21	27/8284 (0.3%)
1	B	0.85	7/6121 (0.1%)	1.21	28/8284 (0.3%)
1	C	0.85	7/6121 (0.1%)	1.21	28/8284 (0.3%)
1	D	0.85	7/6121 (0.1%)	1.21	27/8284 (0.3%)
All	All	0.85	28/24484 (0.1%)	1.21	110/33136 (0.3%)

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	18
1	B	0	18
1	C	0	18
1	D	0	18
All	All	0	72

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	LEU	C-O	-9.07	1.12	1.24
1	A	341	LEU	C-O	-9.06	1.12	1.24
1	B	341	LEU	C-O	-9.06	1.12	1.24
1	D	341	LEU	C-O	-9.06	1.12	1.24
1	A	642	PHE	C-O	-7.64	1.15	1.24
1	B	642	PHE	C-O	-7.64	1.15	1.24
1	C	642	PHE	C-O	-7.64	1.15	1.24
1	D	642	PHE	C-O	-7.64	1.15	1.24
1	A	415	PRO	N-CD	-7.62	1.37	1.47
1	B	415	PRO	N-CD	-7.62	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	PRO	N-CD	-7.62	1.37	1.47
1	D	415	PRO	N-CD	-7.62	1.37	1.47
1	A	346	ILE	C-O	-7.19	1.15	1.24
1	B	346	ILE	C-O	-7.19	1.15	1.24
1	C	346	ILE	C-O	-7.19	1.15	1.24
1	D	346	ILE	C-O	-7.19	1.15	1.24
1	A	492	LEU	C-O	-6.59	1.16	1.24
1	B	492	LEU	C-O	-6.59	1.16	1.24
1	C	492	LEU	C-O	-6.59	1.16	1.24
1	D	492	LEU	C-O	-6.59	1.16	1.24
1	D	139	GLU	C-O	-5.17	1.18	1.24
1	A	139	GLU	C-O	-5.14	1.18	1.24
1	C	139	GLU	C-O	-5.14	1.18	1.24
1	B	139	GLU	C-O	-5.11	1.18	1.24
1	A	833	ILE	C-O	-5.08	1.18	1.23
1	B	833	ILE	C-O	-5.08	1.18	1.23
1	C	833	ILE	C-O	-5.08	1.18	1.23
1	D	833	ILE	C-O	-5.04	1.18	1.23

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	ASP	N-CA-C	-10.18	101.18	114.31
1	C	680	ASP	N-CA-C	-10.18	101.18	114.31
1	B	680	ASP	N-CA-C	-10.17	101.19	114.31
1	D	680	ASP	N-CA-C	-10.17	101.19	114.31
1	B	642	PHE	CA-C-O	-9.89	110.07	120.55
1	D	642	PHE	CA-C-O	-9.88	110.08	120.55
1	A	642	PHE	CA-C-O	-9.86	110.10	120.55
1	C	642	PHE	CA-C-O	-9.86	110.10	120.55
1	D	492	LEU	N-CA-C	-8.63	101.95	111.36
1	A	492	LEU	N-CA-C	-8.63	101.95	111.36
1	B	492	LEU	N-CA-C	-8.63	101.95	111.36
1	C	492	LEU	N-CA-C	-8.63	101.95	111.36
1	B	139	GLU	CA-C-O	-8.12	111.86	120.63
1	A	139	GLU	CA-C-O	-8.08	111.91	120.63
1	C	139	GLU	CA-C-O	-8.08	111.91	120.63
1	D	139	GLU	CA-C-O	-8.04	111.95	120.63
1	B	677	ILE	N-CA-C	6.92	117.19	107.37
1	C	677	ILE	N-CA-C	6.92	117.19	107.37
1	A	677	ILE	N-CA-C	6.91	117.18	107.37
1	A	833	ILE	CA-C-O	-6.90	112.73	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	833	ILE	CA-C-O	-6.90	112.73	120.32
1	C	833	ILE	CA-C-O	-6.90	112.73	120.32
1	D	677	ILE	N-CA-C	6.89	117.16	107.37
1	D	833	ILE	CA-C-O	-6.88	112.75	120.32
1	A	138	CYS	O-C-N	6.87	129.43	122.08
1	C	138	CYS	O-C-N	6.87	129.43	122.08
1	B	138	CYS	O-C-N	6.85	129.41	122.08
1	D	138	CYS	O-C-N	6.84	129.40	122.08
1	A	681	SER	N-CA-C	-6.57	105.13	113.01
1	B	681	SER	N-CA-C	-6.55	105.14	113.01
1	C	681	SER	N-CA-C	-6.54	105.16	113.01
1	D	681	SER	N-CA-C	-6.54	105.16	113.01
1	A	833	ILE	CA-C-N	6.54	129.88	120.79
1	A	833	ILE	C-N-CA	6.54	129.88	120.79
1	B	833	ILE	CA-C-N	6.54	129.88	120.79
1	B	833	ILE	C-N-CA	6.54	129.88	120.79
1	C	833	ILE	CA-C-N	6.54	129.88	120.79
1	C	833	ILE	C-N-CA	6.54	129.88	120.79
1	D	833	ILE	CA-C-N	6.54	129.88	120.79
1	D	833	ILE	C-N-CA	6.54	129.88	120.79
1	A	364	ALA	CA-C-O	-6.31	113.73	120.42
1	D	364	ALA	CA-C-O	-6.31	113.73	120.42
1	C	491	PHE	CA-C-O	-6.30	111.49	119.31
1	C	364	ALA	CA-C-O	-6.30	113.74	120.42
1	B	364	ALA	CA-C-O	-6.29	113.75	120.42
1	C	393	PHE	CA-C-O	-6.29	113.26	120.24
1	D	491	PHE	CA-C-O	-6.28	111.53	119.31
1	A	491	PHE	CA-C-O	-6.27	111.53	119.31
1	B	491	PHE	CA-C-O	-6.27	111.53	119.31
1	A	393	PHE	CA-C-O	-6.27	113.28	120.24
1	B	393	PHE	CA-C-O	-6.27	113.28	120.24
1	D	393	PHE	CA-C-O	-6.25	113.31	120.24
1	A	346	ILE	CA-C-O	-6.13	113.11	120.78
1	B	346	ILE	CA-C-O	-6.13	113.11	120.78
1	C	346	ILE	CA-C-O	-6.13	113.11	120.78
1	D	346	ILE	CA-C-O	-6.13	113.11	120.78
1	B	588	PHE	CA-C-O	-6.10	114.42	120.82
1	D	588	PHE	CA-C-O	-6.10	114.42	120.82
1	A	588	PHE	CA-C-O	-6.07	114.44	120.82
1	C	588	PHE	CA-C-O	-6.07	114.44	120.82
1	D	481	ILE	CA-C-O	-5.88	115.30	121.41
1	A	481	ILE	CA-C-O	-5.86	115.32	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ILE	CA-C-O	-5.86	115.32	121.41
1	C	481	ILE	CA-C-O	-5.86	115.32	121.41
1	D	363	LEU	N-CA-C	-5.67	105.10	111.28
1	A	363	LEU	N-CA-C	-5.66	105.11	111.28
1	B	363	LEU	N-CA-C	-5.66	105.11	111.28
1	C	363	LEU	N-CA-C	-5.66	105.11	111.28
1	C	642	PHE	CA-C-N	5.66	127.69	120.56
1	C	642	PHE	C-N-CA	5.66	127.69	120.56
1	A	670	ILE	CA-C-O	-5.64	115.19	121.17
1	B	670	ILE	CA-C-O	-5.64	115.19	121.17
1	C	670	ILE	CA-C-O	-5.64	115.19	121.17
1	D	670	ILE	CA-C-O	-5.64	115.19	121.17
1	A	642	PHE	CA-C-N	5.64	127.67	120.56
1	A	642	PHE	C-N-CA	5.64	127.67	120.56
1	B	642	PHE	CA-C-N	5.64	127.67	120.56
1	B	642	PHE	C-N-CA	5.64	127.67	120.56
1	D	642	PHE	CA-C-N	5.64	127.67	120.56
1	D	642	PHE	C-N-CA	5.64	127.67	120.56
1	C	619	LYS	N-CA-CB	5.55	118.37	110.16
1	D	619	LYS	N-CA-CB	5.54	118.36	110.16
1	A	619	LYS	N-CA-CB	5.53	118.34	110.16
1	A	642	PHE	O-C-N	5.53	127.98	122.12
1	B	619	LYS	N-CA-CB	5.53	118.34	110.16
1	B	642	PHE	O-C-N	5.53	127.98	122.12
1	C	642	PHE	O-C-N	5.53	127.98	122.12
1	D	642	PHE	O-C-N	5.53	127.98	122.12
1	C	361	PRO	N-CA-C	-5.43	107.08	113.86
1	A	361	PRO	N-CA-C	-5.42	107.08	113.86
1	D	361	PRO	N-CA-C	-5.42	107.08	113.86
1	B	361	PRO	N-CA-C	-5.40	107.11	113.86
1	B	421	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	421	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	421	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	421	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	611	PHE	N-CA-CB	-5.08	103.24	110.46
1	A	611	PHE	N-CA-CB	-5.07	103.26	110.46
1	C	611	PHE	N-CA-CB	-5.07	103.26	110.46
1	D	611	PHE	N-CA-CB	-5.06	103.28	110.46
1	B	37	THR	CA-C-O	-5.03	115.88	121.81
1	C	818	LEU	CA-C-O	-5.02	115.53	120.90
1	B	256	LYS	CA-C-O	-5.02	115.73	121.00
1	C	256	LYS	CA-C-O	-5.02	115.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	LYS	CA-C-O	-5.02	115.73	121.00
1	A	256	LYS	CA-C-O	-5.01	115.73	121.00
1	B	139	GLU	O-C-N	5.01	127.44	122.12
1	C	37	THR	CA-C-O	-5.01	115.90	121.81
1	A	37	THR	CA-C-O	-5.00	115.91	121.81
1	D	37	THR	CA-C-O	-5.00	115.91	121.81

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	308	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	374	ARG	Sidechain
1	A	407	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	428	ARG	Sidechain
1	A	526	ARG	Sidechain
1	A	552	ARG	Sidechain
1	A	572	ARG	Sidechain
1	A	748	ARG	Sidechain
1	A	781	ARG	Sidechain
1	A	785	ARG	Sidechain
1	A	815	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	132	ARG	Sidechain
1	B	188	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	308	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	374	ARG	Sidechain
1	B	407	ARG	Sidechain
1	B	42	ARG	Sidechain
1	B	428	ARG	Sidechain
1	B	526	ARG	Sidechain
1	B	552	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	572	ARG	Sidechain
1	B	748	ARG	Sidechain
1	B	781	ARG	Sidechain
1	B	785	ARG	Sidechain
1	B	815	ARG	Sidechain
1	C	101	ARG	Sidechain
1	C	132	ARG	Sidechain
1	C	188	ARG	Sidechain
1	C	212	ARG	Sidechain
1	C	23	ARG	Sidechain
1	C	308	ARG	Sidechain
1	C	32	ARG	Sidechain
1	C	374	ARG	Sidechain
1	C	407	ARG	Sidechain
1	C	42	ARG	Sidechain
1	C	428	ARG	Sidechain
1	C	526	ARG	Sidechain
1	C	552	ARG	Sidechain
1	C	572	ARG	Sidechain
1	C	748	ARG	Sidechain
1	C	781	ARG	Sidechain
1	C	785	ARG	Sidechain
1	C	815	ARG	Sidechain
1	D	101	ARG	Sidechain
1	D	132	ARG	Sidechain
1	D	188	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	23	ARG	Sidechain
1	D	308	ARG	Sidechain
1	D	32	ARG	Sidechain
1	D	374	ARG	Sidechain
1	D	407	ARG	Sidechain
1	D	42	ARG	Sidechain
1	D	428	ARG	Sidechain
1	D	526	ARG	Sidechain
1	D	552	ARG	Sidechain
1	D	572	ARG	Sidechain
1	D	748	ARG	Sidechain
1	D	781	ARG	Sidechain
1	D	785	ARG	Sidechain
1	D	815	ARG	Sidechain

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	5990	0	6037	84	0
1	B	5990	0	6037	84	0
1	C	5990	0	6037	83	0
1	D	5990	0	6037	82	0
2	A	171	0	0	5	0
2	B	130	0	0	5	0
2	C	130	0	0	5	0
2	D	89	0	0	5	0
All	All	24480	0	24148	316	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 6.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:VAL:O	1:B:665:MET:HG2	1.67	0.94
1:D:661:VAL:O	1:D:665:MET:HG2	1.68	0.94
1:A:661:VAL:O	1:A:665:MET:HG2	1.67	0.93
1:C:661:VAL:O	1:C:665:MET:HG2	1.68	0.92
1:D:577:ILE:HD11	1:D:670:ILE:HD11	1.61	0.83
1:C:577:ILE:HD11	1:C:670:ILE:HD11	1.61	0.82
1:A:577:ILE:HD11	1:A:670:ILE:HD11	1.61	0.82
1:B:577:ILE:HD11	1:B:670:ILE:HD11	1.61	0.81
1:B:405:SER:O	1:B:406:ASP:OD1	2.07	0.73
1:A:405:SER:O	1:A:406:ASP:OD1	2.07	0.72
1:C:405:SER:O	1:C:406:ASP:OD1	2.07	0.72
1:B:449:MET:HG2	1:B:477:LEU:HD22	1.72	0.72
1:A:666:LEU:HD12	1:A:667:ILE:N	2.05	0.71
1:D:405:SER:O	1:D:406:ASP:OD1	2.07	0.71
1:D:666:LEU:HD12	1:D:667:ILE:N	2.05	0.71
1:A:449:MET:HG2	1:A:477:LEU:HD22	1.72	0.71
1:D:449:MET:HG2	1:D:477:LEU:HD22	1.72	0.70
1:C:666:LEU:HD12	1:C:667:ILE:N	2.05	0.70
1:C:449:MET:HG2	1:C:477:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LEU:HD12	1:B:667:ILE:N	2.05	0.70
1:B:465:ILE:HG12	1:B:466:LEU:H	1.58	0.69
1:D:465:ILE:HG12	1:D:466:LEU:H	1.57	0.69
1:D:533:ASP:HB3	1:D:536:ILE:HD12	1.76	0.68
1:A:465:ILE:HG12	1:A:466:LEU:H	1.58	0.68
1:C:465:ILE:HG12	1:C:466:LEU:H	1.58	0.68
1:C:533:ASP:HB3	1:C:536:ILE:HD12	1.76	0.67
1:A:533:ASP:HB3	1:A:536:ILE:HD12	1.76	0.67
1:A:420:THR:HG23	1:A:426:ILE:HA	1.77	0.67
1:B:533:ASP:HB3	1:B:536:ILE:HD12	1.76	0.67
1:D:420:THR:HG23	1:D:426:ILE:HA	1.77	0.67
1:B:420:THR:HG23	1:B:426:ILE:HA	1.77	0.67
1:C:420:THR:HG23	1:C:426:ILE:HA	1.77	0.65
1:D:341:LEU:HD23	1:D:349:LYS:HA	1.80	0.64
1:C:341:LEU:HD23	1:C:349:LYS:HA	1.80	0.63
1:B:341:LEU:HD23	1:B:349:LYS:HA	1.80	0.62
1:A:341:LEU:HD23	1:A:349:LYS:HA	1.80	0.62
1:A:445:VAL:HG21	1:A:484:PHE:HE2	1.65	0.62
1:D:445:VAL:HG21	1:D:484:PHE:HE2	1.65	0.62
1:C:445:VAL:HG21	1:C:484:PHE:HE2	1.65	0.61
1:B:445:VAL:HG21	1:B:484:PHE:HE2	1.65	0.61
1:C:489:LEU:HA	1:C:492:LEU:HD12	1.83	0.61
1:A:357:ALA:HA	1:A:360:LEU:HD12	1.83	0.61
1:B:646:ILE:HG23	1:C:544:ILE:HD11	1.82	0.61
1:A:544:ILE:HD11	1:D:646:ILE:HG23	1.82	0.61
1:B:357:ALA:HA	1:B:360:LEU:HD12	1.83	0.61
1:A:277:CYS:SG	1:A:286:ILE:HD12	2.41	0.61
1:A:646:ILE:HG23	1:B:544:ILE:HD11	1.83	0.61
1:B:489:LEU:HA	1:B:492:LEU:HD12	1.83	0.61
1:C:357:ALA:HA	1:C:360:LEU:HD12	1.83	0.61
1:A:489:LEU:HA	1:A:492:LEU:HD12	1.83	0.60
1:B:277:CYS:SG	1:B:286:ILE:HD12	2.41	0.60
1:C:162:THR:HB	1:C:163:PRO:HD2	1.84	0.60
1:D:357:ALA:HA	1:D:360:LEU:HD12	1.83	0.60
1:D:277:CYS:SG	1:D:286:ILE:HD12	2.41	0.60
1:C:646:ILE:HG23	1:D:544:ILE:HD11	1.82	0.60
1:D:489:LEU:HA	1:D:492:LEU:HD12	1.83	0.60
1:B:162:THR:HB	1:B:163:PRO:HD2	1.84	0.60
1:C:277:CYS:SG	1:C:286:ILE:HD12	2.41	0.59
1:C:664:ASN:O	1:C:665:MET:HE2	2.03	0.59
1:D:664:ASN:O	1:D:665:MET:HE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:THR:HB	1:D:163:PRO:HD2	1.84	0.59
1:A:162:THR:HB	1:A:163:PRO:HD2	1.84	0.58
1:A:664:ASN:O	1:A:665:MET:HE2	2.03	0.58
1:B:664:ASN:O	1:B:665:MET:HE2	2.03	0.58
1:C:414:LEU:HD23	1:C:415:PRO:HD2	1.86	0.57
1:D:414:LEU:HD23	1:D:415:PRO:HD2	1.86	0.57
1:A:667:ILE:HG22	1:D:664:ASN:ND2	2.19	0.57
1:A:664:ASN:ND2	1:B:667:ILE:HG22	2.20	0.57
1:A:703:LEU:HD12	1:A:704:PRO:HD2	1.87	0.57
1:B:703:LEU:HD12	1:B:704:PRO:HD2	1.87	0.57
1:B:414:LEU:HD23	1:B:415:PRO:HD2	1.86	0.56
1:A:414:LEU:HD23	1:A:415:PRO:HD2	1.86	0.56
1:B:664:ASN:ND2	1:C:667:ILE:HG22	2.21	0.56
1:B:175:VAL:HA	1:B:178:MET:HE3	1.87	0.56
1:C:703:LEU:HD12	1:C:704:PRO:HD2	1.87	0.56
1:D:175:VAL:HA	1:D:178:MET:HE3	1.87	0.56
1:A:175:VAL:HA	1:A:178:MET:HE3	1.87	0.55
1:C:175:VAL:HA	1:C:178:MET:HE3	1.87	0.55
1:C:664:ASN:ND2	1:D:667:ILE:HG22	2.21	0.55
1:D:703:LEU:HD12	1:D:704:PRO:HD2	1.87	0.55
1:B:666:LEU:HD12	1:B:666:LEU:C	2.32	0.55
1:C:666:LEU:HD12	1:C:666:LEU:C	2.32	0.55
1:D:666:LEU:HD12	1:D:666:LEU:C	2.32	0.55
2:C:902:UNL:C34	2:C:902:UNL:C12	2.85	0.55
2:B:902:UNL:C34	2:B:902:UNL:C12	2.85	0.55
1:B:356:VAL:HG11	1:B:387:VAL:HG13	1.89	0.55
2:D:902:UNL:C34	2:D:902:UNL:C12	2.85	0.54
2:A:902:UNL:C12	2:A:902:UNL:C33	2.86	0.54
2:B:902:UNL:C13	2:B:902:UNL:C33	2.85	0.54
1:C:78:LEU:HB2	1:C:99:LEU:HD11	1.90	0.54
2:D:902:UNL:C12	2:D:902:UNL:C33	2.86	0.54
1:D:78:LEU:HB2	1:D:99:LEU:HD11	1.90	0.54
1:D:545:ALA:HA	1:D:548:LEU:HD12	1.90	0.54
1:A:545:ALA:HA	1:A:548:LEU:HD12	1.90	0.54
1:A:664:ASN:HD21	1:B:667:ILE:HG22	1.73	0.54
2:C:902:UNL:C34	2:C:902:UNL:C13	2.85	0.54
1:D:356:VAL:HG11	1:D:387:VAL:HG13	1.89	0.54
1:A:667:ILE:HG22	1:D:664:ASN:HD21	1.72	0.54
1:A:666:LEU:HD12	1:A:666:LEU:C	2.32	0.54
2:B:902:UNL:C34	2:B:902:UNL:C13	2.85	0.54
2:B:902:UNL:C12	2:B:902:UNL:C33	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:902:UNL:C33	2:D:902:UNL:C13	2.85	0.54
2:A:902:UNL:C12	2:A:902:UNL:C34	2.85	0.54
2:A:902:UNL:C33	2:A:902:UNL:C13	2.85	0.54
2:D:902:UNL:C34	2:D:902:UNL:C13	2.85	0.54
1:C:356:VAL:HG11	1:C:387:VAL:HG13	1.89	0.54
1:A:34:THR:O	1:A:35:SER:C	2.51	0.54
2:A:902:UNL:C13	2:A:902:UNL:C34	2.85	0.53
2:C:902:UNL:C12	2:C:902:UNL:C33	2.86	0.53
1:A:78:LEU:HB2	1:A:99:LEU:HD11	1.90	0.53
1:B:545:ALA:HA	1:B:548:LEU:HD12	1.90	0.53
1:C:664:ASN:HD21	1:D:667:ILE:HG22	1.73	0.53
1:B:34:THR:O	1:B:35:SER:C	2.51	0.53
1:B:78:LEU:HB2	1:B:99:LEU:HD11	1.90	0.53
1:C:545:ALA:HA	1:C:548:LEU:HD12	1.90	0.53
1:C:34:THR:O	1:C:35:SER:C	2.51	0.53
2:C:902:UNL:C13	2:C:902:UNL:C33	2.85	0.53
1:A:434:PHE:HB3	1:A:439:MET:HE1	1.91	0.53
1:A:356:VAL:HG11	1:A:387:VAL:HG13	1.89	0.53
1:A:376:GLY:HA2	1:A:379:LEU:HD12	1.91	0.53
1:C:376:GLY:HA2	1:C:379:LEU:HD12	1.91	0.53
1:D:34:THR:O	1:D:35:SER:C	2.51	0.53
1:B:613:THR:HG22	1:B:615:GLU:H	1.75	0.52
1:B:434:PHE:HB3	1:B:439:MET:HE1	1.91	0.52
1:D:414:LEU:CD2	1:D:415:PRO:HD2	2.39	0.52
1:B:664:ASN:HD21	1:C:667:ILE:HG22	1.73	0.52
1:C:613:THR:HG22	1:C:615:GLU:H	1.75	0.52
1:D:422:TYR:O	1:D:423:PRO:C	2.53	0.52
1:C:416:ASN:HA	1:C:527:ASP:HB2	1.92	0.52
1:C:422:TYR:O	1:C:423:PRO:C	2.53	0.52
1:B:376:GLY:HA2	1:B:379:LEU:HD12	1.91	0.52
1:B:416:ASN:HA	1:B:527:ASP:HB2	1.92	0.52
1:C:829:LEU:HD13	1:D:829:LEU:HD23	1.92	0.52
1:D:416:ASN:HA	1:D:527:ASP:HB2	1.92	0.52
1:A:414:LEU:CD2	1:A:415:PRO:HD2	2.39	0.52
1:A:829:LEU:HD23	1:D:829:LEU:HD13	1.92	0.51
1:D:434:PHE:HB3	1:D:439:MET:HE1	1.91	0.51
1:B:422:TYR:O	1:B:423:PRO:C	2.53	0.51
1:B:414:LEU:CD2	1:B:415:PRO:HD2	2.39	0.51
1:C:414:LEU:CD2	1:C:415:PRO:HD2	2.39	0.51
1:A:416:ASN:HA	1:A:527:ASP:HB2	1.92	0.51
1:A:422:TYR:O	1:A:423:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:GLY:HA2	1:D:379:LEU:HD12	1.91	0.51
1:C:448:MET:HB2	1:C:477:LEU:HD21	1.93	0.51
1:C:434:PHE:HB3	1:C:439:MET:HE1	1.91	0.51
1:D:613:THR:HG22	1:D:615:GLU:H	1.75	0.51
1:A:414:LEU:HG	1:A:415:PRO:HD2	1.93	0.51
1:B:448:MET:HB2	1:B:477:LEU:HD21	1.93	0.51
1:B:829:LEU:HD13	1:C:829:LEU:HD23	1.92	0.51
1:B:414:LEU:HG	1:B:415:PRO:HD2	1.93	0.50
1:D:448:MET:HB2	1:D:477:LEU:HD21	1.92	0.50
1:A:613:THR:HG22	1:A:615:GLU:H	1.75	0.50
1:A:448:MET:HB2	1:A:477:LEU:HD21	1.93	0.50
1:C:414:LEU:HG	1:C:415:PRO:HD2	1.93	0.50
1:D:140:GLN:HA	1:D:143:GLN:HG2	1.94	0.50
1:A:829:LEU:HD13	1:B:829:LEU:HD23	1.93	0.49
1:B:435:THR:O	1:B:439:MET:HE2	2.13	0.49
1:A:435:THR:O	1:A:439:MET:HE2	2.13	0.49
1:C:140:GLN:HA	1:C:143:GLN:HG2	1.94	0.49
1:D:414:LEU:HG	1:D:415:PRO:HD2	1.93	0.49
1:A:140:GLN:HA	1:A:143:GLN:HG2	1.93	0.49
1:C:435:THR:O	1:C:439:MET:HE2	2.13	0.48
1:D:435:THR:O	1:D:439:MET:HE2	2.12	0.48
1:D:492:LEU:O	1:D:496:LYS:HG2	2.13	0.48
1:A:573:ALA:CB	1:D:665:MET:SD	3.01	0.48
1:B:492:LEU:O	1:B:496:LYS:HG2	2.13	0.48
1:B:140:GLN:HA	1:B:143:GLN:HG2	1.94	0.48
1:A:492:LEU:O	1:A:496:LYS:HG2	2.13	0.48
1:D:659:VAL:O	1:D:660:VAL:C	2.57	0.48
1:A:659:VAL:O	1:A:660:VAL:C	2.57	0.48
1:B:665:MET:SD	1:C:573:ALA:CB	3.02	0.47
1:B:800:ASN:OD1	1:B:800:ASN:N	2.42	0.47
1:C:492:LEU:O	1:C:496:LYS:HG2	2.13	0.47
1:A:829:LEU:CD2	1:D:829:LEU:HD13	2.45	0.47
1:B:659:VAL:O	1:B:660:VAL:C	2.57	0.47
1:C:448:MET:O	1:C:452:GLU:HG2	2.15	0.47
1:C:659:VAL:O	1:C:660:VAL:C	2.57	0.47
1:C:665:MET:SD	1:D:573:ALA:CB	3.02	0.47
1:B:448:MET:O	1:B:452:GLU:HG2	2.15	0.47
1:A:580:PHE:CE1	1:A:669:MET:HG3	2.50	0.47
1:A:665:MET:SD	1:B:573:ALA:CB	3.03	0.47
1:C:829:LEU:HD13	1:D:829:LEU:CD2	2.45	0.47
1:C:580:PHE:CE1	1:C:669:MET:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:MET:O	1:D:452:GLU:HG2	2.15	0.46
1:D:580:PHE:CE1	1:D:669:MET:HG3	2.50	0.46
1:A:448:MET:O	1:A:452:GLU:HG2	2.15	0.46
1:B:414:LEU:CG	1:B:415:PRO:HD2	2.46	0.46
1:D:667:ILE:HD12	1:D:668:ALA:N	2.31	0.46
1:B:580:PHE:CE1	1:B:669:MET:HG3	2.50	0.46
1:C:445:VAL:HG21	1:C:484:PHE:CE2	2.49	0.46
1:C:667:ILE:HD12	1:C:668:ALA:N	2.31	0.46
1:A:414:LEU:CG	1:A:415:PRO:HD2	2.46	0.46
1:B:829:LEU:HD13	1:C:829:LEU:CD2	2.45	0.46
1:C:414:LEU:CG	1:C:415:PRO:HD2	2.46	0.46
1:D:414:LEU:CG	1:D:415:PRO:HD2	2.46	0.46
1:A:667:ILE:HD12	1:A:668:ALA:N	2.31	0.46
1:D:445:VAL:HG21	1:D:484:PHE:CE2	2.49	0.46
1:A:829:LEU:HD13	1:B:829:LEU:CD2	2.46	0.46
1:B:667:ILE:HD12	1:B:668:ALA:N	2.31	0.45
1:A:445:VAL:HG21	1:A:484:PHE:CE2	2.49	0.45
1:A:106:LEU:HD22	1:A:127:PHE:CE1	2.52	0.45
1:B:445:VAL:HG21	1:B:484:PHE:CE2	2.49	0.44
1:B:106:LEU:HD22	1:B:127:PHE:CE1	2.52	0.44
1:C:106:LEU:HD22	1:C:127:PHE:CE1	2.52	0.44
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.87	0.44
1:B:472:LEU:HD21	1:B:551:SER:HB2	2.00	0.44
1:D:106:LEU:HD22	1:D:127:PHE:CE1	2.52	0.44
1:D:568:ILE:HA	2:D:902:UNL:C6	2.48	0.44
1:A:421:ASP:O	1:A:422:TYR:C	2.61	0.43
1:C:306:LEU:HB3	1:C:309:VAL:HB	2.00	0.43
1:C:563:PHE:O	1:C:564:GLY:C	2.62	0.43
1:B:95:LYS:HE2	1:B:95:LYS:HB2	1.82	0.43
1:C:186:ILE:O	1:C:186:ILE:HG22	2.19	0.43
1:C:421:ASP:O	1:C:422:TYR:C	2.62	0.43
1:A:186:ILE:O	1:A:186:ILE:HG22	2.19	0.43
1:A:472:LEU:HD21	1:A:551:SER:HB2	2.00	0.43
1:A:563:PHE:O	1:A:564:GLY:C	2.62	0.43
1:B:306:LEU:HB3	1:B:309:VAL:HB	2.00	0.43
1:B:421:ASP:O	1:B:422:TYR:C	2.62	0.43
1:A:573:ALA:HB1	1:D:665:MET:SD	2.58	0.43
1:C:568:ILE:HA	2:C:902:UNL:C6	2.49	0.43
1:D:186:ILE:HG22	1:D:186:ILE:O	2.19	0.43
1:D:353:VAL:HG13	1:D:387:VAL:HG23	2.01	0.43
1:B:568:ILE:HA	2:B:902:UNL:C6	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:PHE:O	1:D:564:GLY:C	2.62	0.43
1:C:472:LEU:HD21	1:C:551:SER:HB2	2.00	0.43
1:C:640:HIS:HB3	1:C:643:ILE:HB	2.01	0.42
1:D:421:ASP:O	1:D:422:TYR:C	2.61	0.42
1:D:472:LEU:HD21	1:D:551:SER:HB2	2.00	0.42
1:B:563:PHE:O	1:B:564:GLY:C	2.62	0.42
1:A:568:ILE:HA	2:A:902:UNL:C6	2.49	0.42
1:D:73:MET:HA	1:D:73:MET:HE2	2.01	0.42
1:D:640:HIS:HB3	1:D:643:ILE:HB	2.01	0.42
1:C:353:VAL:HG13	1:C:387:VAL:HG23	2.01	0.42
1:D:267:LYS:HZ2	1:D:317:VAL:HG22	1.84	0.42
1:B:67:VAL:HG21	1:B:96:LYS:CE	2.50	0.42
1:C:636:LEU:HD11	1:C:640:HIS:HB2	2.02	0.42
1:A:353:VAL:HG13	1:A:387:VAL:HG23	2.01	0.42
1:B:186:ILE:HG22	1:B:186:ILE:O	2.19	0.42
1:B:584:PHE:CD1	1:B:584:PHE:C	2.98	0.42
1:B:664:ASN:HA	1:B:667:ILE:HG12	2.02	0.42
1:C:115:VAL:HA	1:C:118:VAL:HG12	2.02	0.42
1:D:67:VAL:HG21	1:D:96:LYS:CE	2.50	0.42
1:D:115:VAL:HA	1:D:118:VAL:HG12	2.02	0.42
1:D:212:ARG:HG3	1:D:212:ARG:HH11	1.84	0.42
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.84	0.42
1:A:554:ALA:HA	1:A:557:LEU:HD13	2.01	0.42
1:C:212:ARG:HH11	1:C:212:ARG:HG3	1.84	0.42
1:C:665:MET:SD	1:D:573:ALA:HB1	2.59	0.42
1:D:532:SER:O	1:D:533:ASP:C	2.63	0.42
1:D:589:PHE:HA	1:D:592:MET:HG3	2.02	0.42
1:A:665:MET:SD	1:B:573:ALA:HB1	2.60	0.42
1:D:261:LYS:HA	1:D:261:LYS:HD3	1.81	0.42
1:D:306:LEU:HB3	1:D:309:VAL:HB	2.00	0.42
1:D:584:PHE:CD1	1:D:584:PHE:C	2.98	0.42
1:A:306:LEU:HB3	1:A:309:VAL:HB	2.00	0.42
1:A:640:HIS:HB3	1:A:643:ILE:HB	2.01	0.42
1:B:212:ARG:HG3	1:B:212:ARG:HH11	1.84	0.42
1:B:554:ALA:HA	1:B:557:LEU:HD13	2.01	0.42
1:B:636:LEU:HD11	1:B:640:HIS:HB2	2.02	0.42
1:B:704:PRO:HG2	1:B:707:PHE:HB2	2.02	0.42
1:C:584:PHE:CD1	1:C:584:PHE:C	2.98	0.42
1:C:704:PRO:HG2	1:C:707:PHE:HB2	2.02	0.42
1:D:664:ASN:HA	1:D:667:ILE:HG12	2.02	0.42
1:B:532:SER:O	1:B:533:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:MET:SD	1:C:573:ALA:HB1	2.59	0.41
1:C:67:VAL:HG21	1:C:96:LYS:CE	2.50	0.41
1:C:833:ILE:HD13	1:D:832:LEU:HA	2.02	0.41
1:A:67:VAL:HG21	1:A:96:LYS:CE	2.50	0.41
1:A:832:LEU:HA	1:D:833:ILE:HD13	2.02	0.41
1:B:115:VAL:HA	1:B:118:VAL:HG12	2.02	0.41
1:D:636:LEU:HD11	1:D:640:HIS:HB2	2.02	0.41
1:A:23:ARG:HD3	1:B:181:MET:HE3	2.02	0.41
1:A:73:MET:HE2	1:A:73:MET:HA	2.01	0.41
1:C:73:MET:HE2	1:C:73:MET:HA	2.01	0.41
1:A:532:SER:O	1:A:533:ASP:C	2.63	0.41
1:B:353:VAL:HG13	1:B:387:VAL:HG23	2.01	0.41
1:C:532:SER:O	1:C:533:ASP:C	2.63	0.41
1:A:115:VAL:HA	1:A:118:VAL:HG12	2.02	0.41
1:A:267:LYS:HZ2	1:A:317:VAL:HG22	1.85	0.41
1:A:589:PHE:HA	1:A:592:MET:HG3	2.02	0.41
1:B:267:LYS:HZ2	1:B:317:VAL:HG22	1.86	0.41
1:B:364:ALA:O	1:B:368:TRP:CG	2.74	0.41
1:B:589:PHE:HA	1:B:592:MET:HG3	2.02	0.41
1:C:261:LYS:HA	1:C:261:LYS:HD3	1.81	0.41
1:C:267:LYS:HZ2	1:C:317:VAL:HG22	1.86	0.41
1:C:554:ALA:HA	1:C:557:LEU:HD13	2.01	0.41
1:D:554:ALA:HA	1:D:557:LEU:HD13	2.01	0.41
1:A:636:LEU:HD11	1:A:640:HIS:HB2	2.02	0.41
1:A:642:PHE:O	1:A:646:ILE:HG12	2.21	0.41
1:B:642:PHE:O	1:B:646:ILE:HG12	2.21	0.41
1:B:640:HIS:HB3	1:B:643:ILE:HB	2.01	0.41
1:C:664:ASN:HA	1:C:667:ILE:HG12	2.02	0.41
1:A:364:ALA:O	1:A:368:TRP:CG	2.74	0.41
1:A:584:PHE:CD1	1:A:584:PHE:C	2.98	0.41
1:B:23:ARG:HD3	1:C:181:MET:HE3	2.03	0.41
1:C:30:ASN:HB2	1:C:72:TYR:HA	2.03	0.41
1:D:30:ASN:HB2	1:D:72:TYR:HA	2.03	0.41
1:D:704:PRO:HG2	1:D:707:PHE:HB2	2.02	0.41
1:C:364:ALA:O	1:C:368:TRP:CG	2.74	0.41
1:C:589:PHE:HA	1:C:592:MET:HG3	2.02	0.41
1:A:666:LEU:CD1	1:D:664:ASN:OD1	2.69	0.40
1:A:704:PRO:HG2	1:A:707:PHE:HB2	2.02	0.40
1:A:705:PRO:N	1:A:706:PRO:HD2	2.36	0.40
1:C:659:VAL:HG13	1:C:663:LEU:HD22	2.03	0.40
1:D:642:PHE:O	1:D:646:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASN:HB2	1:A:72:TYR:HA	2.03	0.40
1:D:828:GLU:HG3	1:D:832:LEU:HD13	2.04	0.40
1:B:686:LYS:HD3	1:B:689:ARG:HH21	1.86	0.40
1:B:705:PRO:N	1:B:706:PRO:HD2	2.36	0.40
1:A:578:PHE:HA	1:A:581:MET:HG2	2.04	0.40
1:A:557:LEU:N	1:A:558:PRO:HD2	2.37	0.40
1:A:686:LYS:HD3	1:A:689:ARG:HH21	1.86	0.40
1:B:73:MET:HE2	1:B:73:MET:HA	2.01	0.40
1:C:516:PRO:HA	1:C:517:PRO:HD3	1.98	0.40
1:C:828:GLU:HG3	1:C:832:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/820 (90%)	641 (87%)	85 (12%)	13 (2%)	6	29
1	B	739/820 (90%)	642 (87%)	84 (11%)	13 (2%)	6	29
1	C	739/820 (90%)	642 (87%)	84 (11%)	13 (2%)	6	29
1	D	739/820 (90%)	642 (87%)	84 (11%)	13 (2%)	6	29
All	All	2956/3280 (90%)	2567 (87%)	337 (11%)	52 (2%)	9	29

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	660	VAL
1	B	660	VAL
1	C	660	VAL
1	D	660	VAL
1	A	632	THR

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Mol	Chain	Res	Type
1	A	659	VAL
1	B	632	THR
1	B	659	VAL
1	C	632	THR
1	C	659	VAL
1	D	632	THR
1	D	659	VAL
1	A	129	ALA
1	B	129	ALA
1	C	129	ALA
1	D	129	ALA
1	A	35	SER
1	A	125	PRO
1	A	464	TYR
1	A	641	LYS
1	B	35	SER
1	B	125	PRO
1	B	464	TYR
1	B	641	LYS
1	C	35	SER
1	C	125	PRO
1	C	464	TYR
1	C	641	LYS
1	D	35	SER
1	D	125	PRO
1	D	464	TYR
1	D	641	LYS
1	A	468	LEU
1	B	468	LEU
1	C	468	LEU
1	D	468	LEU
1	A	163	PRO
1	A	406	ASP
1	B	163	PRO
1	B	406	ASP
1	C	163	PRO
1	C	406	ASP
1	D	163	PRO
1	D	406	ASP
1	A	465	ILE
1	B	465	ILE
1	C	465	ILE

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Mol	Chain	Res	Type
1	D	465	ILE
1	A	423	PRO
1	B	423	PRO
1	C	423	PRO
1	D	423	PRO

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	656/726 (90%)	643 (98%)	13 (2%)	48	68
1	B	656/726 (90%)	643 (98%)	13 (2%)	48	68
1	C	656/726 (90%)	643 (98%)	13 (2%)	48	68
1	D	656/726 (90%)	643 (98%)	13 (2%)	48	68
All	All	2624/2904 (90%)	2572 (98%)	52 (2%)	48	68

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	GLU
1	A	399	LEU
1	A	419	VAL
1	A	467	GLN
1	A	468	LEU
1	A	474	PHE
1	A	553	ILE
1	A	562	SER
1	A	601	TYR
1	A	602	TYR
1	A	612	THR
1	A	636	LEU
1	A	640	HIS
1	B	174	GLU
1	B	399	LEU
1	B	419	VAL

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Mol	Chain	Res	Type
1	B	467	GLN
1	B	468	LEU
1	B	474	PHE
1	B	553	ILE
1	B	562	SER
1	B	601	TYR
1	B	602	TYR
1	B	612	THR
1	B	636	LEU
1	B	640	HIS
1	C	174	GLU
1	C	399	LEU
1	C	419	VAL
1	C	467	GLN
1	C	468	LEU
1	C	474	PHE
1	C	553	ILE
1	C	562	SER
1	C	601	TYR
1	C	602	TYR
1	C	612	THR
1	C	636	LEU
1	C	640	HIS
1	D	174	GLU
1	D	399	LEU
1	D	419	VAL
1	D	467	GLN
1	D	468	LEU
1	D	474	PHE
1	D	553	ILE
1	D	562	SER
1	D	601	TYR
1	D	602	TYR
1	D	612	THR
1	D	636	LEU
1	D	640	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	671	ASN

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Mol	Chain	Res	Type
1	B	30	ASN
1	B	671	ASN
1	C	30	ASN
1	C	671	ASN
1	D	30	ASN
1	D	671	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

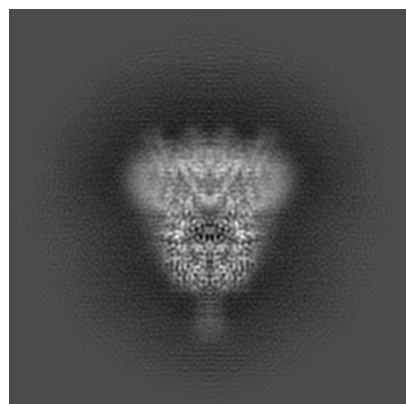
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70724. These allow visual inspection of the internal detail of the map and identification of artifacts.

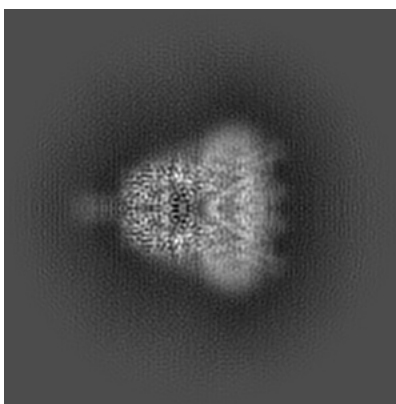
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

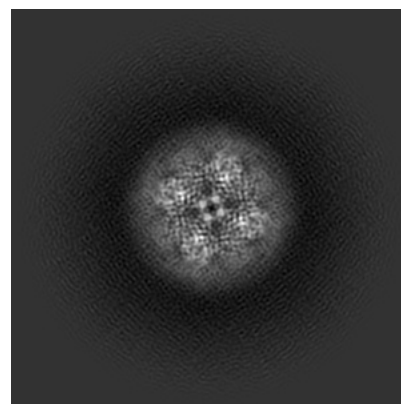
6.1.1 Primary map



X

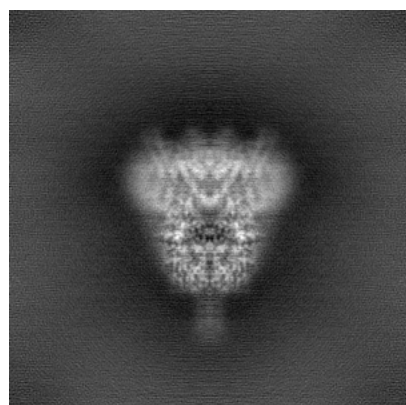


Y

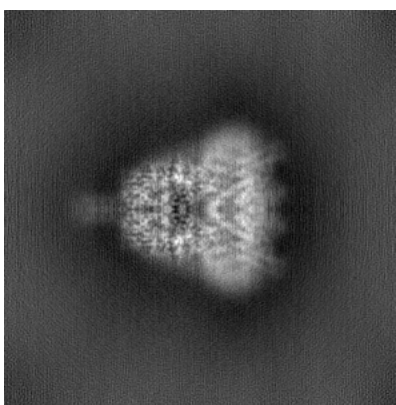


Z

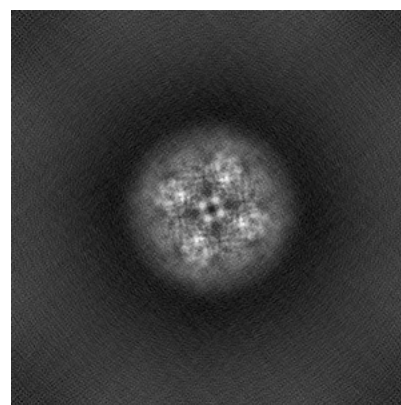
6.1.2 Raw map



X



Y

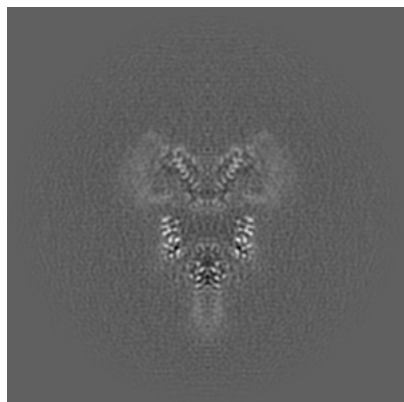


Z

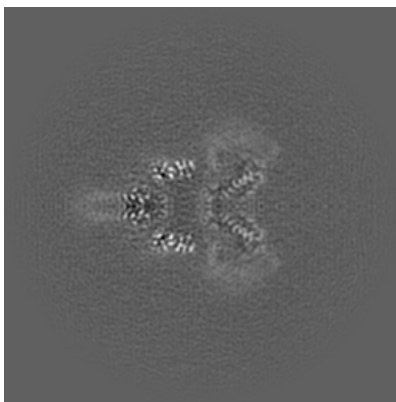
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

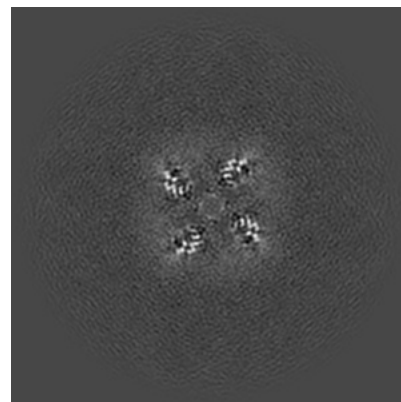
6.2.1 Primary map



X Index: 150

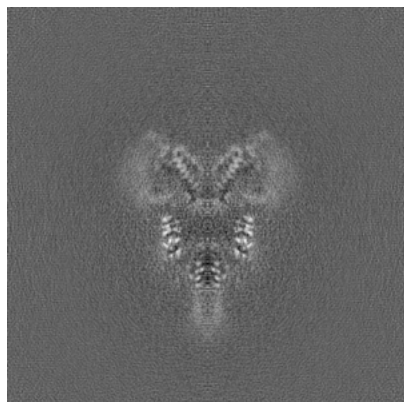


Y Index: 150

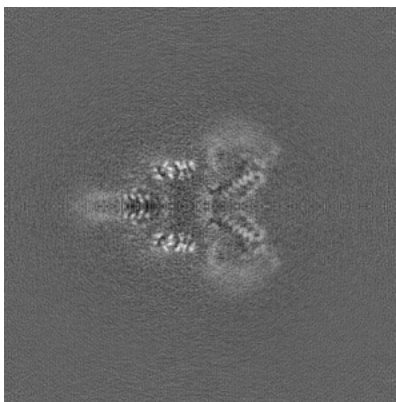


Z Index: 150

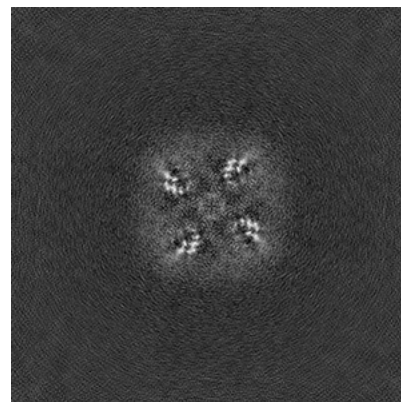
6.2.2 Raw map



X Index: 150



Y Index: 150

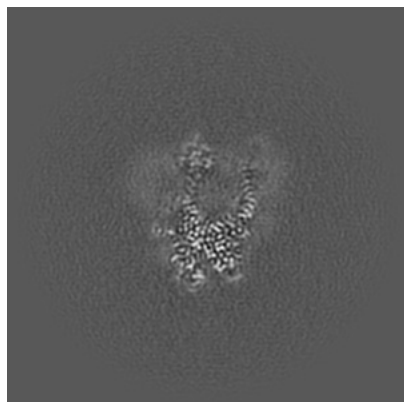


Z Index: 150

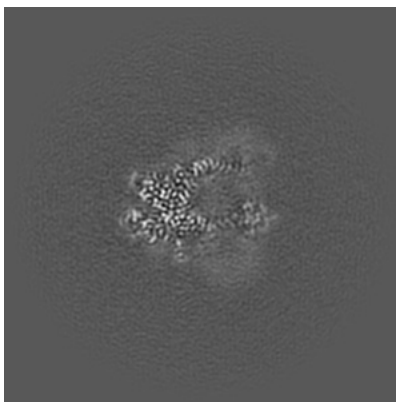
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

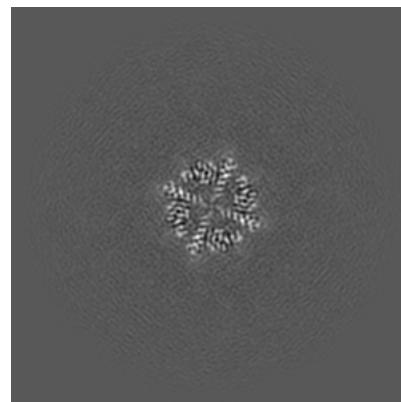
6.3.1 Primary map



X Index: 172

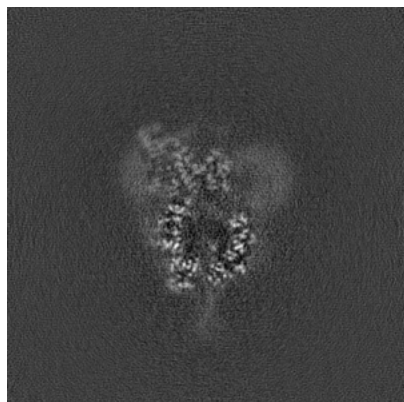


Y Index: 128

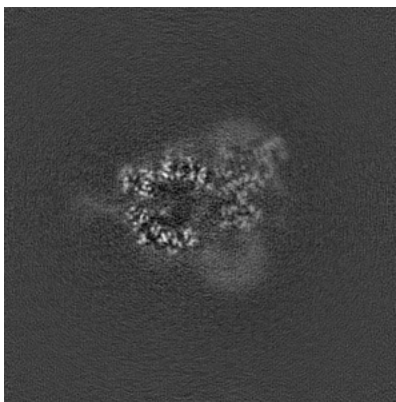


Z Index: 121

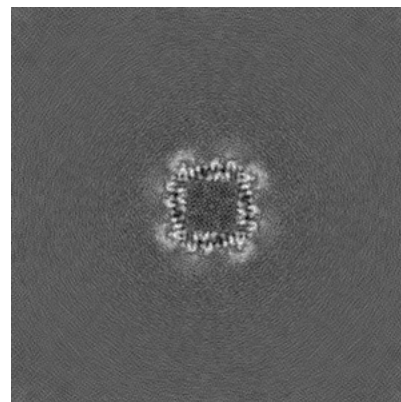
6.3.2 Raw map



X Index: 139



Y Index: 139

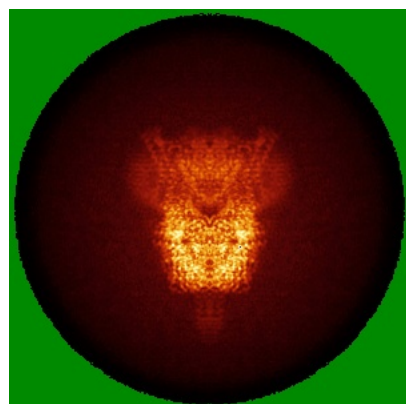


Z Index: 131

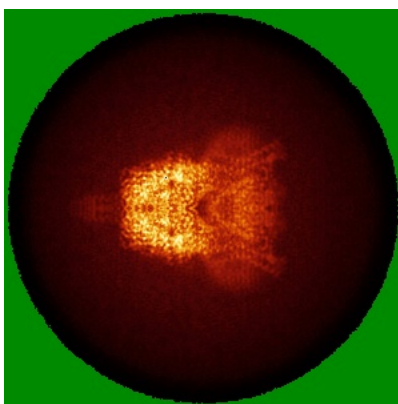
The images above show the largest variance slices of the map in three orthogonal directions.

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

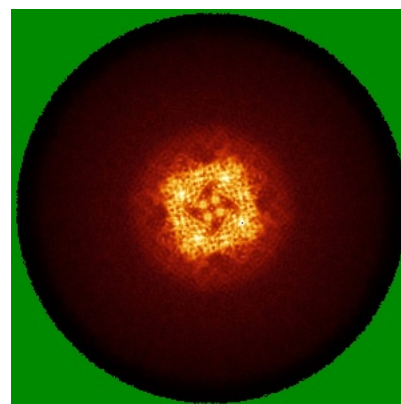
6.4.1 Primary map



X

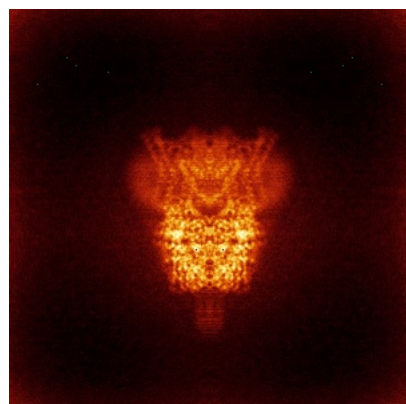


Y

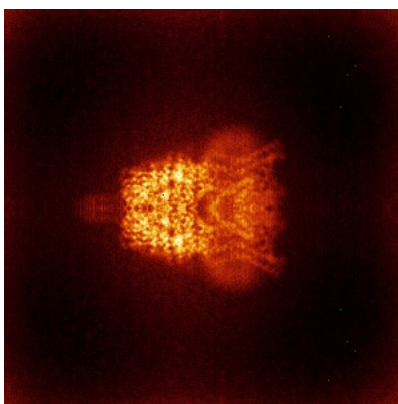


Z

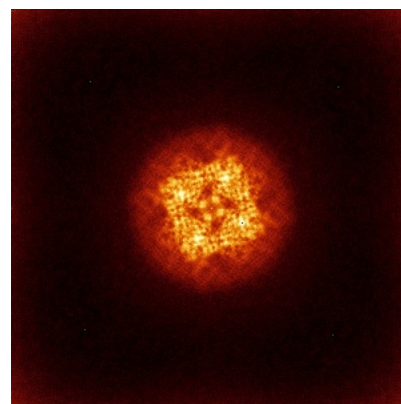
6.4.2 Raw map



X



Y

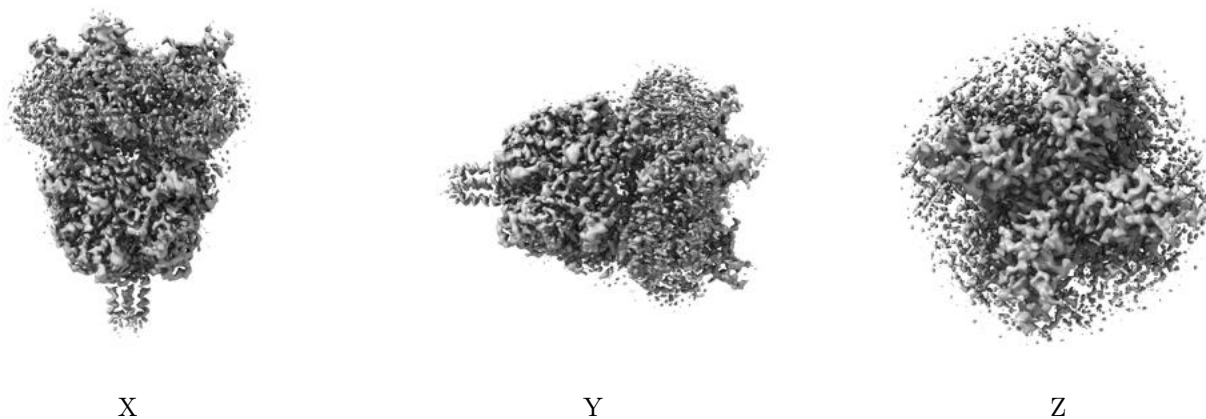


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

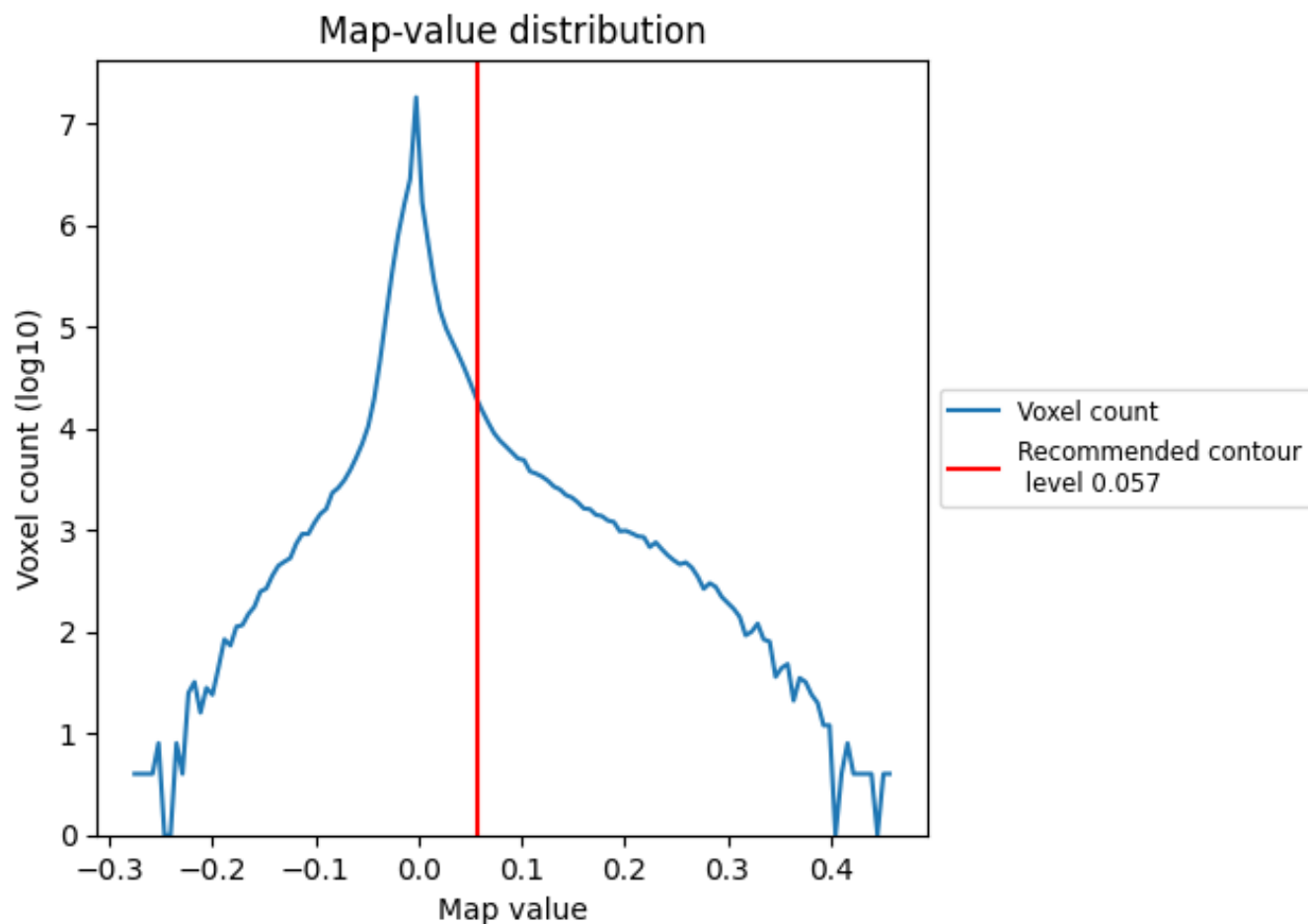
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

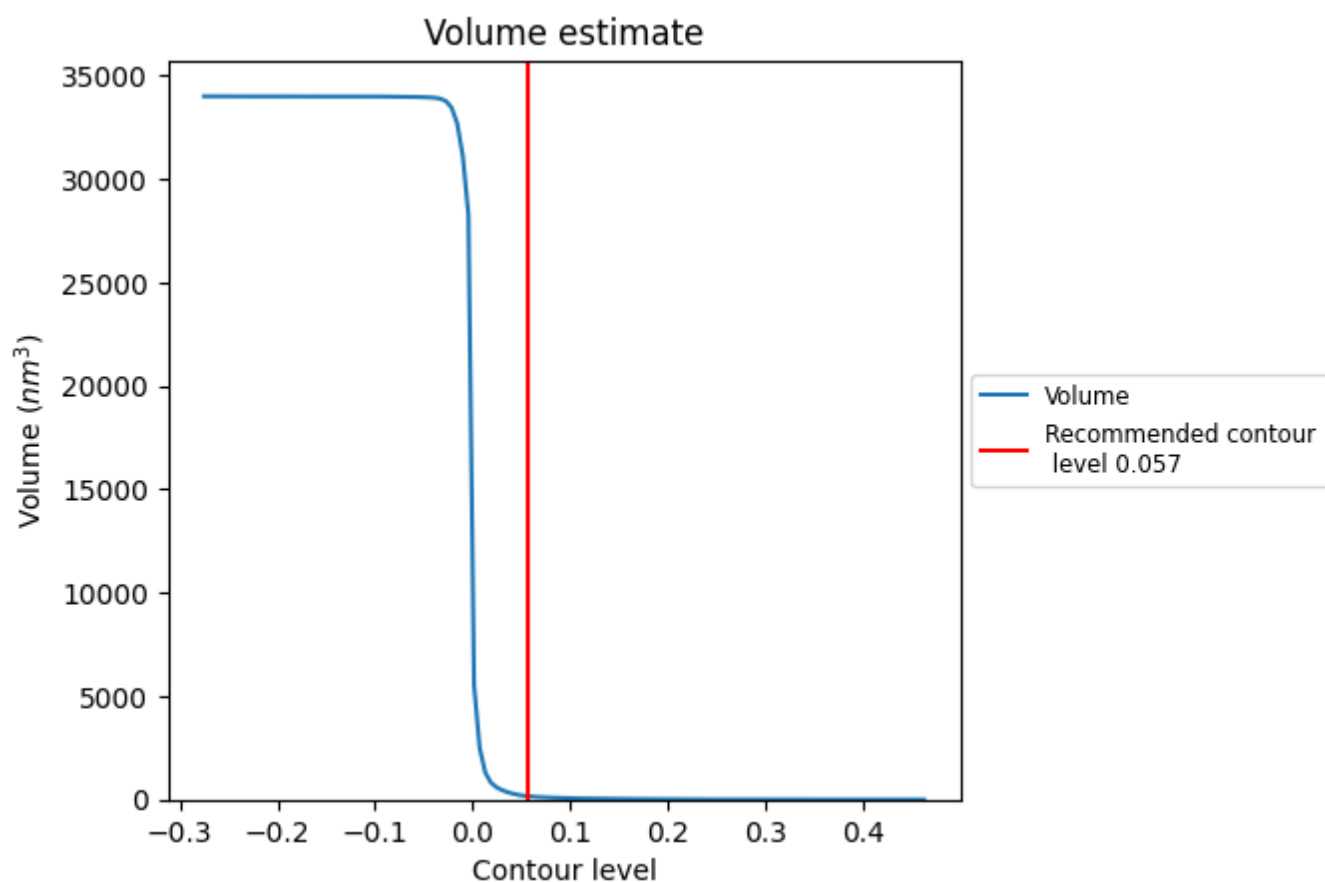
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

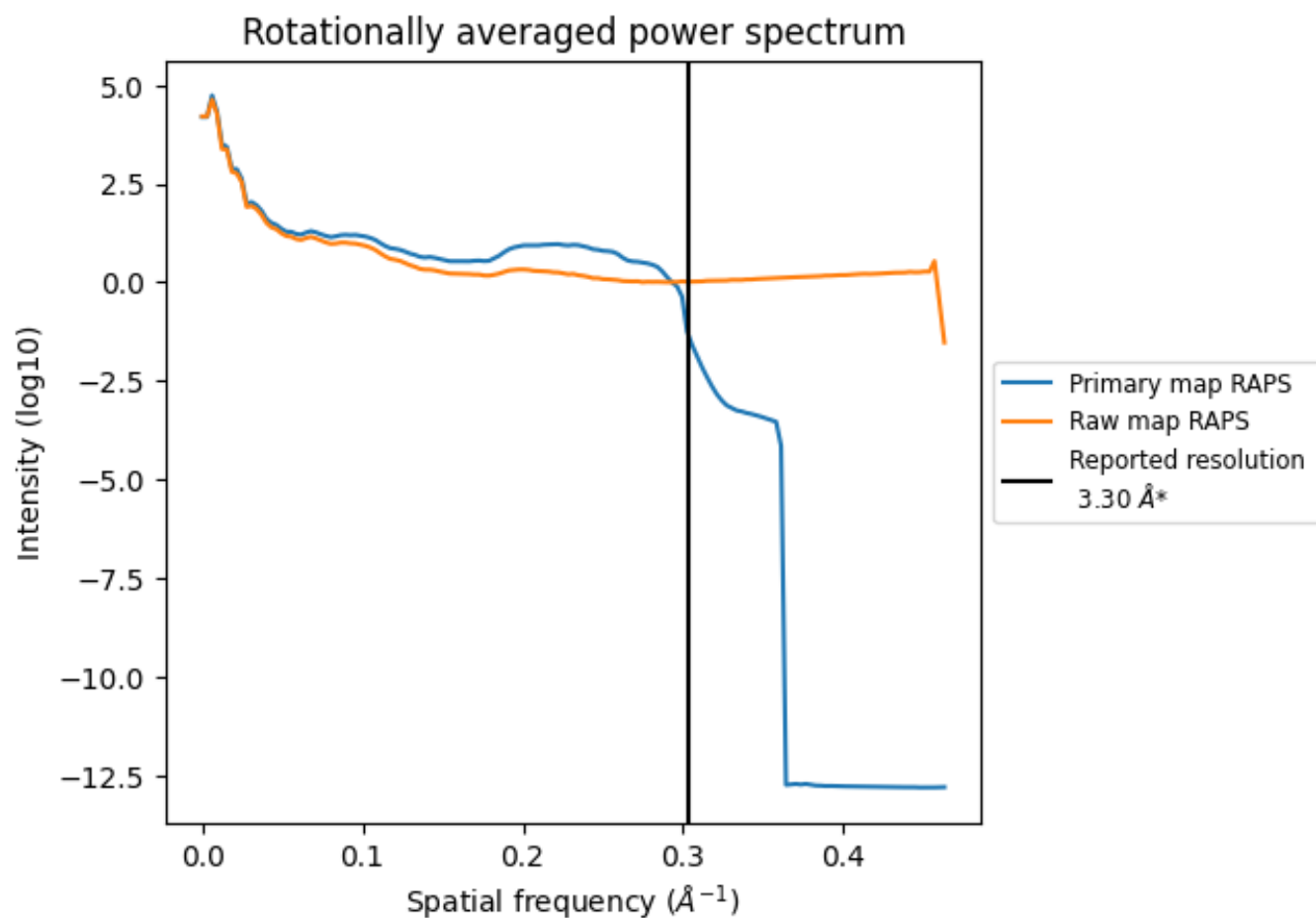
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 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 ⓘ

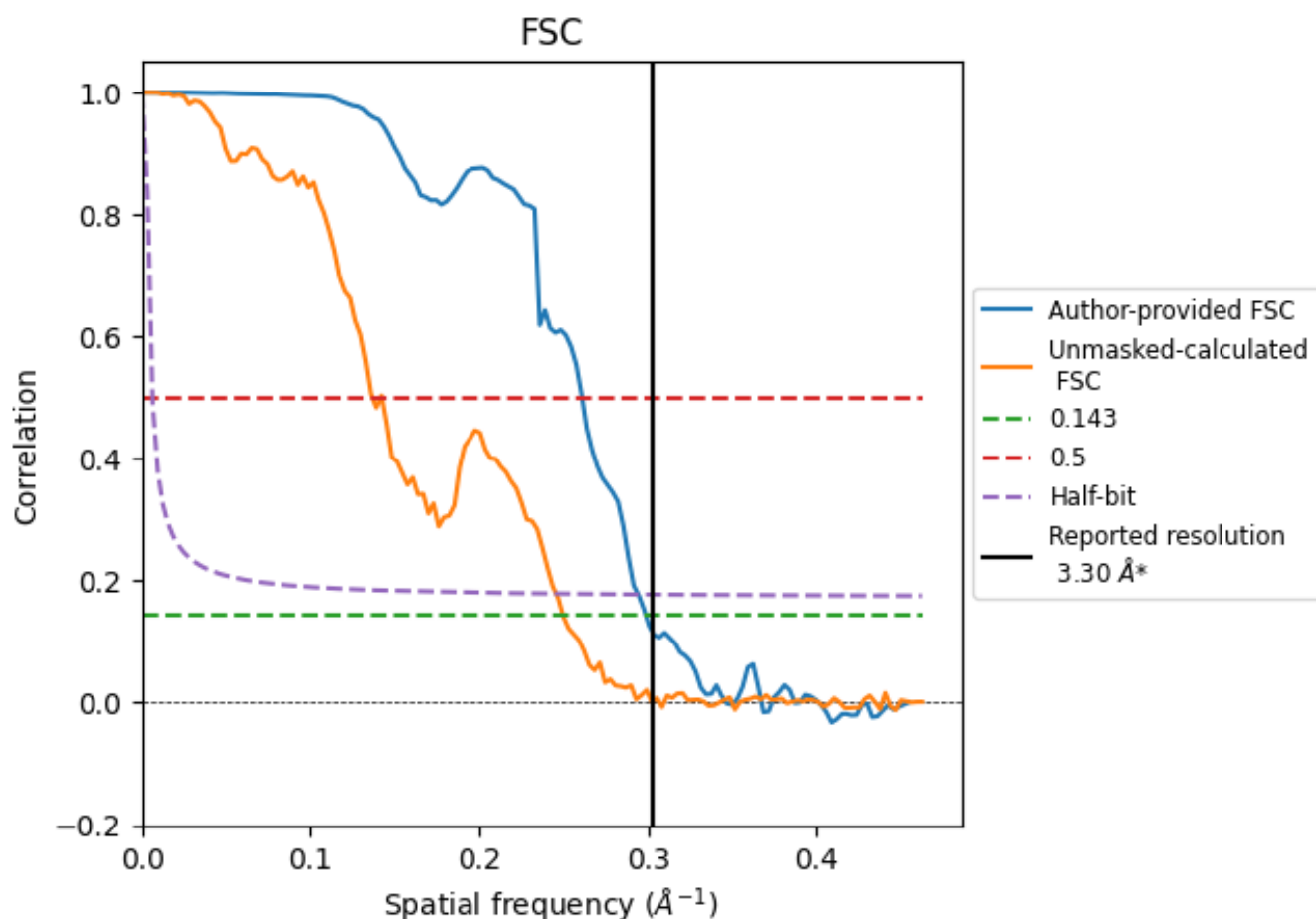


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

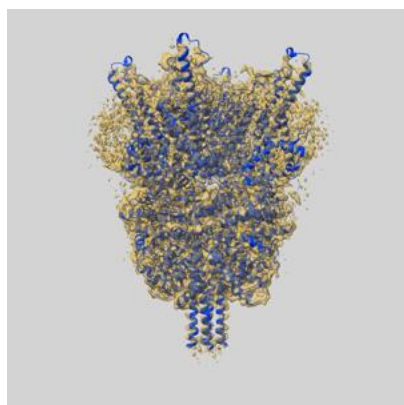
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.83	3.40
Unmasked-calculated*	4.00	7.32	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.3 by more than 10 %

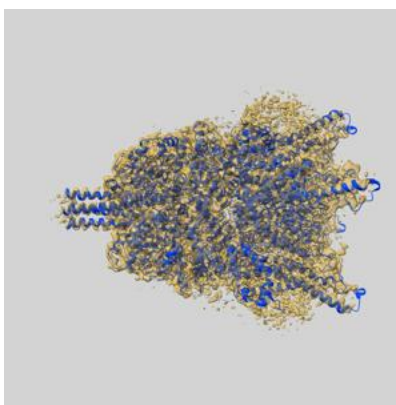
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70724 and PDB model 9OPU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

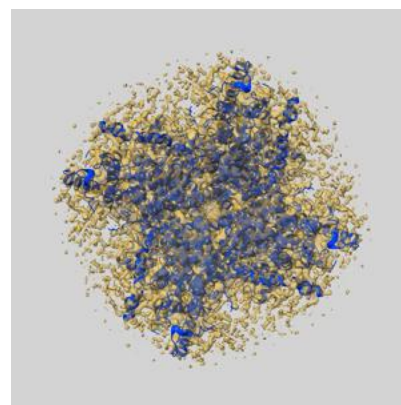
9.1 Map-model overlay [i](#)



X



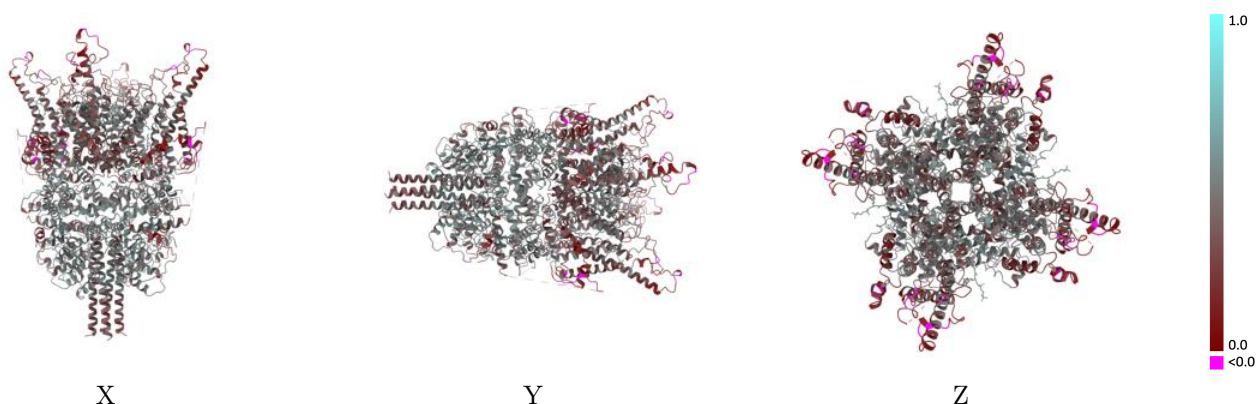
Y



Z

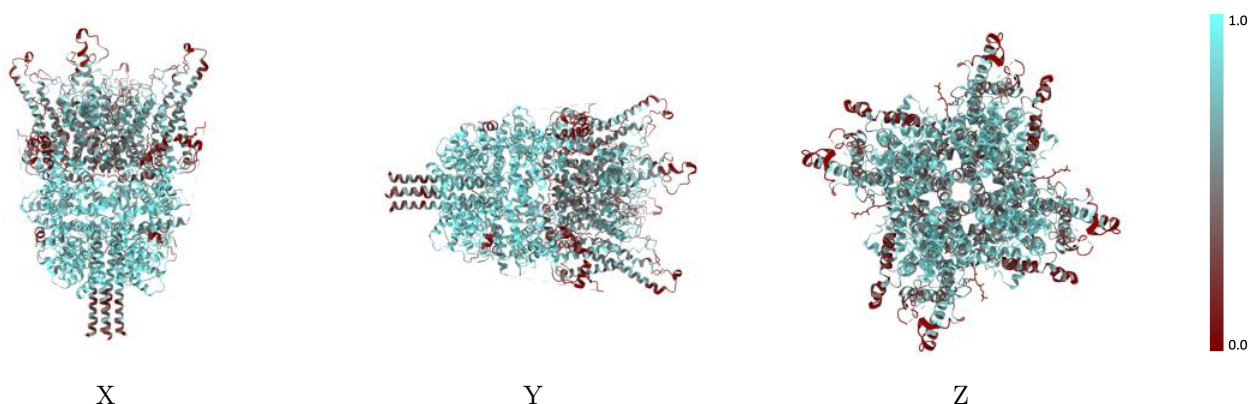
The images above show the 3D surface view of the map at the recommended contour level 0.057 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



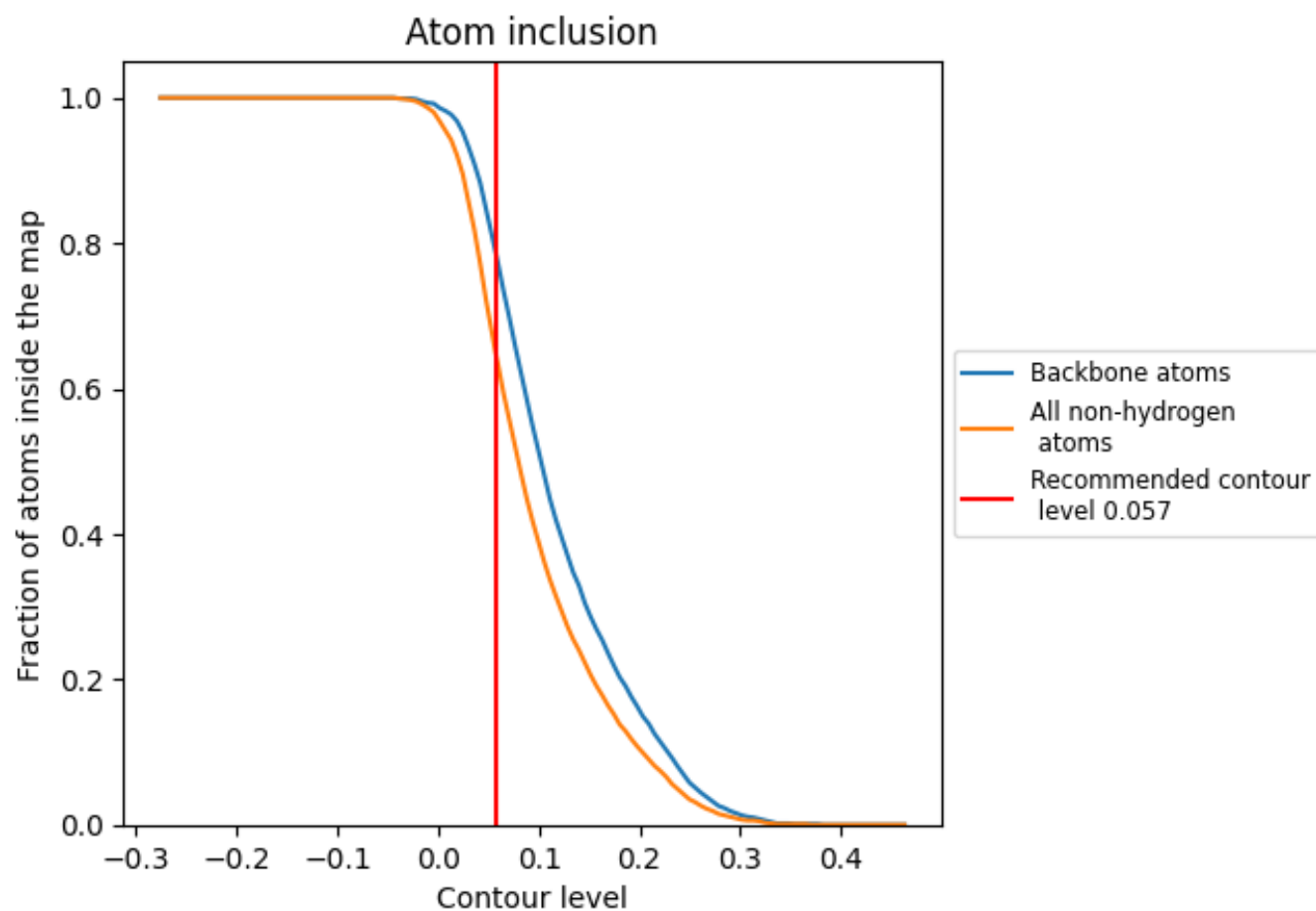
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.057).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6500	<div></div> 0.3980
A	<div></div> 0.6460	<div></div> 0.3990
B	<div></div> 0.6510	<div></div> 0.3990
C	<div></div> 0.6510	<div></div> 0.3990
D	<div></div> 0.6540	<div></div> 0.3970

