



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:48 AM UTC

PDB ID : 9J84 / pdb_00009j84
EMDB ID : EMD-61215
Title : Structural mechanism of human TRPM3 ion channel inhibition
Authors : Yang, T.T.; Cheng, X.Y.
Deposited on : 2024-08-20
Resolution : 4.21 Å(reported)

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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

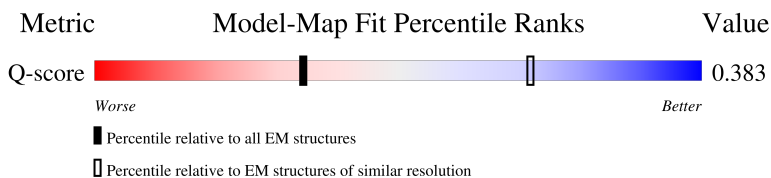
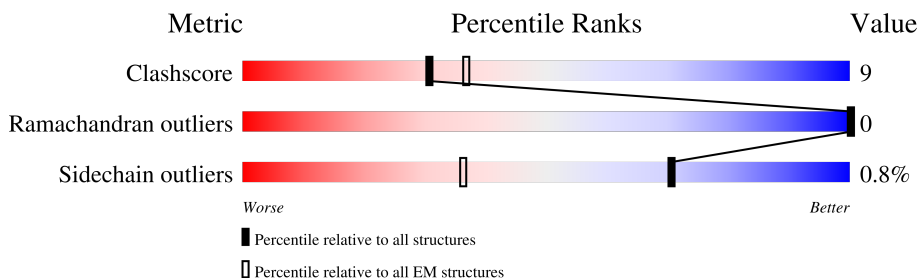
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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	4806 (3.71 - 4.71)

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	1610	
1	B	1610	
1	C	1610	
1	D	1610	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19280 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 Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily M member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	619	Total	C	N	O	S	0	0
			4791	3138	789	827	37		
1	B	619	Total	C	N	O	S	0	0
			4791	3138	789	827	37		
1	C	619	Total	C	N	O	S	0	0
			4791	3138	789	827	37		
1	D	619	Total	C	N	O	S	0	0
			4791	3138	789	827	37		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-289	ALA	-	expression tag	UNP P0AEX9
A	-288	THR	-	expression tag	UNP P0AEX9
A	-287	MET	-	expression tag	UNP P0AEX9
A	-286	GLY	-	expression tag	UNP P0AEX9
A	-285	MET	-	expression tag	UNP P0AEX9
A	-284	GLY	-	expression tag	UNP P0AEX9
A	-283	SER	-	expression tag	UNP P0AEX9
A	-282	SER	-	expression tag	UNP P0AEX9
A	-281	HIS	-	expression tag	UNP P0AEX9
A	-280	HIS	-	expression tag	UNP P0AEX9
A	-279	HIS	-	expression tag	UNP P0AEX9
A	-278	HIS	-	expression tag	UNP P0AEX9
A	-277	HIS	-	expression tag	UNP P0AEX9
A	-276	HIS	-	expression tag	UNP P0AEX9
A	-275	GLY	-	expression tag	UNP P0AEX9
A	-274	SER	-	expression tag	UNP P0AEX9
A	-273	SER	-	expression tag	UNP P0AEX9
A	-272	MET	-	expression tag	UNP P0AEX9
A	95	ASN	-	linker	UNP P0AEX9
A	96	SER	-	linker	UNP P0AEX9
A	97	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	98	SER	-	linker	UNP P0AEX9
A	99	ASN	-	linker	UNP P0AEX9
A	100	ASN	-	linker	UNP P0AEX9
A	101	ASN	-	linker	UNP P0AEX9
A	102	ASN	-	linker	UNP P0AEX9
A	103	ASN	-	linker	UNP P0AEX9
A	104	ASN	-	linker	UNP P0AEX9
A	105	ASN	-	linker	UNP P0AEX9
A	106	ASN	-	linker	UNP P0AEX9
A	107	ASN	-	linker	UNP P0AEX9
A	108	ASN	-	linker	UNP P0AEX9
A	109	LEU	-	linker	UNP P0AEX9
A	110	GLY	-	linker	UNP P0AEX9
A	111	ILE	-	linker	UNP P0AEX9
A	112	GLU	-	linker	UNP P0AEX9
A	113	LEU	-	linker	UNP P0AEX9
A	114	GLU	-	linker	UNP P0AEX9
A	115	VAL	-	linker	UNP P0AEX9
A	116	LEU	-	linker	UNP P0AEX9
A	117	PHE	-	linker	UNP P0AEX9
A	118	GLN	-	linker	UNP P0AEX9
A	119	GLY	-	linker	UNP P0AEX9
A	120	PRO	-	linker	UNP P0AEX9
B	-289	ALA	-	expression tag	UNP P0AEX9
B	-288	THR	-	expression tag	UNP P0AEX9
B	-287	MET	-	expression tag	UNP P0AEX9
B	-286	GLY	-	expression tag	UNP P0AEX9
B	-285	MET	-	expression tag	UNP P0AEX9
B	-284	GLY	-	expression tag	UNP P0AEX9
B	-283	SER	-	expression tag	UNP P0AEX9
B	-282	SER	-	expression tag	UNP P0AEX9
B	-281	HIS	-	expression tag	UNP P0AEX9
B	-280	HIS	-	expression tag	UNP P0AEX9
B	-279	HIS	-	expression tag	UNP P0AEX9
B	-278	HIS	-	expression tag	UNP P0AEX9
B	-277	HIS	-	expression tag	UNP P0AEX9
B	-276	HIS	-	expression tag	UNP P0AEX9
B	-275	GLY	-	expression tag	UNP P0AEX9
B	-274	SER	-	expression tag	UNP P0AEX9
B	-273	SER	-	expression tag	UNP P0AEX9
B	-272	MET	-	expression tag	UNP P0AEX9
B	95	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	96	SER	-	linker	UNP P0AEX9
B	97	SER	-	linker	UNP P0AEX9
B	98	SER	-	linker	UNP P0AEX9
B	99	ASN	-	linker	UNP P0AEX9
B	100	ASN	-	linker	UNP P0AEX9
B	101	ASN	-	linker	UNP P0AEX9
B	102	ASN	-	linker	UNP P0AEX9
B	103	ASN	-	linker	UNP P0AEX9
B	104	ASN	-	linker	UNP P0AEX9
B	105	ASN	-	linker	UNP P0AEX9
B	106	ASN	-	linker	UNP P0AEX9
B	107	ASN	-	linker	UNP P0AEX9
B	108	ASN	-	linker	UNP P0AEX9
B	109	LEU	-	linker	UNP P0AEX9
B	110	GLY	-	linker	UNP P0AEX9
B	111	ILE	-	linker	UNP P0AEX9
B	112	GLU	-	linker	UNP P0AEX9
B	113	LEU	-	linker	UNP P0AEX9
B	114	GLU	-	linker	UNP P0AEX9
B	115	VAL	-	linker	UNP P0AEX9
B	116	LEU	-	linker	UNP P0AEX9
B	117	PHE	-	linker	UNP P0AEX9
B	118	GLN	-	linker	UNP P0AEX9
B	119	GLY	-	linker	UNP P0AEX9
B	120	PRO	-	linker	UNP P0AEX9
C	-289	ALA	-	expression tag	UNP P0AEX9
C	-288	THR	-	expression tag	UNP P0AEX9
C	-287	MET	-	expression tag	UNP P0AEX9
C	-286	GLY	-	expression tag	UNP P0AEX9
C	-285	MET	-	expression tag	UNP P0AEX9
C	-284	GLY	-	expression tag	UNP P0AEX9
C	-283	SER	-	expression tag	UNP P0AEX9
C	-282	SER	-	expression tag	UNP P0AEX9
C	-281	HIS	-	expression tag	UNP P0AEX9
C	-280	HIS	-	expression tag	UNP P0AEX9
C	-279	HIS	-	expression tag	UNP P0AEX9
C	-278	HIS	-	expression tag	UNP P0AEX9
C	-277	HIS	-	expression tag	UNP P0AEX9
C	-276	HIS	-	expression tag	UNP P0AEX9
C	-275	GLY	-	expression tag	UNP P0AEX9
C	-274	SER	-	expression tag	UNP P0AEX9
C	-273	SER	-	expression tag	UNP P0AEX9

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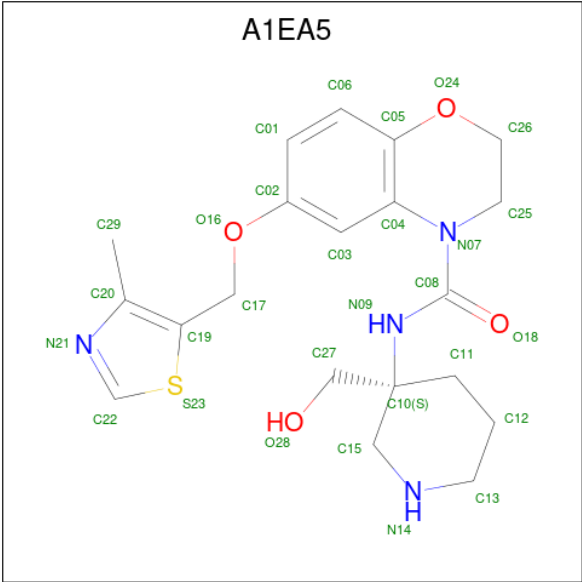
Chain	Residue	Modelled	Actual	Comment	Reference
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C	96	SER	-	linker	UNP P0AEX9
C	97	SER	-	linker	UNP P0AEX9
C	98	SER	-	linker	UNP P0AEX9
C	99	ASN	-	linker	UNP P0AEX9
C	100	ASN	-	linker	UNP P0AEX9
C	101	ASN	-	linker	UNP P0AEX9
C	102	ASN	-	linker	UNP P0AEX9
C	103	ASN	-	linker	UNP P0AEX9
C	104	ASN	-	linker	UNP P0AEX9
C	105	ASN	-	linker	UNP P0AEX9
C	106	ASN	-	linker	UNP P0AEX9
C	107	ASN	-	linker	UNP P0AEX9
C	108	ASN	-	linker	UNP P0AEX9
C	109	LEU	-	linker	UNP P0AEX9
C	110	GLY	-	linker	UNP P0AEX9
C	111	ILE	-	linker	UNP P0AEX9
C	112	GLU	-	linker	UNP P0AEX9
C	113	LEU	-	linker	UNP P0AEX9
C	114	GLU	-	linker	UNP P0AEX9
C	115	VAL	-	linker	UNP P0AEX9
C	116	LEU	-	linker	UNP P0AEX9
C	117	PHE	-	linker	UNP P0AEX9
C	118	GLN	-	linker	UNP P0AEX9
C	119	GLY	-	linker	UNP P0AEX9
C	120	PRO	-	linker	UNP P0AEX9
D	-289	ALA	-	expression tag	UNP P0AEX9
D	-288	THR	-	expression tag	UNP P0AEX9
D	-287	MET	-	expression tag	UNP P0AEX9
D	-286	GLY	-	expression tag	UNP P0AEX9
D	-285	MET	-	expression tag	UNP P0AEX9
D	-284	GLY	-	expression tag	UNP P0AEX9
D	-283	SER	-	expression tag	UNP P0AEX9
D	-282	SER	-	expression tag	UNP P0AEX9
D	-281	HIS	-	expression tag	UNP P0AEX9
D	-280	HIS	-	expression tag	UNP P0AEX9
D	-279	HIS	-	expression tag	UNP P0AEX9
D	-278	HIS	-	expression tag	UNP P0AEX9
D	-277	HIS	-	expression tag	UNP P0AEX9
D	-276	HIS	-	expression tag	UNP P0AEX9
D	-275	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-274	SER	-	expression tag	UNP P0AEX9
D	-273	SER	-	expression tag	UNP P0AEX9
D	-272	MET	-	expression tag	UNP P0AEX9
D	95	ASN	-	linker	UNP P0AEX9
D	96	SER	-	linker	UNP P0AEX9
D	97	SER	-	linker	UNP P0AEX9
D	98	SER	-	linker	UNP P0AEX9
D	99	ASN	-	linker	UNP P0AEX9
D	100	ASN	-	linker	UNP P0AEX9
D	101	ASN	-	linker	UNP P0AEX9
D	102	ASN	-	linker	UNP P0AEX9
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D	104	ASN	-	linker	UNP P0AEX9
D	105	ASN	-	linker	UNP P0AEX9
D	106	ASN	-	linker	UNP P0AEX9
D	107	ASN	-	linker	UNP P0AEX9
D	108	ASN	-	linker	UNP P0AEX9
D	109	LEU	-	linker	UNP P0AEX9
D	110	GLY	-	linker	UNP P0AEX9
D	111	ILE	-	linker	UNP P0AEX9
D	112	GLU	-	linker	UNP P0AEX9
D	113	LEU	-	linker	UNP P0AEX9
D	114	GLU	-	linker	UNP P0AEX9
D	115	VAL	-	linker	UNP P0AEX9
D	116	LEU	-	linker	UNP P0AEX9
D	117	PHE	-	linker	UNP P0AEX9
D	118	GLN	-	linker	UNP P0AEX9
D	119	GLY	-	linker	UNP P0AEX9
D	120	PRO	-	linker	UNP P0AEX9

- Molecule 2 is {N}-[(3 {S})-3-(hydroxymethyl)piperidin-3-yl]-6-[(4-methyl-1,3-thiazol-5-yl)methoxy]-2,3-dihydro-1,4-benzoxazine-4-carboxamide (CCD ID: A1EA5) (formula: C₂₀H₂₆N₄O₄S) (labeled as "Ligand of Interest" by depositor).

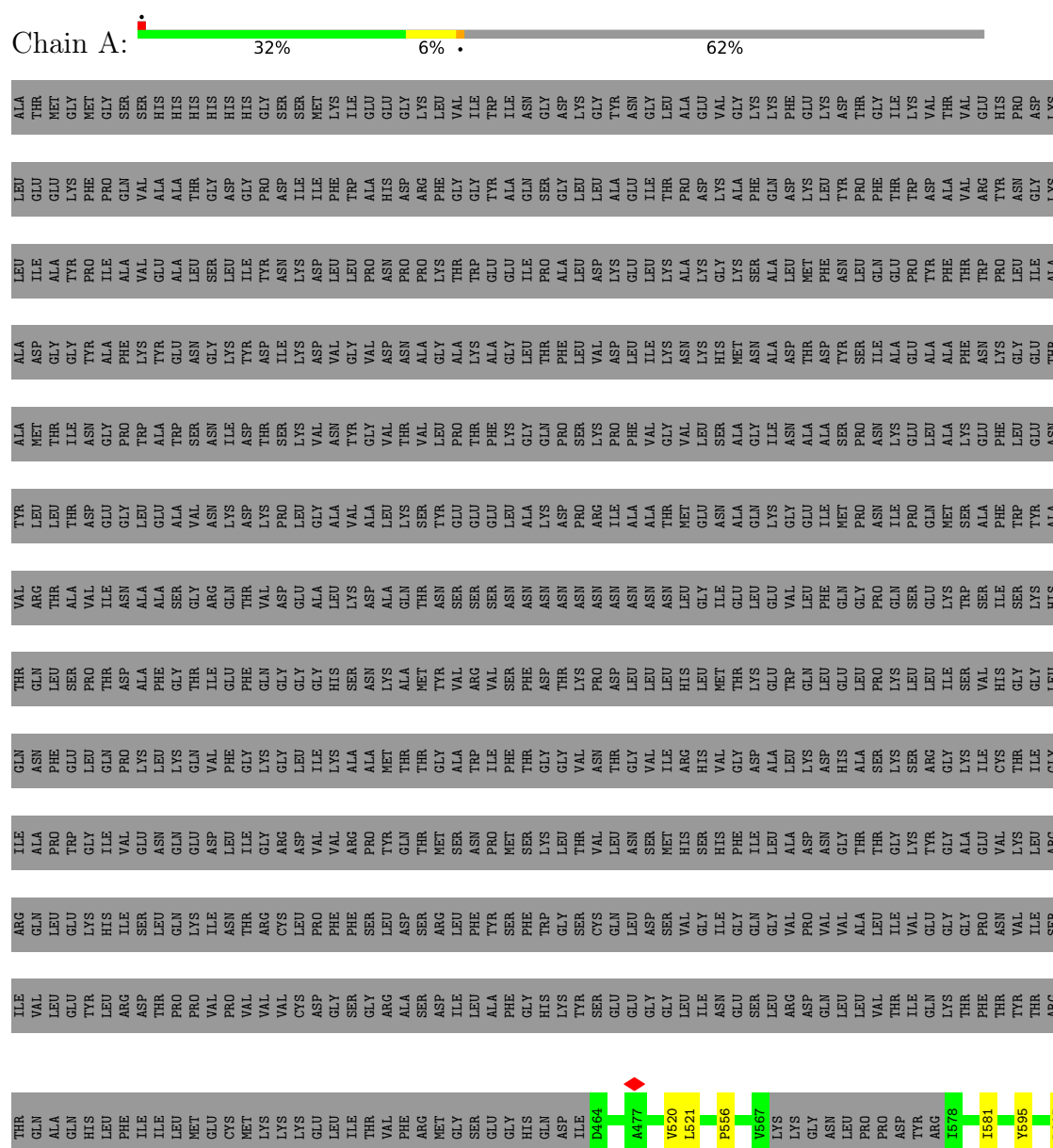


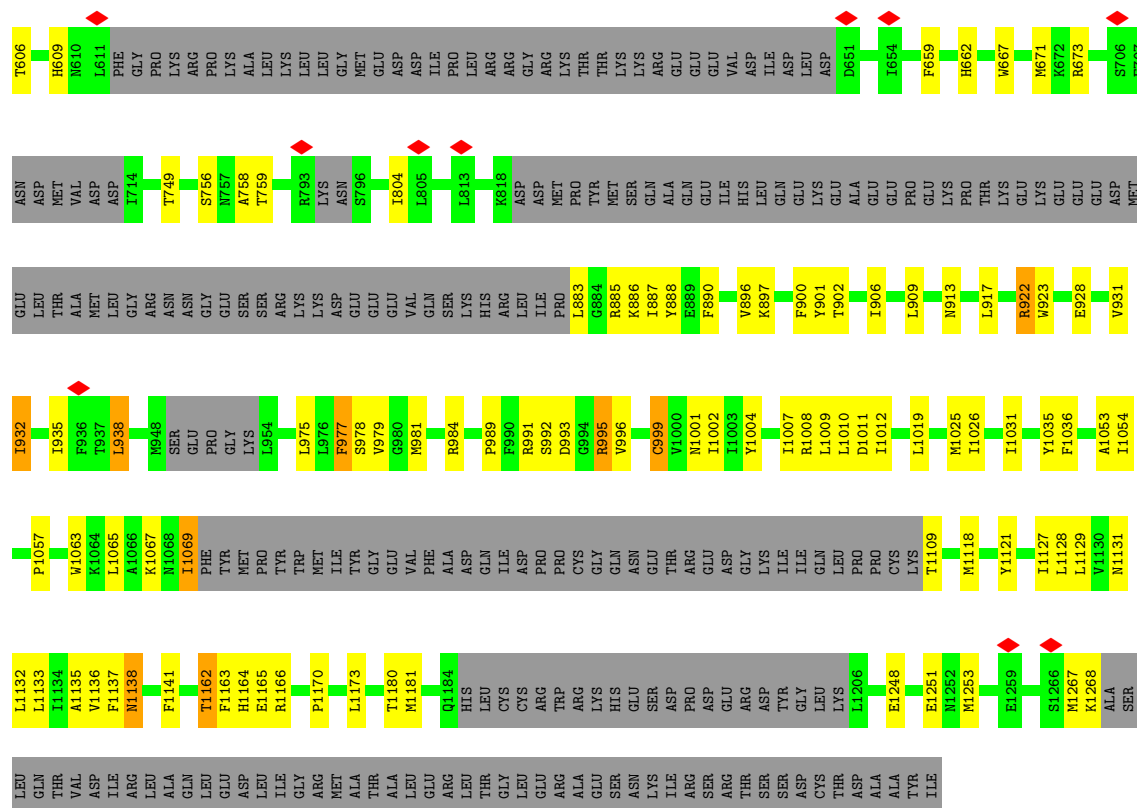
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			29	20	4	4	1	
2	B	1	Total	C	N	O	S	0
			29	20	4	4	1	
2	C	1	Total	C	N	O	S	0
			29	20	4	4	1	
2	D	1	Total	C	N	O	S	0
			29	20	4	4	1	

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.

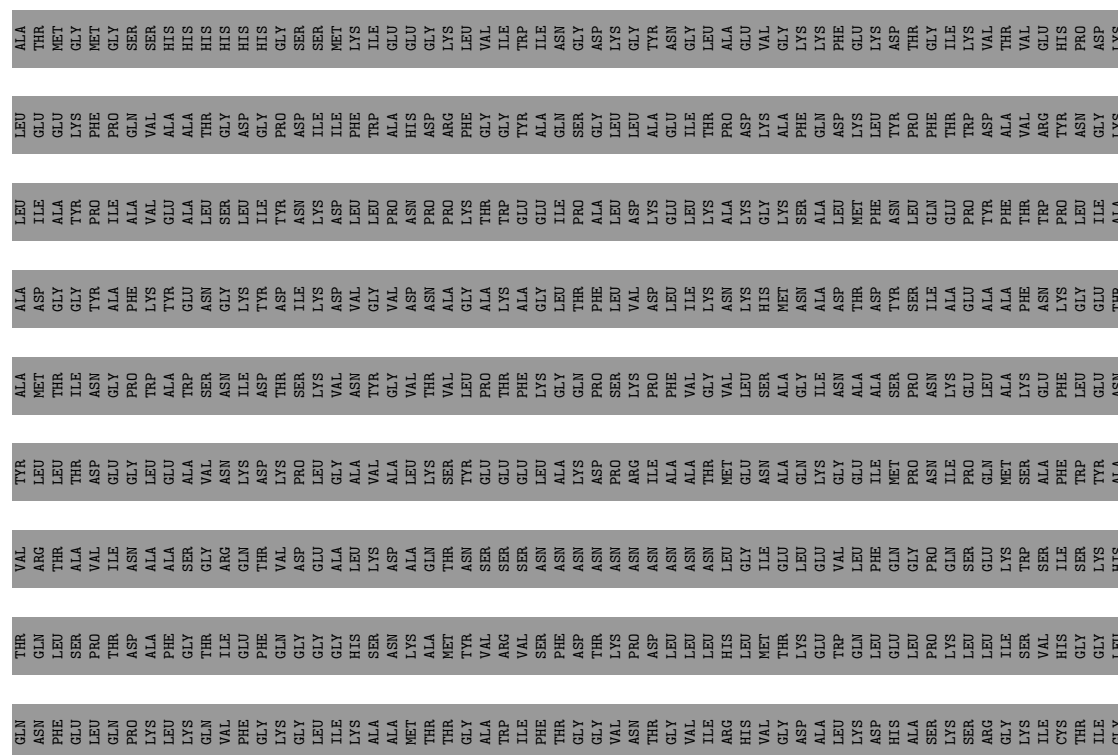
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily M member 3

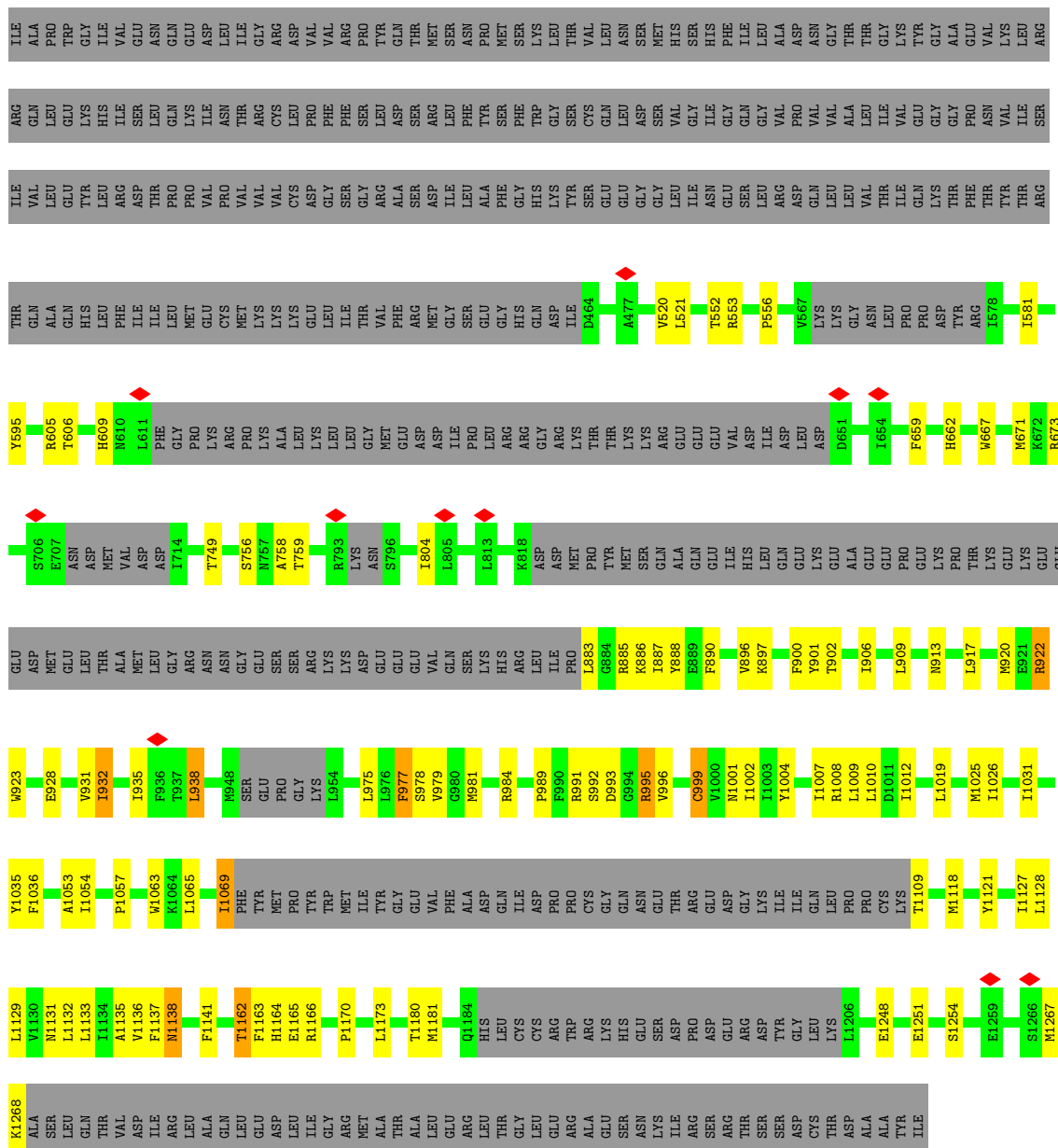




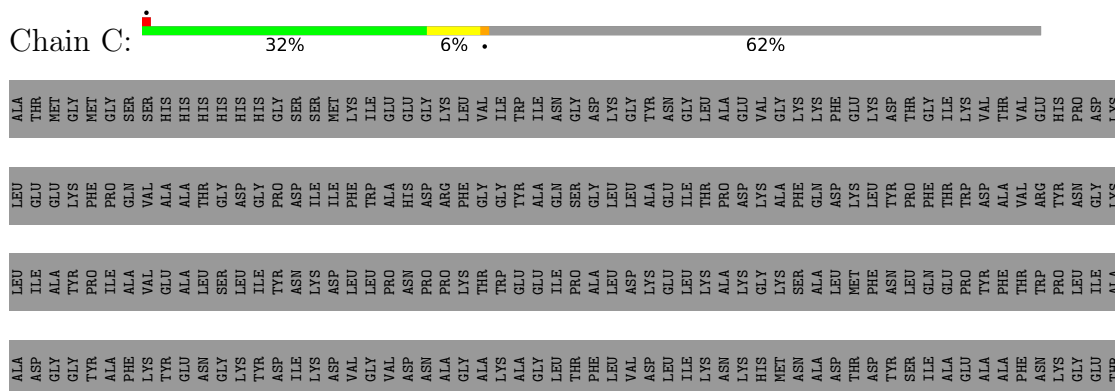
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily M member 3

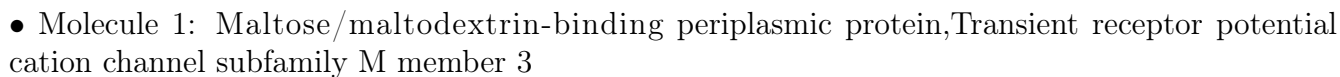
Chain B: 32% 6% 62%





- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily M member 3









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.13	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.474	Depositor
Minimum map value	-0.875	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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: A1EA5

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	0.74	13/4898 (0.3%)	1.00	27/6662 (0.4%)
1	B	0.74	13/4898 (0.3%)	1.00	25/6662 (0.4%)
1	C	0.74	13/4898 (0.3%)	1.01	25/6662 (0.4%)
1	D	0.74	13/4898 (0.3%)	1.01	25/6662 (0.4%)
All	All	0.74	52/19592 (0.3%)	1.00	102/26648 (0.4%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1162	THR	C-N	-18.73	1.05	1.33
1	B	1162	THR	C-N	-18.73	1.05	1.33
1	C	1162	THR	C-N	-18.73	1.05	1.33
1	D	1162	THR	C-N	-18.72	1.05	1.33
1	C	1163	PHE	C-N	11.64	1.49	1.34
1	A	1163	PHE	C-N	11.63	1.49	1.34
1	B	1163	PHE	C-N	11.63	1.49	1.34
1	D	1163	PHE	C-N	11.62	1.49	1.34
1	D	922	ARG	C-N	-11.40	1.17	1.32
1	A	922	ARG	C-N	-11.37	1.17	1.32
1	B	922	ARG	C-N	-11.37	1.17	1.32
1	C	922	ARG	C-N	-11.36	1.17	1.32
1	D	1164	HIS	C-N	10.21	1.49	1.33
1	A	1164	HIS	C-N	10.18	1.49	1.33
1	B	1164	HIS	C-N	10.18	1.49	1.33
1	C	1164	HIS	C-N	10.18	1.49	1.33
1	B	923	TRP	C-N	-9.63	1.21	1.33
1	D	923	TRP	C-N	-9.63	1.21	1.33
1	C	923	TRP	C-N	-9.61	1.21	1.33
1	A	923	TRP	C-N	-9.61	1.21	1.33
1	B	1128	LEU	C-N	-9.59	1.20	1.33
1	A	1128	LEU	C-N	-9.55	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1128	LEU	C-N	-9.50	1.20	1.33
1	D	1128	LEU	C-N	-9.47	1.20	1.33
1	D	1129	LEU	C-N	8.99	1.45	1.33
1	B	759	THR	C-N	-8.94	1.22	1.34
1	C	759	THR	C-N	-8.94	1.22	1.34
1	A	1129	LEU	C-N	8.93	1.45	1.33
1	B	1129	LEU	C-N	8.92	1.45	1.33
1	A	759	THR	C-N	-8.89	1.22	1.34
1	D	759	THR	C-N	-8.89	1.22	1.34
1	C	1129	LEU	C-N	8.88	1.45	1.33
1	B	758	ALA	C-N	-8.39	1.21	1.33
1	C	758	ALA	C-N	-8.39	1.21	1.33
1	D	758	ALA	C-N	-8.39	1.21	1.33
1	A	758	ALA	C-N	-8.34	1.21	1.33
1	D	1180	THR	C-N	-8.19	1.23	1.33
1	A	1180	THR	C-N	-8.15	1.23	1.33
1	C	1180	THR	C-N	-8.15	1.23	1.33
1	B	1180	THR	C-N	-7.77	1.22	1.33
1	D	1181	MET	C-N	6.33	1.41	1.34
1	A	1181	MET	C-N	6.31	1.41	1.34
1	C	1181	MET	C-N	6.31	1.41	1.34
1	B	1181	MET	C-N	6.28	1.41	1.34
1	A	1138	ASN	C-N	-6.28	1.25	1.33
1	C	1138	ASN	C-N	-6.28	1.25	1.33
1	B	1138	ASN	C-N	-6.19	1.25	1.33
1	D	1138	ASN	C-N	-6.19	1.25	1.33
1	A	999	CYS	C-N	-5.82	1.26	1.33
1	D	999	CYS	C-N	-5.82	1.26	1.33
1	C	999	CYS	C-N	-5.74	1.26	1.33
1	B	999	CYS	C-N	-5.73	1.26	1.33

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1162	THR	O-C-N	-17.22	102.14	122.11
1	B	1162	THR	O-C-N	-17.22	102.14	122.11
1	C	1162	THR	O-C-N	-17.20	102.15	122.11
1	D	1162	THR	O-C-N	-17.19	102.17	122.11
1	D	1164	HIS	O-C-N	9.19	132.67	122.20
1	A	1164	HIS	O-C-N	9.15	132.63	122.20
1	B	1164	HIS	O-C-N	9.15	132.63	122.20
1	C	1164	HIS	O-C-N	9.15	132.63	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	977	PHE	N-CA-C	-8.94	102.08	113.16
1	D	977	PHE	N-CA-C	-8.94	102.08	113.16
1	C	977	PHE	N-CA-C	-8.92	102.10	113.16
1	B	977	PHE	N-CA-C	-8.91	102.11	113.16
1	D	1163	PHE	CA-C-N	-8.45	108.04	120.38
1	D	1163	PHE	C-N-CA	-8.45	108.04	120.38
1	B	1163	PHE	CA-C-N	-8.43	108.07	120.38
1	B	1163	PHE	C-N-CA	-8.43	108.07	120.38
1	C	1163	PHE	CA-C-N	-8.43	108.07	120.38
1	C	1163	PHE	C-N-CA	-8.43	108.07	120.38
1	A	1163	PHE	CA-C-N	-8.43	108.08	120.38
1	A	1163	PHE	C-N-CA	-8.43	108.08	120.38
1	A	922	ARG	O-C-N	-8.26	112.55	122.22
1	B	922	ARG	O-C-N	-8.26	112.55	122.22
1	D	922	ARG	O-C-N	-8.26	112.56	122.22
1	C	922	ARG	O-C-N	-8.22	112.60	122.22
1	D	1128	LEU	O-C-N	-7.34	112.39	122.30
1	C	1128	LEU	O-C-N	-7.34	112.39	122.30
1	B	1128	LEU	O-C-N	-7.32	112.42	122.30
1	A	1128	LEU	O-C-N	-7.29	112.45	122.30
1	A	902	THR	N-CA-C	-7.08	105.57	114.56
1	D	902	THR	N-CA-C	-7.08	105.57	114.56
1	B	902	THR	N-CA-C	-7.06	105.59	114.56
1	C	902	THR	N-CA-C	-7.05	105.60	114.56
1	A	1162	THR	CA-C-N	6.26	132.09	121.14
1	A	1162	THR	C-N-CA	6.26	132.09	121.14
1	B	1162	THR	CA-C-N	6.26	132.09	121.14
1	B	1162	THR	C-N-CA	6.26	132.09	121.14
1	C	1162	THR	CA-C-N	6.26	132.09	121.14
1	C	1162	THR	C-N-CA	6.26	132.09	121.14
1	D	1162	THR	CA-C-N	6.25	132.08	121.14
1	D	1162	THR	C-N-CA	6.25	132.08	121.14
1	A	758	ALA	O-C-N	-6.17	115.14	123.15
1	D	758	ALA	O-C-N	-6.12	115.19	123.15
1	B	758	ALA	O-C-N	-6.12	115.20	123.15
1	C	758	ALA	O-C-N	-6.11	115.20	123.15
1	C	1063	TRP	N-CA-C	-6.09	105.11	112.54
1	D	1063	TRP	N-CA-C	-6.08	105.12	112.54
1	B	1063	TRP	N-CA-C	-6.04	105.17	112.54
1	A	1063	TRP	N-CA-C	-6.04	105.17	112.54
1	B	995	ARG	N-CA-C	-5.79	105.05	111.71
1	A	995	ARG	N-CA-C	-5.74	105.11	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	995	ARG	N-CA-C	-5.74	105.11	111.71
1	D	995	ARG	N-CA-C	-5.72	105.13	111.71
1	A	1180	THR	O-C-N	-5.61	115.36	122.27
1	C	1180	THR	O-C-N	-5.57	115.42	122.27
1	B	1180	THR	O-C-N	-5.56	115.43	122.27
1	D	1180	THR	O-C-N	-5.55	115.45	122.27
1	C	1163	PHE	N-CA-C	5.46	119.66	112.89
1	A	749	THR	N-CA-C	5.46	117.31	111.36
1	A	1163	PHE	N-CA-C	5.45	119.65	112.89
1	D	1163	PHE	N-CA-C	5.45	119.65	112.89
1	B	1163	PHE	N-CA-C	5.45	119.64	112.89
1	B	749	THR	N-CA-C	5.44	117.29	111.36
1	D	749	THR	N-CA-C	5.44	117.29	111.36
1	C	749	THR	N-CA-C	5.42	117.26	111.36
1	A	1031	ILE	CA-C-N	5.40	127.51	120.28
1	A	1031	ILE	C-N-CA	5.40	127.51	120.28
1	B	1031	ILE	CA-C-N	5.40	127.51	120.28
1	B	1031	ILE	C-N-CA	5.40	127.51	120.28
1	C	1031	ILE	CA-C-N	5.39	127.51	120.28
1	C	1031	ILE	C-N-CA	5.39	127.51	120.28
1	D	1031	ILE	CA-C-N	5.38	127.49	120.28
1	D	1031	ILE	C-N-CA	5.38	127.49	120.28
1	B	938	LEU	N-CA-C	-5.35	105.45	111.28
1	C	938	LEU	N-CA-C	-5.33	105.47	111.28
1	D	938	LEU	N-CA-C	-5.33	105.47	111.28
1	A	938	LEU	N-CA-C	-5.32	105.49	111.28
1	C	1138	ASN	N-CA-C	-5.21	107.57	114.04
1	A	1165	GLU	N-CA-C	5.21	119.48	113.18
1	B	1165	GLU	N-CA-C	5.21	119.48	113.18
1	A	1138	ASN	N-CA-C	-5.21	107.58	114.04
1	D	1165	GLU	N-CA-C	5.21	119.48	113.18
1	B	1138	ASN	N-CA-C	-5.20	107.59	114.04
1	C	1165	GLU	N-CA-C	5.19	119.46	113.18
1	C	1026	ILE	N-CA-C	-5.18	105.34	110.62
1	D	1138	ASN	N-CA-C	-5.18	107.62	114.04
1	A	1026	ILE	N-CA-C	-5.17	105.35	110.62
1	B	1026	ILE	N-CA-C	-5.16	105.36	110.62
1	D	1026	ILE	N-CA-C	-5.16	105.36	110.62
1	C	759	THR	CA-C-N	5.11	127.63	120.28
1	C	759	THR	C-N-CA	5.11	127.63	120.28
1	A	759	THR	CA-C-N	5.09	127.62	120.28
1	A	759	THR	C-N-CA	5.09	127.62	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	759	THR	CA-C-N	5.08	127.60	120.28
1	D	759	THR	C-N-CA	5.08	127.60	120.28
1	B	759	THR	CA-C-N	5.07	127.58	120.28
1	B	759	THR	C-N-CA	5.07	127.58	120.28
1	A	989	PRO	N-CA-C	-5.04	105.61	113.78
1	C	989	PRO	N-CA-C	-5.04	105.62	113.78
1	B	989	PRO	N-CA-C	-5.01	105.66	113.78
1	D	989	PRO	N-CA-C	-5.01	105.66	113.78
1	A	1129	LEU	CA-C-N	-5.00	113.61	120.46
1	A	1129	LEU	C-N-CA	-5.00	113.61	120.46

There are no chirality outliers.

There are no planarity outliers.

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	4791	0	4646	114	0
1	B	4791	0	4646	124	0
1	C	4791	0	4646	114	0
1	D	4791	0	4646	109	0
2	A	29	0	0	4	0
2	B	29	0	0	4	0
2	C	29	0	0	4	0
2	D	29	0	0	4	0
All	All	19280	0	18584	337	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 9.

All (337) 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:C:1268:LYS:HG3	1:D:1267:MET:SD	1.16	1.69
1:B:1268:LYS:HG3	1:C:1267:MET:SD	1.18	1.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:LYS:HG3	1:B:1267:MET:SD	1.18	1.65
1:A:1267:MET:CE	1:D:1268:LYS:HA	1.25	1.61
1:C:1268:LYS:HA	1:D:1267:MET:CE	1.24	1.59
1:A:1268:LYS:HA	1:B:1267:MET:CE	1.27	1.56
1:B:1268:LYS:HA	1:C:1267:MET:CE	1.27	1.55
1:D:901:TYR:CB	1:D:1166:ARG:HH12	1.26	1.48
1:C:1268:LYS:CG	1:D:1267:MET:SD	2.02	1.47
1:A:1054:ILE:CG1	1:B:999:CYS:SG	2.03	1.47
1:A:901:TYR:CB	1:A:1166:ARG:HH12	1.26	1.46
1:C:901:TYR:CB	1:C:1166:ARG:HH12	1.26	1.46
1:A:1268:LYS:CG	1:B:1267:MET:SD	2.04	1.45
1:B:901:TYR:CB	1:B:1166:ARG:HH12	1.26	1.45
1:B:1054:ILE:CG1	1:C:999:CYS:SG	2.04	1.43
1:B:1268:LYS:CG	1:C:1267:MET:SD	2.04	1.43
1:A:1054:ILE:HD11	1:B:999:CYS:SG	1.66	1.35
1:B:1054:ILE:HD11	1:C:999:CYS:SG	1.64	1.35
1:B:1054:ILE:CD1	1:C:999:CYS:SG	2.18	1.30
1:A:1054:ILE:CD1	1:B:999:CYS:SG	2.18	1.30
1:A:901:TYR:CB	1:A:1166:ARG:NH1	1.99	1.26
1:B:901:TYR:CB	1:B:1166:ARG:NH1	1.99	1.25
1:D:901:TYR:CB	1:D:1166:ARG:NH1	1.99	1.23
1:C:901:TYR:CB	1:C:1166:ARG:NH1	1.99	1.22
1:C:1268:LYS:CA	1:D:1267:MET:CE	2.17	1.22
1:C:1268:LYS:CA	1:D:1267:MET:HE2	1.70	1.20
1:A:1268:LYS:CA	1:B:1267:MET:CE	2.20	1.20
1:A:1267:MET:CE	1:D:1268:LYS:CA	2.17	1.19
1:A:1268:LYS:CA	1:B:1267:MET:HE2	1.72	1.19
1:B:1268:LYS:CA	1:C:1267:MET:CE	2.20	1.18
1:B:1268:LYS:CA	1:C:1267:MET:HE2	1.72	1.18
1:A:1268:LYS:HA	1:B:1267:MET:HE1	1.24	1.18
1:A:1267:MET:HE2	1:D:1268:LYS:CA	1.70	1.17
1:B:1053:ALA:O	1:C:995:ARG:NH2	1.79	1.15
1:C:1053:ALA:O	1:D:995:ARG:NH2	1.78	1.15
1:A:995:ARG:NH2	1:D:1053:ALA:O	1.80	1.14
1:A:1053:ALA:O	1:B:995:ARG:NH2	1.81	1.13
1:A:1267:MET:HE1	1:D:1268:LYS:HA	1.21	1.12
1:C:1268:LYS:HA	1:D:1267:MET:HE1	1.23	1.12
1:B:1268:LYS:HA	1:C:1267:MET:HE1	1.26	1.12
1:A:1054:ILE:HG13	1:B:999:CYS:SG	1.87	1.10
1:B:1054:ILE:HG13	1:C:999:CYS:SG	1.89	1.10
1:A:1054:ILE:HG12	1:B:999:CYS:SG	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:ILE:HG12	1:C:999:CYS:SG	1.89	1.02
1:C:1268:LYS:CB	1:D:1267:MET:SD	2.56	0.94
1:C:1268:LYS:HA	1:D:1267:MET:HE2	0.94	0.93
1:B:1268:LYS:HA	1:C:1267:MET:HE2	0.94	0.93
1:A:1268:LYS:HA	1:B:1267:MET:HE2	0.96	0.93
1:A:1267:MET:HE2	1:D:1268:LYS:HA	0.95	0.92
1:A:1268:LYS:CB	1:B:1267:MET:SD	2.59	0.91
1:B:1268:LYS:CB	1:C:1267:MET:SD	2.58	0.90
1:A:1019:LEU:HD21	1:D:1035:TYR:HD1	1.37	0.89
1:A:1035:TYR:HD1	1:B:1019:LEU:HD21	1.37	0.87
1:C:1035:TYR:HD1	1:D:1019:LEU:HD21	1.37	0.87
1:C:1109:THR:CG2	1:D:992:SER:HB2	2.06	0.86
1:B:1035:TYR:HD1	1:C:1019:LEU:HD21	1.38	0.85
1:B:1109:THR:CG2	1:C:992:SER:HB2	2.06	0.85
1:A:1012:ILE:HG12	2:A:1401:A1EA5:C06	2.07	0.85
1:C:1012:ILE:HG12	2:C:1401:A1EA5:C06	2.07	0.85
1:B:1012:ILE:HG12	2:B:1401:A1EA5:C06	2.07	0.85
1:D:1012:ILE:HG12	2:D:1401:A1EA5:C06	2.07	0.84
1:A:1109:THR:CG2	1:B:992:SER:HB2	2.08	0.83
1:A:992:SER:HB2	1:D:1109:THR:CG2	2.08	0.82
1:A:1025:MET:SD	1:D:1132:LEU:HD11	2.22	0.80
1:C:1109:THR:HG23	1:D:992:SER:HB2	1.64	0.78
1:C:1132:LEU:HD11	1:D:1025:MET:SD	2.24	0.78
1:A:992:SER:HB2	1:D:1109:THR:HG23	1.66	0.78
1:A:1019:LEU:HD21	1:D:1035:TYR:CD1	2.19	0.77
1:A:1035:TYR:CD1	1:B:1019:LEU:HD21	2.19	0.77
1:B:1109:THR:HG23	1:C:992:SER:HB2	1.66	0.77
1:D:938:LEU:HD11	2:D:1401:A1EA5:S23	2.25	0.77
1:C:938:LEU:HD11	2:C:1401:A1EA5:S23	2.25	0.77
1:C:1035:TYR:CD1	1:D:1019:LEU:HD21	2.19	0.77
1:A:1132:LEU:HD11	1:B:1025:MET:SD	2.25	0.77
1:A:938:LEU:HD11	2:A:1401:A1EA5:S23	2.25	0.76
1:B:1035:TYR:CD1	1:C:1019:LEU:HD21	2.20	0.75
1:B:938:LEU:HD11	2:B:1401:A1EA5:S23	2.25	0.75
1:A:995:ARG:HH12	1:D:1057:PRO:HA	1.51	0.74
1:B:1132:LEU:HD11	1:C:1025:MET:SD	2.27	0.74
1:A:1109:THR:HG23	1:B:992:SER:HB2	1.68	0.74
1:A:1137:PHE:O	1:D:1135:ALA:HB2	1.88	0.73
1:C:1057:PRO:HA	1:D:995:ARG:HH12	1.54	0.72
1:A:1135:ALA:HB2	1:B:1137:PHE:O	1.89	0.72
1:C:1135:ALA:HB2	1:D:1137:PHE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:PRO:HA	1:B:995:ARG:HH12	1.54	0.71
1:B:1008:ARG:O	1:B:1009:LEU:C	2.34	0.70
1:B:1135:ALA:HB2	1:C:1137:PHE:O	1.92	0.70
1:C:1008:ARG:O	1:C:1009:LEU:C	2.34	0.70
1:D:1008:ARG:O	1:D:1009:LEU:C	2.34	0.70
1:B:1057:PRO:HA	1:C:995:ARG:HH12	1.58	0.67
1:A:1008:ARG:O	1:A:1009:LEU:C	2.34	0.67
1:C:977:PHE:HB2	1:C:1001:ASN:HD21	1.61	0.66
1:B:1109:THR:HG21	1:C:992:SER:HB2	1.76	0.66
1:A:977:PHE:HB2	1:A:1001:ASN:HD21	1.61	0.66
1:C:1268:LYS:CA	1:D:1267:MET:HE1	2.07	0.66
1:C:1109:THR:HG21	1:D:992:SER:HB2	1.76	0.65
1:D:977:PHE:HB2	1:D:1001:ASN:HD21	1.61	0.65
1:B:977:PHE:HB2	1:B:1001:ASN:HD21	1.61	0.65
1:A:1109:THR:HG21	1:B:992:SER:HB2	1.78	0.65
1:C:901:TYR:CB	1:C:1166:ARG:CZ	2.76	0.64
1:A:1267:MET:HE1	1:D:1268:LYS:CA	2.05	0.64
1:A:992:SER:HB2	1:D:1109:THR:HG21	1.78	0.63
1:D:901:TYR:CB	1:D:1166:ARG:CZ	2.76	0.63
1:A:977:PHE:HB2	1:A:1001:ASN:ND2	2.14	0.63
1:C:977:PHE:HB2	1:C:1001:ASN:ND2	2.14	0.63
1:B:901:TYR:CB	1:B:1166:ARG:CZ	2.76	0.62
1:D:977:PHE:HB2	1:D:1001:ASN:ND2	2.14	0.62
1:C:1268:LYS:CB	1:D:1267:MET:CE	2.78	0.62
1:A:901:TYR:CB	1:A:1166:ARG:CZ	2.76	0.62
1:B:900:PHE:HE2	1:B:1170:PRO:HD3	1.65	0.61
1:D:1009:LEU:O	1:D:1010:LEU:C	2.44	0.61
1:A:1009:LEU:O	1:A:1010:LEU:C	2.44	0.61
1:B:977:PHE:HB2	1:B:1001:ASN:ND2	2.14	0.61
1:A:900:PHE:HE2	1:A:1170:PRO:HD3	1.65	0.61
1:A:1268:LYS:CB	1:B:1267:MET:CE	2.79	0.60
1:A:1138:ASN:OD1	1:D:1138:ASN:OD1	2.19	0.60
1:C:900:PHE:HE2	1:C:1170:PRO:HD3	1.65	0.60
1:C:1009:LEU:O	1:C:1010:LEU:C	2.44	0.60
1:A:887:ILE:O	1:A:890:PHE:N	2.35	0.60
1:B:1009:LEU:O	1:B:1010:LEU:C	2.44	0.60
1:D:900:PHE:HE2	1:D:1170:PRO:HD3	1.65	0.60
1:C:887:ILE:O	1:C:890:PHE:N	2.35	0.60
1:B:887:ILE:O	1:B:890:PHE:N	2.35	0.59
1:A:932:ILE:HD12	1:A:981:MET:HG3	1.85	0.59
1:B:1138:ASN:OD1	1:C:1138:ASN:OD1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:PHE:O	1:D:1135:ALA:CB	2.50	0.59
1:A:1138:ASN:OD1	1:B:1138:ASN:OD1	2.20	0.58
1:B:1268:LYS:CB	1:C:1267:MET:CE	2.81	0.58
1:C:1138:ASN:OD1	1:D:1138:ASN:OD1	2.20	0.58
1:B:932:ILE:HD12	1:B:981:MET:HG3	1.85	0.58
1:D:887:ILE:O	1:D:890:PHE:N	2.35	0.58
1:B:1268:LYS:CA	1:C:1267:MET:HE1	2.10	0.58
1:D:932:ILE:HD12	1:D:981:MET:HG3	1.85	0.58
1:A:1135:ALA:CB	1:B:1137:PHE:O	2.51	0.58
1:A:520:VAL:HG23	1:A:521:LEU:HG	1.86	0.58
1:C:1004:TYR:HA	1:C:1007:ILE:HG22	1.86	0.58
1:C:1135:ALA:CB	1:D:1137:PHE:O	2.52	0.58
1:C:932:ILE:HD12	1:C:981:MET:HG3	1.85	0.58
1:B:520:VAL:HG23	1:B:521:LEU:HG	1.86	0.57
1:C:520:VAL:HG23	1:C:521:LEU:HG	1.86	0.57
1:A:995:ARG:NH1	1:D:1057:PRO:HA	2.19	0.57
1:A:1268:LYS:CD	1:B:1267:MET:SD	2.89	0.57
1:C:659:PHE:HB3	1:C:662:HIS:HD2	1.70	0.57
1:A:1268:LYS:CA	1:B:1267:MET:HE1	2.08	0.57
1:D:520:VAL:HG23	1:D:521:LEU:HG	1.86	0.57
1:D:1004:TYR:HA	1:D:1007:ILE:HG22	1.86	0.57
1:A:659:PHE:HB3	1:A:662:HIS:HD2	1.70	0.57
1:A:1004:TYR:HA	1:A:1007:ILE:HG22	1.86	0.56
1:B:1135:ALA:CB	1:C:1137:PHE:O	2.53	0.56
1:B:659:PHE:HB3	1:B:662:HIS:HD2	1.70	0.56
1:B:932:ILE:HG23	1:B:981:MET:HE2	1.88	0.56
1:C:932:ILE:HG23	1:C:981:MET:HE2	1.88	0.56
1:B:1004:TYR:HA	1:B:1007:ILE:HG22	1.86	0.56
1:D:932:ILE:HG23	1:D:981:MET:HE2	1.88	0.56
1:A:932:ILE:HG23	1:A:981:MET:HE2	1.88	0.56
1:D:900:PHE:CE2	1:D:1170:PRO:HD3	2.41	0.56
1:C:900:PHE:CE2	1:C:1170:PRO:HD3	2.41	0.56
1:C:804:ILE:HD13	1:C:900:PHE:HB2	1.89	0.55
1:D:659:PHE:HB3	1:D:662:HIS:HD2	1.70	0.55
1:A:900:PHE:CE2	1:A:1170:PRO:HD3	2.41	0.55
1:D:804:ILE:HD13	1:D:900:PHE:HB2	1.89	0.55
1:A:993:ASP:O	1:A:996:VAL:HB	2.07	0.55
1:A:1141:PHE:CE1	1:D:1136:VAL:HG12	2.42	0.55
1:B:900:PHE:CE2	1:B:1170:PRO:HD3	2.41	0.55
1:B:804:ILE:HD13	1:B:900:PHE:HB2	1.89	0.55
1:C:1268:LYS:CD	1:D:1267:MET:SD	2.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:993:ASP:O	1:D:996:VAL:HB	2.07	0.54
1:A:804:ILE:HD13	1:A:900:PHE:HB2	1.89	0.54
1:C:993:ASP:O	1:C:996:VAL:HB	2.07	0.54
1:B:993:ASP:O	1:B:996:VAL:HB	2.07	0.54
1:A:1170:PRO:HG2	1:A:1173:LEU:HB2	1.90	0.54
1:C:1170:PRO:HG2	1:C:1173:LEU:HB2	1.90	0.54
1:B:978:SER:O	1:B:979:VAL:C	2.50	0.53
1:B:1170:PRO:HG2	1:B:1173:LEU:HB2	1.90	0.53
1:D:1170:PRO:HG2	1:D:1173:LEU:HB2	1.90	0.53
1:A:1057:PRO:HA	1:B:995:ARG:NH1	2.22	0.53
1:A:667:TRP:NE1	1:A:671:MET:SD	2.82	0.53
1:C:581:ILE:HG21	1:C:605:ARG:HH12	1.74	0.52
1:D:978:SER:O	1:D:979:VAL:C	2.50	0.52
1:C:1057:PRO:HA	1:D:995:ARG:NH1	2.21	0.52
1:A:581:ILE:HG21	1:A:605:ARG:HH12	1.74	0.52
1:D:667:TRP:NE1	1:D:671:MET:SD	2.82	0.52
1:C:1136:VAL:HG12	1:D:1141:PHE:CE1	2.44	0.52
1:B:667:TRP:NE1	1:B:671:MET:SD	2.82	0.52
1:A:978:SER:O	1:A:979:VAL:C	2.50	0.52
1:B:581:ILE:HG21	1:B:605:ARG:HH12	1.74	0.52
1:B:1133:LEU:HD11	1:B:1137:PHE:CZ	2.45	0.52
1:C:1133:LEU:HD11	1:C:1137:PHE:CZ	2.45	0.52
1:C:667:TRP:NE1	1:C:671:MET:SD	2.82	0.52
1:A:1136:VAL:HG12	1:B:1141:PHE:CE1	2.44	0.51
1:D:1133:LEU:HD11	1:D:1137:PHE:CZ	2.45	0.51
1:D:581:ILE:HG21	1:D:605:ARG:HH12	1.74	0.51
1:B:1268:LYS:CD	1:C:1267:MET:SD	2.92	0.51
1:A:1133:LEU:HD11	1:A:1137:PHE:CZ	2.45	0.51
1:C:978:SER:O	1:C:979:VAL:C	2.50	0.50
1:A:1136:VAL:O	1:A:1137:PHE:HD1	1.95	0.50
1:B:1136:VAL:HG12	1:C:1141:PHE:CE1	2.47	0.50
1:C:1136:VAL:O	1:C:1137:PHE:HD1	1.95	0.50
1:D:606:THR:O	1:D:609:HIS:ND1	2.35	0.50
1:B:1136:VAL:O	1:B:1137:PHE:HD1	1.95	0.49
1:B:885:ARG:C	1:B:887:ILE:N	2.69	0.49
1:A:1012:ILE:HA	2:A:1401:A1EA5:C26	2.42	0.49
1:C:606:THR:O	1:C:609:HIS:ND1	2.35	0.49
1:C:595:TYR:CE1	1:C:756:SER:HB3	2.48	0.49
1:B:595:TYR:CE1	1:B:756:SER:HB3	2.48	0.49
1:B:1012:ILE:HA	2:B:1401:A1EA5:C26	2.42	0.49
1:D:1012:ILE:HA	2:D:1401:A1EA5:C26	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TYR:CE1	1:A:756:SER:HB3	2.48	0.49
1:C:1008:ARG:C	1:C:1010:LEU:N	2.70	0.49
1:B:922:ARG:HA	1:B:991:ARG:HH12	1.78	0.49
1:B:606:THR:O	1:B:609:HIS:ND1	2.35	0.49
1:C:922:ARG:HA	1:C:991:ARG:HH12	1.78	0.49
1:C:1012:ILE:HA	2:C:1401:A1EA5:C26	2.42	0.49
1:D:1008:ARG:C	1:D:1010:LEU:N	2.70	0.49
1:B:556:PRO:HD3	1:B:673:ARG:HH21	1.78	0.48
1:B:1057:PRO:HA	1:C:995:ARG:NH1	2.25	0.48
1:C:556:PRO:HD3	1:C:673:ARG:HH21	1.78	0.48
1:A:922:ARG:HA	1:A:991:ARG:HH12	1.78	0.48
1:D:1136:VAL:O	1:D:1137:PHE:HD1	1.95	0.48
1:A:606:THR:O	1:A:609:HIS:ND1	2.35	0.48
1:D:922:ARG:HA	1:D:991:ARG:HH12	1.78	0.48
1:D:595:TYR:CE1	1:D:756:SER:HB3	2.48	0.48
1:A:556:PRO:HD3	1:A:673:ARG:HH21	1.78	0.48
1:D:977:PHE:O	1:D:977:PHE:CD1	2.67	0.47
1:A:1118:MET:O	1:A:1121:TYR:HB3	2.15	0.47
1:B:1036:PHE:HE2	1:B:1136:VAL:HG21	1.79	0.47
1:B:1118:MET:O	1:B:1121:TYR:HB3	2.14	0.47
1:D:556:PRO:HD3	1:D:673:ARG:HH21	1.78	0.47
1:B:977:PHE:O	1:B:977:PHE:CD1	2.67	0.47
1:D:1036:PHE:HE2	1:D:1136:VAL:HG21	1.79	0.47
1:A:977:PHE:CD1	1:A:977:PHE:O	2.67	0.47
1:C:977:PHE:CD1	1:C:977:PHE:O	2.67	0.47
1:D:975:LEU:HD23	1:D:975:LEU:HA	1.79	0.47
1:A:1036:PHE:HE2	1:A:1136:VAL:HG21	1.79	0.47
1:C:1118:MET:O	1:C:1121:TYR:HB3	2.15	0.47
1:C:1036:PHE:HE2	1:C:1136:VAL:HG21	1.79	0.47
1:D:1118:MET:O	1:D:1121:TYR:HB3	2.15	0.47
1:B:1008:ARG:C	1:B:1010:LEU:N	2.70	0.46
1:A:1008:ARG:C	1:A:1010:LEU:N	2.70	0.46
1:C:1268:LYS:HB2	1:D:1267:MET:SD	2.51	0.46
1:A:917:LEU:HB3	1:D:1065:LEU:HD21	1.97	0.46
1:D:885:ARG:C	1:D:887:ILE:N	2.69	0.46
1:A:1035:TYR:CD1	1:B:1019:LEU:CD2	2.96	0.46
1:A:1053:ALA:O	1:B:995:ARG:CZ	2.60	0.46
1:D:913:ASN:OD1	1:D:1002:ILE:HD11	2.16	0.46
1:D:1007:ILE:HD12	1:D:1007:ILE:HA	1.78	0.46
1:C:913:ASN:OD1	1:C:1002:ILE:HD11	2.16	0.46
1:A:1127:ILE:O	1:A:1131:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:ASN:OD1	1:B:1002:ILE:HD11	2.16	0.46
1:A:885:ARG:C	1:A:887:ILE:N	2.69	0.45
1:A:913:ASN:OD1	1:A:1002:ILE:HD11	2.16	0.45
1:C:1127:ILE:O	1:C:1131:ASN:ND2	2.49	0.45
1:C:1133:LEU:HD11	1:C:1137:PHE:CE2	2.52	0.45
1:B:996:VAL:O	1:B:999:CYS:HB3	2.16	0.45
1:A:996:VAL:O	1:A:999:CYS:HB3	2.16	0.45
1:B:1127:ILE:O	1:B:1131:ASN:ND2	2.49	0.45
1:D:1069:ILE:HD13	1:D:1069:ILE:HA	1.84	0.45
1:B:1133:LEU:HD11	1:B:1137:PHE:CE2	2.52	0.45
1:C:996:VAL:O	1:C:999:CYS:HB3	2.16	0.45
1:D:996:VAL:O	1:D:999:CYS:HB3	2.16	0.45
1:A:1267:MET:HE2	1:D:1268:LYS:N	2.26	0.45
1:D:1133:LEU:HD11	1:D:1137:PHE:CE2	2.52	0.45
1:A:906:ILE:HD13	1:A:906:ILE:HA	1.90	0.44
1:A:975:LEU:O	1:A:978:SER:HB3	2.18	0.44
1:C:885:ARG:C	1:C:887:ILE:N	2.69	0.44
1:A:975:LEU:HD23	1:A:975:LEU:HA	1.79	0.44
1:C:1065:LEU:HD21	1:D:917:LEU:HB3	2.00	0.44
1:D:975:LEU:O	1:D:978:SER:HB3	2.18	0.44
1:D:1127:ILE:O	1:D:1131:ASN:ND2	2.49	0.44
1:A:883:LEU:C	1:A:885:ARG:H	2.26	0.44
1:A:1019:LEU:CD2	1:D:1035:TYR:CD1	2.96	0.44
1:C:1268:LYS:N	1:D:1267:MET:HE2	2.25	0.44
1:B:975:LEU:O	1:B:978:SER:HB3	2.18	0.44
1:B:1053:ALA:O	1:C:995:ARG:CZ	2.58	0.44
1:C:920:MET:SD	1:C:984:ARG:NH1	2.84	0.44
1:A:1133:LEU:HD11	1:A:1137:PHE:CE2	2.52	0.44
1:C:975:LEU:O	1:C:978:SER:HB3	2.18	0.44
1:C:1248:GLU:HA	1:C:1251:GLU:HG2	2.00	0.44
1:A:1065:LEU:HD21	1:B:917:LEU:HB3	2.00	0.44
1:B:1248:GLU:HA	1:B:1251:GLU:HG2	2.00	0.44
1:C:1035:TYR:CD1	1:D:1019:LEU:CD2	2.96	0.43
1:A:1268:LYS:HB2	1:B:1267:MET:SD	2.53	0.43
1:A:1248:GLU:HA	1:A:1251:GLU:HG2	2.00	0.43
1:D:883:LEU:C	1:D:885:ARG:H	2.26	0.43
1:A:995:ARG:CZ	1:D:1053:ALA:O	2.59	0.43
1:C:1053:ALA:O	1:D:995:ARG:CZ	2.57	0.43
1:D:920:MET:SD	1:D:984:ARG:NH1	2.85	0.43
1:A:1268:LYS:N	1:B:1267:MET:HE2	2.28	0.43
1:B:883:LEU:C	1:B:885:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:ILE:HD13	1:B:1069:ILE:HA	1.84	0.43
1:D:1248:GLU:HA	1:D:1251:GLU:HG2	2.00	0.43
1:B:885:ARG:O	1:B:886:LYS:C	2.61	0.43
1:A:935:ILE:HD13	1:A:935:ILE:HA	1.87	0.43
1:B:920:MET:SD	1:B:984:ARG:NH1	2.84	0.43
1:C:885:ARG:O	1:C:886:LYS:C	2.61	0.43
1:C:975:LEU:HD23	1:C:975:LEU:HA	1.79	0.42
1:C:1162:THR:HG21	2:C:1401:A1EA5:C27	2.49	0.42
1:B:975:LEU:HD23	1:B:975:LEU:HA	1.79	0.42
1:C:1254:SER:HB3	1:D:1253:MET:SD	2.59	0.42
1:B:1268:LYS:N	1:C:1267:MET:HE2	2.27	0.42
1:C:883:LEU:C	1:C:885:ARG:H	2.26	0.42
1:D:896:VAL:O	1:D:897:LYS:C	2.63	0.42
1:B:896:VAL:O	1:B:897:LYS:C	2.62	0.42
1:C:906:ILE:HD13	1:C:906:ILE:HA	1.90	0.42
1:D:1162:THR:HG21	2:D:1401:A1EA5:C27	2.49	0.42
1:A:1162:THR:HG21	2:A:1401:A1EA5:C27	2.49	0.42
1:B:1162:THR:HG21	2:B:1401:A1EA5:C27	2.49	0.42
1:A:1268:LYS:CB	1:B:1267:MET:HE2	2.43	0.42
1:A:896:VAL:O	1:A:897:LYS:C	2.62	0.41
1:A:1067:LYS:HD2	1:A:1067:LYS:HA	1.97	0.41
1:A:1069:ILE:HD13	1:A:1069:ILE:HA	1.84	0.41
1:A:1253:MET:SD	1:D:1254:SER:HB3	2.60	0.41
1:B:928:GLU:OE1	1:B:984:ARG:NH2	2.54	0.41
1:C:928:GLU:OE1	1:C:984:ARG:NH2	2.53	0.41
1:A:885:ARG:O	1:A:886:LYS:C	2.61	0.41
1:A:928:GLU:OE1	1:A:984:ARG:NH2	2.54	0.41
1:D:885:ARG:O	1:D:886:LYS:C	2.61	0.41
1:D:906:ILE:HD13	1:D:906:ILE:HA	1.90	0.41
1:D:928:GLU:OE1	1:D:984:ARG:NH2	2.53	0.41
1:B:1065:LEU:HD21	1:C:917:LEU:HB3	2.03	0.41
1:C:1030:MET:O	1:C:1031:ILE:C	2.64	0.41
1:B:1268:LYS:HB2	1:C:1267:MET:SD	2.54	0.41
1:A:1253:MET:HE2	1:D:1250:VAL:HG13	2.03	0.41
1:B:581:ILE:HG21	1:B:605:ARG:NH1	2.36	0.41
1:D:923:TRP:HA	1:D:924:PRO:HD3	1.87	0.41
1:D:1010:LEU:O	1:D:1011:ASP:C	2.63	0.41
1:B:935:ILE:HD13	1:B:935:ILE:HA	1.87	0.41
1:C:896:VAL:O	1:C:897:LYS:C	2.63	0.41
1:A:887:ILE:O	1:A:888:TYR:C	2.63	0.40
1:A:1010:LEU:O	1:A:1011:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:LEU:HA	1:A:1136:VAL:HG22	2.03	0.40
1:B:552:THR:OG1	1:B:553:ARG:N	2.55	0.40
1:B:887:ILE:O	1:B:888:TYR:C	2.63	0.40
1:B:906:ILE:HD13	1:B:906:ILE:HA	1.90	0.40
1:B:977:PHE:O	1:B:977:PHE:CG	2.75	0.40
1:B:1254:SER:HB3	1:C:1253:MET:SD	2.61	0.40
1:D:1067:LYS:HD2	1:D:1067:LYS:HA	1.97	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	601/1610 (37%)	581 (97%)	20 (3%)	0	100	100
1	B	557/1610 (35%)	540 (97%)	17 (3%)	0	100	100
1	C	448/1610 (28%)	433 (97%)	15 (3%)	0	100	100
1	D	574/1610 (36%)	555 (97%)	19 (3%)	0	100	100
All	All	2180/6440 (34%)	2109 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	486/1398 (35%)	482 (99%)	4 (1%)	73	77
1	B	486/1398 (35%)	482 (99%)	4 (1%)	73	77
1	C	486/1398 (35%)	482 (99%)	4 (1%)	73	77
1	D	486/1398 (35%)	482 (99%)	4 (1%)	73	77
All	All	1944/5592 (35%)	1928 (99%)	16 (1%)	70	77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	909	LEU
1	A	931	VAL
1	A	932	ILE
1	A	1069	ILE
1	B	909	LEU
1	B	931	VAL
1	B	932	ILE
1	B	1069	ILE
1	C	909	LEU
1	C	931	VAL
1	C	932	ILE
1	C	1069	ILE
1	D	909	LEU
1	D	931	VAL
1	D	932	ILE
1	D	1069	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	GLN
1	A	662	HIS
1	A	683	HIS
1	A	719	ASN
1	A	757	ASN
1	A	769	HIS
1	A	988	GLN
1	A	1001	ASN
1	A	1138	ASN
1	A	1217	HIS
1	B	538	HIS

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Mol	Chain	Res	Type
1	B	662	HIS
1	B	683	HIS
1	B	757	ASN
1	B	769	HIS
1	B	988	GLN
1	B	1217	HIS
1	C	538	HIS
1	C	662	HIS
1	C	683	HIS
1	C	719	ASN
1	C	757	ASN
1	C	769	HIS
1	C	988	GLN
1	C	1138	ASN
1	C	1217	HIS
1	D	662	HIS
1	D	683	HIS
1	D	719	ASN
1	D	757	ASN
1	D	769	HIS
1	D	988	GLN
1	D	1217	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EA5	C	1401	-	30,32,32	2.73	7 (23%)	37,45,45	3.29	12 (32%)
2	A1EA5	B	1401	-	30,32,32	2.72	7 (23%)	37,45,45	3.30	12 (32%)
2	A1EA5	A	1401	-	30,32,32	2.72	7 (23%)	37,45,45	3.30	12 (32%)
2	A1EA5	D	1401	-	30,32,32	2.72	7 (23%)	37,45,45	3.29	12 (32%)

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
2	A1EA5	C	1401	-	-	6/17/37/37	1/4/4/4
2	A1EA5	B	1401	-	-	6/17/37/37	1/4/4/4
2	A1EA5	A	1401	-	-	6/17/37/37	1/4/4/4
2	A1EA5	D	1401	-	-	6/17/37/37	1/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	A1EA5	O24-C05	8.70	1.47	1.37
2	B	1401	A1EA5	O24-C05	8.70	1.47	1.37
2	C	1401	A1EA5	O24-C05	8.70	1.47	1.37
2	D	1401	A1EA5	O24-C05	8.70	1.47	1.37
2	A	1401	A1EA5	C08-N09	6.04	1.48	1.37
2	B	1401	A1EA5	C08-N09	6.04	1.48	1.37
2	C	1401	A1EA5	C08-N09	6.04	1.48	1.37
2	D	1401	A1EA5	C08-N09	6.04	1.48	1.37
2	C	1401	A1EA5	C25-N07	-5.50	1.38	1.47
2	A	1401	A1EA5	C25-N07	-5.48	1.38	1.47
2	B	1401	A1EA5	C25-N07	-5.48	1.38	1.47
2	D	1401	A1EA5	C25-N07	-5.44	1.38	1.47
2	C	1401	A1EA5	C08-N07	4.59	1.48	1.39
2	A	1401	A1EA5	C08-N07	4.55	1.48	1.39
2	B	1401	A1EA5	C08-N07	4.55	1.48	1.39
2	D	1401	A1EA5	C08-N07	4.53	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	A1EA5	O18-C08	-3.66	1.16	1.23
2	B	1401	A1EA5	O18-C08	-3.66	1.16	1.23
2	C	1401	A1EA5	O18-C08	-3.63	1.16	1.23
2	D	1401	A1EA5	O18-C08	-3.63	1.16	1.23
2	C	1401	A1EA5	C11-C10	-3.32	1.48	1.53
2	D	1401	A1EA5	C11-C10	-3.32	1.48	1.53
2	B	1401	A1EA5	C11-C10	-3.30	1.48	1.53
2	A	1401	A1EA5	C11-C10	-3.28	1.48	1.53
2	A	1401	A1EA5	C27-C10	2.28	1.56	1.53
2	D	1401	A1EA5	C27-C10	2.28	1.56	1.53
2	C	1401	A1EA5	C27-C10	2.26	1.56	1.53
2	B	1401	A1EA5	C27-C10	2.22	1.56	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	A1EA5	S23-C22-N21	-11.19	106.46	116.08
2	B	1401	A1EA5	S23-C22-N21	-11.19	106.46	116.08
2	C	1401	A1EA5	S23-C22-N21	-11.18	106.47	116.08
2	D	1401	A1EA5	S23-C22-N21	-11.17	106.48	116.08
2	B	1401	A1EA5	C17-C19-S23	9.57	129.03	116.57
2	A	1401	A1EA5	C17-C19-S23	9.56	129.02	116.57
2	C	1401	A1EA5	C17-C19-S23	9.54	128.98	116.57
2	D	1401	A1EA5	C17-C19-S23	9.54	128.98	116.57
2	B	1401	A1EA5	C22-S23-C19	8.20	98.08	89.55
2	C	1401	A1EA5	C22-S23-C19	8.20	98.08	89.55
2	A	1401	A1EA5	C22-S23-C19	8.19	98.07	89.55
2	D	1401	A1EA5	C22-S23-C19	8.19	98.07	89.55
2	B	1401	A1EA5	C26-O24-C05	-4.67	105.46	113.67
2	A	1401	A1EA5	C26-O24-C05	-4.66	105.47	113.67
2	D	1401	A1EA5	C26-O24-C05	-4.64	105.51	113.67
2	C	1401	A1EA5	C26-O24-C05	-4.63	105.52	113.67
2	A	1401	A1EA5	C22-N21-C20	4.19	115.42	110.71
2	B	1401	A1EA5	C22-N21-C20	4.19	115.42	110.71
2	C	1401	A1EA5	C22-N21-C20	4.14	115.37	110.71
2	D	1401	A1EA5	C22-N21-C20	4.14	115.37	110.71
2	B	1401	A1EA5	C11-C10-C15	3.83	111.58	109.04
2	C	1401	A1EA5	C11-C10-C15	3.81	111.57	109.04
2	D	1401	A1EA5	C11-C10-C15	3.81	111.57	109.04
2	A	1401	A1EA5	C11-C10-C15	3.74	111.53	109.04
2	D	1401	A1EA5	O16-C17-C19	-3.68	100.78	110.83
2	B	1401	A1EA5	O16-C17-C19	-3.68	100.79	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	A1EA5	O16-C17-C19	-3.67	100.82	110.83
2	A	1401	A1EA5	O16-C17-C19	-3.66	100.82	110.83
2	C	1401	A1EA5	O24-C05-C04	-3.07	116.25	122.07
2	D	1401	A1EA5	O24-C05-C04	-3.06	116.26	122.07
2	A	1401	A1EA5	O24-C05-C04	-3.06	116.27	122.07
2	B	1401	A1EA5	O24-C05-C04	-3.05	116.30	122.07
2	B	1401	A1EA5	O24-C05-C06	2.69	121.18	116.89
2	A	1401	A1EA5	O24-C05-C06	2.68	121.16	116.89
2	C	1401	A1EA5	O24-C05-C06	2.68	121.16	116.89
2	D	1401	A1EA5	O24-C05-C06	2.68	121.16	116.89
2	A	1401	A1EA5	C10-N09-C08	-2.25	120.41	125.18
2	C	1401	A1EA5	C10-N09-C08	-2.25	120.41	125.18
2	D	1401	A1EA5	C10-N09-C08	-2.25	120.41	125.18
2	B	1401	A1EA5	C10-N09-C08	-2.25	120.42	125.18
2	A	1401	A1EA5	C03-C04-N07	2.25	124.88	121.85
2	B	1401	A1EA5	C03-C04-N07	2.25	124.88	121.85
2	B	1401	A1EA5	C11-C12-C13	2.24	112.03	109.58
2	C	1401	A1EA5	C03-C04-N07	2.22	124.84	121.85
2	D	1401	A1EA5	C03-C04-N07	2.22	124.84	121.85
2	A	1401	A1EA5	C11-C12-C13	2.22	112.01	109.58
2	C	1401	A1EA5	C11-C12-C13	2.18	111.97	109.58
2	D	1401	A1EA5	C11-C12-C13	2.18	111.97	109.58

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	A1EA5	C15-C10-C27-O28
2	B	1401	A1EA5	C15-C10-C27-O28
2	C	1401	A1EA5	C15-C10-C27-O28
2	D	1401	A1EA5	C15-C10-C27-O28
2	A	1401	A1EA5	C01-C02-O16-C17
2	A	1401	A1EA5	C03-C02-O16-C17
2	B	1401	A1EA5	C01-C02-O16-C17
2	B	1401	A1EA5	C03-C02-O16-C17
2	C	1401	A1EA5	C01-C02-O16-C17
2	C	1401	A1EA5	C03-C02-O16-C17
2	D	1401	A1EA5	C01-C02-O16-C17
2	D	1401	A1EA5	C03-C02-O16-C17
2	A	1401	A1EA5	C19-C17-O16-C02
2	B	1401	A1EA5	C19-C17-O16-C02
2	C	1401	A1EA5	C19-C17-O16-C02

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Mol	Chain	Res	Type	Atoms
2	D	1401	A1EA5	C19-C17-O16-C02
2	A	1401	A1EA5	N09-C10-C27-O28
2	A	1401	A1EA5	C11-C10-C27-O28
2	B	1401	A1EA5	N09-C10-C27-O28
2	B	1401	A1EA5	C11-C10-C27-O28
2	C	1401	A1EA5	N09-C10-C27-O28
2	C	1401	A1EA5	C11-C10-C27-O28
2	D	1401	A1EA5	N09-C10-C27-O28
2	D	1401	A1EA5	C11-C10-C27-O28

All (4) ring outliers are listed below:

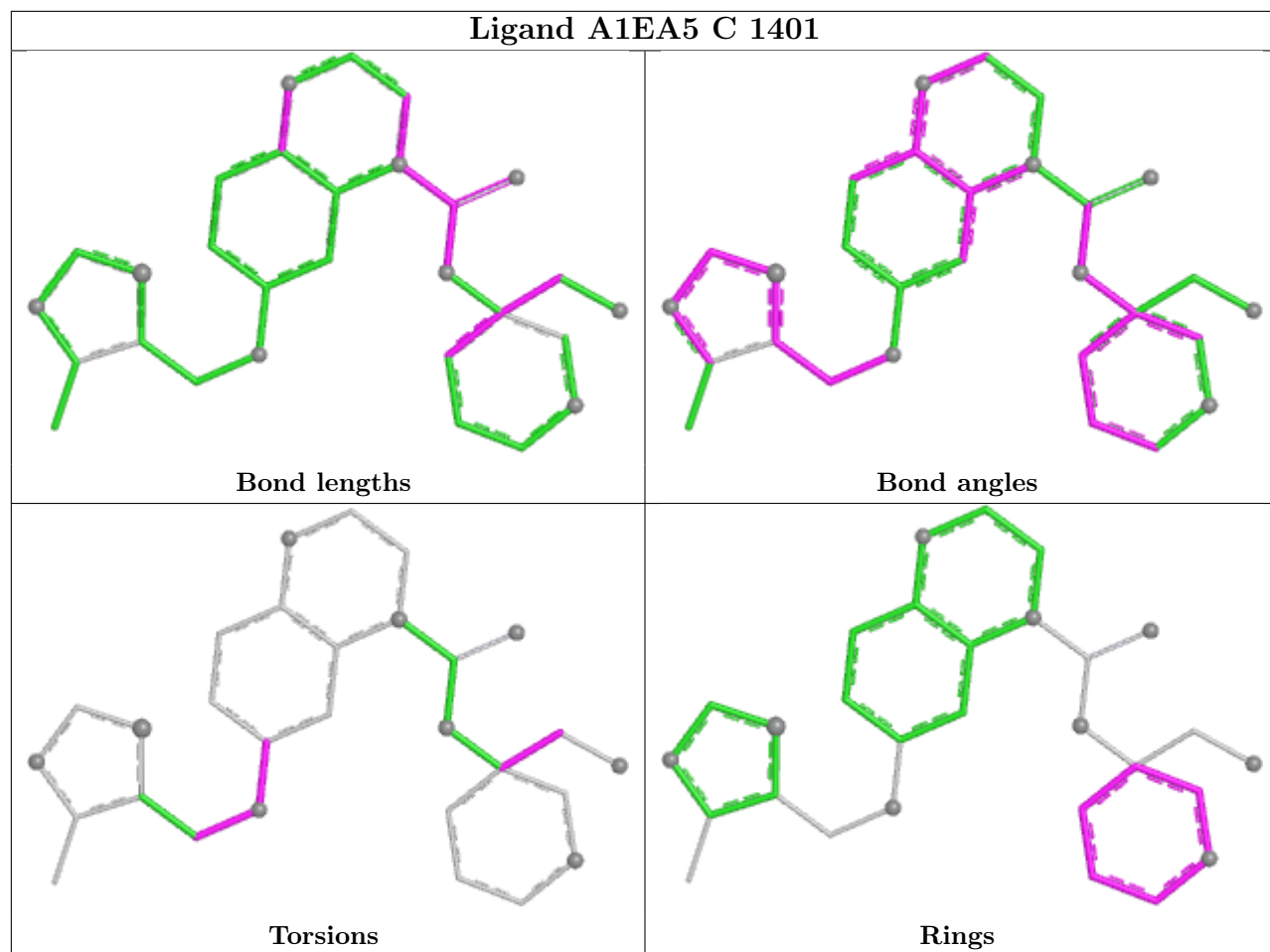
Mol	Chain	Res	Type	Atoms
2	C	1401	A1EA5	C10-C11-C12-C13-C15-N14
2	D	1401	A1EA5	C10-C11-C12-C13-C15-N14
2	A	1401	A1EA5	C10-C11-C12-C13-C15-N14
2	B	1401	A1EA5	C10-C11-C12-C13-C15-N14

4 monomers are involved in 16 short contacts:

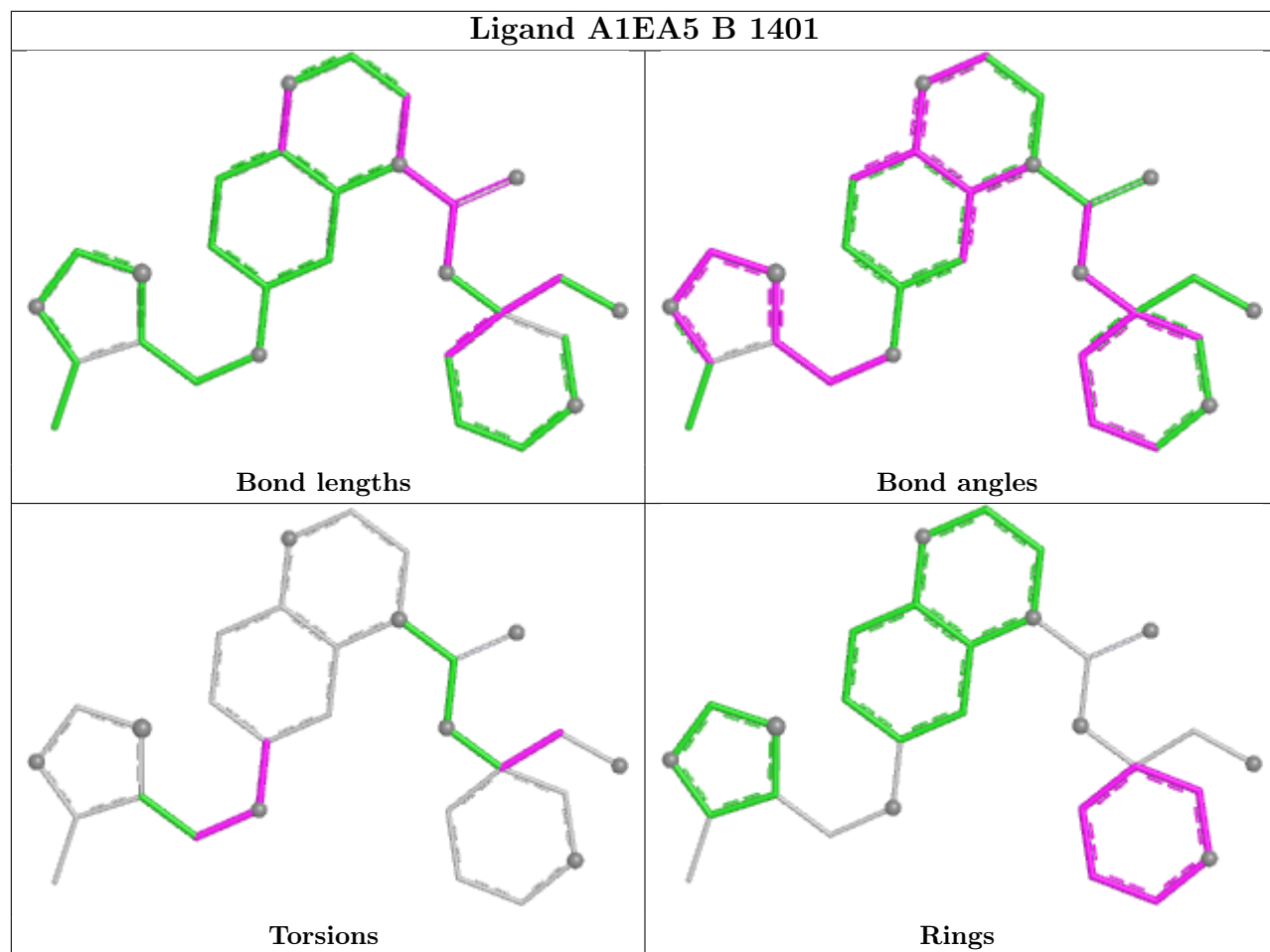
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1401	A1EA5	4	0
2	B	1401	A1EA5	4	0
2	A	1401	A1EA5	4	0
2	D	1401	A1EA5	4	0

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.

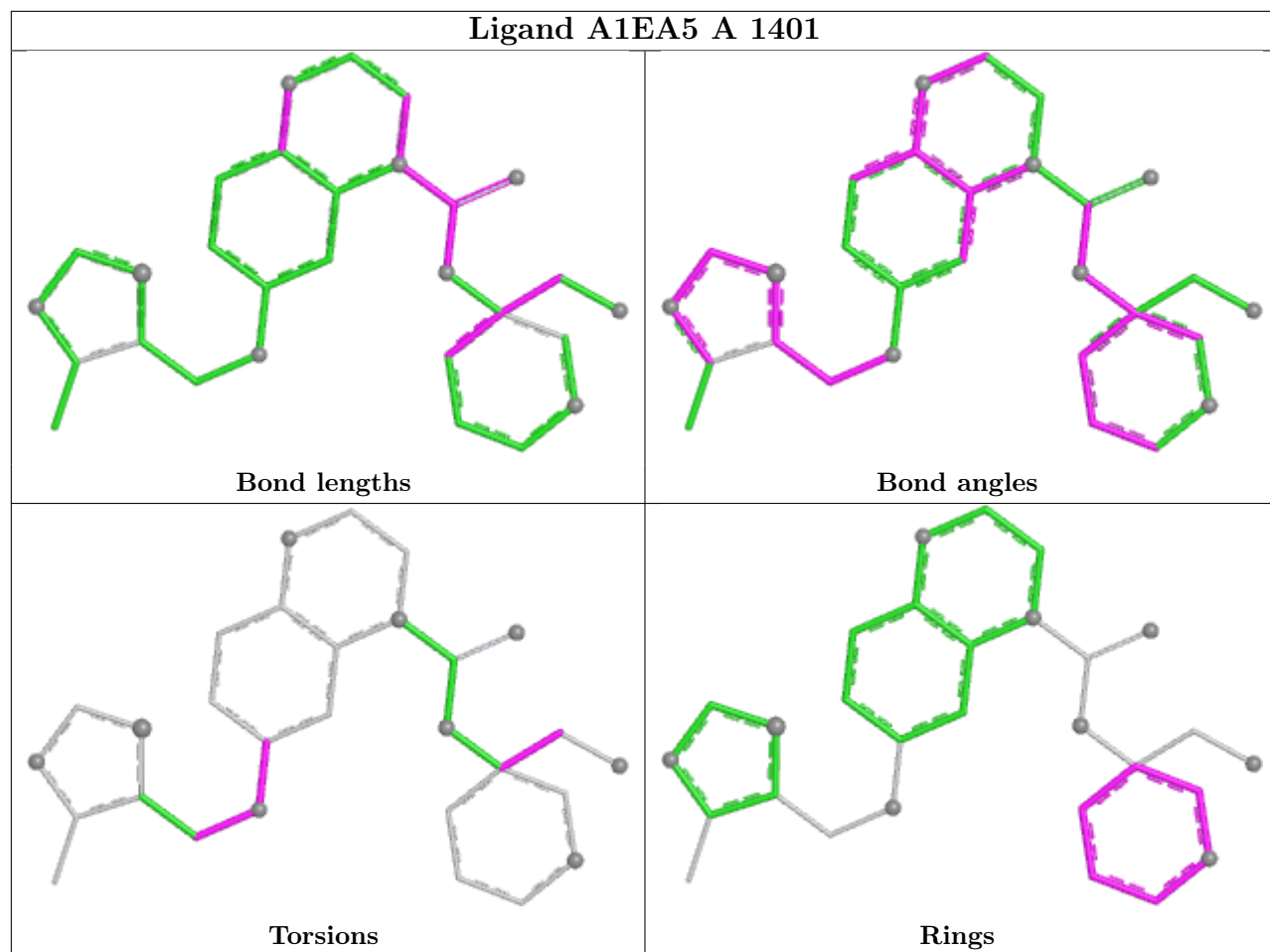
Ligand A1EA5 C 1401

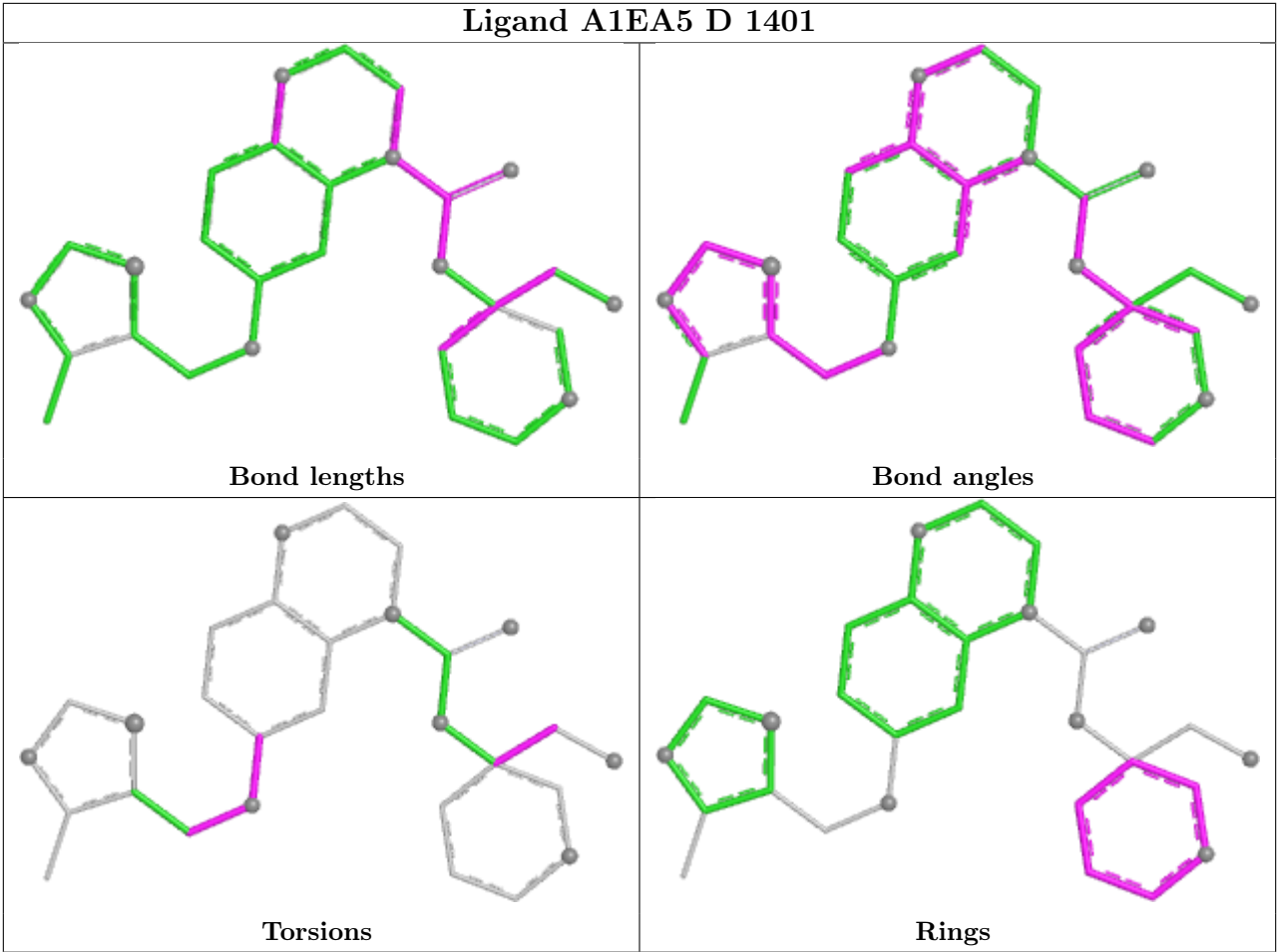


Ligand A1EA5 B 1401



Ligand A1EA5 A 1401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	3
1	C	3
1	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1128:LEU	C	1129:LEU	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1128:LEU	C	1129:LEU	N	1.20
1	C	1128:LEU	C	1129:LEU	N	1.20
1	D	1128:LEU	C	1129:LEU	N	1.20
1	A	922:ARG	C	923:TRP	N	1.17
1	B	922:ARG	C	923:TRP	N	1.17
1	C	922:ARG	C	923:TRP	N	1.17
1	D	922:ARG	C	923:TRP	N	1.17
1	D	1162:THR	C	1163:PHE	N	1.06
1	A	1162:THR	C	1163:PHE	N	1.05
1	B	1162:THR	C	1163:PHE	N	1.05
1	C	1162:THR	C	1163:PHE	N	1.05

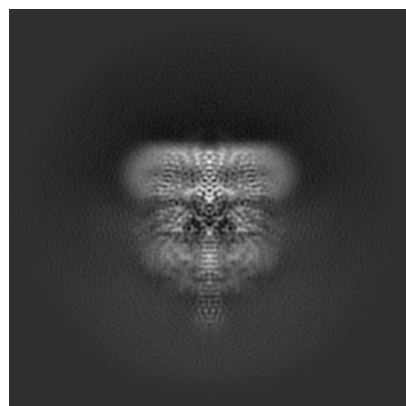
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61215. These allow visual inspection of the internal detail of the map and identification of artifacts.

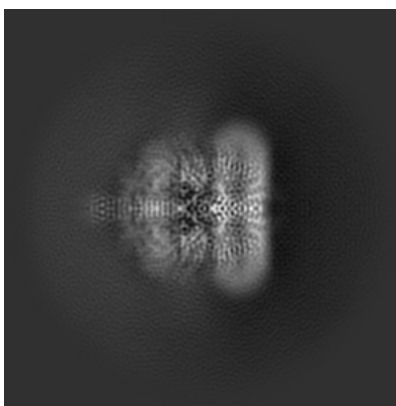
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

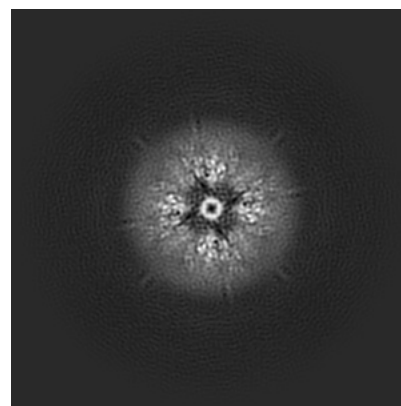
6.1.1 Primary map



X

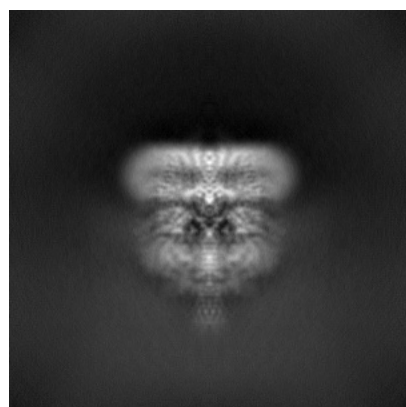


Y

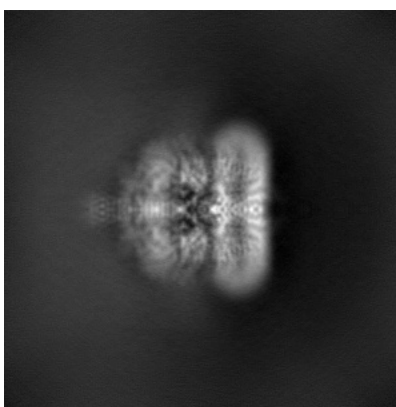


Z

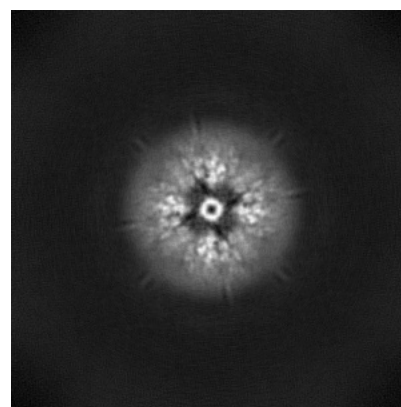
6.1.2 Raw map



X



Y

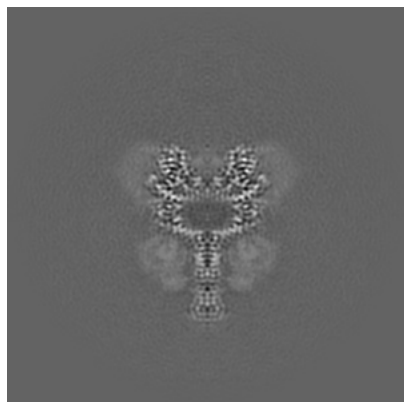


Z

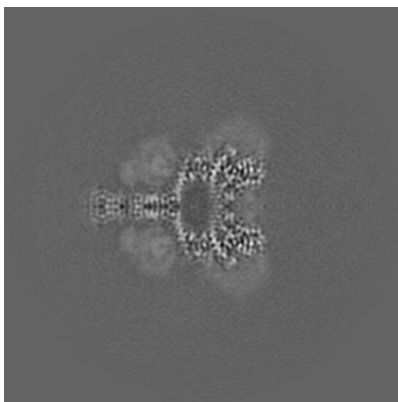
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

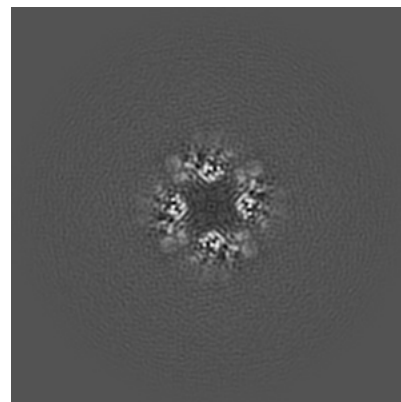
6.2.1 Primary map



X Index: 200

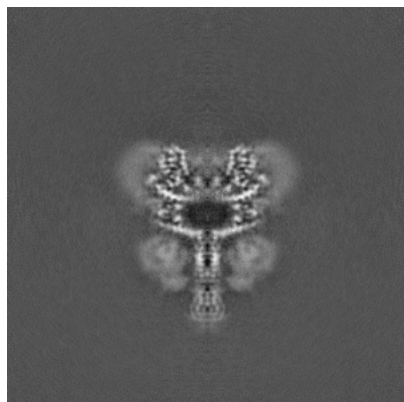


Y Index: 200

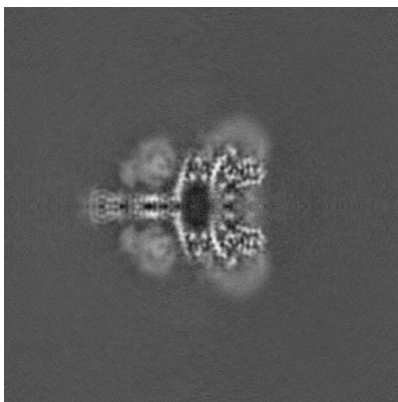


Z Index: 200

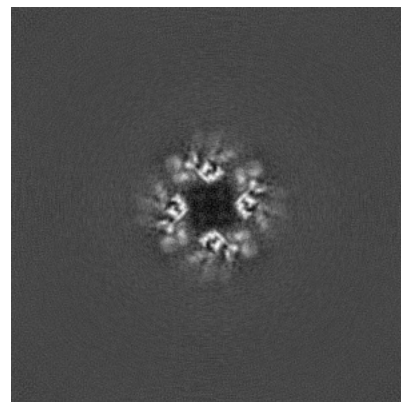
6.2.2 Raw map



X Index: 200



Y Index: 200

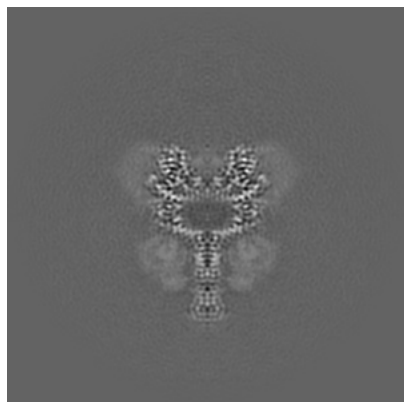


Z Index: 200

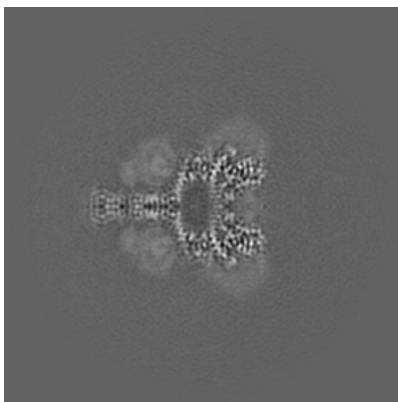
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

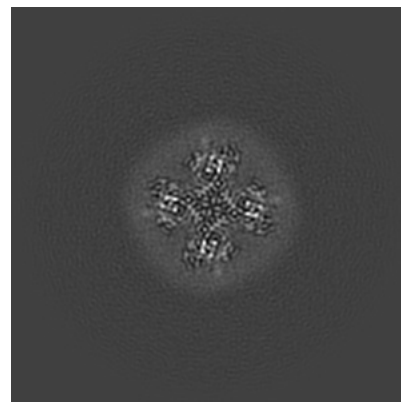
6.3.1 Primary map



X Index: 200

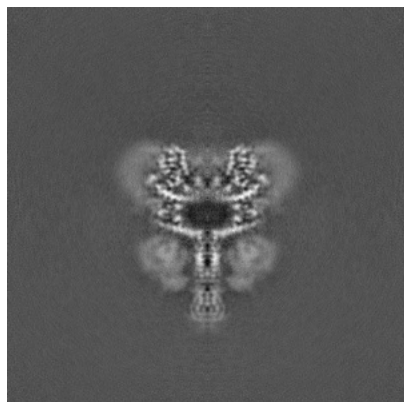


Y Index: 200

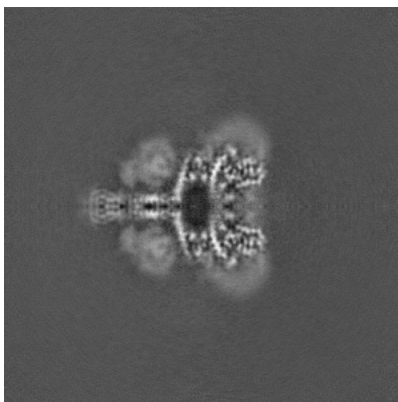


Z Index: 220

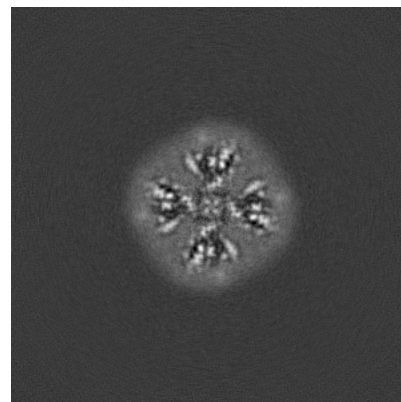
6.3.2 Raw map



X Index: 200



Y Index: 200

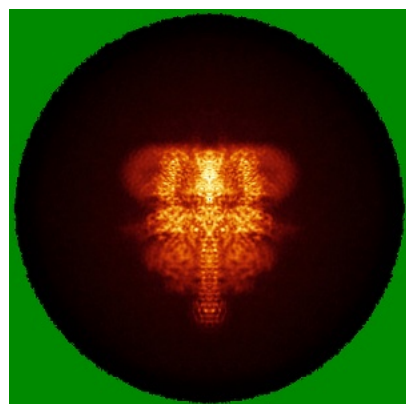


Z Index: 216

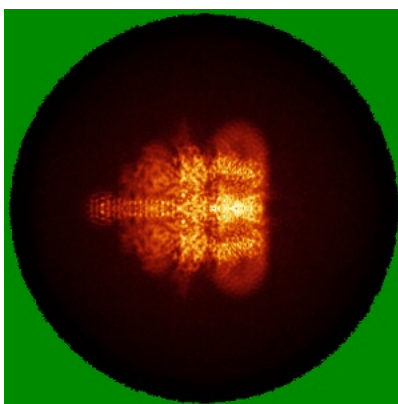
The images above show the largest variance slices of the map in three orthogonal directions.

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

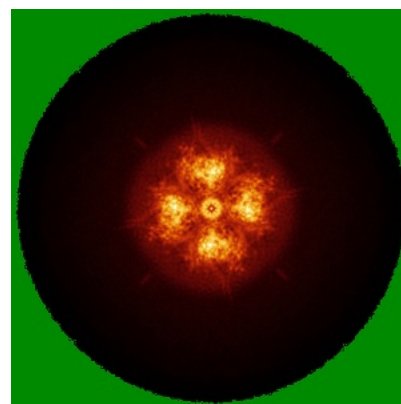
6.4.1 Primary map



X

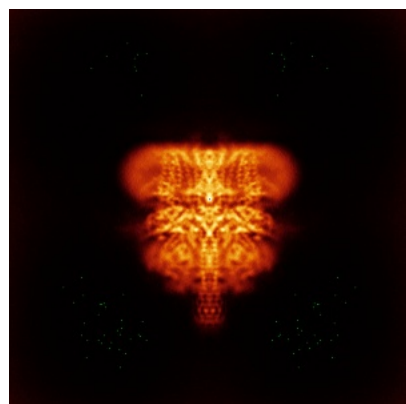


Y

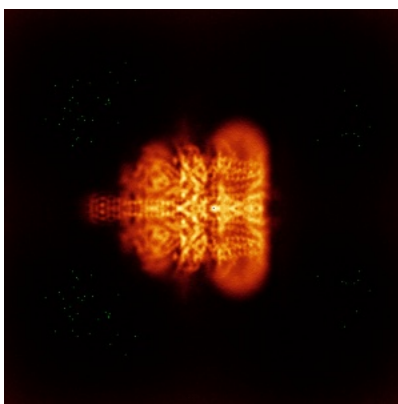


Z

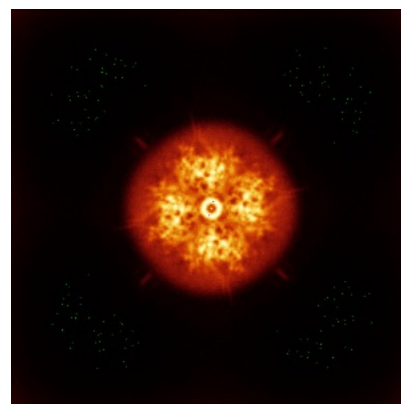
6.4.2 Raw map



X



Y

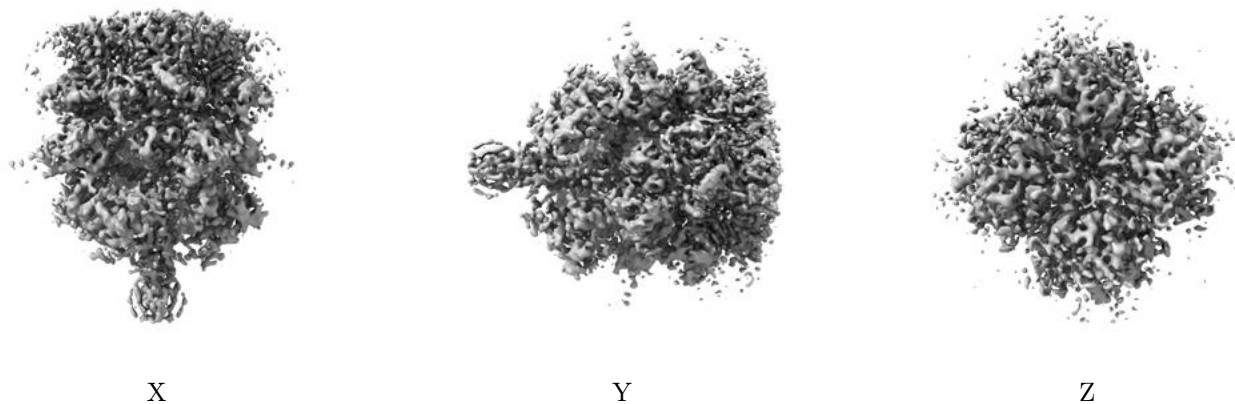


Z

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.

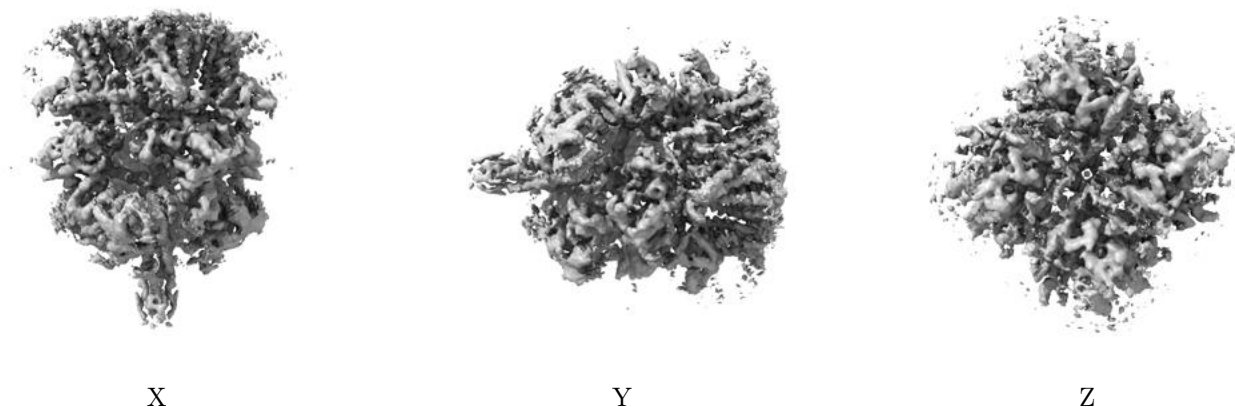
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

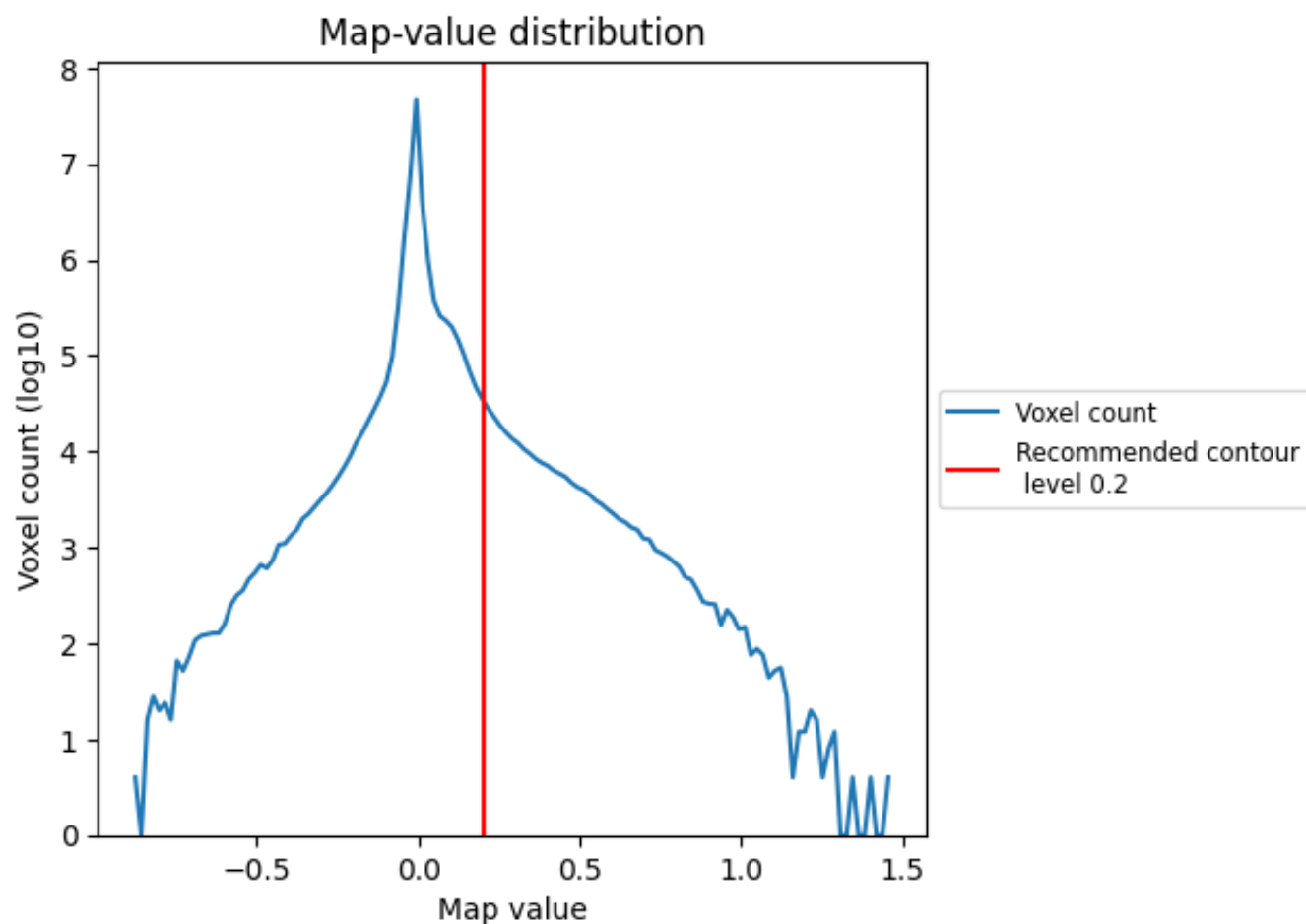
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

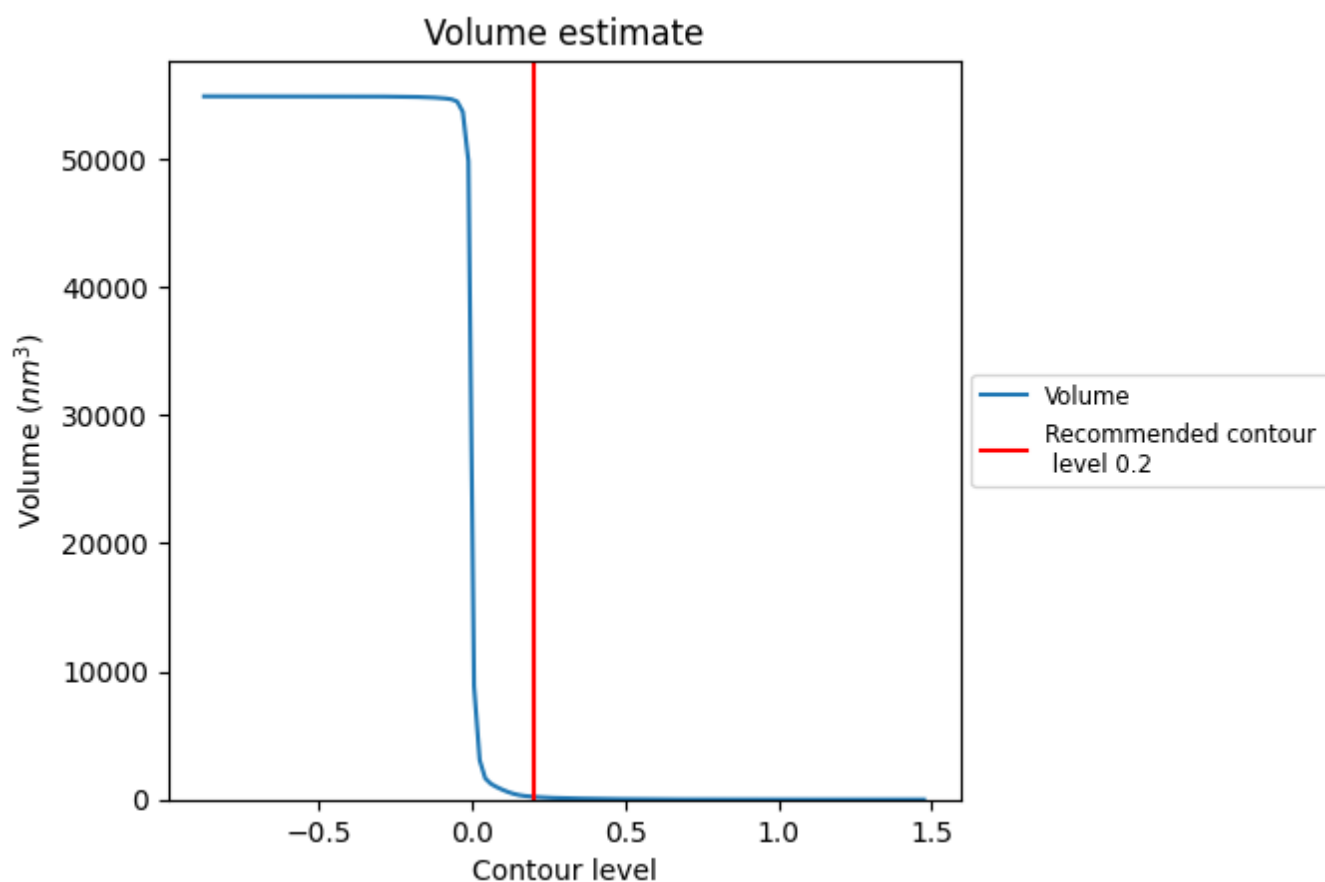
This section contains the results of statistical analysis of the map.

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.

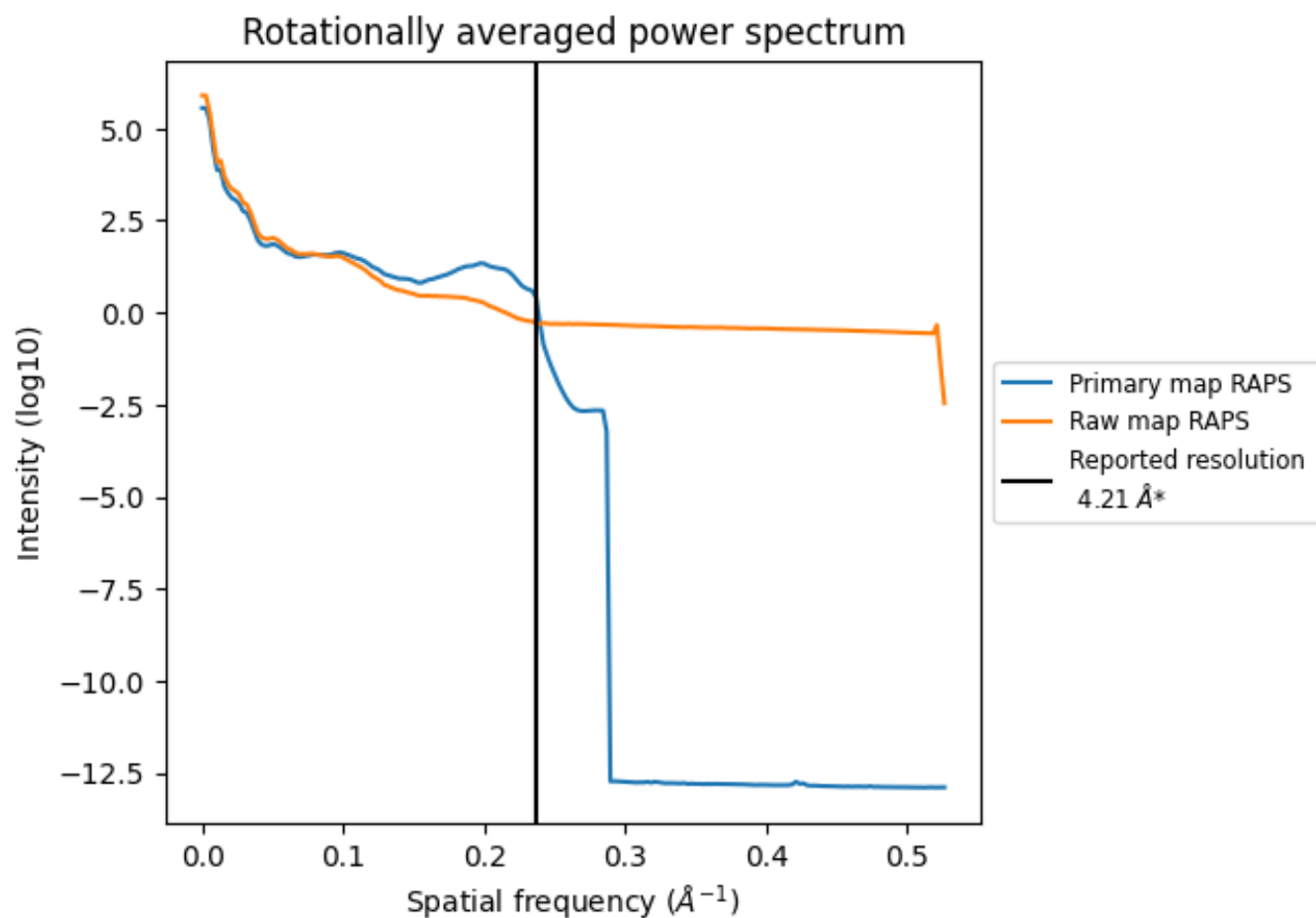
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 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 ⓘ

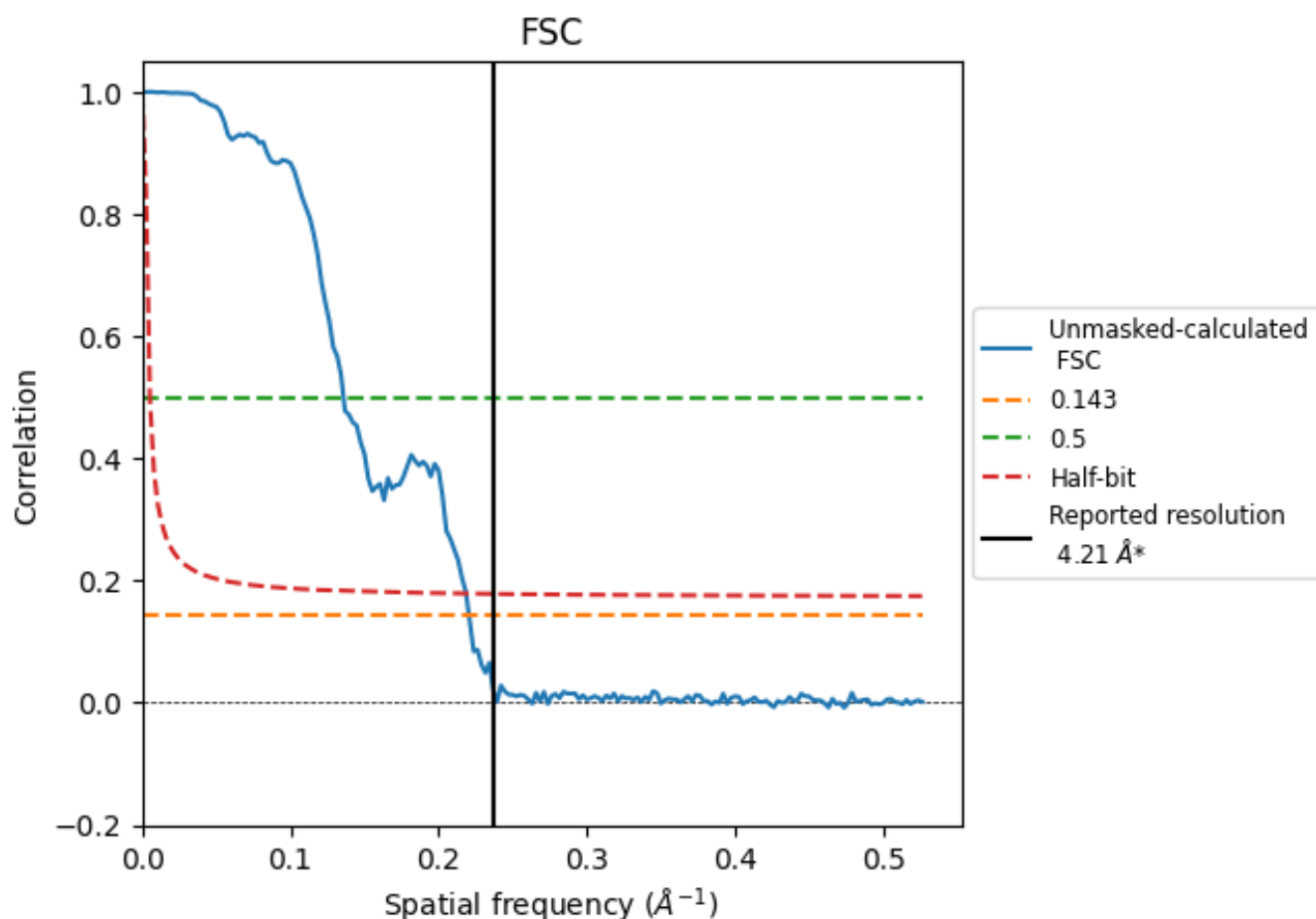


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.54	7.36	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

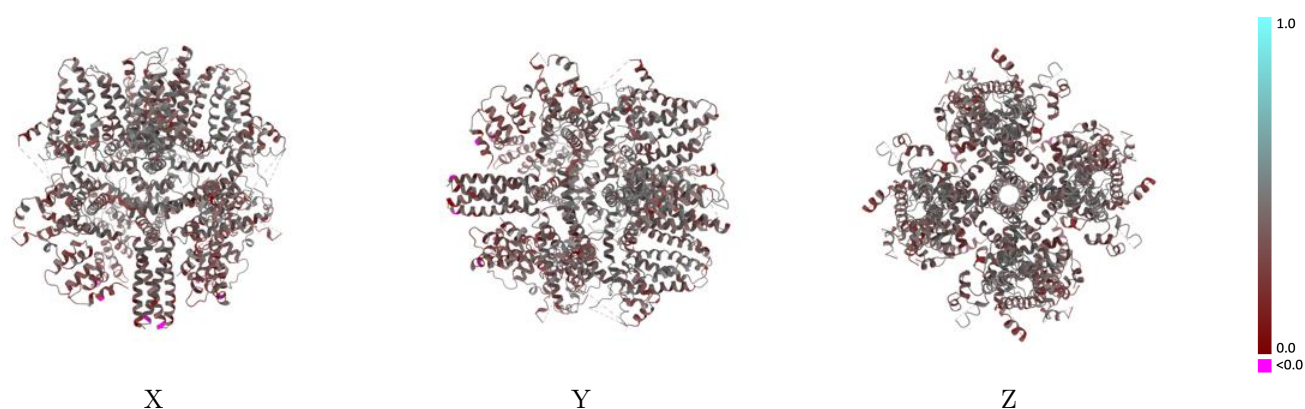
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61215 and PDB model 9J84. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

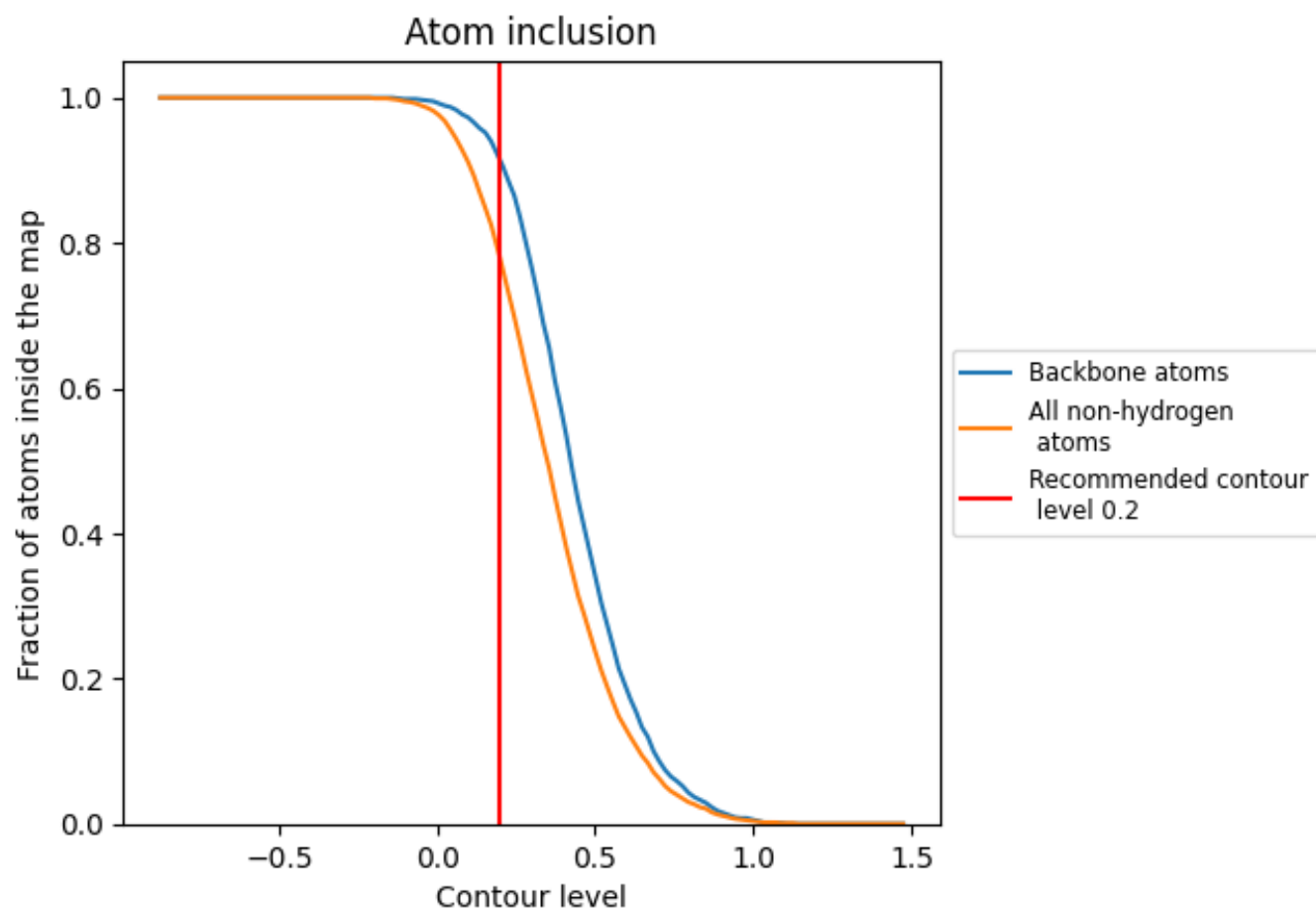


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.3830
A	0.7780	0.3830
B	0.7780	0.3830
C	0.7780	0.3830
D	0.7780	0.3840

