



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 07:23 pm BST

PDB ID : 9T5M / pdb_00009t5m
EMDB ID : EMD-55589
Title : Structure of mouse full-length LRRC8D
Authors : Lehmann, E.F.; Deneka, D.; Stierli, F.; Rutz, S.; Dutzler, R.
Deposited on : 2025-11-05
Resolution : 2.99 Å(reported)

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:

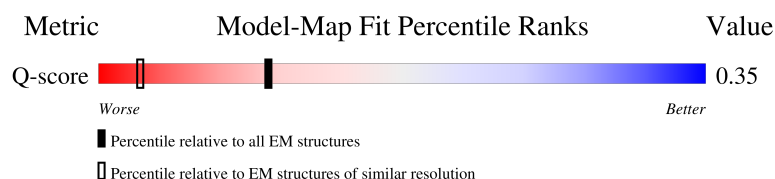
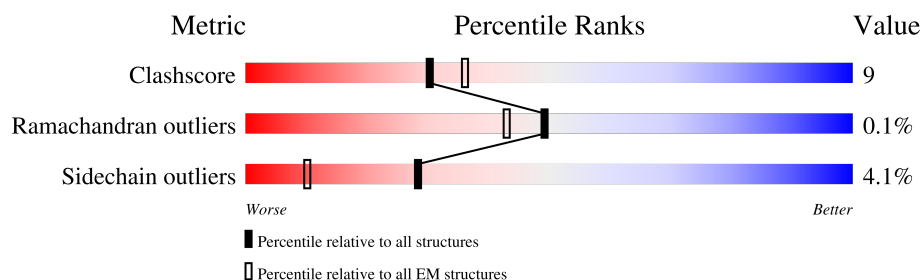
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.99 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	13287 (2.49 - 3.49)

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	924	
1	B	924	
1	C	924	
1	D	924	

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Mol	Chain	Length	Quality of chain
1	E	924	
1	F	924	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34368 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 Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		
1	C	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		
1	B	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		
1	D	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		
1	F	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		
1	E	702	Total	C	N	O	S	1	0
			5728	3729	951	1013	35		

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8BGR2
A	1	SER	-	expression tag	UNP Q8BGR2
A	61N	VAL	ILE	conflict	UNP Q8BGR2
A	63O	VAL	ALA	conflict	UNP Q8BGR2
A	313	VAL	LEU	conflict	UNP Q8BGR2
A	347	ILE	THR	conflict	UNP Q8BGR2
A	859	ALA	-	expression tag	UNP Q8BGR2
A	860	LEU	-	expression tag	UNP Q8BGR2
A	861	GLU	-	expression tag	UNP Q8BGR2
A	862	VAL	-	expression tag	UNP Q8BGR2
A	863	LEU	-	expression tag	UNP Q8BGR2
A	864	PHE	-	expression tag	UNP Q8BGR2
A	865	GLN	-	expression tag	UNP Q8BGR2
A	866	GLY	-	expression tag	UNP Q8BGR2
A	867	PRO	-	expression tag	UNP Q8BGR2
A	868	GLN	-	expression tag	UNP Q8BGR2
A	869	GLY	-	expression tag	UNP Q8BGR2
A	870	THR	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	871	GLU	-	expression tag	UNP Q8BGR2
A	872	GLN	-	expression tag	UNP Q8BGR2
A	873	LYS	-	expression tag	UNP Q8BGR2
A	874	LEU	-	expression tag	UNP Q8BGR2
A	875	ILE	-	expression tag	UNP Q8BGR2
A	876	SER	-	expression tag	UNP Q8BGR2
A	877	GLU	-	expression tag	UNP Q8BGR2
A	878	GLU	-	expression tag	UNP Q8BGR2
A	879	ASP	-	expression tag	UNP Q8BGR2
A	880	LEU	-	expression tag	UNP Q8BGR2
A	881	ARG	-	expression tag	UNP Q8BGR2
A	882	GLY	-	expression tag	UNP Q8BGR2
A	883	ALA	-	expression tag	UNP Q8BGR2
A	884	SER	-	expression tag	UNP Q8BGR2
A	885	MET	-	expression tag	UNP Q8BGR2
A	886	ASP	-	expression tag	UNP Q8BGR2
A	887	GLU	-	expression tag	UNP Q8BGR2
A	888	LYS	-	expression tag	UNP Q8BGR2
A	889	THR	-	expression tag	UNP Q8BGR2
A	890	THR	-	expression tag	UNP Q8BGR2
A	891	GLY	-	expression tag	UNP Q8BGR2
A	892	TRP	-	expression tag	UNP Q8BGR2
A	893	ARG	-	expression tag	UNP Q8BGR2
A	894	GLY	-	expression tag	UNP Q8BGR2
A	895	GLY	-	expression tag	UNP Q8BGR2
A	896	HIS	-	expression tag	UNP Q8BGR2
A	897	VAL	-	expression tag	UNP Q8BGR2
A	898	VAL	-	expression tag	UNP Q8BGR2
A	899	GLU	-	expression tag	UNP Q8BGR2
A	900	GLY	-	expression tag	UNP Q8BGR2
A	901	LEU	-	expression tag	UNP Q8BGR2
A	902	ALA	-	expression tag	UNP Q8BGR2
A	903	GLY	-	expression tag	UNP Q8BGR2
A	904	GLU	-	expression tag	UNP Q8BGR2
A	905	LEU	-	expression tag	UNP Q8BGR2
A	906	GLU	-	expression tag	UNP Q8BGR2
A	907	GLN	-	expression tag	UNP Q8BGR2
A	908	LEU	-	expression tag	UNP Q8BGR2
A	909	ARG	-	expression tag	UNP Q8BGR2
A	910	ALA	-	expression tag	UNP Q8BGR2
A	911	ARG	-	expression tag	UNP Q8BGR2
A	912	LEU	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	913	GLU	-	expression tag	UNP Q8BGR2
A	914	HIS	-	expression tag	UNP Q8BGR2
A	915	HIS	-	expression tag	UNP Q8BGR2
A	916	PRO	-	expression tag	UNP Q8BGR2
A	917	GLN	-	expression tag	UNP Q8BGR2
A	918	GLY	-	expression tag	UNP Q8BGR2
A	919	GLN	-	expression tag	UNP Q8BGR2
A	920	ARG	-	expression tag	UNP Q8BGR2
A	921	GLU	-	expression tag	UNP Q8BGR2
A	922	PRO	-	expression tag	UNP Q8BGR2
C	0	MET	-	initiating methionine	UNP Q8BGR2
C	1	SER	-	expression tag	UNP Q8BGR2
C	61N	VAL	ILE	conflict	UNP Q8BGR2
C	63O	VAL	ALA	conflict	UNP Q8BGR2
C	313	VAL	LEU	conflict	UNP Q8BGR2
C	347	ILE	THR	conflict	UNP Q8BGR2
C	859	ALA	-	expression tag	UNP Q8BGR2
C	860	LEU	-	expression tag	UNP Q8BGR2
C	861	GLU	-	expression tag	UNP Q8BGR2
C	862	VAL	-	expression tag	UNP Q8BGR2
C	863	LEU	-	expression tag	UNP Q8BGR2
C	864	PHE	-	expression tag	UNP Q8BGR2
C	865	GLN	-	expression tag	UNP Q8BGR2
C	866	GLY	-	expression tag	UNP Q8BGR2
C	867	PRO	-	expression tag	UNP Q8BGR2
C	868	GLN	-	expression tag	UNP Q8BGR2
C	869	GLY	-	expression tag	UNP Q8BGR2
C	870	THR	-	expression tag	UNP Q8BGR2
C	871	GLU	-	expression tag	UNP Q8BGR2
C	872	GLN	-	expression tag	UNP Q8BGR2
C	873	LYS	-	expression tag	UNP Q8BGR2
C	874	LEU	-	expression tag	UNP Q8BGR2
C	875	ILE	-	expression tag	UNP Q8BGR2
C	876	SER	-	expression tag	UNP Q8BGR2
C	877	GLU	-	expression tag	UNP Q8BGR2
C	878	GLU	-	expression tag	UNP Q8BGR2
C	879	ASP	-	expression tag	UNP Q8BGR2
C	880	LEU	-	expression tag	UNP Q8BGR2
C	881	ARG	-	expression tag	UNP Q8BGR2
C	882	GLY	-	expression tag	UNP Q8BGR2
C	883	ALA	-	expression tag	UNP Q8BGR2
C	884	SER	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	885	MET	-	expression tag	UNP Q8BGR2
C	886	ASP	-	expression tag	UNP Q8BGR2
C	887	GLU	-	expression tag	UNP Q8BGR2
C	888	LYS	-	expression tag	UNP Q8BGR2
C	889	THR	-	expression tag	UNP Q8BGR2
C	890	THR	-	expression tag	UNP Q8BGR2
C	891	GLY	-	expression tag	UNP Q8BGR2
C	892	TRP	-	expression tag	UNP Q8BGR2
C	893	ARG	-	expression tag	UNP Q8BGR2
C	894	GLY	-	expression tag	UNP Q8BGR2
C	895	GLY	-	expression tag	UNP Q8BGR2
C	896	HIS	-	expression tag	UNP Q8BGR2
C	897	VAL	-	expression tag	UNP Q8BGR2
C	898	VAL	-	expression tag	UNP Q8BGR2
C	899	GLU	-	expression tag	UNP Q8BGR2
C	900	GLY	-	expression tag	UNP Q8BGR2
C	901	LEU	-	expression tag	UNP Q8BGR2
C	902	ALA	-	expression tag	UNP Q8BGR2
C	903	GLY	-	expression tag	UNP Q8BGR2
C	904	GLU	-	expression tag	UNP Q8BGR2
C	905	LEU	-	expression tag	UNP Q8BGR2
C	906	GLU	-	expression tag	UNP Q8BGR2
C	907	GLN	-	expression tag	UNP Q8BGR2
C	908	LEU	-	expression tag	UNP Q8BGR2
C	909	ARG	-	expression tag	UNP Q8BGR2
C	910	ALA	-	expression tag	UNP Q8BGR2
C	911	ARG	-	expression tag	UNP Q8BGR2
C	912	LEU	-	expression tag	UNP Q8BGR2
C	913	GLU	-	expression tag	UNP Q8BGR2
C	914	HIS	-	expression tag	UNP Q8BGR2
C	915	HIS	-	expression tag	UNP Q8BGR2
C	916	PRO	-	expression tag	UNP Q8BGR2
C	917	GLN	-	expression tag	UNP Q8BGR2
C	918	GLY	-	expression tag	UNP Q8BGR2
C	919	GLN	-	expression tag	UNP Q8BGR2
C	920	ARG	-	expression tag	UNP Q8BGR2
C	921	GLU	-	expression tag	UNP Q8BGR2
C	922	PRO	-	expression tag	UNP Q8BGR2
B	0	MET	-	initiating methionine	UNP Q8BGR2
B	1	SER	-	expression tag	UNP Q8BGR2
B	61N	VAL	ILE	conflict	UNP Q8BGR2
B	63O	VAL	ALA	conflict	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	313	VAL	LEU	conflict	UNP Q8BGR2
B	347	ILE	THR	conflict	UNP Q8BGR2
B	859	ALA	-	expression tag	UNP Q8BGR2
B	860	LEU	-	expression tag	UNP Q8BGR2
B	861	GLU	-	expression tag	UNP Q8BGR2
B	862	VAL	-	expression tag	UNP Q8BGR2
B	863	LEU	-	expression tag	UNP Q8BGR2
B	864	PHE	-	expression tag	UNP Q8BGR2
B	865	GLN	-	expression tag	UNP Q8BGR2
B	866	GLY	-	expression tag	UNP Q8BGR2
B	867	PRO	-	expression tag	UNP Q8BGR2
B	868	GLN	-	expression tag	UNP Q8BGR2
B	869	GLY	-	expression tag	UNP Q8BGR2
B	870	THR	-	expression tag	UNP Q8BGR2
B	871	GLU	-	expression tag	UNP Q8BGR2
B	872	GLN	-	expression tag	UNP Q8BGR2
B	873	LYS	-	expression tag	UNP Q8BGR2
B	874	LEU	-	expression tag	UNP Q8BGR2
B	875	ILE	-	expression tag	UNP Q8BGR2
B	876	SER	-	expression tag	UNP Q8BGR2
B	877	GLU	-	expression tag	UNP Q8BGR2
B	878	GLU	-	expression tag	UNP Q8BGR2
B	879	ASP	-	expression tag	UNP Q8BGR2
B	880	LEU	-	expression tag	UNP Q8BGR2
B	881	ARG	-	expression tag	UNP Q8BGR2
B	882	GLY	-	expression tag	UNP Q8BGR2
B	883	ALA	-	expression tag	UNP Q8BGR2
B	884	SER	-	expression tag	UNP Q8BGR2
B	885	MET	-	expression tag	UNP Q8BGR2
B	886	ASP	-	expression tag	UNP Q8BGR2
B	887	GLU	-	expression tag	UNP Q8BGR2
B	888	LYS	-	expression tag	UNP Q8BGR2
B	889	THR	-	expression tag	UNP Q8BGR2
B	890	THR	-	expression tag	UNP Q8BGR2
B	891	GLY	-	expression tag	UNP Q8BGR2
B	892	TRP	-	expression tag	UNP Q8BGR2
B	893	ARG	-	expression tag	UNP Q8BGR2
B	894	GLY	-	expression tag	UNP Q8BGR2
B	895	GLY	-	expression tag	UNP Q8BGR2
B	896	HIS	-	expression tag	UNP Q8BGR2
B	897	VAL	-	expression tag	UNP Q8BGR2
B	898	VAL	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	GLU	-	expression tag	UNP Q8BGR2
B	900	GLY	-	expression tag	UNP Q8BGR2
B	901	LEU	-	expression tag	UNP Q8BGR2
B	902	ALA	-	expression tag	UNP Q8BGR2
B	903	GLY	-	expression tag	UNP Q8BGR2
B	904	GLU	-	expression tag	UNP Q8BGR2
B	905	LEU	-	expression tag	UNP Q8BGR2
B	906	GLU	-	expression tag	UNP Q8BGR2
B	907	GLN	-	expression tag	UNP Q8BGR2
B	908	LEU	-	expression tag	UNP Q8BGR2
B	909	ARG	-	expression tag	UNP Q8BGR2
B	910	ALA	-	expression tag	UNP Q8BGR2
B	911	ARG	-	expression tag	UNP Q8BGR2
B	912	LEU	-	expression tag	UNP Q8BGR2
B	913	GLU	-	expression tag	UNP Q8BGR2
B	914	HIS	-	expression tag	UNP Q8BGR2
B	915	HIS	-	expression tag	UNP Q8BGR2
B	916	PRO	-	expression tag	UNP Q8BGR2
B	917	GLN	-	expression tag	UNP Q8BGR2
B	918	GLY	-	expression tag	UNP Q8BGR2
B	919	GLN	-	expression tag	UNP Q8BGR2
B	920	ARG	-	expression tag	UNP Q8BGR2
B	921	GLU	-	expression tag	UNP Q8BGR2
B	922	PRO	-	expression tag	UNP Q8BGR2
D	0	MET	-	initiating methionine	UNP Q8BGR2
D	1	SER	-	expression tag	UNP Q8BGR2
D	61N	VAL	ILE	conflict	UNP Q8BGR2
D	63O	VAL	ALA	conflict	UNP Q8BGR2
D	313	VAL	LEU	conflict	UNP Q8BGR2
D	347	ILE	THR	conflict	UNP Q8BGR2
D	859	ALA	-	expression tag	UNP Q8BGR2
D	860	LEU	-	expression tag	UNP Q8BGR2
D	861	GLU	-	expression tag	UNP Q8BGR2
D	862	VAL	-	expression tag	UNP Q8BGR2
D	863	LEU	-	expression tag	UNP Q8BGR2
D	864	PHE	-	expression tag	UNP Q8BGR2
D	865	GLN	-	expression tag	UNP Q8BGR2
D	866	GLY	-	expression tag	UNP Q8BGR2
D	867	PRO	-	expression tag	UNP Q8BGR2
D	868	GLN	-	expression tag	UNP Q8BGR2
D	869	GLY	-	expression tag	UNP Q8BGR2
D	870	THR	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	871	GLU	-	expression tag	UNP Q8BGR2
D	872	GLN	-	expression tag	UNP Q8BGR2
D	873	LYS	-	expression tag	UNP Q8BGR2
D	874	LEU	-	expression tag	UNP Q8BGR2
D	875	ILE	-	expression tag	UNP Q8BGR2
D	876	SER	-	expression tag	UNP Q8BGR2
D	877	GLU	-	expression tag	UNP Q8BGR2
D	878	GLU	-	expression tag	UNP Q8BGR2
D	879	ASP	-	expression tag	UNP Q8BGR2
D	880	LEU	-	expression tag	UNP Q8BGR2
D	881	ARG	-	expression tag	UNP Q8BGR2
D	882	GLY	-	expression tag	UNP Q8BGR2
D	883	ALA	-	expression tag	UNP Q8BGR2
D	884	SER	-	expression tag	UNP Q8BGR2
D	885	MET	-	expression tag	UNP Q8BGR2
D	886	ASP	-	expression tag	UNP Q8BGR2
D	887	GLU	-	expression tag	UNP Q8BGR2
D	888	LYS	-	expression tag	UNP Q8BGR2
D	889	THR	-	expression tag	UNP Q8BGR2
D	890	THR	-	expression tag	UNP Q8BGR2
D	891	GLY	-	expression tag	UNP Q8BGR2
D	892	TRP	-	expression tag	UNP Q8BGR2
D	893	ARG	-	expression tag	UNP Q8BGR2
D	894	GLY	-	expression tag	UNP Q8BGR2
D	895	GLY	-	expression tag	UNP Q8BGR2
D	896	HIS	-	expression tag	UNP Q8BGR2
D	897	VAL	-	expression tag	UNP Q8BGR2
D	898	VAL	-	expression tag	UNP Q8BGR2
D	899	GLU	-	expression tag	UNP Q8BGR2
D	900	GLY	-	expression tag	UNP Q8BGR2
D	901	LEU	-	expression tag	UNP Q8BGR2
D	902	ALA	-	expression tag	UNP Q8BGR2
D	903	GLY	-	expression tag	UNP Q8BGR2
D	904	GLU	-	expression tag	UNP Q8BGR2
D	905	LEU	-	expression tag	UNP Q8BGR2
D	906	GLU	-	expression tag	UNP Q8BGR2
D	907	GLN	-	expression tag	UNP Q8BGR2
D	908	LEU	-	expression tag	UNP Q8BGR2
D	909	ARG	-	expression tag	UNP Q8BGR2
D	910	ALA	-	expression tag	UNP Q8BGR2
D	911	ARG	-	expression tag	UNP Q8BGR2
D	912	LEU	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	913	GLU	-	expression tag	UNP Q8BGR2
D	914	HIS	-	expression tag	UNP Q8BGR2
D	915	HIS	-	expression tag	UNP Q8BGR2
D	916	PRO	-	expression tag	UNP Q8BGR2
D	917	GLN	-	expression tag	UNP Q8BGR2
D	918	GLY	-	expression tag	UNP Q8BGR2
D	919	GLN	-	expression tag	UNP Q8BGR2
D	920	ARG	-	expression tag	UNP Q8BGR2
D	921	GLU	-	expression tag	UNP Q8BGR2
D	922	PRO	-	expression tag	UNP Q8BGR2
F	0	MET	-	initiating methionine	UNP Q8BGR2
F	1	SER	-	expression tag	UNP Q8BGR2
F	61N	VAL	ILE	conflict	UNP Q8BGR2
F	63O	VAL	ALA	conflict	UNP Q8BGR2
F	313	VAL	LEU	conflict	UNP Q8BGR2
F	347	ILE	THR	conflict	UNP Q8BGR2
F	859	ALA	-	expression tag	UNP Q8BGR2
F	860	LEU	-	expression tag	UNP Q8BGR2
F	861	GLU	-	expression tag	UNP Q8BGR2
F	862	VAL	-	expression tag	UNP Q8BGR2
F	863	LEU	-	expression tag	UNP Q8BGR2
F	864	PHE	-	expression tag	UNP Q8BGR2
F	865	GLN	-	expression tag	UNP Q8BGR2
F	866	GLY	-	expression tag	UNP Q8BGR2
F	867	PRO	-	expression tag	UNP Q8BGR2
F	868	GLN	-	expression tag	UNP Q8BGR2
F	869	GLY	-	expression tag	UNP Q8BGR2
F	870	THR	-	expression tag	UNP Q8BGR2
F	871	GLU	-	expression tag	UNP Q8BGR2
F	872	GLN	-	expression tag	UNP Q8BGR2
F	873	LYS	-	expression tag	UNP Q8BGR2
F	874	LEU	-	expression tag	UNP Q8BGR2
F	875	ILE	-	expression tag	UNP Q8BGR2
F	876	SER	-	expression tag	UNP Q8BGR2
F	877	GLU	-	expression tag	UNP Q8BGR2
F	878	GLU	-	expression tag	UNP Q8BGR2
F	879	ASP	-	expression tag	UNP Q8BGR2
F	880	LEU	-	expression tag	UNP Q8BGR2
F	881	ARG	-	expression tag	UNP Q8BGR2
F	882	GLY	-	expression tag	UNP Q8BGR2
F	883	ALA	-	expression tag	UNP Q8BGR2
F	884	SER	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	885	MET	-	expression tag	UNP Q8BGR2
F	886	ASP	-	expression tag	UNP Q8BGR2
F	887	GLU	-	expression tag	UNP Q8BGR2
F	888	LYS	-	expression tag	UNP Q8BGR2
F	889	THR	-	expression tag	UNP Q8BGR2
F	890	THR	-	expression tag	UNP Q8BGR2
F	891	GLY	-	expression tag	UNP Q8BGR2
F	892	TRP	-	expression tag	UNP Q8BGR2
F	893	ARG	-	expression tag	UNP Q8BGR2
F	894	GLY	-	expression tag	UNP Q8BGR2
F	895	GLY	-	expression tag	UNP Q8BGR2
F	896	HIS	-	expression tag	UNP Q8BGR2
F	897	VAL	-	expression tag	UNP Q8BGR2
F	898	VAL	-	expression tag	UNP Q8BGR2
F	899	GLU	-	expression tag	UNP Q8BGR2
F	900	GLY	-	expression tag	UNP Q8BGR2
F	901	LEU	-	expression tag	UNP Q8BGR2
F	902	ALA	-	expression tag	UNP Q8BGR2
F	903	GLY	-	expression tag	UNP Q8BGR2
F	904	GLU	-	expression tag	UNP Q8BGR2
F	905	LEU	-	expression tag	UNP Q8BGR2
F	906	GLU	-	expression tag	UNP Q8BGR2
F	907	GLN	-	expression tag	UNP Q8BGR2
F	908	LEU	-	expression tag	UNP Q8BGR2
F	909	ARG	-	expression tag	UNP Q8BGR2
F	910	ALA	-	expression tag	UNP Q8BGR2
F	911	ARG	-	expression tag	UNP Q8BGR2
F	912	LEU	-	expression tag	UNP Q8BGR2
F	913	GLU	-	expression tag	UNP Q8BGR2
F	914	HIS	-	expression tag	UNP Q8BGR2
F	915	HIS	-	expression tag	UNP Q8BGR2
F	916	PRO	-	expression tag	UNP Q8BGR2
F	917	GLN	-	expression tag	UNP Q8BGR2
F	918	GLY	-	expression tag	UNP Q8BGR2
F	919	GLN	-	expression tag	UNP Q8BGR2
F	920	ARG	-	expression tag	UNP Q8BGR2
F	921	GLU	-	expression tag	UNP Q8BGR2
F	922	PRO	-	expression tag	UNP Q8BGR2
E	0	MET	-	initiating methionine	UNP Q8BGR2
E	1	SER	-	expression tag	UNP Q8BGR2
E	61N	VAL	ILE	conflict	UNP Q8BGR2
E	63O	VAL	ALA	conflict	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	313	VAL	LEU	conflict	UNP Q8BGR2
E	347	ILE	THR	conflict	UNP Q8BGR2
E	859	ALA	-	expression tag	UNP Q8BGR2
E	860	LEU	-	expression tag	UNP Q8BGR2
E	861	GLU	-	expression tag	UNP Q8BGR2
E	862	VAL	-	expression tag	UNP Q8BGR2
E	863	LEU	-	expression tag	UNP Q8BGR2
E	864	PHE	-	expression tag	UNP Q8BGR2
E	865	GLN	-	expression tag	UNP Q8BGR2
E	866	GLY	-	expression tag	UNP Q8BGR2
E	867	PRO	-	expression tag	UNP Q8BGR2
E	868	GLN	-	expression tag	UNP Q8BGR2
E	869	GLY	-	expression tag	UNP Q8BGR2
E	870	THR	-	expression tag	UNP Q8BGR2
E	871	GLU	-	expression tag	UNP Q8BGR2
E	872	GLN	-	expression tag	UNP Q8BGR2
E	873	LYS	-	expression tag	UNP Q8BGR2
E	874	LEU	-	expression tag	UNP Q8BGR2
E	875	ILE	-	expression tag	UNP Q8BGR2
E	876	SER	-	expression tag	UNP Q8BGR2
E	877	GLU	-	expression tag	UNP Q8BGR2
E	878	GLU	-	expression tag	UNP Q8BGR2
E	879	ASP	-	expression tag	UNP Q8BGR2
E	880	LEU	-	expression tag	UNP Q8BGR2
E	881	ARG	-	expression tag	UNP Q8BGR2
E	882	GLY	-	expression tag	UNP Q8BGR2
E	883	ALA	-	expression tag	UNP Q8BGR2
E	884	SER	-	expression tag	UNP Q8BGR2
E	885	MET	-	expression tag	UNP Q8BGR2
E	886	ASP	-	expression tag	UNP Q8BGR2
E	887	GLU	-	expression tag	UNP Q8BGR2
E	888	LYS	-	expression tag	UNP Q8BGR2
E	889	THR	-	expression tag	UNP Q8BGR2
E	890	THR	-	expression tag	UNP Q8BGR2
E	891	GLY	-	expression tag	UNP Q8BGR2
E	892	TRP	-	expression tag	UNP Q8BGR2
E	893	ARG	-	expression tag	UNP Q8BGR2
E	894	GLY	-	expression tag	UNP Q8BGR2
E	895	GLY	-	expression tag	UNP Q8BGR2
E	896	HIS	-	expression tag	UNP Q8BGR2
E	897	VAL	-	expression tag	UNP Q8BGR2
E	898	VAL	-	expression tag	UNP Q8BGR2

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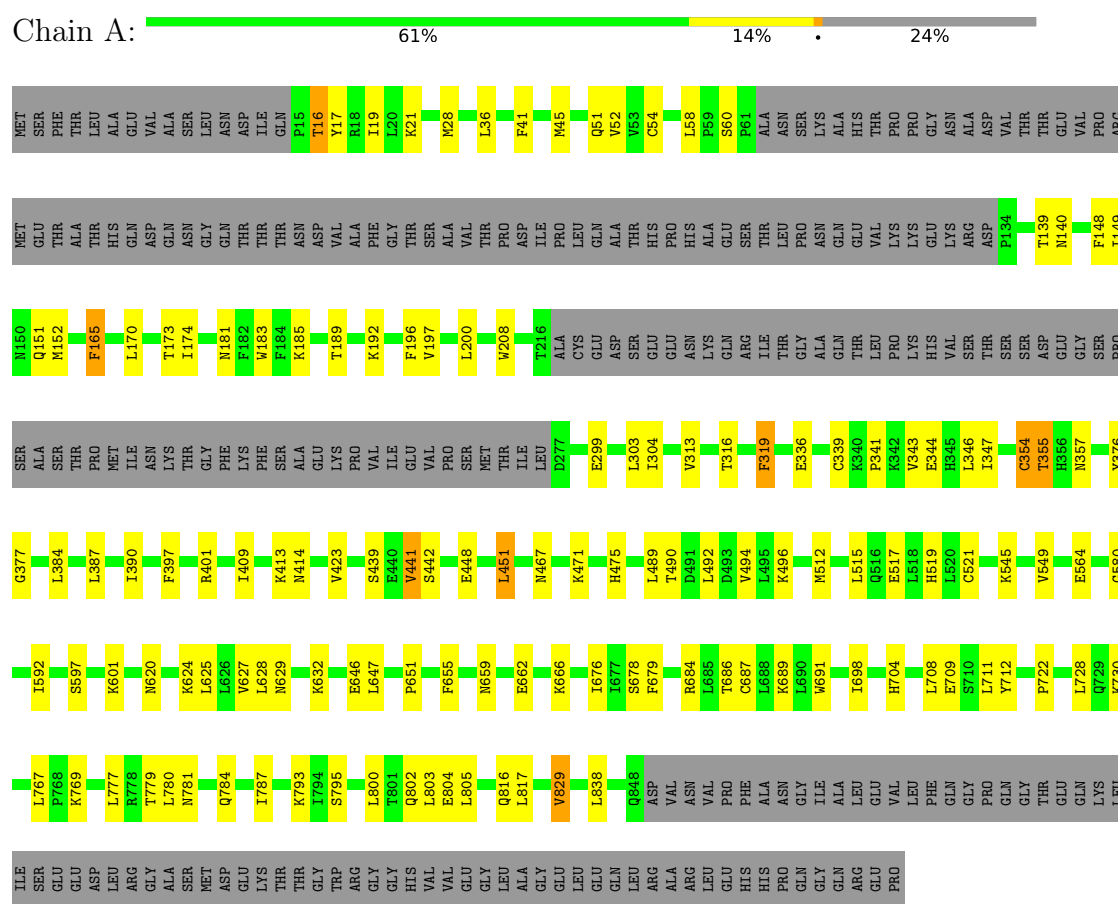
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Chain	Residue	Modelled	Actual	Comment	Reference
E	899	GLU	-	expression tag	UNP Q8BGR2
E	900	GLY	-	expression tag	UNP Q8BGR2
E	901	LEU	-	expression tag	UNP Q8BGR2
E	902	ALA	-	expression tag	UNP Q8BGR2
E	903	GLY	-	expression tag	UNP Q8BGR2
E	904	GLU	-	expression tag	UNP Q8BGR2
E	905	LEU	-	expression tag	UNP Q8BGR2
E	906	GLU	-	expression tag	UNP Q8BGR2
E	907	GLN	-	expression tag	UNP Q8BGR2
E	908	LEU	-	expression tag	UNP Q8BGR2
E	909	ARG	-	expression tag	UNP Q8BGR2
E	910	ALA	-	expression tag	UNP Q8BGR2
E	911	ARG	-	expression tag	UNP Q8BGR2
E	912	LEU	-	expression tag	UNP Q8BGR2
E	913	GLU	-	expression tag	UNP Q8BGR2
E	914	HIS	-	expression tag	UNP Q8BGR2
E	915	HIS	-	expression tag	UNP Q8BGR2
E	916	PRO	-	expression tag	UNP Q8BGR2
E	917	GLN	-	expression tag	UNP Q8BGR2
E	918	GLY	-	expression tag	UNP Q8BGR2
E	919	GLN	-	expression tag	UNP Q8BGR2
E	920	ARG	-	expression tag	UNP Q8BGR2
E	921	GLU	-	expression tag	UNP Q8BGR2
E	922	PRO	-	expression tag	UNP Q8BGR2

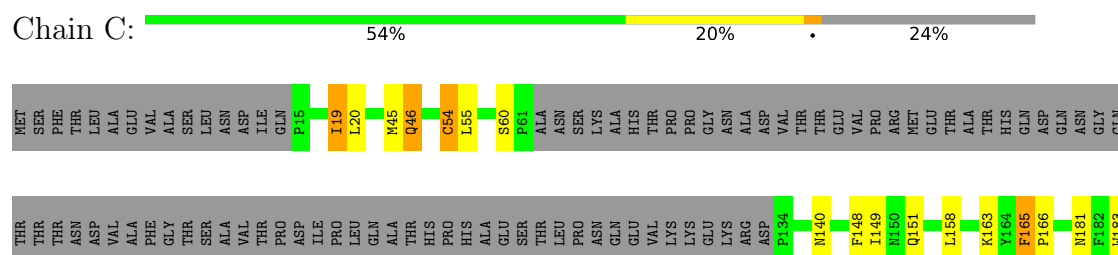
3 Residue-property plots

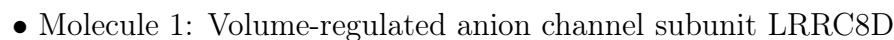
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Volume-regulated anion channel subunit LRRC8D

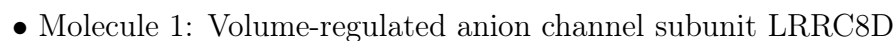


• Molecule 1: Volume-regulated anion channel subunit LRRC8D





MET	K138	THR	THR	MET
GLU	T139	GLU	GLU	GLU
VAL	H140	VAL	VAL	PHE
THR	L141	PRO	PRO	THR
ARG	Q145	ARG	ARG	LEU
ALA	Q145	MET	MET	ALA
GLU	F148	GLU	GLU	LEU
VAL	F148	THR	THR	VAL
ALA	I149	ALA	ALA	ALA
SER	I149	SER	SER	SER
HIS	F165	HIS	HIS	LEU
GLN	L170	GLN	GLN	ASN
ASP	L170	ASP	ASP	ASP
ILE	T173	ILE	ILE	ASP
ASN	T173	ASN	ASN	GLN
GLN	L176	GLY	GLY	P15
GLY	L176	GLN	GLN	T16
THR	H183	THR	THR	Y17
THR	P187	THR	THR	R18
ASN	P187	ASN	ASN	I19
ASP	P187	ASP	ASP	L20
VAL	S206	VAL	VAL	K21
ALA	P207	ALA	ALA	W24
PHE	W208	PHE	PHE	D25
GLY	T209	GLY	GLY	M28
THR	T209	THR	THR	
SER	T216	SER	SER	M37
ALA	T216	ALA	ALA	V86
VAL	CYS	VAL	VAL	V86
THR	GLU	THR	THR	A39
PRO	ASP	PRO	PRO	I40
ASP	ASP	ASP	ASP	F41
ILE	R292	ILE	ILE	M45
PRO	GLU	PRO	PRO	
LEU	GLU	LEU	LEU	Q51
GLN	ASN	GLN	GLN	V52
ALA	V313	ALA	ALA	V53
THR	L489	THR	THR	C54
HIS	T316	HIS	HIS	L58
PRO	A317	PRO	PRO	P59
THR	K318	THR	THR	S80
GLY	F319	GLY	GLY	P81
ALA	E336	ALA	ALA	ALA
GLN	E336	GLN	GLN	THR
THR	C339	THR	THR	THR
LEU	E339	LEU	LEU	ASN
PRO	K340	PRO	PRO	SER
LYS	P341	LYS	LYS	LYS
HIS	L518	HIS	HIS	ALA
VAL	L520	VAL	VAL	ALA
HIS	C521	HIS	HIS	THR
THR	E344	THR	THR	THR
LYS	H345	LYS	LYS	PRO
SER	L346	SER	SER	PRO
GLU	I347	GLU	GLU	GLY
ASN	V549	ASN	ASN	GLY
ASP	V556	ASP	ASP	ASP
GLY	E350	GLY	GLY	ALA
ASP	V351	ASP	ASP	ALA
SER	E564	SER	SER	VAL
PRO	C361	PRO	PRO	THR





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	530537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.285	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.537	Depositor
Minimum map value	-0.601	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.111	Depositor
Map size ($\text{\AA}$)	437.47202, 437.47202, 437.47202	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/5860	0.25	0/7934
1	B	0.12	0/5860	0.26	0/7934
1	C	0.12	0/5860	0.27	2/7934 (0.0%)
1	D	0.09	0/5860	0.22	0/7934
1	E	0.10	0/5860	0.24	0/7934
1	F	0.11	0/5860	0.26	2/7934 (0.0%)
All	All	0.11	0/35160	0.25	4/47604 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	511	GLN	CA-C-N	5.40	131.43	121.70
1	F	511	GLN	C-N-CA	5.40	131.43	121.70
1	C	511	GLN	CA-C-N	5.38	131.39	121.70
1	C	511	GLN	C-N-CA	5.38	131.39	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5728	0	5887	67	0
1	B	5728	0	5887	81	0
1	C	5728	0	5887	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5728	0	5887	109	0
1	E	5728	0	5887	120	0
1	F	5728	0	5887	125	0
All	All	34368	0	35322	625	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 (625) 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:E:149:ILE:HD11	1:E:347:ILE:HG13	1.64	0.80
1:F:149:ILE:HD11	1:F:347:ILE:HG13	1.64	0.79
1:C:712:TYR:HA	1:C:735:ASP:HB3	1.64	0.79
1:B:149:ILE:HD11	1:B:347:ILE:HG13	1.63	0.79
1:A:149:ILE:HD11	1:A:347:ILE:HG13	1.64	0.78
1:B:601:LYS:HG3	1:B:627:VAL:HB	1.67	0.77
1:D:149:ILE:HD11	1:D:347:ILE:HG13	1.67	0.75
1:F:710:SER:HA	1:F:733:CYS:HB3	1.69	0.74
1:C:661:GLN:HG2	1:C:684:ARG:HB3	1.71	0.73
1:C:625:LEU:HB3	1:C:647:LEU:HD21	1.70	0.73
1:C:753:ASN:HA	1:C:776:LYS:HD2	1.69	0.72
1:D:521:CYS:HA	1:D:545:LYS:HB3	1.71	0.72
1:F:676:ILE:HD13	1:F:702:ILE:HG22	1.71	0.71
1:E:58:LEU:HD22	1:E:137:ARG:HD3	1.73	0.71
1:B:467:ASN:HD21	1:B:471:LYS:HB2	1.56	0.71
1:C:676:ILE:HD13	1:C:702:ILE:HG22	1.71	0.70
1:C:748:ILE:HG22	1:C:770:GLN:HE21	1.57	0.70
1:C:149:ILE:HD11	1:C:347:ILE:HG13	1.72	0.69
1:C:487:PHE:HE2	1:C:506:PRO:HD2	1.57	0.69
1:F:753:ASN:HA	1:F:776:LYS:HD2	1.74	0.69
1:A:512[A]:MET:HE2	1:A:515:LEU:HB2	1.74	0.69
1:E:521:CYS:HA	1:E:545:LYS:HB3	1.75	0.69
1:F:721:LEU:HB2	1:F:745:PRO:HG2	1.75	0.68
1:C:707:ASN:HA	1:C:730:LYS:HD2	1.75	0.68
1:D:496:LYS:HA	1:D:519:HIS:HB2	1.75	0.67
1:E:148:PHE:HE2	1:E:343:VAL:HG11	1.59	0.67
1:C:503:ALA:HB3	1:C:525:ALA:HA	1.77	0.67
1:F:595:VAL:HB	1:F:618:ILE:HA	1.77	0.67
1:F:748:ILE:HG22	1:F:770:GLN:HE21	1.59	0.67
1:A:467:ASN:HD21	1:A:471:LYS:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:732:ARG:HA	1:E:754:LEU:HA	1.76	0.67
1:F:691:TRP:HA	1:F:716:ASN:HD21	1.60	0.67
1:B:686:THR:HA	1:B:708:LEU:HA	1.76	0.66
1:D:455:TRP:HA	1:D:459:LYS:HD3	1.78	0.66
1:F:783:GLY:HA2	1:F:808:ASN:HD21	1.61	0.66
1:E:536:ARG:HG3	1:E:559:LEU:HA	1.77	0.66
1:F:707:ASN:HA	1:F:730:LYS:HD2	1.79	0.65
1:C:709:GLU:HA	1:C:731:LEU:HA	1.79	0.65
1:F:563:ARG:HD2	1:F:591:LYS:HD3	1.79	0.65
1:D:753:ASN:HA	1:D:776:LYS:HD2	1.78	0.65
1:A:601:LYS:HG3	1:A:627:VAL:HB	1.78	0.65
1:F:496:LYS:HA	1:F:519:HIS:HB2	1.79	0.65
1:E:571:LEU:HB2	1:E:599:LEU:HD21	1.78	0.64
1:C:721:LEU:HB2	1:C:745:PRO:HG2	1.78	0.64
1:F:649:ARG:HH21	1:F:671:ARG:HE	1.46	0.64
1:F:566:TYR:HA	1:F:594:HIS:HB3	1.79	0.64
1:A:777:LEU:HD21	1:A:780:LEU:HD13	1.79	0.63
1:E:794:ILE:HD12	1:E:797:LEU:HD23	1.79	0.63
1:C:735:ASP:HB2	1:C:758:HIS:HD2	1.63	0.62
1:D:662:GLU:HG2	1:D:687:CYS:HB3	1.81	0.62
1:D:794:ILE:HD12	1:D:797:LEU:HD23	1.80	0.62
1:C:299:GLU:HG3	1:C:413:LYS:HD2	1.81	0.62
1:F:601:LYS:HG3	1:F:627:VAL:HB	1.82	0.62
1:E:299:GLU:HB2	1:E:413:LYS:HB2	1.82	0.62
1:B:299:GLU:HB2	1:B:413:LYS:HB2	1.82	0.62
1:E:707:ASN:HA	1:E:730:LYS:HD2	1.81	0.62
1:E:728:LEU:HD12	1:E:731:LEU:HD22	1.81	0.62
1:E:560:LYS:HG3	1:E:588:ARG:HB2	1.82	0.62
1:B:24:TRP:CD1	1:B:383:THR:HG1	2.18	0.61
1:F:475:HIS:HA	1:F:496:LYS:HB2	1.82	0.61
1:E:753:ASN:HA	1:E:776:LYS:HD2	1.82	0.61
1:C:803:LEU:HD11	1:C:828:LEU:HD12	1.82	0.61
1:B:662:GLU:HG2	1:B:687:CYS:HB3	1.81	0.61
1:A:521:CYS:HA	1:A:545:LYS:HB3	1.82	0.61
1:D:176:LEU:HD21	1:D:318:LYS:HD3	1.82	0.61
1:D:543:HIS:HA	1:D:566:TYR:HB2	1.81	0.61
1:B:659:ASN:HA	1:B:684:ARG:HD2	1.83	0.60
1:C:490:THR:HA	1:C:512[A]:MET:H	1.65	0.60
1:D:58:LEU:HD22	1:D:137:ARG:HD3	1.82	0.60
1:E:543:HIS:HA	1:E:566:TYR:HB2	1.83	0.60
1:C:710:SER:HA	1:C:733:CYS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:HG21	1:A:580:GLY:HA3	1.82	0.60
1:C:691:TRP:HA	1:C:716:ASN:HD21	1.66	0.60
1:F:521:CYS:HA	1:F:545:LYS:HB2	1.82	0.60
1:F:781:ASN:HA	1:F:804:GLU:HB3	1.84	0.60
1:C:780:LEU:HB2	1:C:803:LEU:HA	1.84	0.60
1:B:28:MET:HB3	1:B:379:ILE:HD11	1.84	0.60
1:D:28:MET:HB3	1:D:379:ILE:HD11	1.84	0.60
1:B:708:LEU:HD21	1:B:728:LEU:HD13	1.84	0.59
1:A:769:LYS:HE3	1:A:793:LYS:HD2	1.84	0.59
1:E:734:LEU:HB2	1:E:754:LEU:HD11	1.83	0.59
1:D:572:ASN:HB2	1:D:599:LEU:HD23	1.83	0.59
1:B:148:PHE:HE2	1:B:343:VAL:HG11	1.66	0.59
1:B:350:GLU:HG2	1:B:351:VAL:HG23	1.84	0.59
1:C:601:LYS:HG3	1:C:627:VAL:HB	1.84	0.59
1:C:676:ILE:HG13	1:C:679:PHE:HD2	1.68	0.59
1:B:805:LEU:HB3	1:B:830:VAL:HG12	1.85	0.59
1:D:721:LEU:HB2	1:D:745:PRO:HG2	1.85	0.59
1:B:758:HIS:HA	1:B:781:ASN:HB2	1.85	0.58
1:B:521:CYS:HA	1:B:545:LYS:HB3	1.84	0.58
1:F:795:SER:HB3	1:F:816:GLN:HB3	1.84	0.58
1:E:578:MET:HE3	1:E:601:LYS:HB3	1.86	0.58
1:E:721:LEU:HB2	1:E:745:PRO:HG2	1.85	0.58
1:F:148:PHE:HE2	1:F:343:VAL:HG11	1.69	0.58
1:F:196:PHE:HB2	1:F:419:LEU:HD21	1.86	0.58
1:E:509:ILE:HD13	1:E:535:LEU:HD11	1.86	0.58
1:C:148:PHE:HE2	1:C:343:VAL:HG11	1.68	0.58
1:B:494:VAL:HG22	1:B:517:GLU:HB3	1.84	0.58
1:E:755:GLN:HA	1:E:777:LEU:HA	1.85	0.58
1:D:506:PRO:HA	1:D:528:GLU:HB2	1.84	0.58
1:F:682:LEU:HD12	1:F:685:LEU:HD22	1.86	0.57
1:E:617:VAL:HG13	1:E:641:GLU:HB2	1.86	0.57
1:A:192:LYS:HB2	1:A:304:ILE:HD11	1.85	0.57
1:C:755:GLN:HA	1:C:777:LEU:HA	1.84	0.57
1:C:781:ASN:HA	1:C:804:GLU:HB3	1.87	0.57
1:C:536:ARG:HG3	1:C:560:LYS:H	1.69	0.57
1:D:494:VAL:HG22	1:D:517:GLU:HB3	1.86	0.57
1:F:592:ILE:HG23	1:F:615:LYS:HD3	1.87	0.57
1:E:578:MET:HG3	1:E:599:LEU:HD22	1.87	0.57
1:A:316:THR:HG21	1:A:384:LEU:HD11	1.87	0.57
1:C:723:THR:HA	1:C:726:PHE:HD2	1.69	0.57
1:B:58:LEU:HD11	1:B:139:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:VAL:HG21	1:E:631:LEU:HG	1.87	0.57
1:A:686:THR:HA	1:A:708:LEU:HA	1.87	0.56
1:D:707:ASN:HA	1:D:730:LYS:HD2	1.86	0.56
1:F:200:LEU:HD21	1:F:430:TYR:HB3	1.86	0.56
1:C:511:GLN:H	1:C:512[A]:MET:HB2	1.70	0.56
1:C:543:HIS:HA	1:C:566:TYR:HB2	1.86	0.56
1:C:673:ILE:HG21	1:C:690:LEU:HD13	1.87	0.56
1:E:192:LYS:HE2	1:E:298:VAL:HG12	1.88	0.56
1:E:489:LEU:HB3	1:E:492:LEU:HD23	1.86	0.56
1:D:778:ARG:HA	1:D:800:LEU:HA	1.86	0.56
1:F:503:ALA:HB3	1:F:525:ALA:HA	1.86	0.56
1:D:460:LEU:HD22	1:D:474:LEU:HD21	1.86	0.56
1:B:455:TRP:HA	1:B:459:LYS:HD3	1.87	0.56
1:E:590:LEU:HD21	1:E:593:LEU:HD13	1.88	0.56
1:B:54:CYS:HA	1:B:354:CYS:HA	1.86	0.56
1:A:54:CYS:HA	1:A:354:CYS:HA	1.88	0.56
1:D:732:ARG:HA	1:D:754:LEU:HA	1.86	0.56
1:B:795:SER:HB3	1:B:816:GLN:HB3	1.87	0.55
1:C:581:LEU:HD22	1:C:603:PRO:HB3	1.88	0.55
1:B:628:LEU:HD22	1:B:651:PRO:HG3	1.89	0.55
1:D:790:LEU:HD23	1:D:814:PRO:HD2	1.88	0.55
1:D:777:LEU:HD21	1:D:780:LEU:HD13	1.88	0.55
1:D:489:LEU:HB3	1:D:492:LEU:HD23	1.89	0.55
1:B:186:TYR:HD1	1:B:187:PRO:HD2	1.71	0.55
1:B:625:LEU:HB3	1:B:647:LEU:HD21	1.88	0.55
1:D:655:PHE:HZ	1:D:675:GLU:HB3	1.71	0.55
1:B:277:ASP:HA	1:B:280:ASP:HB3	1.88	0.55
1:F:464:VAL:HG22	1:F:474:LEU:HB2	1.87	0.55
1:D:767:LEU:HB2	1:D:791:PRO:HG2	1.88	0.55
1:D:186:TYR:HD1	1:D:187:PRO:HD2	1.72	0.55
1:E:804:GLU:HA	1:E:829:VAL:HG23	1.89	0.55
1:C:587:LEU:HD22	1:C:590:LEU:HD22	1.89	0.54
1:F:587:LEU:HD23	1:F:590:LEU:HD13	1.87	0.54
1:E:640:LEU:HD22	1:E:657:LEU:HD11	1.89	0.54
1:B:176:LEU:HD21	1:B:318:LYS:HD3	1.89	0.54
1:D:779:THR:HA	1:D:802:GLN:HB3	1.88	0.54
1:E:744:ILE:HD11	1:E:759:ILE:HD13	1.89	0.54
1:D:409:ILE:HD13	1:D:439:SER:HB2	1.90	0.54
1:F:650:ILE:HG23	1:F:654:ILE:HD12	1.89	0.54
1:E:46:GLN:HG3	1:E:166:PRO:HG2	1.88	0.54
1:D:781:ASN:HA	1:D:804:GLU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:GLN:HB2	1:F:512[A]:MET:HB2	1.90	0.54
1:D:755:GLN:HA	1:D:777:LEU:HA	1.89	0.54
1:C:401:ARG:HD3	1:C:409:ILE:H	1.73	0.54
1:A:662:GLU:HG2	1:A:687:CYS:HB3	1.88	0.54
1:F:661:GLN:HG2	1:F:684:ARG:HB3	1.91	0.54
1:F:655:PHE:HZ	1:F:675:GLU:HB3	1.74	0.53
1:E:208:TRP:HH2	1:E:442:SER:HB2	1.72	0.53
1:E:783:GLY:HA2	1:E:808:ASN:HD21	1.73	0.53
1:B:707:ASN:HA	1:B:730:LYS:HD2	1.91	0.53
1:E:54:CYS:HA	1:E:354:CYS:HA	1.89	0.53
1:E:186:TYR:HD1	1:E:187:PRO:HD2	1.74	0.53
1:C:158:LEU:HB2	1:C:163:LYS:HD2	1.89	0.53
1:C:732:ARG:HA	1:C:754:LEU:HA	1.91	0.53
1:B:825:LYS:HB2	1:B:846:LEU:HB3	1.90	0.53
1:E:702:ILE:HG13	1:E:728:LEU:HD21	1.90	0.53
1:B:800:LEU:HD21	1:B:803:LEU:HB2	1.91	0.53
1:A:490:THR:HA	1:A:512[A]:MET:HG3	1.91	0.53
1:D:299:GLU:HB2	1:D:413:LYS:HB2	1.90	0.53
1:D:723:THR:HG23	1:D:747:GLU:HG2	1.90	0.53
1:E:58:LEU:HD11	1:E:139:THR:HG22	1.90	0.53
1:C:467:ASN:HD21	1:C:471:LYS:HB2	1.73	0.52
1:C:662:GLU:HG2	1:C:687:CYS:HB3	1.91	0.52
1:B:581:LEU:HB3	1:B:605:ASN:HB3	1.90	0.52
1:F:183:TRP:HB2	1:F:307:LEU:HG	1.91	0.52
1:F:536:ARG:HG3	1:F:560:LYS:H	1.74	0.52
1:C:585:ARG:HB2	1:C:608:ASP:HB3	1.90	0.52
1:C:599:LEU:H	1:C:599:LEU:HD23	1.72	0.52
1:E:24:TRP:CD1	1:E:383:THR:HG1	2.27	0.52
1:A:16:THR:HA	1:A:197:VAL:HG11	1.91	0.52
1:C:673:ILE:HG13	1:C:699:PRO:HD3	1.91	0.52
1:C:759:ILE:HD11	1:C:782:LEU:HD23	1.91	0.52
1:E:192:LYS:HB2	1:E:304:ILE:HD11	1.92	0.52
1:E:572:ASN:HB2	1:E:599:LEU:HD23	1.91	0.52
1:A:208:TRP:HH2	1:A:442:SER:HB2	1.75	0.52
1:C:721:LEU:HD21	1:C:736:VAL:HG11	1.92	0.52
1:E:778:ARG:HA	1:E:800:LEU:HA	1.90	0.52
1:C:401:ARG:HB3	1:C:407:SER:HA	1.91	0.52
1:D:590:LEU:HD23	1:D:609:VAL:HG11	1.92	0.52
1:A:475:HIS:HA	1:A:496:LYS:HB3	1.91	0.52
1:D:702:ILE:HG12	1:D:725:VAL:HG23	1.92	0.52
1:F:599:LEU:HD23	1:F:599:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:813:LEU:HD11	1:F:830:VAL:HG11	1.91	0.52
1:E:797:LEU:HB3	1:E:800:LEU:HB2	1.91	0.52
1:A:494:VAL:HG22	1:A:517:GLU:HB3	1.92	0.52
1:B:703:THR:HA	1:B:728:LEU:HD21	1.91	0.52
1:E:19:ILE:HD11	1:E:423:VAL:HG13	1.92	0.51
1:E:723:THR:HG23	1:E:747:GLU:HG2	1.91	0.51
1:C:181:ASN:HB3	1:C:184:PHE:HB2	1.92	0.51
1:C:731:LEU:HD23	1:C:751:LEU:HD13	1.92	0.51
1:C:758:HIS:HA	1:C:781:ASN:HB2	1.92	0.51
1:D:345:HIS:CD2	1:D:346:LEU:HD13	2.45	0.51
1:A:496:LYS:HA	1:A:519:HIS:HB2	1.93	0.51
1:C:830:VAL:HB	1:C:834:LEU:HD12	1.93	0.51
1:B:549:VAL:HG21	1:B:580:GLY:HA3	1.92	0.51
1:C:564:GLU:HG2	1:C:592:ILE:HD12	1.92	0.51
1:C:667:SER:H	1:C:692:HIS:HB2	1.76	0.51
1:D:773:LYS:HD3	1:D:796:GLN:HE22	1.74	0.51
1:F:58:LEU:HD11	1:F:139:THR:HG22	1.92	0.51
1:E:461:ARG:HH11	1:E:489:LEU:HD22	1.75	0.51
1:E:657:LEU:HB2	1:E:660:LEU:HB2	1.92	0.51
1:F:19:ILE:HG23	1:F:20:LEU:HD22	1.91	0.51
1:C:151:GLN:HG2	1:D:357:ASN:HD22	1.76	0.51
1:C:689:LYS:HA	1:C:712:TYR:HB2	1.93	0.51
1:C:805:LEU:HB2	1:C:830:VAL:HG12	1.93	0.51
1:E:673:ILE:HD13	1:E:695:ILE:HD13	1.93	0.51
1:C:768:PRO:HG2	1:C:771:LEU:HB2	1.91	0.51
1:F:629:ASN:HA	1:F:632:LYS:HE2	1.93	0.51
1:F:706:LYS:HA	1:F:728:LEU:HD22	1.92	0.51
1:E:655:PHE:HZ	1:E:675:GLU:HB3	1.77	0.50
1:B:790:LEU:HD23	1:B:814:PRO:HD2	1.94	0.50
1:F:409:ILE:HG13	1:F:410:PRO:HD2	1.93	0.50
1:E:496:LYS:HA	1:E:519:HIS:HB2	1.93	0.50
1:A:804:GLU:HA	1:A:829:VAL:HG23	1.93	0.50
1:C:46:GLN:HG3	1:C:166:PRO:HG2	1.93	0.50
1:E:544:VAL:HG11	1:E:552:ILE:HG23	1.94	0.50
1:C:511:GLN:HB2	1:C:512[A]:MET:HB2	1.93	0.50
1:C:783:GLY:HA2	1:C:808:ASN:HD21	1.77	0.50
1:D:578:MET:HE3	1:D:601:LYS:HB3	1.94	0.50
1:F:625:LEU:HB3	1:F:647:LEU:HD21	1.92	0.50
1:D:629:ASN:HA	1:D:632:LYS:HE2	1.94	0.49
1:D:192:LYS:HE2	1:D:304:ILE:HD11	1.93	0.49
1:C:200:LEU:HD21	1:C:423:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ASN:HD22	1:F:151:GLN:HG3	1.78	0.49
1:C:588:ARG:HB2	1:C:589:HIS:CE1	2.46	0.49
1:D:46:GLN:HG3	1:D:166:PRO:HG2	1.93	0.49
1:A:409:ILE:HD13	1:A:439:SER:HB2	1.93	0.49
1:C:19:ILE:HD11	1:C:423:VAL:HG13	1.94	0.49
1:C:812:ARG:HG3	1:C:837:THR:HB	1.95	0.49
1:B:769:LYS:HE3	1:B:793:LYS:HD2	1.93	0.49
1:D:509:ILE:HD13	1:D:535:LEU:HD11	1.93	0.49
1:F:490:THR:HG22	1:F:512[A]:MET:H	1.76	0.49
1:C:676:ILE:HG21	1:C:702:ILE:HG22	1.94	0.49
1:C:840:LEU:HA	1:C:843:LYS:HE2	1.95	0.49
1:B:815:ALA:HB2	1:B:839:PRO:HG2	1.95	0.49
1:D:339:CYS:SG	1:D:341:PRO:HD3	2.53	0.49
1:D:691:TRP:HA	1:D:716:ASN:HD21	1.76	0.49
1:C:45:MET:HG2	1:C:361:MET:HG2	1.95	0.49
1:C:295:ARG:HE	1:C:413:LYS:HE2	1.78	0.49
1:C:345:HIS:CD2	1:C:346:LEU:HD13	2.48	0.49
1:D:728:LEU:HD12	1:D:731:LEU:HD22	1.95	0.49
1:D:795:SER:HB3	1:D:816:GLN:HB3	1.95	0.49
1:F:397:PHE:HB3	1:F:409:ILE:HG21	1.94	0.49
1:F:662:GLU:HA	1:F:687:CYS:HB3	1.94	0.49
1:A:339:CYS:SG	1:A:341:PRO:HD3	2.53	0.49
1:C:549:VAL:HG21	1:C:580:GLY:HA3	1.95	0.49
1:D:749:GLY:HA3	1:D:770:GLN:HB3	1.95	0.49
1:E:662:GLU:HG2	1:E:687:CYS:HB3	1.95	0.49
1:A:151:GLN:HG3	1:B:357:ASN:HD22	1.76	0.48
1:A:795:SER:HB3	1:A:816:GLN:HB3	1.94	0.48
1:C:780:LEU:HB3	1:C:782:LEU:HD11	1.95	0.48
1:B:345:HIS:CD2	1:B:346:LEU:HD13	2.48	0.48
1:D:319:PHE:CE1	1:D:377:GLY:HA3	2.47	0.48
1:D:587:LEU:HD12	1:D:590:LEU:HD22	1.95	0.48
1:D:54:CYS:HA	1:D:354:CYS:HA	1.95	0.48
1:E:494:VAL:HG22	1:E:517:GLU:HB3	1.94	0.48
1:D:708:LEU:HD21	1:D:728:LEU:HD13	1.94	0.48
1:E:28:MET:HB3	1:E:379:ILE:HD11	1.94	0.48
1:E:345:HIS:CD2	1:E:346:LEU:HD13	2.48	0.48
1:F:709:GLU:HA	1:F:731:LEU:HA	1.95	0.48
1:A:148:PHE:HE2	1:A:343:VAL:HG11	1.79	0.48
1:C:537:ASP:HA	1:C:561:ASN:HD22	1.78	0.48
1:C:726:PHE:CD2	1:C:747:GLU:HB2	2.49	0.48
1:D:805:LEU:HD21	1:D:810:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:732:ARG:HA	1:F:754:LEU:HA	1.95	0.48
1:B:564:GLU:HG2	1:B:592:ILE:HD12	1.96	0.48
1:D:58:LEU:HD21	1:D:139:THR:HG22	1.96	0.48
1:F:339:CYS:SG	1:F:341:PRO:HD3	2.54	0.48
1:C:440:GLU:H	1:C:440:GLU:CD	2.22	0.48
1:C:795:SER:HB3	1:C:816:GLN:HB3	1.95	0.48
1:D:464:VAL:HG22	1:D:474:LEU:HB2	1.94	0.48
1:E:16:THR:HA	1:E:197:VAL:HG11	1.96	0.48
1:A:659:ASN:HA	1:A:684:ARG:HD2	1.95	0.47
1:A:708:LEU:HD23	1:A:708:LEU:H	1.78	0.47
1:F:527:VAL:HG21	1:F:532:PHE:HB2	1.95	0.47
1:A:817:LEU:HD21	1:A:838:LEU:HD21	1.95	0.47
1:C:723:THR:HG23	1:C:747:GLU:HG2	1.96	0.47
1:C:804:GLU:HA	1:C:829:VAL:HB	1.95	0.47
1:D:148:PHE:HE2	1:D:343:VAL:HG11	1.80	0.47
1:F:712:TYR:HA	1:F:735:ASP:HB3	1.95	0.47
1:F:804:GLU:HA	1:F:829:VAL:HB	1.95	0.47
1:D:628:LEU:HD23	1:D:631:LEU:HD12	1.95	0.47
1:A:189:THR:HB	1:A:304:ILE:HG12	1.97	0.47
1:C:735:ASP:HB2	1:C:758:HIS:CD2	2.48	0.47
1:C:779:THR:HA	1:C:802:GLN:HB3	1.96	0.47
1:B:804:GLU:HA	1:B:829:VAL:HG23	1.96	0.47
1:F:696:VAL:HG12	1:F:717:LYS:HB2	1.97	0.47
1:F:723:THR:HA	1:F:726:PHE:HD2	1.79	0.47
1:C:181:ASN:H	1:C:185:LYS:HZ3	1.61	0.47
1:B:319:PHE:CE1	1:B:377:GLY:HA3	2.50	0.47
1:F:723:THR:HG23	1:F:747:GLU:HG2	1.97	0.47
1:F:738:TYR:CD1	1:F:761:GLY:HA3	2.49	0.47
1:A:676:ILE:HG13	1:A:679:PHE:HD2	1.79	0.47
1:B:339:CYS:SG	1:B:341:PRO:HD3	2.54	0.47
1:B:461:ARG:HH11	1:B:489:LEU:HD22	1.79	0.47
1:B:649:ARG:HH21	1:B:671:ARG:H	1.63	0.47
1:B:742:SER:HA	1:B:763:LYS:HB2	1.96	0.47
1:B:781:ASN:HA	1:B:804:GLU:HB3	1.97	0.47
1:E:587:LEU:HD12	1:E:590:LEU:HD22	1.96	0.47
1:A:313:VAL:HA	1:A:316:THR:HG22	1.96	0.47
1:D:651:PRO:HG2	1:D:654:ILE:HG13	1.97	0.47
1:A:767:LEU:HD11	1:A:787:ILE:HD13	1.97	0.47
1:A:781:ASN:HA	1:A:804:GLU:HB3	1.97	0.47
1:C:805:LEU:HD13	1:C:810:LEU:HD22	1.96	0.47
1:E:767:LEU:HB2	1:E:791:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:ILE:HG12	1:B:725:VAL:HG23	1.97	0.46
1:C:545:LYS:HG2	1:C:568:ILE:HB	1.97	0.46
1:C:577:LYS:HG3	1:C:579:ILE:HG12	1.97	0.46
1:B:777:LEU:HD21	1:B:780:LEU:HD13	1.97	0.46
1:D:676:ILE:HG13	1:D:679:PHE:HD2	1.79	0.46
1:F:288:PHE:HD1	1:F:292:ARG:HH22	1.62	0.46
1:E:564:GLU:HG2	1:E:592:ILE:HB	1.96	0.46
1:E:673:ILE:HG21	1:E:690:LEU:HD13	1.97	0.46
1:B:208:TRP:HH2	1:B:442:SER:HB2	1.81	0.46
1:D:710:SER:HA	1:D:733:CYS:HB3	1.97	0.46
1:A:800:LEU:HD21	1:A:803:LEU:HB2	1.98	0.46
1:C:817:LEU:HD12	1:C:838:LEU:HD21	1.98	0.46
1:D:341:PRO:HB2	1:D:343:VAL:HG22	1.97	0.46
1:E:341:PRO:HB2	1:E:343:VAL:HG22	1.96	0.46
1:C:55:LEU:HD21	1:B:145:GLN:HG2	1.97	0.46
1:C:511:GLN:H	1:C:512[A]:MET:CB	2.27	0.46
1:C:703:THR:HA	1:C:728:LEU:HD21	1.98	0.46
1:B:779:THR:HG22	1:B:802:GLN:HB3	1.97	0.46
1:D:711:LEU:HD22	1:D:713:PHE:HE2	1.80	0.46
1:D:767:LEU:HD11	1:D:787:ILE:HD13	1.97	0.46
1:F:165:PHE:HZ	1:F:326:THR:HG22	1.80	0.46
1:E:196:PHE:HE2	1:E:423:VAL:HG21	1.81	0.46
1:A:564:GLU:HG2	1:A:592:ILE:HD12	1.96	0.46
1:C:505:ILE:HB	1:C:527:VAL:HG12	1.97	0.46
1:C:690:LEU:HB2	1:C:713:PHE:CE1	2.51	0.46
1:D:467:ASN:HD22	1:D:473:GLU:HB2	1.80	0.46
1:F:37:MET:HE1	1:E:174:ILE:HG21	1.97	0.46
1:F:52:VAL:HG12	1:F:356:HIS:HA	1.98	0.46
1:F:691:TRP:H	1:F:691:TRP:CD1	2.33	0.46
1:F:341:PRO:HB2	1:F:343:VAL:HG22	1.98	0.46
1:C:698:ILE:HG22	1:C:702:ILE:HG21	1.97	0.46
1:D:16:THR:HA	1:D:197:VAL:HG11	1.97	0.46
1:D:734:LEU:HB2	1:D:754:LEU:HD11	1.97	0.46
1:F:319:PHE:CE1	1:F:377:GLY:HA3	2.51	0.46
1:C:794:ILE:HD12	1:C:797:LEU:HD12	1.97	0.45
1:E:733:CYS:HA	1:E:756:HIS:HB2	1.97	0.45
1:C:412:VAL:HB	1:C:416:PHE:HB3	1.97	0.45
1:F:186:TYR:HD1	1:F:187:PRO:HD2	1.80	0.45
1:A:489:LEU:HB3	1:A:492:LEU:HD23	1.98	0.45
1:C:521:CYS:HA	1:C:545:LYS:HB2	1.98	0.45
1:C:401:ARG:HD3	1:C:409:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ILE:HD11	1:C:722:PRO:HG2	1.98	0.45
1:B:17:TYR:O	1:B:21:LYS:HG2	2.16	0.45
1:D:455:TRP:CD1	1:D:455:TRP:H	2.35	0.45
1:F:194:GLU:HA	1:F:197:VAL:HG12	1.98	0.45
1:A:319:PHE:CE1	1:A:377:GLY:HA3	2.51	0.45
1:E:339:CYS:SG	1:E:341:PRO:HD3	2.56	0.45
1:C:454:GLU:HG3	1:C:455:TRP:CD1	2.52	0.45
1:C:779:THR:HG23	1:C:802:GLN:HG2	1.99	0.45
1:F:54:CYS:HA	1:F:354:CYS:HA	1.97	0.45
1:F:345:HIS:CD2	1:F:346:LEU:HD13	2.52	0.45
1:F:702:ILE:HD11	1:F:722:PRO:HG2	1.99	0.45
1:F:751:LEU:HB3	1:F:754:LEU:HB2	1.99	0.45
1:E:781:ASN:HA	1:E:804:GLU:HB3	1.98	0.45
1:A:36:LEU:HB2	1:A:173:THR:HG21	1.99	0.45
1:C:733:CYS:HA	1:C:756:HIS:HB2	1.99	0.45
1:D:601:LYS:HG3	1:D:627:VAL:HB	1.99	0.45
1:F:483:PRO:HB2	1:F:486:VAL:HG23	1.98	0.45
1:E:467:ASN:HD21	1:E:471:LYS:HB2	1.82	0.45
1:A:58:LEU:HD11	1:A:139:THR:HG22	1.98	0.45
1:A:625:LEU:HB3	1:A:647:LEU:HD21	1.99	0.45
1:C:165:PHE:HD1	1:C:165:PHE:HA	1.69	0.45
1:D:553:PRO:HB2	1:D:556:VAL:HG13	1.97	0.45
1:C:341:PRO:HB2	1:C:343:VAL:HG22	1.99	0.45
1:C:494:VAL:HG22	1:C:517:GLU:HB3	1.99	0.45
1:F:607:THR:HA	1:F:610:ALA:HB2	1.98	0.45
1:E:466:ARG:HB3	1:E:470:ASP:HA	1.98	0.45
1:B:767:LEU:HD11	1:B:787:ILE:HD13	1.98	0.44
1:D:736:VAL:HG23	1:D:759:ILE:HG22	1.97	0.44
1:F:498:GLU:HA	1:F:521:CYS:HB3	1.98	0.44
1:F:673:ILE:HG21	1:F:690:LEU:HD13	1.98	0.44
1:E:138:LYS:C	1:E:140:ASN:H	2.25	0.44
1:C:151:GLN:NE2	1:D:357:ASN:HB2	2.32	0.44
1:D:797:LEU:HB3	1:D:800:LEU:HB2	2.00	0.44
1:E:578:MET:HE3	1:E:601:LYS:HE2	1.98	0.44
1:E:593:LEU:HD23	1:E:606:ILE:HG23	1.98	0.44
1:E:651:PRO:HG2	1:E:654:ILE:HG13	1.99	0.44
1:C:563:ARG:HD2	1:B:807:GLY:HA3	1.99	0.44
1:D:36:LEU:HA	1:D:173:THR:HG21	1.98	0.44
1:F:553:PRO:HB2	1:F:556:VAL:HG23	1.98	0.44
1:E:805:LEU:HD21	1:E:810:LEU:HD22	2.00	0.44
1:C:339:CYS:SG	1:C:341:PRO:HD3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:LYS:HG2	1:C:712:TYR:CD2	2.52	0.44
1:A:709:GLU:HG2	1:A:730:LYS:HB3	1.98	0.44
1:A:779:THR:HG22	1:A:802:GLN:HB3	2.00	0.44
1:B:767:LEU:HB3	1:B:771:LEU:HD21	2.00	0.44
1:D:673:ILE:HD13	1:D:695:ILE:HD13	1.99	0.44
1:F:578:MET:HB3	1:F:581:LEU:HD11	1.99	0.44
1:F:673:ILE:HG13	1:F:699:PRO:HD3	1.98	0.44
1:E:464:VAL:HG22	1:E:474:LEU:HB2	1.99	0.44
1:E:749:GLY:HA3	1:E:770:GLN:HB3	1.99	0.44
1:A:200:LEU:HD21	1:A:423:VAL:HG11	1.98	0.44
1:D:661:GLN:HG2	1:D:684:ARG:HB3	2.00	0.44
1:C:670:ILE:H	1:C:693:ASN:HB3	1.83	0.44
1:F:634:MET:O	1:F:657:LEU:HD22	2.17	0.44
1:E:512[A]:MET:HE2	1:E:515:LEU:HA	2.00	0.44
1:A:28:MET:HB2	1:A:376:TYR:CE2	2.52	0.44
1:C:666:LYS:HE3	1:C:692:HIS:CE1	2.53	0.44
1:B:318:LYS:HE3	1:B:318:LYS:HB2	1.71	0.44
1:F:192:LYS:HE2	1:F:298:VAL:HG12	1.99	0.44
1:F:365:LEU:HD12	1:F:365:LEU:HA	1.82	0.44
1:F:737:SER:HA	1:F:762:ASN:HD21	1.82	0.44
1:A:299:GLU:HB2	1:A:413:LYS:HB2	2.00	0.43
1:C:340:LYS:HE3	1:C:340:LYS:HB2	1.76	0.43
1:D:416:PHE:HD1	1:D:416:PHE:HA	1.72	0.43
1:D:659:ASN:HA	1:D:684:ARG:HD2	1.99	0.43
1:A:708:LEU:HD21	1:A:728:LEU:HD13	2.00	0.43
1:D:578:MET:HG3	1:D:599:LEU:HD22	2.00	0.43
1:D:673:ILE:HG13	1:D:699:PRO:HD3	2.01	0.43
1:D:800:LEU:HD21	1:D:803:LEU:HB2	2.00	0.43
1:F:496:LYS:HG2	1:F:519:HIS:CG	2.53	0.43
1:E:17:TYR:O	1:E:21:LYS:HG2	2.18	0.43
1:A:341:PRO:HB2	1:A:343:VAL:HG22	1.99	0.43
1:B:676:ILE:HG13	1:B:679:PHE:HD2	1.83	0.43
1:B:790:LEU:HB2	1:B:810:LEU:HD21	2.01	0.43
1:C:714:SER:HA	1:C:737:SER:O	2.18	0.43
1:C:578:MET:HE1	1:C:600:THR:H	1.82	0.43
1:B:313:VAL:HA	1:B:316:THR:HG22	2.00	0.43
1:B:393:LYS:HB3	1:B:414:ASN:HA	2.01	0.43
1:B:673:ILE:HG21	1:B:690:LEU:HD13	1.99	0.43
1:D:412:VAL:HB	1:D:416:PHE:HB3	2.00	0.43
1:E:553:PRO:HB2	1:E:556:VAL:HG13	2.00	0.43
1:E:659:ASN:HA	1:E:684:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:HIS:NE2	1:F:322:ILE:HD13	2.33	0.43
1:F:759:ILE:HD11	1:F:782:LEU:HD23	2.00	0.43
1:F:806:LYS:HG3	1:F:829:VAL:HG12	2.01	0.43
1:E:673:ILE:HG13	1:E:699:PRO:HD3	2.00	0.43
1:E:722:PRO:HG2	1:E:725:VAL:HB	2.00	0.43
1:E:773:LYS:HD3	1:E:796:GLN:HE22	1.84	0.43
1:B:652:HIS:HA	1:B:655:PHE:CD1	2.53	0.43
1:D:313:VAL:HA	1:D:316:THR:HG22	2.00	0.43
1:D:536:ARG:HG3	1:D:560:LYS:H	1.84	0.43
1:F:490:THR:HA	1:F:512[A]:MET:HA	2.00	0.43
1:F:733:CYS:HA	1:F:756:HIS:HB2	2.01	0.43
1:A:181:ASN:O	1:A:185:LYS:HG2	2.18	0.43
1:A:629:ASN:HA	1:A:632:LYS:HE2	2.01	0.43
1:C:406:PHE:CE2	1:C:442:SER:HB3	2.54	0.43
1:D:413:LYS:HD2	1:D:413:LYS:HA	1.87	0.43
1:F:777:LEU:HB3	1:F:780:LEU:HD21	1.99	0.43
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.88	0.43
1:F:357:ASN:HB2	1:E:151:GLN:NE2	2.34	0.43
1:F:711:LEU:HG	1:F:731:LEU:HD11	2.01	0.43
1:E:767:LEU:HD11	1:E:787:ILE:HD13	2.00	0.43
1:C:726:PHE:HA	1:C:751:LEU:HD21	2.00	0.43
1:D:564:GLU:HG2	1:D:592:ILE:HD12	2.01	0.43
1:F:299:GLU:CD	1:F:413:LYS:HZ3	2.26	0.43
1:E:28:MET:HB2	1:E:376:TYR:CE1	2.54	0.43
1:E:301:SER:O	1:E:415:ASP:HB2	2.19	0.43
1:E:313:VAL:HA	1:E:316:THR:HG22	2.00	0.43
1:E:736:VAL:HG23	1:E:759:ILE:HG22	2.00	0.43
1:A:624:LYS:HA	1:A:646:GLU:HB3	2.01	0.42
1:B:652:HIS:HA	1:B:655:PHE:HD1	1.83	0.42
1:D:427:ASP:HB3	1:D:430:TYR:HD1	1.85	0.42
1:F:455:TRP:HZ2	1:F:479:LEU:HD21	1.84	0.42
1:F:676:ILE:HA	1:F:679:PHE:CD2	2.54	0.42
1:E:560:LYS:HE2	1:E:588:ARG:HG3	2.00	0.42
1:F:735:ASP:HB2	1:F:758:HIS:HD2	1.84	0.42
1:E:309:VAL:HG22	1:E:387:LEU:HD23	2.01	0.42
1:E:427:ASP:HB3	1:E:430:TYR:HD1	1.84	0.42
1:E:779:THR:HA	1:E:802:GLN:HB3	2.02	0.42
1:A:597:SER:O	1:A:620:ASN:HA	2.19	0.42
1:C:648:GLU:HB3	1:C:671:ARG:HH12	1.84	0.42
1:C:650:ILE:HG23	1:C:654:ILE:HD12	2.00	0.42
1:D:373:ILE:HD13	1:D:373:ILE:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:TYR:O	1:F:21:LYS:HG3	2.20	0.42
1:F:487:PHE:CE2	1:F:506:PRO:HD2	2.55	0.42
1:E:760:THR:HA	1:E:783:GLY:O	2.19	0.42
1:A:165:PHE:HD1	1:A:165:PHE:HA	1.71	0.42
1:A:196:PHE:HE2	1:A:423:VAL:HG21	1.83	0.42
1:A:401:ARG:HG3	1:A:409:ILE:HG12	2.00	0.42
1:C:290:LYS:HE3	1:C:290:LYS:HB2	1.91	0.42
1:E:49:LYS:O	1:E:358:MET:HB3	2.20	0.42
1:C:652:HIS:HA	1:C:655:PHE:HD1	1.84	0.42
1:B:496:LYS:HG3	1:B:519:HIS:HB2	2.02	0.42
1:B:578:MET:HE3	1:B:601:LYS:HE2	2.01	0.42
1:B:719:GLU:O	1:B:741:ILE:HA	2.20	0.42
1:D:498:GLU:HA	1:D:521:CYS:HB2	2.01	0.42
1:F:521:CYS:SG	1:F:545:LYS:HD2	2.59	0.42
1:F:690:LEU:HB2	1:F:713:PHE:CD1	2.54	0.42
1:E:526:LYS:HA	1:E:555:TRP:HE1	1.84	0.42
1:E:777:LEU:HD21	1:E:780:LEU:HD13	2.01	0.42
1:A:689:LYS:HA	1:A:712:TYR:HB2	2.02	0.42
1:C:54:CYS:HA	1:C:354:CYS:HA	2.00	0.42
1:C:416:PHE:HD1	1:C:416:PHE:HA	1.68	0.42
1:D:401:ARG:HG3	1:D:409:ILE:HG12	2.02	0.42
1:F:496:LYS:HE2	1:F:519:HIS:CE1	2.55	0.42
1:E:490:THR:HG22	1:E:511:GLN:HG2	2.01	0.42
1:A:17:TYR:O	1:A:21:LYS:HG2	2.19	0.42
1:A:628:LEU:HD22	1:A:651:PRO:HG3	2.00	0.42
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.90	0.42
1:C:186:TYR:CE2	1:C:188:LYS:HB2	2.55	0.42
1:C:299:GLU:HA	1:C:413:LYS:HG3	2.01	0.42
1:B:666:LYS:HB2	1:B:691:TRP:HE1	1.85	0.42
1:D:196:PHE:HE2	1:D:423:VAL:HG21	1.84	0.42
1:D:650:ILE:HG23	1:D:654:ILE:HD12	2.01	0.42
1:D:769:LYS:HE3	1:D:793:LYS:HD3	2.01	0.42
1:E:358:MET:HE3	1:E:358:MET:HB2	1.89	0.42
1:A:666:LYS:HB2	1:A:691:TRP:HE1	1.85	0.42
1:C:19:ILE:HD13	1:C:20:LEU:HD22	2.01	0.42
1:C:659:ASN:HA	1:C:684:ARG:HD2	2.00	0.42
1:B:206:SER:HB3	1:B:209:THR:HG23	2.01	0.42
1:D:760:THR:HA	1:D:783:GLY:O	2.19	0.42
1:F:636:ASN:HB2	1:E:833:GLN:CD	2.44	0.42
1:F:677:ILE:HB	1:F:701:SER:HB2	2.01	0.42
1:F:784:GLN:NE2	1:F:807:GLY:HA3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:LYS:HB2	1:F:340:LYS:HE3	1.78	0.42
1:E:703:THR:HB	1:E:724:ALA:HB1	2.02	0.42
1:D:463:HIS:HD2	1:D:474:LEU:HD12	1.84	0.41
1:D:563:ARG:HA	1:D:589:HIS:O	2.19	0.41
1:F:19:ILE:HD11	1:F:423:VAL:HG13	2.02	0.41
1:C:192:LYS:H	1:C:192:LYS:HG2	1.71	0.41
1:C:757:LEU:HB3	1:C:780:LEU:HD23	2.01	0.41
1:B:496:LYS:HA	1:B:519:HIS:HB2	2.02	0.41
1:F:46:GLN:O	1:F:50:ASP:HB2	2.20	0.41
1:F:288:PHE:CE1	1:F:443:GLU:HB2	2.55	0.41
1:E:174:ILE:HD13	1:E:174:ILE:HA	1.89	0.41
1:E:469:GLN:HB2	1:E:471:LYS:HE2	2.02	0.41
1:A:41:PHE:O	1:A:45:MET:HG2	2.20	0.41
1:A:439:SER:OG	1:A:441:VAL:HG13	2.20	0.41
1:C:624:LYS:HA	1:C:645:CYS:O	2.20	0.41
1:B:578:MET:O	1:B:581:LEU:HG	2.21	0.41
1:B:617:VAL:HG13	1:B:641:GLU:HB2	2.03	0.41
1:E:601:LYS:HG3	1:E:627:VAL:HB	2.02	0.41
1:E:790:LEU:HD23	1:E:814:PRO:HD2	2.01	0.41
1:B:37:MET:HE3	1:B:37:MET:HB3	1.97	0.41
1:B:592:ILE:HG12	1:B:615:LYS:HB3	2.02	0.41
1:B:649:ARG:NH2	1:B:672:THR:H	2.18	0.41
1:F:36:LEU:HA	1:F:173:THR:HG21	2.02	0.41
1:E:208:TRP:CH2	1:E:442:SER:HB2	2.52	0.41
1:E:677:ILE:HD13	1:E:701:SER:HB2	2.02	0.41
1:E:689:LYS:HG2	1:E:712:TYR:CD1	2.55	0.41
1:C:319:PHE:CE1	1:C:377:GLY:HA3	2.55	0.41
1:D:512[A]:MET:HE2	1:D:515:LEU:HA	2.02	0.41
1:F:301:SER:O	1:F:415:ASP:HB2	2.19	0.41
1:E:768:PRO:HG2	1:E:771:LEU:HD23	2.01	0.41
1:A:52:VAL:HA	1:A:355:THR:O	2.21	0.41
1:A:174:ILE:HD13	1:A:174:ILE:HA	1.95	0.41
1:C:194:GLU:HA	1:C:197:VAL:HG12	2.02	0.41
1:B:341:PRO:HB2	1:B:343:VAL:HG22	2.01	0.41
1:D:602:VAL:HG21	1:D:631:LEU:HG	2.02	0.41
1:F:384:LEU:HD23	1:F:384:LEU:HA	1.92	0.41
1:C:358:MET:HE2	1:C:358:MET:HB3	1.88	0.41
1:C:765:ASP:O	1:C:787:ILE:HA	2.20	0.41
1:D:25:ASP:HA	1:D:28:MET:HG2	2.03	0.41
1:D:546:PHE:CZ	1:D:552:ILE:HD11	2.56	0.41
1:F:427:ASP:OD2	1:F:429:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:735:ASP:OD1	1:F:758:HIS:HB2	2.21	0.41
1:E:544:VAL:HG12	1:E:546:PHE:HD2	1.85	0.41
1:A:448:GLU:HA	1:A:451:LEU:HD23	2.03	0.41
1:B:39:ALA:HB1	1:B:170:LEU:HD22	2.01	0.41
1:D:527:VAL:HG21	1:D:532:PHE:HB2	2.02	0.41
1:E:285:LYS:NZ	1:E:447:ARG:HB3	2.36	0.41
1:C:647:LEU:O	1:C:668:ASN:HB3	2.21	0.41
1:C:733:CYS:HB2	1:C:756:HIS:HD2	1.85	0.41
1:B:401:ARG:HD3	1:B:409:ILE:H	1.86	0.41
1:D:571:LEU:HB2	1:D:599:LEU:HD21	2.03	0.41
1:F:473:GLU:HA	1:F:494:VAL:HB	2.03	0.41
1:F:676:ILE:HG13	1:F:679:PHE:HD2	1.86	0.41
1:F:682:LEU:HB2	1:F:685:LEU:HB2	2.03	0.41
1:F:702:ILE:HD12	1:F:725:VAL:HB	2.03	0.41
1:F:780:LEU:HB3	1:F:782:LEU:HD11	2.03	0.41
1:E:170:LEU:HD22	1:E:170:LEU:HA	1.97	0.41
1:E:319:PHE:CE1	1:E:377:GLY:HA3	2.56	0.41
1:E:691:TRP:HA	1:E:716:ASN:HD21	1.86	0.41
1:E:691:TRP:CD1	1:E:691:TRP:H	2.38	0.41
1:C:664:ASP:HA	1:C:689:LYS:O	2.21	0.41
1:C:666:LYS:HB2	1:C:691:TRP:HE1	1.85	0.41
1:C:680:GLN:HB3	1:C:704:HIS:HB3	2.03	0.41
1:B:614:THR:HA	1:B:637:VAL:HA	2.03	0.41
1:B:661:GLN:HA	1:B:685:LEU:HA	2.02	0.41
1:B:814:PRO:HB2	1:B:816:GLN:OE1	2.21	0.41
1:D:301:SER:O	1:D:415:ASP:HB2	2.21	0.41
1:F:279:LYS:O	1:F:283:GLN:HG2	2.21	0.41
1:E:817:LEU:HD21	1:E:838:LEU:HD21	2.03	0.41
1:A:698:ILE:HB	1:A:722:PRO:HG3	2.02	0.40
1:D:20:LEU:HB3	1:D:183:TRP:HH2	1.86	0.40
1:D:497:LEU:HB3	1:D:500:ILE:HD12	2.02	0.40
1:E:36:LEU:HA	1:E:173:THR:HG21	2.03	0.40
1:E:615:LYS:HG3	1:E:639:GLU:HB2	2.03	0.40
1:C:628:LEU:HD22	1:C:651:PRO:HG3	2.03	0.40
1:B:778:ARG:HA	1:B:800:LEU:HA	2.02	0.40
1:D:483:PRO:O	1:D:486:VAL:HG12	2.21	0.40
1:D:768:PRO:HG2	1:D:771:LEU:HD23	2.02	0.40
1:F:711:LEU:HB3	1:F:713:PHE:CE2	2.56	0.40
1:E:149:ILE:HD13	1:E:149:ILE:HA	1.90	0.40
1:E:320:ILE:HD13	1:E:320:ILE:HA	1.95	0.40
1:A:655:PHE:CE1	1:A:678:SER:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:O	1:B:45:MET:HG2	2.21	0.40
1:F:587:LEU:HB3	1:F:590:LEU:HB2	2.03	0.40
1:F:755:GLN:HA	1:F:777:LEU:HA	2.03	0.40
1:E:141:LEU:HD12	1:E:141:LEU:HA	1.93	0.40
1:E:539:LEU:HG	1:E:562:LEU:HD13	2.03	0.40
1:C:390:ILE:HD12	1:C:390:ILE:HA	1.96	0.40
1:B:773:LYS:HD3	1:B:796:GLN:HE22	1.86	0.40
1:D:19:ILE:HD11	1:D:423:VAL:HG13	2.04	0.40
1:D:503:ALA:HB3	1:D:525:ALA:HA	2.02	0.40
1:D:790:LEU:HD12	1:D:791:PRO:HD2	2.04	0.40
1:F:557:TYR:CD1	1:F:582:GLU:HB2	2.57	0.40
1:F:693:ASN:HB2	1:F:695:ILE:HG13	2.03	0.40
1:E:642:LEU:HD12	1:E:654:ILE:HD11	2.02	0.40
1:D:41:PHE:O	1:D:45:MET:HG2	2.22	0.40
1:D:578:MET:HB3	1:D:581:LEU:HD11	2.04	0.40
1:F:138:LYS:C	1:F:140:ASN:H	2.28	0.40
1:F:309:VAL:HG22	1:F:387:LEU:HD23	2.03	0.40
1:F:840:LEU:HA	1:F:843:LYS:HE2	2.04	0.40
1:E:708:LEU:HD21	1:E:728: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	697/924 (75%)	676 (97%)	20 (3%)	1 (0%)	48	80
1	B	697/924 (75%)	669 (96%)	27 (4%)	1 (0%)	48	80
1	C	697/924 (75%)	662 (95%)	34 (5%)	1 (0%)	48	80
1	D	697/924 (75%)	671 (96%)	25 (4%)	1 (0%)	48	80
1	E	697/924 (75%)	676 (97%)	20 (3%)	1 (0%)	48	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	697/924 (75%)	671 (96%)	25 (4%)	1 (0%)	48	80
All	All	4182/5544 (75%)	4025 (96%)	151 (4%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	60	SER
1	A	60	SER
1	C	60	SER
1	B	60	SER
1	F	60	SER
1	E	60	SER

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	655/842 (78%)	630 (96%)	25 (4%)	29	63
1	B	655/842 (78%)	625 (95%)	30 (5%)	24	58
1	C	655/842 (78%)	625 (95%)	30 (5%)	24	58
1	D	655/842 (78%)	634 (97%)	21 (3%)	34	67
1	E	655/842 (78%)	629 (96%)	26 (4%)	28	62
1	F	655/842 (78%)	625 (95%)	30 (5%)	24	58
All	All	3930/5052 (78%)	3768 (96%)	162 (4%)	28	61

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	19	ILE
1	A	51	GLN
1	A	140	ASN
1	A	152	MET

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Mol	Chain	Res	Type
1	A	165	PHE
1	A	170	LEU
1	A	183	TRP
1	A	303	LEU
1	A	319	PHE
1	A	336	GLU
1	A	344	GLU
1	A	346	LEU
1	A	354	CYS
1	A	355	THR
1	A	387	LEU
1	A	390	ILE
1	A	397	PHE
1	A	414	ASN
1	A	441	VAL
1	A	451	LEU
1	A	704	HIS
1	A	784	GLN
1	A	805	LEU
1	A	829	VAL
1	C	19	ILE
1	C	46	GLN
1	C	54	CYS
1	C	140	ASN
1	C	165	PHE
1	C	183	TRP
1	C	184	PHE
1	C	280	ASP
1	C	293	LYS
1	C	319	PHE
1	C	330	VAL
1	C	346	LEU
1	C	354	CYS
1	C	355	THR
1	C	365	LEU
1	C	387	LEU
1	C	390	ILE
1	C	392	LEU
1	C	413	LYS
1	C	416	PHE
1	C	441	VAL
1	C	459	LYS

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Mol	Chain	Res	Type
1	C	512[A]	MET
1	C	512[B]	MET
1	C	513	THR
1	C	677	ILE
1	C	698	ILE
1	C	705	VAL
1	C	728	LEU
1	C	782	LEU
1	B	16	THR
1	B	17	TYR
1	B	19	ILE
1	B	20	LEU
1	B	25	ASP
1	B	51	GLN
1	B	53	VAL
1	B	138	LYS
1	B	141	LEU
1	B	165	PHE
1	B	173	THR
1	B	183	TRP
1	B	280	ASP
1	B	292	ARG
1	B	319	PHE
1	B	336	GLU
1	B	344	GLU
1	B	346	LEU
1	B	354	CYS
1	B	355	THR
1	B	365	LEU
1	B	379	ILE
1	B	387	LEU
1	B	390	ILE
1	B	441	VAL
1	B	492	LEU
1	B	556	VAL
1	B	728	LEU
1	B	734	LEU
1	B	829	VAL
1	D	16	THR
1	D	17	TYR
1	D	19	ILE
1	D	20	LEU

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Mol	Chain	Res	Type
1	D	51	GLN
1	D	53	VAL
1	D	60	SER
1	D	141	LEU
1	D	173	THR
1	D	183	TRP
1	D	319	PHE
1	D	336	GLU
1	D	344	GLU
1	D	346	LEU
1	D	354	CYS
1	D	355	THR
1	D	397	PHE
1	D	416	PHE
1	D	725	VAL
1	D	817	LEU
1	D	829	VAL
1	F	19	ILE
1	F	27	PHE
1	F	51	GLN
1	F	54	CYS
1	F	141	LEU
1	F	165	PHE
1	F	183	TRP
1	F	184	PHE
1	F	293	LYS
1	F	300	ASP
1	F	319	PHE
1	F	325	TYR
1	F	336	GLU
1	F	346	LEU
1	F	354	CYS
1	F	355	THR
1	F	365	LEU
1	F	390	ILE
1	F	392	LEU
1	F	397	PHE
1	F	409	ILE
1	F	420	LEU
1	F	463	HIS
1	F	512[A]	MET
1	F	512[B]	MET

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Mol	Chain	Res	Type
1	F	513	THR
1	F	637	VAL
1	F	673	ILE
1	F	677	ILE
1	F	705	VAL
1	E	19	ILE
1	E	20	LEU
1	E	25	ASP
1	E	46	GLN
1	E	51	GLN
1	E	53	VAL
1	E	60	SER
1	E	141	LEU
1	E	165	PHE
1	E	170	LEU
1	E	183	TRP
1	E	195	HIS
1	E	303	LEU
1	E	319	PHE
1	E	336	GLU
1	E	344	GLU
1	E	346	LEU
1	E	354	CYS
1	E	365	LEU
1	E	387	LEU
1	E	397	PHE
1	E	441	VAL
1	E	454	GLU
1	E	725	VAL
1	E	734	LEU
1	E	829	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	311	GLN
1	A	357	ASN
1	A	414	ASN
1	A	425	GLN
1	A	511	GLN
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	629	ASN
1	A	704	HIS
1	A	740	ASN
1	A	833	GLN
1	C	145	GLN
1	C	155	HIS
1	C	462	GLN
1	C	522	HIS
1	C	561	ASN
1	C	570	ASN
1	C	572	ASN
1	C	707	ASN
1	C	752	GLN
1	C	770	GLN
1	C	784	GLN
1	C	796	GLN
1	B	155	HIS
1	B	172	HIS
1	B	181	ASN
1	B	357	ASN
1	B	463	HIS
1	B	467	ASN
1	B	511	GLN
1	B	629	ASN
1	B	784	GLN
1	B	799	GLN
1	D	140	ASN
1	D	145	GLN
1	D	181	ASN
1	D	357	ASN
1	D	453	HIS
1	D	570	ASN
1	D	594	HIS
1	D	819	GLN
1	F	155	HIS
1	F	462	GLN
1	F	463	HIS
1	F	511	GLN
1	F	519	HIS
1	F	522	HIS
1	F	543	HIS
1	F	572	ASN

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Mol	Chain	Res	Type
1	F	629	ASN
1	F	707	ASN
1	F	716	ASN
1	F	770	GLN
1	F	796	GLN
1	E	145	GLN
1	E	181	ASN
1	E	195	HIS
1	E	311	GLN
1	E	784	GLN
1	E	808	ASN
1	E	819	GLN
1	E	833	GLN

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](#)

There are no ligands in this entry.

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.

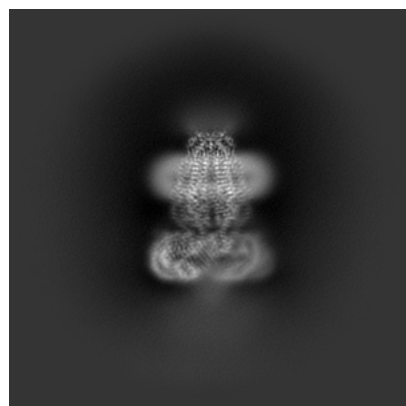
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55589. These allow visual inspection of the internal detail of the map and identification of artifacts.

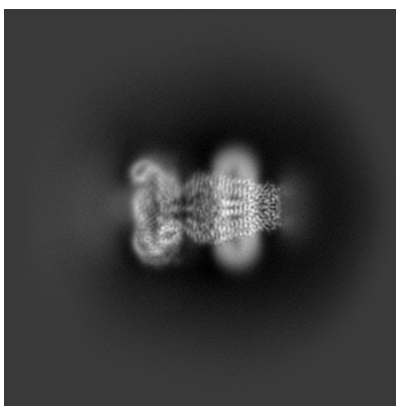
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

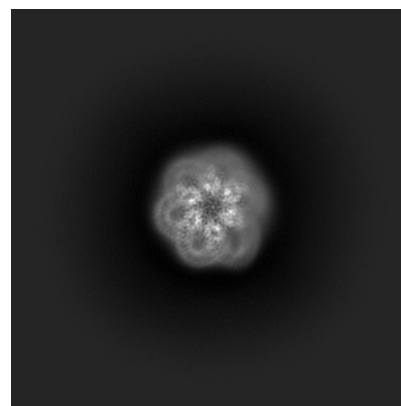
6.1.1 Primary map



X

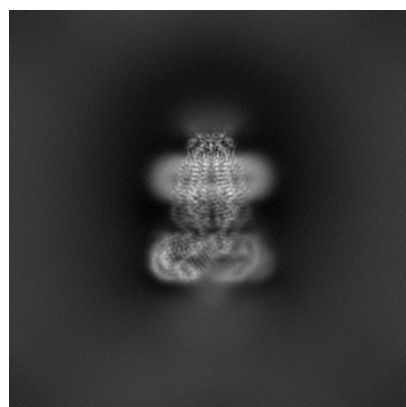


Y

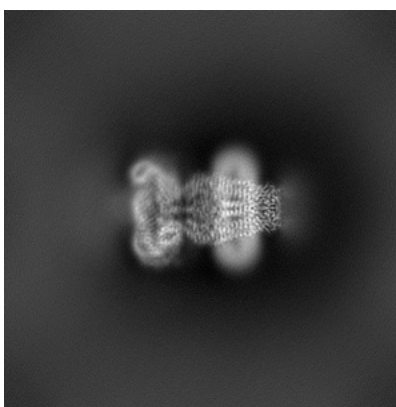


Z

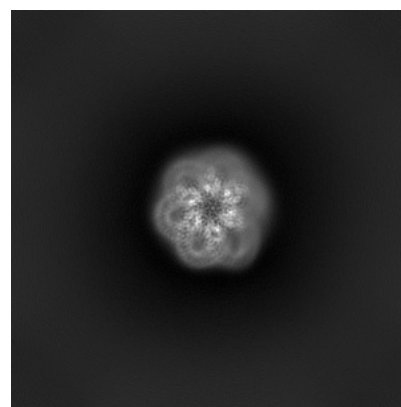
6.1.2 Raw map



X



Y

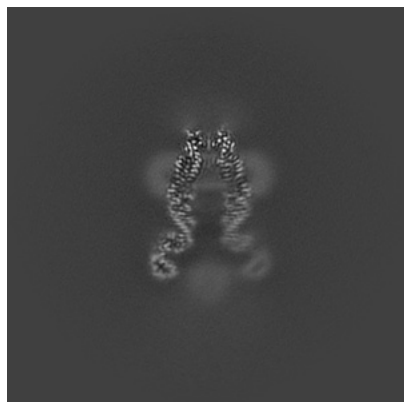


Z

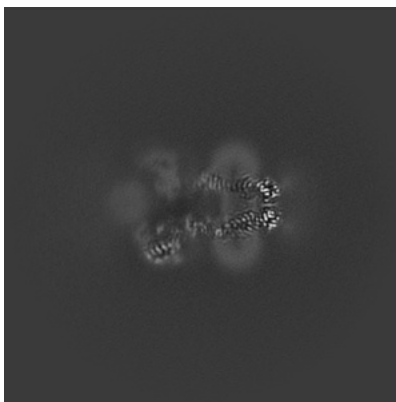
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

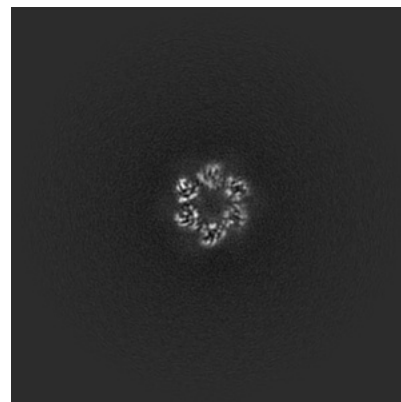
6.2.1 Primary map



X Index: 168

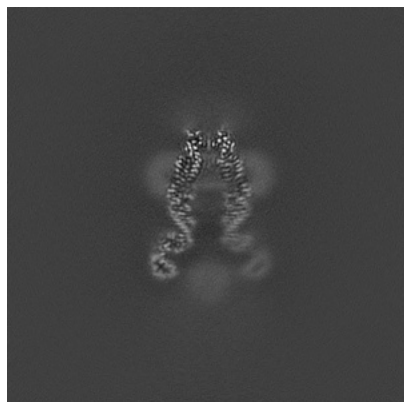


Y Index: 168

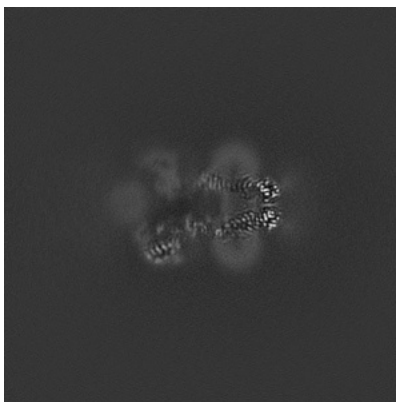


Z Index: 168

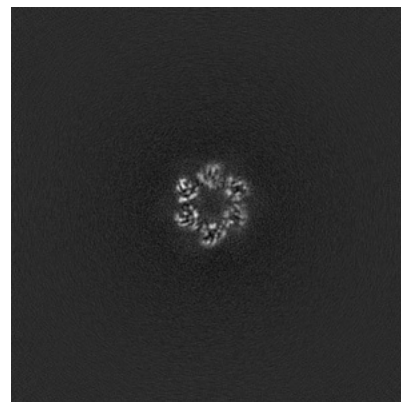
6.2.2 Raw map



X Index: 168



Y Index: 168

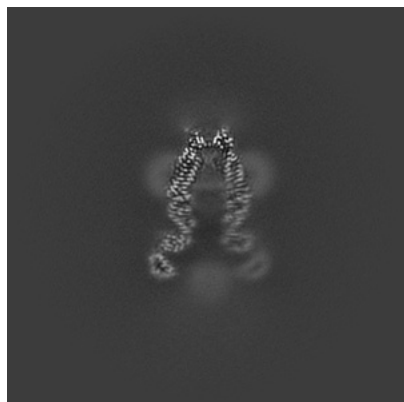


Z Index: 168

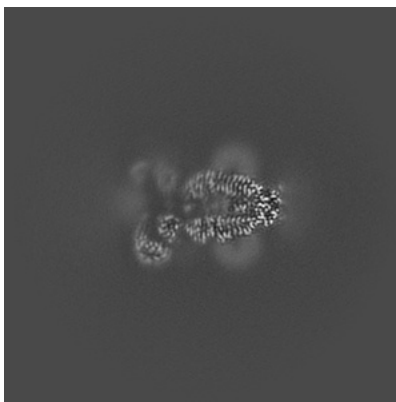
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

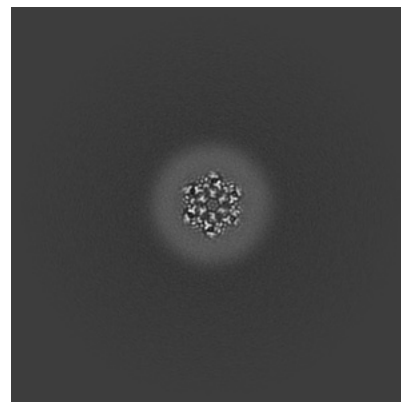
6.3.1 Primary map



X Index: 166

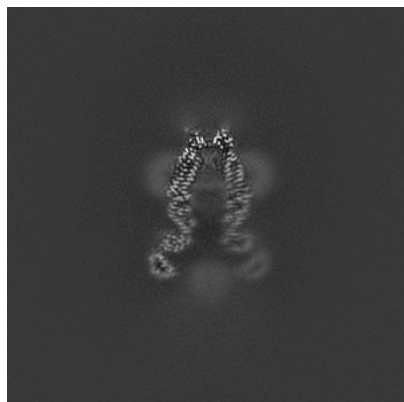


Y Index: 157

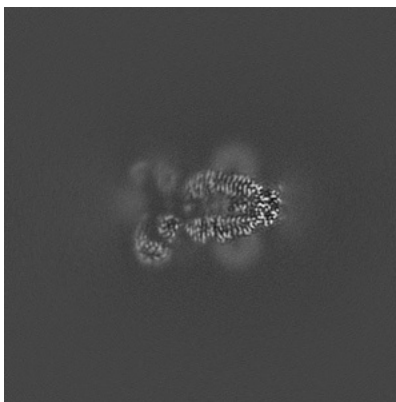


Z Index: 206

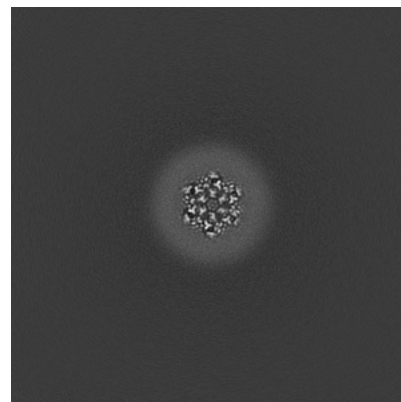
6.3.2 Raw map



X Index: 166



Y Index: 157

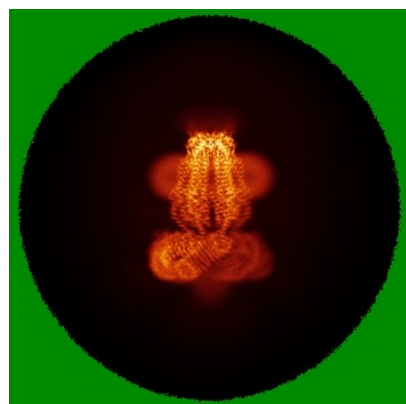


Z Index: 206

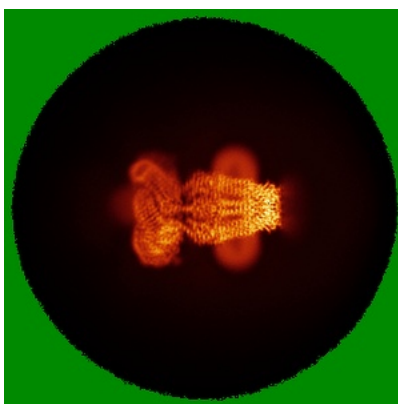
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

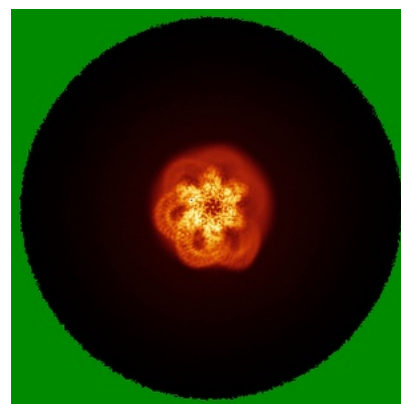
6.4.1 Primary map



X

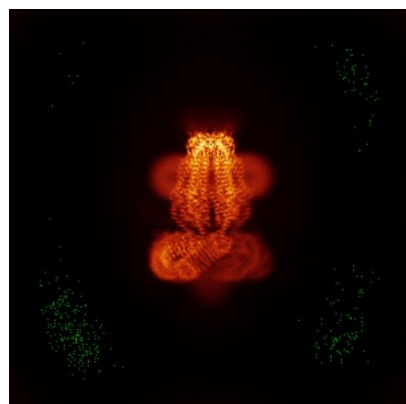


Y

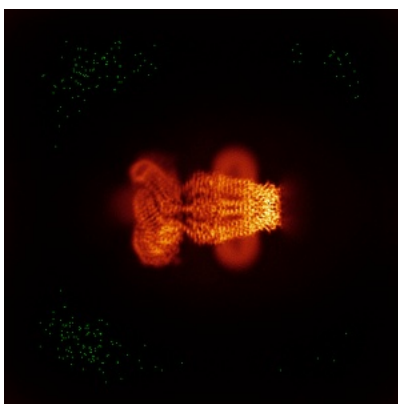


Z

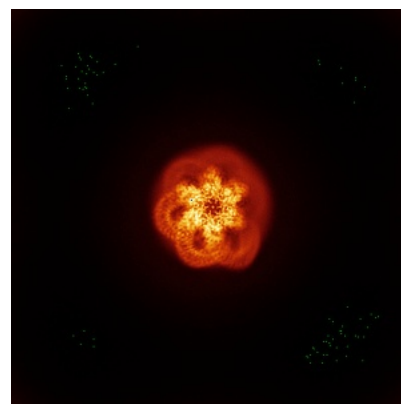
6.4.2 Raw map



X



Y

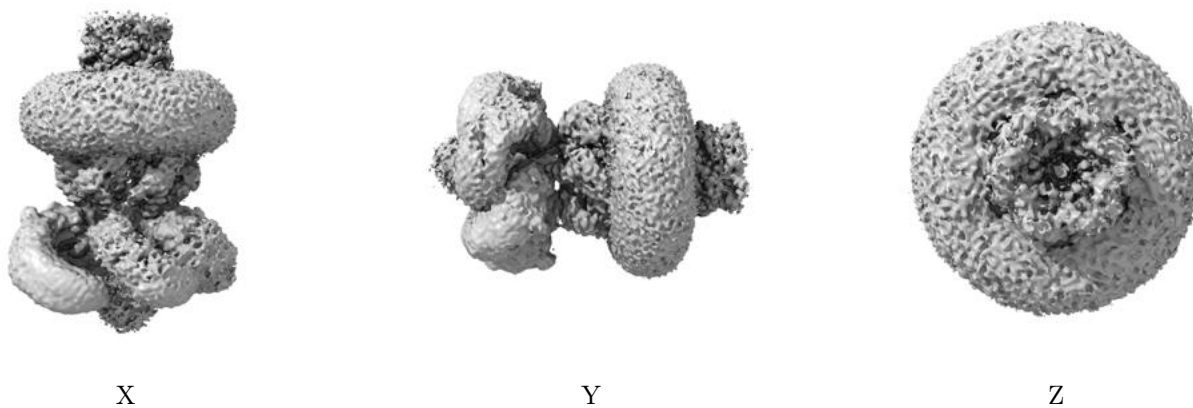


Z

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.

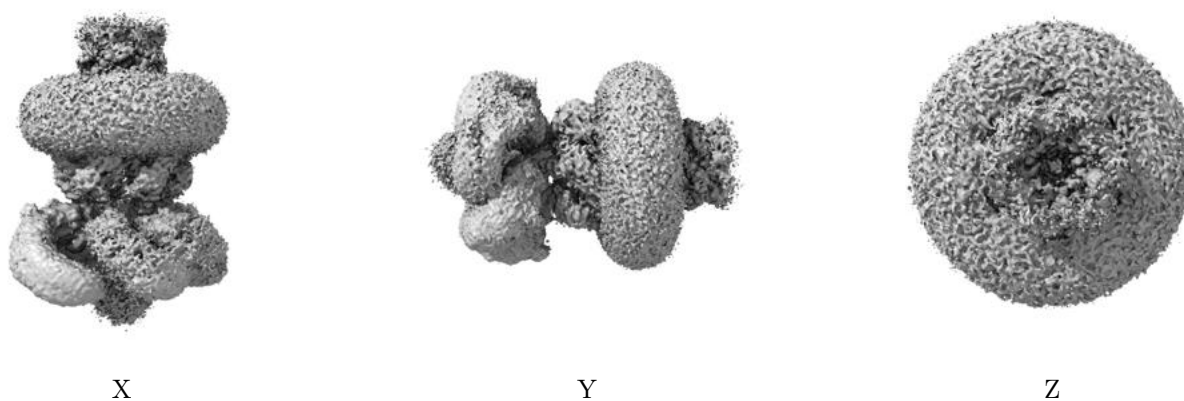
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.111. 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.

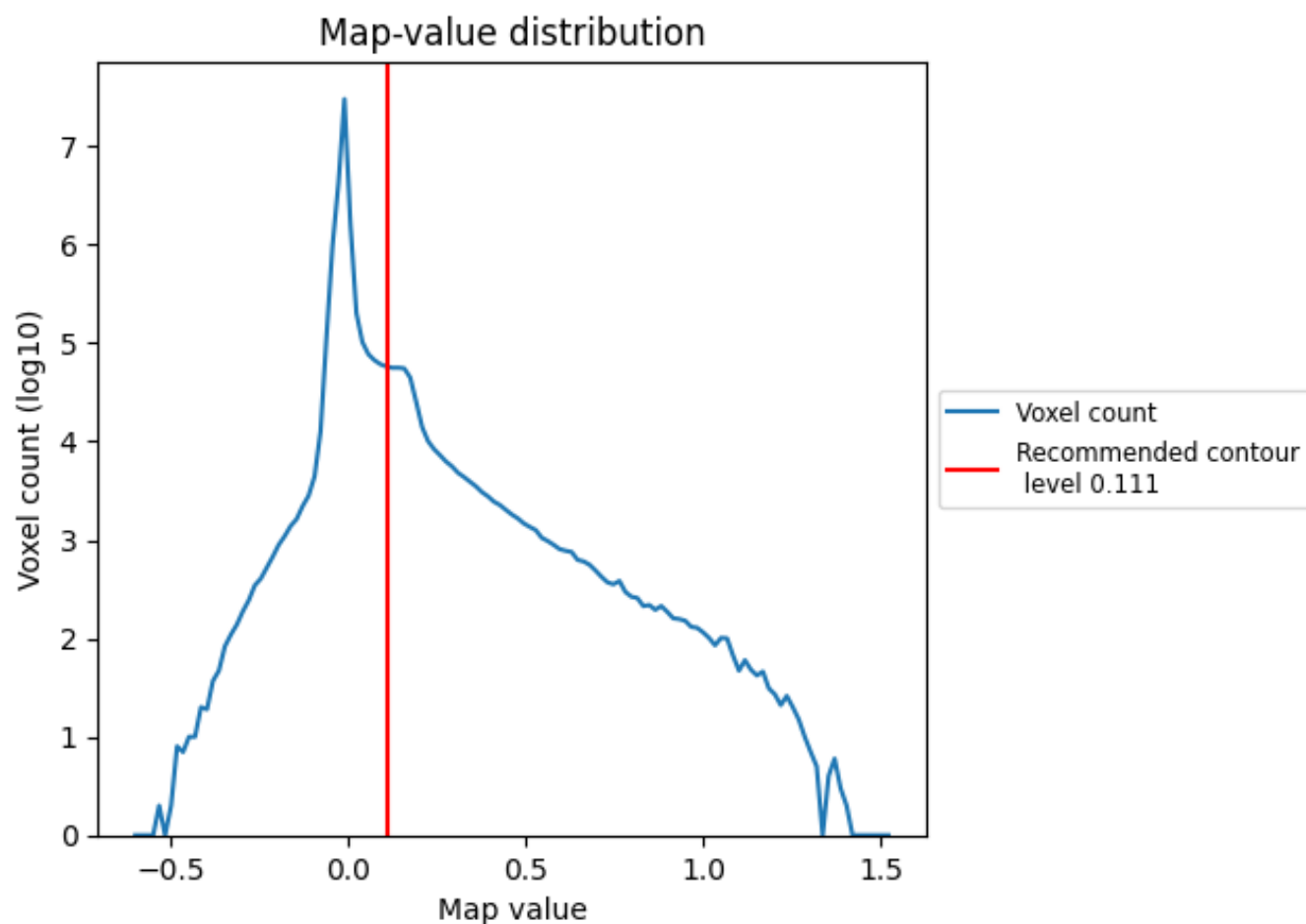
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

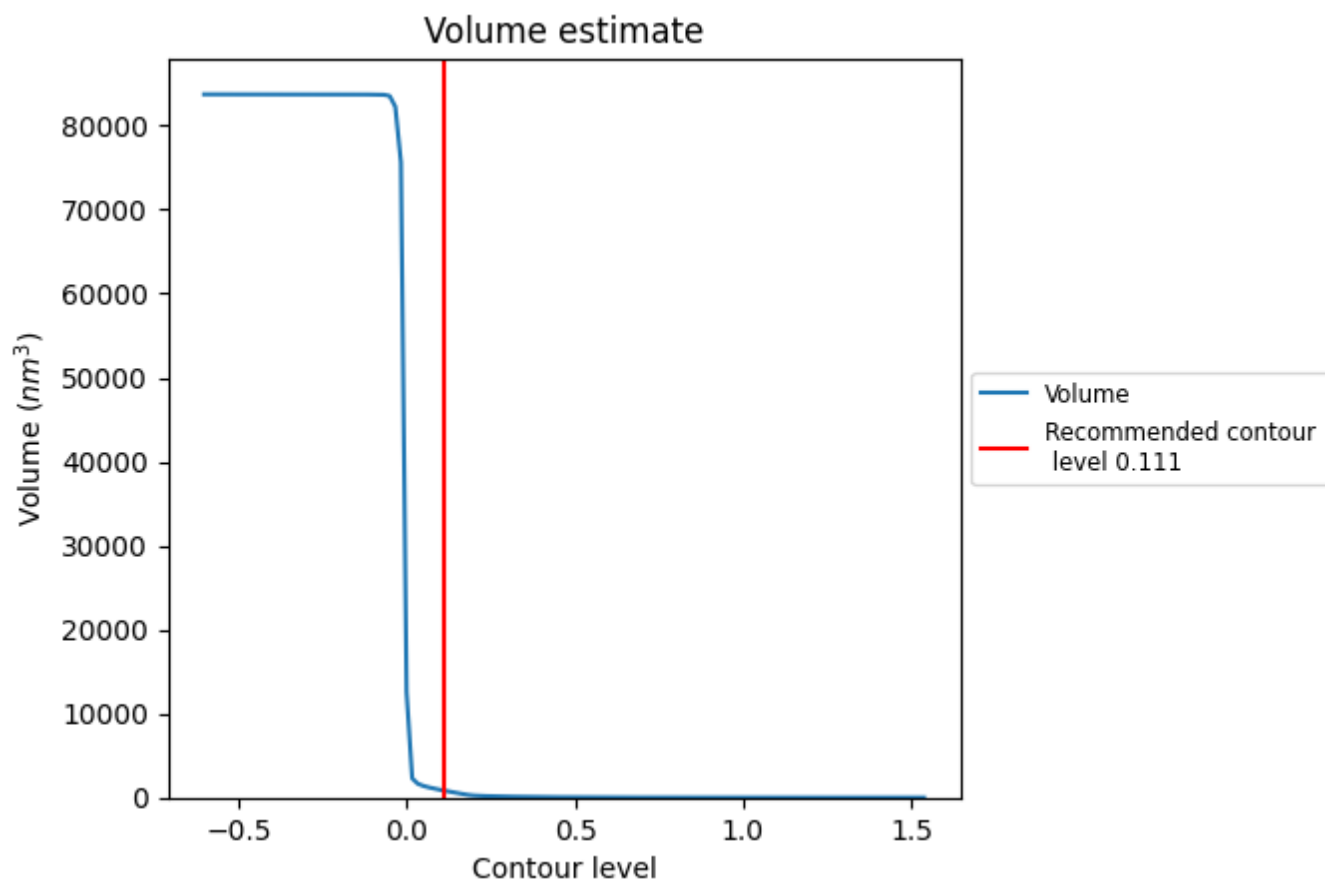
This section contains the results of statistical analysis of the map.

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.

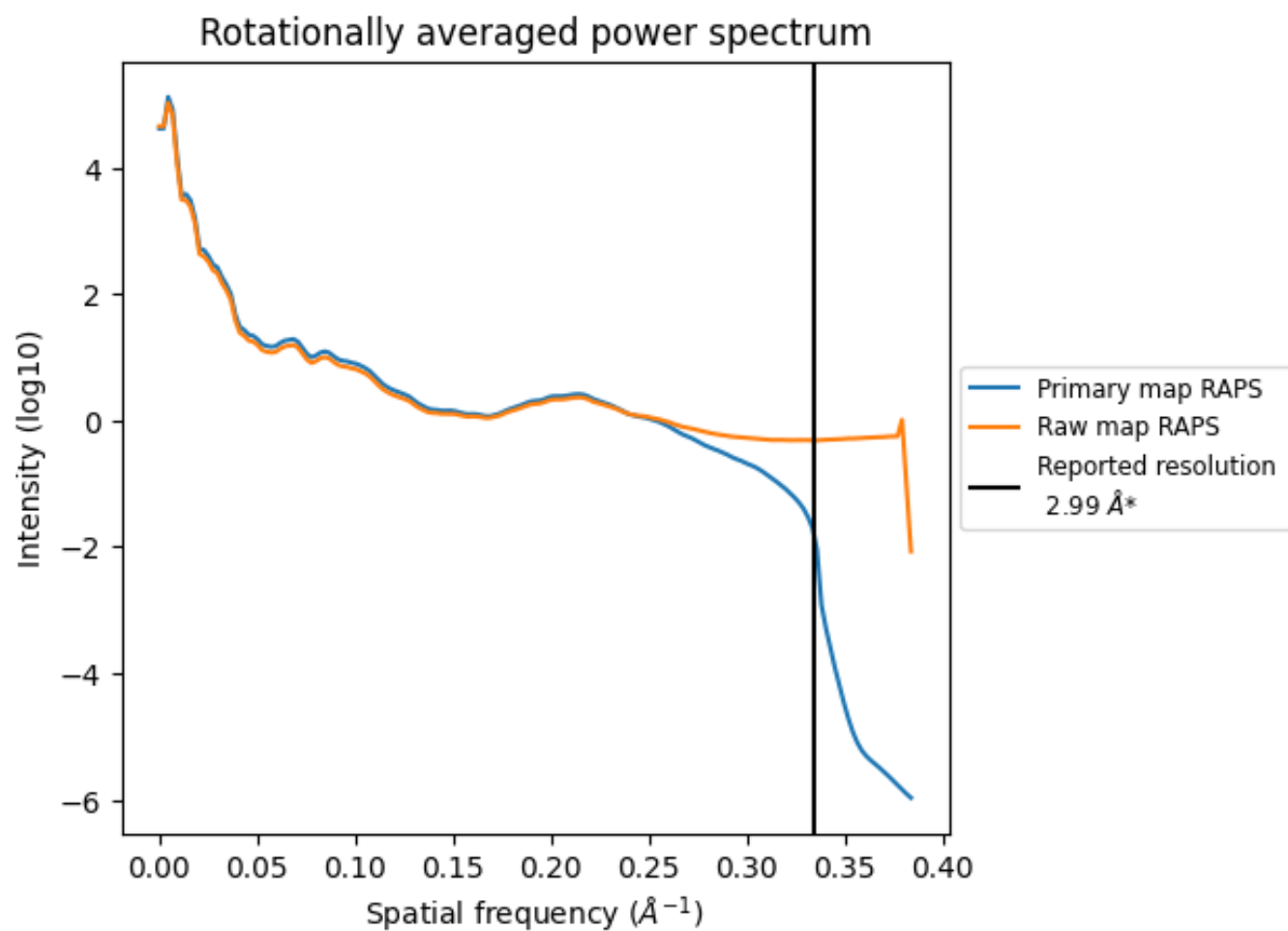
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 835 nm^3 ; this corresponds to an approximate mass of 754 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 [i](#)

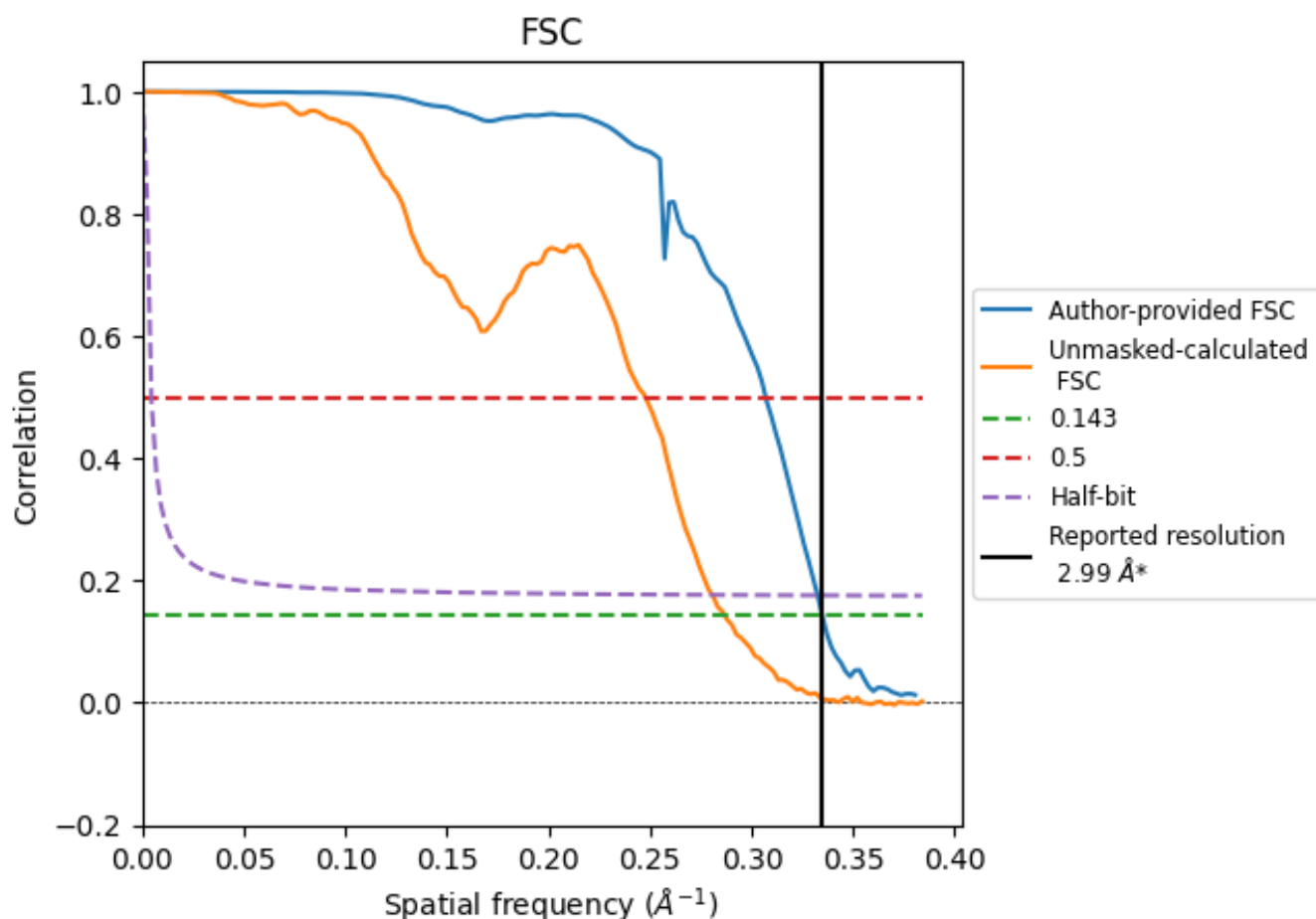


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

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 0.334 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

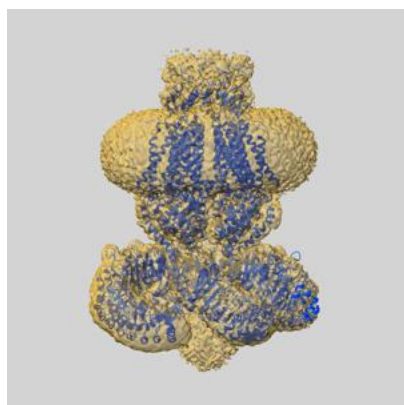
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.26	3.01
Unmasked-calculated*	3.49	4.04	3.56

*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 3.49 differs from the reported value 2.99 by more than 10 %

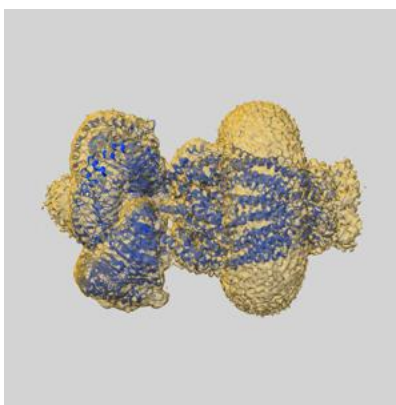
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55589 and PDB model 9T5M. Per-residue inclusion information can be found in section 3 on page 15.

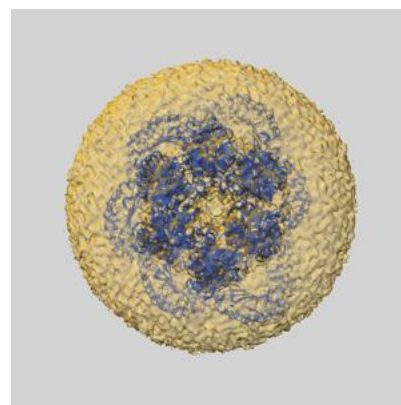
9.1 Map-model overlay [i](#)



X



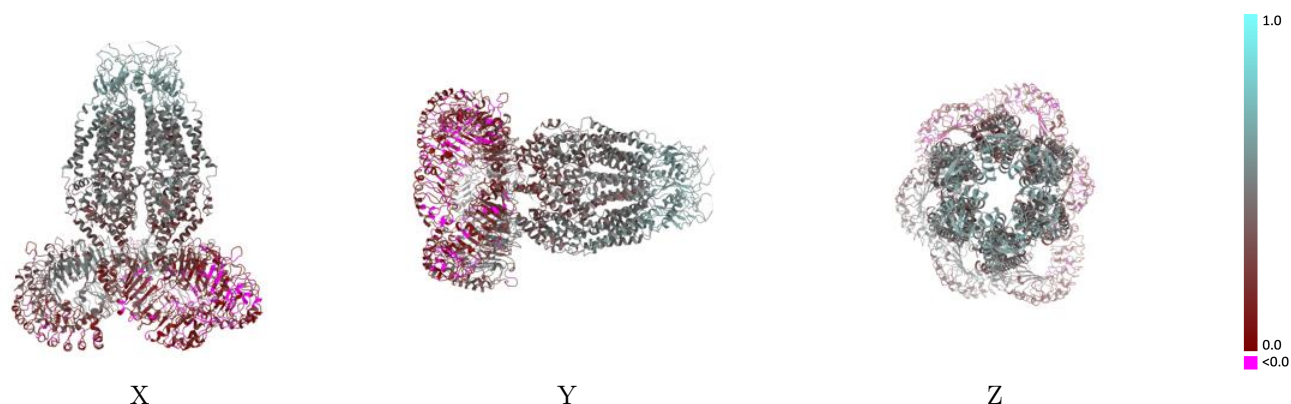
Y



Z

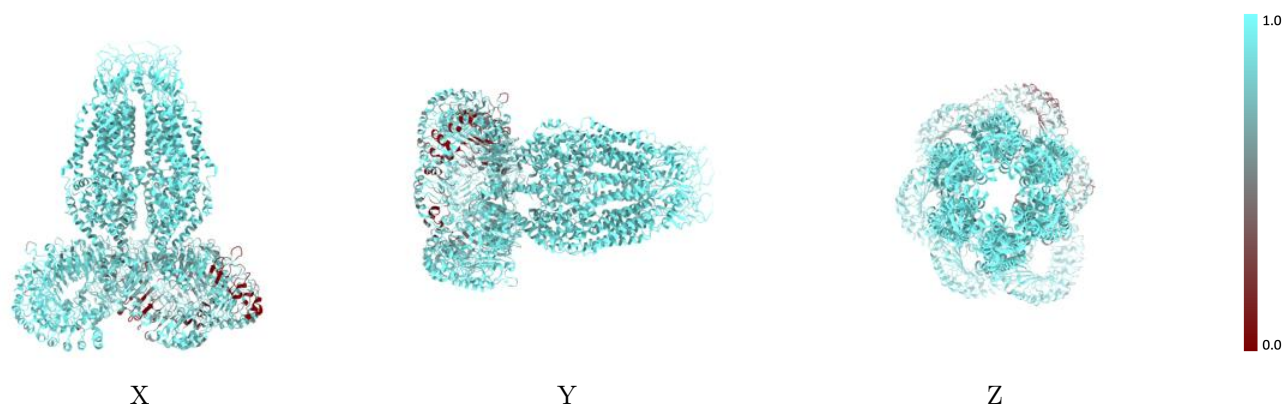
The images above show the 3D surface view of the map at the recommended contour level 0.111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



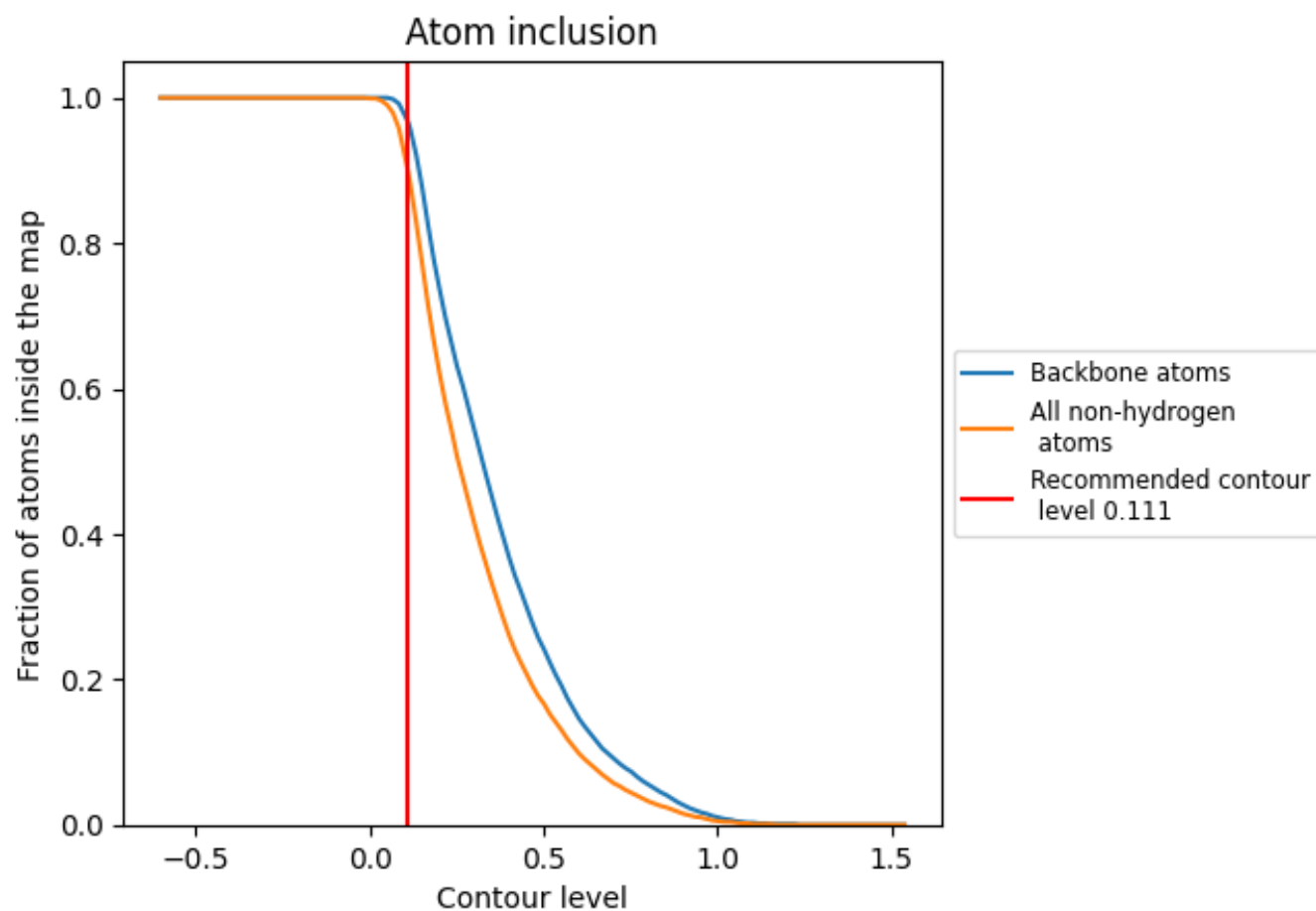
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.111).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.3500
A	0.9610	0.4510
B	0.9630	0.4470
C	0.9490	0.3720
D	0.8250	0.2920
E	0.8120	0.2740
F	0.8700	0.2640

