



Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 08:31 AM EDT

PDB ID : 9Y9C / pdb_00009y9c
EMDB ID : EMD-72693
Title : Cryo-EM map of the in vitro reconstituted RAZR:GP77 complex with AlphaFold-predicted models fitted into the density.
Authors : Lyu, Y.; Zhang, T.; Laub, M.; Ghanbarpour, A.
Deposited on : 2025-09-14
Resolution : 3.50 Å(reported)
Based on initial model : .

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

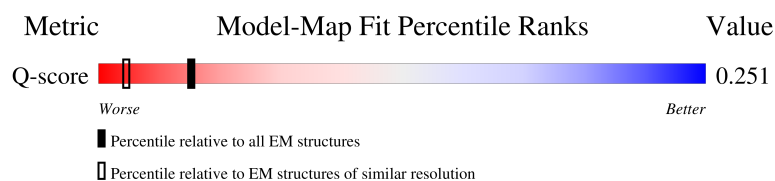
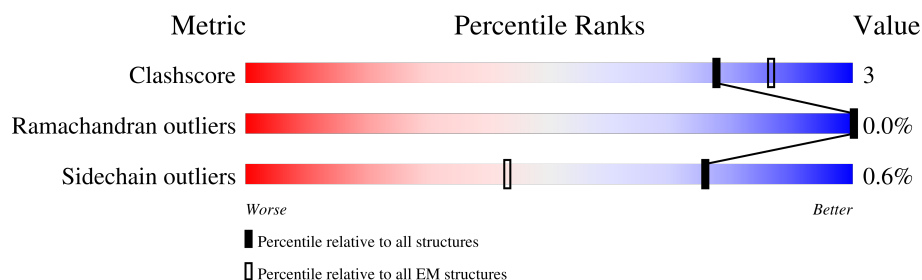
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



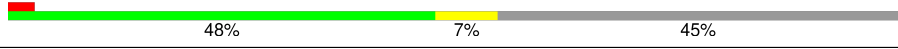
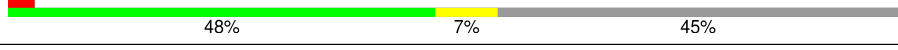
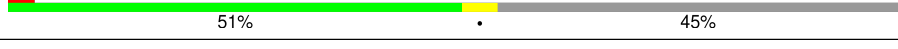
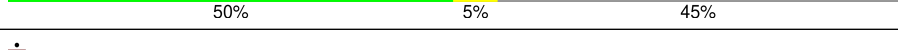
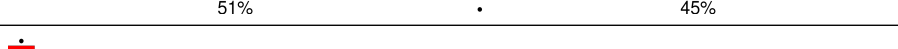
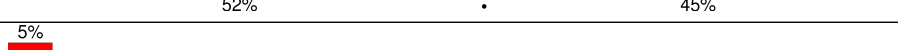
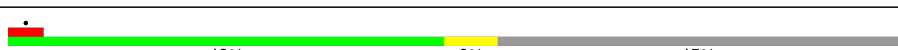
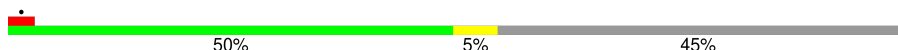
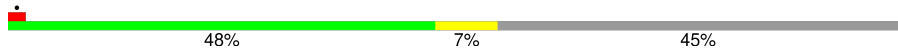
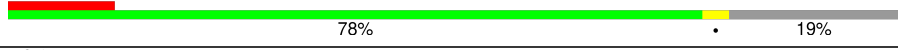
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	IA	227	
1	IB	227	
1	IC	227	
1	ID	227	

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Mol	Chain	Length	Quality of chain
1	IE	227	
1	IF	227	
1	IG	227	
1	IH	227	
1	II	227	
1	IJ	227	
1	IK	227	
1	IL	227	
1	IM	227	
1	IN	227	
1	IO	227	
1	IP	227	
1	IQ	227	
1	IR	227	
1	IS	227	
1	IT	227	
1	IU	227	
1	IV	227	
1	IW	227	
1	IX	227	
2	OA	219	
2	OB	219	
2	OC	219	
2	OD	219	
2	OE	219	

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Mol	Chain	Length	Quality of chain
2	OF	219	
2	OG	219	
2	OH	219	
2	OI	219	
2	OJ	219	
2	OK	219	
2	OL	219	
2	OM	219	
2	ON	219	
2	OO	219	
2	OP	219	
2	OQ	219	
2	OR	219	
2	OS	219	
2	OT	219	
2	OU	219	
2	OV	219	
2	OW	219	
2	OX	219	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 112779 atoms, of which 55949 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 Gp77.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	IA	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IB	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IC	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	ID	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IE	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IF	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IG	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IH	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	II	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IJ	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IK	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IL	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IM	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IN	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IO	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IP	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IQ	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	IR	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IS	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IT	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IU	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IV	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IW	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		
1	IX	125	Total	C	H	N	O	S	0	0
			1972	623	986	172	186	5		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IA	218	GLY	-	expression tag	UNP A0AAE8YXX1
IA	219	SER	-	expression tag	UNP A0AAE8YXX1
IA	220	SER	-	expression tag	UNP A0AAE8YXX1
IA	221	GLY	-	expression tag	UNP A0AAE8YXX1
IA	222	HIS	-	expression tag	UNP A0AAE8YXX1
IA	223	HIS	-	expression tag	UNP A0AAE8YXX1
IA	224	HIS	-	expression tag	UNP A0AAE8YXX1
IA	225	HIS	-	expression tag	UNP A0AAE8YXX1
IA	226	HIS	-	expression tag	UNP A0AAE8YXX1
IA	227	HIS	-	expression tag	UNP A0AAE8YXX1
IB	218	GLY	-	expression tag	UNP A0AAE8YXX1
IB	219	SER	-	expression tag	UNP A0AAE8YXX1
IB	220	SER	-	expression tag	UNP A0AAE8YXX1
IB	221	GLY	-	expression tag	UNP A0AAE8YXX1
IB	222	HIS	-	expression tag	UNP A0AAE8YXX1
IB	223	HIS	-	expression tag	UNP A0AAE8YXX1
IB	224	HIS	-	expression tag	UNP A0AAE8YXX1
IB	225	HIS	-	expression tag	UNP A0AAE8YXX1
IB	226	HIS	-	expression tag	UNP A0AAE8YXX1
IB	227	HIS	-	expression tag	UNP A0AAE8YXX1
IC	218	GLY	-	expression tag	UNP A0AAE8YXX1
IC	219	SER	-	expression tag	UNP A0AAE8YXX1
IC	220	SER	-	expression tag	UNP A0AAE8YXX1
IC	221	GLY	-	expression tag	UNP A0AAE8YXX1
IC	222	HIS	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IC	223	HIS	-	expression tag	UNP A0AAE8YXX1
IC	224	HIS	-	expression tag	UNP A0AAE8YXX1
IC	225	HIS	-	expression tag	UNP A0AAE8YXX1
IC	226	HIS	-	expression tag	UNP A0AAE8YXX1
IC	227	HIS	-	expression tag	UNP A0AAE8YXX1
ID	218	GLY	-	expression tag	UNP A0AAE8YXX1
ID	219	SER	-	expression tag	UNP A0AAE8YXX1
ID	220	SER	-	expression tag	UNP A0AAE8YXX1
ID	221	GLY	-	expression tag	UNP A0AAE8YXX1
ID	222	HIS	-	expression tag	UNP A0AAE8YXX1
ID	223	HIS	-	expression tag	UNP A0AAE8YXX1
ID	224	HIS	-	expression tag	UNP A0AAE8YXX1
ID	225	HIS	-	expression tag	UNP A0AAE8YXX1
ID	226	HIS	-	expression tag	UNP A0AAE8YXX1
ID	227	HIS	-	expression tag	UNP A0AAE8YXX1
IE	218	GLY	-	expression tag	UNP A0AAE8YXX1
IE	219	SER	-	expression tag	UNP A0AAE8YXX1
IE	220	SER	-	expression tag	UNP A0AAE8YXX1
IE	221	GLY	-	expression tag	UNP A0AAE8YXX1
IE	222	HIS	-	expression tag	UNP A0AAE8YXX1
IE	223	HIS	-	expression tag	UNP A0AAE8YXX1
IE	224	HIS	-	expression tag	UNP A0AAE8YXX1
IE	225	HIS	-	expression tag	UNP A0AAE8YXX1
IE	226	HIS	-	expression tag	UNP A0AAE8YXX1
IE	227	HIS	-	expression tag	UNP A0AAE8YXX1
IF	218	GLY	-	expression tag	UNP A0AAE8YXX1
IF	219	SER	-	expression tag	UNP A0AAE8YXX1
IF	220	SER	-	expression tag	UNP A0AAE8YXX1
IF	221	GLY	-	expression tag	UNP A0AAE8YXX1
IF	222	HIS	-	expression tag	UNP A0AAE8YXX1
IF	223	HIS	-	expression tag	UNP A0AAE8YXX1
IF	224	HIS	-	expression tag	UNP A0AAE8YXX1
IF	225	HIS	-	expression tag	UNP A0AAE8YXX1
IF	226	HIS	-	expression tag	UNP A0AAE8YXX1
IF	227	HIS	-	expression tag	UNP A0AAE8YXX1
IG	218	GLY	-	expression tag	UNP A0AAE8YXX1
IG	219	SER	-	expression tag	UNP A0AAE8YXX1
IG	220	SER	-	expression tag	UNP A0AAE8YXX1
IG	221	GLY	-	expression tag	UNP A0AAE8YXX1
IG	222	HIS	-	expression tag	UNP A0AAE8YXX1
IG	223	HIS	-	expression tag	UNP A0AAE8YXX1
IG	224	HIS	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IG	225	HIS	-	expression tag	UNP A0AAE8YXX1
IG	226	HIS	-	expression tag	UNP A0AAE8YXX1
IG	227	HIS	-	expression tag	UNP A0AAE8YXX1
IH	218	GLY	-	expression tag	UNP A0AAE8YXX1
IH	219	SER	-	expression tag	UNP A0AAE8YXX1
IH	220	SER	-	expression tag	UNP A0AAE8YXX1
IH	221	GLY	-	expression tag	UNP A0AAE8YXX1
IH	222	HIS	-	expression tag	UNP A0AAE8YXX1
IH	223	HIS	-	expression tag	UNP A0AAE8YXX1
IH	224	HIS	-	expression tag	UNP A0AAE8YXX1
IH	225	HIS	-	expression tag	UNP A0AAE8YXX1
IH	226	HIS	-	expression tag	UNP A0AAE8YXX1
IH	227	HIS	-	expression tag	UNP A0AAE8YXX1
II	218	GLY	-	expression tag	UNP A0AAE8YXX1
II	219	SER	-	expression tag	UNP A0AAE8YXX1
II	220	SER	-	expression tag	UNP A0AAE8YXX1
II	221	GLY	-	expression tag	UNP A0AAE8YXX1
II	222	HIS	-	expression tag	UNP A0AAE8YXX1
II	223	HIS	-	expression tag	UNP A0AAE8YXX1
II	224	HIS	-	expression tag	UNP A0AAE8YXX1
II	225	HIS	-	expression tag	UNP A0AAE8YXX1
II	226	HIS	-	expression tag	UNP A0AAE8YXX1
II	227	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	218	GLY	-	expression tag	UNP A0AAE8YXX1
IJ	219	SER	-	expression tag	UNP A0AAE8YXX1
IJ	220	SER	-	expression tag	UNP A0AAE8YXX1
IJ	221	GLY	-	expression tag	UNP A0AAE8YXX1
IJ	222	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	223	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	224	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	225	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	226	HIS	-	expression tag	UNP A0AAE8YXX1
IJ	227	HIS	-	expression tag	UNP A0AAE8YXX1
IK	218	GLY	-	expression tag	UNP A0AAE8YXX1
IK	219	SER	-	expression tag	UNP A0AAE8YXX1
IK	220	SER	-	expression tag	UNP A0AAE8YXX1
IK	221	GLY	-	expression tag	UNP A0AAE8YXX1
IK	222	HIS	-	expression tag	UNP A0AAE8YXX1
IK	223	HIS	-	expression tag	UNP A0AAE8YXX1
IK	224	HIS	-	expression tag	UNP A0AAE8YXX1
IK	225	HIS	-	expression tag	UNP A0AAE8YXX1
IK	226	HIS	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IK	227	HIS	-	expression tag	UNP A0AAE8YXX1
IL	218	GLY	-	expression tag	UNP A0AAE8YXX1
IL	219	SER	-	expression tag	UNP A0AAE8YXX1
IL	220	SER	-	expression tag	UNP A0AAE8YXX1
IL	221	GLY	-	expression tag	UNP A0AAE8YXX1
IL	222	HIS	-	expression tag	UNP A0AAE8YXX1
IL	223	HIS	-	expression tag	UNP A0AAE8YXX1
IL	224	HIS	-	expression tag	UNP A0AAE8YXX1
IL	225	HIS	-	expression tag	UNP A0AAE8YXX1
IL	226	HIS	-	expression tag	UNP A0AAE8YXX1
IL	227	HIS	-	expression tag	UNP A0AAE8YXX1
IM	218	GLY	-	expression tag	UNP A0AAE8YXX1
IM	219	SER	-	expression tag	UNP A0AAE8YXX1
IM	220	SER	-	expression tag	UNP A0AAE8YXX1
IM	221	GLY	-	expression tag	UNP A0AAE8YXX1
IM	222	HIS	-	expression tag	UNP A0AAE8YXX1
IM	223	HIS	-	expression tag	UNP A0AAE8YXX1
IM	224	HIS	-	expression tag	UNP A0AAE8YXX1
IM	225	HIS	-	expression tag	UNP A0AAE8YXX1
IM	226	HIS	-	expression tag	UNP A0AAE8YXX1
IM	227	HIS	-	expression tag	UNP A0AAE8YXX1
IN	218	GLY	-	expression tag	UNP A0AAE8YXX1
IN	219	SER	-	expression tag	UNP A0AAE8YXX1
IN	220	SER	-	expression tag	UNP A0AAE8YXX1
IN	221	GLY	-	expression tag	UNP A0AAE8YXX1
IN	222	HIS	-	expression tag	UNP A0AAE8YXX1
IN	223	HIS	-	expression tag	UNP A0AAE8YXX1
IN	224	HIS	-	expression tag	UNP A0AAE8YXX1
IN	225	HIS	-	expression tag	UNP A0AAE8YXX1
IN	226	HIS	-	expression tag	UNP A0AAE8YXX1
IN	227	HIS	-	expression tag	UNP A0AAE8YXX1
IO	218	GLY	-	expression tag	UNP A0AAE8YXX1
IO	219	SER	-	expression tag	UNP A0AAE8YXX1
IO	220	SER	-	expression tag	UNP A0AAE8YXX1
IO	221	GLY	-	expression tag	UNP A0AAE8YXX1
IO	222	HIS	-	expression tag	UNP A0AAE8YXX1
IO	223	HIS	-	expression tag	UNP A0AAE8YXX1
IO	224	HIS	-	expression tag	UNP A0AAE8YXX1
IO	225	HIS	-	expression tag	UNP A0AAE8YXX1
IO	226	HIS	-	expression tag	UNP A0AAE8YXX1
IO	227	HIS	-	expression tag	UNP A0AAE8YXX1
IP	218	GLY	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IP	219	SER	-	expression tag	UNP A0AAE8YXX1
IP	220	SER	-	expression tag	UNP A0AAE8YXX1
IP	221	GLY	-	expression tag	UNP A0AAE8YXX1
IP	222	HIS	-	expression tag	UNP A0AAE8YXX1
IP	223	HIS	-	expression tag	UNP A0AAE8YXX1
IP	224	HIS	-	expression tag	UNP A0AAE8YXX1
IP	225	HIS	-	expression tag	UNP A0AAE8YXX1
IP	226	HIS	-	expression tag	UNP A0AAE8YXX1
IP	227	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	218	GLY	-	expression tag	UNP A0AAE8YXX1
IQ	219	SER	-	expression tag	UNP A0AAE8YXX1
IQ	220	SER	-	expression tag	UNP A0AAE8YXX1
IQ	221	GLY	-	expression tag	UNP A0AAE8YXX1
IQ	222	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	223	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	224	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	225	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	226	HIS	-	expression tag	UNP A0AAE8YXX1
IQ	227	HIS	-	expression tag	UNP A0AAE8YXX1
IR	218	GLY	-	expression tag	UNP A0AAE8YXX1
IR	219	SER	-	expression tag	UNP A0AAE8YXX1
IR	220	SER	-	expression tag	UNP A0AAE8YXX1
IR	221	GLY	-	expression tag	UNP A0AAE8YXX1
IR	222	HIS	-	expression tag	UNP A0AAE8YXX1
IR	223	HIS	-	expression tag	UNP A0AAE8YXX1
IR	224	HIS	-	expression tag	UNP A0AAE8YXX1
IR	225	HIS	-	expression tag	UNP A0AAE8YXX1
IR	226	HIS	-	expression tag	UNP A0AAE8YXX1
IR	227	HIS	-	expression tag	UNP A0AAE8YXX1
IS	218	GLY	-	expression tag	UNP A0AAE8YXX1
IS	219	SER	-	expression tag	UNP A0AAE8YXX1
IS	220	SER	-	expression tag	UNP A0AAE8YXX1
IS	221	GLY	-	expression tag	UNP A0AAE8YXX1
IS	222	HIS	-	expression tag	UNP A0AAE8YXX1
IS	223	HIS	-	expression tag	UNP A0AAE8YXX1
IS	224	HIS	-	expression tag	UNP A0AAE8YXX1
IS	225	HIS	-	expression tag	UNP A0AAE8YXX1
IS	226	HIS	-	expression tag	UNP A0AAE8YXX1
IS	227	HIS	-	expression tag	UNP A0AAE8YXX1
IT	218	GLY	-	expression tag	UNP A0AAE8YXX1
IT	219	SER	-	expression tag	UNP A0AAE8YXX1
IT	220	SER	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IT	221	GLY	-	expression tag	UNP A0AAE8YXX1
IT	222	HIS	-	expression tag	UNP A0AAE8YXX1
IT	223	HIS	-	expression tag	UNP A0AAE8YXX1
IT	224	HIS	-	expression tag	UNP A0AAE8YXX1
IT	225	HIS	-	expression tag	UNP A0AAE8YXX1
IT	226	HIS	-	expression tag	UNP A0AAE8YXX1
IT	227	HIS	-	expression tag	UNP A0AAE8YXX1
IU	218	GLY	-	expression tag	UNP A0AAE8YXX1
IU	219	SER	-	expression tag	UNP A0AAE8YXX1
IU	220	SER	-	expression tag	UNP A0AAE8YXX1
IU	221	GLY	-	expression tag	UNP A0AAE8YXX1
IU	222	HIS	-	expression tag	UNP A0AAE8YXX1
IU	223	HIS	-	expression tag	UNP A0AAE8YXX1
IU	224	HIS	-	expression tag	UNP A0AAE8YXX1
IU	225	HIS	-	expression tag	UNP A0AAE8YXX1
IU	226	HIS	-	expression tag	UNP A0AAE8YXX1
IU	227	HIS	-	expression tag	UNP A0AAE8YXX1
IV	218	GLY	-	expression tag	UNP A0AAE8YXX1
IV	219	SER	-	expression tag	UNP A0AAE8YXX1
IV	220	SER	-	expression tag	UNP A0AAE8YXX1
IV	221	GLY	-	expression tag	UNP A0AAE8YXX1
IV	222	HIS	-	expression tag	UNP A0AAE8YXX1
IV	223	HIS	-	expression tag	UNP A0AAE8YXX1
IV	224	HIS	-	expression tag	UNP A0AAE8YXX1
IV	225	HIS	-	expression tag	UNP A0AAE8YXX1
IV	226	HIS	-	expression tag	UNP A0AAE8YXX1
IV	227	HIS	-	expression tag	UNP A0AAE8YXX1
IW	218	GLY	-	expression tag	UNP A0AAE8YXX1
IW	219	SER	-	expression tag	UNP A0AAE8YXX1
IW	220	SER	-	expression tag	UNP A0AAE8YXX1
IW	221	GLY	-	expression tag	UNP A0AAE8YXX1
IW	222	HIS	-	expression tag	UNP A0AAE8YXX1
IW	223	HIS	-	expression tag	UNP A0AAE8YXX1
IW	224	HIS	-	expression tag	UNP A0AAE8YXX1
IW	225	HIS	-	expression tag	UNP A0AAE8YXX1
IW	226	HIS	-	expression tag	UNP A0AAE8YXX1
IW	227	HIS	-	expression tag	UNP A0AAE8YXX1
IX	218	GLY	-	expression tag	UNP A0AAE8YXX1
IX	219	SER	-	expression tag	UNP A0AAE8YXX1
IX	220	SER	-	expression tag	UNP A0AAE8YXX1
IX	221	GLY	-	expression tag	UNP A0AAE8YXX1
IX	222	HIS	-	expression tag	UNP A0AAE8YXX1

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Chain	Residue	Modelled	Actual	Comment	Reference
IX	223	HIS	-	expression tag	UNP A0AAE8YXX1
IX	224	HIS	-	expression tag	UNP A0AAE8YXX1
IX	225	HIS	-	expression tag	UNP A0AAE8YXX1
IX	226	HIS	-	expression tag	UNP A0AAE8YXX1
IX	227	HIS	-	expression tag	UNP A0AAE8YXX1

- Molecule 2 is a protein called DUF4145 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	OA	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OB	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OC	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OD	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OE	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OF	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OG	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OH	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OI	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OJ	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OK	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OL	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OM	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	ON	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OO	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OP	177	Total	C	H	N	O	S	0	0
			2718	865	1339	244	257	13		
2	OQ	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	OR	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OS	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OT	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OU	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OV	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		
2	OW	177	Total	C	H	N	O	S	0	0
			2726	867	1345	244	257	13		
2	OX	177	Total	C	H	N	O	S	0	0
			2727	867	1346	244	257	13		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	OA	1	Total	Zn	0
			1	1	
3	OB	1	Total	Zn	0
			1	1	
3	OC	1	Total	Zn	0
			1	1	
3	OD	1	Total	Zn	0
			1	1	
3	OE	1	Total	Zn	0
			1	1	
3	OF	1	Total	Zn	0
			1	1	
3	OG	1	Total	Zn	0
			1	1	
3	OH	1	Total	Zn	0
			1	1	
3	OI	1	Total	Zn	0
			1	1	
3	OJ	1	Total	Zn	0
			1	1	
3	OK	1	Total	Zn	0
			1	1	
3	OL	1	Total	Zn	0
			1	1	

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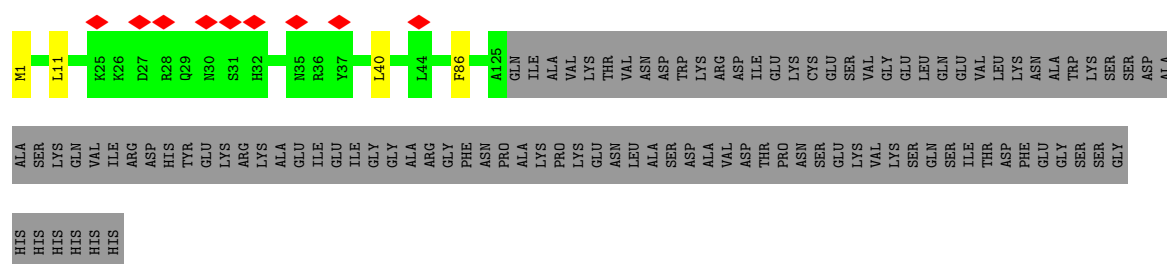
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Mol	Chain	Residues	Atoms		AltConf
3	OM	1	Total 1	Zn 1	0
3	ON	1	Total 1	Zn 1	0
3	OO	1	Total 1	Zn 1	0
3	OP	1	Total 1	Zn 1	0
3	OQ	1	Total 1	Zn 1	0
3	OR	1	Total 1	Zn 1	0
3	OS	1	Total 1	Zn 1	0
3	OT	1	Total 1	Zn 1	0
3	OU	1	Total 1	Zn 1	0
3	OV	1	Total 1	Zn 1	0
3	OW	1	Total 1	Zn 1	0
3	OX	1	Total 1	Zn 1	0

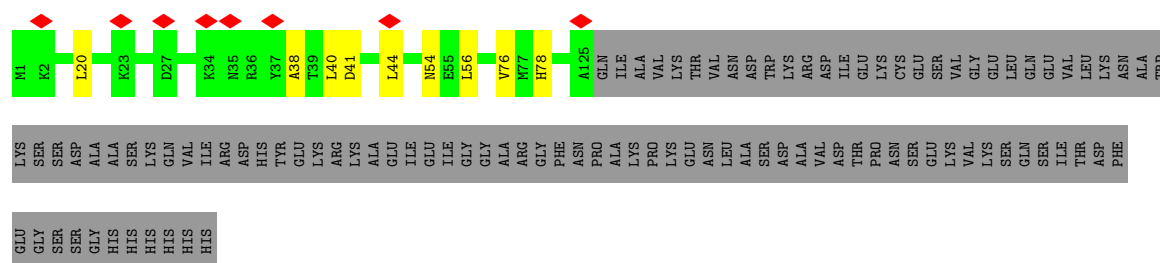
Chain ID:



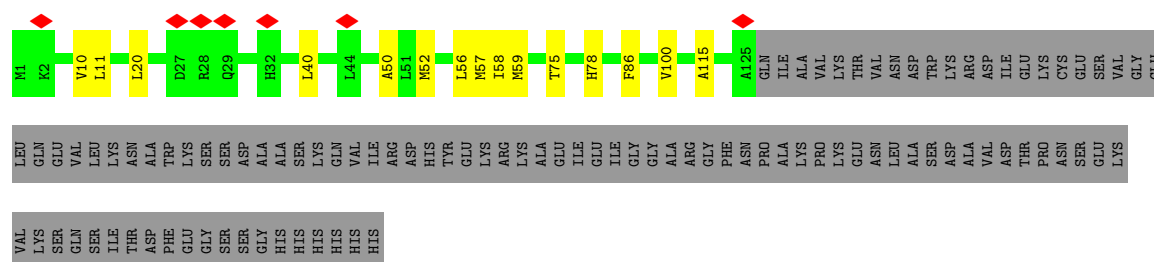
Chain IE: 53% 45%



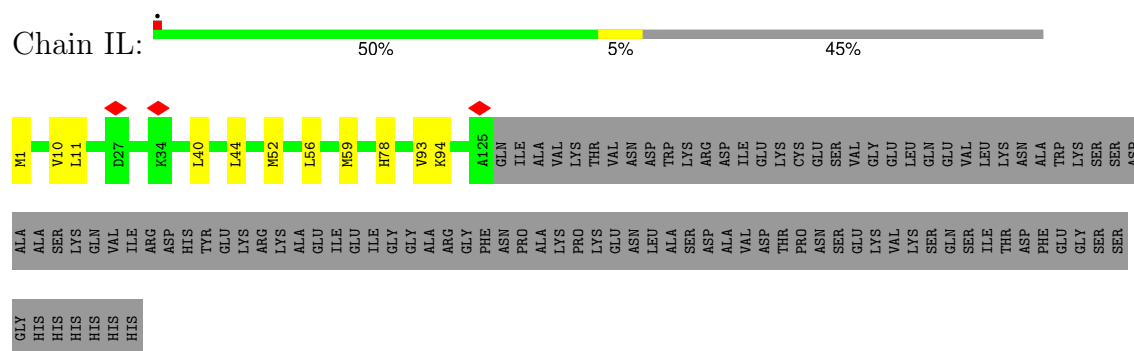
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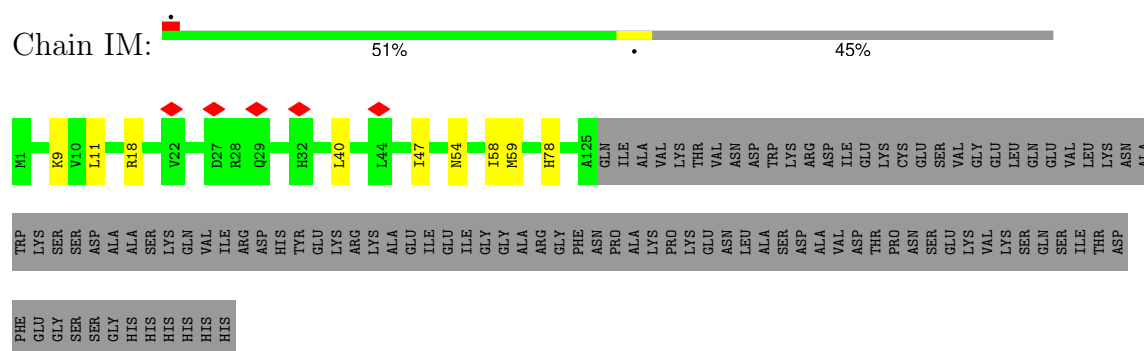
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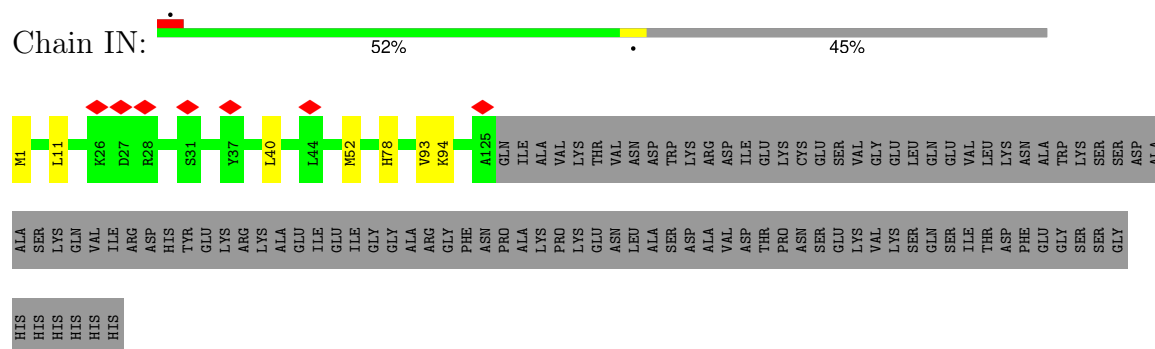
● Molecule 1: Gp77



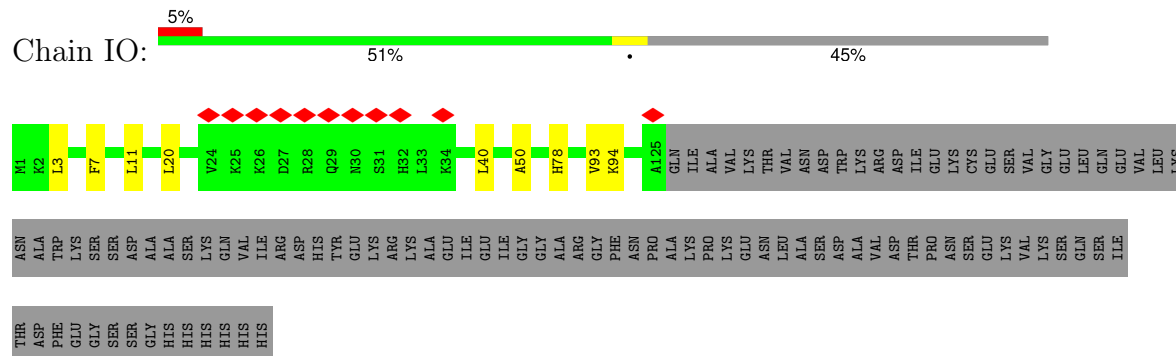
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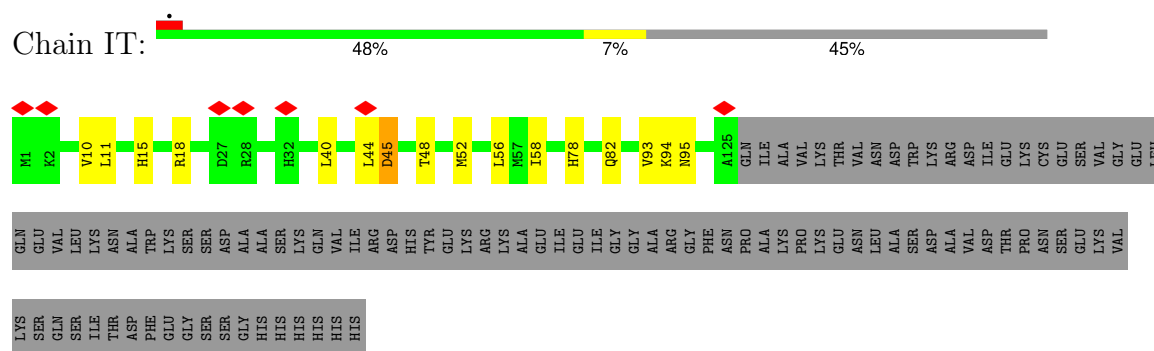
● Molecule 1: Gp77



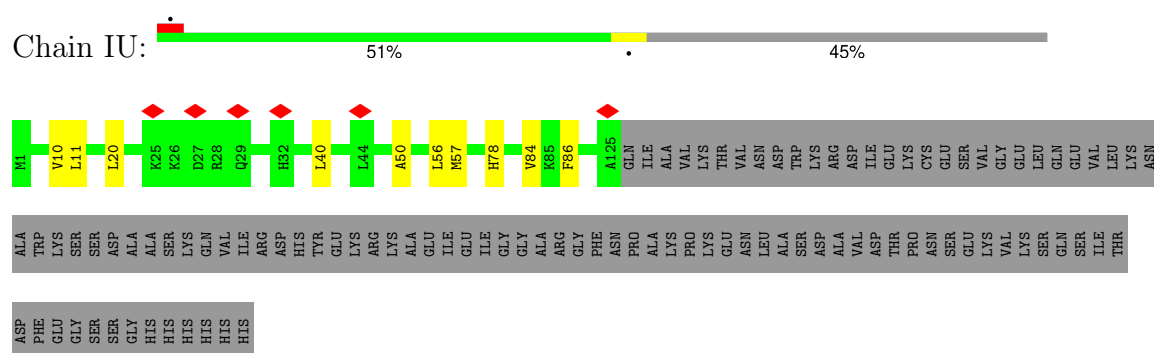
● Molecule 1: Gp77



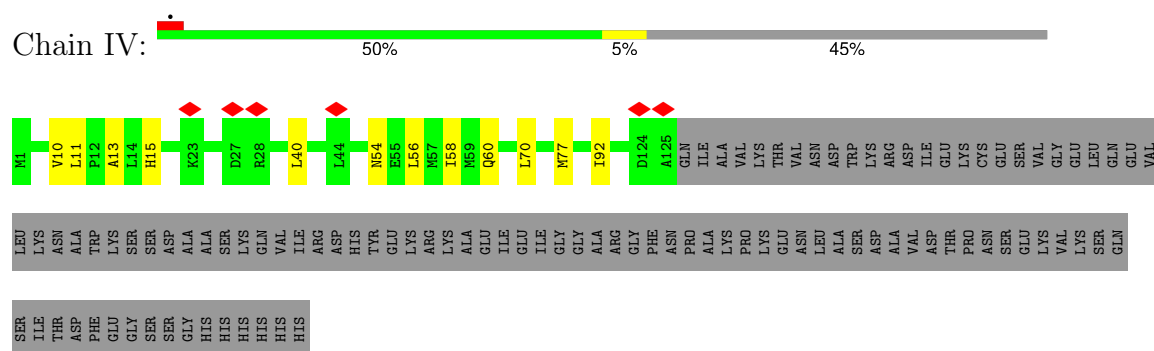
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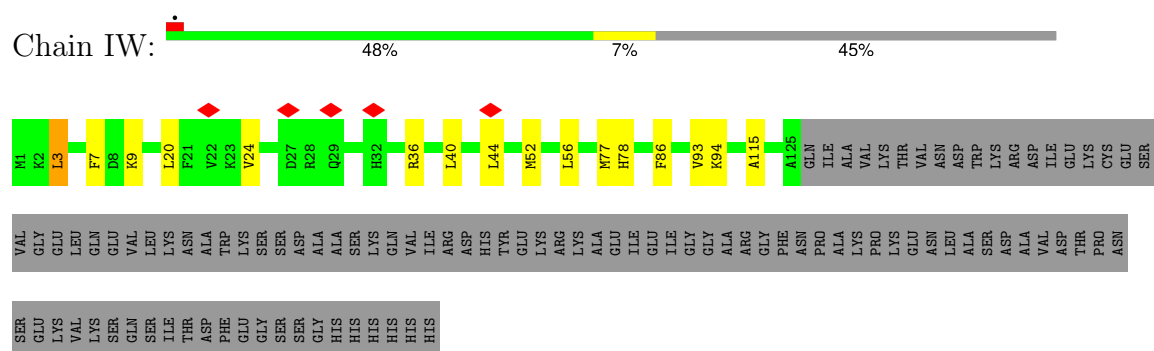
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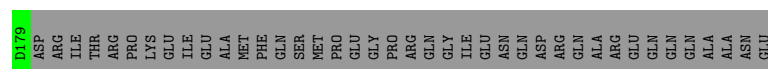


● Molecule 1: Gp77

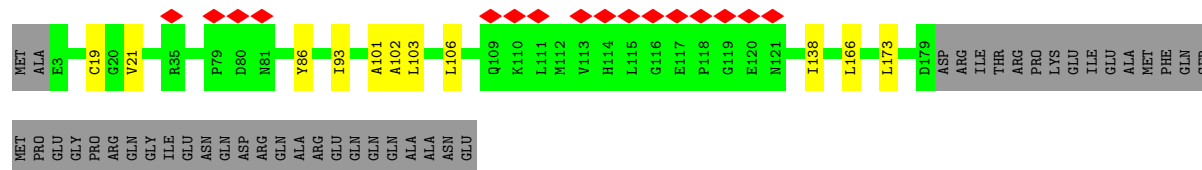
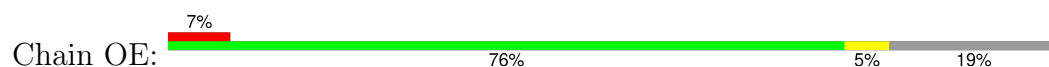


● Molecule 1: Gp77

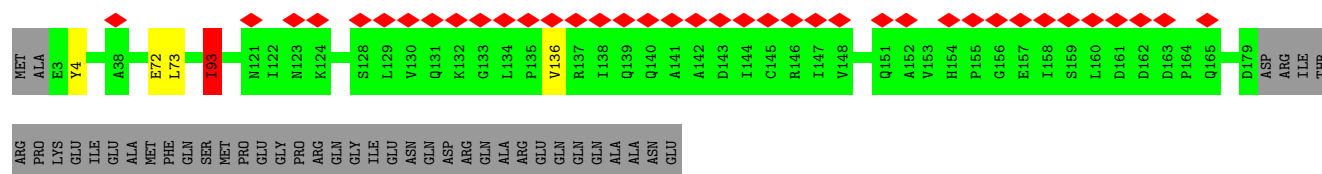
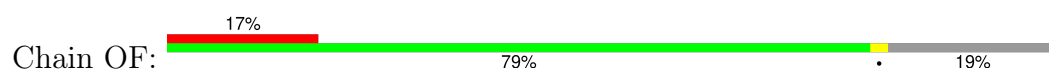




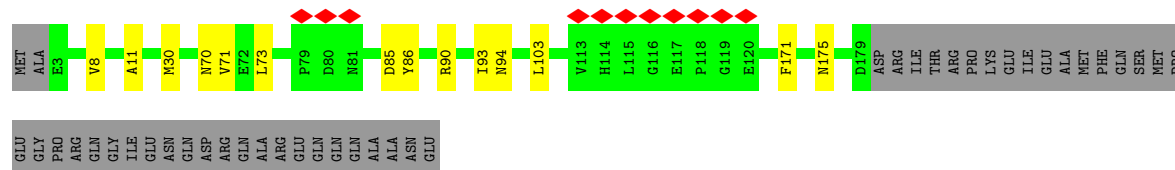
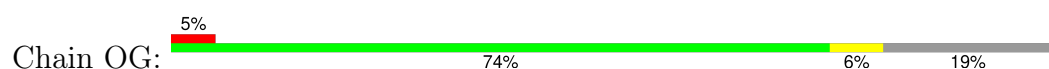
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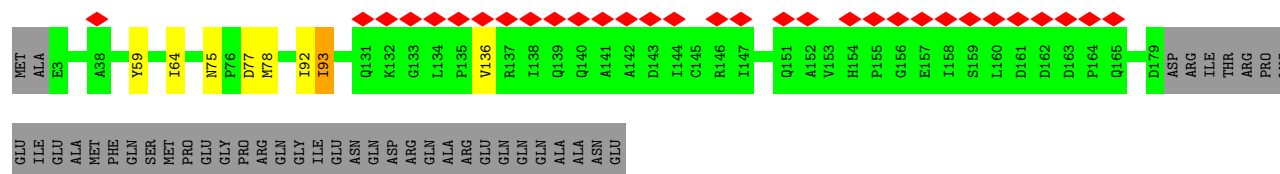
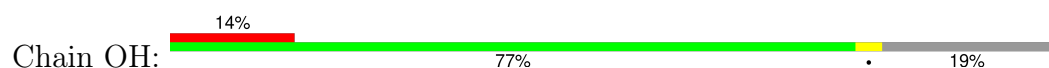
- Molecule 2: DUF4145 domain-containing protein



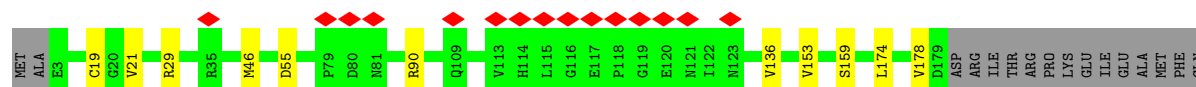
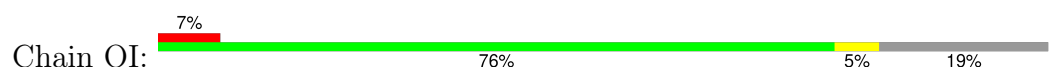
- Molecule 2: DUF4145 domain-containing protein



- Molecule 2: DUF4145 domain-containing protein



- Molecule 2: DUF4145 domain-containing protein



SER MET PRO GLY PRO ARG GLN ILE GLU ASN GLN ASP ARG GLN ALA ARG GLU GLN GLN ALA ASN GLU

- Molecule 2: DUF4145 domain-containing protein

Chain OJ: 14% 75% 6% 19%

MET ALA E3 F26 S33 A38 Y59 T64 M78 C82 N123 K124 Q131 K132 G133 L134 P135 V136 R137 I138 Q139 Q140 A141 A142 D143 I144 C145 R146 I147 N150 Q151 H154 P155 G156 E157 I158 S159 L160 D161 D162 D163 P164 Q165 I176 I177 V178 D179 ASP

ARG ILE THR ARG LYS GLU ILE GLU ALA MET PHE GLN SER MET PRO GLU PRO ARG GLN ILE GLU ASN GLN ASP ARG GLN ALA ASN GLU

- Molecule 2: DUF4145 domain-containing protein

Chain OK: 7% 75% 5% 19%

MET ALA E3 V21 H51 A56 Y59 M63 T64 P79 D80 N81 I93 N94 L104 L111 M112 V113 H114 L115 G116 E117 P118 G119 N121 I122 N123 K124 G133 A152 L170 D179 ASP ARG ILE THR ARG LYS PRO GLU ILE GLU ALA MET PHE GLN

SER MET PRO GLY PRO ARG GLN ILE GLU ALA MET PHE GLN SER MET PRO GLU PRO ARG GLN ILE GLU ASN GLN ASP ARG GLN ALA ASN GLU

- Molecule 2: DUF4145 domain-containing protein

Chain OL: 15% 78% 19%

MET ALA E3 Y4 K30 L37 A38 K83 H87 P118 K124 S128 Q131 K132 G133 L134 P135 V136 R137 I138 Q139 Q140 A141 A142 D143 I144 C145 R146 I147 H154 P155 G156 E157 I158 S159 L160 D161 D162 P164 Q165 H168 D179 ASP ARG ILE THR ARG PRO

LYS GLU ILE GLU ALA MET PHE GLN SER MET PRO GLU GLY PRO ARG GLN ILE GLU ASN ASP GLN ALA ARG GLU GLN GLN ALA ALA ASN GLU

- Molecule 2: DUF4145 domain-containing protein

Chain OM: 5% 75% 5% 19%

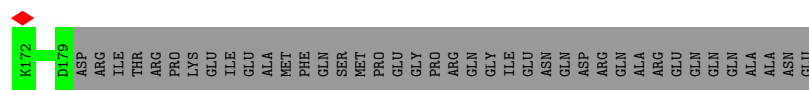
MET ALA E3 C19 G20 V21 R28 R29 M30 R35 A56 M63 P79 D80 N81 I93 N94 V113 H114 L115 G116 E117 P118 K124 D125 I126 R127 V136 A152 D179 ASP ARG ILE THR ARG PRO LYS GLU ILE GLU ALA MET PHE GLN SER MET PRO GLU

GLY PRO ARG GLN GLY ILE ASN GLN ASP ARG GLN ALA ARG GLN GLN ALA ALA ASN GLU

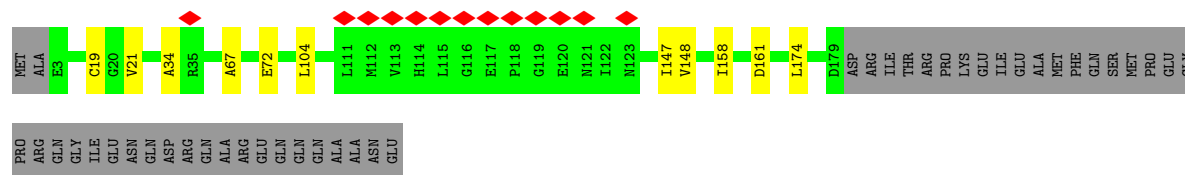
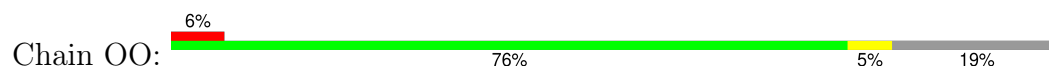
- Molecule 2: DUF4145 domain-containing protein

Chain ON: 19% 78% 19%

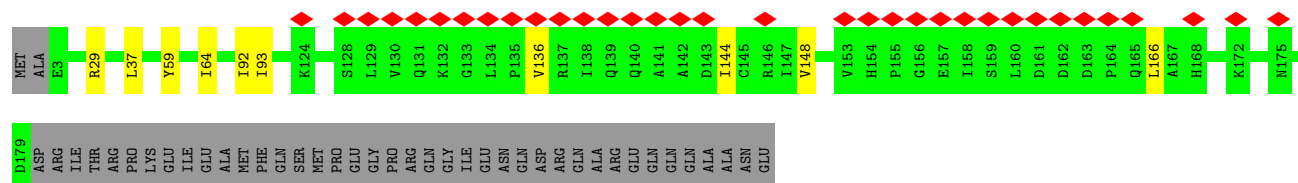
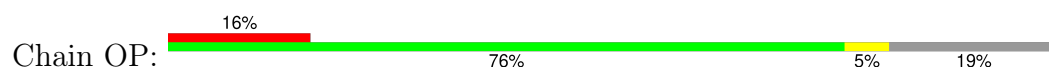
MET ALA E3 Y4 R29 A38 M62 I93 L115 P118 K124 D125 S128 L129 V130 Q131 K132 G133 L134 P135 V136 R137 I138 Q139 Q140 A141 A142 D143 I144 C145 R146 I147 N150 Q151 A152 V153 H154 P155 G156 E157 I158 S159 L160 D161 D162 D163 P164 Q165 H168



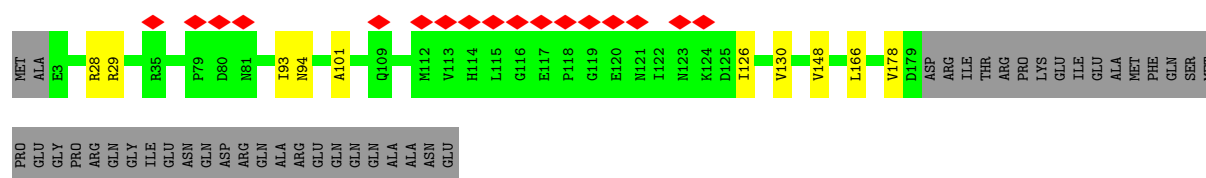
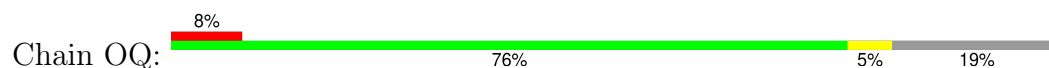
- Molecule 2: DUF4145 domain-containing protein



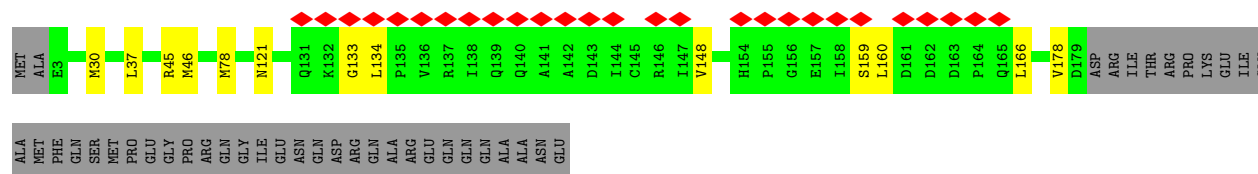
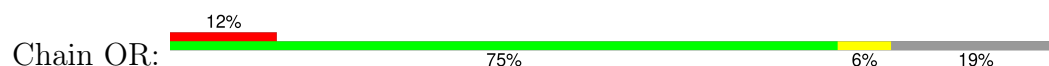
- Molecule 2: DUF4145 domain-containing protein



- Molecule 2: DUF4145 domain-containing protein

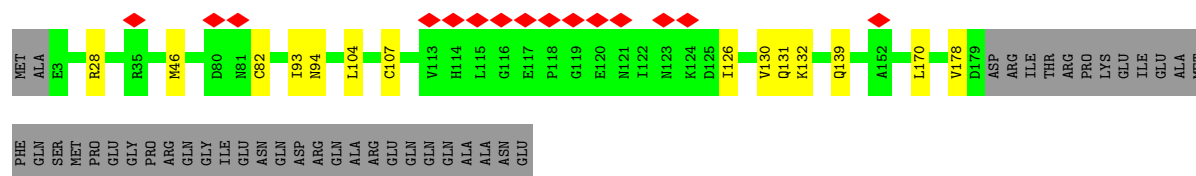


- Molecule 2: DUF4145 domain-containing protein

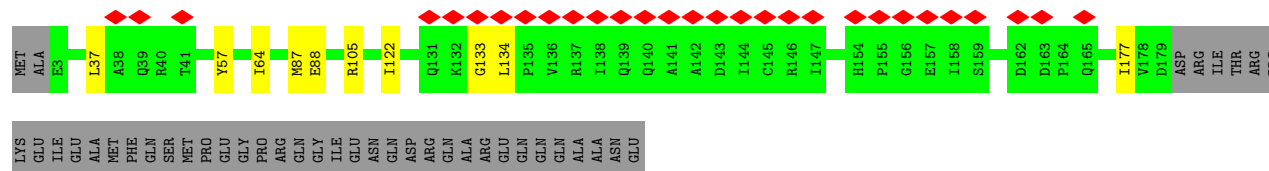
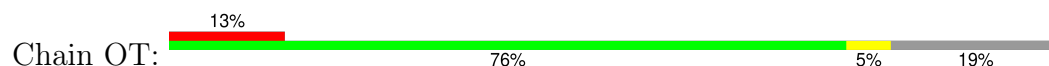


- Molecule 2: DUF4145 domain-containing protein

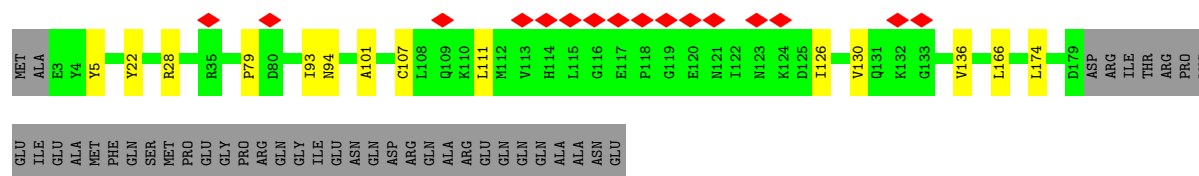
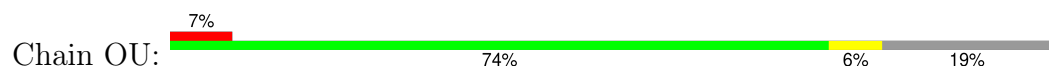




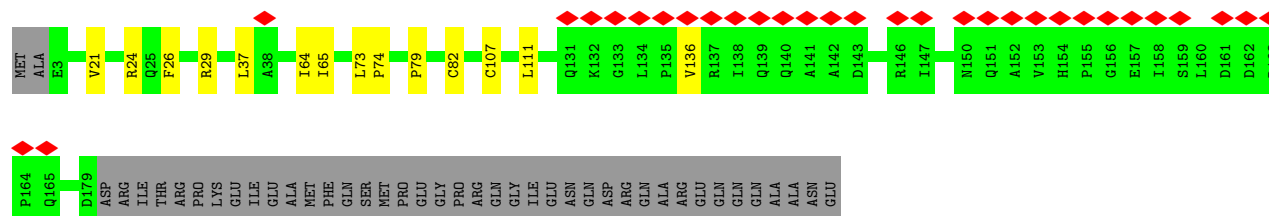
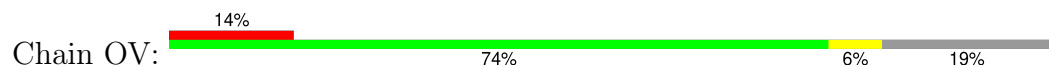
- Molecule 2: DUF4145 domain-containing protein



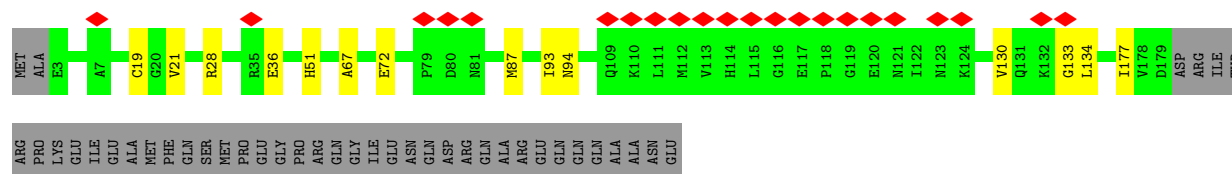
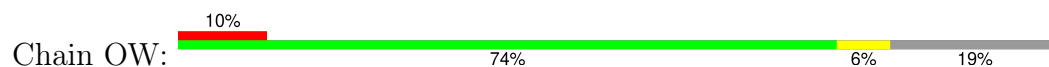
- Molecule 2: DUF4145 domain-containing protein



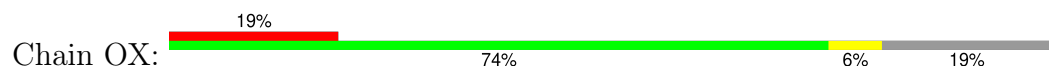
- Molecule 2: DUF4145 domain-containing protein

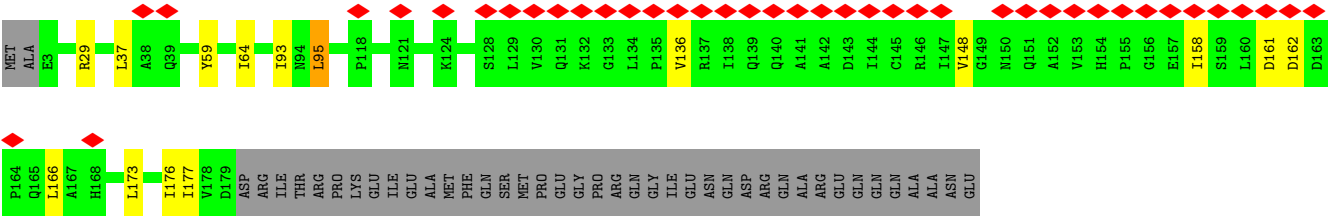


- Molecule 2: DUF4145 domain-containing protein



- Molecule 2: DUF4145 domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.18	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.828	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0777	Depositor
Map size ($\text{\AA}$)	653.972, 653.972, 653.972	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4863, 1.4863, 1.4863	Depositor

5 Model quality

5.1 Standard geometry

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

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	IA	0.13	0/1004	0.33	0/1355
1	IB	0.15	0/1004	0.39	0/1355
1	IC	0.14	0/1004	0.35	0/1355
1	ID	0.15	0/1004	0.39	0/1355
1	IE	0.16	0/1004	0.37	0/1355
1	IF	0.13	0/1004	0.35	0/1355
1	IG	0.15	0/1004	0.37	0/1355
1	IH	0.15	0/1004	0.39	0/1355
1	II	0.14	0/1004	0.35	0/1355
1	IJ	0.14	0/1004	0.37	0/1355
1	IK	0.12	0/1004	0.32	0/1355
1	IL	0.15	0/1004	0.39	0/1355
1	IM	0.15	0/1004	0.37	0/1355
1	IN	0.15	0/1004	0.40	0/1355
1	IO	0.12	0/1004	0.32	0/1355
1	IP	0.17	0/1004	0.45	0/1355
1	IQ	0.15	0/1004	0.38	0/1355
1	IR	0.15	0/1004	0.35	0/1355
1	IS	0.13	0/1004	0.37	0/1355
1	IT	0.16	0/1004	0.41	0/1355
1	IU	0.14	0/1004	0.34	0/1355
1	IV	0.16	0/1004	0.39	0/1355
1	IW	0.14	0/1004	0.40	0/1355
1	IX	0.14	0/1004	0.37	0/1355
2	OA	0.14	0/1411	0.36	0/1913
2	OB	0.14	0/1411	0.36	0/1913
2	OC	0.16	0/1411	0.35	0/1913
2	OD	0.16	0/1411	0.39	0/1913
2	OE	0.13	0/1411	0.32	0/1913
2	OF	0.15	0/1411	0.35	0/1913
2	OG	0.14	0/1411	0.33	0/1913
2	OH	0.13	0/1411	0.32	0/1913

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	OI	0.17	0/1411	0.34	0/1913
2	OJ	0.15	0/1411	0.35	0/1913
2	OK	0.14	0/1411	0.33	0/1913
2	OL	0.19	0/1411	0.40	0/1913
2	OM	0.14	0/1411	0.34	0/1913
2	ON	0.15	0/1411	0.36	0/1913
2	OO	0.13	0/1411	0.33	0/1913
2	OP	0.15	0/1409	0.36	0/1910
2	OQ	0.13	0/1411	0.33	0/1913
2	OR	0.15	0/1411	0.35	0/1913
2	OS	0.14	0/1411	0.33	0/1913
2	OT	0.14	0/1411	0.34	0/1913
2	OU	0.12	0/1411	0.30	0/1913
2	OV	0.16	0/1411	0.37	0/1913
2	OW	0.16	0/1411	0.39	0/1913
2	OX	0.15	0/1411	0.38	0/1913
All	All	0.15	0/57958	0.36	0/78429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	IA	986	986	986	8	0
1	IB	986	986	986	10	0
1	IC	986	986	986	10	0
1	ID	986	986	986	11	0
1	IE	986	986	986	5	0
1	IF	986	986	986	6	0
1	IG	986	986	986	13	0
1	IH	986	986	986	15	0
1	II	986	986	986	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IJ	986	986	986	8	0
1	IK	986	986	986	4	0
1	IL	986	986	986	9	0
1	IM	986	986	986	9	0
1	IN	986	986	986	6	0
1	IO	986	986	986	7	0
1	IP	986	986	986	14	0
1	IQ	986	986	986	11	0
1	IR	986	986	986	5	0
1	IS	986	986	986	12	0
1	IT	986	986	986	13	0
1	IU	986	986	986	8	0
1	IV	986	986	986	9	0
1	IW	986	986	986	10	0
1	IX	986	986	986	5	0
2	OA	1381	1345	1342	8	0
2	OB	1381	1346	1342	6	0
2	OC	1381	1345	1341	8	0
2	OD	1381	1346	1342	6	0
2	OE	1381	1345	1341	6	0
2	OF	1381	1346	1342	3	0
2	OG	1381	1345	1342	10	0
2	OH	1381	1346	1342	6	0
2	OI	1381	1345	1341	9	0
2	OJ	1381	1346	1342	6	0
2	OK	1381	1345	1342	6	0
2	OL	1381	1346	1342	4	0
2	OM	1381	1345	1341	8	0
2	ON	1381	1346	1342	5	0
2	OO	1381	1345	1341	7	0
2	OP	1379	1339	1335	8	0
2	OQ	1381	1345	1341	8	0
2	OR	1381	1346	1342	10	0
2	OS	1381	1345	1342	9	0
2	OT	1381	1346	1342	6	0
2	OU	1381	1345	1342	8	0
2	OV	1381	1346	1342	10	0
2	OW	1381	1345	1342	9	0
2	OX	1381	1346	1342	12	0
3	OA	1	0	0	0	0
3	OB	1	0	0	0	0
3	OC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	OD	1	0	0	0	0
3	OE	1	0	0	0	0
3	OF	1	0	0	0	0
3	OG	1	0	0	0	0
3	OH	1	0	0	0	0
3	OI	1	0	0	0	0
3	OJ	1	0	0	0	0
3	OK	1	0	0	0	0
3	OL	1	0	0	0	0
3	OM	1	0	0	0	0
3	ON	1	0	0	0	0
3	OO	1	0	0	0	0
3	OP	1	0	0	0	0
3	OQ	1	0	0	0	0
3	OR	1	0	0	0	0
3	OS	1	0	0	0	0
3	OT	1	0	0	0	0
3	OU	1	0	0	0	0
3	OV	1	0	0	0	0
3	OW	1	0	0	0	0
3	OX	1	0	0	0	0
All	All	56830	55949	55859	331	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 3.

All (331) 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)
2:OW:67:ALA:HB1	2:OW:87:MET:HE1	1.62	0.80
1:IR:40:LEU:HD21	1:IR:44:LEU:HD22	1.70	0.74
1:IU:20:LEU:HD11	1:IU:50:ALA:HB1	1.73	0.71
1:IN:52:MET:HE3	1:IN:52:MET:HA	1.74	0.69
1:IJ:93:VAL:HG23	1:IJ:94:LYS:HG3	1.75	0.69
2:OI:174:LEU:HD23	2:OI:174:LEU:O	1.92	0.69
1:IU:10:VAL:HG23	1:IU:56:LEU:HD21	1.78	0.66
2:OA:21:VAL:HG11	2:OA:51:HIS:ND1	2.11	0.66
1:IO:40:LEU:HD12	1:IO:40:LEU:O	1.96	0.66
2:OR:37:LEU:HD21	2:OS:28:ARG:NH1	2.13	0.64
2:OQ:126:ILE:O	2:OQ:130:VAL:HG23	1.97	0.64
1:IQ:17:ALA:HB2	1:IQ:54:ASN:HD22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:130:VAL:HG12	2:OA:139:GLN:NE2	2.14	0.63
1:IT:52:MET:HE3	1:IT:52:MET:HA	1.81	0.63
1:IM:47:ILE:HD11	1:IM:58:ILE:HD12	1.80	0.63
2:OI:153:VAL:HG22	2:OI:159:SER:HB2	1.81	0.63
2:OQ:148:VAL:HG11	2:OQ:166:LEU:HD13	1.81	0.63
2:OO:174:LEU:O	2:OO:174:LEU:HD23	1.98	0.62
2:OH:93:ILE:HD11	2:OI:90:ARG:HB3	1.81	0.62
2:OC:56:ALA:HB1	2:OC:63:MET:HE1	1.81	0.62
2:OC:174:LEU:O	2:OC:174:LEU:HD23	1.99	0.62
1:IT:40:LEU:HD21	1:IT:44:LEU:HD22	1.79	0.62
1:IK:78:HIS:O	1:IL:11:LEU:HD23	2.01	0.61
2:OD:158:ILE:HD12	2:OD:161:ASP:HB2	1.83	0.60
1:IV:13:ALA:HB1	1:IV:54:ASN:OD1	2.02	0.60
2:OP:148:VAL:HG21	2:OP:166:LEU:HD11	1.82	0.60
2:OU:174:LEU:HD23	2:OU:174:LEU:O	2.02	0.60
1:II:57:MET:HE1	1:IJ:15:HIS:HA	1.83	0.59
2:OU:22:TYR:HE1	2:OV:21:VAL:HG22	1.67	0.59
1:IA:67:VAL:O	1:IA:92:ILE:HD11	2.02	0.59
1:IQ:59:MET:SD	1:IR:1:MET:HE1	2.42	0.59
1:IF:40:LEU:HD21	1:IF:44:LEU:HD22	1.84	0.59
2:OE:86:TYR:HA	2:OE:103:LEU:HD11	1.84	0.58
1:IH:57:MET:HE1	1:II:15:HIS:HA	1.84	0.58
2:OM:56:ALA:HB1	2:OM:63:MET:HE1	1.85	0.58
2:OW:130:VAL:HG22	2:OW:177:ILE:HD11	1.84	0.58
2:OX:158:ILE:HD12	2:OX:161:ASP:HB2	1.85	0.58
1:IP:40:LEU:CD2	1:IP:44:LEU:HD22	2.35	0.57
1:IG:57:MET:HE1	1:IH:15:HIS:HA	1.86	0.57
2:OP:37:LEU:HD11	2:OQ:28:ARG:CD	2.34	0.57
1:IQ:3:LEU:HD11	1:IQ:84:VAL:HG12	1.87	0.57
2:OW:19:CYS:HB2	2:OW:21:VAL:HG12	1.87	0.57
1:IR:78:HIS:O	1:IS:11:LEU:HD23	2.05	0.57
1:IG:10:VAL:HG23	1:IG:56:LEU:HD21	1.86	0.56
1:IH:20:LEU:HD21	2:OI:29:ARG:NH2	2.21	0.56
1:IQ:78:HIS:O	1:IR:11:LEU:HD23	2.06	0.56
1:IU:78:HIS:O	1:IV:11:LEU:HD23	2.05	0.55
2:OX:148:VAL:HG11	2:OX:166:LEU:HD11	1.88	0.55
1:IP:60:GLN:OE1	1:IP:74:THR:HG23	2.06	0.55
2:OO:67:ALA:HB3	2:OO:72:GLU:OE1	2.05	0.55
2:OD:77:ASP:CG	2:OD:78:MET:HE2	2.31	0.55
2:OU:101:ALA:HB2	2:OU:166:LEU:HD11	1.88	0.55
1:IO:78:HIS:O	1:IP:11:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OV:73:LEU:HD12	2:OV:74:PRO:HD2	1.89	0.54
1:IP:78:HIS:O	1:IQ:11:LEU:HD23	2.08	0.54
1:IC:17:ALA:HB2	1:IC:54:ASN:OD1	2.08	0.54
1:IA:11:LEU:HD23	1:IX:78:HIS:O	2.08	0.53
1:IG:20:LEU:HD11	1:IG:50:ALA:HB1	1.89	0.53
2:OI:19:CYS:HB2	2:OI:21:VAL:HG12	1.89	0.53
1:IP:70:LEU:CB	1:IP:92:ILE:HD11	2.38	0.53
1:IT:10:VAL:HG23	1:IT:56:LEU:HD21	1.90	0.53
2:OC:113:VAL:HG23	2:OC:118:PRO:O	2.08	0.53
2:OX:148:VAL:HG11	2:OX:166:LEU:CD1	2.39	0.53
2:OE:19:CYS:HB2	2:OE:21:VAL:HG12	1.89	0.53
2:OG:70:ASN:OD1	2:OG:71:VAL:HG13	2.07	0.53
2:OD:158:ILE:HD11	2:OD:162:ASP:HB2	1.90	0.52
2:OQ:178:VAL:HG12	2:OQ:178:VAL:O	2.09	0.52
2:OR:159:SER:O	2:OR:160:LEU:HD23	2.10	0.52
1:IB:78:HIS:O	1:IC:11:LEU:HD23	2.09	0.52
1:IK:20:LEU:O	1:IK:20:LEU:HD12	2.10	0.52
1:IO:20:LEU:HD11	1:IO:50:ALA:HB1	1.92	0.52
1:IJ:78:HIS:O	1:IK:11:LEU:HD23	2.09	0.51
1:IS:52:MET:HE1	1:IT:18:ARG:HG3	1.91	0.51
2:OP:59:TYR:N	2:OP:64:ILE:HD11	2.25	0.51
2:OX:29:ARG:HD3	2:OX:29:ARG:H	1.75	0.51
1:IB:70:LEU:CB	1:IB:92:ILE:HD11	2.40	0.51
1:IU:57:MET:HE1	1:IV:15:HIS:HA	1.93	0.51
2:OM:19:CYS:HB2	2:OM:21:VAL:HG12	1.93	0.51
1:IQ:54:ASN:OD1	1:IQ:54:ASN:O	2.28	0.51
1:IG:59:MET:HE2	1:IH:1:MET:SD	2.50	0.51
2:OK:79:PRO:HD3	2:OK:111:LEU:HD13	1.91	0.51
2:OO:104:LEU:HD21	2:OO:174:LEU:HD11	1.93	0.51
1:IL:52:MET:HE3	1:IM:18:ARG:HB3	1.93	0.51
2:OW:67:ALA:HB3	2:OW:72:GLU:OE1	2.11	0.51
1:IL:78:HIS:O	1:IM:11:LEU:HD23	2.10	0.51
1:IS:40:LEU:HD11	1:IS:44:LEU:HD22	1.93	0.51
2:OQ:101:ALA:HB2	2:OQ:166:LEU:HD11	1.92	0.51
2:OB:40:ARG:NE	2:OC:46:MET:HE1	2.26	0.50
1:ID:59:MET:CE	1:IE:1:MET:HE2	2.41	0.50
1:IW:20:LEU:O	1:IW:20:LEU:HD12	2.10	0.50
1:IC:57:MET:HE1	1:ID:15:HIS:HA	1.92	0.50
1:IM:78:HIS:O	1:IN:11:LEU:HD23	2.12	0.50
2:OV:29:ARG:H	2:OV:29:ARG:HD3	1.76	0.50
1:IW:86:PHE:CE2	1:IW:115:ALA:HB1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OK:21:VAL:HG11	2:OK:51:HIS:ND1	2.26	0.50
2:OL:30:MET:HE1	2:OM:30:MET:HE2	1.93	0.50
1:IT:40:LEU:CD2	1:IT:44:LEU:HD22	2.42	0.49
2:OV:37:LEU:HD21	2:OW:28:ARG:NH1	2.26	0.49
2:OI:46:MET:HE2	2:OI:55:ASP:OD2	2.12	0.49
2:OM:124:LYS:O	2:OM:124:LYS:HD3	2.12	0.49
1:IA:78:HIS:O	1:IB:11:LEU:HD23	2.12	0.49
1:IU:84:VAL:HG23	1:IU:86:PHE:HE1	1.77	0.49
2:OR:148:VAL:CG1	2:OR:166:LEU:HD13	2.42	0.49
2:OU:79:PRO:HG2	2:OU:111:LEU:HD22	1.94	0.49
1:ID:59:MET:HE2	1:IE:1:MET:HE2	1.94	0.49
1:IL:40:LEU:CD2	1:IL:44:LEU:HD22	2.43	0.49
1:IP:20:LEU:HD11	2:OQ:29:ARG:NH1	2.28	0.49
2:OF:72:GLU:O	2:OF:73:LEU:HD22	2.12	0.49
1:IH:47:ILE:O	1:IH:51:LEU:HD23	2.12	0.49
2:OG:85:ASP:O	2:OG:103:LEU:HD11	2.13	0.49
1:IT:10:VAL:HG12	1:IT:82:GLN:OE1	2.11	0.49
1:IA:20:LEU:HD11	1:IA:50:ALA:HB1	1.94	0.49
1:ID:40:LEU:O	1:ID:40:LEU:HD12	2.12	0.49
1:IV:77:MET:HE3	1:IV:77:MET:HA	1.95	0.49
2:OR:30:MET:HE3	2:OR:46:MET:CG	2.43	0.49
2:OD:77:ASP:OD1	2:OD:78:MET:HE2	2.13	0.49
1:IB:10:VAL:HG23	1:IB:56:LEU:HD21	1.95	0.49
1:ID:13:ALA:HB1	1:ID:54:ASN:OD1	2.13	0.49
2:OG:73:LEU:HD12	2:OG:175:ASN:HD21	1.78	0.49
2:OH:92:ILE:C	2:OH:93:ILE:HD12	2.37	0.49
2:OR:30:MET:HE1	2:OR:45:ARG:C	2.38	0.49
1:IS:40:LEU:CD1	1:IS:44:LEU:HD22	2.43	0.48
1:IQ:70:LEU:CB	1:IQ:92:ILE:HD11	2.43	0.48
1:IT:78:HIS:O	1:IU:11:LEU:HD23	2.12	0.48
2:OE:138:ILE:HD11	2:OE:173:LEU:HD11	1.95	0.48
2:OP:29:ARG:HD3	2:OP:29:ARG:H	1.79	0.48
2:OR:178:VAL:HG12	2:OR:178:VAL:O	2.12	0.48
1:ID:78:HIS:O	1:IE:11:LEU:HD23	2.14	0.48
1:IN:78:HIS:O	1:IO:11:LEU:HD23	2.13	0.48
1:IW:3:LEU:HD12	1:IW:7:PHE:HB3	1.95	0.48
2:OI:178:VAL:HG12	2:OI:178:VAL:O	2.13	0.48
2:OJ:158:ILE:HD11	2:OJ:162:ASP:HB2	1.95	0.48
2:OM:93:ILE:HG23	2:OM:94:ASN:H	1.79	0.48
2:OV:24:ARG:HG3	2:OV:24:ARG:O	2.14	0.48
2:OX:173:LEU:HD12	2:OX:176:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:24:VAL:HG21	1:IA:36:ARG:CD	2.44	0.48
1:IG:52:MET:HE1	1:IH:18:ARG:CB	2.44	0.48
1:IO:3:LEU:HD12	1:IO:7:PHE:HB3	1.94	0.48
1:IJ:13:ALA:HB1	1:IJ:54:ASN:OD1	2.14	0.48
2:ON:158:ILE:HD12	2:ON:161:ASP:HB2	1.95	0.48
2:OT:177:ILE:HG22	2:OT:177:ILE:O	2.13	0.48
1:IL:40:LEU:HD21	1:IL:44:LEU:HD22	1.96	0.48
2:OS:132:LYS:O	2:OS:132:LYS:HG3	2.13	0.47
1:IU:20:LEU:HD12	1:IU:20:LEU:C	2.39	0.47
1:IF:56:LEU:HD22	1:IF:76:VAL:CG1	2.44	0.47
2:ON:62:ASN:ND2	2:ON:93:ILE:HD11	2.30	0.47
1:IC:20:LEU:HD11	1:IC:50:ALA:HB1	1.96	0.47
2:OC:90:ARG:HD2	2:OC:90:ARG:O	2.15	0.47
2:OK:56:ALA:HB1	2:OK:63:MET:HE1	1.97	0.47
2:OK:59:TYR:HB3	2:OK:64:ILE:HD11	1.97	0.47
2:OP:144:ILE:O	2:OP:166:LEU:HD13	2.15	0.47
1:IP:70:LEU:HB3	1:IP:92:ILE:HD11	1.97	0.47
1:IT:44:LEU:HD23	1:IT:45:ASP:OD1	2.15	0.46
2:OG:86:TYR:HA	2:OG:103:LEU:HD21	1.96	0.46
1:ID:59:MET:HE3	1:IE:86:PHE:HE1	1.81	0.46
2:OE:138:ILE:CD1	2:OE:173:LEU:HD11	2.45	0.46
2:OX:93:ILE:HG23	2:OX:93:ILE:O	2.15	0.46
1:IC:10:VAL:HG23	1:IC:56:LEU:HD21	1.98	0.46
2:OS:93:ILE:HG23	2:OS:94:ASN:H	1.80	0.46
2:OW:21:VAL:HG11	2:OW:51:HIS:ND1	2.30	0.46
1:IS:57:MET:HE2	1:IT:15:HIS:ND1	2.31	0.46
2:OJ:158:ILE:HD12	2:OJ:161:ASP:HB2	1.96	0.46
1:IN:93:VAL:HG23	1:IN:94:LYS:N	2.30	0.46
1:IQ:16:LYS:O	1:IQ:20:LEU:HD13	2.16	0.46
1:IP:3:LEU:HD12	1:IP:84:VAL:HG12	1.98	0.46
1:IR:54:ASN:CG	1:IR:54:ASN:O	2.59	0.46
2:OT:87:MET:HE3	2:OT:88:GLU:OE2	2.16	0.46
2:OX:95:LEU:HD23	2:OX:95:LEU:O	2.16	0.46
1:IP:16:LYS:O	1:IP:20:LEU:HD13	2.16	0.45
2:OA:28:ARG:NH1	2:OX:37:LEU:HD21	2.31	0.45
2:OG:90:ARG:HG3	2:OG:90:ARG:O	2.16	0.45
2:OG:73:LEU:HD13	2:OG:171:PHE:O	2.16	0.45
2:OK:104:LEU:CD1	2:OK:170:LEU:HD13	2.47	0.45
2:ON:29:ARG:HH21	2:OO:34:ALA:HB1	1.81	0.45
2:OV:79:PRO:CG	2:OV:111:LEU:HD13	2.47	0.45
1:IA:18:ARG:HB3	1:IX:52:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IL:10:VAL:HG23	1:IL:56:LEU:HD21	1.99	0.45
1:IP:40:LEU:HD21	1:IP:44:LEU:HD22	1.98	0.45
1:IX:20:LEU:HD12	1:IX:20:LEU:O	2.17	0.45
1:IA:40:LEU:C	1:IA:40:LEU:HD12	2.42	0.45
1:IO:20:LEU:C	1:IO:20:LEU:HD12	2.42	0.45
1:IS:51:LEU:HD22	1:IS:56:LEU:HB3	1.98	0.45
1:IS:78:HIS:O	1:IT:11:LEU:HD23	2.16	0.45
1:IW:93:VAL:HG23	1:IW:94:LYS:HG3	1.99	0.45
2:OA:19:CYS:HB2	2:OA:21:VAL:HG12	1.99	0.45
2:OT:57:TYR:O	2:OT:64:ILE:HD12	2.17	0.45
2:OT:133:GLY:O	2:OT:134:LEU:HD22	2.16	0.45
1:IL:93:VAL:HG23	1:IL:94:LYS:N	2.32	0.45
2:OB:30:MET:HE1	2:OC:44:PHE:CE2	2.52	0.44
2:ON:62:ASN:OD1	2:ON:62:ASN:O	2.34	0.44
1:IW:78:HIS:O	1:IX:11:LEU:HD23	2.17	0.44
1:IW:40:LEU:CD1	1:IW:44:LEU:HD22	2.48	0.44
2:OG:8:VAL:O	2:OG:11:ALA:HB3	2.17	0.44
2:OS:93:ILE:HG23	2:OS:94:ASN:N	2.32	0.44
1:IG:100:VAL:HG11	1:IH:90:ILE:HD12	1.98	0.44
2:OL:37:LEU:HD21	2:OM:28:ARG:NH1	2.32	0.44
2:OX:136:VAL:HG13	2:OX:136:VAL:O	2.18	0.44
2:OA:21:VAL:HG11	2:OA:51:HIS:CE1	2.52	0.44
1:IF:38:ALA:HB1	1:IF:41:ASP:OD1	2.18	0.44
1:IG:40:LEU:HD12	1:IG:40:LEU:O	2.18	0.44
2:OB:121:ASN:OD1	2:OB:121:ASN:O	2.36	0.44
2:OO:147:ILE:HG13	2:OO:148:VAL:HG23	1.99	0.44
2:OX:59:TYR:N	2:OX:64:ILE:HD11	2.33	0.44
1:IH:93:VAL:HG23	1:IH:94:LYS:N	2.32	0.43
2:OT:37:LEU:HD21	2:OU:28:ARG:NH1	2.32	0.43
2:OT:105:ARG:HD3	2:OT:122:ILE:HD13	1.99	0.43
1:IG:20:LEU:C	1:IG:20:LEU:HD12	2.43	0.43
1:IT:48:THR:HG22	1:IT:58:ILE:CD1	2.48	0.43
1:IF:40:LEU:C	1:IF:40:LEU:HD23	2.43	0.43
1:II:57:MET:HE1	1:IJ:15:HIS:CA	2.48	0.43
1:IS:9:LYS:HA	1:IS:9:LYS:HE2	2.00	0.43
1:IS:77:MET:HE3	1:IS:77:MET:HA	2.00	0.43
1:IC:78:HIS:O	1:ID:11:LEU:HD23	2.18	0.43
1:IP:41:ASP:OD2	1:IP:41:ASP:O	2.35	0.43
2:OE:101:ALA:HB2	2:OE:166:LEU:HD12	1.99	0.43
1:IJ:70:LEU:HD23	1:IJ:70:LEU:C	2.44	0.43
1:IM:9:LYS:HE2	1:IM:9:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IV:70:LEU:CB	1:IV:92:ILE:HD11	2.48	0.43
1:IW:24:VAL:HG21	1:IW:36:ARG:CD	2.49	0.43
1:IB:70:LEU:HB2	1:IB:92:ILE:HD11	2.00	0.43
1:IB:93:VAL:HG23	1:IB:94:LYS:N	2.34	0.43
1:IT:93:VAL:HG23	1:IT:94:LYS:N	2.32	0.43
1:IW:56:LEU:HD23	1:IW:77:MET:O	2.19	0.43
1:IG:57:MET:HE1	1:IH:15:HIS:CA	2.48	0.43
1:IC:10:VAL:HG12	1:IC:82:GLN:OE1	2.18	0.43
1:IK:76:VAL:HG22	1:IK:84:VAL:HG22	2.00	0.43
1:IL:1:MET:H1	1:IL:1:MET:HE2	1.84	0.43
1:IV:10:VAL:HG23	1:IV:56:LEU:HD21	1.99	0.43
1:IW:52:MET:HE3	1:IW:52:MET:HA	2.01	0.43
2:OE:102:ALA:O	2:OE:106:LEU:HD12	2.19	0.43
1:IH:54:ASN:O	1:IH:54:ASN:CG	2.62	0.43
1:IS:40:LEU:HD12	1:IS:40:LEU:C	2.44	0.43
1:IX:40:LEU:C	1:IX:40:LEU:HD23	2.44	0.43
2:OW:93:ILE:HG23	2:OW:94:ASN:H	1.84	0.43
1:IE:40:LEU:C	1:IE:40:LEU:HD12	2.44	0.42
1:IT:95:ASN:OD1	1:IT:95:ASN:O	2.37	0.42
2:OG:93:ILE:HG23	2:OG:94:ASN:H	1.84	0.42
2:OO:19:CYS:HB2	2:OO:21:VAL:HG12	2.01	0.42
2:OU:136:VAL:HG12	2:OU:136:VAL:O	2.18	0.42
1:IB:56:LEU:HD23	1:IB:77:MET:O	2.19	0.42
1:IH:40:LEU:C	1:IH:40:LEU:HD23	2.44	0.42
2:OA:147:ILE:HG13	2:OA:148:VAL:HG23	2.00	0.42
2:OR:78:MET:HA	2:OR:78:MET:HE2	2.00	0.42
1:IG:78:HIS:O	1:IH:11:LEU:HD23	2.19	0.42
1:IS:93:VAL:HG23	1:IS:94:LYS:HG3	2.02	0.42
1:IV:58:ILE:HD11	1:IV:60:GLN:HE21	1.83	0.42
2:OH:59:TYR:N	2:OH:64:ILE:HD11	2.34	0.42
2:OP:92:ILE:C	2:OP:93:ILE:HD12	2.44	0.42
1:ID:93:VAL:HG23	1:ID:94:LYS:CG	2.49	0.42
1:IS:20:LEU:HD11	1:IS:50:ALA:CB	2.49	0.42
2:OU:126:ILE:O	2:OU:130:VAL:HG23	2.19	0.42
1:II:78:HIS:O	1:IJ:11:LEU:HD23	2.19	0.42
2:OJ:78:MET:HA	2:OJ:78:MET:HE2	2.01	0.42
2:OP:136:VAL:O	2:OP:136:VAL:HG13	2.20	0.42
2:OS:178:VAL:HG12	2:OS:178:VAL:O	2.19	0.42
2:OV:82:CYS:HB2	2:OV:107:CYS:HB2	1.96	0.42
2:OJ:136:VAL:HG13	2:OJ:136:VAL:O	2.19	0.42
1:ID:54:ASN:CG	1:ID:54:ASN:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IH:77:MET:HE1	1:II:1:MET:HE2	2.01	0.42
1:II:40:LEU:HD12	1:II:40:LEU:C	2.45	0.42
2:OG:93:ILE:HG23	2:OG:94:ASN:N	2.35	0.42
2:OH:93:ILE:HD12	2:OH:93:ILE:N	2.35	0.42
2:OM:126:ILE:HG23	2:OM:127:ARG:HD2	2.00	0.42
2:OS:126:ILE:O	2:OS:130:VAL:HG23	2.20	0.42
2:OX:158:ILE:HD11	2:OX:162:ASP:HB2	2.01	0.42
1:II:10:VAL:HG23	1:II:56:LEU:HD21	2.01	0.42
1:IQ:40:LEU:C	1:IQ:40:LEU:HD12	2.45	0.42
2:OB:29:ARG:H	2:OB:29:ARG:HD3	1.85	0.42
2:OK:93:ILE:HG23	2:OK:94:ASN:H	1.84	0.42
2:OL:83:LYS:O	2:OL:87:MET:SD	2.78	0.42
2:OP:37:LEU:HD11	2:OQ:28:ARG:HD3	2.00	0.42
2:OS:104:LEU:HD12	2:OS:170:LEU:HD13	2.01	0.42
1:IA:20:LEU:C	1:IA:20:LEU:HD12	2.45	0.42
1:ID:93:VAL:HG23	1:ID:94:LYS:N	2.34	0.42
2:OF:136:VAL:O	2:OF:136:VAL:HG13	2.20	0.42
1:IG:86:PHE:CZ	1:IG:115:ALA:HB1	2.54	0.42
2:OI:136:VAL:O	2:OI:136:VAL:HG12	2.20	0.42
2:OR:30:MET:HE3	2:OR:46:MET:HG2	2.02	0.42
1:IV:54:ASN:CG	1:IV:54:ASN:O	2.63	0.41
2:OL:136:VAL:O	2:OL:136:VAL:HG13	2.19	0.41
2:OV:136:VAL:O	2:OV:136:VAL:HG13	2.20	0.41
1:IG:52:MET:HE1	1:IH:18:ARG:HB3	2.01	0.41
1:IC:40:LEU:HD12	1:IC:40:LEU:C	2.45	0.41
1:IP:47:ILE:O	1:IP:51:LEU:HD23	2.19	0.41
2:OH:136:VAL:HG13	2:OH:136:VAL:O	2.21	0.41
2:OV:79:PRO:HG3	2:OV:111:LEU:HD13	2.03	0.41
1:IF:78:HIS:O	1:IG:11:LEU:HD23	2.20	0.41
1:IP:120:GLN:O	1:IP:120:GLN:CG	2.69	0.41
2:OJ:59:TYR:N	2:OJ:64:ILE:HD11	2.35	0.41
2:ON:136:VAL:O	2:ON:136:VAL:HG13	2.20	0.41
2:OS:28:ARG:HE	2:OS:46:MET:HE3	1.85	0.41
2:OW:133:GLY:C	2:OW:134:LEU:HD22	2.45	0.41
2:OB:109:GLN:HG2	2:OB:122:ILE:HD11	2.02	0.41
2:OR:121:ASN:OD1	2:OR:121:ASN:O	2.38	0.41
1:IL:52:MET:HE1	1:IM:18:ARG:HH11	1.86	0.41
1:IM:54:ASN:O	1:IM:54:ASN:CG	2.63	0.41
1:IQ:86:PHE:CE1	1:IQ:115:ALA:HB1	2.55	0.41
2:OW:36:GLU:OE2	2:OW:36:GLU:N	2.53	0.41
1:IH:77:MET:CE	1:II:1:MET:HE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IM:40:LEU:C	1:IM:40:LEU:HD12	2.45	0.41
1:IO:93:VAL:HG23	1:IO:94:LYS:N	2.36	0.41
1:IP:57:MET:HE1	1:IQ:15:HIS:HA	2.03	0.41
1:IW:9:LYS:HA	1:IW:9:LYS:HE2	2.02	0.41
2:OA:93:ILE:HG23	2:OA:94:ASN:H	1.85	0.41
2:OB:30:MET:HE1	2:OC:44:PHE:HE2	1.86	0.41
2:OH:75:ASN:OD1	2:OH:77:ASP:OD1	2.38	0.41
2:OS:131:GLN:OE1	2:OS:139:GLN:OE1	2.38	0.41
2:OU:93:ILE:HG23	2:OU:94:ASN:H	1.86	0.41
2:OD:24:ARG:O	2:OD:24:ARG:HG3	2.20	0.41
2:OF:93:ILE:HD12	2:OG:90:ARG:HE	1.86	0.41
2:OR:133:GLY:O	2:OR:134:LEU:HD22	2.21	0.41
1:IF:54:ASN:CG	1:IF:54:ASN:O	2.64	0.40
1:IB:57:MET:HE1	1:IC:15:HIS:HA	2.02	0.40
1:IM:59:MET:HE2	1:IN:1:MET:SD	2.62	0.40
1:IN:40:LEU:HD23	1:IN:40:LEU:C	2.46	0.40
1:IU:40:LEU:C	1:IU:40:LEU:HD12	2.46	0.40
2:OX:176:ILE:HD12	2:OX:177:ILE:HD12	2.03	0.40
1:IJ:54:ASN:O	1:IJ:54:ASN:CG	2.64	0.40
1:IV:40:LEU:HD12	1:IV:40:LEU:C	2.46	0.40
2:OA:136:VAL:O	2:OA:136:VAL:HG12	2.21	0.40
2:OC:19:CYS:HB2	2:OC:21:VAL:HG12	2.03	0.40
2:OI:19:CYS:CB	2:OI:21:VAL:HG12	2.50	0.40
2:OJ:177:ILE:HD11	2:OJ:179:ASP:CG	2.47	0.40
2:OM:136:VAL:HG12	2:OM:136:VAL:O	2.22	0.40
2:OV:64:ILE:HB	2:OV:65:ILE:HD12	2.03	0.40
1:IB:77:MET:HE3	1:IC:3:LEU:HD21	2.04	0.40
1:II:24:VAL:HG21	1:II:36:ARG:HD2	2.03	0.40
2:OD:136:VAL:O	2:OD:136:VAL:HG13	2.21	0.40
1:IB:95:ASN:O	1:IB:95:ASN:OD1	2.40	0.40
2:OO:158:ILE:HD12	2:OO:161:ASP:HB2	2.02	0.40
2:OQ:93:ILE:HG23	2:OQ:94:ASN:H	1.86	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	IA	123/227 (54%)	122 (99%)	1 (1%)	0	100	100
1	IB	123/227 (54%)	122 (99%)	1 (1%)	0	100	100
1	IC	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	ID	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IE	123/227 (54%)	122 (99%)	1 (1%)	0	100	100
1	IF	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IG	123/227 (54%)	123 (100%)	0	0	100	100
1	IH	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	II	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IJ	123/227 (54%)	123 (100%)	0	0	100	100
1	IK	123/227 (54%)	123 (100%)	0	0	100	100
1	IL	123/227 (54%)	123 (100%)	0	0	100	100
1	IM	123/227 (54%)	123 (100%)	0	0	100	100
1	IN	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IO	123/227 (54%)	123 (100%)	0	0	100	100
1	IP	123/227 (54%)	123 (100%)	0	0	100	100
1	IQ	123/227 (54%)	123 (100%)	0	0	100	100
1	IR	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IS	123/227 (54%)	123 (100%)	0	0	100	100
1	IT	123/227 (54%)	122 (99%)	1 (1%)	0	100	100
1	IU	123/227 (54%)	123 (100%)	0	0	100	100
1	IV	123/227 (54%)	121 (98%)	2 (2%)	0	100	100
1	IW	123/227 (54%)	123 (100%)	0	0	100	100
1	IX	123/227 (54%)	122 (99%)	1 (1%)	0	100	100
2	OA	175/219 (80%)	171 (98%)	4 (2%)	0	100	100
2	OB	175/219 (80%)	171 (98%)	4 (2%)	0	100	100
2	OC	175/219 (80%)	169 (97%)	6 (3%)	0	100	100
2	OD	175/219 (80%)	174 (99%)	1 (1%)	0	100	100
2	OE	175/219 (80%)	172 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	OF	175/219 (80%)	174 (99%)	0	1 (1%)	21	54
2	OG	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OH	175/219 (80%)	170 (97%)	5 (3%)	0	100	100
2	OI	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OJ	175/219 (80%)	172 (98%)	2 (1%)	1 (1%)	21	54
2	OK	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OL	175/219 (80%)	173 (99%)	2 (1%)	0	100	100
2	OM	175/219 (80%)	173 (99%)	2 (1%)	0	100	100
2	ON	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OO	175/219 (80%)	173 (99%)	2 (1%)	0	100	100
2	OP	175/219 (80%)	174 (99%)	1 (1%)	0	100	100
2	OQ	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OR	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OS	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OT	175/219 (80%)	174 (99%)	1 (1%)	0	100	100
2	OU	175/219 (80%)	173 (99%)	2 (1%)	0	100	100
2	OV	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
2	OW	175/219 (80%)	171 (98%)	4 (2%)	0	100	100
2	OX	175/219 (80%)	172 (98%)	3 (2%)	0	100	100
All	All	7152/10704 (67%)	7063 (99%)	87 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	OJ	176	ILE
2	OF	93	ILE

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	IA	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IB	107/194 (55%)	107 (100%)	0	100	100
1	IC	107/194 (55%)	104 (97%)	3 (3%)	38	61
1	ID	107/194 (55%)	107 (100%)	0	100	100
1	IE	107/194 (55%)	107 (100%)	0	100	100
1	IF	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IG	107/194 (55%)	105 (98%)	2 (2%)	50	68
1	IH	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	II	107/194 (55%)	107 (100%)	0	100	100
1	IJ	107/194 (55%)	107 (100%)	0	100	100
1	IK	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IL	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IM	107/194 (55%)	107 (100%)	0	100	100
1	IN	107/194 (55%)	107 (100%)	0	100	100
1	IO	107/194 (55%)	107 (100%)	0	100	100
1	IP	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IQ	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IR	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IS	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IT	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IU	107/194 (55%)	107 (100%)	0	100	100
1	IV	107/194 (55%)	107 (100%)	0	100	100
1	IW	107/194 (55%)	106 (99%)	1 (1%)	70	76
1	IX	107/194 (55%)	107 (100%)	0	100	100
2	OA	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OB	147/183 (80%)	147 (100%)	0	100	100
2	OC	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OD	147/183 (80%)	147 (100%)	0	100	100
2	OE	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OF	147/183 (80%)	145 (99%)	2 (1%)	59	71
2	OG	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OH	147/183 (80%)	145 (99%)	2 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	OI	147/183 (80%)	147 (100%)	0	100	100
2	OJ	147/183 (80%)	144 (98%)	3 (2%)	48	67
2	OK	147/183 (80%)	147 (100%)	0	100	100
2	OL	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OM	147/183 (80%)	147 (100%)	0	100	100
2	ON	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OO	147/183 (80%)	147 (100%)	0	100	100
2	OP	146/183 (80%)	146 (100%)	0	100	100
2	OQ	147/183 (80%)	147 (100%)	0	100	100
2	OR	147/183 (80%)	147 (100%)	0	100	100
2	OS	147/183 (80%)	145 (99%)	2 (1%)	59	71
2	OT	147/183 (80%)	147 (100%)	0	100	100
2	OU	147/183 (80%)	145 (99%)	2 (1%)	59	71
2	OV	147/183 (80%)	146 (99%)	1 (1%)	76	78
2	OW	147/183 (80%)	147 (100%)	0	100	100
2	OX	147/183 (80%)	146 (99%)	1 (1%)	76	78
All	All	6095/9048 (67%)	6060 (99%)	35 (1%)	76	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	IA	3	LEU
1	IC	3	LEU
1	IC	26	LYS
1	IC	51	LEU
1	IF	20	LEU
1	IG	58	ILE
1	IG	75	THR
1	IH	48	THR
1	IK	75	THR
1	IL	59	MET
1	IP	20	LEU
1	IQ	3	LEU
1	IR	40	LEU
1	IS	56	LEU
1	IT	45	ASP

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Mol	Chain	Res	Type
1	IW	3	LEU
2	OA	62	ASN
2	OC	107	CYS
2	OE	93	ILE
2	OF	4	TYR
2	OF	93	ILE
2	OG	30	MET
2	OH	78	MET
2	OH	93	ILE
2	OJ	26	PHE
2	OJ	33	SER
2	OJ	82	CYS
2	OL	4	TYR
2	ON	4	TYR
2	OS	82	CYS
2	OS	107	CYS
2	OU	5	TYR
2	OU	107	CYS
2	OV	26	PHE
2	OX	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	ID	60	GLN
1	IE	29	GLN
1	IE	78	HIS
1	IK	35	ASN
1	IL	15	HIS
1	IM	15	HIS
1	IO	95	ASN
1	IQ	54	ASN
1	IR	30	ASN
1	IW	54	ASN
2	OA	131	GLN
2	OA	168	HIS
2	OD	62	ASN
2	OF	70	ASN
2	OF	94	ASN
2	OG	39	GLN
2	OG	121	ASN
2	OG	168	HIS

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Continued from previous page...

Mol	Chain	Res	Type
2	OG	175	ASN
2	OJ	168	HIS
2	OK	168	HIS
2	OL	139	GLN
2	OL	150	ASN
2	ON	62	ASN
2	OO	121	ASN
2	OP	139	GLN
2	OQ	51	HIS
2	OQ	121	ASN
2	OQ	131	GLN
2	OQ	168	HIS
2	OT	51	HIS
2	OT	75	ASN
2	OU	39	GLN
2	OW	121	ASN
2	OX	139	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](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

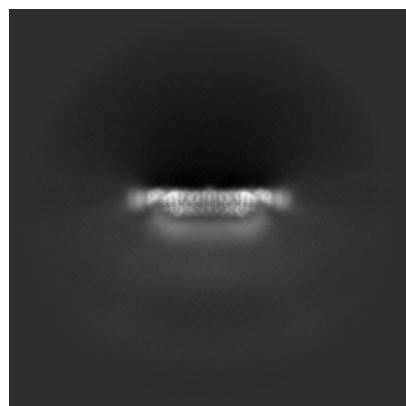
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72693. These allow visual inspection of the internal detail of the map and identification of artifacts.

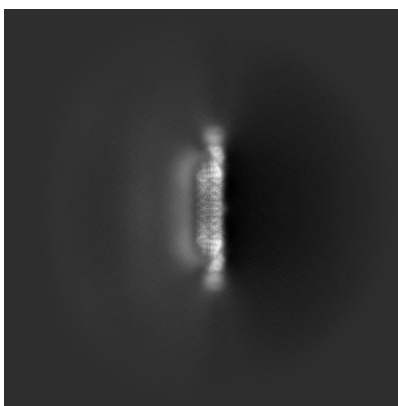
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

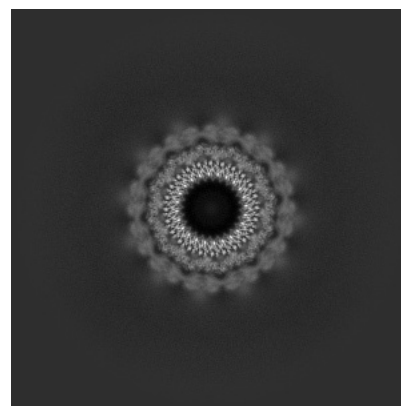
6.1.1 Primary map



X

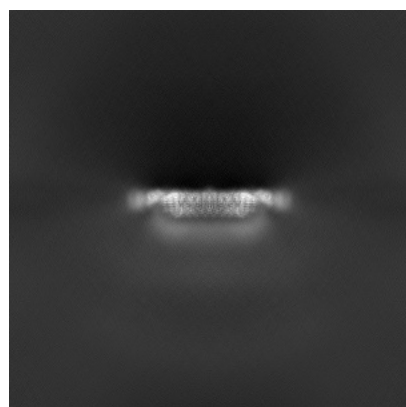


Y

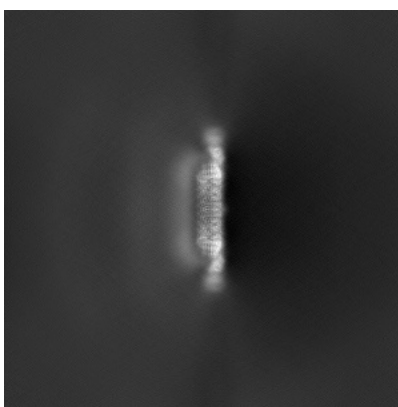


Z

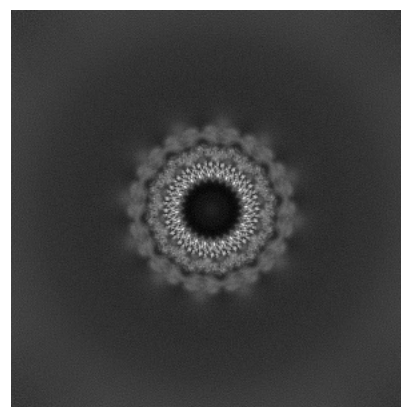
6.1.2 Raw map



X



Y

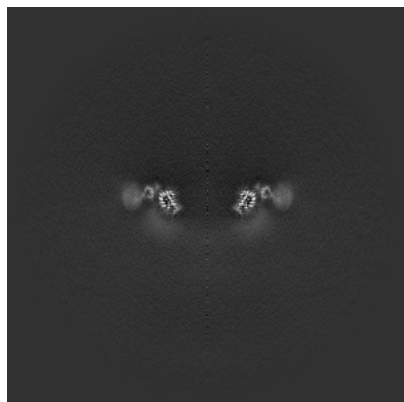


Z

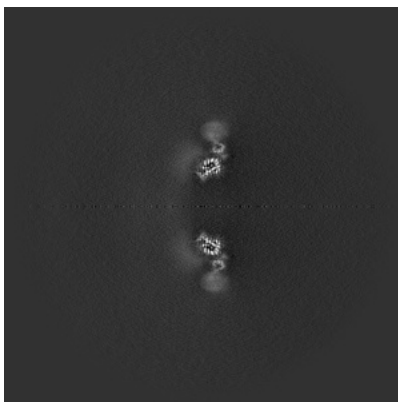
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

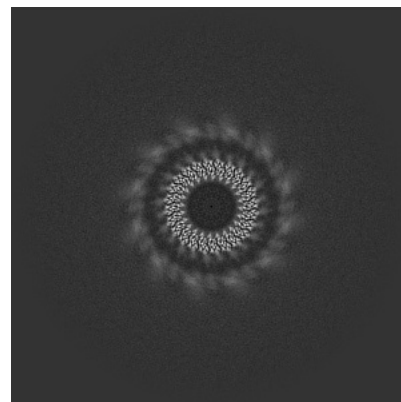
6.2.1 Primary map



X Index: 220

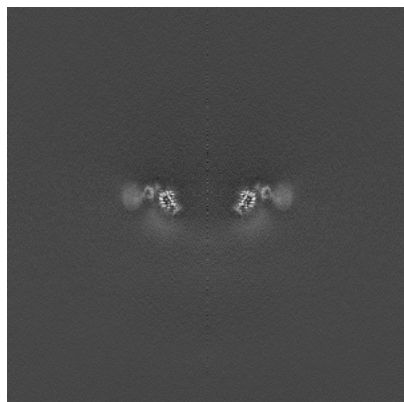


Y Index: 220

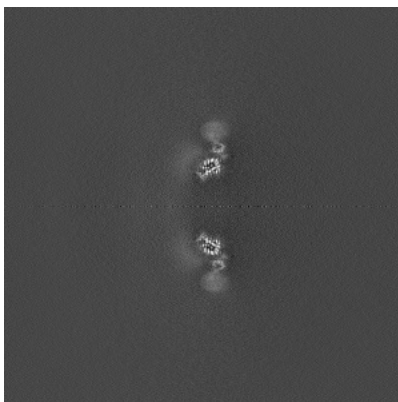


Z Index: 220

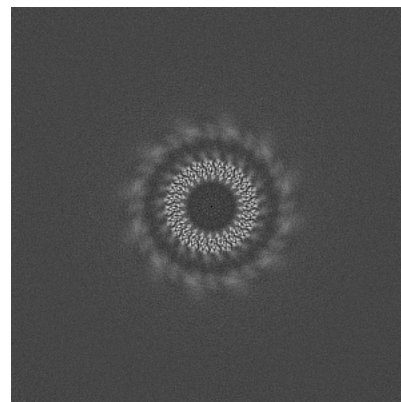
6.2.2 Raw map



X Index: 220



Y Index: 220

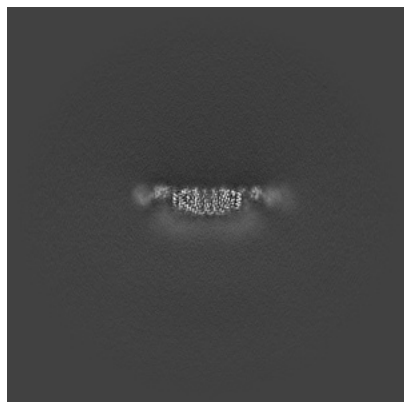


Z Index: 220

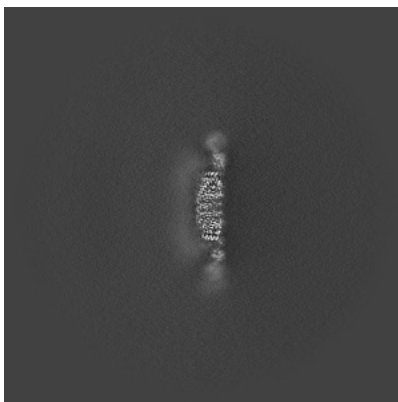
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

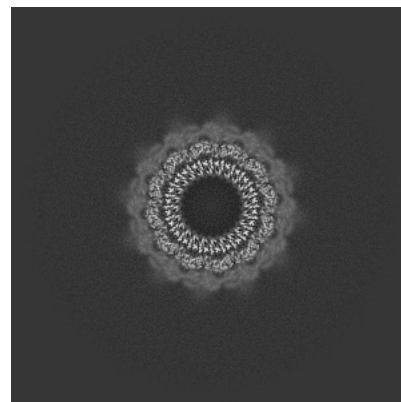
6.3.1 Primary map



X Index: 184

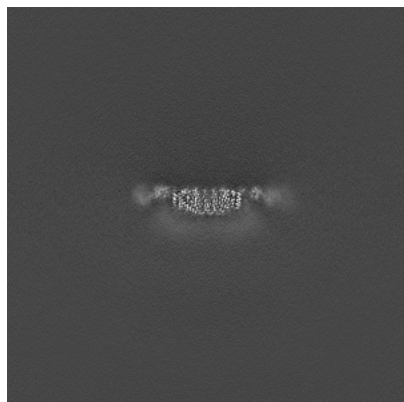


Y Index: 184

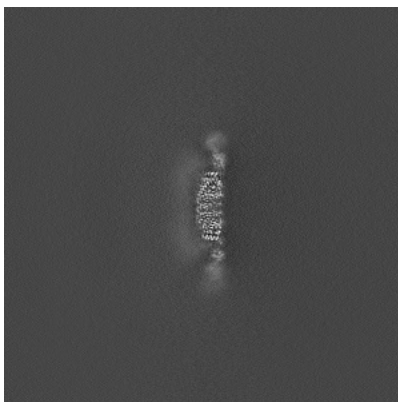


Z Index: 234

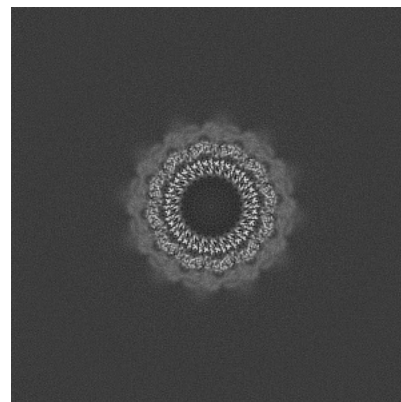
6.3.2 Raw map



X Index: 184



Y Index: 184

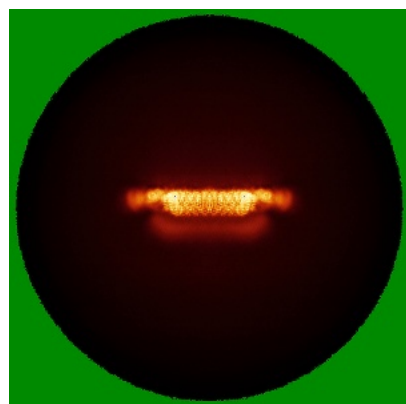


Z Index: 234

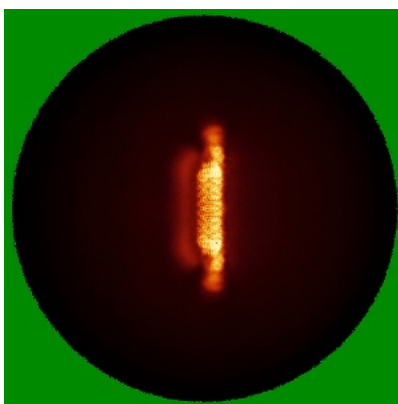
The images above show the largest variance slices of the map in three orthogonal directions.

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

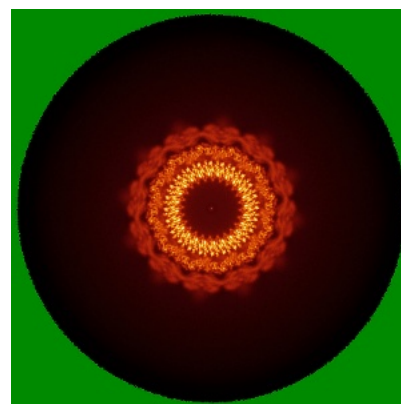
6.4.1 Primary map



X

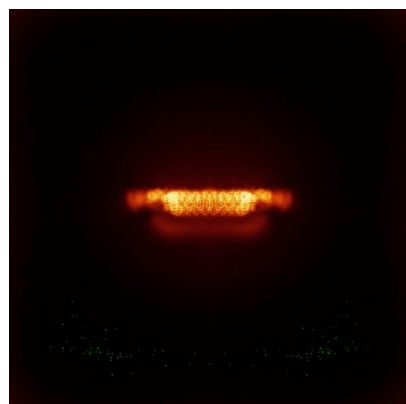


Y

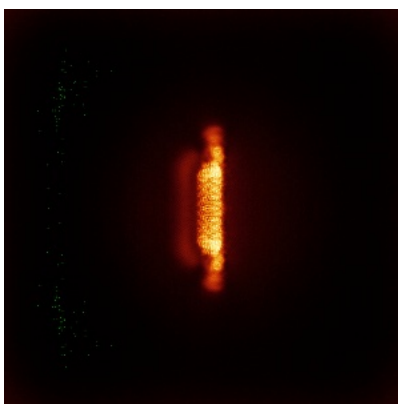


Z

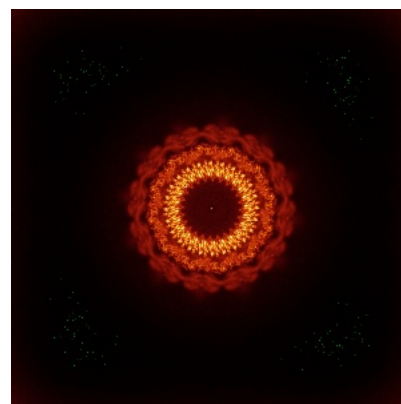
6.4.2 Raw map



X



Y

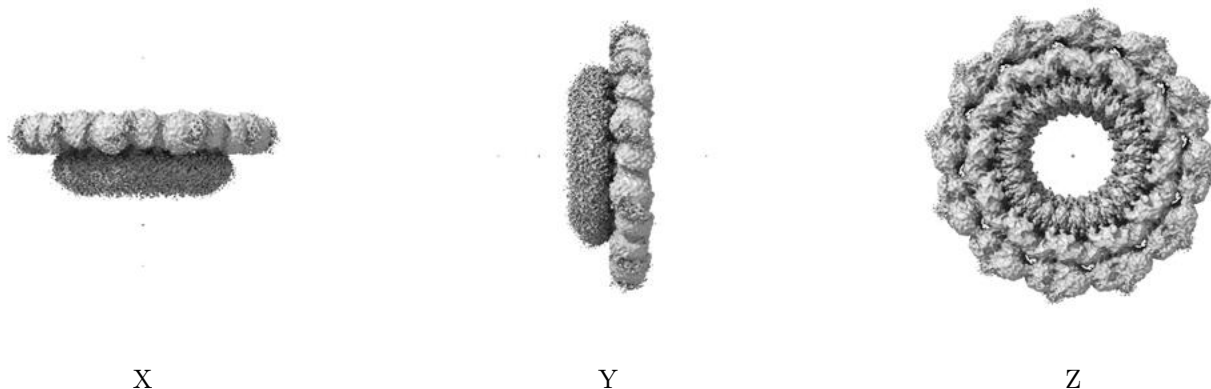


Z

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.

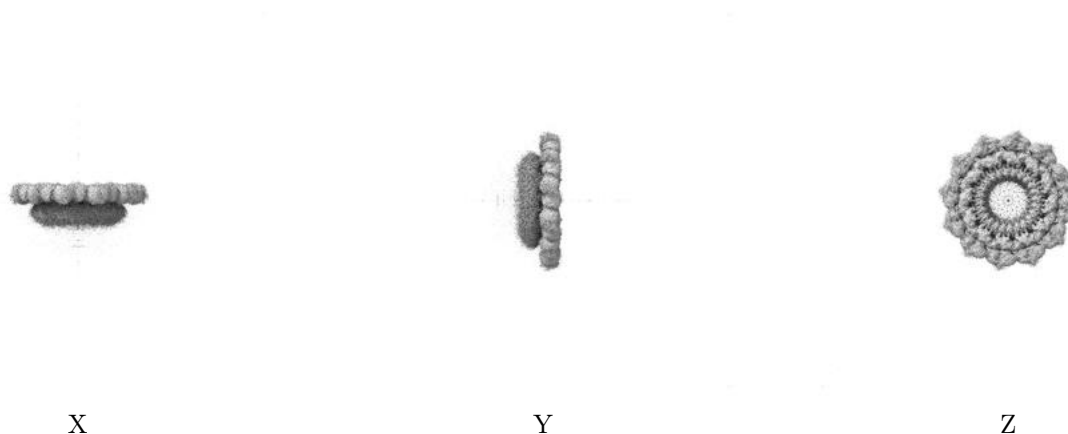
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0777. 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.

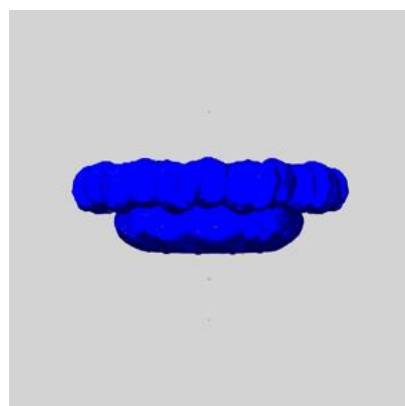
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

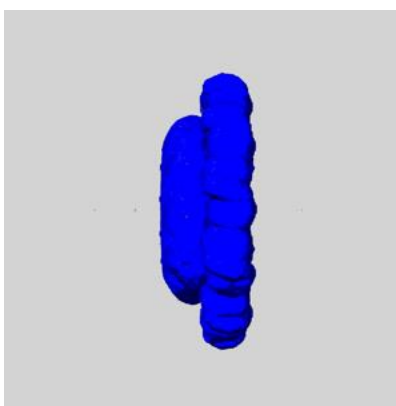
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

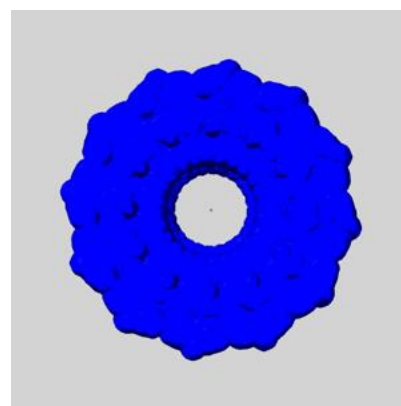
6.6.1 emd_72693_msk_1.map [i](#)



X



Y

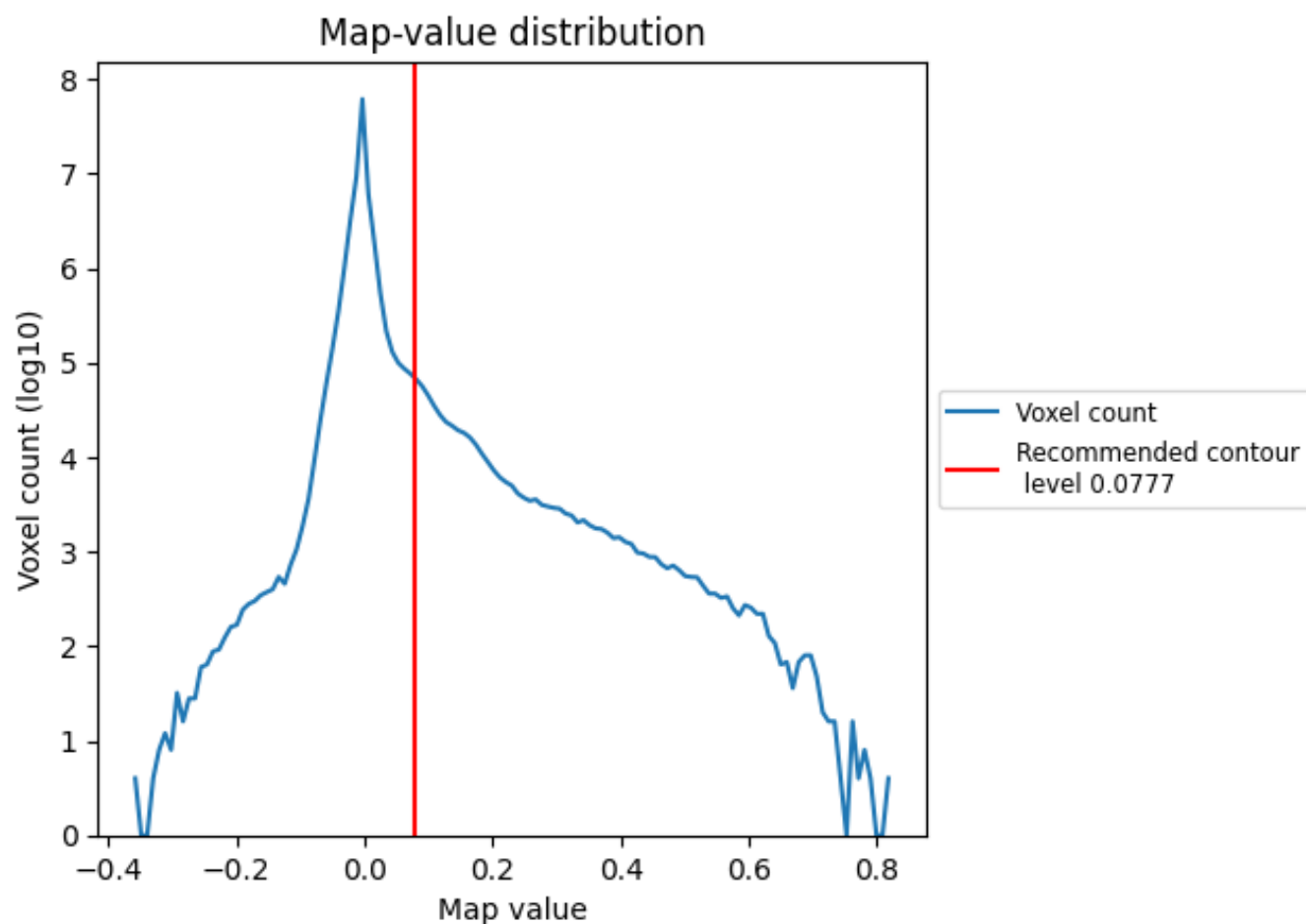


Z

7 Map analysis [i](#)

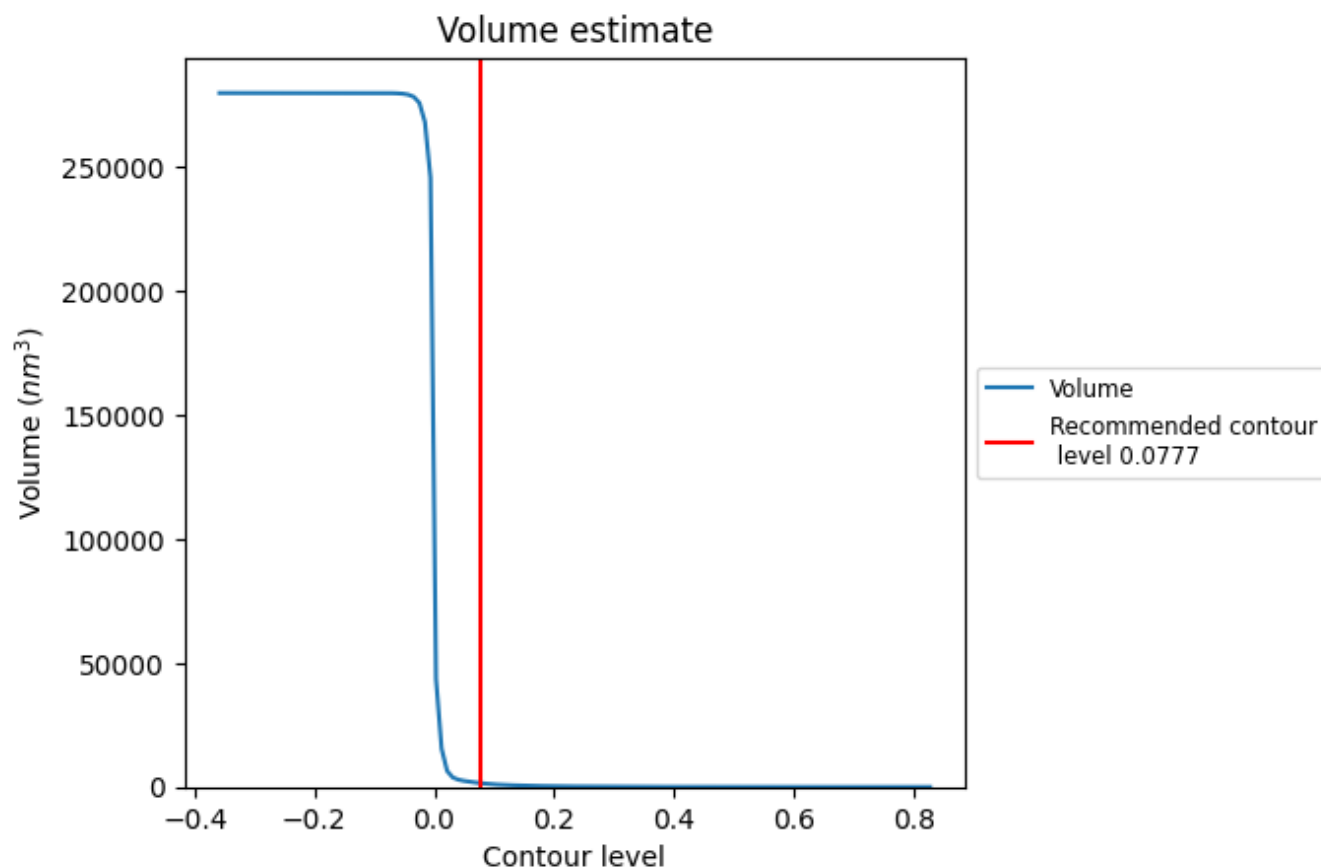
This section contains the results of statistical analysis of the map.

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.

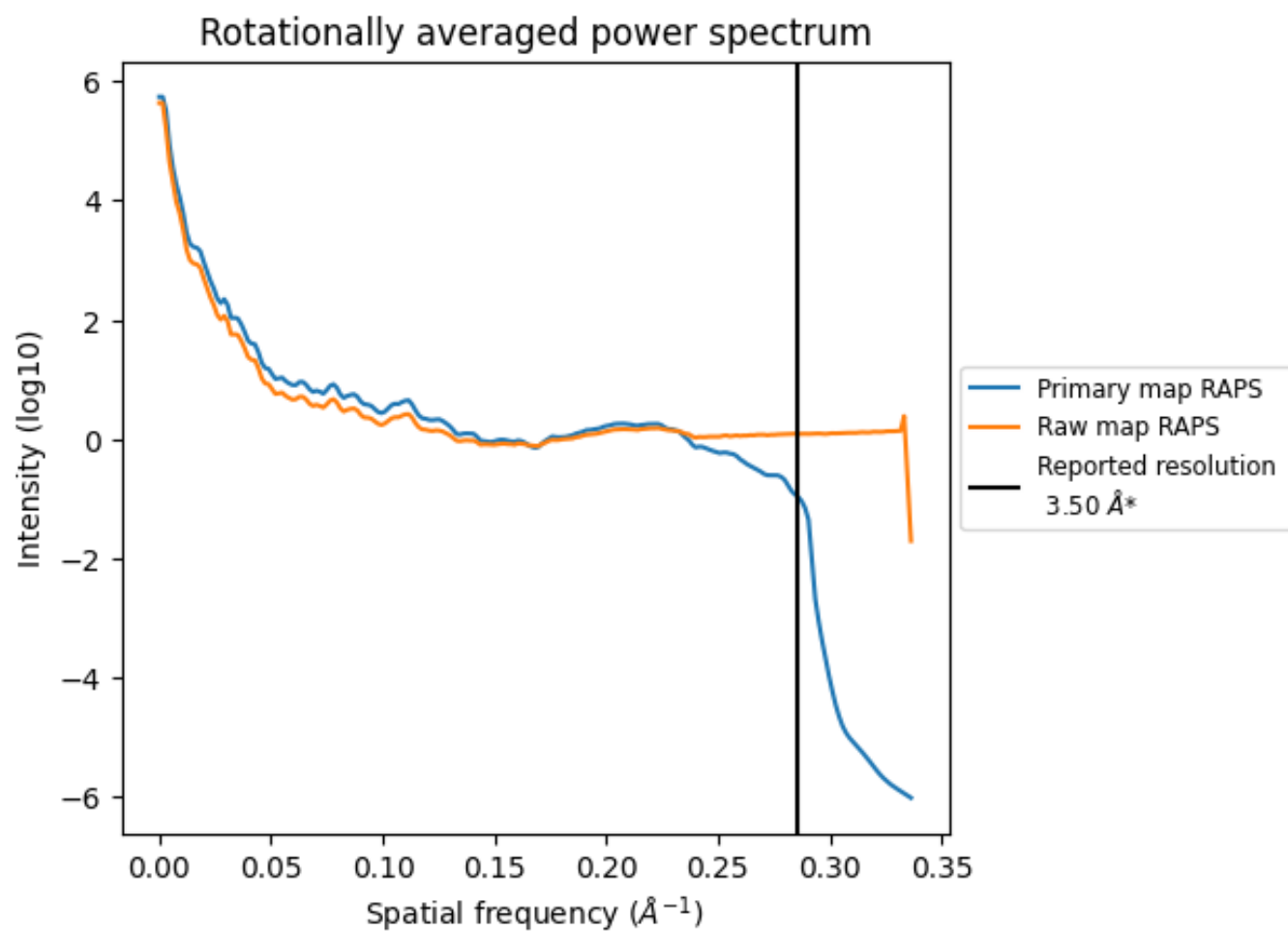
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1542 nm^3 ; this corresponds to an approximate mass of 1393 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 ⓘ

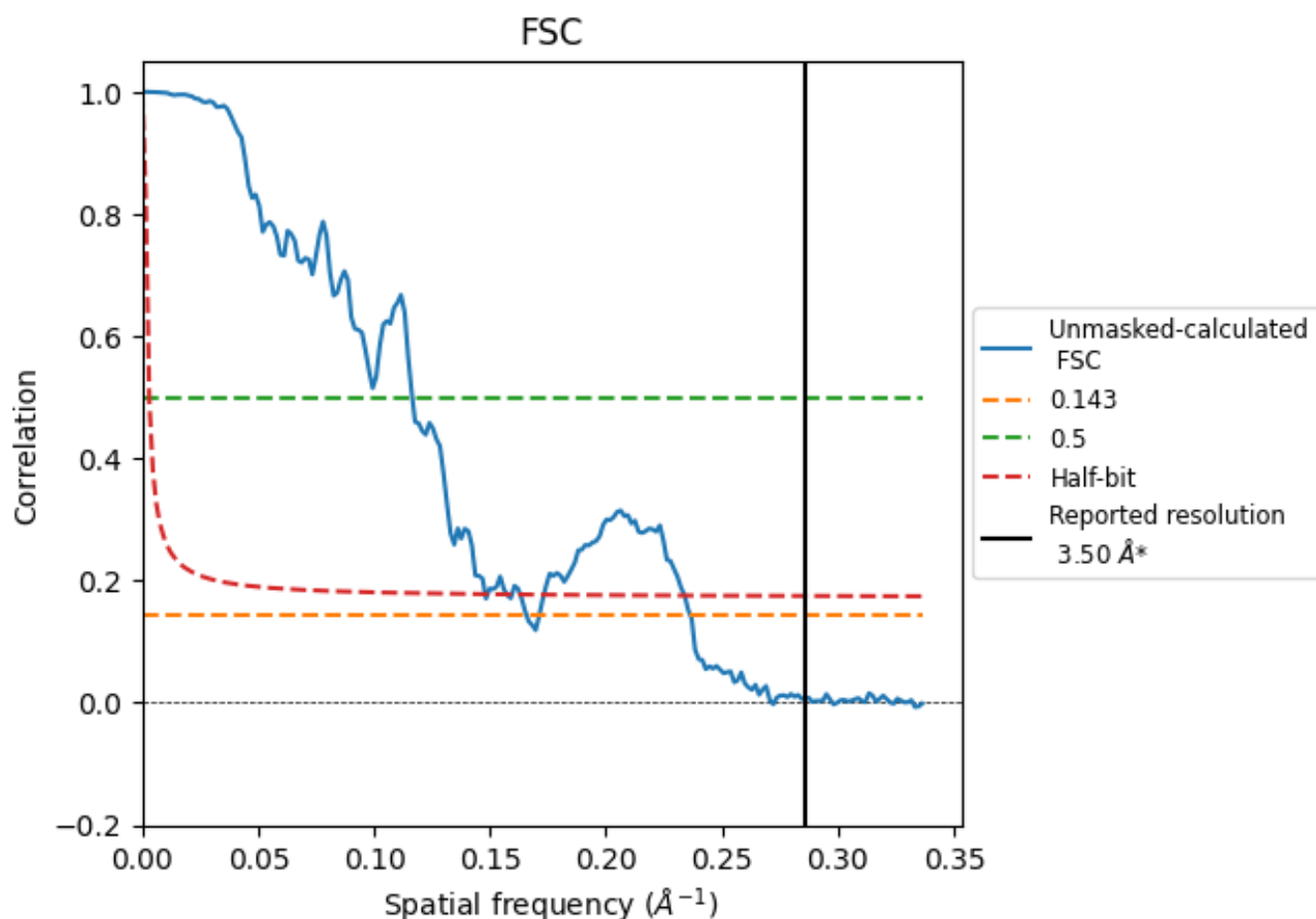


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

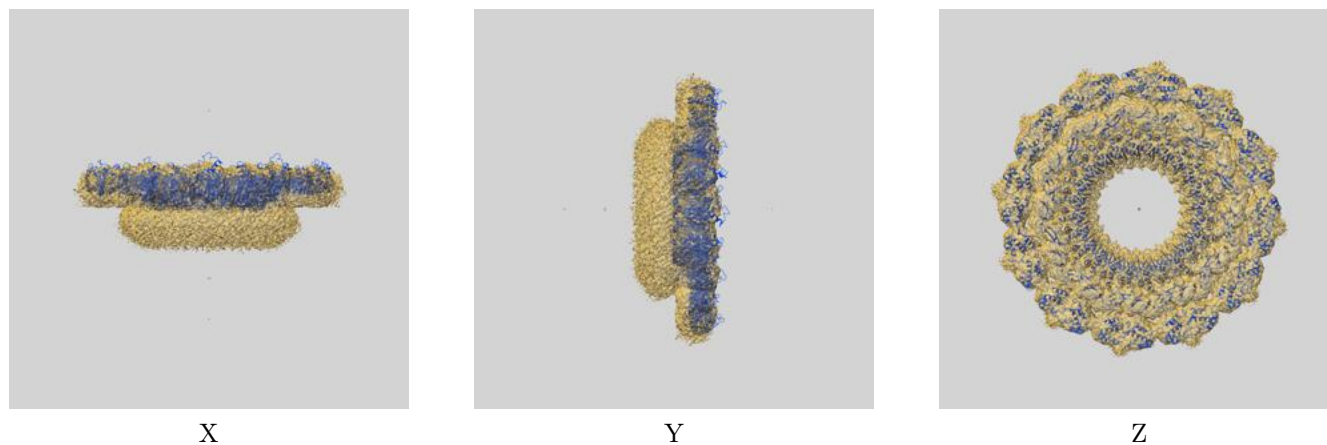
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.03	8.58	6.76

*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 6.03 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

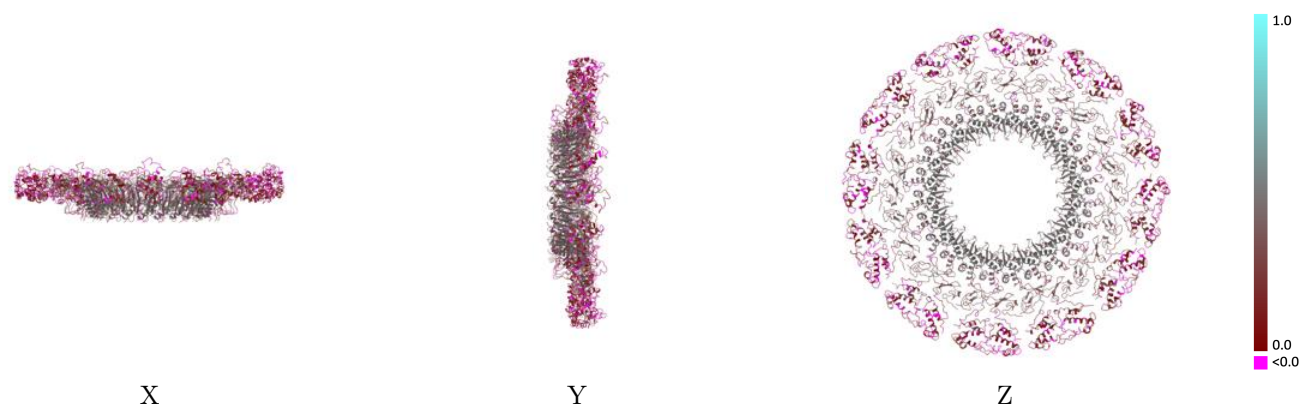
This section contains information regarding the fit between EMDB map EMD-72693 and PDB model 9Y9C. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



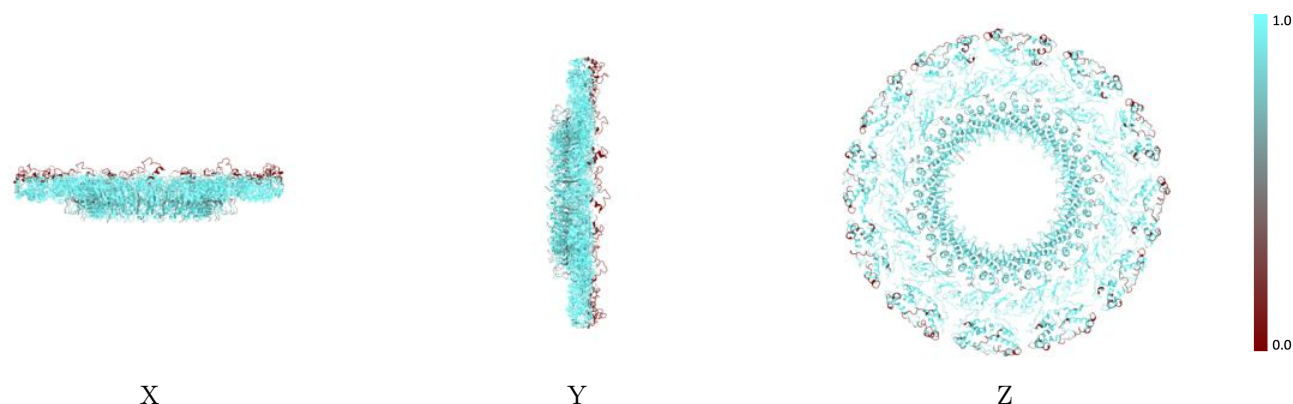
The images above show the 3D surface view of the map at the recommended contour level 0.0777 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



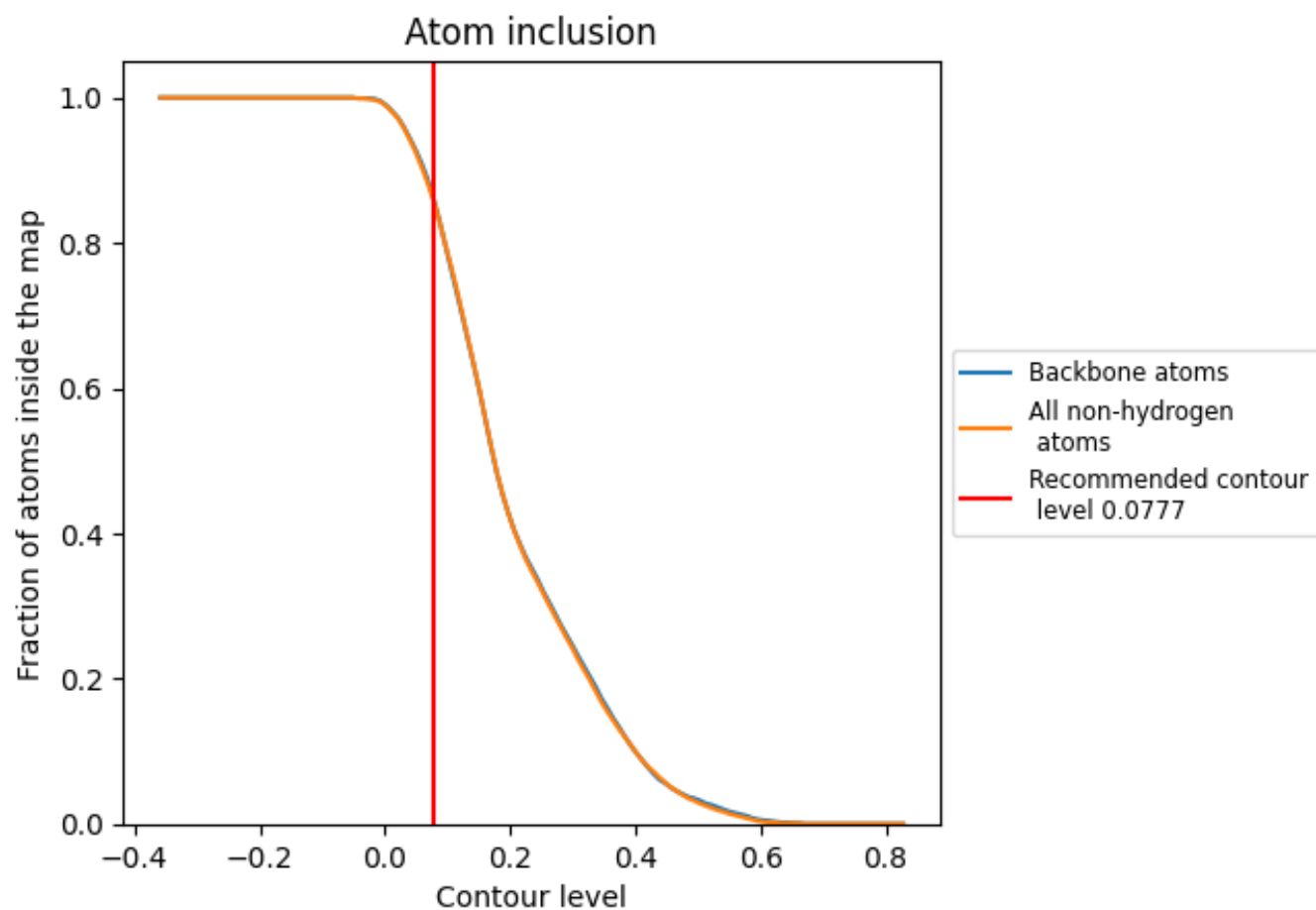
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0777).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.0777) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.2510
IA	 0.8990	 0.3640
IB	 0.9040	 0.3530
IC	 0.8990	 0.3590
ID	 0.9070	 0.3540
IE	 0.8900	 0.3510
IF	 0.8980	 0.3450
IG	 0.9040	 0.3510
IH	 0.8940	 0.3490
II	 0.9070	 0.3600
IJ	 0.8990	 0.3480
IK	 0.9010	 0.3670
IL	 0.9070	 0.3430
IM	 0.9010	 0.3680
IN	 0.9030	 0.3540
IO	 0.8740	 0.3520
IP	 0.8900	 0.3520
IQ	 0.8960	 0.3650
IR	 0.9130	 0.3510
IS	 0.8870	 0.3560
IT	 0.8860	 0.3460
IU	 0.9010	 0.3560
IV	 0.9070	 0.3480
IW	 0.9060	 0.3620
IX	 0.8940	 0.3470
OA	 0.8420	 0.1960
OB	 0.8190	 0.1540
OC	 0.9070	 0.1950
OD	 0.7590	 0.1450
OE	 0.8940	 0.2040
OF	 0.7700	 0.1520
OG	 0.9160	 0.2120
OH	 0.8020	 0.1600
OI	 0.9070	 0.2020
OJ	 0.7930	 0.1590



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Chain	Atom inclusion	Q-score
OK	 0.8910	 0.2050
OL	 0.7990	 0.1490
OM	 0.9320	 0.1940
ON	 0.7500	 0.1500
OO	 0.9050	 0.2060
OP	 0.7950	 0.1650
OQ	 0.8840	 0.2050
OR	 0.8220	 0.1670
OS	 0.9040	 0.1950
OT	 0.7990	 0.1440
OU	 0.8940	 0.2070
OV	 0.8100	 0.1650
OW	 0.8740	 0.2000
OX	 0.7620	 0.1450