



Full wwPDB EM Validation Report ⓘ

Oct 29, 2024 – 04:33 PM EDT

PDB ID : 8TQK
EMDB ID : EMD-41506
Title : Human parainfluenza virus type 3 prefusion F trimer in complex with rPIV3-18 Fab
Authors : Otrelo-Cardoso, A.R.; Jardetzky, T.S.
Deposited on : 2023-08-07
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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

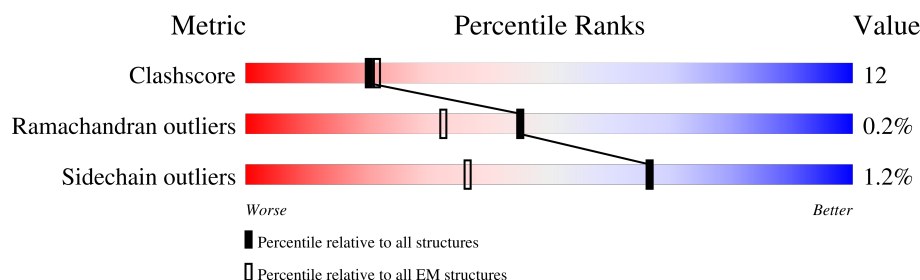
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	224	
1	F	224	
1	H	224	
2	E	214	
2	G	214	
2	L	214	
3	A	516	
3	B	516	

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Mol	Chain	Length	Quality of chain
3	C	516	 A horizontal bar chart showing the quality of chain C. The bar is divided into three segments: green (67%), yellow (14%), and grey (19%). A small red dot is at the beginning of the green segment.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29229 atoms, of which 14504 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 Heavy chain Fab rPIV3-18.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	116	Total	C	H	N	O	S	0	0
			1757	569	860	154	169	5		
1	F	116	Total	C	H	N	O	S	0	0
			1765	571	864	154	171	5		
1	H	116	Total	C	H	N	O	S	0	0
			1740	566	849	151	169	5		

- Molecule 2 is a protein called Light chain Fab rPIV3-28.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	105	Total	C	H	N	O	S	0	0
			1528	509	720	137	159	3		
2	G	105	Total	C	H	N	O	S	0	0
			1527	510	716	137	161	3		
2	L	104	Total	C	H	N	O	S	0	0
			1514	509	711	133	158	3		

- Molecule 3 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	417	Total	C	H	N	O	S	0	0
			6440	2027	3238	535	622	18		
3	B	415	Total	C	H	N	O	S	0	0
			6463	2027	3265	535	620	16		
3	C	418	Total	C	H	N	O	S	0	0
			6495	2034	3281	537	625	18		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	CYS	GLN	engineered mutation	UNP A0A059QA82
A	168	CYS	LEU	engineered mutation	UNP A0A059QA82
A	213	CYS	ILE	engineered mutation	UNP A0A059QA82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	230	CYS	GLY	engineered mutation	UNP A0A059QA82
A	463	VAL	ALA	engineered mutation	UNP A0A059QA82
A	474	TYR	ILE	engineered mutation	UNP A0A059QA82
A	482	SER	-	expression tag	UNP A0A059QA82
A	483	ALA	-	expression tag	UNP A0A059QA82
A	484	ILE	-	expression tag	UNP A0A059QA82
A	485	GLU	-	expression tag	UNP A0A059QA82
A	486	ASP	-	expression tag	UNP A0A059QA82
A	487	LYS	-	expression tag	UNP A0A059QA82
A	488	ILE	-	expression tag	UNP A0A059QA82
A	489	GLU	-	expression tag	UNP A0A059QA82
A	490	GLU	-	expression tag	UNP A0A059QA82
A	491	ILE	-	expression tag	UNP A0A059QA82
A	492	LEU	-	expression tag	UNP A0A059QA82
A	493	SER	-	expression tag	UNP A0A059QA82
A	494	LYS	-	expression tag	UNP A0A059QA82
A	495	ILE	-	expression tag	UNP A0A059QA82
A	496	TYR	-	expression tag	UNP A0A059QA82
A	497	HIS	-	expression tag	UNP A0A059QA82
A	498	ILE	-	expression tag	UNP A0A059QA82
A	499	GLU	-	expression tag	UNP A0A059QA82
A	500	ASN	-	expression tag	UNP A0A059QA82
A	501	GLU	-	expression tag	UNP A0A059QA82
A	502	ILE	-	expression tag	UNP A0A059QA82
A	503	ALA	-	expression tag	UNP A0A059QA82
A	504	ARG	-	expression tag	UNP A0A059QA82
A	505	ILE	-	expression tag	UNP A0A059QA82
A	506	LYS	-	expression tag	UNP A0A059QA82
A	507	LYS	-	expression tag	UNP A0A059QA82
A	508	LEU	-	expression tag	UNP A0A059QA82
A	509	ILE	-	expression tag	UNP A0A059QA82
A	510	GLY	-	expression tag	UNP A0A059QA82
A	511	GLU	-	expression tag	UNP A0A059QA82
A	512	ALA	-	expression tag	UNP A0A059QA82
A	513	PRO	-	expression tag	UNP A0A059QA82
A	514	GLY	-	expression tag	UNP A0A059QA82
A	515	SER	-	expression tag	UNP A0A059QA82
A	516	GLU	-	expression tag	UNP A0A059QA82
A	517	ASN	-	expression tag	UNP A0A059QA82
A	518	LEU	-	expression tag	UNP A0A059QA82
A	519	TYR	-	expression tag	UNP A0A059QA82
A	520	PHE	-	expression tag	UNP A0A059QA82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	521	GLN	-	expression tag	UNP A0A059QA82
A	522	GLY	-	expression tag	UNP A0A059QA82
A	523	GLY	-	expression tag	UNP A0A059QA82
A	524	SER	-	expression tag	UNP A0A059QA82
A	525	GLY	-	expression tag	UNP A0A059QA82
A	526	SER	-	expression tag	UNP A0A059QA82
A	527	HIS	-	expression tag	UNP A0A059QA82
A	528	HIS	-	expression tag	UNP A0A059QA82
A	529	HIS	-	expression tag	UNP A0A059QA82
A	530	HIS	-	expression tag	UNP A0A059QA82
A	531	HIS	-	expression tag	UNP A0A059QA82
A	532	HIS	-	expression tag	UNP A0A059QA82
A	533	HIS	-	expression tag	UNP A0A059QA82
A	534	HIS	-	expression tag	UNP A0A059QA82
B	162	CYS	GLN	engineered mutation	UNP A0A059QA82
B	168	CYS	LEU	engineered mutation	UNP A0A059QA82
B	213	CYS	ILE	engineered mutation	UNP A0A059QA82
B	230	CYS	GLY	engineered mutation	UNP A0A059QA82
B	463	VAL	ALA	engineered mutation	UNP A0A059QA82
B	474	TYR	ILE	engineered mutation	UNP A0A059QA82
B	482	SER	-	expression tag	UNP A0A059QA82
B	483	ALA	-	expression tag	UNP A0A059QA82
B	484	ILE	-	expression tag	UNP A0A059QA82
B	485	GLU	-	expression tag	UNP A0A059QA82
B	486	ASP	-	expression tag	UNP A0A059QA82
B	487	LYS	-	expression tag	UNP A0A059QA82
B	488	ILE	-	expression tag	UNP A0A059QA82
B	489	GLU	-	expression tag	UNP A0A059QA82
B	490	GLU	-	expression tag	UNP A0A059QA82
B	491	ILE	-	expression tag	UNP A0A059QA82
B	492	LEU	-	expression tag	UNP A0A059QA82
B	493	SER	-	expression tag	UNP A0A059QA82
B	494	LYS	-	expression tag	UNP A0A059QA82
B	495	ILE	-	expression tag	UNP A0A059QA82
B	496	TYR	-	expression tag	UNP A0A059QA82
B	497	HIS	-	expression tag	UNP A0A059QA82
B	498	ILE	-	expression tag	UNP A0A059QA82
B	499	GLU	-	expression tag	UNP A0A059QA82
B	500	ASN	-	expression tag	UNP A0A059QA82
B	501	GLU	-	expression tag	UNP A0A059QA82
B	502	ILE	-	expression tag	UNP A0A059QA82
B	503	ALA	-	expression tag	UNP A0A059QA82

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Chain	Residue	Modelled	Actual	Comment	Reference
B	504	ARG	-	expression tag	UNP A0A059QA82
B	505	ILE	-	expression tag	UNP A0A059QA82
B	506	LYS	-	expression tag	UNP A0A059QA82
B	507	LYS	-	expression tag	UNP A0A059QA82
B	508	LEU	-	expression tag	UNP A0A059QA82
B	509	ILE	-	expression tag	UNP A0A059QA82
B	510	GLY	-	expression tag	UNP A0A059QA82
B	511	GLU	-	expression tag	UNP A0A059QA82
B	512	ALA	-	expression tag	UNP A0A059QA82
B	513	PRO	-	expression tag	UNP A0A059QA82
B	514	GLY	-	expression tag	UNP A0A059QA82
B	515	SER	-	expression tag	UNP A0A059QA82
B	516	GLU	-	expression tag	UNP A0A059QA82
B	517	ASN	-	expression tag	UNP A0A059QA82
B	518	LEU	-	expression tag	UNP A0A059QA82
B	519	TYR	-	expression tag	UNP A0A059QA82
B	520	PHE	-	expression tag	UNP A0A059QA82
B	521	GLN	-	expression tag	UNP A0A059QA82
B	522	GLY	-	expression tag	UNP A0A059QA82
B	523	GLY	-	expression tag	UNP A0A059QA82
B	524	SER	-	expression tag	UNP A0A059QA82
B	525	GLY	-	expression tag	UNP A0A059QA82
B	526	SER	-	expression tag	UNP A0A059QA82
B	527	HIS	-	expression tag	UNP A0A059QA82
B	528	HIS	-	expression tag	UNP A0A059QA82
B	529	HIS	-	expression tag	UNP A0A059QA82
B	530	HIS	-	expression tag	UNP A0A059QA82
B	531	HIS	-	expression tag	UNP A0A059QA82
B	532	HIS	-	expression tag	UNP A0A059QA82
B	533	HIS	-	expression tag	UNP A0A059QA82
B	534	HIS	-	expression tag	UNP A0A059QA82
C	162	CYS	GLN	engineered mutation	UNP A0A059QA82
C	168	CYS	LEU	engineered mutation	UNP A0A059QA82
C	213	CYS	ILE	engineered mutation	UNP A0A059QA82
C	230	CYS	GLY	engineered mutation	UNP A0A059QA82
C	463	VAL	ALA	engineered mutation	UNP A0A059QA82
C	474	TYR	ILE	engineered mutation	UNP A0A059QA82
C	482	SER	-	expression tag	UNP A0A059QA82
C	483	ALA	-	expression tag	UNP A0A059QA82
C	484	ILE	-	expression tag	UNP A0A059QA82
C	485	GLU	-	expression tag	UNP A0A059QA82
C	486	ASP	-	expression tag	UNP A0A059QA82

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Chain	Residue	Modelled	Actual	Comment	Reference
C	487	LYS	-	expression tag	UNP A0A059QA82
C	488	ILE	-	expression tag	UNP A0A059QA82
C	489	GLU	-	expression tag	UNP A0A059QA82
C	490	GLU	-	expression tag	UNP A0A059QA82
C	491	ILE	-	expression tag	UNP A0A059QA82
C	492	LEU	-	expression tag	UNP A0A059QA82
C	493	SER	-	expression tag	UNP A0A059QA82
C	494	LYS	-	expression tag	UNP A0A059QA82
C	495	ILE	-	expression tag	UNP A0A059QA82
C	496	TYR	-	expression tag	UNP A0A059QA82
C	497	HIS	-	expression tag	UNP A0A059QA82
C	498	ILE	-	expression tag	UNP A0A059QA82
C	499	GLU	-	expression tag	UNP A0A059QA82
C	500	ASN	-	expression tag	UNP A0A059QA82
C	501	GLU	-	expression tag	UNP A0A059QA82
C	502	ILE	-	expression tag	UNP A0A059QA82
C	503	ALA	-	expression tag	UNP A0A059QA82
C	504	ARG	-	expression tag	UNP A0A059QA82
C	505	ILE	-	expression tag	UNP A0A059QA82
C	506	LYS	-	expression tag	UNP A0A059QA82
C	507	LYS	-	expression tag	UNP A0A059QA82
C	508	LEU	-	expression tag	UNP A0A059QA82
C	509	ILE	-	expression tag	UNP A0A059QA82
C	510	GLY	-	expression tag	UNP A0A059QA82
C	511	GLU	-	expression tag	UNP A0A059QA82
C	512	ALA	-	expression tag	UNP A0A059QA82
C	513	PRO	-	expression tag	UNP A0A059QA82
C	514	GLY	-	expression tag	UNP A0A059QA82
C	515	SER	-	expression tag	UNP A0A059QA82
C	516	GLU	-	expression tag	UNP A0A059QA82
C	517	ASN	-	expression tag	UNP A0A059QA82
C	518	LEU	-	expression tag	UNP A0A059QA82
C	519	TYR	-	expression tag	UNP A0A059QA82
C	520	PHE	-	expression tag	UNP A0A059QA82
C	521	GLN	-	expression tag	UNP A0A059QA82
C	522	GLY	-	expression tag	UNP A0A059QA82
C	523	GLY	-	expression tag	UNP A0A059QA82
C	524	SER	-	expression tag	UNP A0A059QA82
C	525	GLY	-	expression tag	UNP A0A059QA82
C	526	SER	-	expression tag	UNP A0A059QA82
C	527	HIS	-	expression tag	UNP A0A059QA82
C	528	HIS	-	expression tag	UNP A0A059QA82

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Chain	Residue	Modelled	Actual	Comment	Reference
C	529	HIS	-	expression tag	UNP A0A059QA82
C	530	HIS	-	expression tag	UNP A0A059QA82
C	531	HIS	-	expression tag	UNP A0A059QA82
C	532	HIS	-	expression tag	UNP A0A059QA82
C	533	HIS	-	expression tag	UNP A0A059QA82
C	534	HIS	-	expression tag	UNP A0A059QA82

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.267	Depositor
Minimum map value	-0.499	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	275.2, 275.2, 275.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	D	0.34	1/918 (0.1%)	0.61	0/1239
1	F	0.32	0/922	0.61	0/1244
1	H	0.31	0/912	0.58	0/1232
2	E	0.33	0/829	0.66	1/1128 (0.1%)
2	G	0.37	0/832	0.68	1/1132 (0.1%)
2	L	0.37	0/825	0.63	0/1123
3	A	0.31	0/3240	0.58	0/4391
3	B	0.30	0/3238	0.60	0/4389
3	C	0.31	0/3252	0.57	0/4406
All	All	0.32	1/14968 (0.0%)	0.60	2/20284 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	PRO	N-CD	5.10	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	81	ASP	CB-CG-OD2	5.26	123.04	118.30
2	E	81	ASP	CB-CG-OD2	5.23	123.01	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	D	897	860	859	50	0
1	F	901	864	861	27	0
1	H	891	849	846	6	0
2	E	808	720	772	25	0
2	G	811	716	770	39	0
2	L	803	711	763	24	0
3	A	3202	3238	3262	78	0
3	B	3198	3265	3270	83	0
3	C	3214	3281	3281	74	0
All	All	14725	14504	14684	349	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 (349) 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:E:13:ALA:O	2:E:105:GLU:OE1	1.63	1.14
2:G:92:ASN:ND2	3:C:191:GLY:HA3	1.69	1.07
2:L:89:GLN:NE2	2:L:96:TRP:CE3	2.25	1.03
2:L:89:GLN:HE22	2:L:96:TRP:HE3	1.07	0.95
1:D:22:CYS:SG	1:D:92:CYS:CB	2.58	0.92
2:E:23:CYS:HG	2:E:88:CYS:HG	1.15	0.89
3:C:348:LEU:HD13	3:C:352:MET:SD	2.12	0.89
3:A:210:LEU:O	3:A:211:THR:OG1	1.90	0.89
3:B:210:LEU:O	3:B:211:THR:OG1	1.92	0.88
3:B:422:ILE:HG22	3:B:423:ASN:H	1.40	0.87
3:C:33:ASN:OD1	3:C:34:SER:N	2.08	0.86
2:E:61:ARG:NH2	2:E:82:ASP:OD2	2.08	0.86
1:D:98:TRP:CZ3	3:B:192:CYS:HB2	2.11	0.85
2:L:4:MET:CE	2:L:23:CYS:SG	2.64	0.85
2:L:39:LYS:NZ	2:L:83:PHE:CE1	2.44	0.85
2:L:8:PRO:O	2:L:102:THR:HG22	1.77	0.84
2:L:23:CYS:HG	2:L:88:CYS:HG	1.05	0.84
2:G:92:ASN:HD22	3:C:191:GLY:HA3	1.41	0.84
1:D:66:ARG:O	1:D:82(A):SER:OG	1.96	0.84
3:B:422:ILE:HG22	3:B:423:ASN:N	1.93	0.83
2:G:92:ASN:ND2	3:C:191:GLY:CA	2.43	0.80
3:B:309:TYR:HD2	3:B:368:VAL:HG22	1.47	0.80
1:D:33:VAL:CG2	3:B:61:ASN:OD1	2.30	0.79
3:A:58:GLU:OE1	3:A:58:GLU:N	2.16	0.79
3:A:237:THR:HG21	3:A:242:ILE:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HG21	3:B:61:ASN:OD1	1.84	0.78
2:L:4:MET:HE2	2:L:23:CYS:SG	2.24	0.78
2:E:103:ARG:HG3	2:E:103:ARG:HH11	1.49	0.76
3:B:446:ASN:OD1	3:B:446:ASN:O	2.04	0.76
1:D:22:CYS:SG	1:D:92:CYS:HB3	2.24	0.75
3:A:460:LEU:HD11	3:B:456:ILE:HG23	1.69	0.74
3:A:379:VAL:HG12	3:B:122:VAL:HG22	1.69	0.74
3:B:422:ILE:CG2	3:B:423:ASN:H	2.01	0.73
2:G:92:ASN:HD22	3:C:191:GLY:CA	2.03	0.72
3:A:418:ASN:O	3:A:419:THR:HG23	1.90	0.72
2:L:4:MET:SD	2:L:90:GLN:HB3	2.30	0.72
1:D:58:PHE:CE1	3:B:188:ALA:HB1	2.26	0.71
2:L:8:PRO:O	2:L:102:THR:CG2	2.39	0.70
3:B:309:TYR:CD2	3:B:368:VAL:HG22	2.27	0.70
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.26	0.69
3:B:394:CYS:SG	3:B:395:ASN:N	2.64	0.69
3:B:124:THR:OG1	3:B:127:GLN:OE1	2.09	0.69
3:C:244:THR:HG23	3:C:245:THR:N	2.07	0.69
3:A:309:TYR:HD2	3:A:368:VAL:HG22	1.57	0.69
1:D:57:THR:HG22	1:D:57:THR:O	1.93	0.69
2:E:46:ILE:HD12	2:E:46:ILE:O	1.93	0.68
3:A:428:ASN:HB2	3:B:116:GLY:O	1.94	0.68
3:C:312:LEU:HD21	3:C:356:LEU:HD21	1.74	0.68
2:L:4:MET:HE3	2:L:23:CYS:SG	2.34	0.68
1:D:22:CYS:HG	1:D:92:CYS:CB	2.03	0.67
2:E:103:ARG:HG3	2:E:103:ARG:NH1	2.06	0.67
3:A:378:PHE:HB3	3:A:383:VAL:HG12	1.76	0.67
1:D:65:GLY:O	1:D:82(B):ARG:NH2	2.28	0.66
2:L:89:GLN:NE2	2:L:96:TRP:HE3	1.74	0.66
3:C:304:GLN:O	3:C:304:GLN:HG3	1.94	0.66
2:G:92:ASN:ND2	3:C:192:CYS:N	2.43	0.66
3:A:457:SER:O	3:A:461:ASN:ND2	2.28	0.66
2:E:89:GLN:OE1	2:E:98:PHE:CE1	2.49	0.66
3:A:459:GLU:O	3:A:463:VAL:HG23	1.96	0.65
3:B:414:HIS:NE2	3:B:431:LYS:HA	2.12	0.65
3:B:422:ILE:CG2	3:B:423:ASN:N	2.58	0.65
2:G:93:THR:HG22	3:C:191:GLY:N	2.13	0.64
2:G:93:THR:HG22	3:C:191:GLY:CA	2.27	0.64
1:D:98:TRP:CE3	3:B:63:CYS:HB2	2.33	0.64
3:A:418:ASN:O	3:A:419:THR:CG2	2.46	0.64
1:D:22:CYS:HG	1:D:92:CYS:HG	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:422:ILE:HG22	3:B:423:ASN:OD1	1.98	0.63
3:A:378:PHE:CG	3:B:118:ILE:HD12	2.33	0.63
3:A:378:PHE:CD2	3:B:118:ILE:HD12	2.33	0.63
3:B:454:ILE:O	3:B:458:ILE:HD12	1.99	0.62
3:A:454:ILE:O	3:A:458:ILE:HD12	1.99	0.62
3:A:430:ASN:HB2	3:B:117:THR:HG22	1.80	0.62
2:E:82:ASP:OD1	2:E:86:TYR:OH	2.17	0.62
3:A:72:LYS:HD3	3:A:274:TYR:CE1	2.34	0.62
3:B:175:VAL:HG23	3:B:175:VAL:O	1.99	0.61
3:C:297:ASP:OD1	3:C:298:SER:N	2.33	0.61
3:A:237:THR:CG2	3:A:242:ILE:HG13	2.30	0.61
3:C:244:THR:HG23	3:C:245:THR:H	1.66	0.61
1:D:4:LEU:HD12	1:D:102:VAL:CG1	2.31	0.61
1:D:45:LEU:O	2:E:98:PHE:CD2	2.53	0.61
1:F:105:GLN:O	1:F:105:GLN:NE2	2.34	0.61
3:C:309:TYR:HD2	3:C:368:VAL:HG22	1.66	0.60
3:A:237:THR:HG21	3:A:242:ILE:CG1	2.30	0.60
3:A:464:LYS:O	3:A:468:GLU:HG3	2.01	0.60
2:E:33:LEU:HD11	2:E:88:CYS:SG	2.42	0.60
2:G:93:THR:CG2	3:C:191:GLY:CA	2.80	0.60
3:A:78:LEU:HD12	3:A:211:THR:HG23	1.83	0.60
1:D:33:VAL:HG23	3:B:61:ASN:OD1	2.01	0.60
2:L:39:LYS:NZ	2:L:83:PHE:CD1	2.70	0.60
3:A:251:TYR:OH	3:A:283:PRO:O	2.20	0.60
1:D:58:PHE:HE1	3:B:188:ALA:HB1	1.65	0.60
1:D:99:ASP:HB3	3:B:65:ASP:OD2	2.02	0.60
3:A:351:GLU:OE1	3:A:351:GLU:N	2.34	0.59
3:C:251:TYR:OH	3:C:283:PRO:O	2.19	0.59
3:A:430:ASN:HB2	3:B:117:THR:CG2	2.33	0.59
3:A:307:GLU:OE1	3:A:375:ARG:NH2	2.35	0.59
2:G:92:ASN:ND2	3:C:192:CYS:H	2.01	0.58
3:B:92:VAL:O	3:B:119:ALA:HB3	2.04	0.58
3:B:422:ILE:O	3:B:424:GLY:N	2.36	0.58
3:B:467:LEU:HD12	3:B:468:GLU:N	2.19	0.58
2:E:34:THR:HG1	2:E:91:PHE:HE1	1.50	0.58
1:F:98:TRP:CE3	3:C:63:CYS:HB2	2.37	0.58
3:A:383:VAL:HG22	3:A:412:ILE:HD11	1.85	0.58
3:C:351:GLU:OE1	3:C:351:GLU:N	2.37	0.58
1:D:82:MET:HG2	1:D:82(C):LEU:HD21	1.85	0.58
2:E:105:GLU:O	2:E:105:GLU:HG2	2.04	0.58
3:C:151:ILE:HG22	3:C:159:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:PHE:CE1	3:B:188:ALA:CB	2.86	0.57
2:G:92:ASN:HD22	2:G:92:ASN:C	2.08	0.57
3:A:406:ASP:OD2	3:A:406:ASP:N	2.38	0.57
3:C:92:VAL:O	3:C:118:ILE:O	2.23	0.57
3:C:177:ASP:OD1	3:C:178:TYR:N	2.37	0.56
2:E:23:CYS:CB	2:E:88:CYS:SG	2.93	0.56
1:F:83:ARG:HG2	1:F:84:ALA:H	1.70	0.56
3:A:87:LYS:HD2	3:A:87:LYS:N	2.21	0.56
2:G:102:THR:O	2:G:102:THR:OG1	2.21	0.56
2:L:19:VAL:CG2	2:L:78:LEU:HD11	2.36	0.56
2:G:93:THR:HG22	3:C:191:GLY:HA2	1.88	0.56
2:G:96:TRP:N	2:G:96:TRP:CD1	2.73	0.55
2:E:34:THR:OG1	2:E:91:PHE:HE1	1.90	0.55
3:A:328:VAL:HG12	3:A:328:VAL:O	2.06	0.55
3:A:309:TYR:CD2	3:A:368:VAL:HG22	2.39	0.54
1:F:5:LEU:O	1:F:22:CYS:SG	2.66	0.54
2:G:21:ILE:CG2	2:G:102:THR:HG21	2.37	0.54
3:B:65:ASP:OD1	3:B:66:GLN:N	2.41	0.54
3:A:131:ALA:O	3:A:135:VAL:HG23	2.07	0.54
3:C:163:SER:O	3:C:163:SER:OG	2.22	0.54
3:A:163:SER:O	3:A:163:SER:OG	2.25	0.54
3:C:244:THR:CG2	3:C:245:THR:N	2.70	0.53
1:D:47:TRP:CD1	2:E:96:TRP:HB2	2.44	0.53
3:B:177:ASP:OD1	3:B:178:TYR:N	2.41	0.53
3:B:314:SER:HG	3:B:315:HIS:CE1	2.25	0.53
3:B:154:THR:HG22	3:B:156:LYS:H	1.72	0.53
3:B:262:ILE:HD12	3:B:262:ILE:O	2.08	0.53
3:A:130:ALA:O	3:A:134:LEU:HD22	2.09	0.53
3:C:226:ILE:O	3:C:226:ILE:HG22	2.09	0.53
3:C:244:THR:CG2	3:C:245:THR:H	2.22	0.53
3:C:454:ILE:O	3:C:458:ILE:HD12	2.09	0.53
1:F:66:ARG:NH2	1:F:86:ASP:OD2	2.42	0.53
3:C:237:THR:HG23	3:C:238:ASN:HD22	1.74	0.53
3:C:397:ILE:HD11	3:C:426:LEU:HD11	1.91	0.52
1:F:11:LEU:HD13	1:F:12:VAL:N	2.25	0.52
1:F:99:ASP:OD1	1:F:100:TYR:N	2.37	0.52
3:A:426:LEU:HD11	3:B:114:VAL:HG22	1.91	0.52
3:A:28:VAL:HG12	3:A:28:VAL:O	2.09	0.52
1:D:55:GLU:N	1:D:55:GLU:OE1	2.43	0.52
3:A:426:LEU:HD12	3:B:114:VAL:O	2.10	0.52
1:D:12:VAL:HG22	1:D:13:ARG:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:THR:HG22	1:F:81:GLU:HB3	1.90	0.52
1:D:45:LEU:HB3	2:E:98:PHE:CZ	2.45	0.52
1:F:95:MET:SD	2:G:96:TRP:HZ2	2.33	0.52
3:B:153:ASP:O	3:B:153:ASP:OD2	2.28	0.52
3:C:467:LEU:HD12	3:C:468:GLU:N	2.25	0.52
1:D:52:THR:HG21	3:B:59:ASP:OD2	2.11	0.51
2:E:6:GLN:HB2	2:E:22:THR:O	2.11	0.51
2:G:4:MET:HG2	2:G:97:THR:HG22	1.93	0.51
3:C:210:LEU:O	3:C:211:THR:OG1	2.22	0.51
2:E:79:GLN:HG3	2:E:80:PRO:HD2	1.93	0.51
3:A:378:PHE:CD2	3:B:118:ILE:CD1	2.94	0.51
2:G:91:PHE:HD1	2:G:91:PHE:O	1.94	0.50
3:A:328:VAL:O	3:A:328:VAL:CG1	2.58	0.50
3:C:337:SER:OG	3:C:338:TYR:N	2.44	0.50
2:L:19:VAL:HG21	2:L:78:LEU:HD11	1.93	0.50
2:L:39:LYS:NZ	2:L:83:PHE:HE1	2.08	0.50
3:B:114:VAL:O	3:B:114:VAL:HG13	2.12	0.50
3:C:378:PHE:CD1	3:C:383:VAL:HG12	2.47	0.50
1:D:22:CYS:SG	1:D:92:CYS:HB2	2.46	0.50
2:G:7:SER:O	2:G:22:THR:HG22	2.12	0.50
3:C:147:LEU:C	3:C:147:LEU:HD13	2.31	0.50
1:F:83:ARG:HG2	1:F:84:ALA:N	2.27	0.50
3:B:83:TYR:CD2	3:B:271:LEU:HD22	2.47	0.49
3:B:351:GLU:N	3:B:351:GLU:OE1	2.45	0.49
3:C:268:ASP:OD1	3:C:269:VAL:N	2.45	0.49
1:D:22:CYS:HB3	1:D:92:CYS:HG	1.76	0.49
2:G:94:TYR:CE2	3:C:187:ILE:O	2.65	0.49
3:B:394:CYS:O	3:B:395:ASN:C	2.51	0.49
3:A:459:GLU:HA	3:A:459:GLU:OE1	2.13	0.49
3:A:293:ILE:HG12	3:A:317:MET:HB2	1.94	0.48
1:D:5:LEU:HD23	1:D:6:GLU:N	2.28	0.48
2:G:92:ASN:HD21	3:C:191:GLY:HA3	1.66	0.48
3:C:394:CYS:SG	3:C:395:ASN:N	2.87	0.48
1:D:45:LEU:HB3	2:E:98:PHE:CE2	2.48	0.48
2:E:36:TYR:HE1	2:E:89:GLN:HB3	1.78	0.48
3:B:437:PHE:CG	3:B:437:PHE:O	2.67	0.48
1:D:40:ALA:HB3	1:D:43:LYS:HB2	1.95	0.48
3:C:51:LEU:HD13	3:C:278:LEU:HD13	1.95	0.48
1:D:98:TRP:CE3	3:B:192:CYS:HB2	2.47	0.48
1:F:95:MET:SD	2:G:96:TRP:CZ2	3.07	0.48
1:F:96:PHE:CZ	2:G:49:TYR:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:ASP:O	3:C:273:ASP:OD2	2.32	0.47
1:D:22:CYS:CB	1:D:92:CYS:HG	2.27	0.47
3:A:115:ILE:HD12	3:C:426:LEU:O	2.14	0.47
3:C:378:PHE:HD1	3:C:383:VAL:HG12	1.79	0.47
3:B:151:ILE:HD12	3:B:151:ILE:O	2.14	0.47
3:B:291:THR:O	3:B:291:THR:CG2	2.62	0.47
3:C:334:ALA:HB3	3:C:337:SER:O	2.14	0.47
3:A:238:ASN:OD1	3:A:238:ASN:C	2.53	0.47
1:F:19:ARG:HD3	1:F:81:GLU:HB2	1.96	0.47
3:B:147:LEU:HD22	3:B:161:VAL:CG2	2.45	0.47
3:A:213:CYS:SG	3:A:230:CYS:CB	3.03	0.47
3:B:205:GLN:HA	3:B:205:GLN:OE1	2.14	0.47
3:B:366:THR:HG22	3:B:449:VAL:HG23	1.97	0.47
2:E:23:CYS:SG	2:E:71:PHE:HB2	2.55	0.46
1:F:100(A):ASP:OD1	1:F:100(B):THR:N	2.48	0.46
1:D:15:GLY:N	1:D:82(C):LEU:O	2.49	0.46
2:L:29:VAL:HG21	2:L:90:GLN:HB2	1.97	0.46
1:H:56:ARG:O	1:H:57:THR:OG1	2.32	0.46
3:A:72:LYS:HD3	3:A:274:TYR:CZ	2.50	0.46
3:B:143:ASP:OD2	3:B:143:ASP:N	2.48	0.46
3:B:199:LEU:HD23	3:B:203:LEU:HG	1.98	0.46
3:B:348:LEU:HD22	3:B:352:MET:SD	2.55	0.46
1:F:67:PHE:N	1:F:67:PHE:CD1	2.83	0.46
3:C:153:ASP:OD1	3:C:153:ASP:N	2.46	0.46
3:A:336:SER:O	3:A:336:SER:OG	2.32	0.46
3:A:177:ASP:OD1	3:A:177:ASP:N	2.47	0.46
3:C:383:VAL:CG2	3:C:420:ILE:HD13	2.46	0.46
3:A:397:ILE:HD11	3:A:426:LEU:CD2	2.46	0.46
3:A:147:LEU:HD13	3:A:147:LEU:O	2.16	0.46
3:A:394:CYS:SG	3:A:395:ASN:N	2.87	0.46
3:B:437:PHE:O	3:B:437:PHE:CD2	2.69	0.46
3:C:146:LYS:HZ3	3:C:146:LYS:HB2	1.81	0.46
3:C:237:THR:HG23	3:C:238:ASN:ND2	2.30	0.46
1:D:58:PHE:CZ	3:B:188:ALA:HB2	2.52	0.45
2:G:92:ASN:ND2	3:C:191:GLY:C	2.70	0.45
2:L:83:PHE:O	2:L:83:PHE:CG	2.69	0.45
1:D:98:TRP:CD1	1:D:98:TRP:N	2.83	0.45
3:A:128:ILE:HD13	3:A:128:ILE:N	2.31	0.45
3:C:59:ASP:OD1	3:C:59:ASP:O	2.34	0.45
3:C:311:PRO:O	3:C:312:LEU:HD12	2.16	0.45
1:D:22:CYS:HG	1:D:92:CYS:HB3	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:153:ASP:O	3:B:154:THR:OG1	2.23	0.45
1:F:4:LEU:HB3	1:F:22:CYS:SG	2.56	0.45
2:L:83:PHE:CD1	2:L:83:PHE:O	2.70	0.45
2:G:91:PHE:O	2:G:91:PHE:CD1	2.70	0.45
1:D:29:PHE:O	1:D:29:PHE:CG	2.70	0.45
1:H:49:SER:OG	1:H:50:SER:N	2.50	0.45
2:L:9:SER:O	2:L:102:THR:HA	2.16	0.45
3:B:140:ALA:O	3:B:144:ILE:HG12	2.17	0.45
3:B:147:LEU:HD22	3:B:161:VAL:HG22	1.98	0.45
3:C:304:GLN:O	3:C:305:ASN:HB2	2.15	0.45
1:D:4:LEU:HD12	1:D:102:VAL:HG11	1.99	0.45
2:G:93:THR:CG2	3:C:191:GLY:HA2	2.45	0.45
3:B:59:ASP:OD2	3:B:59:ASP:C	2.55	0.45
1:F:73:ASN:OD1	1:F:73:ASN:N	2.48	0.45
1:D:102:VAL:HG12	1:D:103:TRP:N	2.32	0.44
2:G:24:ARG:NH1	2:G:70:GLU:OE2	2.49	0.44
2:L:4:MET:HE2	2:L:23:CYS:HG	1.81	0.44
2:L:58:VAL:HG13	2:L:59:PRO:HD2	1.98	0.44
3:B:307:GLU:OE2	3:B:375:ARG:NH2	2.49	0.44
1:D:33:VAL:HG22	1:D:52:THR:HG23	1.99	0.44
3:B:378:PHE:HD1	3:B:383:VAL:HG12	1.82	0.44
3:C:394:CYS:HA	3:C:421:GLY:H	1.82	0.44
3:A:161:VAL:O	3:A:168:CYS:HA	2.17	0.44
3:C:278:LEU:HD12	3:C:278:LEU:N	2.31	0.44
1:F:103:TRP:HE1	2:G:44:PRO:HD2	1.83	0.44
3:B:33:ASN:OD1	3:B:34:SER:N	2.50	0.44
3:C:445:LEU:O	3:C:446:ASN:OD1	2.36	0.44
1:F:81:GLU:OE2	1:F:82:MET:O	2.36	0.44
3:B:293:ILE:HG21	3:B:338:TYR:CE2	2.53	0.44
1:D:57:THR:O	1:D:57:THR:CG2	2.64	0.44
1:D:58:PHE:HE1	3:B:188:ALA:CB	2.27	0.44
2:G:25:ALA:O	2:G:69:THR:HG23	2.18	0.44
2:G:93:THR:HG23	3:C:191:GLY:CA	2.48	0.44
2:L:76:SER:OG	2:L:77:SER:N	2.50	0.44
3:C:78:LEU:HD13	3:C:211:THR:HG22	1.99	0.44
1:D:52:THR:HG22	3:B:59:ASP:OD1	2.17	0.43
3:A:65:ASP:O	3:A:66:GLN:HB2	2.19	0.43
3:C:368:VAL:HG13	3:C:373:VAL:CG2	2.48	0.43
1:H:86:ASP:N	1:H:86:ASP:OD1	2.51	0.43
3:A:115:ILE:HD12	3:A:115:ILE:N	2.33	0.43
3:A:379:VAL:HG23	3:A:380:ASN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:VAL:HG11	3:C:312:LEU:HD23	2.00	0.43
1:D:29:PHE:O	1:D:71:ARG:NH2	2.52	0.43
3:A:79:ILE:HG23	3:A:269:VAL:HG11	2.00	0.43
3:A:378:PHE:CZ	3:B:128:ILE:HD12	2.53	0.43
3:A:394:CYS:O	3:A:395:ASN:C	2.56	0.43
3:B:413:THR:O	3:B:414:HIS:HB3	2.18	0.43
2:G:67:SER:OG	2:G:68:GLY:N	2.51	0.43
3:A:78:LEU:HD23	3:A:78:LEU:O	2.18	0.43
3:C:76:ASP:HA	3:C:79:ILE:HG22	1.99	0.43
3:B:118:ILE:HG22	3:B:119:ALA:O	2.18	0.43
2:L:19:VAL:HG23	2:L:78:LEU:CD1	2.48	0.43
3:A:79:ILE:HG22	3:A:271:LEU:HD13	2.01	0.43
3:B:291:THR:O	3:B:291:THR:HG23	2.19	0.43
1:F:7:SER:HB2	1:F:21:SER:O	2.19	0.43
3:A:118:ILE:O	3:A:119:ALA:HB3	2.19	0.43
3:A:147:LEU:HD13	3:A:147:LEU:C	2.40	0.43
3:A:418:ASN:C	3:A:419:THR:HG23	2.38	0.43
3:B:147:LEU:HD12	3:B:147:LEU:O	2.19	0.43
2:E:89:GLN:OE1	2:E:98:PHE:CZ	2.72	0.43
1:H:2:VAL:N	1:H:25:SER:O	2.52	0.43
3:A:115:ILE:HD12	3:A:115:ILE:H	1.83	0.43
2:E:103:ARG:HH11	2:E:103:ARG:CG	2.22	0.42
3:C:28:VAL:HG11	3:C:360:ILE:HG23	2.01	0.42
2:G:92:ASN:ND2	2:G:92:ASN:C	2.72	0.42
2:G:92:ASN:HD21	3:C:191:GLY:C	2.22	0.42
2:G:92:ASN:HD21	3:C:192:CYS:N	2.14	0.42
1:F:99:ASP:O	2:G:50:LYS:NZ	2.50	0.42
3:C:28:VAL:HG23	3:C:30:VAL:HG23	2.01	0.42
3:B:151:ILE:O	3:B:152:ARG:C	2.57	0.42
3:C:270:ASP:O	3:C:271:LEU:HB2	2.19	0.42
1:F:29:PHE:CD1	1:F:29:PHE:C	2.93	0.42
2:L:19:VAL:HG23	2:L:78:LEU:HD11	2.02	0.42
1:F:6:GLU:O	1:F:7:SER:OG	2.27	0.42
3:B:251:TYR:OH	3:B:283:PRO:O	2.37	0.42
3:C:467:LEU:HD12	3:C:467:LEU:C	2.39	0.42
1:D:52:THR:HG22	1:D:53:SER:N	2.35	0.42
1:D:52:THR:CG2	3:B:59:ASP:OD2	2.68	0.42
2:G:93:THR:CG2	3:C:191:GLY:N	2.81	0.42
3:A:78:LEU:HD12	3:A:211:THR:CG2	2.49	0.42
1:F:47:TRP:CZ3	2:G:95:SER:OG	2.59	0.41
1:H:69:VAL:HG12	1:H:80:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:LEU:HD12	2:E:89:GLN:O	2.20	0.41
3:A:176:GLN:HA	3:A:176:GLN:OE1	2.20	0.41
3:A:289:LEU:HD12	3:A:290:ASN:HB2	2.02	0.41
3:B:181:LYS:HB3	3:B:182:GLU:OE1	2.20	0.41
1:D:28:THR:HG21	1:D:31:LYS:NZ	2.35	0.41
3:A:28:VAL:O	3:A:28:VAL:CG1	2.67	0.41
3:A:417:CYS:O	3:A:429:THR:HG21	2.19	0.41
3:A:289:LEU:HD12	3:A:289:LEU:C	2.41	0.41
3:A:356:LEU:N	3:A:356:LEU:CD2	2.83	0.41
3:A:415:LYS:N	3:A:415:LYS:HE2	2.35	0.41
3:B:383:VAL:HG21	3:B:420:ILE:HD13	2.01	0.41
1:F:82(C):LEU:HD23	1:F:83:ARG:O	2.21	0.41
3:B:147:LEU:HD12	3:B:151:ILE:HG23	2.02	0.41
3:B:456:ILE:H	3:B:456:ILE:HG13	1.60	0.41
1:F:39:GLN:O	1:F:39:GLN:HG2	2.21	0.41
2:G:35:TRP:CH2	2:G:88:CYS:HB3	2.55	0.41
3:A:38:MET:HB3	3:A:291:THR:HG21	2.03	0.41
3:B:459:GLU:O	3:B:463:VAL:HG22	2.21	0.41
3:C:383:VAL:HG21	3:C:420:ILE:HD13	2.03	0.41
1:F:68:THR:CG2	1:F:81:GLU:HB3	2.51	0.41
3:C:394:CYS:HA	3:C:420:ILE:HA	2.02	0.41
3:A:92:VAL:O	3:A:119:ALA:HB3	2.20	0.40
3:A:383:VAL:HG13	3:A:420:ILE:HD11	2.03	0.40
3:B:383:VAL:CG2	3:B:420:ILE:HD13	2.51	0.40
3:A:348:LEU:HD22	3:A:352:MET:CE	2.50	0.40
3:A:460:LEU:O	3:A:464:LYS:HG3	2.21	0.40
1:D:59:TYR:OH	1:D:67:PHE:O	2.35	0.40
2:G:21:ILE:HG21	2:G:102:THR:HG21	2.03	0.40
2:G:93:THR:C	2:G:95:SER:N	2.75	0.40
3:C:59:ASP:OD1	3:C:59:ASP:C	2.59	0.40
3:C:80:ILE:HB	3:C:81:PRO:HD3	2.03	0.40
1:D:35:ALA:HB1	1:D:49:SER:O	2.21	0.40
1:D:42:GLY:O	1:D:43:LYS:HD2	2.22	0.40
3:A:428:ASN:C	3:A:429:THR:HG22	2.42	0.40
3:A:464:LYS:O	3:A:467:LEU:HG	2.20	0.40
3:C:394:CYS:CA	3:C:420:ILE:HA	2.51	0.40
1:D:47:TRP:CZ3	2:E:95:SER:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	114/224 (51%)	111 (97%)	3 (3%)	0	100	100
1	F	114/224 (51%)	110 (96%)	4 (4%)	0	100	100
1	H	114/224 (51%)	111 (97%)	3 (3%)	0	100	100
2	E	103/214 (48%)	100 (97%)	3 (3%)	0	100	100
2	G	103/214 (48%)	98 (95%)	5 (5%)	0	100	100
2	L	102/214 (48%)	96 (94%)	6 (6%)	0	100	100
3	A	405/516 (78%)	385 (95%)	18 (4%)	2 (0%)	25	60
3	B	405/516 (78%)	378 (93%)	27 (7%)	0	100	100
3	C	406/516 (79%)	375 (92%)	30 (7%)	1 (0%)	44	75
All	All	1866/2862 (65%)	1764 (94%)	99 (5%)	3 (0%)	45	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	174	SER
3	C	174	SER
3	A	236	ARG

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	D	92/189 (49%)	90 (98%)	2 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	93/189 (49%)	93 (100%)	0	100	100
1	H	91/189 (48%)	88 (97%)	3 (3%)	33	64
2	E	89/189 (47%)	88 (99%)	1 (1%)	70	86
2	G	90/189 (48%)	86 (96%)	4 (4%)	24	57
2	L	89/189 (47%)	85 (96%)	4 (4%)	23	56
3	A	366/457 (80%)	363 (99%)	3 (1%)	79	90
3	B	366/457 (80%)	364 (100%)	2 (0%)	86	93
3	C	369/457 (81%)	368 (100%)	1 (0%)	91	96
All	All	1645/2505 (66%)	1625 (99%)	20 (1%)	66	85

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	100(D)	ASP
1	D	103	TRP
2	E	97	THR
2	G	82	ASP
2	G	90	GLN
2	G	92	ASN
2	G	97	THR
1	H	82(A)	SER
1	H	100(D)	ASP
1	H	100(E)	PHE
2	L	78	LEU
2	L	81	ASP
2	L	97	THR
2	L	105	GLU
3	A	214	PHE
3	A	235	TYR
3	A	357	SER
3	B	414	HIS
3	B	419	THR
3	C	472	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	6	GLN

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Mol	Chain	Res	Type
2	E	38	HIS
2	E	90	GLN
2	G	92	ASN
3	C	238	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

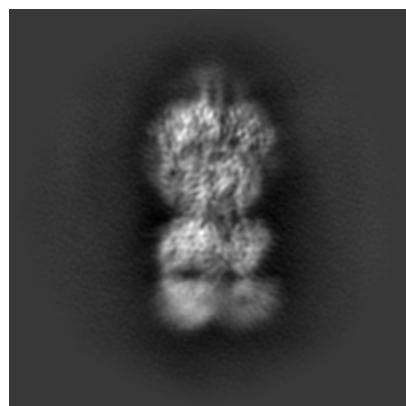
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41506. These allow visual inspection of the internal detail of the map and identification of artifacts.

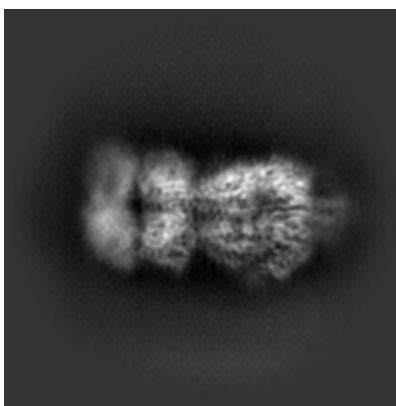
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

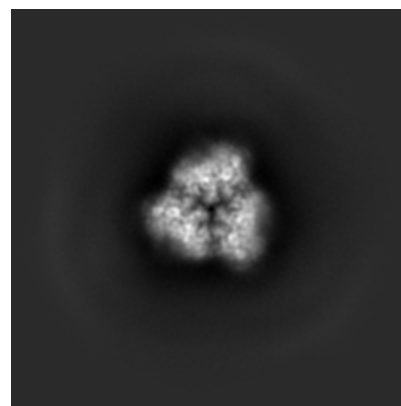
6.1.1 Primary map



X

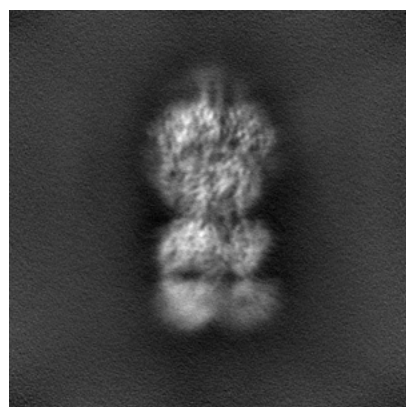


Y

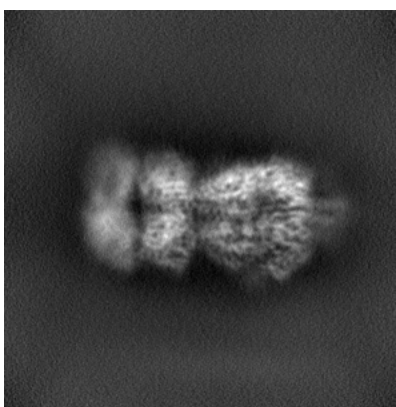


Z

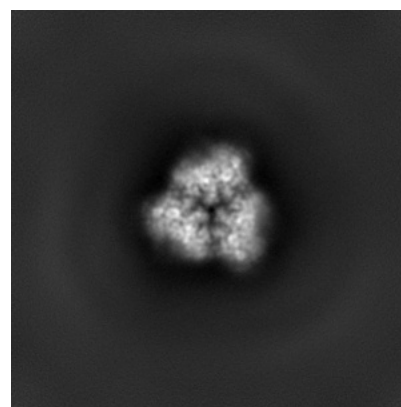
6.1.2 Raw map



X



Y

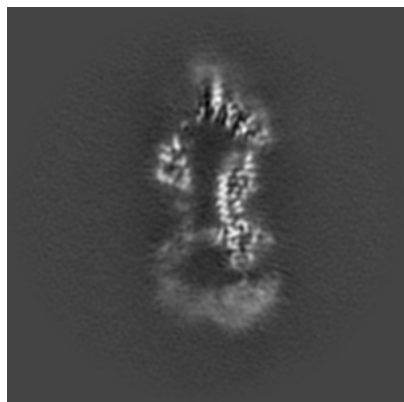


Z

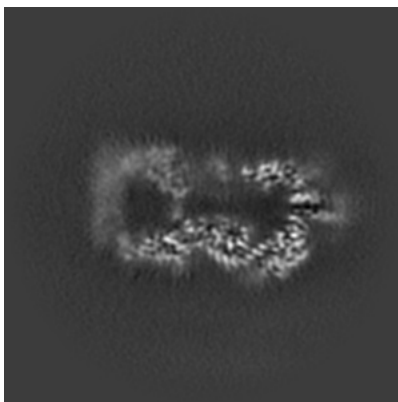
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

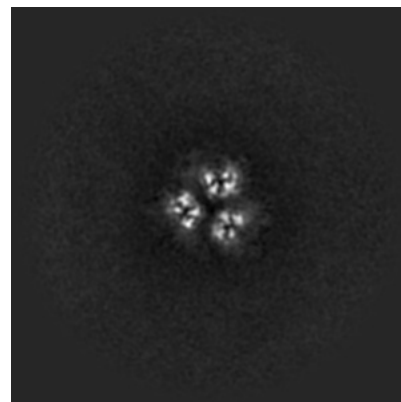
6.2.1 Primary map



X Index: 160

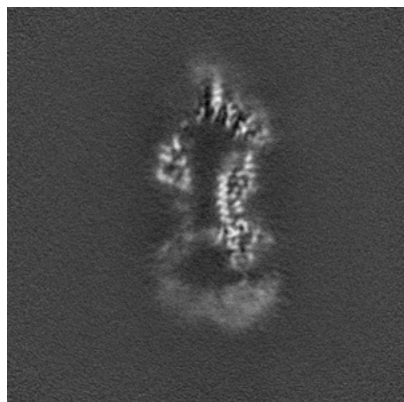


Y Index: 160

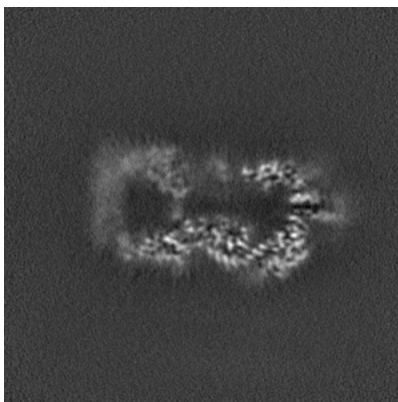


Z Index: 160

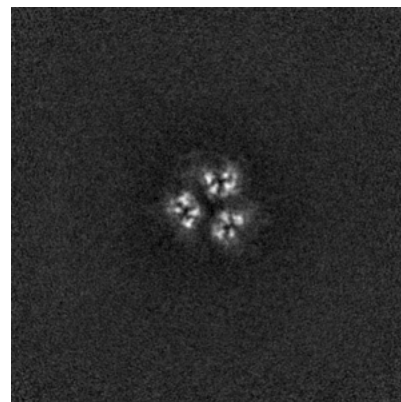
6.2.2 Raw map



X Index: 160



Y Index: 160

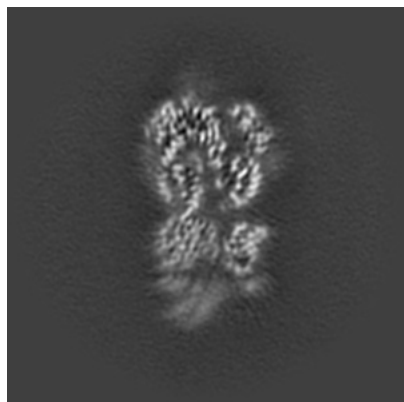


Z Index: 160

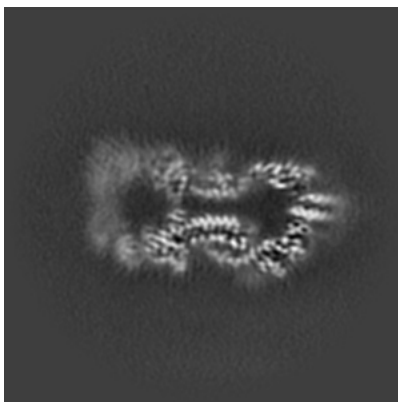
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

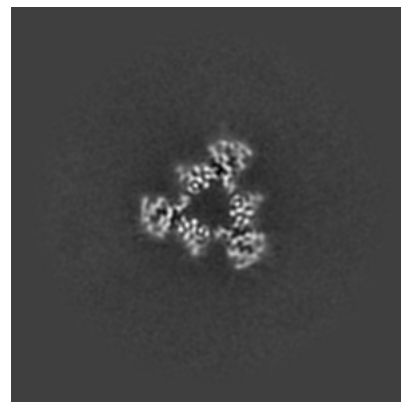
6.3.1 Primary map



X Index: 180

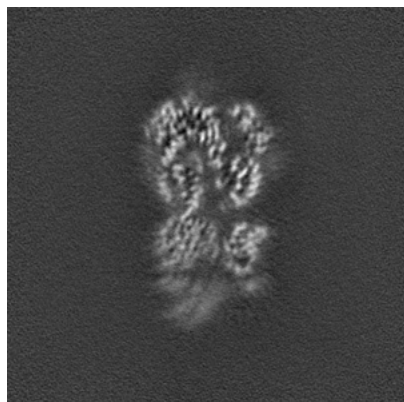


Y Index: 155

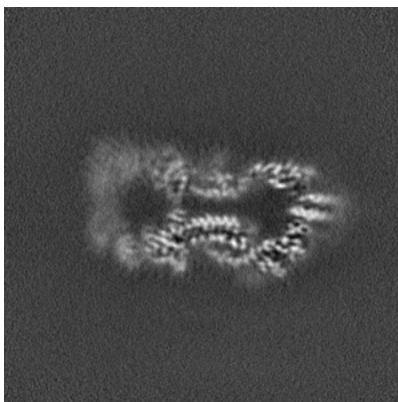


Z Index: 219

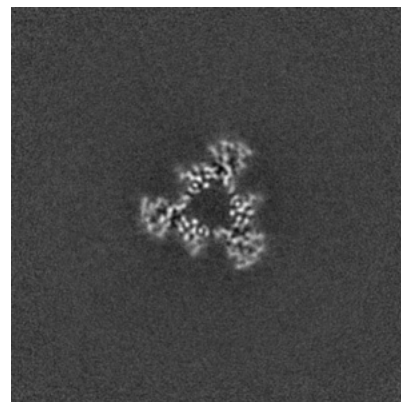
6.3.2 Raw map



X Index: 180



Y Index: 155

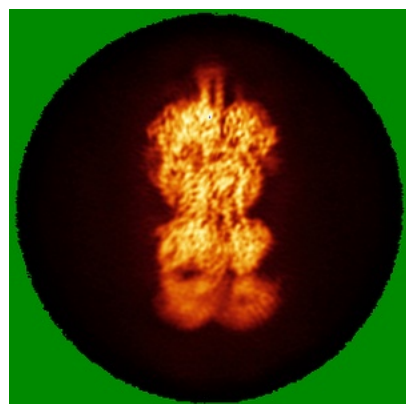


Z Index: 220

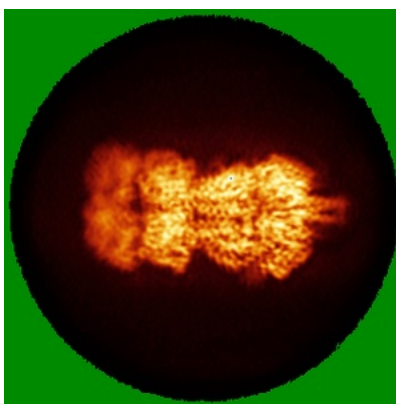
The images above show the largest variance slices of the map in three orthogonal directions.

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

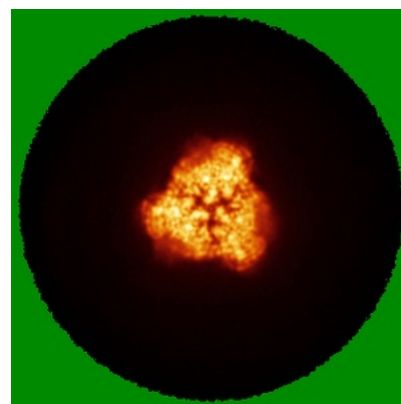
6.4.1 Primary map



X

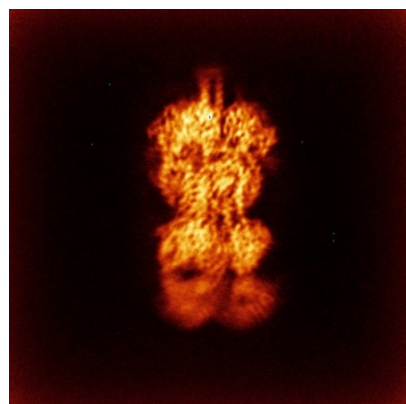


Y

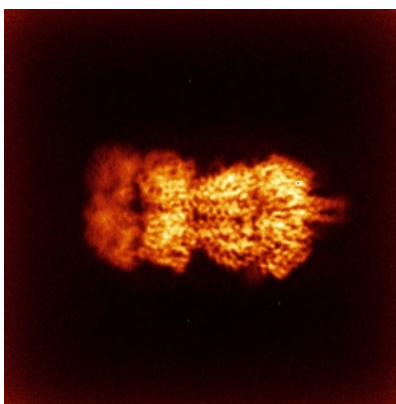


Z

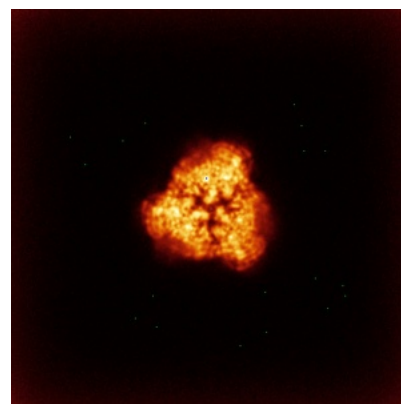
6.4.2 Raw map



X



Y

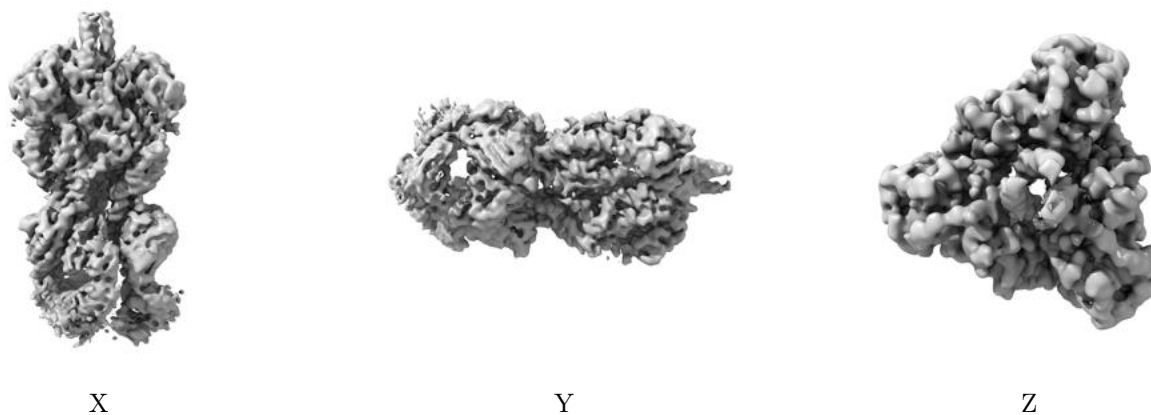


Z

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.

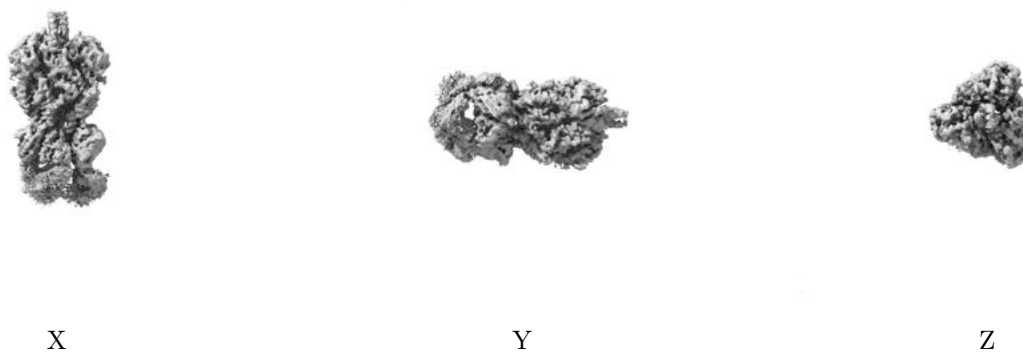
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

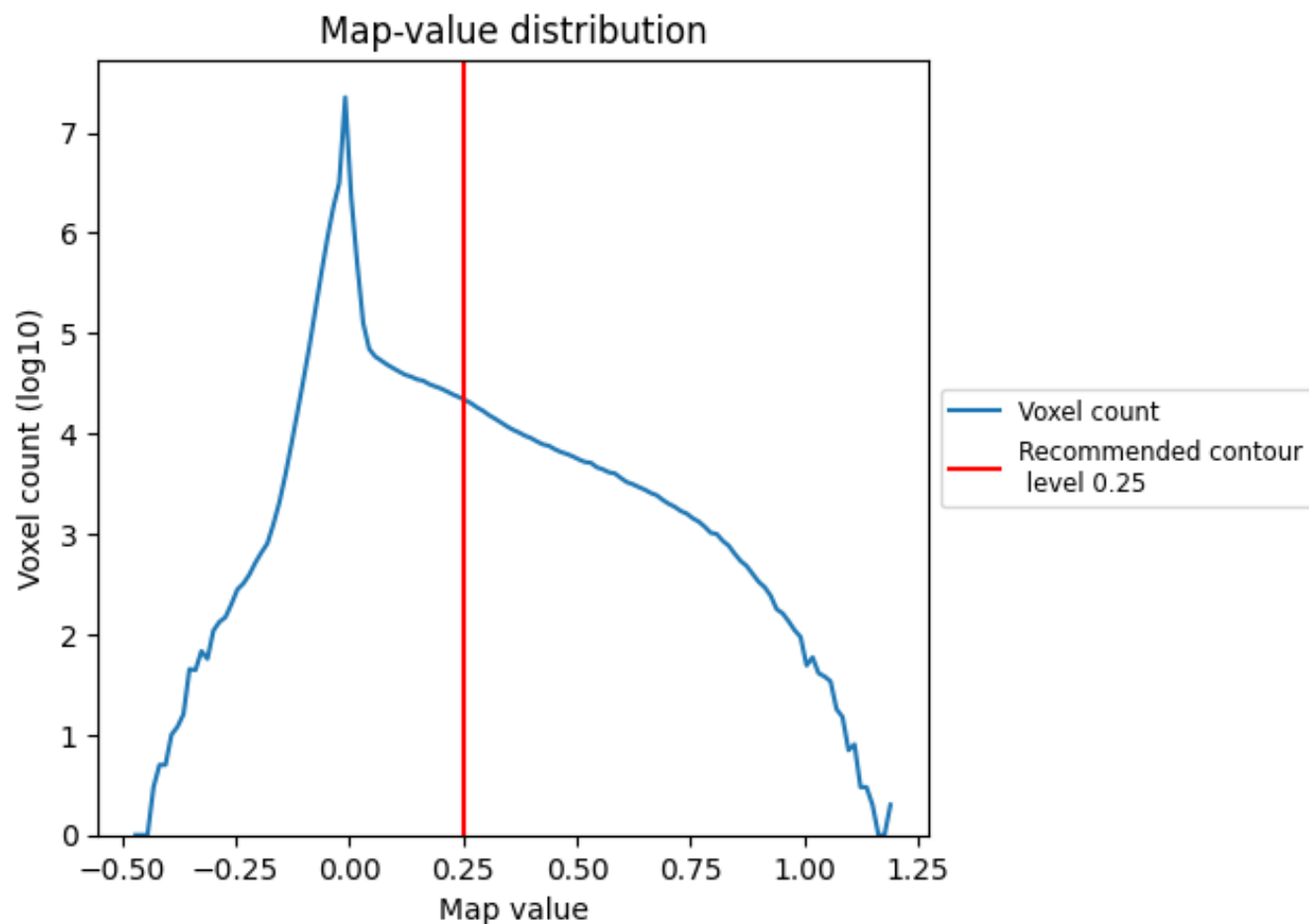
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

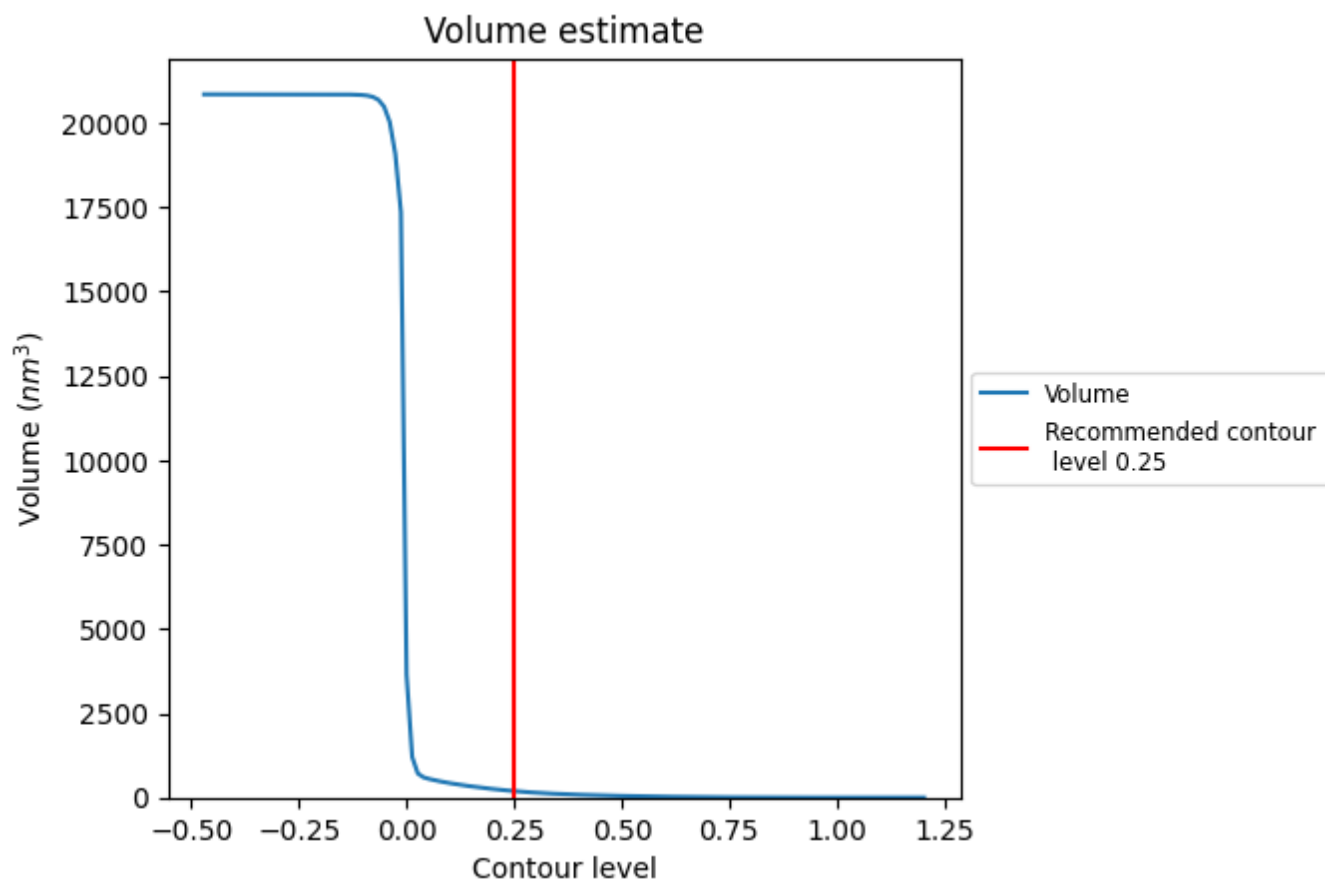
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

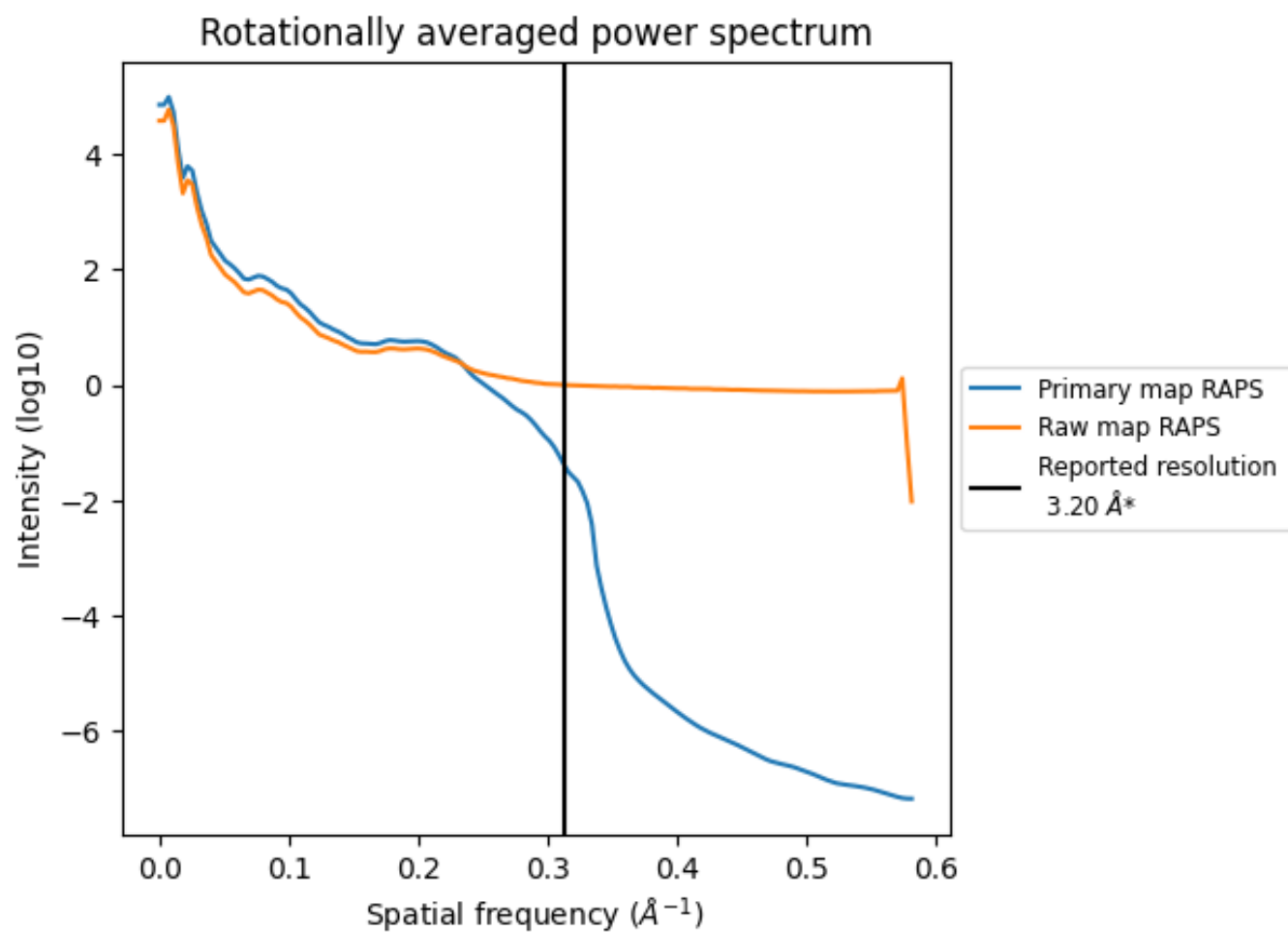
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 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 ⓘ

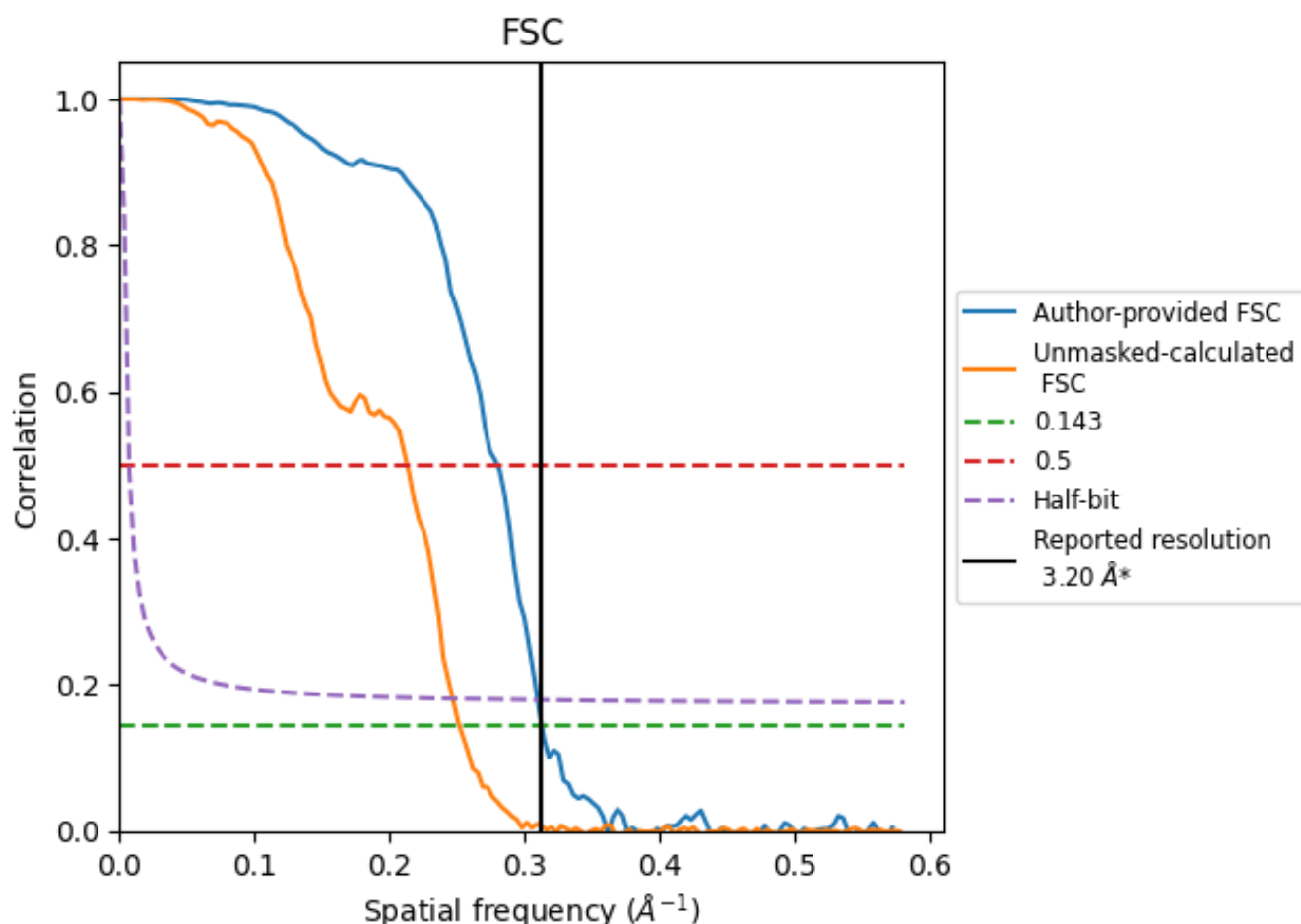


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

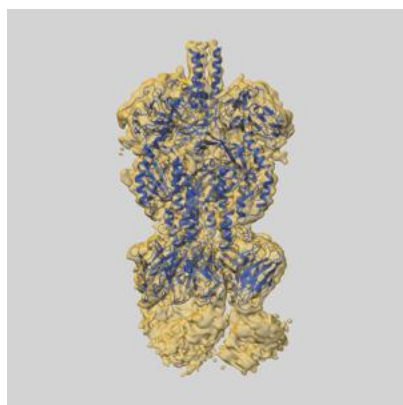
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.58	3.23
Unmasked-calculated*	3.97	4.69	4.05

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

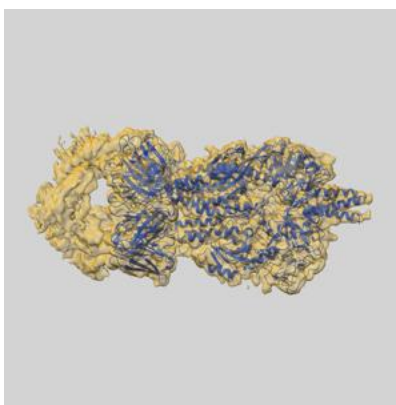
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41506 and PDB model 8TQK. Per-residue inclusion information can be found in section [3](#) on page [10](#).

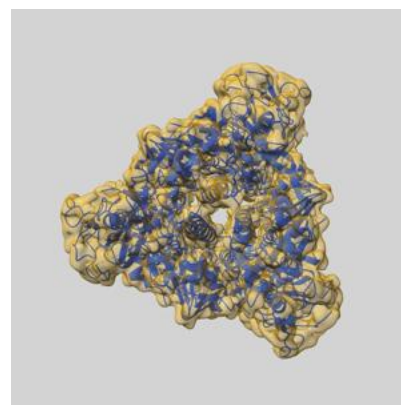
9.1 Map-model overlay [i](#)



X



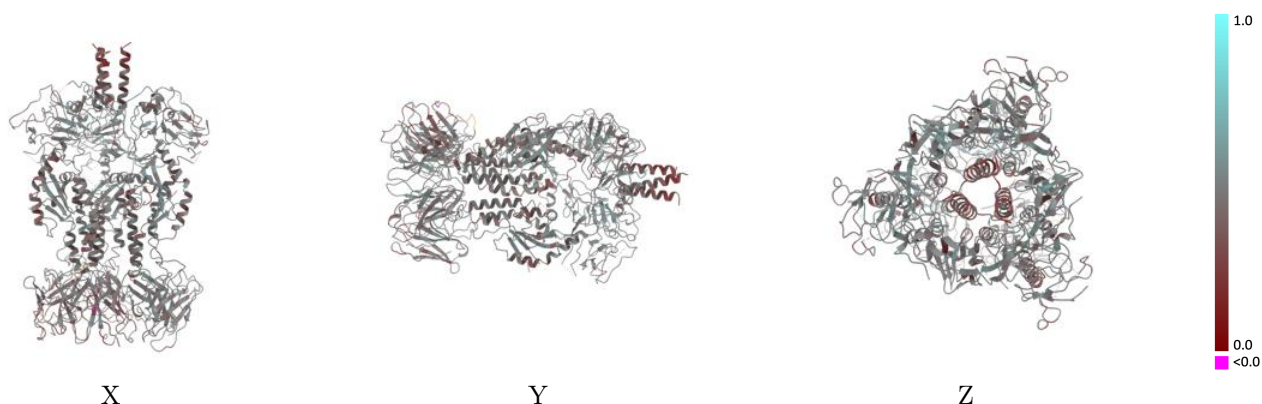
Y



Z

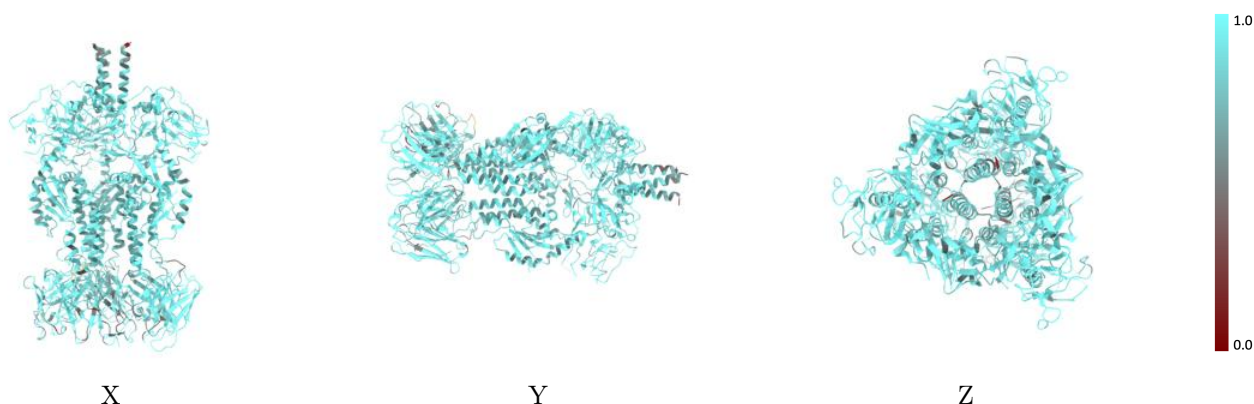
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



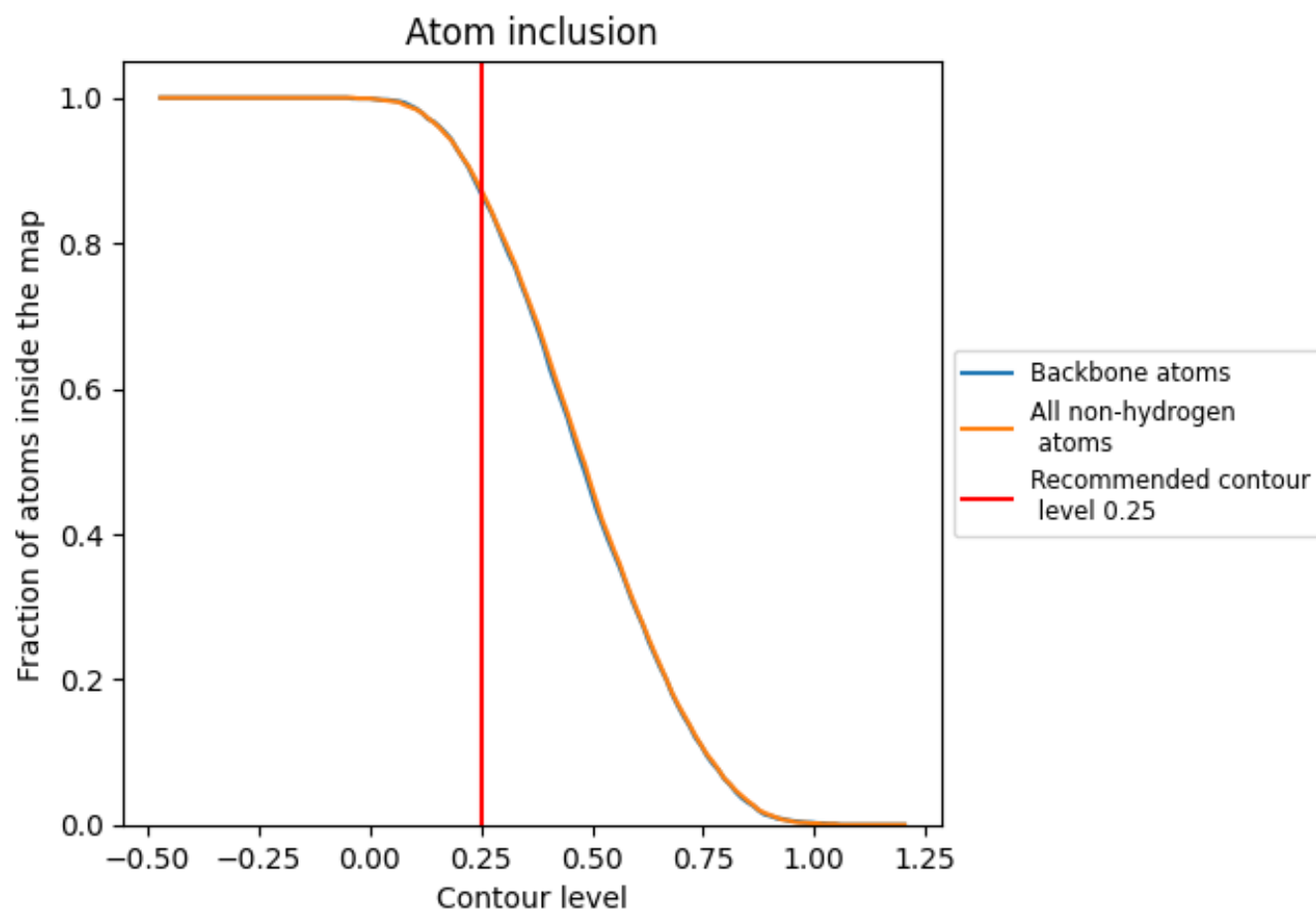
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8740	<div><div></div></div> 0.4510
A	<div><div></div></div> 0.8900	<div><div></div></div> 0.4590
B	<div><div></div></div> 0.8770	<div><div></div></div> 0.4550
C	<div><div></div></div> 0.8870	<div><div></div></div> 0.4590
D	<div><div></div></div> 0.8580	<div><div></div></div> 0.4100
E	<div><div></div></div> 0.7740	<div><div></div></div> 0.3900
F	<div><div></div></div> 0.9030	<div><div></div></div> 0.4530
G	<div><div></div></div> 0.8850	<div><div></div></div> 0.4320
H	<div><div></div></div> 0.9100	<div><div></div></div> 0.4720
L	<div><div></div></div> 0.9100	<div><div></div></div> 0.4650

1.0

0.0

<0.0