



Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 01:04 PM EST

PDB ID : 8DO4
EMDB ID : EMD-27590
Title : Prefusion-stabilized Nipah virus fusion protein, dimer of trimers
Authors : Byrne, P.O.; Blade, E.G.; McLellan, J.S.
Deposited on : 2022-07-12
Resolution : 3.20 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

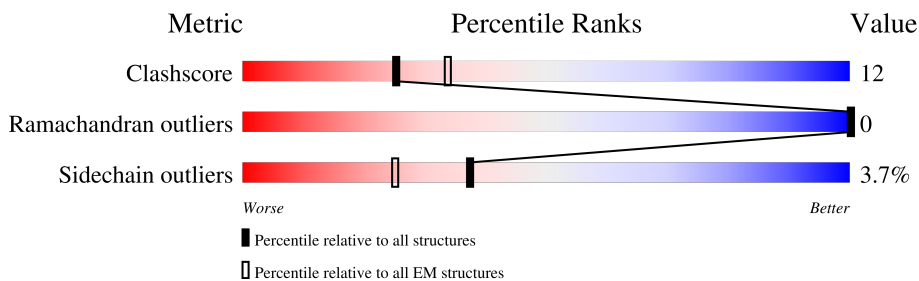
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	543	
1	B	543	
1	C	543	
1	D	543	
1	E	543	
1	G	543	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 20163 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	436	3348	2121	548	657	22	0	0
1	B	442	3393	2149	557	665	22	0	0
1	C	435	3343	2118	547	656	22	0	0
1	D	442	3393	2149	557	665	22	0	0
1	E	435	3343	2118	547	656	22	0	0
1	G	435	3343	2118	547	656	22	0	0

There are 504 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	expression tag	UNP Q9IH63
A	6	TYR	-	expression tag	UNP Q9IH63
A	7	SER	-	expression tag	UNP Q9IH63
A	8	MET	-	expression tag	UNP Q9IH63
A	9	GLN	-	expression tag	UNP Q9IH63
A	10	LEU	-	expression tag	UNP Q9IH63
A	11	ALA	-	expression tag	UNP Q9IH63
A	12	SER	-	expression tag	UNP Q9IH63
A	13	CYS	-	expression tag	UNP Q9IH63
A	14	VAL	-	expression tag	UNP Q9IH63
A	15	THR	-	expression tag	UNP Q9IH63
A	16	LEU	-	expression tag	UNP Q9IH63
A	17	THR	-	expression tag	UNP Q9IH63
A	18	LEU	-	expression tag	UNP Q9IH63
A	19	VAL	-	expression tag	UNP Q9IH63
A	20	LEU	-	expression tag	UNP Q9IH63
A	21	LEU	-	expression tag	UNP Q9IH63
A	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ASN	-	expression tag	UNP Q9IH63
A	24	SER	-	expression tag	UNP Q9IH63
A	25	GLN	-	expression tag	UNP Q9IH63
A	104	CYS	LEU	conflict	UNP Q9IH63
A	114	CYS	ILE	conflict	UNP Q9IH63
A	172	PHE	LEU	conflict	UNP Q9IH63
A	191	PRO	SER	conflict	UNP Q9IH63
A	489	LYS	-	expression tag	UNP Q9IH63
A	490	LEU	-	expression tag	UNP Q9IH63
A	491	MET	-	expression tag	UNP Q9IH63
A	492	LYS	-	expression tag	UNP Q9IH63
A	493	GLN	-	expression tag	UNP Q9IH63
A	494	ILE	-	expression tag	UNP Q9IH63
A	495	GLU	-	expression tag	UNP Q9IH63
A	496	ASP	-	expression tag	UNP Q9IH63
A	497	LYS	-	expression tag	UNP Q9IH63
A	498	ILE	-	expression tag	UNP Q9IH63
A	499	GLU	-	expression tag	UNP Q9IH63
A	500	GLU	-	expression tag	UNP Q9IH63
A	501	ILE	-	expression tag	UNP Q9IH63
A	502	LEU	-	expression tag	UNP Q9IH63
A	503	SER	-	expression tag	UNP Q9IH63
A	504	LYS	-	expression tag	UNP Q9IH63
A	505	ILE	-	expression tag	UNP Q9IH63
A	506	TYR	-	expression tag	UNP Q9IH63
A	507	HIS	-	expression tag	UNP Q9IH63
A	508	ILE	-	expression tag	UNP Q9IH63
A	509	GLU	-	expression tag	UNP Q9IH63
A	510	ASN	-	expression tag	UNP Q9IH63
A	511	GLU	-	expression tag	UNP Q9IH63
A	512	ILE	-	expression tag	UNP Q9IH63
A	513	ALA	-	expression tag	UNP Q9IH63
A	514	ARG	-	expression tag	UNP Q9IH63
A	515	ILE	-	expression tag	UNP Q9IH63
A	516	LYS	-	expression tag	UNP Q9IH63
A	517	LYS	-	expression tag	UNP Q9IH63
A	518	LEU	-	expression tag	UNP Q9IH63
A	519	ILE	-	expression tag	UNP Q9IH63
A	520	GLY	-	expression tag	UNP Q9IH63
A	521	GLU	-	expression tag	UNP Q9IH63
A	522	ALA	-	expression tag	UNP Q9IH63
A	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	GLY	-	expression tag	UNP Q9IH63
A	525	GLY	-	expression tag	UNP Q9IH63
A	526	LEU	-	expression tag	UNP Q9IH63
A	527	VAL	-	expression tag	UNP Q9IH63
A	528	PRO	-	expression tag	UNP Q9IH63
A	529	ARG	-	expression tag	UNP Q9IH63
A	530	GLY	-	expression tag	UNP Q9IH63
A	531	SER	-	expression tag	UNP Q9IH63
A	532	HIS	-	expression tag	UNP Q9IH63
A	533	HIS	-	expression tag	UNP Q9IH63
A	534	HIS	-	expression tag	UNP Q9IH63
A	535	HIS	-	expression tag	UNP Q9IH63
A	536	HIS	-	expression tag	UNP Q9IH63
A	537	HIS	-	expression tag	UNP Q9IH63
A	538	SER	-	expression tag	UNP Q9IH63
A	539	ALA	-	expression tag	UNP Q9IH63
A	540	TRP	-	expression tag	UNP Q9IH63
A	541	SER	-	expression tag	UNP Q9IH63
A	542	HIS	-	expression tag	UNP Q9IH63
A	543	PRO	-	expression tag	UNP Q9IH63
A	544	GLN	-	expression tag	UNP Q9IH63
A	545	PHE	-	expression tag	UNP Q9IH63
A	546	GLU	-	expression tag	UNP Q9IH63
A	547	LYS	-	expression tag	UNP Q9IH63
B	5	MET	-	expression tag	UNP Q9IH63
B	6	TYR	-	expression tag	UNP Q9IH63
B	7	SER	-	expression tag	UNP Q9IH63
B	8	MET	-	expression tag	UNP Q9IH63
B	9	GLN	-	expression tag	UNP Q9IH63
B	10	LEU	-	expression tag	UNP Q9IH63
B	11	ALA	-	expression tag	UNP Q9IH63
B	12	SER	-	expression tag	UNP Q9IH63
B	13	CYS	-	expression tag	UNP Q9IH63
B	14	VAL	-	expression tag	UNP Q9IH63
B	15	THR	-	expression tag	UNP Q9IH63
B	16	LEU	-	expression tag	UNP Q9IH63
B	17	THR	-	expression tag	UNP Q9IH63
B	18	LEU	-	expression tag	UNP Q9IH63
B	19	VAL	-	expression tag	UNP Q9IH63
B	20	LEU	-	expression tag	UNP Q9IH63
B	21	LEU	-	expression tag	UNP Q9IH63
B	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ASN	-	expression tag	UNP Q9IH63
B	24	SER	-	expression tag	UNP Q9IH63
B	25	GLN	-	expression tag	UNP Q9IH63
B	104	CYS	LEU	conflict	UNP Q9IH63
B	114	CYS	ILE	conflict	UNP Q9IH63
B	172	PHE	LEU	conflict	UNP Q9IH63
B	191	PRO	SER	conflict	UNP Q9IH63
B	489	LYS	-	expression tag	UNP Q9IH63
B	490	LEU	-	expression tag	UNP Q9IH63
B	491	MET	-	expression tag	UNP Q9IH63
B	492	LYS	-	expression tag	UNP Q9IH63
B	493	GLN	-	expression tag	UNP Q9IH63
B	494	ILE	-	expression tag	UNP Q9IH63
B	495	GLU	-	expression tag	UNP Q9IH63
B	496	ASP	-	expression tag	UNP Q9IH63
B	497	LYS	-	expression tag	UNP Q9IH63
B	498	ILE	-	expression tag	UNP Q9IH63
B	499	GLU	-	expression tag	UNP Q9IH63
B	500	GLU	-	expression tag	UNP Q9IH63
B	501	ILE	-	expression tag	UNP Q9IH63
B	502	LEU	-	expression tag	UNP Q9IH63
B	503	SER	-	expression tag	UNP Q9IH63
B	504	LYS	-	expression tag	UNP Q9IH63
B	505	ILE	-	expression tag	UNP Q9IH63
B	506	TYR	-	expression tag	UNP Q9IH63
B	507	HIS	-	expression tag	UNP Q9IH63
B	508	ILE	-	expression tag	UNP Q9IH63
B	509	GLU	-	expression tag	UNP Q9IH63
B	510	ASN	-	expression tag	UNP Q9IH63
B	511	GLU	-	expression tag	UNP Q9IH63
B	512	ILE	-	expression tag	UNP Q9IH63
B	513	ALA	-	expression tag	UNP Q9IH63
B	514	ARG	-	expression tag	UNP Q9IH63
B	515	ILE	-	expression tag	UNP Q9IH63
B	516	LYS	-	expression tag	UNP Q9IH63
B	517	LYS	-	expression tag	UNP Q9IH63
B	518	LEU	-	expression tag	UNP Q9IH63
B	519	ILE	-	expression tag	UNP Q9IH63
B	520	GLY	-	expression tag	UNP Q9IH63
B	521	GLU	-	expression tag	UNP Q9IH63
B	522	ALA	-	expression tag	UNP Q9IH63
B	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	GLY	-	expression tag	UNP Q9IH63
B	525	GLY	-	expression tag	UNP Q9IH63
B	526	LEU	-	expression tag	UNP Q9IH63
B	527	VAL	-	expression tag	UNP Q9IH63
B	528	PRO	-	expression tag	UNP Q9IH63
B	529	ARG	-	expression tag	UNP Q9IH63
B	530	GLY	-	expression tag	UNP Q9IH63
B	531	SER	-	expression tag	UNP Q9IH63
B	532	HIS	-	expression tag	UNP Q9IH63
B	533	HIS	-	expression tag	UNP Q9IH63
B	534	HIS	-	expression tag	UNP Q9IH63
B	535	HIS	-	expression tag	UNP Q9IH63
B	536	HIS	-	expression tag	UNP Q9IH63
B	537	HIS	-	expression tag	UNP Q9IH63
B	538	SER	-	expression tag	UNP Q9IH63
B	539	ALA	-	expression tag	UNP Q9IH63
B	540	TRP	-	expression tag	UNP Q9IH63
B	541	SER	-	expression tag	UNP Q9IH63
B	542	HIS	-	expression tag	UNP Q9IH63
B	543	PRO	-	expression tag	UNP Q9IH63
B	544	GLN	-	expression tag	UNP Q9IH63
B	545	PHE	-	expression tag	UNP Q9IH63
B	546	GLU	-	expression tag	UNP Q9IH63
B	547	LYS	-	expression tag	UNP Q9IH63
C	5	MET	-	expression tag	UNP Q9IH63
C	6	TYR	-	expression tag	UNP Q9IH63
C	7	SER	-	expression tag	UNP Q9IH63
C	8	MET	-	expression tag	UNP Q9IH63
C	9	GLN	-	expression tag	UNP Q9IH63
C	10	LEU	-	expression tag	UNP Q9IH63
C	11	ALA	-	expression tag	UNP Q9IH63
C	12	SER	-	expression tag	UNP Q9IH63
C	13	CYS	-	expression tag	UNP Q9IH63
C	14	VAL	-	expression tag	UNP Q9IH63
C	15	THR	-	expression tag	UNP Q9IH63
C	16	LEU	-	expression tag	UNP Q9IH63
C	17	THR	-	expression tag	UNP Q9IH63
C	18	LEU	-	expression tag	UNP Q9IH63
C	19	VAL	-	expression tag	UNP Q9IH63
C	20	LEU	-	expression tag	UNP Q9IH63
C	21	LEU	-	expression tag	UNP Q9IH63
C	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	ASN	-	expression tag	UNP Q9IH63
C	24	SER	-	expression tag	UNP Q9IH63
C	25	GLN	-	expression tag	UNP Q9IH63
C	104	CYS	LEU	conflict	UNP Q9IH63
C	114	CYS	ILE	conflict	UNP Q9IH63
C	172	PHE	LEU	conflict	UNP Q9IH63
C	191	PRO	SER	conflict	UNP Q9IH63
C	489	LYS	-	expression tag	UNP Q9IH63
C	490	LEU	-	expression tag	UNP Q9IH63
C	491	MET	-	expression tag	UNP Q9IH63
C	492	LYS	-	expression tag	UNP Q9IH63
C	493	GLN	-	expression tag	UNP Q9IH63
C	494	ILE	-	expression tag	UNP Q9IH63
C	495	GLU	-	expression tag	UNP Q9IH63
C	496	ASP	-	expression tag	UNP Q9IH63
C	497	LYS	-	expression tag	UNP Q9IH63
C	498	ILE	-	expression tag	UNP Q9IH63
C	499	GLU	-	expression tag	UNP Q9IH63
C	500	GLU	-	expression tag	UNP Q9IH63
C	501	ILE	-	expression tag	UNP Q9IH63
C	502	LEU	-	expression tag	UNP Q9IH63
C	503	SER	-	expression tag	UNP Q9IH63
C	504	LYS	-	expression tag	UNP Q9IH63
C	505	ILE	-	expression tag	UNP Q9IH63
C	506	TYR	-	expression tag	UNP Q9IH63
C	507	HIS	-	expression tag	UNP Q9IH63
C	508	ILE	-	expression tag	UNP Q9IH63
C	509	GLU	-	expression tag	UNP Q9IH63
C	510	ASN	-	expression tag	UNP Q9IH63
C	511	GLU	-	expression tag	UNP Q9IH63
C	512	ILE	-	expression tag	UNP Q9IH63
C	513	ALA	-	expression tag	UNP Q9IH63
C	514	ARG	-	expression tag	UNP Q9IH63
C	515	ILE	-	expression tag	UNP Q9IH63
C	516	LYS	-	expression tag	UNP Q9IH63
C	517	LYS	-	expression tag	UNP Q9IH63
C	518	LEU	-	expression tag	UNP Q9IH63
C	519	ILE	-	expression tag	UNP Q9IH63
C	520	GLY	-	expression tag	UNP Q9IH63
C	521	GLU	-	expression tag	UNP Q9IH63
C	522	ALA	-	expression tag	UNP Q9IH63
C	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	524	GLY	-	expression tag	UNP Q9IH63
C	525	GLY	-	expression tag	UNP Q9IH63
C	526	LEU	-	expression tag	UNP Q9IH63
C	527	VAL	-	expression tag	UNP Q9IH63
C	528	PRO	-	expression tag	UNP Q9IH63
C	529	ARG	-	expression tag	UNP Q9IH63
C	530	GLY	-	expression tag	UNP Q9IH63
C	531	SER	-	expression tag	UNP Q9IH63
C	532	HIS	-	expression tag	UNP Q9IH63
C	533	HIS	-	expression tag	UNP Q9IH63
C	534	HIS	-	expression tag	UNP Q9IH63
C	535	HIS	-	expression tag	UNP Q9IH63
C	536	HIS	-	expression tag	UNP Q9IH63
C	537	HIS	-	expression tag	UNP Q9IH63
C	538	SER	-	expression tag	UNP Q9IH63
C	539	ALA	-	expression tag	UNP Q9IH63
C	540	TRP	-	expression tag	UNP Q9IH63
C	541	SER	-	expression tag	UNP Q9IH63
C	542	HIS	-	expression tag	UNP Q9IH63
C	543	PRO	-	expression tag	UNP Q9IH63
C	544	GLN	-	expression tag	UNP Q9IH63
C	545	PHE	-	expression tag	UNP Q9IH63
C	546	GLU	-	expression tag	UNP Q9IH63
C	547	LYS	-	expression tag	UNP Q9IH63
D	5	MET	-	expression tag	UNP Q9IH63
D	6	TYR	-	expression tag	UNP Q9IH63
D	7	SER	-	expression tag	UNP Q9IH63
D	8	MET	-	expression tag	UNP Q9IH63
D	9	GLN	-	expression tag	UNP Q9IH63
D	10	LEU	-	expression tag	UNP Q9IH63
D	11	ALA	-	expression tag	UNP Q9IH63
D	12	SER	-	expression tag	UNP Q9IH63
D	13	CYS	-	expression tag	UNP Q9IH63
D	14	VAL	-	expression tag	UNP Q9IH63
D	15	THR	-	expression tag	UNP Q9IH63
D	16	LEU	-	expression tag	UNP Q9IH63
D	17	THR	-	expression tag	UNP Q9IH63
D	18	LEU	-	expression tag	UNP Q9IH63
D	19	VAL	-	expression tag	UNP Q9IH63
D	20	LEU	-	expression tag	UNP Q9IH63
D	21	LEU	-	expression tag	UNP Q9IH63
D	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	23	ASN	-	expression tag	UNP Q9IH63
D	24	SER	-	expression tag	UNP Q9IH63
D	25	GLN	-	expression tag	UNP Q9IH63
D	104	CYS	LEU	conflict	UNP Q9IH63
D	114	CYS	ILE	conflict	UNP Q9IH63
D	172	PHE	LEU	conflict	UNP Q9IH63
D	191	PRO	SER	conflict	UNP Q9IH63
D	489	LYS	-	expression tag	UNP Q9IH63
D	490	LEU	-	expression tag	UNP Q9IH63
D	491	MET	-	expression tag	UNP Q9IH63
D	492	LYS	-	expression tag	UNP Q9IH63
D	493	GLN	-	expression tag	UNP Q9IH63
D	494	ILE	-	expression tag	UNP Q9IH63
D	495	GLU	-	expression tag	UNP Q9IH63
D	496	ASP	-	expression tag	UNP Q9IH63
D	497	LYS	-	expression tag	UNP Q9IH63
D	498	ILE	-	expression tag	UNP Q9IH63
D	499	GLU	-	expression tag	UNP Q9IH63
D	500	GLU	-	expression tag	UNP Q9IH63
D	501	ILE	-	expression tag	UNP Q9IH63
D	502	LEU	-	expression tag	UNP Q9IH63
D	503	SER	-	expression tag	UNP Q9IH63
D	504	LYS	-	expression tag	UNP Q9IH63
D	505	ILE	-	expression tag	UNP Q9IH63
D	506	TYR	-	expression tag	UNP Q9IH63
D	507	HIS	-	expression tag	UNP Q9IH63
D	508	ILE	-	expression tag	UNP Q9IH63
D	509	GLU	-	expression tag	UNP Q9IH63
D	510	ASN	-	expression tag	UNP Q9IH63
D	511	GLU	-	expression tag	UNP Q9IH63
D	512	ILE	-	expression tag	UNP Q9IH63
D	513	ALA	-	expression tag	UNP Q9IH63
D	514	ARG	-	expression tag	UNP Q9IH63
D	515	ILE	-	expression tag	UNP Q9IH63
D	516	LYS	-	expression tag	UNP Q9IH63
D	517	LYS	-	expression tag	UNP Q9IH63
D	518	LEU	-	expression tag	UNP Q9IH63
D	519	ILE	-	expression tag	UNP Q9IH63
D	520	GLY	-	expression tag	UNP Q9IH63
D	521	GLU	-	expression tag	UNP Q9IH63
D	522	ALA	-	expression tag	UNP Q9IH63
D	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	524	GLY	-	expression tag	UNP Q9IH63
D	525	GLY	-	expression tag	UNP Q9IH63
D	526	LEU	-	expression tag	UNP Q9IH63
D	527	VAL	-	expression tag	UNP Q9IH63
D	528	PRO	-	expression tag	UNP Q9IH63
D	529	ARG	-	expression tag	UNP Q9IH63
D	530	GLY	-	expression tag	UNP Q9IH63
D	531	SER	-	expression tag	UNP Q9IH63
D	532	HIS	-	expression tag	UNP Q9IH63
D	533	HIS	-	expression tag	UNP Q9IH63
D	534	HIS	-	expression tag	UNP Q9IH63
D	535	HIS	-	expression tag	UNP Q9IH63
D	536	HIS	-	expression tag	UNP Q9IH63
D	537	HIS	-	expression tag	UNP Q9IH63
D	538	SER	-	expression tag	UNP Q9IH63
D	539	ALA	-	expression tag	UNP Q9IH63
D	540	TRP	-	expression tag	UNP Q9IH63
D	541	SER	-	expression tag	UNP Q9IH63
D	542	HIS	-	expression tag	UNP Q9IH63
D	543	PRO	-	expression tag	UNP Q9IH63
D	544	GLN	-	expression tag	UNP Q9IH63
D	545	PHE	-	expression tag	UNP Q9IH63
D	546	GLU	-	expression tag	UNP Q9IH63
D	547	LYS	-	expression tag	UNP Q9IH63
E	5	MET	-	expression tag	UNP Q9IH63
E	6	TYR	-	expression tag	UNP Q9IH63
E	7	SER	-	expression tag	UNP Q9IH63
E	8	MET	-	expression tag	UNP Q9IH63
E	9	GLN	-	expression tag	UNP Q9IH63
E	10	LEU	-	expression tag	UNP Q9IH63
E	11	ALA	-	expression tag	UNP Q9IH63
E	12	SER	-	expression tag	UNP Q9IH63
E	13	CYS	-	expression tag	UNP Q9IH63
E	14	VAL	-	expression tag	UNP Q9IH63
E	15	THR	-	expression tag	UNP Q9IH63
E	16	LEU	-	expression tag	UNP Q9IH63
E	17	THR	-	expression tag	UNP Q9IH63
E	18	LEU	-	expression tag	UNP Q9IH63
E	19	VAL	-	expression tag	UNP Q9IH63
E	20	LEU	-	expression tag	UNP Q9IH63
E	21	LEU	-	expression tag	UNP Q9IH63
E	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	23	ASN	-	expression tag	UNP Q9IH63
E	24	SER	-	expression tag	UNP Q9IH63
E	25	GLN	-	expression tag	UNP Q9IH63
E	104	CYS	LEU	conflict	UNP Q9IH63
E	114	CYS	ILE	conflict	UNP Q9IH63
E	172	PHE	LEU	conflict	UNP Q9IH63
E	191	PRO	SER	conflict	UNP Q9IH63
E	489	LYS	-	expression tag	UNP Q9IH63
E	490	LEU	-	expression tag	UNP Q9IH63
E	491	MET	-	expression tag	UNP Q9IH63
E	492	LYS	-	expression tag	UNP Q9IH63
E	493	GLN	-	expression tag	UNP Q9IH63
E	494	ILE	-	expression tag	UNP Q9IH63
E	495	GLU	-	expression tag	UNP Q9IH63
E	496	ASP	-	expression tag	UNP Q9IH63
E	497	LYS	-	expression tag	UNP Q9IH63
E	498	ILE	-	expression tag	UNP Q9IH63
E	499	GLU	-	expression tag	UNP Q9IH63
E	500	GLU	-	expression tag	UNP Q9IH63
E	501	ILE	-	expression tag	UNP Q9IH63
E	502	LEU	-	expression tag	UNP Q9IH63
E	503	SER	-	expression tag	UNP Q9IH63
E	504	LYS	-	expression tag	UNP Q9IH63
E	505	ILE	-	expression tag	UNP Q9IH63
E	506	TYR	-	expression tag	UNP Q9IH63
E	507	HIS	-	expression tag	UNP Q9IH63
E	508	ILE	-	expression tag	UNP Q9IH63
E	509	GLU	-	expression tag	UNP Q9IH63
E	510	ASN	-	expression tag	UNP Q9IH63
E	511	GLU	-	expression tag	UNP Q9IH63
E	512	ILE	-	expression tag	UNP Q9IH63
E	513	ALA	-	expression tag	UNP Q9IH63
E	514	ARG	-	expression tag	UNP Q9IH63
E	515	ILE	-	expression tag	UNP Q9IH63
E	516	LYS	-	expression tag	UNP Q9IH63
E	517	LYS	-	expression tag	UNP Q9IH63
E	518	LEU	-	expression tag	UNP Q9IH63
E	519	ILE	-	expression tag	UNP Q9IH63
E	520	GLY	-	expression tag	UNP Q9IH63
E	521	GLU	-	expression tag	UNP Q9IH63
E	522	ALA	-	expression tag	UNP Q9IH63
E	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	524	GLY	-	expression tag	UNP Q9IH63
E	525	GLY	-	expression tag	UNP Q9IH63
E	526	LEU	-	expression tag	UNP Q9IH63
E	527	VAL	-	expression tag	UNP Q9IH63
E	528	PRO	-	expression tag	UNP Q9IH63
E	529	ARG	-	expression tag	UNP Q9IH63
E	530	GLY	-	expression tag	UNP Q9IH63
E	531	SER	-	expression tag	UNP Q9IH63
E	532	HIS	-	expression tag	UNP Q9IH63
E	533	HIS	-	expression tag	UNP Q9IH63
E	534	HIS	-	expression tag	UNP Q9IH63
E	535	HIS	-	expression tag	UNP Q9IH63
E	536	HIS	-	expression tag	UNP Q9IH63
E	537	HIS	-	expression tag	UNP Q9IH63
E	538	SER	-	expression tag	UNP Q9IH63
E	539	ALA	-	expression tag	UNP Q9IH63
E	540	TRP	-	expression tag	UNP Q9IH63
E	541	SER	-	expression tag	UNP Q9IH63
E	542	HIS	-	expression tag	UNP Q9IH63
E	543	PRO	-	expression tag	UNP Q9IH63
E	544	GLN	-	expression tag	UNP Q9IH63
E	545	PHE	-	expression tag	UNP Q9IH63
E	546	GLU	-	expression tag	UNP Q9IH63
E	547	LYS	-	expression tag	UNP Q9IH63
G	5	MET	-	expression tag	UNP Q9IH63
G	6	TYR	-	expression tag	UNP Q9IH63
G	7	SER	-	expression tag	UNP Q9IH63
G	8	MET	-	expression tag	UNP Q9IH63
G	9	GLN	-	expression tag	UNP Q9IH63
G	10	LEU	-	expression tag	UNP Q9IH63
G	11	ALA	-	expression tag	UNP Q9IH63
G	12	SER	-	expression tag	UNP Q9IH63
G	13	CYS	-	expression tag	UNP Q9IH63
G	14	VAL	-	expression tag	UNP Q9IH63
G	15	THR	-	expression tag	UNP Q9IH63
G	16	LEU	-	expression tag	UNP Q9IH63
G	17	THR	-	expression tag	UNP Q9IH63
G	18	LEU	-	expression tag	UNP Q9IH63
G	19	VAL	-	expression tag	UNP Q9IH63
G	20	LEU	-	expression tag	UNP Q9IH63
G	21	LEU	-	expression tag	UNP Q9IH63
G	22	VAL	-	expression tag	UNP Q9IH63

Continued on next page...

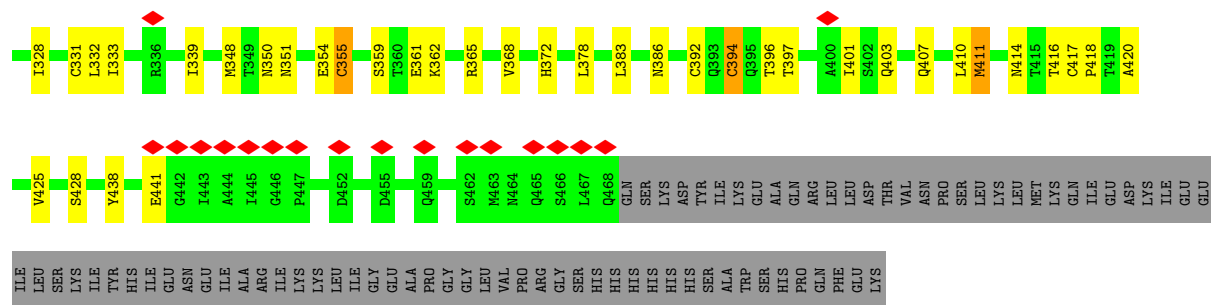
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	23	ASN	-	expression tag	UNP Q9IH63
G	24	SER	-	expression tag	UNP Q9IH63
G	25	GLN	-	expression tag	UNP Q9IH63
G	104	CYS	LEU	conflict	UNP Q9IH63
G	114	CYS	ILE	conflict	UNP Q9IH63
G	172	PHE	LEU	conflict	UNP Q9IH63
G	191	PRO	SER	conflict	UNP Q9IH63
G	489	LYS	-	expression tag	UNP Q9IH63
G	490	LEU	-	expression tag	UNP Q9IH63
G	491	MET	-	expression tag	UNP Q9IH63
G	492	LYS	-	expression tag	UNP Q9IH63
G	493	GLN	-	expression tag	UNP Q9IH63
G	494	ILE	-	expression tag	UNP Q9IH63
G	495	GLU	-	expression tag	UNP Q9IH63
G	496	ASP	-	expression tag	UNP Q9IH63
G	497	LYS	-	expression tag	UNP Q9IH63
G	498	ILE	-	expression tag	UNP Q9IH63
G	499	GLU	-	expression tag	UNP Q9IH63
G	500	GLU	-	expression tag	UNP Q9IH63
G	501	ILE	-	expression tag	UNP Q9IH63
G	502	LEU	-	expression tag	UNP Q9IH63
G	503	SER	-	expression tag	UNP Q9IH63
G	504	LYS	-	expression tag	UNP Q9IH63
G	505	ILE	-	expression tag	UNP Q9IH63
G	506	TYR	-	expression tag	UNP Q9IH63
G	507	HIS	-	expression tag	UNP Q9IH63
G	508	ILE	-	expression tag	UNP Q9IH63
G	509	GLU	-	expression tag	UNP Q9IH63
G	510	ASN	-	expression tag	UNP Q9IH63
G	511	GLU	-	expression tag	UNP Q9IH63
G	512	ILE	-	expression tag	UNP Q9IH63
G	513	ALA	-	expression tag	UNP Q9IH63
G	514	ARG	-	expression tag	UNP Q9IH63
G	515	ILE	-	expression tag	UNP Q9IH63
G	516	LYS	-	expression tag	UNP Q9IH63
G	517	LYS	-	expression tag	UNP Q9IH63
G	518	LEU	-	expression tag	UNP Q9IH63
G	519	ILE	-	expression tag	UNP Q9IH63
G	520	GLY	-	expression tag	UNP Q9IH63
G	521	GLU	-	expression tag	UNP Q9IH63
G	522	ALA	-	expression tag	UNP Q9IH63
G	523	PRO	-	expression tag	UNP Q9IH63

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	524	GLY	-	expression tag	UNP Q9IH63
G	525	GLY	-	expression tag	UNP Q9IH63
G	526	LEU	-	expression tag	UNP Q9IH63
G	527	VAL	-	expression tag	UNP Q9IH63
G	528	PRO	-	expression tag	UNP Q9IH63
G	529	ARG	-	expression tag	UNP Q9IH63
G	530	GLY	-	expression tag	UNP Q9IH63
G	531	SER	-	expression tag	UNP Q9IH63
G	532	HIS	-	expression tag	UNP Q9IH63
G	533	HIS	-	expression tag	UNP Q9IH63
G	534	HIS	-	expression tag	UNP Q9IH63
G	535	HIS	-	expression tag	UNP Q9IH63
G	536	HIS	-	expression tag	UNP Q9IH63
G	537	HIS	-	expression tag	UNP Q9IH63
G	538	SER	-	expression tag	UNP Q9IH63
G	539	ALA	-	expression tag	UNP Q9IH63
G	540	TRP	-	expression tag	UNP Q9IH63
G	541	SER	-	expression tag	UNP Q9IH63
G	542	HIS	-	expression tag	UNP Q9IH63
G	543	PRO	-	expression tag	UNP Q9IH63
G	544	GLN	-	expression tag	UNP Q9IH63
G	545	PHE	-	expression tag	UNP Q9IH63
G	546	GLU	-	expression tag	UNP Q9IH63
G	547	LYS	-	expression tag	UNP Q9IH63



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	534823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.082	Depositor
Minimum map value	-0.742	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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	0.33	0/3397	0.53	0/4616
1	B	0.36	0/3443	0.58	0/4680
1	C	0.30	0/3392	0.48	0/4609
1	D	0.37	0/3443	0.58	1/4680 (0.0%)
1	E	0.30	0/3392	0.50	0/4609
1	G	0.31	0/3392	0.50	0/4609
All	All	0.33	0/20459	0.53	1/27803 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	ASP	CB-CG-OD1	6.06	123.76	118.30

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	3348	0	3394	73	0
1	B	3393	0	3444	93	0
1	C	3343	0	3389	84	0
1	D	3393	0	3444	103	0
1	E	3343	0	3389	74	0
1	G	3343	0	3389	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20163	0	20449	468	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 12.

All (468) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HG3	1:D:216:PRO:CG	1.66	1.25
1:A:258:GLU:CG	1:D:216:PRO:HG2	1.80	1.10
1:A:258:GLU:HG3	1:D:216:PRO:HG2	0.87	0.87
1:B:421:VAL:HG22	1:B:426:ILE:HG12	1.60	0.84
1:A:258:GLU:CG	1:D:216:PRO:CG	2.48	0.82
1:B:157:ALA:HB2	1:B:177:ASP:HB2	1.60	0.81
1:G:268:TYR:HB3	1:G:277:ILE:HD12	1.64	0.79
1:D:256:LEU:HD23	1:D:285:LEU:HD23	1.65	0.78
1:G:190:ILE:HG13	1:G:191:PRO:HD2	1.64	0.78
1:A:244:ARG:NH2	1:D:200:ASP:OD1	2.17	0.78
1:B:244:ARG:NH2	1:C:200:ASP:OD1	2.18	0.76
1:C:327:GLU:HB2	1:C:344:TYR:HB3	1.67	0.76
1:G:303:ASN:OD1	1:G:365:ARG:NH1	2.17	0.76
1:G:35:LYS:NZ	1:G:441:GLU:O	2.19	0.76
1:A:395:GLN:HA	1:D:109:ARG:HH21	1.51	0.75
1:B:179:ILE:HG12	1:B:183:LEU:HD12	1.68	0.74
1:C:404:SER:OG	1:C:406:GLU:OE1	2.06	0.74
1:G:328:ILE:HD11	1:G:333:ILE:HD13	1.68	0.73
1:B:109:ARG:HB2	1:E:395:GLN:HB2	1.70	0.72
1:D:302:ASN:HD22	1:D:388:ILE:HG21	1.54	0.72
1:D:44:ARG:NH2	1:D:295:GLU:OE1	2.23	0.72
1:C:33:LEU:HD22	1:C:38:LEU:HD12	1.72	0.71
1:A:258:GLU:HB2	1:A:332:LEU:HD22	1.72	0.71
1:A:317:LEU:HD13	1:A:326:ILE:HD12	1.73	0.71
1:C:47:LYS:HB3	1:C:285:LEU:HD12	1.72	0.70
1:G:154:THR:HG21	1:G:171:VAL:HG11	1.73	0.70
1:B:148:LYS:NZ	1:B:270:ASP:OD2	2.23	0.70
1:C:324:SER:HA	1:C:348:MET:HG3	1.74	0.70
1:C:36:ILE:HD11	1:C:360:THR:HB	1.73	0.69
1:D:288:ILE:HG21	1:D:319:ARG:HH11	1.57	0.69
1:C:148:LYS:HZ2	1:C:275:TYR:HE2	1.40	0.69
1:G:394:CYS:HB3	1:G:401:ILE:HD11	1.75	0.69
1:G:189:LYS:HE3	1:G:189:LYS:HA	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:O	1:B:186:THR:OG1	2.11	0.68
1:C:154:THR:HG21	1:C:171:VAL:HG11	1.75	0.68
1:D:253:PHE:HA	1:D:256:LEU:HD12	1.75	0.67
1:A:342:GLN:OE1	1:G:372:HIS:NE2	2.28	0.67
1:E:49:LYS:HD2	1:E:283:PRO:HG3	1.76	0.66
1:B:173:THR:HG21	1:B:176:GLN:HG2	1.76	0.66
1:B:258:GLU:HG2	1:C:216:PRO:HG2	1.77	0.66
1:D:361:GLU:OE2	1:D:362:LYS:NZ	2.28	0.66
1:D:175:LEU:HD11	1:D:206:TYR:CD2	2.31	0.65
1:A:35:LYS:HE3	1:A:438:TYR:CE1	2.32	0.65
1:B:254:ASP:CG	1:C:82:ARG:HH12	1.99	0.65
1:B:204:SER:OG	1:E:244:ARG:NH1	2.27	0.65
1:A:258:GLU:OE2	1:D:211:LEU:HD22	1.97	0.64
1:A:398:GLY:HA2	1:D:109:ARG:HH22	1.61	0.64
1:G:392:CYS:HB2	1:G:401:ILE:HB	1.80	0.64
1:A:176:GLN:NE2	1:A:180:ASN:OD1	2.23	0.64
1:G:103:ASP:OD1	1:G:135:TYR:OH	2.15	0.63
1:E:30:TYR:CD2	1:E:40:LYS:HG3	2.33	0.63
1:B:291:ALA:HB2	1:B:319:ARG:HG3	1.80	0.62
1:C:435:SER:OG	1:C:437:ASN:OD1	2.17	0.62
1:A:58:VAL:HG22	1:A:277:ILE:HG22	1.81	0.62
1:G:403:GLN:HB2	1:G:410:LEU:HD22	1.80	0.62
1:D:421:VAL:HG12	1:D:426:ILE:HA	1.82	0.62
1:G:35:LYS:HE2	1:G:438:TYR:HE1	1.64	0.62
1:A:70:GLN:N	1:A:70:GLN:OE1	2.33	0.62
1:G:135:TYR:HA	1:G:138:MET:HG3	1.80	0.62
1:A:267:ILE:HG13	1:A:277:ILE:HG13	1.80	0.62
1:D:435:SER:OG	1:D:437:ASN:OD1	2.19	0.61
1:D:306:SER:OG	1:D:308:TRP:NE1	2.34	0.61
1:G:258:GLU:HB3	1:G:332:LEU:HD22	1.81	0.61
1:C:258:GLU:HB3	1:C:332:LEU:HD22	1.81	0.61
1:D:244:ARG:NH2	1:G:200:ASP:OD1	2.33	0.61
1:D:293:ILE:HG21	1:D:338:VAL:HG21	1.82	0.61
1:C:95:GLU:HA	1:C:98:LYS:HB2	1.83	0.61
1:D:382:VAL:HG23	1:D:413:ASP:HB3	1.83	0.60
1:A:186:THR:HB	1:A:190:ILE:HG23	1.83	0.60
1:G:47:LYS:HB2	1:G:285:LEU:HD12	1.83	0.60
1:G:193:LYS:HG3	1:G:193:LYS:O	2.01	0.60
1:B:238:ASN:OD1	1:C:204:SER:OG	2.18	0.60
1:A:351:ASN:HA	1:A:354:GLU:OE1	2.01	0.60
1:D:285:LEU:HD11	1:D:339:ILE:HG23	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:HD3	1:B:110:LEU:N	2.16	0.60
1:C:124:THR:HG22	1:C:127:GLN:OE1	2.01	0.60
1:E:293:ILE:HG12	1:E:317:LEU:HD12	1.84	0.60
1:D:28:LEU:HD22	1:D:356:LEU:HD12	1.84	0.59
1:D:101:THR:HB	1:D:135:TYR:CD2	2.37	0.59
1:B:310:SER:HA	1:B:365:ARG:HA	1.85	0.59
1:D:61:MET:O	1:D:79:TYR:OH	2.20	0.59
1:C:144:ILE:HG21	1:C:277:ILE:HD12	1.84	0.59
1:E:259:SER:O	1:E:341:ASN:ND2	2.29	0.59
1:G:372:HIS:CG	1:G:372:HIS:O	2.56	0.58
1:A:156:GLU:HB2	1:A:159:VAL:HG22	1.84	0.58
1:C:58:VAL:HG11	1:C:151:ILE:HD13	1.86	0.58
1:E:393:GLN:HB3	1:E:400:ALA:HA	1.86	0.58
1:B:30:TYR:CD1	1:B:40:LYS:HB2	2.39	0.58
1:D:210:LEU:HD11	1:D:214:PHE:CD2	2.39	0.58
1:D:77:GLU:O	1:D:81:THR:HG23	2.04	0.58
1:G:35:LYS:HE2	1:G:438:TYR:CE1	2.39	0.58
1:A:44:ARG:HB2	1:A:293:ILE:HB	1.85	0.58
1:G:205:LYS:NZ	1:G:209:ASP:OD1	2.37	0.58
1:E:394:CYS:HA	1:E:420:ALA:HA	1.86	0.58
1:A:258:GLU:OE2	1:D:211:LEU:HB3	2.04	0.57
1:E:414:ASN:HD21	1:E:431:LYS:HB2	1.69	0.57
1:B:306:SER:OG	1:B:308:TRP:NE1	2.37	0.57
1:A:291:ALA:HB2	1:A:319:ARG:HG3	1.85	0.57
1:D:302:ASN:ND2	1:D:388:ILE:HG21	2.19	0.57
1:B:318:VAL:HG22	1:B:323:ILE:HG22	1.86	0.57
1:E:44:ARG:NE	1:E:334:THR:O	2.31	0.57
1:D:214:PHE:CE2	1:D:234:ALA:HB2	2.39	0.57
1:C:96:ILE:HG22	1:C:120:ILE:HD13	1.87	0.57
1:D:254:ASP:HB3	1:G:216:PRO:HG3	1.86	0.57
1:A:303:ASN:HD21	1:A:445:ILE:HG21	1.70	0.56
1:B:77:GLU:O	1:B:81:THR:HG23	2.05	0.56
1:B:210:LEU:HG	1:B:214:PHE:HB2	1.86	0.56
1:B:414:ASN:HD21	1:B:431:LYS:NZ	2.01	0.56
1:C:255:ASP:HB3	1:C:339:ILE:HG13	1.87	0.56
1:C:328:ILE:HG12	1:C:333:ILE:HG12	1.87	0.56
1:G:403:GLN:HG3	1:G:410:LEU:HD13	1.86	0.56
1:C:426:ILE:O	1:E:115:MET:N	2.32	0.56
1:A:268:TYR:HB3	1:A:277:ILE:HG12	1.87	0.56
1:G:403:GLN:NE2	1:G:407:GLN:O	2.39	0.56
1:G:68:MET:HE1	1:G:179:ILE:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LYS:HD2	1:C:283:PRO:HG3	1.87	0.56
1:D:383:LEU:HD23	1:D:412:ILE:HD12	1.87	0.55
1:C:332:LEU:HD21	1:E:216:PRO:HB2	1.89	0.55
1:D:173:THR:HB	1:D:176:GLN:HB2	1.88	0.55
1:E:61:MET:HE1	1:E:276:ILE:HG23	1.87	0.55
1:E:200:ASP:O	1:E:204:SER:OG	2.20	0.55
1:C:287:GLU:OE2	1:C:289:GLN:NE2	2.28	0.55
1:A:231:ILE:HD13	1:A:278:VAL:HG11	1.89	0.55
1:D:38:LEU:HD21	1:D:310:SER:HB3	1.89	0.55
1:B:353:ARG:O	1:B:357:THR:HG23	2.07	0.55
1:C:94:LEU:HD11	1:C:266:ILE:HG22	1.89	0.55
1:G:191:PRO:C	1:G:193:LYS:H	2.10	0.55
1:B:240:GLU:HB3	1:C:204:SER:HB2	1.88	0.54
1:G:95:GLU:HA	1:G:98:LYS:HB2	1.89	0.54
1:B:109:ARG:CZ	1:E:421:VAL:HG11	2.36	0.54
1:C:255:ASP:HA	1:C:332:LEU:HD23	1.87	0.54
1:G:350:ASN:O	1:G:354:GLU:HG2	2.08	0.54
1:C:148:LYS:HD2	1:C:275:TYR:CE2	2.42	0.54
1:D:291:ALA:HB2	1:D:319:ARG:HD3	1.89	0.54
1:D:63:PRO:HD3	1:D:175:LEU:HD13	1.89	0.54
1:B:173:THR:HB	1:B:176:GLN:HB2	1.90	0.54
1:C:327:GLU:HB3	1:C:330:PHE:CE1	2.43	0.54
1:D:383:LEU:HD21	1:D:422:LEU:HD11	1.90	0.54
1:D:387:CYS:HB2	1:D:403:GLN:HB2	1.89	0.54
1:E:103:ASP:OD1	1:E:135:TYR:OH	2.18	0.54
1:B:313:PRO:HD3	1:E:454:VAL:HG11	1.90	0.54
1:G:68:MET:CE	1:G:183:LEU:HB3	2.38	0.54
1:A:353:ARG:O	1:A:357:THR:HG23	2.08	0.54
1:E:156:GLU:HB2	1:E:159:VAL:HG22	1.90	0.54
1:B:325:ASN:ND2	1:B:348:MET:HG3	2.23	0.53
1:C:135:TYR:HA	1:C:138:MET:SD	2.48	0.53
1:C:454:VAL:HG13	1:E:311:ILE:HG22	1.90	0.53
1:B:127:GLN:OE1	1:B:222:VAL:HB	2.08	0.53
1:C:350:ASN:O	1:C:354:GLU:HG2	2.09	0.53
1:D:29:HIS:CD2	1:D:32:LYS:HZ3	2.26	0.53
1:C:49:LYS:HB2	1:C:283:PRO:HB2	1.89	0.53
1:E:94:LEU:HD11	1:E:266:ILE:HG22	1.90	0.53
1:B:231:ILE:HD13	1:B:278:VAL:HG11	1.91	0.53
1:D:210:LEU:HD11	1:D:214:PHE:HD2	1.74	0.53
1:G:141:ALA:O	1:G:144:ILE:HG22	2.09	0.53
1:G:307:GLU:HG2	1:G:368:VAL:HB	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:O	1:D:138:MET:HB3	2.09	0.53
1:A:47:LYS:HD3	1:A:287:GLU:HG3	1.91	0.52
1:E:350:ASN:O	1:E:354:GLU:HG2	2.09	0.52
1:G:394:CYS:SG	1:G:397:THR:OG1	2.63	0.52
1:B:268:TYR:CZ	1:B:270:ASP:HB2	2.43	0.52
1:B:302:ASN:ND2	1:B:386:ASN:OD1	2.42	0.52
1:D:84:ASN:ND2	1:D:274:TYR:OH	2.42	0.52
1:D:454:VAL:HG13	1:G:311:ILE:HG22	1.92	0.52
1:D:310:SER:HA	1:D:365:ARG:HA	1.90	0.52
1:B:122:ILE:HD13	1:E:379:SER:HA	1.91	0.52
1:B:270:ASP:OD1	1:B:272:SER:N	2.42	0.52
1:G:49:LYS:HD2	1:G:283:PRO:HG3	1.91	0.52
1:B:109:ARG:HD2	1:E:421:VAL:HG21	1.91	0.52
1:C:60:LYS:NZ	1:C:154:THR:OG1	2.32	0.52
1:D:320:ASN:HB3	1:D:322:LEU:HD22	1.91	0.52
1:B:61:MET:O	1:B:79:TYR:OH	2.28	0.52
1:C:79:TYR:CG	1:C:203:LEU:HD23	2.44	0.52
1:D:210:LEU:HG	1:D:214:PHE:HB2	1.91	0.52
1:G:68:MET:CE	1:G:179:ILE:HG23	2.40	0.52
1:D:179:ILE:O	1:D:184:VAL:HG23	2.10	0.51
1:C:100:ASN:HB3	1:C:116:ALA:HB3	1.91	0.51
1:C:310:SER:HA	1:C:365:ARG:HA	1.92	0.51
1:G:75:VAL:HG11	1:G:200:ASP:HB2	1.92	0.51
1:B:351:ASN:OD1	1:E:462:SER:OG	2.20	0.51
1:G:58:VAL:HG11	1:G:151:ILE:HD13	1.91	0.51
1:G:147:LEU:HD11	1:G:163:GLU:HA	1.93	0.51
1:G:184:VAL:O	1:G:187:ILE:HG22	2.10	0.51
1:G:300:SER:O	1:G:386:ASN:ND2	2.43	0.51
1:A:258:GLU:HG3	1:D:216:PRO:CD	2.35	0.51
1:D:193:LYS:O	1:D:197:LEU:HG	2.10	0.51
1:B:203:LEU:O	1:B:207:LEU:HD23	2.11	0.51
1:E:354:GLU:HB2	1:E:362:LYS:HE3	1.92	0.51
1:B:302:ASN:N	1:B:302:ASN:HD22	2.08	0.51
1:D:101:THR:HB	1:D:135:TYR:HD2	1.75	0.51
1:D:258:GLU:HB3	1:D:332:LEU:HD22	1.91	0.51
1:G:60:LYS:NZ	1:G:154:THR:OG1	2.32	0.51
1:A:311:ILE:HG13	1:A:364:PRO:HG2	1.93	0.51
1:C:33:LEU:HB3	1:C:38:LEU:HB2	1.92	0.51
1:E:231:ILE:HD13	1:E:278:VAL:HG11	1.92	0.51
1:B:342:GLN:HG3	1:E:372:HIS:ND1	2.26	0.50
1:A:91:LYS:O	1:A:95:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LYS:NZ	1:B:441:GLU:O	2.35	0.50
1:E:147:LEU:HD11	1:E:163:GLU:HA	1.94	0.50
1:B:70:GLN:HE22	1:B:187:ILE:HG13	1.76	0.50
1:D:179:ILE:HG12	1:D:183:LEU:HD12	1.93	0.50
1:D:173:THR:HG21	1:D:176:GLN:OE1	2.11	0.50
1:E:79:TYR:CG	1:E:203:LEU:HD23	2.46	0.50
1:A:113:VAL:HG22	1:A:135:TYR:HD2	1.76	0.50
1:A:369:VAL:HG23	1:D:347:PRO:HG3	1.93	0.50
1:B:33:LEU:HB3	1:B:38:LEU:HB2	1.93	0.50
1:D:30:TYR:CD2	1:D:40:LYS:HB2	2.47	0.50
1:G:378:LEU:HD13	1:G:383:LEU:HD13	1.93	0.50
1:A:28:LEU:HB2	1:A:30:TYR:CE1	2.47	0.49
1:A:30:TYR:CD2	1:A:40:LYS:HD3	2.46	0.49
1:C:124:THR:OG1	1:C:125:ALA:N	2.44	0.49
1:D:222:VAL:O	1:D:265:GLN:NE2	2.45	0.49
1:E:375:ARG:HD3	1:E:390:VAL:HG13	1.94	0.49
1:E:141:ALA:HA	1:E:144:ILE:HG22	1.95	0.49
1:D:52:PRO:HA	1:D:283:PRO:HA	1.95	0.49
1:D:102:HIS:O	1:D:114:CYS:N	2.35	0.49
1:B:268:TYR:CE2	1:B:270:ASP:HB2	2.48	0.49
1:E:113:VAL:HG22	1:E:135:TYR:HD2	1.77	0.49
1:A:37:GLY:O	1:A:299:VAL:N	2.45	0.49
1:B:394:CYS:HB2	1:B:401:ILE:HD11	1.94	0.49
1:A:35:LYS:HB2	1:A:443:ILE:HD13	1.94	0.49
1:A:252:ASP:HB3	1:A:285:LEU:HD12	1.95	0.49
1:C:103:ASP:OD1	1:C:135:TYR:OH	2.31	0.49
1:E:258:GLU:HB3	1:E:332:LEU:HD22	1.94	0.49
1:B:70:GLN:HE22	1:B:187:ILE:CG1	2.26	0.49
1:B:359:SER:OG	1:B:362:LYS:NZ	2.31	0.48
1:D:253:PHE:HA	1:D:256:LEU:CD1	2.41	0.48
1:G:61:MET:HE2	1:G:83:LEU:HD11	1.96	0.48
1:G:310:SER:HA	1:G:365:ARG:HA	1.94	0.48
1:E:79:TYR:CD2	1:E:203:LEU:HD23	2.48	0.48
1:E:387:CYS:N	1:E:403:GLN:OE1	2.46	0.48
1:A:435:SER:OG	1:A:437:ASN:OD1	2.32	0.48
1:D:231:ILE:HD13	1:D:278:VAL:HG11	1.96	0.48
1:E:129:THR:O	1:E:132:VAL:HG12	2.12	0.48
1:E:37:GLY:HA2	1:E:409:LEU:HD11	1.95	0.48
1:G:303:ASN:HD22	1:G:304:ASP:N	2.12	0.48
1:G:207:LEU:O	1:G:211:LEU:HD23	2.14	0.48
1:A:311:ILE:HD11	1:A:449:VAL:HG21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HD21	1:B:422:LEU:HD11	1.94	0.48
1:C:61:MET:O	1:C:79:TYR:OH	2.30	0.48
1:G:285:LEU:HD11	1:G:339:ILE:HG23	1.95	0.48
1:G:414:ASN:HA	1:G:418:PRO:HA	1.96	0.48
1:C:75:VAL:HG11	1:C:200:ASP:HB2	1.94	0.48
1:C:255:ASP:HA	1:C:332:LEU:CD2	2.44	0.48
1:A:382:VAL:HG23	1:A:413:ASP:HB3	1.95	0.48
1:B:172:PHE:HB3	1:B:235:PHE:CE1	2.49	0.47
1:E:194:GLN:O	1:E:194:GLN:NE2	2.46	0.47
1:A:132:VAL:HG21	1:G:425:VAL:HB	1.95	0.47
1:A:44:ARG:NE	1:A:334:THR:O	2.30	0.47
1:B:253:PHE:HA	1:B:256:LEU:HD12	1.97	0.47
1:B:293:ILE:HG21	1:B:338:VAL:HG21	1.96	0.47
1:B:411:MET:HB2	1:B:411:MET:HE3	1.55	0.47
1:B:259:SER:O	1:B:259:SER:OG	2.31	0.47
1:D:47:LYS:HB2	1:D:285:LEU:HD12	1.97	0.47
1:D:350:ASN:O	1:D:354:GLU:HG2	2.14	0.47
1:C:136:GLU:HA	1:C:139:LYS:HD2	1.96	0.47
1:A:186:THR:HB	1:A:190:ILE:CG2	2.44	0.47
1:C:404:SER:OG	1:C:405:GLY:N	2.47	0.47
1:D:255:ASP:OD1	1:D:332:LEU:HD23	2.15	0.47
1:E:394:CYS:HB2	1:E:419:THR:O	2.15	0.47
1:G:324:SER:HA	1:G:348:MET:HG3	1.97	0.47
1:B:109:ARG:CZ	1:B:110:LEU:HB2	2.45	0.47
1:D:175:LEU:O	1:D:179:ILE:HD12	2.15	0.47
1:E:39:VAL:HG12	1:E:297:LEU:HB2	1.96	0.47
1:G:361:GLU:OE1	1:G:361:GLU:N	2.40	0.47
1:B:109:ARG:NH1	1:B:110:LEU:HB2	2.30	0.47
1:D:108:VAL:HG23	1:D:109:ARG:H	1.80	0.47
1:D:323:ILE:O	1:D:353:ARG:NH1	2.47	0.47
1:B:412:ILE:O	1:B:429:LEU:HD13	2.14	0.47
1:A:240:GLU:HB2	1:D:204:SER:HB3	1.96	0.46
1:E:307:GLU:HG2	1:E:368:VAL:HB	1.97	0.46
1:B:109:ARG:HB2	1:E:395:GLN:CB	2.44	0.46
1:A:190:ILE:HG22	1:G:185:PRO:HG3	1.97	0.46
1:A:387:CYS:N	1:A:403:GLN:OE1	2.48	0.46
1:B:323:ILE:HD11	1:B:353:ARG:HG3	1.96	0.46
1:B:388:ILE:HG13	1:B:389:SER:N	2.31	0.46
1:E:411:MET:HB2	1:E:438:TYR:CE2	2.51	0.46
1:B:193:LYS:NZ	1:B:197:LEU:HG	2.30	0.46
1:B:308:TRP:HZ3	1:B:448:PRO:HB3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:TRP:HZ3	1:D:448:PRO:HB3	1.79	0.46
1:B:200:ASP:OD1	1:E:244:ARG:NH2	2.49	0.46
1:E:35:LYS:HG3	1:E:443:ILE:HG12	1.97	0.46
1:B:435:SER:OG	1:B:437:ASN:OD1	2.34	0.46
1:C:222:VAL:O	1:C:265:GLN:NE2	2.45	0.46
1:C:325:ASN:ND2	1:C:348:MET:HG2	2.30	0.46
1:D:94:LEU:HD23	1:D:222:VAL:HG22	1.97	0.46
1:E:47:LYS:HG2	1:E:287:GLU:HA	1.98	0.46
1:G:61:MET:O	1:G:79:TYR:OH	2.31	0.46
1:G:141:ALA:HA	1:G:144:ILE:HG22	1.98	0.46
1:C:396:THR:HG21	1:C:418:PRO:HD2	1.97	0.46
1:G:199:LEU:HD23	1:G:203:LEU:HD13	1.98	0.46
1:A:396:THR:HG23	1:A:397:THR:HG23	1.97	0.45
1:G:416:THR:OG1	1:G:417:CYS:N	2.49	0.45
1:A:95:GLU:HA	1:A:98:LYS:HB2	1.97	0.45
1:C:239:TYR:CE1	1:C:257:LEU:HD21	2.51	0.45
1:G:163:GLU:HG3	1:G:164:THR:HG23	1.97	0.45
1:G:302:ASN:OD1	1:G:303:ASN:N	2.49	0.45
1:B:97:TYR:CD1	1:B:222:VAL:HG21	2.51	0.45
1:B:403:GLN:HB2	1:B:410:LEU:HD22	1.98	0.45
1:G:173:THR:HG21	1:G:176:GLN:HG2	1.98	0.45
1:E:35:LYS:HE3	1:E:438:TYR:CE1	2.50	0.45
1:A:97:TYR:O	1:A:101:THR:HG23	2.16	0.45
1:A:303:ASN:ND2	1:A:445:ILE:HG12	2.31	0.45
1:D:109:ARG:C	1:D:111:ALA:N	2.70	0.45
1:E:28:LEU:HB2	1:E:30:TYR:CE1	2.52	0.45
1:A:308:TRP:HZ3	1:A:448:PRO:HB3	1.81	0.45
1:E:35:LYS:CE	1:E:438:TYR:HE1	2.29	0.45
1:G:73:GLY:HA3	1:G:196:GLU:OE2	2.16	0.45
1:A:186:THR:HG22	1:A:189:LYS:HZ2	1.82	0.45
1:C:327:GLU:CB	1:C:344:TYR:HB3	2.42	0.45
1:G:331:CYS:HB3	1:G:339:ILE:O	2.17	0.45
1:B:394:CYS:SG	1:B:395:GLN:N	2.90	0.45
1:C:176:GLN:OE1	1:C:180:ASN:ND2	2.50	0.45
1:C:327:GLU:HB2	1:C:344:TYR:CB	2.42	0.45
1:D:109:ARG:HG3	1:D:110:LEU:H	1.82	0.45
1:E:416:THR:HG23	1:E:417:CYS:H	1.81	0.45
1:B:35:LYS:HB2	1:B:443:ILE:HD13	1.99	0.45
1:C:394:CYS:SG	1:C:396:THR:HG22	2.57	0.45
1:G:351:ASN:OD1	1:G:362:LYS:NZ	2.47	0.45
1:G:295:GLU:HG3	1:G:315:PHE:CE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ILE:HA	1:C:331:CYS:HB2	1.99	0.44
1:C:387:CYS:HB2	1:C:403:GLN:HB2	1.99	0.44
1:D:258:GLU:HB2	1:G:216:PRO:HG2	2.00	0.44
1:D:379:SER:O	1:D:382:VAL:HG12	2.17	0.44
1:E:239:TYR:HE1	1:E:257:LEU:HD21	1.82	0.44
1:E:365:ARG:NE	1:E:446:GLY:O	2.30	0.44
1:D:148:LYS:NZ	1:D:270:ASP:OD2	2.51	0.44
1:G:52:PRO:HA	1:G:283:PRO:HA	1.99	0.44
1:G:68:MET:HE2	1:G:183:LEU:HB3	1.98	0.44
1:G:394:CYS:HB2	1:G:420:ALA:HA	1.98	0.44
1:D:273:SER:HB2	1:D:275:TYR:HD1	1.82	0.44
1:E:364:PRO:HB2	1:E:449:VAL:HG21	2.00	0.44
1:B:315:PHE:CG	1:B:328:ILE:HD13	2.53	0.44
1:C:371:SER:O	1:C:371:SER:OG	2.35	0.44
1:G:192:CYS:O	1:G:195:THR:N	2.51	0.44
1:B:427:ILE:HG13	1:C:115:MET:HG3	1.99	0.44
1:D:109:ARG:C	1:D:111:ALA:H	2.20	0.44
1:G:144:ILE:HD12	1:G:144:ILE:HA	1.83	0.44
1:E:157:ALA:O	1:E:172:PHE:HA	2.17	0.44
1:E:335:LYS:HA	1:E:335:LYS:HD3	1.71	0.44
1:B:44:ARG:HB3	1:B:337:SER:HA	2.00	0.44
1:C:44:ARG:NH2	1:C:295:GLU:OE1	2.39	0.44
1:B:316:ILE:HG13	1:B:356:LEU:HD21	1.99	0.43
1:C:253:PHE:CD1	1:C:253:PHE:C	2.91	0.43
1:D:175:LEU:HD21	1:D:206:TYR:HB2	1.99	0.43
1:E:35:LYS:HE3	1:E:438:TYR:HE1	1.83	0.43
1:G:410:LEU:HD12	1:G:410:LEU:HA	1.84	0.43
1:D:179:ILE:HA	1:D:183:LEU:HD12	2.00	0.43
1:A:379:SER:O	1:A:382:VAL:HG12	2.17	0.43
1:B:140:ASN:O	1:B:144:ILE:HG13	2.18	0.43
1:C:158:VAL:HG22	1:C:172:PHE:CD1	2.53	0.43
1:D:172:PHE:HB3	1:D:235:PHE:CE1	2.54	0.43
1:G:100:ASN:O	1:G:116:ALA:N	2.42	0.43
1:B:270:ASP:OD1	1:B:273:SER:N	2.43	0.43
1:C:307:GLU:HB2	1:C:368:VAL:HG12	2.00	0.43
1:C:378:LEU:HD13	1:C:383:LEU:HD13	2.01	0.43
1:D:35:LYS:NZ	1:D:441:GLU:HB2	2.34	0.43
1:D:109:ARG:HG3	1:D:110:LEU:HG	1.99	0.43
1:E:52:PRO:HA	1:E:283:PRO:HA	2.00	0.43
1:E:71:CYS:HB3	1:E:192:CYS:HB2	1.65	0.43
1:B:226:MET:SD	1:B:231:ILE:HG13	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:TYR:OH	1:B:270:ASP:HB2	2.17	0.43
1:D:368:VAL:HG21	1:D:373:VAL:HG11	2.01	0.43
1:D:411:MET:HB2	1:D:411:MET:HE3	1.62	0.43
1:A:372:HIS:ND1	1:D:342:GLN:HG3	2.34	0.43
1:A:414:ASN:HA	1:A:418:PRO:HA	2.01	0.43
1:G:69:SER:HA	1:G:72:THR:HG23	2.00	0.43
1:G:158:VAL:HG22	1:G:172:PHE:CD1	2.54	0.43
1:A:244:ARG:NH1	1:D:204:SER:OG	2.52	0.43
1:D:95:GLU:HA	1:D:98:LYS:HB2	2.01	0.43
1:D:410:LEU:HD23	1:D:410:LEU:HA	1.89	0.43
1:E:101:THR:OG1	1:E:115:MET:SD	2.68	0.43
1:G:190:ILE:CG1	1:G:191:PRO:HD2	2.41	0.43
1:G:239:TYR:CE1	1:G:257:LEU:HD21	2.54	0.43
1:A:326:ILE:O	1:A:327:GLU:C	2.57	0.43
1:A:427:ILE:HA	1:D:115:MET:HB2	2.01	0.43
1:B:47:LYS:HG3	1:B:285:LEU:HD22	2.01	0.43
1:B:361:GLU:H	1:B:361:GLU:CD	2.23	0.43
1:D:61:MET:HA	1:D:174:ALA:HB2	2.00	0.43
1:G:175:LEU:HD11	1:G:206:TYR:HB2	2.00	0.43
1:A:257:LEU:HD13	1:A:262:ILE:HD12	2.00	0.42
1:B:323:ILE:HD11	1:B:353:ARG:HA	2.01	0.42
1:C:378:LEU:HD12	1:C:382:VAL:O	2.18	0.42
1:G:69:SER:HA	1:G:72:THR:CG2	2.49	0.42
1:A:240:GLU:OE1	1:A:240:GLU:HA	2.19	0.42
1:C:148:LYS:HD2	1:C:275:TYR:HE2	1.83	0.42
1:C:348:MET:CE	1:C:352:MET:HG2	2.48	0.42
1:D:30:TYR:HD2	1:D:40:LYS:HB2	1.84	0.42
1:D:319:ARG:O	1:D:322:LEU:HB2	2.19	0.42
1:B:258:GLU:OE2	1:C:211:LEU:HD12	2.18	0.42
1:C:318:VAL:HG22	1:C:323:ILE:HG12	2.01	0.42
1:D:240:GLU:HB3	1:G:204:SER:OG	2.18	0.42
1:B:382:VAL:HG23	1:B:413:ASP:HB3	2.00	0.42
1:D:193:LYS:O	1:D:196:GLU:HB3	2.20	0.42
1:G:411:MET:HG3	1:G:438:TYR:HD2	1.84	0.42
1:C:35:LYS:HB3	1:C:443:ILE:HD13	2.01	0.42
1:D:173:THR:CG2	1:D:176:GLN:HB2	2.49	0.42
1:A:175:LEU:HD11	1:A:206:TYR:HB2	2.02	0.42
1:E:35:LYS:HB3	1:E:443:ILE:HG12	2.01	0.42
1:A:116:ALA:HA	1:G:428:SER:OG	2.19	0.42
1:A:391:THR:HB	1:E:393:GLN:NE2	2.34	0.42
1:C:91:LYS:O	1:C:95:GLU:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ILE:HD12	1:C:183:LEU:HD22	2.01	0.42
1:D:255:ASP:OD2	1:D:339:ILE:HG13	2.19	0.42
1:E:447:PRO:HA	1:E:448:PRO:HD3	1.96	0.42
1:B:376:PHE:HB2	1:B:383:LEU:HD11	2.01	0.42
1:C:210:LEU:HD11	1:C:234:ALA:HA	2.02	0.42
1:C:297:LEU:HA	1:C:298:PRO:HD3	1.94	0.42
1:D:259:SER:O	1:D:259:SER:OG	2.35	0.42
1:A:52:PRO:HA	1:A:283:PRO:HA	2.01	0.42
1:C:239:TYR:HE1	1:C:257:LEU:HD21	1.84	0.42
1:E:49:LYS:CD	1:E:283:PRO:HG3	2.46	0.42
1:G:79:TYR:CG	1:G:203:LEU:HD23	2.54	0.42
1:G:138:MET:HA	1:G:141:ALA:HB3	2.01	0.42
1:G:355:CYS:HA	1:G:359:SER:O	2.20	0.42
1:B:260:ASP:N	1:B:260:ASP:OD1	2.53	0.41
1:C:428:SER:OG	1:E:116:ALA:HA	2.20	0.41
1:G:44:ARG:NH2	1:G:295:GLU:OE2	2.40	0.41
1:B:145:ASN:ND2	1:B:268:TYR:CZ	2.88	0.41
1:D:174:ALA:HB3	1:D:175:LEU:HD12	2.00	0.41
1:C:302:ASN:OD1	1:C:303:ASN:N	2.53	0.41
1:C:396:THR:HG23	1:C:397:THR:HG23	2.02	0.41
1:A:351:ASN:ND2	1:A:362:LYS:HD3	2.36	0.41
1:C:355:CYS:HA	1:C:359:SER:O	2.20	0.41
1:E:75:VAL:HG22	1:E:196:GLU:OE2	2.20	0.41
1:G:293:ILE:HG13	1:G:317:LEU:HD13	2.02	0.41
1:G:297:LEU:HA	1:G:298:PRO:HD3	1.95	0.41
1:A:99:ASN:OD1	1:A:99:ASN:N	2.53	0.41
1:A:239:TYR:CE1	1:A:257:LEU:HD21	2.55	0.41
1:C:182:ASN:C	1:C:185:PRO:HD2	2.41	0.41
1:G:328:ILE:HD11	1:G:333:ILE:CD1	2.45	0.41
1:B:33:LEU:HD22	1:B:38:LEU:HD12	2.03	0.41
1:B:178:TYR:OH	1:B:183:LEU:HD11	2.20	0.41
1:C:308:TRP:CZ3	1:C:448:PRO:HB3	2.56	0.41
1:D:79:TYR:CE1	1:D:203:LEU:HD22	2.55	0.41
1:E:375:ARG:NE	1:E:389:SER:OG	2.27	0.41
1:D:388:ILE:N	1:D:403:GLN:OE1	2.51	0.41
1:E:154:THR:HG21	1:E:171:VAL:HG11	2.01	0.41
1:E:239:TYR:CE1	1:E:257:LEU:HD21	2.56	0.41
1:E:267:ILE:HG13	1:E:277:ILE:HG13	2.01	0.41
1:A:258:GLU:CB	1:A:332:LEU:HD22	2.47	0.41
1:B:79:TYR:HE1	1:B:207:LEU:HD21	1.86	0.41
1:C:61:MET:HE2	1:C:83:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ILE:O	1:D:429:LEU:HD13	2.20	0.41
1:E:355:CYS:HA	1:E:359:SER:O	2.21	0.41
1:G:186:THR:O	1:G:190:ILE:HG22	2.21	0.41
1:G:396:THR:OG1	1:G:417:CYS:HB2	2.20	0.41
1:B:172:PHE:HB3	1:B:235:PHE:CD1	2.56	0.41
1:B:437:ASN:ND2	1:B:441:GLU:OE2	2.54	0.41
1:C:379:SER:HA	1:E:122:ILE:HD13	2.02	0.41
1:D:108:VAL:HG23	1:D:109:ARG:N	2.36	0.41
1:E:413:ASP:OD1	1:E:416:THR:HG22	2.21	0.41
1:B:447:PRO:HA	1:B:448:PRO:HD3	1.96	0.40
1:C:267:ILE:HD11	1:C:277:ILE:HG12	2.03	0.40
1:A:398:GLY:HA2	1:D:109:ARG:NH2	2.33	0.40
1:B:388:ILE:HG23	1:B:403:GLN:HB3	2.04	0.40
1:E:414:ASN:HA	1:E:418:PRO:HA	2.02	0.40
1:A:45:LYS:HB3	1:A:45:LYS:HE2	1.88	0.40
1:A:160:LYS:HZ3	1:A:160:LYS:HG3	1.70	0.40
1:A:293:ILE:HG13	1:A:338:VAL:HB	2.03	0.40
1:B:302:ASN:ND2	1:B:302:ASN:N	2.70	0.40
1:D:110:LEU:H	1:D:110:LEU:HG	1.76	0.40
1:B:379:SER:O	1:B:382:VAL:HG12	2.22	0.40
1:E:101:THR:HG21	1:E:135:TYR:HB2	2.04	0.40
1:A:113:VAL:HG21	1:A:132:VAL:HG13	2.03	0.40
1:B:122:ILE:HD13	1:B:122:ILE:HA	1.86	0.40
1:B:176:GLN:OE1	1:B:176:GLN:HA	2.15	0.40
1:C:293:ILE:HG21	1:C:338:VAL:HG21	2.03	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	432/543 (80%)	417 (96%)	15 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/543 (81%)	427 (97%)	13 (3%)	0	100	100
1	C	431/543 (79%)	420 (97%)	11 (3%)	0	100	100
1	D	440/543 (81%)	420 (96%)	20 (4%)	0	100	100
1	E	431/543 (79%)	419 (97%)	12 (3%)	0	100	100
1	G	431/543 (79%)	413 (96%)	18 (4%)	0	100	100
All	All	2605/3258 (80%)	2516 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/483 (80%)	376 (97%)	11 (3%)	43	74
1	B	392/483 (81%)	377 (96%)	15 (4%)	33	67
1	C	387/483 (80%)	372 (96%)	15 (4%)	32	67
1	D	392/483 (81%)	375 (96%)	17 (4%)	29	64
1	E	387/483 (80%)	371 (96%)	16 (4%)	30	66
1	G	387/483 (80%)	374 (97%)	13 (3%)	37	70
All	All	2332/2898 (80%)	2245 (96%)	87 (4%)	37	68

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	138	MET
1	A	142	ASP
1	A	163	GLU
1	A	189	LYS
1	A	190	ILE
1	A	304	ASP
1	A	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	ASN
1	A	355	CYS
1	A	425	VAL
1	B	49	LYS
1	B	58	VAL
1	B	78	ASN
1	B	83	LEU
1	B	156	GLU
1	B	176	GLN
1	B	178	TYR
1	B	182	ASN
1	B	216	PRO
1	B	260	ASP
1	B	261	SER
1	B	290	GLN
1	B	355	CYS
1	B	370	SER
1	B	383	LEU
1	C	51	ASN
1	C	68	MET
1	C	104	CYS
1	C	114	CYS
1	C	140	ASN
1	C	188	ASP
1	C	252	ASP
1	C	253	PHE
1	C	261	SER
1	C	287	GLU
1	C	298	PRO
1	C	300	SER
1	C	326	ILE
1	C	330	PHE
1	C	371	SER
1	D	29	HIS
1	D	31	GLU
1	D	58	VAL
1	D	102	HIS
1	D	110	LEU
1	D	163	GLU
1	D	192	CYS
1	D	254	ASP
1	D	256	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	290	GLN
1	D	322	LEU
1	D	337	SER
1	D	370	SER
1	D	371	SER
1	D	380	ASN
1	D	440	SER
1	D	463	MET
1	E	32	LYS
1	E	74	SER
1	E	104	CYS
1	E	114	CYS
1	E	138	MET
1	E	142	ASP
1	E	189	LYS
1	E	196	GLU
1	E	261	SER
1	E	303	ASN
1	E	304	ASP
1	E	320	ASN
1	E	324	SER
1	E	355	CYS
1	E	399	ARG
1	E	404	SER
1	G	32	LYS
1	G	34	SER
1	G	51	ASN
1	G	104	CYS
1	G	142	ASP
1	G	143	ASN
1	G	189	LYS
1	G	217	ASN
1	G	225	SER
1	G	303	ASN
1	G	355	CYS
1	G	394	CYS
1	G	411	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	ASN
1	B	302	ASN
1	B	386	ASN
1	B	414	ASN
1	D	84	ASN
1	G	176	GLN
1	G	194	GLN
1	G	217	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

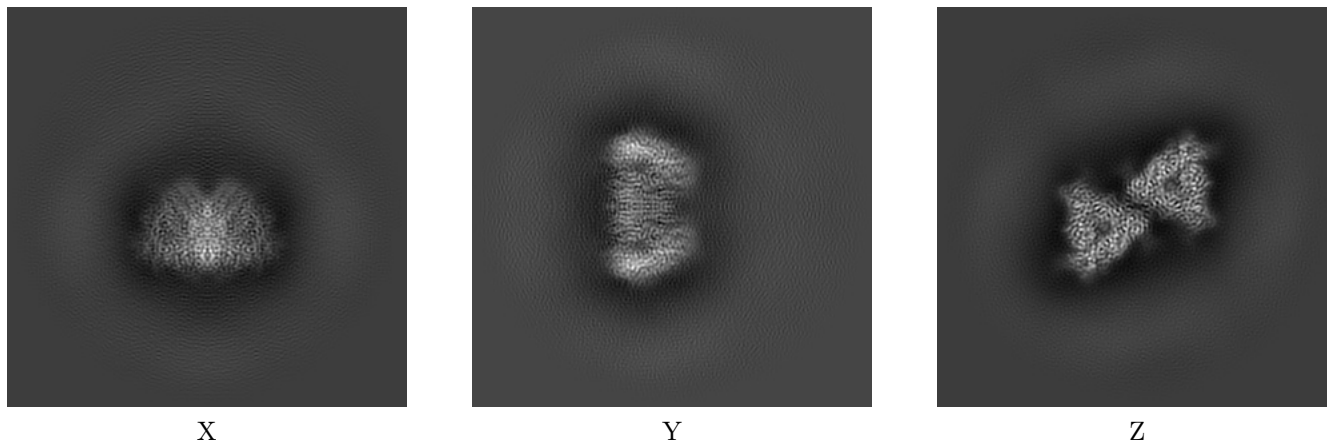
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27590. These allow visual inspection of the internal detail of the map and identification of artifacts.

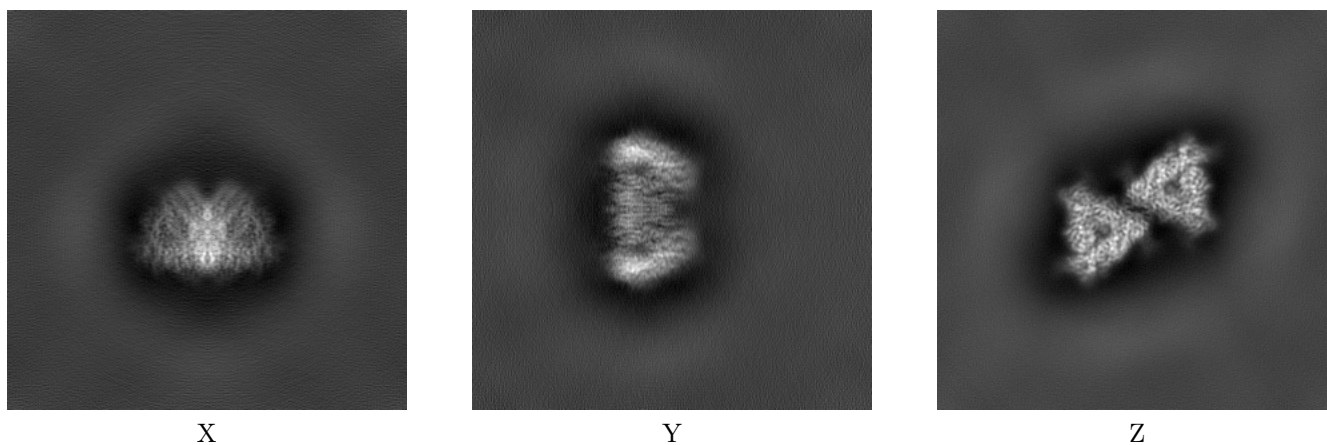
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



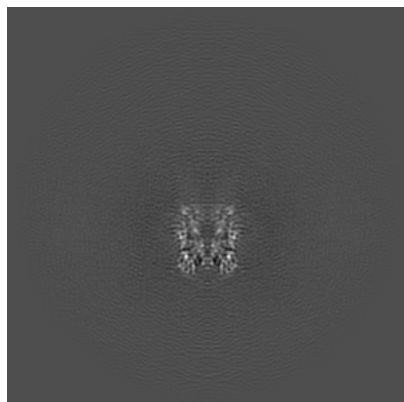
6.1.2 Raw map



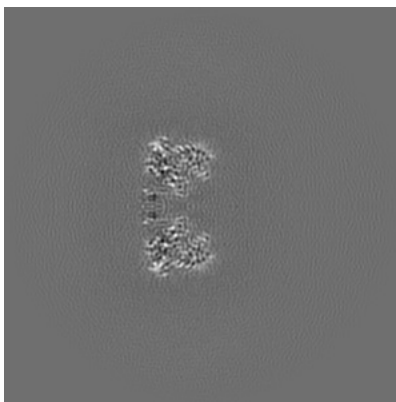
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

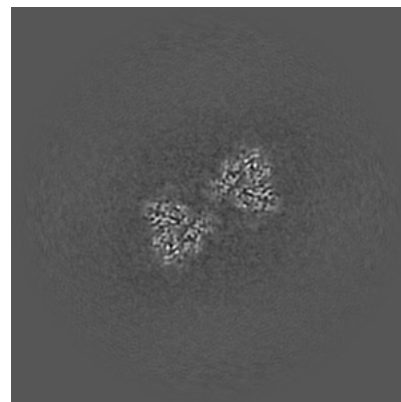
6.2.1 Primary map



X Index: 192

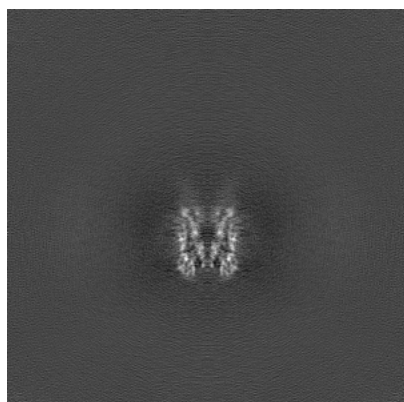


Y Index: 192

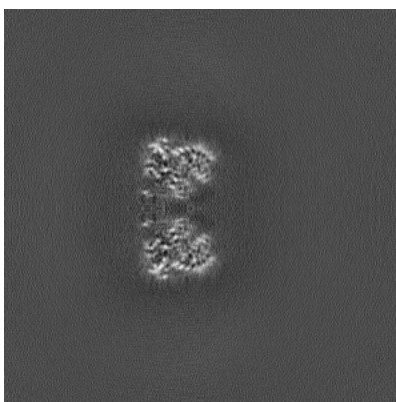


Z Index: 192

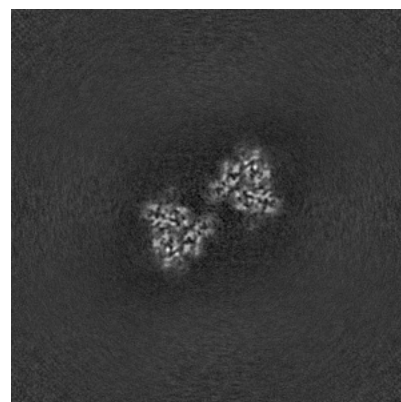
6.2.2 Raw map



X Index: 192



Y Index: 192

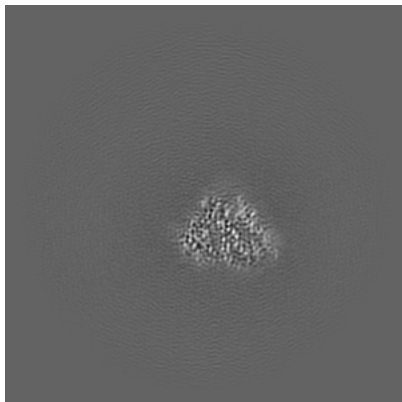


Z Index: 192

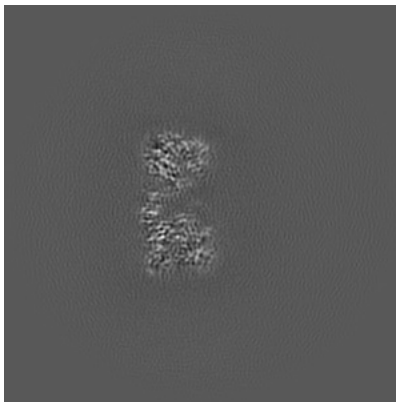
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

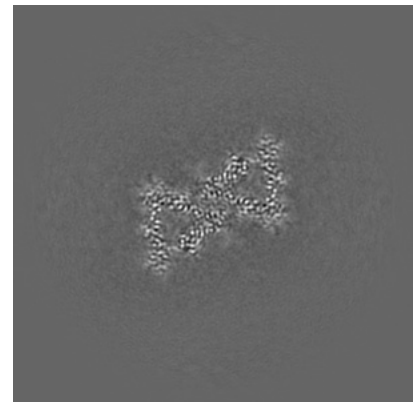
6.3.1 Primary map



X Index: 245

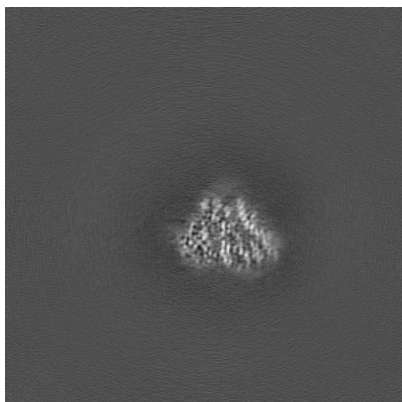


Y Index: 189

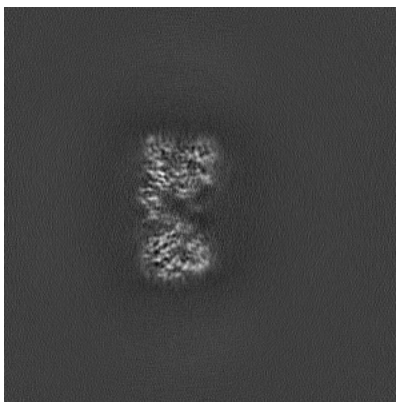


Z Index: 150

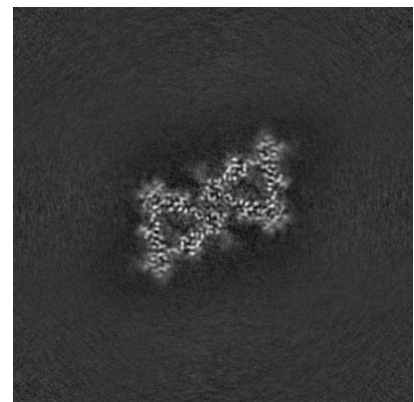
6.3.2 Raw map



X Index: 246



Y Index: 195

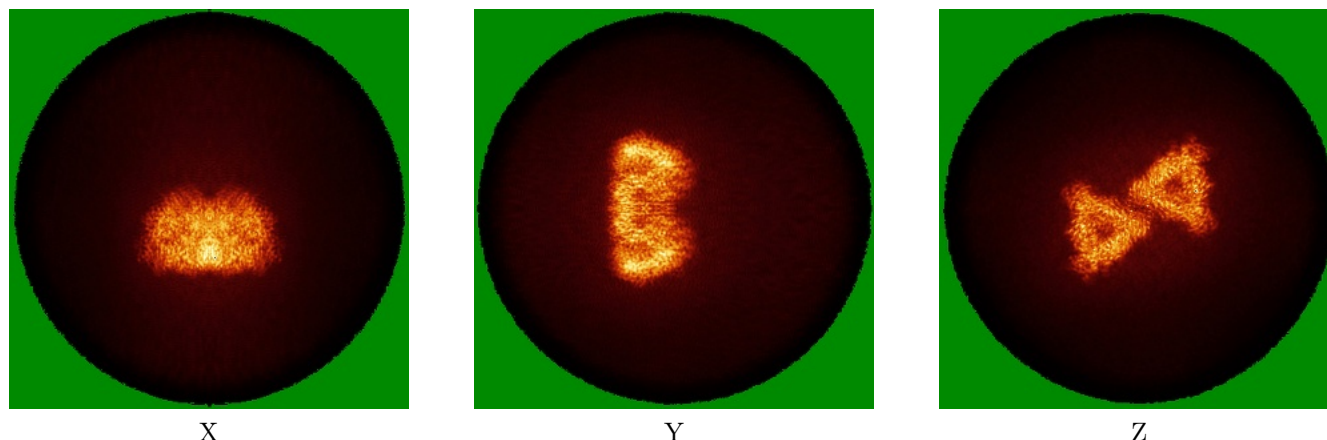


Z Index: 150

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

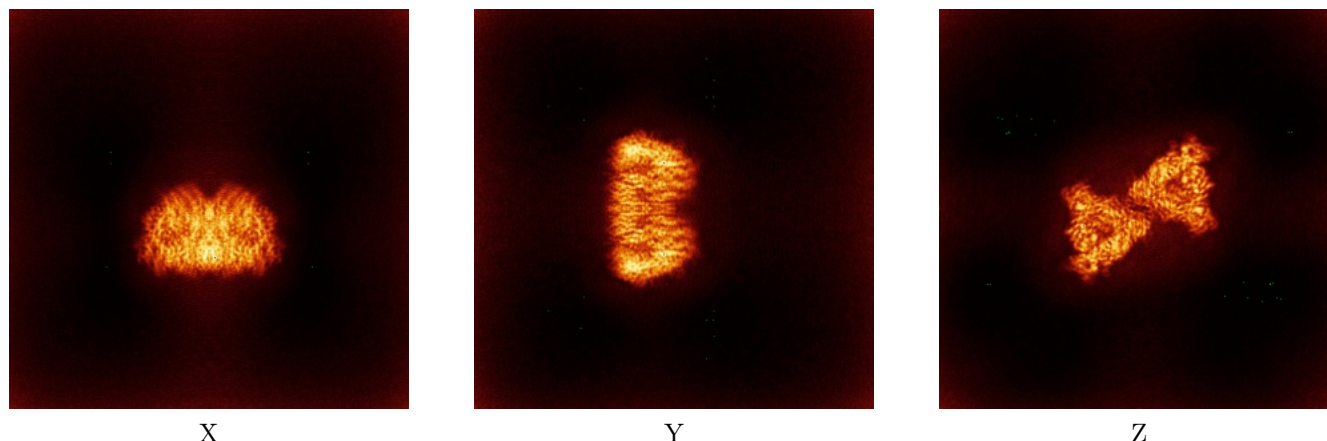


X

Y

Z

6.4.2 Raw map



X

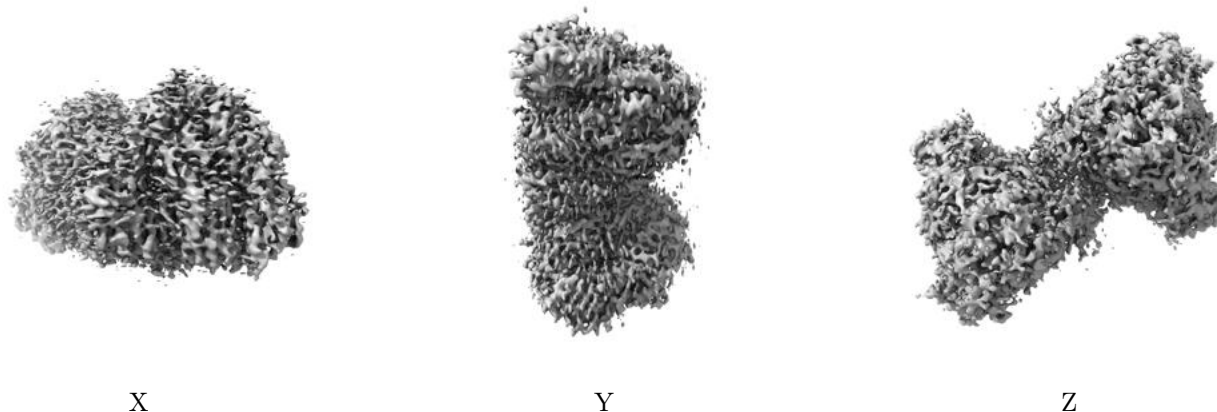
Y

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.

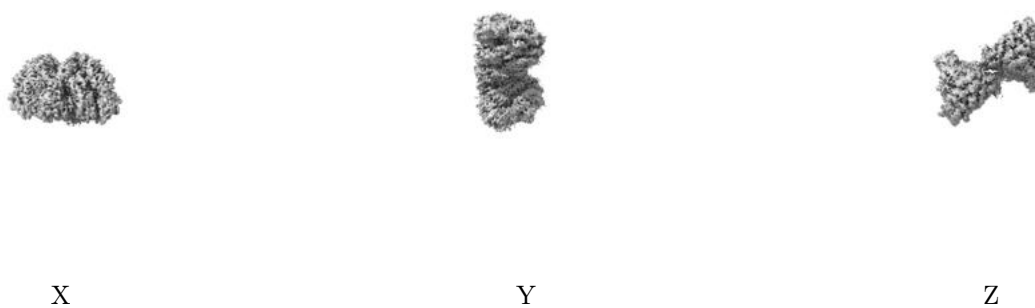
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

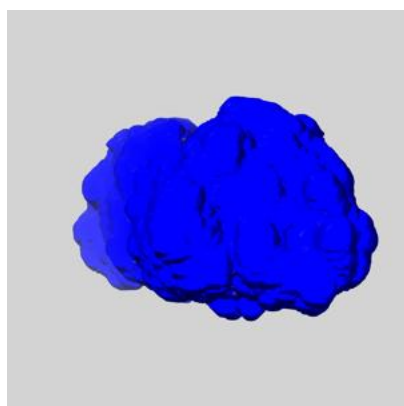
6.6 Mask visualisation [i](#)

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

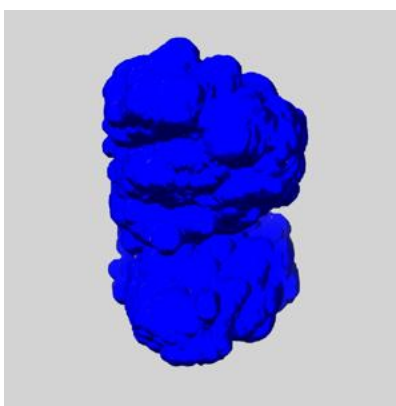
A mask typically either:

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

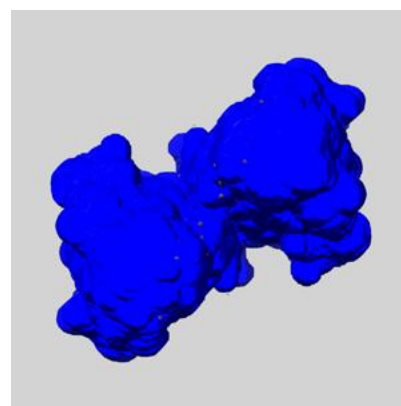
6.6.1 emd_27590_msk_1.map [i](#)



X



Y

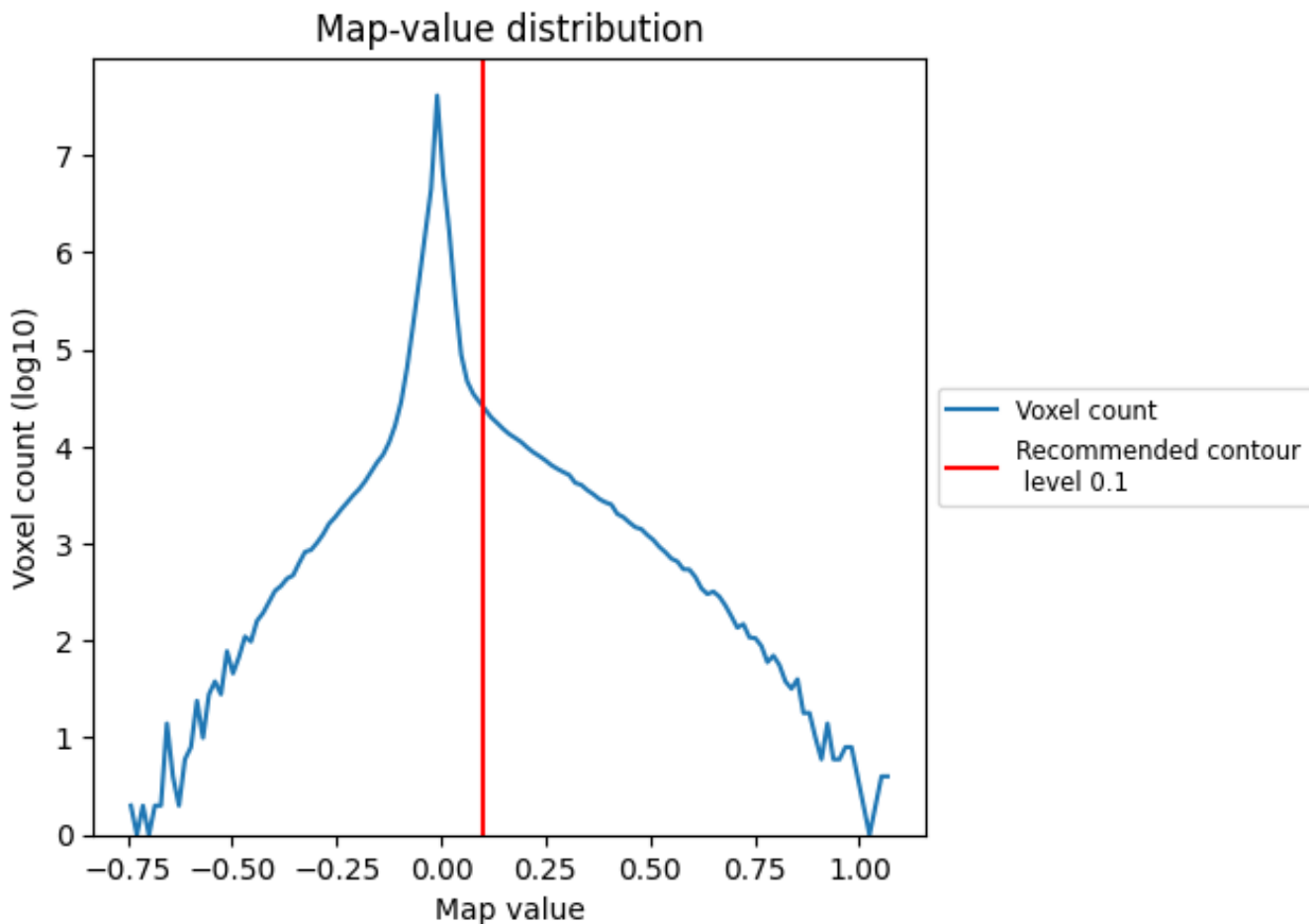


Z

7 Map analysis [i](#)

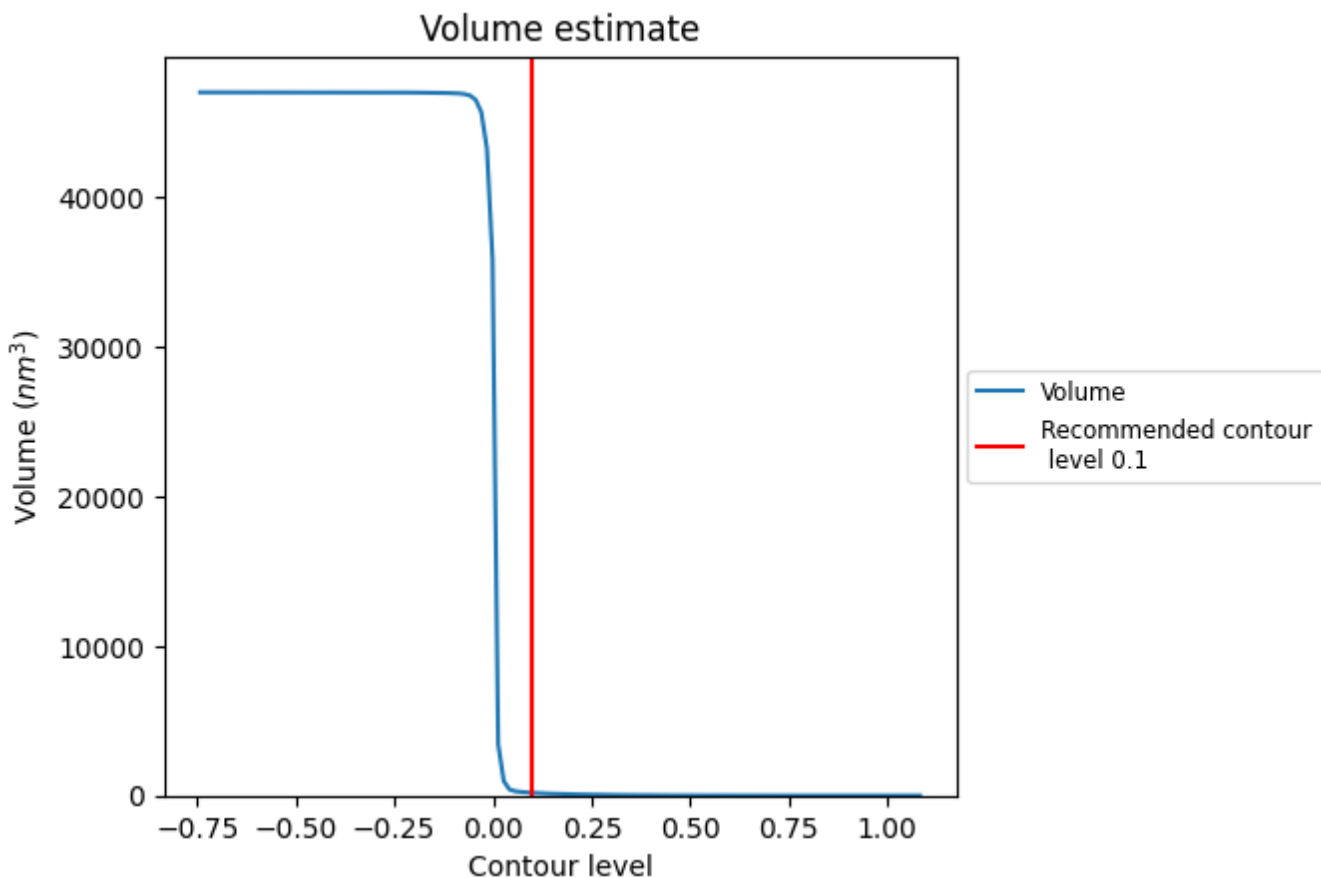
This section contains the results of statistical analysis of the map.

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.

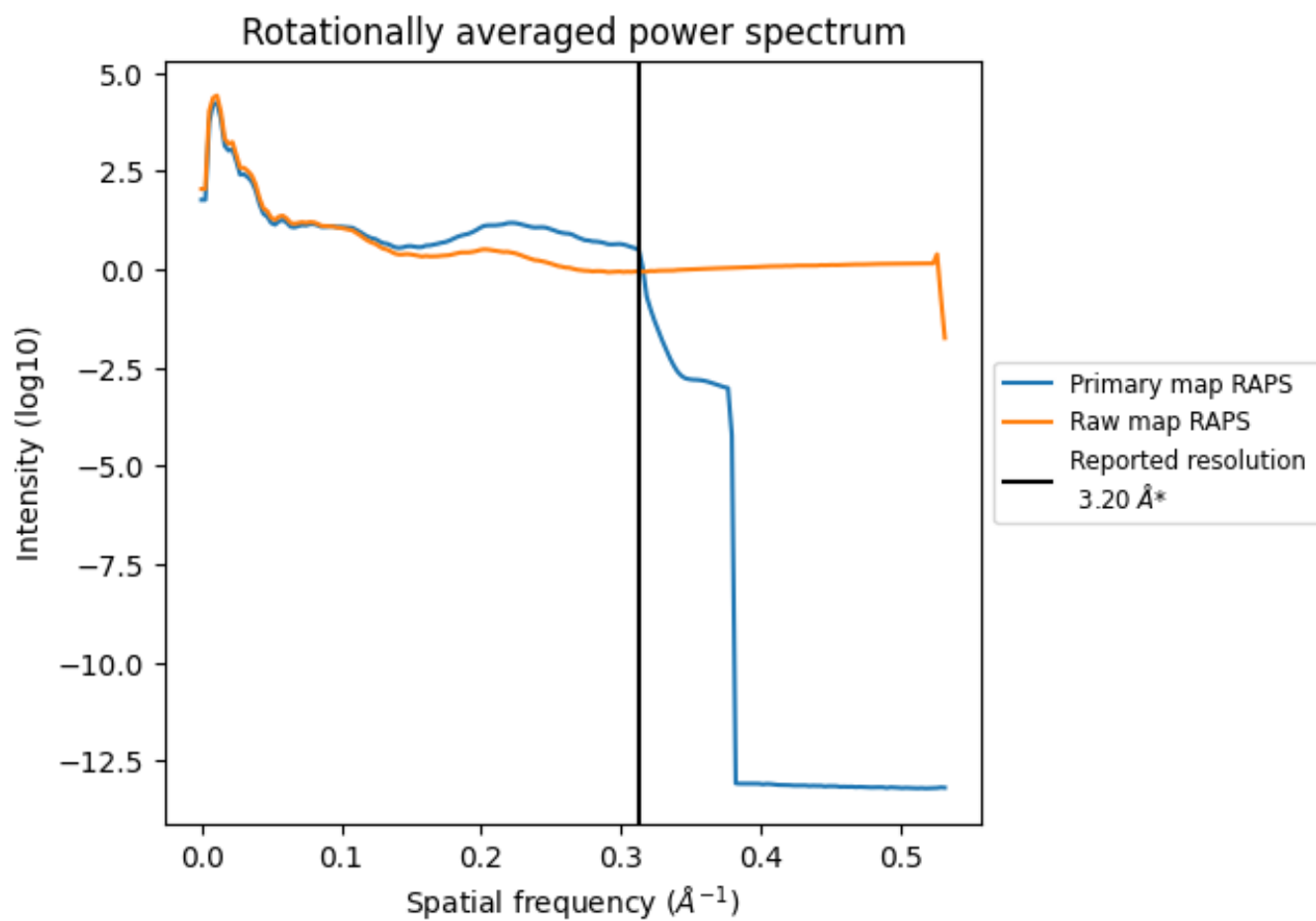
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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

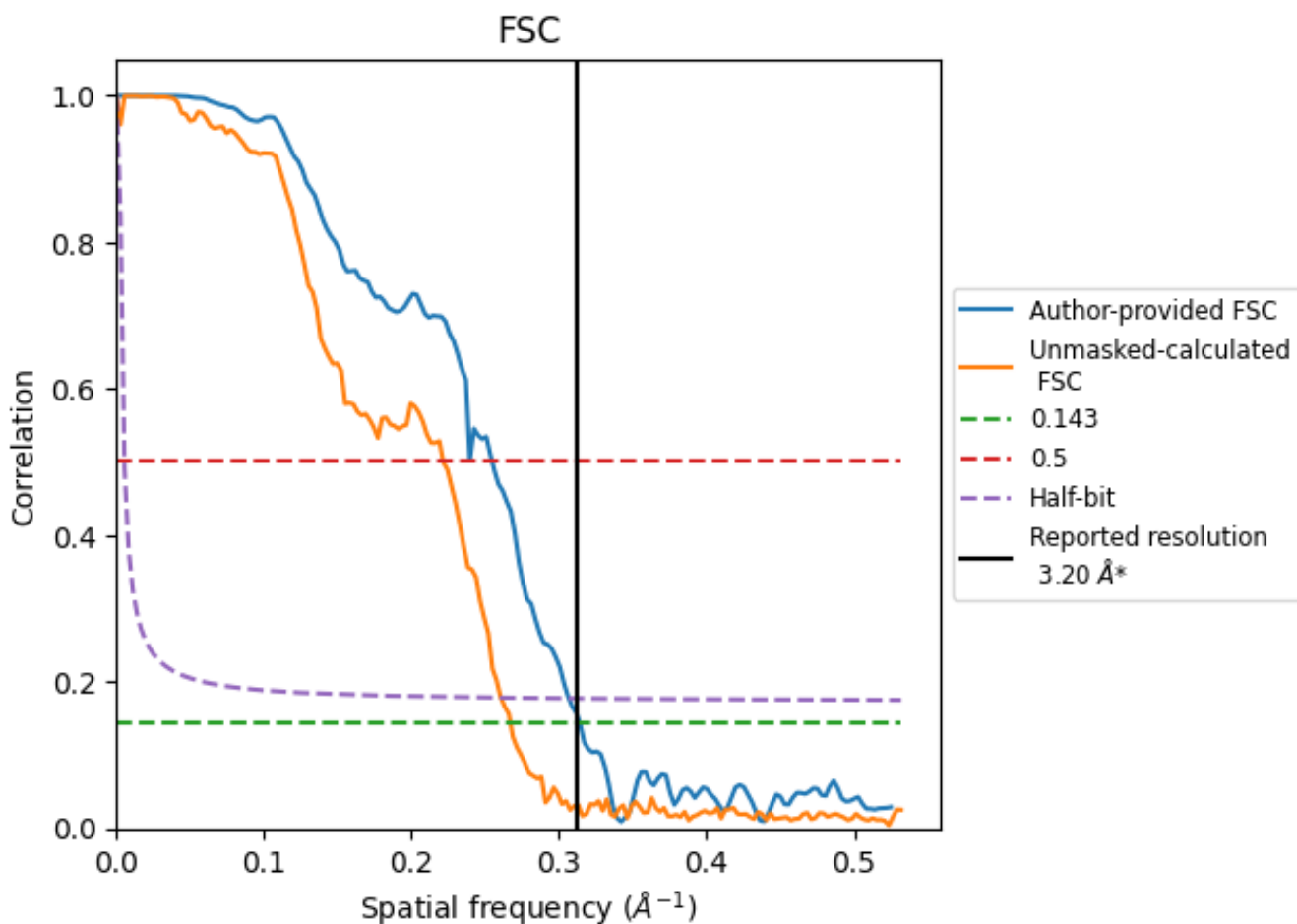


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

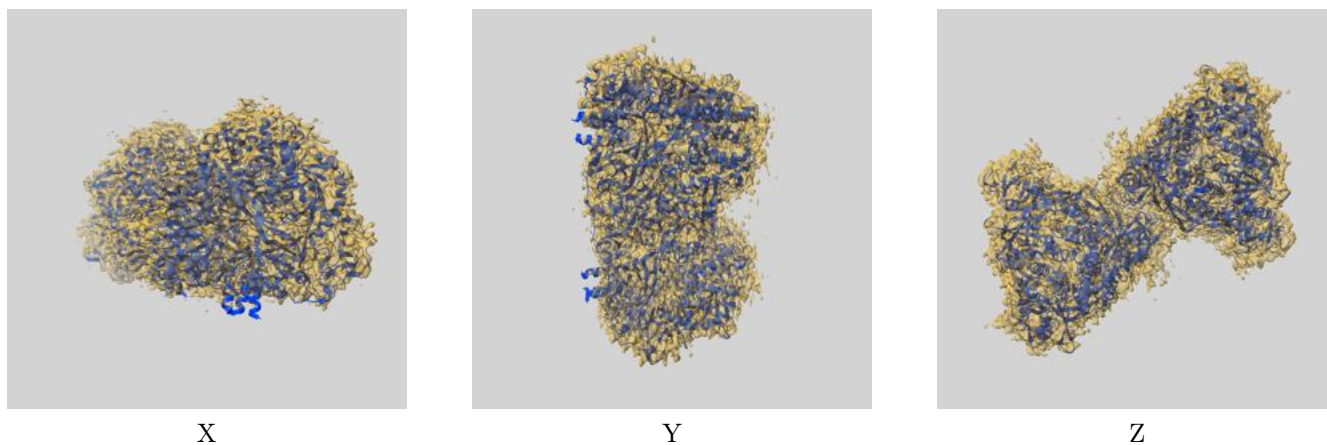
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.93	3.26
Unmasked-calculated*	3.74	4.51	3.84

*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 3.74 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

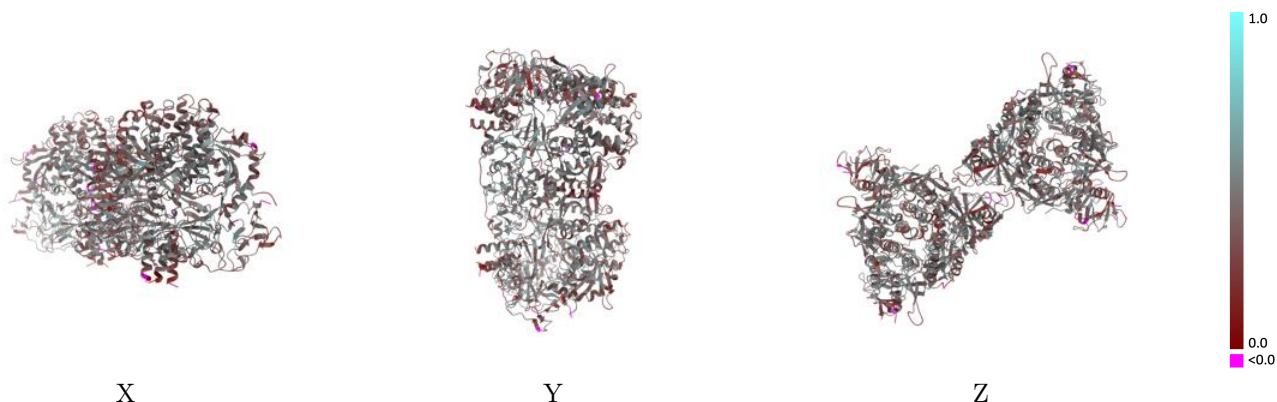
This section contains information regarding the fit between EMDB map EMD-27590 and PDB model 8DO4. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



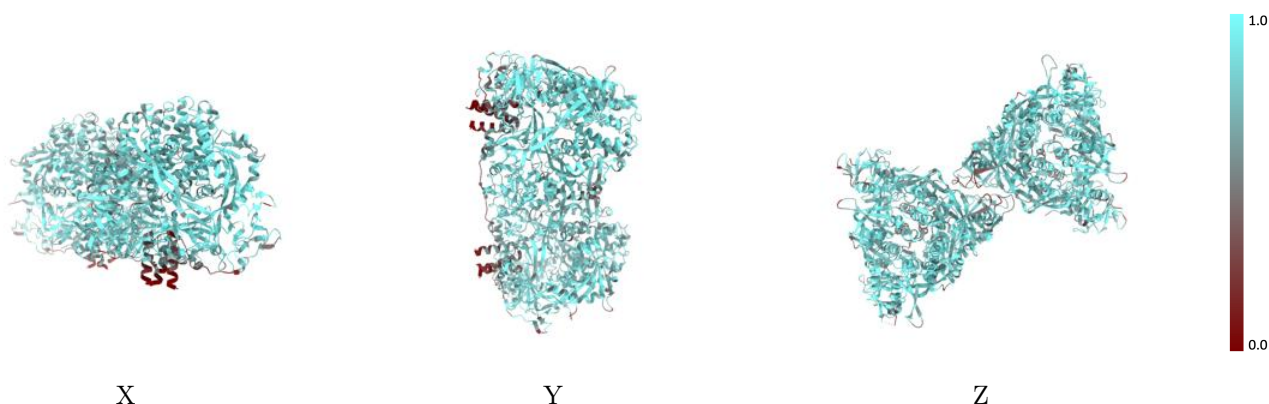
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



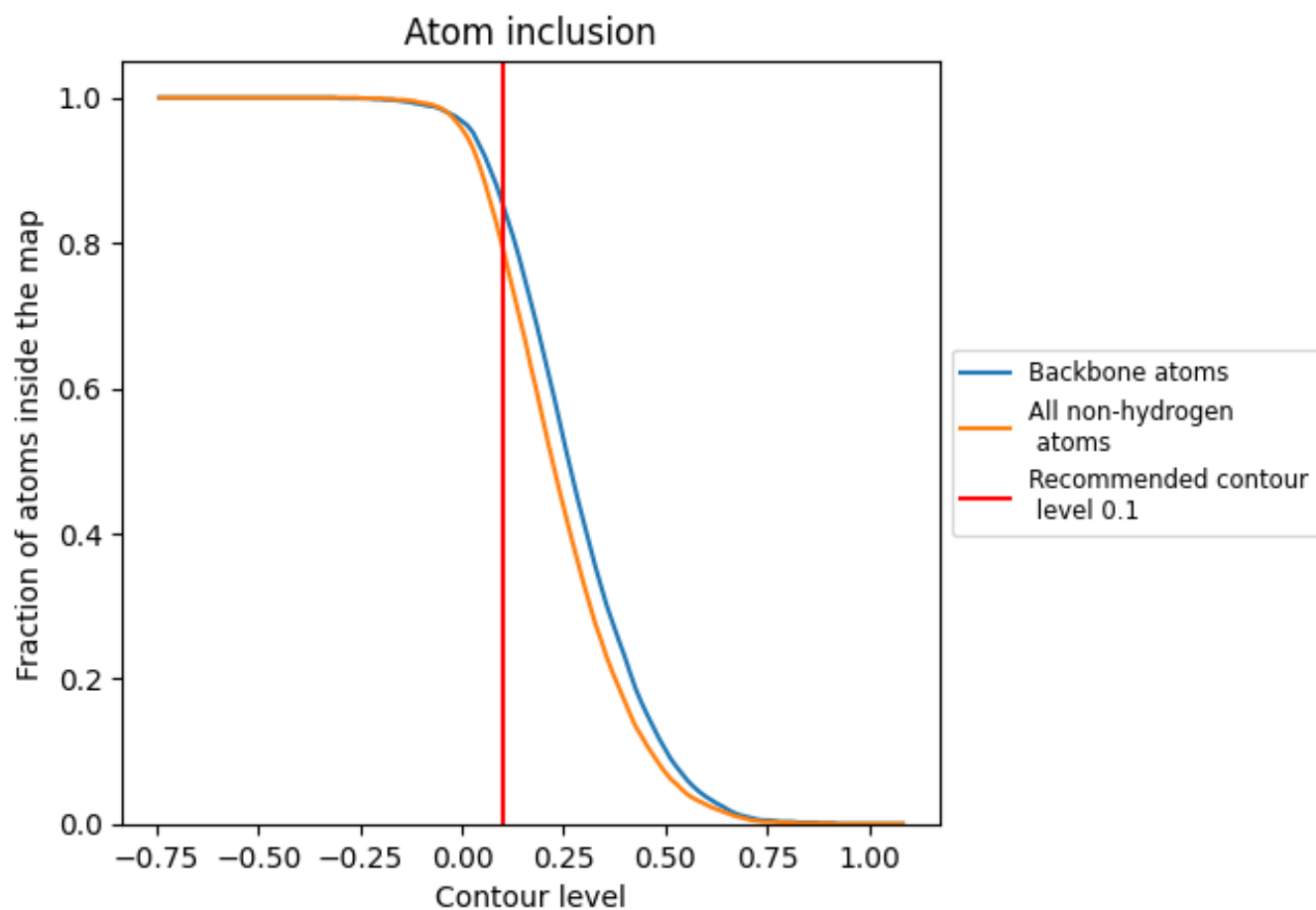
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).















9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.4060
A	 0.8150	 0.4220
B	 0.7860	 0.4000
C	 0.7830	 0.3990
D	 0.7810	 0.3950
E	 0.8170	 0.4240
G	 0.7820	 0.3960

