



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:47 PM EST

PDB ID : 7SJX
EMDB ID : EMD-25165
Title : Cryo-EM Structure of the PR-RT components of the HIV-1 Pol Polyprotein
Authors : Lyumkis, D.; Passos, D.; Arnold, E.; Harrison, J.J.E.K.; Ruiz, F.X.
Deposited on : 2021-10-19
Resolution : 8.20 Å(reported)
Based on initial models : 1DLO, 2HB4, 3BGR

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

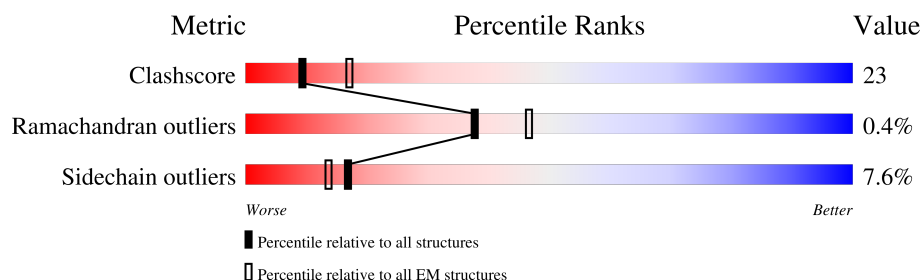
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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	1053	<div> <div>5%</div> <div>39%</div> <div>20%</div> <div>40%</div> </div>
1	B	1053	<div> <div>5%</div> <div>30%</div> <div>15%</div> <div>52%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9215 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	634	Total	C	N	O	S	0	0
			5118	3319	852	935	12		
1	B	503	Total	C	N	O	S	0	0
			4097	2668	678	740	11		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-105	MET	-	initiating methionine	UNP P03366
A	-104	GLY	-	expression tag	UNP P03366
A	-103	SER	-	expression tag	UNP P03366
A	-102	SER	-	expression tag	UNP P03366
A	-101	HIS	-	expression tag	UNP P03366
A	-100	HIS	-	expression tag	UNP P03366
A	-99	HIS	-	expression tag	UNP P03366
A	-98	HIS	-	expression tag	UNP P03366
A	-97	HIS	-	expression tag	UNP P03366
A	-96	HIS	-	expression tag	UNP P03366
A	-95	MET	-	expression tag	UNP P03366
A	-94	ALA	-	expression tag	UNP P03366
A	-93	THR	-	expression tag	UNP P03366
A	-92	VAL	-	expression tag	UNP P03366
A	-91	LYS	-	expression tag	UNP P03366
A	-90	PHE	-	expression tag	UNP P03366
A	-89	LYS	-	expression tag	UNP P03366
A	-88	TYR	-	expression tag	UNP P03366
A	-87	LYS	-	expression tag	UNP P03366
A	-86	GLY	-	expression tag	UNP P03366
A	-85	GLU	-	expression tag	UNP P03366
A	-84	GLU	-	expression tag	UNP P03366
A	-83	LYS	-	expression tag	UNP P03366
A	-82	GLU	-	expression tag	UNP P03366
A	-81	VAL	-	expression tag	UNP P03366
A	-80	ASP	-	expression tag	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-79	ILE	-	expression tag	UNP P03366
A	-78	SER	-	expression tag	UNP P03366
A	-77	LYS	-	expression tag	UNP P03366
A	-76	ILE	-	expression tag	UNP P03366
A	-75	LYS	-	expression tag	UNP P03366
A	-74	LYS	-	expression tag	UNP P03366
A	-73	VAL	-	expression tag	UNP P03366
A	-72	TRP	-	expression tag	UNP P03366
A	-71	ARG	-	expression tag	UNP P03366
A	-70	VAL	-	expression tag	UNP P03366
A	-69	GLY	-	expression tag	UNP P03366
A	-68	LYS	-	expression tag	UNP P03366
A	-67	MET	-	expression tag	UNP P03366
A	-66	ILE	-	expression tag	UNP P03366
A	-65	SER	-	expression tag	UNP P03366
A	-64	PHE	-	expression tag	UNP P03366
A	-63	THR	-	expression tag	UNP P03366
A	-62	TYR	-	expression tag	UNP P03366
A	-61	ASP	-	expression tag	UNP P03366
A	-60	GLU	-	expression tag	UNP P03366
A	-59	GLY	-	expression tag	UNP P03366
A	-58	GLY	-	expression tag	UNP P03366
A	-57	GLY	-	expression tag	UNP P03366
A	-56	LYS	-	expression tag	UNP P03366
A	-55	THR	-	expression tag	UNP P03366
A	-54	GLY	-	expression tag	UNP P03366
A	-53	ARG	-	expression tag	UNP P03366
A	-52	GLY	-	expression tag	UNP P03366
A	-51	ALA	-	expression tag	UNP P03366
A	-50	VAL	-	expression tag	UNP P03366
A	-49	SER	-	expression tag	UNP P03366
A	-48	GLU	-	expression tag	UNP P03366
A	-47	LYS	-	expression tag	UNP P03366
A	-46	ASP	-	expression tag	UNP P03366
A	-45	ALA	-	expression tag	UNP P03366
A	-44	PRO	-	expression tag	UNP P03366
A	-43	LYS	-	expression tag	UNP P03366
A	-42	GLU	-	expression tag	UNP P03366
A	-41	LEU	-	expression tag	UNP P03366
A	-40	LEU	-	expression tag	UNP P03366
A	-39	GLN	-	expression tag	UNP P03366
A	-38	MET	-	expression tag	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-37	LEU	-	expression tag	UNP P03366
A	-36	GLU	-	expression tag	UNP P03366
A	-35	LYS	-	expression tag	UNP P03366
A	-34	GLN	-	expression tag	UNP P03366
A	-33	LYS	-	expression tag	UNP P03366
A	-32	LYS	-	expression tag	UNP P03366
A	-31	ALA	-	expression tag	UNP P03366
A	-30	LEU	-	expression tag	UNP P03366
A	-29	GLU	-	expression tag	UNP P03366
A	-28	VAL	-	expression tag	UNP P03366
A	-27	LEU	-	expression tag	UNP P03366
A	-26	PHE	-	expression tag	UNP P03366
A	-25	GLN	-	expression tag	UNP P03366
A	-24	GLY	-	expression tag	UNP P03366
A	-23	PRO	-	expression tag	UNP P03366
A	-22	MET	-	expression tag	UNP P03366
A	25	ALA	ASP	engineered mutation	UNP P03366
A	641	ASP	LEU	engineered mutation	UNP P03366
A	642	ASP	PHE	engineered mutation	UNP P03366
B	-105	MET	-	initiating methionine	UNP P03366
B	-104	GLY	-	expression tag	UNP P03366
B	-103	SER	-	expression tag	UNP P03366
B	-102	SER	-	expression tag	UNP P03366
B	-101	HIS	-	expression tag	UNP P03366
B	-100	HIS	-	expression tag	UNP P03366
B	-99	HIS	-	expression tag	UNP P03366
B	-98	HIS	-	expression tag	UNP P03366
B	-97	HIS	-	expression tag	UNP P03366
B	-96	HIS	-	expression tag	UNP P03366
B	-95	MET	-	expression tag	UNP P03366
B	-94	ALA	-	expression tag	UNP P03366
B	-93	THR	-	expression tag	UNP P03366
B	-92	VAL	-	expression tag	UNP P03366
B	-91	LYS	-	expression tag	UNP P03366
B	-90	PHE	-	expression tag	UNP P03366
B	-89	LYS	-	expression tag	UNP P03366
B	-88	TYR	-	expression tag	UNP P03366
B	-87	LYS	-	expression tag	UNP P03366
B	-86	GLY	-	expression tag	UNP P03366
B	-85	GLU	-	expression tag	UNP P03366
B	-84	GLU	-	expression tag	UNP P03366
B	-83	LYS	-	expression tag	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-82	GLU	-	expression tag	UNP P03366
B	-81	VAL	-	expression tag	UNP P03366
B	-80	ASP	-	expression tag	UNP P03366
B	-79	ILE	-	expression tag	UNP P03366
B	-78	SER	-	expression tag	UNP P03366
B	-77	LYS	-	expression tag	UNP P03366
B	-76	ILE	-	expression tag	UNP P03366
B	-75	LYS	-	expression tag	UNP P03366
B	-74	LYS	-	expression tag	UNP P03366
B	-73	VAL	-	expression tag	UNP P03366
B	-72	TRP	-	expression tag	UNP P03366
B	-71	ARG	-	expression tag	UNP P03366
B	-70	VAL	-	expression tag	UNP P03366
B	-69	GLY	-	expression tag	UNP P03366
B	-68	LYS	-	expression tag	UNP P03366
B	-67	MET	-	expression tag	UNP P03366
B	-66	ILE	-	expression tag	UNP P03366
B	-65	SER	-	expression tag	UNP P03366
B	-64	PHE	-	expression tag	UNP P03366
B	-63	THR	-	expression tag	UNP P03366
B	-62	TYR	-	expression tag	UNP P03366
B	-61	ASP	-	expression tag	UNP P03366
B	-60	GLU	-	expression tag	UNP P03366
B	-59	GLY	-	expression tag	UNP P03366
B	-58	GLY	-	expression tag	UNP P03366
B	-57	GLY	-	expression tag	UNP P03366
B	-56	LYS	-	expression tag	UNP P03366
B	-55	THR	-	expression tag	UNP P03366
B	-54	GLY	-	expression tag	UNP P03366
B	-53	ARG	-	expression tag	UNP P03366
B	-52	GLY	-	expression tag	UNP P03366
B	-51	ALA	-	expression tag	UNP P03366
B	-50	VAL	-	expression tag	UNP P03366
B	-49	SER	-	expression tag	UNP P03366
B	-48	GLU	-	expression tag	UNP P03366
B	-47	LYS	-	expression tag	UNP P03366
B	-46	ASP	-	expression tag	UNP P03366
B	-45	ALA	-	expression tag	UNP P03366
B	-44	PRO	-	expression tag	UNP P03366
B	-43	LYS	-	expression tag	UNP P03366
B	-42	GLU	-	expression tag	UNP P03366
B	-41	LEU	-	expression tag	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-40	LEU	-	expression tag	UNP P03366
B	-39	GLN	-	expression tag	UNP P03366
B	-38	MET	-	expression tag	UNP P03366
B	-37	LEU	-	expression tag	UNP P03366
B	-36	GLU	-	expression tag	UNP P03366
B	-35	LYS	-	expression tag	UNP P03366
B	-34	GLN	-	expression tag	UNP P03366
B	-33	LYS	-	expression tag	UNP P03366
B	-32	LYS	-	expression tag	UNP P03366
B	-31	ALA	-	expression tag	UNP P03366
B	-30	LEU	-	expression tag	UNP P03366
B	-29	GLU	-	expression tag	UNP P03366
B	-28	VAL	-	expression tag	UNP P03366
B	-27	LEU	-	expression tag	UNP P03366
B	-26	PHE	-	expression tag	UNP P03366
B	-25	GLN	-	expression tag	UNP P03366
B	-24	GLY	-	expression tag	UNP P03366
B	-23	PRO	-	expression tag	UNP P03366
B	-22	MET	-	expression tag	UNP P03366
B	25	ALA	ASP	engineered mutation	UNP P03366
B	635	ASP	LEU	engineered mutation	UNP P03366
B	636	ASP	PHE	engineered mutation	UNP P03366

LEU GLN LYS LYS ILE THR LYS ILE GLN ASN PHE ARG VAL TYR TYR ARG ASP SER ARG ASN PRO LEU TRP LYS GLY PRO ALA LYS LEU LEU TRP LYS GLY GLU GLY ALA VAL VAL VAL ILE GLN ASP ASN SER ASP ILE LYS VAL VAL PRO ARG ARG LYS ALA LYS ILE ILE ARG ASP TYR GLY

LYS GLN MET ALA GLY ASP ASP CYS VAL ALA SER ARG GLN ASP GLU ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27555	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.185	Depositor
Minimum map value	-1.445	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.289	Depositor
Recommended contour level	0.85	Depositor
Map size (\AA)	259.84, 259.84, 259.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.015, 1.015, 1.015	Depositor

5 Model quality

5.1 Standard geometry

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	0.41	0/5244	0.52	0/7119
1	B	0.44	0/4206	0.53	0/5715
All	All	0.42	0/9450	0.52	0/12834

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5118	0	5221	280	0
1	B	4097	0	4176	249	0
All	All	9215	0	9397	420	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 23.

All (420) 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:94:GLY:HA3	1:B:100:PRO:CG	1.38	1.48
1:A:102:SER:HB3	1:A:103:PRO:CD	1.48	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:CYS:SG	1:B:99:PHE:CE1	2.34	1.20
1:A:94:GLY:HA3	1:B:100:PRO:HG2	1.19	1.18
1:A:102:SER:HB3	1:A:103:PRO:HD3	1.23	1.14
1:A:42:TRP:CD1	1:A:57:ARG:HB3	1.86	1.09
1:A:102:SER:CB	1:A:103:PRO:HD3	1.83	1.08
1:A:26:THR:HG22	1:B:26:THR:N	1.69	1.07
1:A:99:PHE:HB2	1:A:100:PRO:HD2	1.35	1.06
1:A:26:THR:HG22	1:B:26:THR:H	0.92	1.06
1:A:94:GLY:CA	1:B:100:PRO:CG	2.34	1.06
1:A:50:ILE:HG22	1:B:49:GLY:CA	1.86	1.04
1:A:63:LEU:HD11	1:A:70:LYS:HE2	1.37	1.04
1:A:95:CYS:SG	1:B:99:PHE:CD1	2.50	1.03
1:B:15:ILE:HD13	1:B:33:LEU:CD1	1.88	1.03
1:A:100:PRO:HB3	1:B:93:ILE:HA	1.40	1.02
1:A:99:PHE:CB	1:A:100:PRO:HD2	1.90	1.02
1:A:32:VAL:HB	1:A:84:ILE:HD11	1.42	1.01
1:A:102:SER:CB	1:A:103:PRO:CD	2.34	0.99
1:A:94:GLY:HA3	1:B:100:PRO:HG3	1.39	0.98
1:A:42:TRP:CD1	1:A:57:ARG:CB	2.46	0.98
1:A:50:ILE:HG22	1:B:49:GLY:HA3	1.45	0.98
1:B:106:THR:HG21	1:B:220:ASP:N	1.78	0.97
1:A:100:PRO:HB3	1:B:93:ILE:CA	1.94	0.97
1:A:94:GLY:HA3	1:B:100:PRO:CD	1.94	0.97
1:A:32:VAL:HB	1:A:84:ILE:CD1	1.96	0.94
1:A:32:VAL:HB	1:A:84:ILE:CG1	1.97	0.94
1:A:102:SER:HB3	1:A:103:PRO:HD2	1.45	0.94
1:A:49:GLY:HA3	1:B:50:ILE:H	1.32	0.93
1:A:26:THR:CG2	1:B:26:THR:H	1.83	0.92
1:A:63:LEU:HD11	1:A:70:LYS:CE	2.01	0.90
1:A:52:GLY:C	1:B:51:GLY:HA3	1.92	0.90
1:A:42:TRP:CG	1:A:57:ARG:HB3	2.06	0.89
1:A:98:ASN:O	1:B:95:CYS:HA	1.71	0.89
1:A:100:PRO:HD3	1:B:93:ILE:HB	1.53	0.89
1:A:42:TRP:CD1	1:A:57:ARG:HA	2.06	0.89
1:A:42:TRP:NE1	1:A:57:ARG:HG2	1.88	0.89
1:A:49:GLY:HA3	1:B:50:ILE:N	1.88	0.89
1:B:15:ILE:HD13	1:B:33:LEU:HD12	1.55	0.89
1:A:33:LEU:HD12	1:A:75:VAL:HG11	1.54	0.88
1:B:90:LEU:HD23	1:B:93:ILE:HD11	1.55	0.88
1:A:100:PRO:CD	1:B:93:ILE:HB	2.04	0.87
1:A:50:ILE:HD13	1:B:47:ILE:CD1	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:CD2	1:B:1:PRO:HD2	2.11	0.86
1:A:52:GLY:O	1:B:51:GLY:HA3	1.75	0.86
1:A:98:ASN:HB2	1:B:96:THR:OG1	1.76	0.85
1:A:94:GLY:CA	1:B:100:PRO:CD	2.54	0.85
1:A:94:GLY:CA	1:B:100:PRO:HG2	2.01	0.85
1:A:99:PHE:CB	1:A:100:PRO:CD	2.54	0.84
1:A:54:ILE:HG12	1:B:50:ILE:O	1.78	0.84
1:A:50:ILE:H	1:B:49:GLY:HA3	1.44	0.83
1:A:42:TRP:CD1	1:A:57:ARG:CA	2.63	0.82
1:A:50:ILE:CD1	1:B:47:ILE:HD11	2.10	0.82
1:A:99:PHE:CE2	1:B:1:PRO:HD2	2.16	0.81
1:A:99:PHE:HB2	1:A:100:PRO:CD	2.12	0.80
1:B:15:ILE:CG2	1:B:20:LYS:HE3	2.11	0.79
1:A:626:ASN:OD1	1:A:626:ASN:N	2.16	0.79
1:B:32:VAL:HG12	1:B:80:THR:HG21	1.64	0.79
1:A:47:ILE:HD12	1:B:50:ILE:HG21	1.64	0.78
1:A:32:VAL:CB	1:A:84:ILE:HD11	2.12	0.78
1:A:100:PRO:HB3	1:B:93:ILE:CB	2.16	0.76
1:B:63:LEU:HD23	1:B:72:ILE:HG12	1.69	0.75
1:B:15:ILE:HG22	1:B:20:LYS:CE	2.16	0.75
1:A:267:TYR:HB2	1:A:274:TYR:HB3	1.69	0.74
1:A:50:ILE:HD13	1:B:47:ILE:HD13	1.68	0.74
1:A:42:TRP:CE2	1:A:57:ARG:HD3	2.23	0.74
1:A:50:ILE:HG12	1:B:54:ILE:HG12	1.69	0.74
1:A:48:GLY:HA2	1:A:53:PHE:CD2	2.23	0.73
1:B:224:ARG:HD3	1:B:246:ASN:HA	1.68	0.73
1:A:42:TRP:HD1	1:A:57:ARG:HA	1.51	0.73
1:A:49:GLY:HA3	1:B:50:ILE:CA	2.17	0.73
1:B:11:VAL:HB	1:B:67:CYS:SG	2.28	0.73
1:B:15:ILE:CD1	1:B:33:LEU:CD1	2.65	0.73
1:A:49:GLY:CA	1:B:50:ILE:H	2.02	0.73
1:B:15:ILE:HG21	1:B:20:LYS:HE3	1.69	0.73
1:B:106:THR:HG21	1:B:220:ASP:H	1.52	0.73
1:A:50:ILE:CG2	1:B:49:GLY:HA3	2.18	0.72
1:B:15:ILE:CG2	1:B:20:LYS:CE	2.67	0.72
1:A:507:TRP:HB3	1:A:607:ILE:HD11	1.69	0.72
1:A:99:PHE:CZ	1:B:3:ILE:HG13	2.24	0.72
1:A:50:ILE:CD1	1:B:47:ILE:CD1	2.67	0.72
1:A:47:ILE:HD11	1:A:54:ILE:HD11	1.71	0.72
1:A:47:ILE:HD12	1:B:50:ILE:CG2	2.18	0.72
1:B:90:LEU:HD22	1:B:95:CYS:SG	2.30	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD12	1:A:75:VAL:CG1	2.19	0.71
1:B:15:ILE:HD13	1:B:33:LEU:HD13	1.73	0.71
1:B:15:ILE:CD1	1:B:33:LEU:HD12	2.20	0.70
1:B:102:SER:OG	1:B:103:PRO:HD3	1.90	0.70
1:A:42:TRP:NE1	1:A:57:ARG:CG	2.54	0.70
1:B:90:LEU:HA	1:B:93:ILE:HD11	1.73	0.70
1:A:43:LYS:HG3	1:A:44:PRO:HD2	1.74	0.70
1:A:32:VAL:HB	1:A:84:ILE:HG13	1.74	0.69
1:A:63:LEU:CD1	1:A:70:LYS:HE2	2.19	0.69
1:A:409:GLU:OE2	1:A:411:GLN:NE2	2.26	0.69
1:B:122:GLN:NE2	1:B:230:THR:O	2.26	0.69
1:B:56:VAL:HG12	1:B:78:GLY:HA3	1.74	0.69
1:A:28:ALA:O	1:A:86:GLY:HA2	1.92	0.69
1:A:480:GLU:HA	1:A:483:TRP:HD1	1.57	0.68
1:B:408:GLN:HB2	1:B:499:LYS:HG2	1.76	0.68
1:A:48:GLY:CA	1:A:53:PHE:CD2	2.76	0.68
1:A:48:GLY:HA2	1:A:53:PHE:HD2	1.59	0.68
1:B:64:ILE:HG21	1:B:89:LEU:HD13	1.76	0.67
1:A:489:ALA:HB1	1:B:439:ASP:OD2	1.95	0.67
1:B:106:THR:CG2	1:B:220:ASP:N	2.56	0.67
1:A:100:PRO:CG	1:B:93:ILE:HB	2.25	0.67
1:A:50:ILE:N	1:B:49:GLY:HA3	2.09	0.66
1:B:189:VAL:HG23	1:B:190:GLN:HG2	1.76	0.66
1:A:118:PRO:HG3	1:A:177:LEU:HD23	1.77	0.66
1:A:95:CYS:HA	1:B:98:ASN:O	1.94	0.66
1:A:50:ILE:CG2	1:B:49:GLY:CA	2.68	0.66
1:A:11:VAL:HB	1:A:67:CYS:HB2	1.77	0.66
1:A:99:PHE:HZ	1:B:3:ILE:CG1	2.10	0.65
1:A:170:LYS:O	1:A:237:GLN:NE2	2.30	0.65
1:A:26:THR:CG2	1:B:25:ALA:HA	2.27	0.64
1:A:33:LEU:CD1	1:A:75:VAL:HG11	2.25	0.64
1:B:107:VAL:CG2	1:B:258:ILE:HD12	2.28	0.64
1:A:51:GLY:HA2	1:B:54:ILE:HG23	1.79	0.64
1:A:42:TRP:CE2	1:A:57:ARG:CD	2.81	0.64
1:A:99:PHE:HB3	1:A:100:PRO:HD2	1.78	0.64
1:B:15:ILE:CG2	1:B:36:MET:SD	2.86	0.63
1:A:26:THR:H	1:B:26:THR:HB	1.63	0.63
1:B:367:LEU:H	1:B:367:LEU:HD23	1.62	0.63
1:A:570:SER:OG	1:A:609:LYS:NZ	2.30	0.63
1:A:95:CYS:SG	1:B:99:PHE:HE1	2.19	0.62
1:A:100:PRO:CB	1:B:93:ILE:HB	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:O	1:A:39:PRO:HD3	2.00	0.62
1:A:26:THR:CG2	1:B:26:THR:N	2.52	0.62
1:A:99:PHE:CE1	1:B:3:ILE:HG13	2.34	0.62
1:A:32:VAL:H	1:A:84:ILE:HG13	1.64	0.62
1:B:196:PRO:HG3	1:B:280:TYR:HB2	1.81	0.62
1:A:42:TRP:HB3	1:A:59:TYR:CE1	2.35	0.62
1:B:15:ILE:HG21	1:B:36:MET:SD	2.40	0.62
1:B:11:VAL:HG11	1:B:67:CYS:SG	2.40	0.62
1:B:123:TRP:HZ2	1:B:160:PHE:HE2	1.46	0.61
1:A:87:ARG:HA	1:A:90:LEU:HB2	1.81	0.61
1:A:445:ASP:OD1	1:A:445:ASP:N	2.29	0.61
1:A:67:CYS:SG	1:A:67:CYS:O	2.58	0.61
1:B:90:LEU:O	1:B:93:ILE:HG13	2.01	0.61
1:A:48:GLY:CA	1:A:53:PHE:HD2	2.12	0.61
1:B:11:VAL:CB	1:B:67:CYS:SG	2.89	0.61
1:B:133:LEU:HG	1:B:161:ALA:HB2	1.83	0.61
1:B:73:GLY:HA3	1:B:89:LEU:HD21	1.82	0.61
1:A:99:PHE:CZ	1:B:3:ILE:CG1	2.84	0.60
1:A:52:GLY:C	1:B:51:GLY:CA	2.68	0.60
1:B:237:GLU:HG3	1:B:238:THR:H	1.66	0.60
1:A:47:ILE:CD1	1:B:50:ILE:HG21	2.32	0.60
1:B:106:THR:HG21	1:B:219:LEU:C	2.22	0.60
1:A:98:ASN:O	1:B:95:CYS:CA	2.50	0.59
1:A:50:ILE:O	1:B:52:GLY:O	2.20	0.59
1:A:59:TYR:HB3	1:A:62:ILE:HD11	1.85	0.59
1:A:26:THR:O	1:A:87:ARG:CG	2.51	0.59
1:A:363:LEU:HD21	1:A:377:THR:HG23	1.84	0.58
1:A:224:PHE:HB3	1:A:230:TYR:HB2	1.85	0.58
1:B:15:ILE:HG22	1:B:20:LYS:CD	2.34	0.58
1:A:50:ILE:CG2	1:B:47:ILE:HD12	2.33	0.58
1:A:50:ILE:HG12	1:B:47:ILE:HD11	1.85	0.58
1:A:99:PHE:HB3	1:A:100:PRO:CD	2.34	0.58
1:B:437:THR:OG1	1:B:438:ASN:N	2.34	0.58
1:A:235:LEU:HD21	1:A:245:ILE:HG23	1.86	0.57
1:A:520:THR:HA	1:A:575:ASN:HB2	1.86	0.57
1:A:50:ILE:HG22	1:B:49:GLY:HA2	1.80	0.57
1:A:51:GLY:HA3	1:B:52:GLY:C	2.24	0.57
1:A:163:LYS:HA	1:A:167:LYS:HA	1.85	0.57
1:B:54:ILE:HD12	1:B:79:PRO:HD2	1.85	0.57
1:B:432:TYR:OH	1:B:445:GLU:OE1	2.23	0.57
1:A:296:LEU:HA	1:A:300:LEU:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:THR:HG22	1:A:580:SER:H	1.69	0.57
1:A:50:ILE:CG1	1:B:47:ILE:HD11	2.34	0.57
1:B:180:ASN:OD1	1:B:253:LYS:N	2.37	0.57
1:A:164:LYS:HD2	1:A:169:ARG:HG3	1.87	0.56
1:A:205:VAL:HB	1:A:208:ALA:HB2	1.87	0.56
1:A:500:THR:OG1	1:A:502:PRO:O	2.23	0.56
1:A:39:PRO:HB2	1:A:59:TYR:CE1	2.41	0.56
1:A:49:GLY:HA3	1:B:50:ILE:CB	2.36	0.56
1:B:11:VAL:CG1	1:B:67:CYS:SG	2.93	0.56
1:A:42:TRP:CZ2	1:A:57:ARG:NE	2.73	0.56
1:A:576:ILE:HB	1:A:614:LEU:HD23	1.88	0.56
1:B:32:VAL:HG12	1:B:80:THR:CG2	2.36	0.56
1:B:204:SER:HG	1:B:297:HIS:CE1	2.22	0.56
1:A:100:PRO:HA	1:B:93:ILE:O	2.06	0.56
1:B:15:ILE:HG12	1:B:36:MET:SD	2.46	0.55
1:A:99:PHE:CE2	1:B:1:PRO:CD	2.89	0.55
1:B:205:VAL:HG23	1:B:317:LEU:HB3	1.89	0.55
1:A:50:ILE:HD11	1:B:54:ILE:HD11	1.89	0.55
1:A:248:SER:O	1:A:251:THR:OG1	2.22	0.55
1:A:321:THR:HG22	1:A:322:VAL:N	2.22	0.54
1:A:466:LYS:HE3	1:B:127:GLU:OE2	2.06	0.54
1:A:580:SER:HG	1:A:583:ALA:H	1.53	0.54
1:B:106:THR:OG1	1:B:218:PRO:O	2.22	0.54
1:A:15:ILE:HG21	1:A:36:MET:SD	2.47	0.54
1:B:13:ILE:HA	1:B:65:GLU:O	2.07	0.54
1:A:19:LEU:C	1:A:20:LYS:CG	2.76	0.54
1:B:457:ILE:HG23	1:B:458:TRP:CD2	2.43	0.54
1:A:14:LYS:HA	1:A:18:GLN:O	2.07	0.54
1:A:47:ILE:CD1	1:B:50:ILE:CG2	2.84	0.54
1:A:143:GLU:O	1:A:145:LYS:NZ	2.37	0.54
1:B:87:ARG:HA	1:B:90:LEU:HB2	1.89	0.54
1:A:89:LEU:HA	1:A:92:GLN:HG3	1.89	0.54
1:B:453:GLU:O	1:B:457:ILE:HG22	2.08	0.54
1:B:443:LEU:HD12	1:B:473:TRP:HZ3	1.73	0.54
1:A:94:GLY:H	1:B:100:PRO:HD2	1.72	0.54
1:A:100:PRO:HB3	1:B:93:ILE:HB	1.83	0.54
1:B:443:LEU:HD12	1:B:473:TRP:CZ3	2.43	0.54
1:A:257:PHE:HE1	1:A:290:GLU:HG3	1.73	0.53
1:A:98:ASN:O	1:B:96:THR:N	2.41	0.53
1:A:42:TRP:CE2	1:A:57:ARG:CG	2.91	0.53
1:A:285:ARG:O	1:A:288:ILE:HG22	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ILE:HG12	1:B:288:VAL:HG12	1.90	0.53
1:A:162:ILE:HG13	1:A:164:LYS:H	1.72	0.53
1:A:28:ALA:O	1:A:86:GLY:CA	2.56	0.53
1:A:49:GLY:HA3	1:B:50:ILE:HB	1.90	0.53
1:A:100:PRO:HG3	1:B:93:ILE:HG22	1.91	0.53
1:A:292:ARG:NH2	1:A:302:THR:OG1	2.42	0.53
1:A:487:TRP:CD1	1:A:488:GLN:HG3	2.44	0.52
1:B:14:LYS:HA	1:B:18:GLN:O	2.09	0.52
1:A:162:ILE:O	1:A:169:ARG:N	2.32	0.52
1:B:15:ILE:CG2	1:B:20:LYS:HD2	2.39	0.52
1:A:99:PHE:HZ	1:B:3:ILE:HG12	1.73	0.52
1:A:105:GLU:HA	1:A:105:GLU:OE1	2.10	0.52
1:B:187:TRP:HB2	1:B:253:LYS:HD3	1.92	0.52
1:A:100:PRO:HG3	1:B:93:ILE:CG2	2.39	0.52
1:A:115:MET:HB3	1:A:180:ARG:HH11	1.74	0.52
1:B:15:ILE:HG22	1:B:20:LYS:HD2	1.90	0.52
1:A:9:PRO:HD2	1:A:23:LEU:HD11	1.92	0.52
1:A:94:GLY:C	1:B:100:PRO:HD3	2.29	0.52
1:A:42:TRP:HE1	1:A:57:ARG:HG2	1.70	0.51
1:A:183:ASP:HB3	1:B:154:PRO:HB3	1.93	0.51
1:B:306:GLN:O	1:B:310:ARG:HB2	2.10	0.51
1:A:153:ASN:N	1:A:153:ASN:OD1	2.41	0.51
1:B:325:GLN:NE2	1:B:503:GLN:OE1	2.36	0.51
1:A:48:GLY:HA3	1:A:53:PHE:CE2	2.45	0.51
1:A:429:ASN:OD1	1:A:432:THR:OG1	2.29	0.51
1:B:123:TRP:CZ2	1:B:160:PHE:HE2	2.28	0.51
1:A:99:PHE:HD2	1:B:1:PRO:HD2	1.72	0.51
1:B:123:TRP:HE1	1:B:160:PHE:HD2	1.58	0.51
1:A:42:TRP:NE1	1:A:57:ARG:CB	2.73	0.51
1:A:191:PRO:HG3	1:A:313:TYR:CG	2.46	0.51
1:A:32:VAL:CG2	1:A:84:ILE:HD11	2.41	0.51
1:A:313:TYR:OH	1:A:350:GLN:OE1	2.28	0.51
1:A:99:PHE:HA	1:B:95:CYS:SG	2.52	0.50
1:A:102:SER:OG	1:A:103:PRO:HD3	2.07	0.50
1:A:277:SER:OG	1:A:284:HIS:ND1	2.36	0.50
1:B:161:ALA:HA	1:B:172:LYS:HA	1.93	0.50
1:B:15:ILE:HG23	1:B:36:MET:SD	2.51	0.50
1:A:42:TRP:CD2	1:A:57:ARG:HD3	2.46	0.50
1:B:102:SER:OG	1:B:103:PRO:CD	2.58	0.50
1:A:327:LEU:HD22	1:A:341:LEU:HD22	1.93	0.50
1:B:397:TYR:HD1	1:B:398:ASP:N	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:O	1:B:86:GLY:HA3	2.11	0.50
1:A:94:GLY:CA	1:B:100:PRO:HD2	2.39	0.50
1:B:297:HIS:O	1:B:301:ILE:HG12	2.12	0.49
1:B:107:VAL:HG23	1:B:258:ILE:HD12	1.94	0.49
1:B:93:ILE:HD12	1:B:95:CYS:SG	2.52	0.49
1:A:3:ILE:HD11	1:B:99:PHE:HE2	1.78	0.49
1:A:570:SER:HB2	1:A:574:VAL:HG11	1.94	0.49
1:A:43:LYS:CG	1:A:44:PRO:HD2	2.41	0.49
1:A:49:GLY:CA	1:B:50:ILE:HB	2.42	0.49
1:B:90:LEU:O	1:B:93:ILE:CG1	2.61	0.49
1:B:90:LEU:HA	1:B:93:ILE:CD1	2.43	0.48
1:A:50:ILE:CG1	1:B:47:ILE:CD1	2.91	0.48
1:A:97:LEU:O	1:A:99:PHE:CE1	2.66	0.48
1:A:360:LEU:HG	1:A:384:LEU:HD11	1.95	0.48
1:B:10:LEU:HA	1:B:23:LEU:HA	1.96	0.48
1:A:5:LEU:HD12	1:B:90:LEU:HB3	1.96	0.48
1:A:32:VAL:N	1:A:84:ILE:HG13	2.27	0.48
1:B:164:LYS:HG3	1:B:165:LYS:HG3	1.95	0.48
1:B:248:LEU:HD22	1:B:252:TRP:HZ3	1.79	0.48
1:A:50:ILE:HG21	1:B:47:ILE:HD12	1.95	0.48
1:B:120:VAL:HG13	1:B:158:PRO:HD3	1.96	0.48
1:A:33:LEU:CD1	1:A:75:VAL:CG1	2.89	0.48
1:A:5:LEU:O	1:B:87:ARG:NH1	2.46	0.48
1:A:9:PRO:HD2	1:A:23:LEU:CD1	2.44	0.48
1:A:94:GLY:N	1:B:100:PRO:HD2	2.29	0.48
1:B:263:MET:O	1:B:266:ILE:N	2.46	0.48
1:A:94:GLY:C	1:B:100:PRO:CD	2.82	0.48
1:A:441:ALA:O	1:A:594:SER:HA	2.13	0.48
1:B:496:PRO:HB2	1:B:498:VAL:HG23	1.96	0.48
1:A:26:THR:O	1:A:87:ARG:HG3	2.14	0.48
1:A:266:ILE:HD13	1:A:275:VAL:HG22	1.95	0.47
1:A:444:ASN:ND2	1:A:590:GLN:O	2.46	0.47
1:A:192:ALA:HB1	1:A:430:LEU:HD12	1.95	0.47
1:A:449:LEU:HD11	1:A:472:LEU:HG	1.95	0.47
1:B:296:GLN:HA	1:B:299:THR:OG1	2.15	0.47
1:B:205:VAL:HG22	1:B:319:PRO:HD3	1.96	0.47
1:B:97:LEU:HB3	1:B:99:PHE:CE1	2.49	0.47
1:B:115:MET:HB3	1:B:182:ARG:HD2	1.96	0.47
1:A:554:THR:O	1:A:558:THR:N	2.42	0.47
1:B:70:LYS:HE2	1:B:72:ILE:HD11	1.97	0.47
1:A:538:TYR:CE1	1:A:546:LYS:HG2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HD21	1:A:612:VAL:HG11	1.96	0.47
1:A:42:TRP:CE2	1:A:57:ARG:HG2	2.46	0.47
1:A:42:TRP:CZ2	1:A:57:ARG:CD	2.98	0.46
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.76	0.46
1:B:300:LYS:HA	1:B:300:LYS:HD3	1.69	0.46
1:A:50:ILE:HG12	1:B:47:ILE:CD1	2.44	0.46
1:A:26:THR:HG22	1:B:25:ALA:HA	1.98	0.46
1:B:9:PRO:HD2	1:B:23:LEU:HD11	1.96	0.46
1:B:90:LEU:CD2	1:B:95:CYS:SG	3.03	0.46
1:B:93:ILE:CD1	1:B:95:CYS:SG	3.03	0.46
1:B:471:GLU:O	1:B:474:GLU:HG2	2.16	0.46
1:B:219:LEU:HD12	1:B:220:ASP:H	1.80	0.46
1:A:49:GLY:HA3	1:B:50:ILE:C	2.35	0.46
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.62	0.45
1:B:133:LEU:HD13	1:B:231:ILE:HG22	1.98	0.45
1:B:64:ILE:CG2	1:B:71:ALA:HB3	2.46	0.45
1:B:107:VAL:HG21	1:B:258:ILE:HD12	1.97	0.45
1:A:50:ILE:HG21	1:B:47:ILE:CD1	2.47	0.45
1:A:590:GLN:N	1:A:591:PRO:HD3	2.31	0.45
1:A:554:THR:HB	1:A:557:LYS:HB2	1.99	0.45
1:B:82:VAL:HG13	1:B:84:ILE:HD11	1.98	0.45
1:A:215:ASP:HB3	1:A:217:ASP:OD1	2.16	0.45
1:B:8:ARG:HB3	1:B:23:LEU:HD13	1.99	0.45
1:A:26:THR:HB	1:B:26:THR:OG1	2.15	0.45
1:A:412:LYS:HD2	1:A:504:VAL:HG22	1.99	0.45
1:B:15:ILE:HG23	1:B:15:ILE:O	2.17	0.45
1:B:64:ILE:HG23	1:B:71:ALA:HB3	1.98	0.45
1:A:5:LEU:HB2	1:B:91:THR:HG23	1.99	0.45
1:B:217:VAL:O	1:B:248:LEU:HG	2.17	0.45
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.78	0.45
1:A:26:THR:O	1:A:87:ARG:HD3	2.16	0.44
1:A:49:GLY:HA3	1:B:51:GLY:N	2.32	0.44
1:B:122:GLN:HE22	1:B:159:VAL:HG12	1.82	0.44
1:A:19:LEU:O	1:A:20:LYS:HG2	2.16	0.44
1:B:441:LYS:HE2	1:B:480:TYR:CZ	2.53	0.44
1:A:42:TRP:HB3	1:A:59:TYR:CZ	2.52	0.44
1:A:328:PRO:HG2	1:A:341:LEU:HD11	2.00	0.44
1:B:162:ILE:HD13	1:B:173:LEU:HD11	2.00	0.44
1:A:493:PRO:O	1:A:495:TRP:HD1	2.00	0.44
1:A:280:GLU:O	1:A:284:HIS:N	2.46	0.44
1:B:149:ILE:HD12	1:B:153:ASN:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:O	1:B:482:GLN:HG2	2.17	0.44
1:B:403:LEU:HD23	1:B:462:PRO:HB3	2.00	0.44
1:B:347:LEU:O	1:B:350:ALA:N	2.49	0.44
1:A:5:LEU:HB2	1:B:91:THR:CG2	2.48	0.43
1:A:161:ALA:HB1	1:A:168:TRP:HB3	1.99	0.43
1:B:85:ILE:HG22	1:B:90:LEU:HG	1.99	0.43
1:A:194:LEU:HD11	1:A:310:TRP:CZ3	2.52	0.43
1:A:274:TYR:HB2	1:A:310:TRP:NE1	2.33	0.43
1:A:487:TRP:O	1:B:409:LYS:HE3	2.17	0.43
1:A:26:THR:O	1:A:87:ARG:CD	2.66	0.43
1:A:42:TRP:CZ2	1:A:57:ARG:HD3	2.53	0.43
1:A:24:LEU:HD13	1:B:97:LEU:HD13	2.00	0.43
1:A:190:HIS:ND1	1:A:191:PRO:HD2	2.33	0.43
1:A:306:PRO:HB2	1:A:307:PRO:HD3	2.00	0.43
1:A:511:GLU:HG3	1:A:513:GLU:H	1.83	0.43
1:B:182:ARG:HA	1:B:182:ARG:HD3	1.81	0.43
1:A:350:GLN:HE21	1:A:350:GLN:HB3	1.57	0.43
1:B:177:ARG:HG3	1:B:486:ILE:HD13	2.01	0.43
1:B:234:ILE:O	1:B:237:GLU:HG2	2.19	0.43
1:A:540:THR:OG1	1:A:544:ARG:N	2.52	0.43
1:B:15:ILE:CG2	1:B:20:LYS:CD	2.96	0.43
1:B:254:GLY:O	1:B:258:ILE:HG12	2.18	0.43
1:A:24:LEU:HA	1:A:85:ILE:HB	2.02	0.42
1:A:32:VAL:CB	1:A:84:ILE:HG13	2.46	0.42
1:A:73:GLY:HA3	1:A:89:LEU:HD21	2.01	0.42
1:A:154:PRO:HD2	1:A:155:TYR:CE2	2.54	0.42
1:B:73:GLY:HA3	1:B:89:LEU:CD2	2.49	0.42
1:B:99:PHE:HA	1:B:100:PRO:HD3	1.74	0.42
1:B:448:GLN:O	1:B:451:THR:HG22	2.19	0.42
1:A:115:MET:SD	1:A:180:ARG:NH1	2.92	0.42
1:B:34:GLU:HB2	1:B:83:ASN:OD1	2.19	0.42
1:A:334:THR:O	1:A:338:ILE:HG13	2.19	0.42
1:A:91:THR:HG22	1:B:5:LEU:HB2	2.02	0.42
1:B:361:GLN:OE1	1:B:361:GLN:N	2.50	0.42
1:A:11:VAL:HG11	1:A:24:LEU:HD11	2.01	0.42
1:A:127:GLU:HA	1:A:130:ILE:HB	2.00	0.42
1:A:137:CYS:SG	1:A:138:THR:N	2.92	0.42
1:B:361:GLN:O	1:B:364:LYS:HB2	2.19	0.42
1:B:486:ILE:HA	1:B:487:PRO:HD3	1.90	0.42
1:A:1:PRO:HD2	1:B:99:PHE:HD2	1.85	0.42
1:A:387:ASN:O	1:A:391:LEU:HG	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HG22	1:B:20:LYS:HE2	2.00	0.42
1:B:82:VAL:HG22	1:B:83:ASN:O	2.20	0.42
1:A:94:GLY:CA	1:B:100:PRO:HG3	2.26	0.42
1:A:491:TRP:HZ3	1:B:476:TRP:NE1	2.18	0.42
1:A:53:PHE:O	1:A:54:ILE:HG23	2.20	0.41
1:A:321:THR:CG2	1:A:322:VAL:N	2.82	0.41
1:A:575:ASN:ND2	1:A:613:TYR:HB3	2.34	0.41
1:B:24:LEU:HA	1:B:85:ILE:HB	2.02	0.41
1:A:100:PRO:HD3	1:B:93:ILE:CB	2.38	0.41
1:B:60:ASP:HA	1:B:74:THR:HA	2.02	0.41
1:B:364:LYS:HB2	1:B:364:LYS:HE3	1.85	0.41
1:A:146:ILE:HG13	1:A:232:TYR:HA	2.02	0.41
1:A:420:TYR:CZ	1:A:435:TYR:HB2	2.55	0.41
1:A:514:PRO:HD3	1:A:613:TYR:CZ	2.55	0.41
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.85	0.41
1:A:425:GLU:HB3	1:A:426:PRO:HD2	2.03	0.41
1:B:360:ARG:HA	1:B:360:ARG:HD2	1.89	0.41
1:A:4:THR:HB	1:A:6:TRP:CD1	2.56	0.41
1:A:50:ILE:CG2	1:B:49:GLY:N	2.83	0.41
1:A:191:PRO:HD3	1:A:313:TYR:CZ	2.54	0.41
1:A:355:ILE:HG23	1:A:387:ASN:HD21	1.86	0.41
1:B:47:ILE:HD11	1:B:54:ILE:HD11	2.02	0.41
1:B:186:PHE:O	1:B:189:VAL:HG22	2.20	0.41
1:B:318:HIS:O	1:B:322:TRP:HE3	2.04	0.41
1:B:397:TYR:HE2	1:B:458:TRP:HB3	1.84	0.41
1:B:193:ILE:HA	1:B:194:PRO:HA	1.79	0.41
1:B:249:PRO:HD2	1:B:252:TRP:HE3	1.86	0.41
1:A:3:ILE:HD11	1:B:99:PHE:CE2	2.56	0.41
1:A:47:ILE:HD12	1:B:50:ILE:HG22	1.98	0.41
1:A:50:ILE:HG12	1:B:54:ILE:CG1	2.44	0.41
1:A:97:LEU:HA	1:B:96:THR:O	2.21	0.41
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.90	0.41
1:A:104:ILE:H	1:A:104:ILE:HG12	1.71	0.41
1:A:437:ARG:HD2	1:A:440:GLY:HA2	2.02	0.41
1:A:486:TYR:HE2	1:A:488:GLN:HB2	1.87	0.41
1:B:64:ILE:HG22	1:B:71:ALA:O	2.21	0.41
1:A:48:GLY:HA3	1:A:53:PHE:CD2	2.53	0.40
1:A:191:PRO:HB2	1:A:320:TRP:CD2	2.56	0.40
1:A:321:THR:HG22	1:A:322:VAL:H	1.86	0.40
1:B:36:MET:HB2	1:B:36:MET:HE2	1.82	0.40
1:B:270:PHE:CE2	1:B:304:LEU:HD23	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:HG13	1:B:501:TRP:CH2	2.56	0.40
1:A:160:PHE:HE2	1:A:173:ASP:HB2	1.87	0.40
1:A:47:ILE:HG12	1:A:56:VAL:HG11	2.03	0.40
1:A:146:ILE:HG23	1:A:230:TYR:HB3	2.03	0.40
1:A:205:VAL:HG22	1:A:271:ASP:O	2.21	0.40
1:B:231:ILE:HD11	1:B:243:TYR:HE2	1.86	0.40
1:A:257:PHE:CE2	1:A:291:LEU:HD13	2.57	0.40
1:B:102:SER:H	1:B:103:PRO:HD2	1.85	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	624/1053 (59%)	586 (94%)	35 (6%)	3 (0%)	29	69
1	B	495/1053 (47%)	473 (96%)	21 (4%)	1 (0%)	47	81
All	All	1119/2106 (53%)	1059 (95%)	56 (5%)	4 (0%)	38	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	SER
1	A	103	PRO
1	A	28	ALA
1	B	100	PRO

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	560/909 (62%)	521 (93%)	39 (7%)	15	40
1	B	452/909 (50%)	414 (92%)	38 (8%)	11	33
All	All	1012/1818 (56%)	935 (92%)	77 (8%)	17	37

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	20	LYS
1	A	36	MET
1	A	41	ARG
1	A	55	LYS
1	A	64	ILE
1	A	93	ILE
1	A	99	PHE
1	A	101	ILE
1	A	102	SER
1	A	104	ILE
1	A	106	THR
1	A	116	ASP
1	A	119	LYS
1	A	128	GLU
1	A	137	CYS
1	A	153	ASN
1	A	185	TRP
1	A	209	TYR
1	A	231	GLN
1	A	311	MET
1	A	326	VAL
1	A	329	GLU
1	A	350	GLN
1	A	430	LEU
1	A	454	GLN
1	A	455	LYS
1	A	483	TRP
1	A	497	PHE
1	A	500	THR
1	A	503	LEU
1	A	505	LYS
1	A	509	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	515	ILE
1	A	535	LYS
1	A	620	HIS
1	A	623	ILE
1	A	626	ASN
1	A	632	LEU
1	B	15	ILE
1	B	20	LYS
1	B	31	THR
1	B	34	GLU
1	B	65	GLU
1	B	120	VAL
1	B	128	GLU
1	B	133	LEU
1	B	148	LYS
1	B	155	TYR
1	B	160	PHE
1	B	168	THR
1	B	182	ARG
1	B	191	LEU
1	B	242	ARG
1	B	266	ILE
1	B	270	PHE
1	B	274	ASN
1	B	284	ASP
1	B	288	VAL
1	B	296	GLN
1	B	300	LYS
1	B	308	LEU
1	B	310	ARG
1	B	322	TRP
1	B	335	TRP
1	B	397	TYR
1	B	426	ASN
1	B	437	THR
1	B	439	ASP
1	B	443	LEU
1	B	461	THR
1	B	472	THR
1	B	475	THR
1	B	480	TYR
1	B	486	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	489	TRP
1	B	494	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	122	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

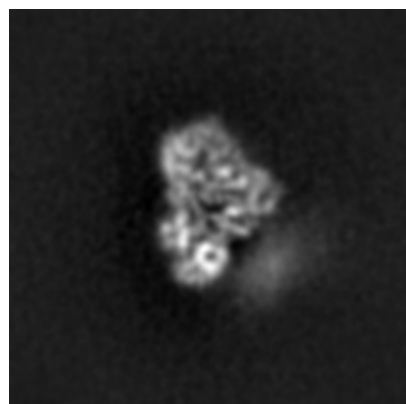
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25165. These allow visual inspection of the internal detail of the map and identification of artifacts.

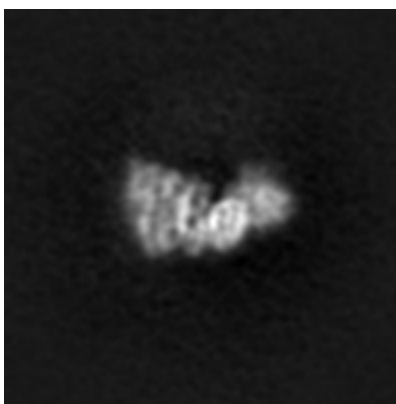
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

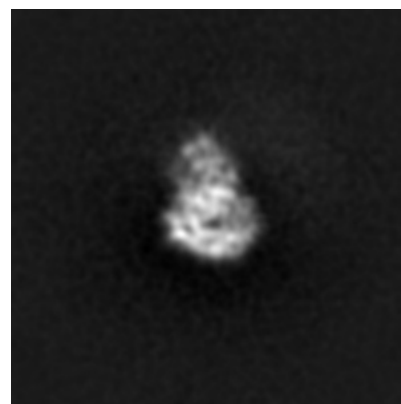
6.1.1 Primary map



X

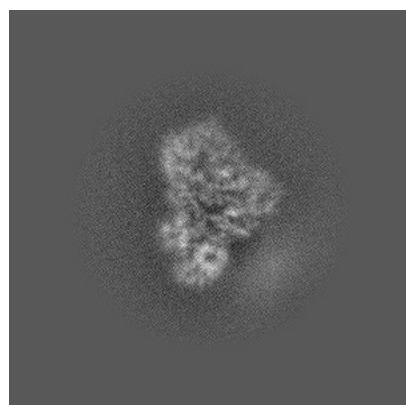


Y

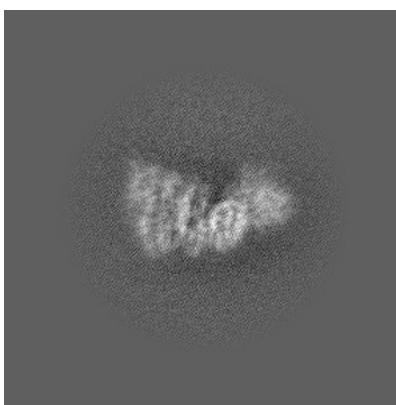


Z

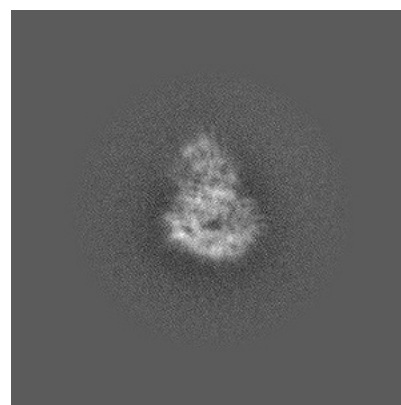
6.1.2 Raw map



X



Y

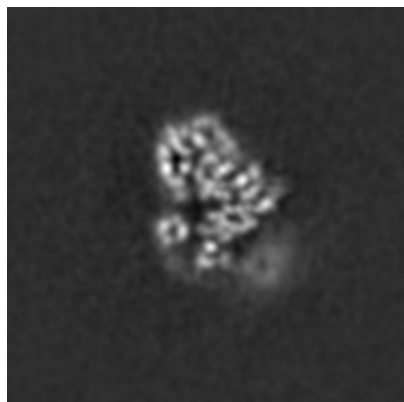


Z

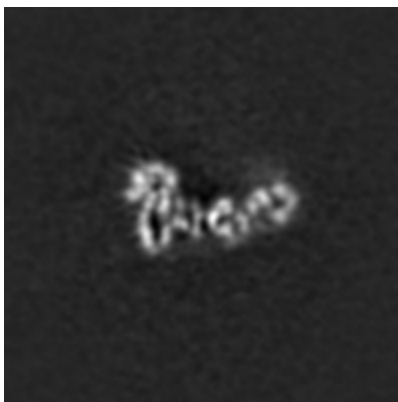
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

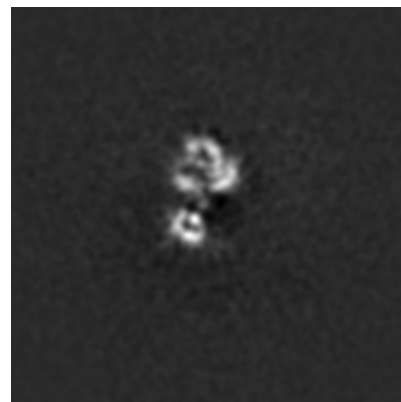
6.2.1 Primary map



X Index: 128

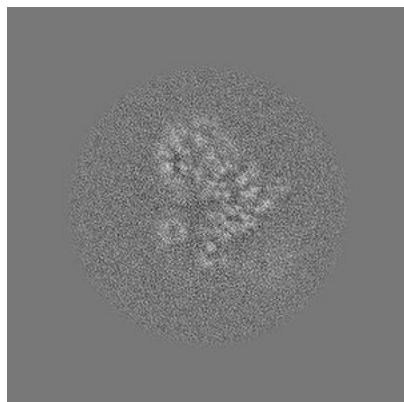


Y Index: 128

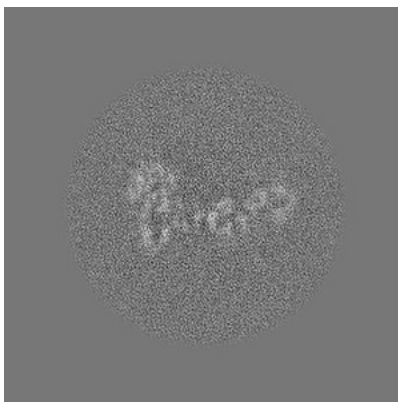


Z Index: 128

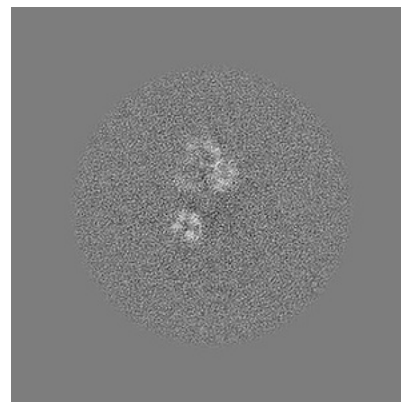
6.2.2 Raw map



X Index: 128



Y Index: 128

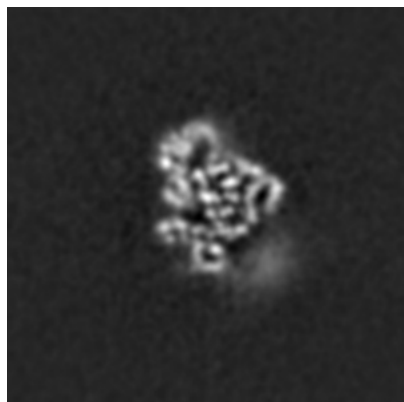


Z Index: 128

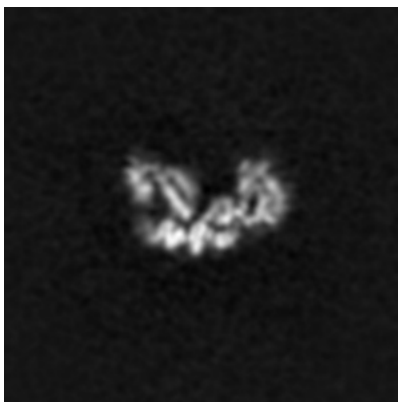
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

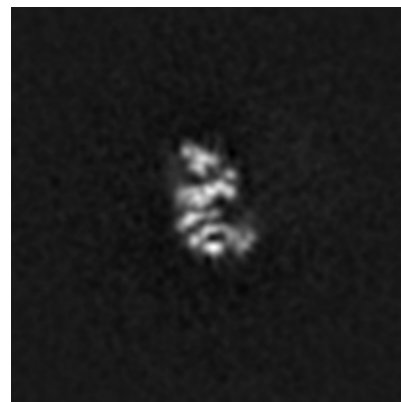
6.3.1 Primary map



X Index: 122

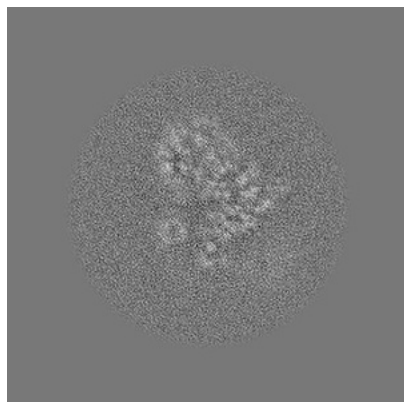


Y Index: 111

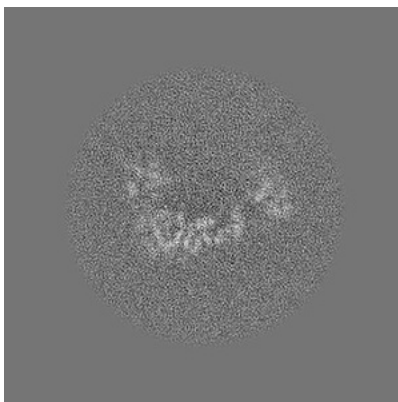


Z Index: 151

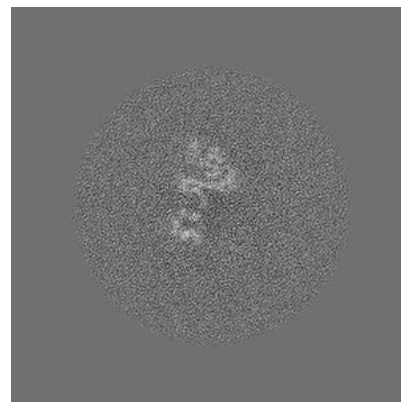
6.3.2 Raw map



X Index: 128



Y Index: 120

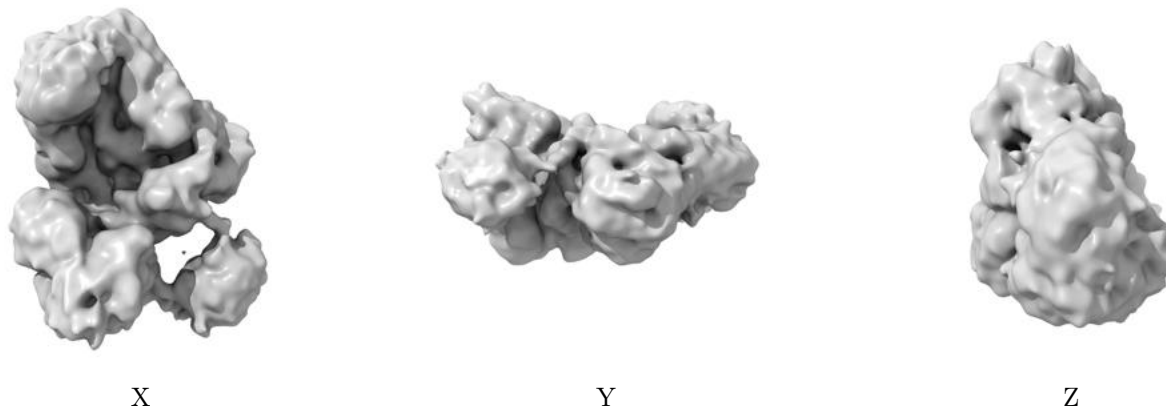


Z Index: 126

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

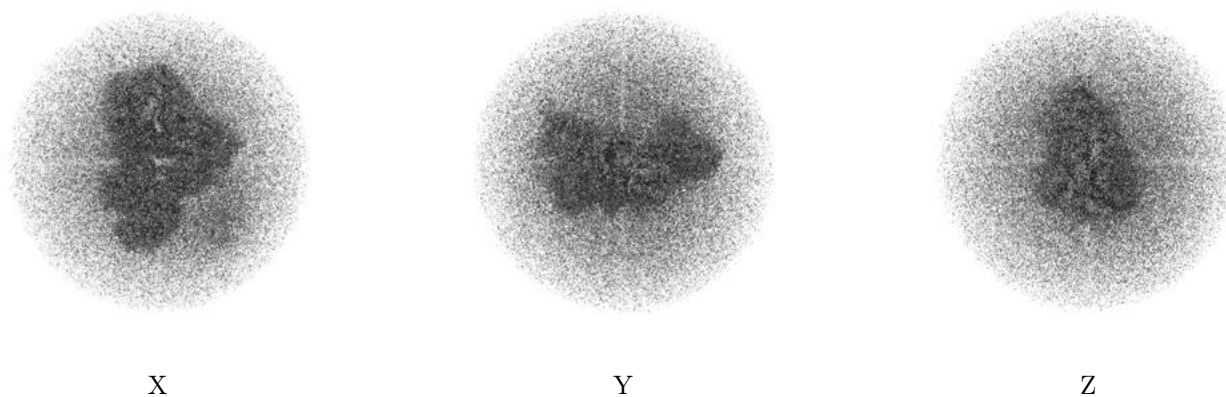
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

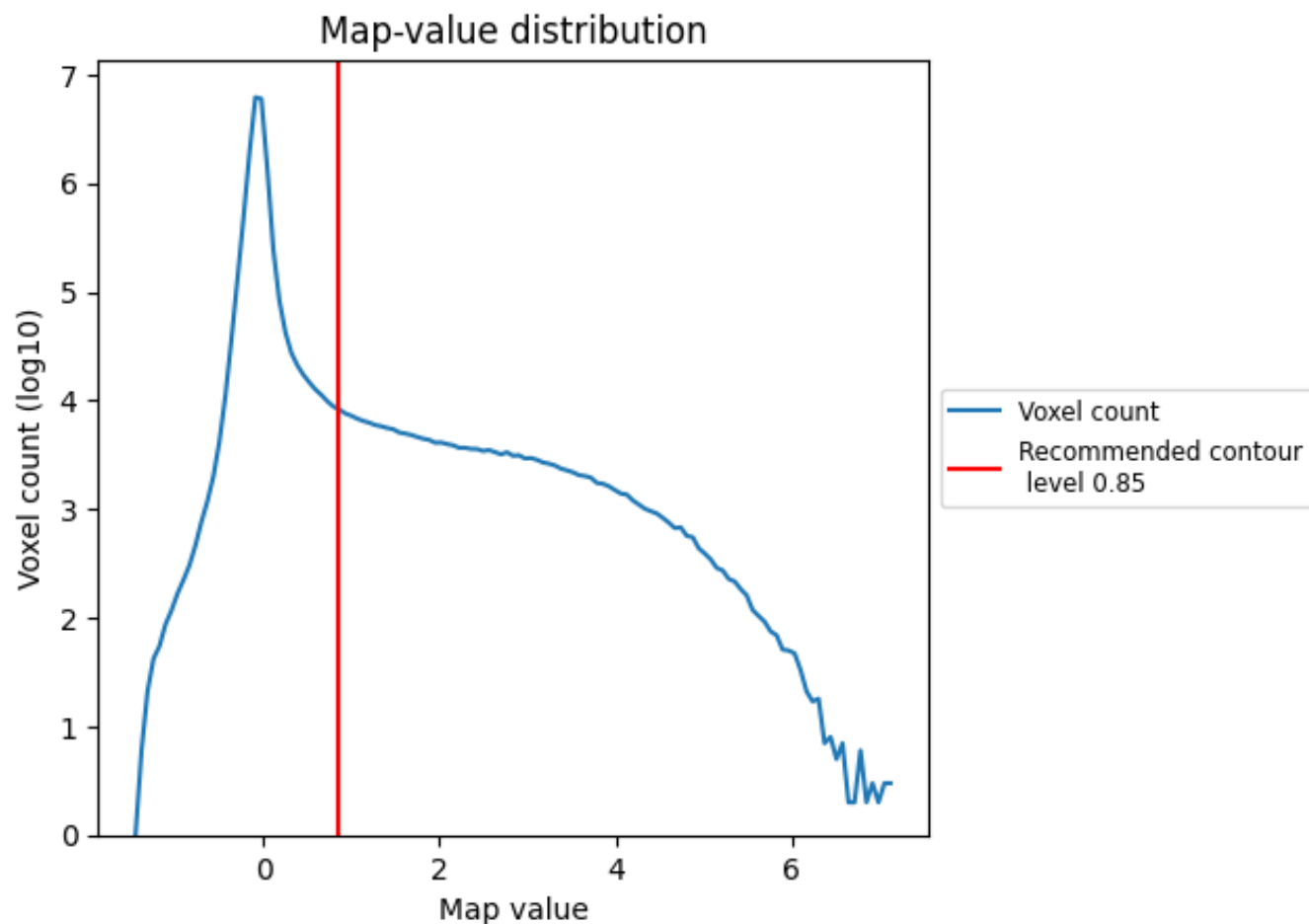
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

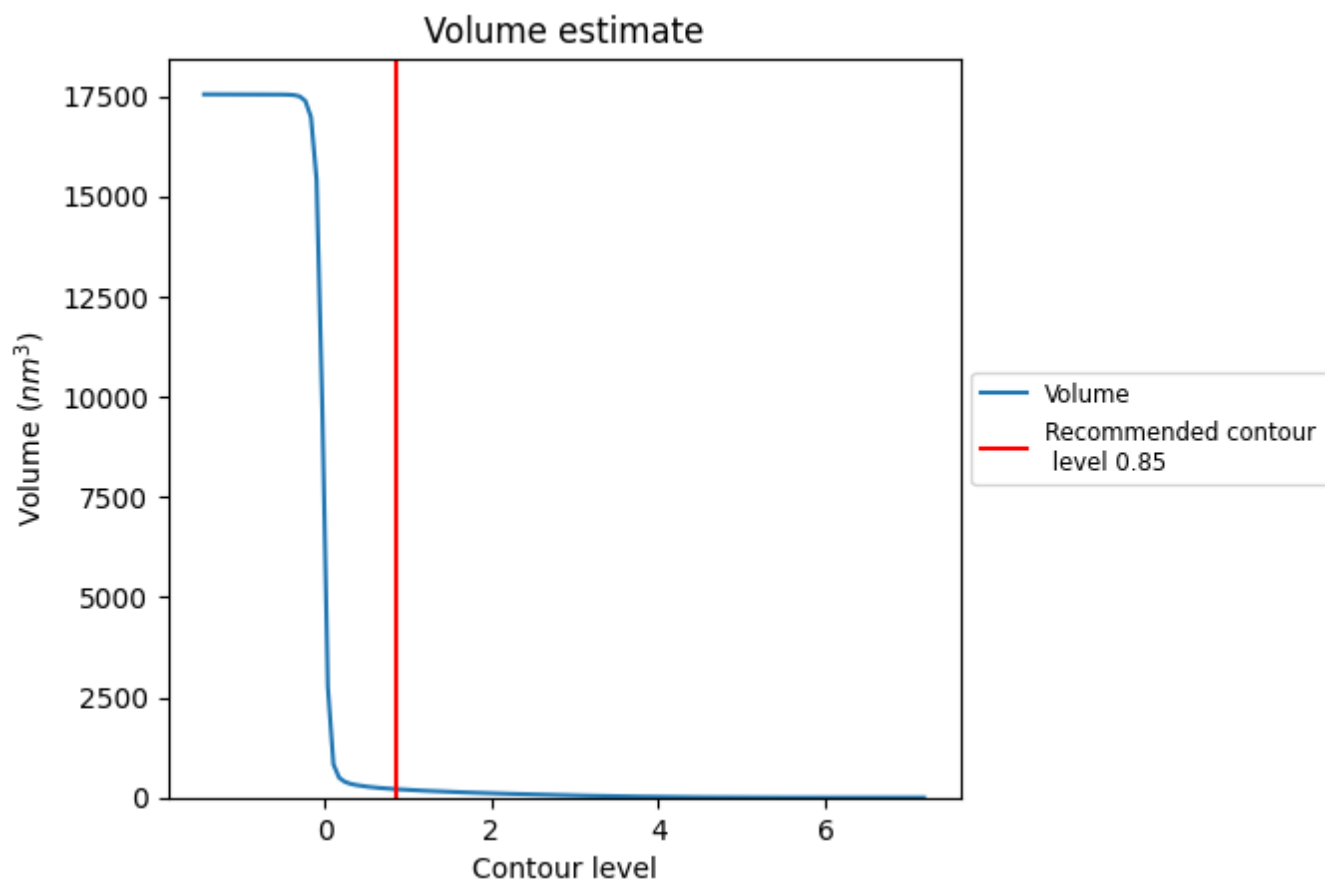
This section contains the results of statistical analysis of the map.

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.

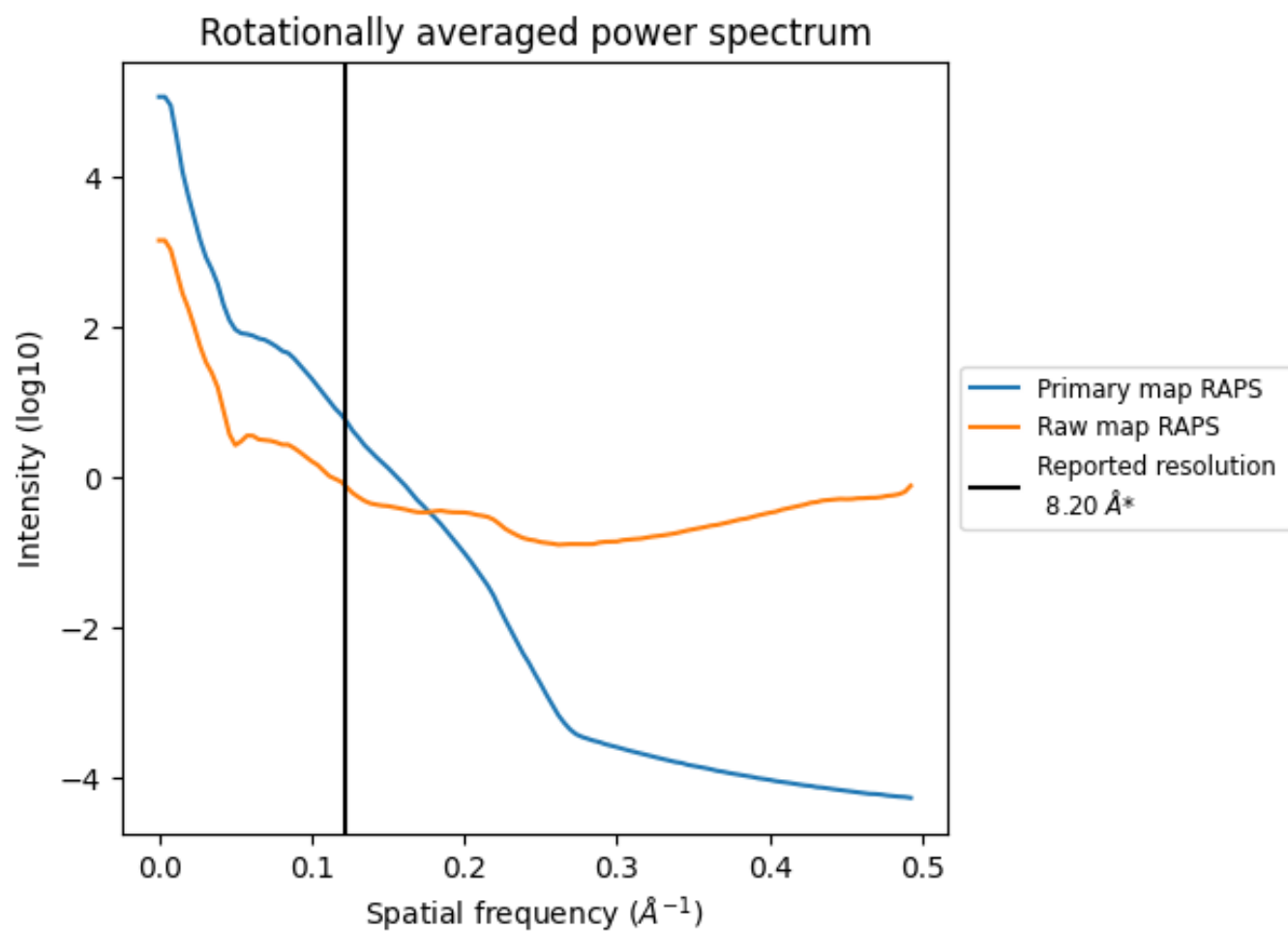
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm^3 ; this corresponds to an approximate mass of 190 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 ⓘ

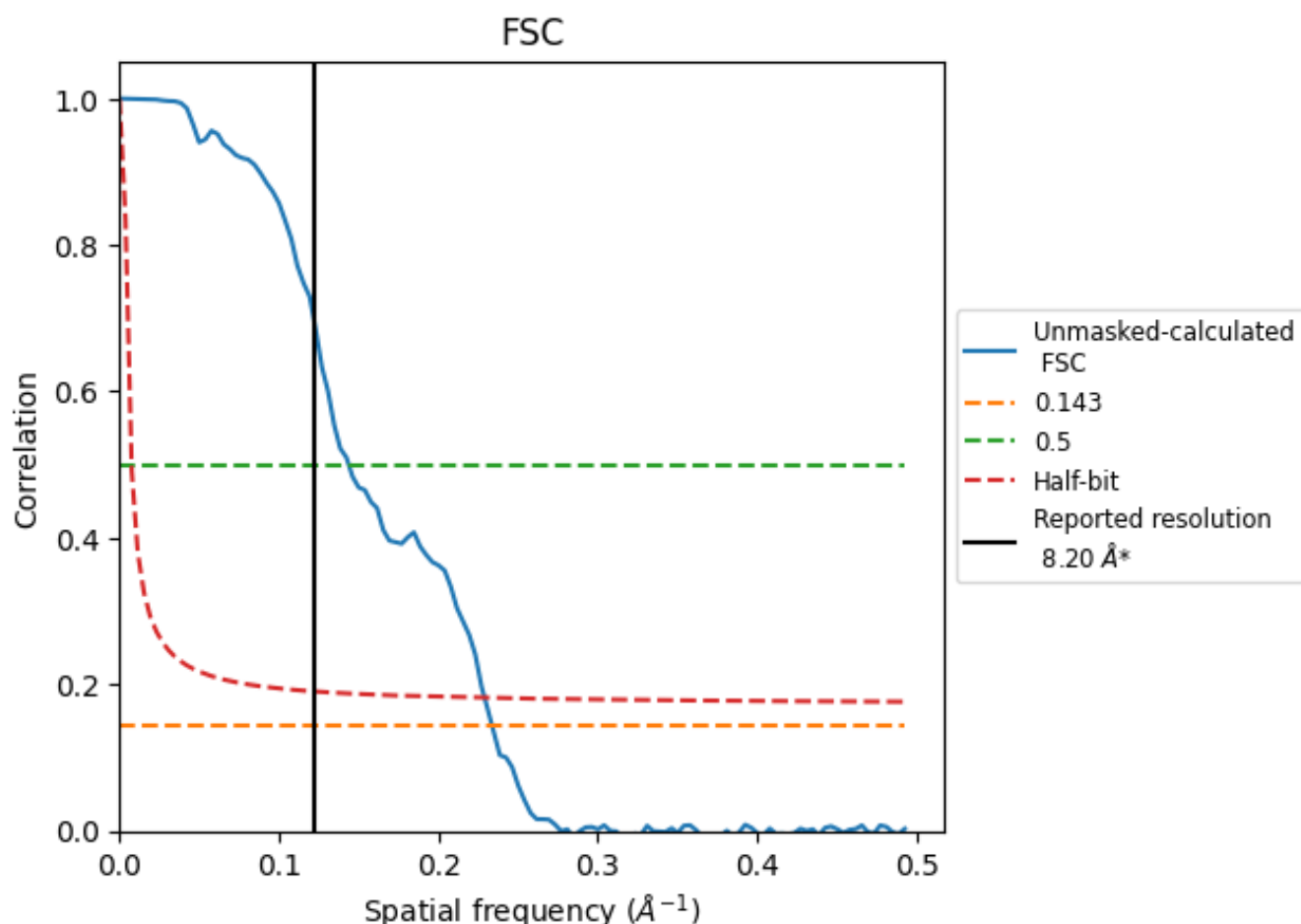


*Reported resolution corresponds to spatial frequency of 0.122 \AA^{-1}

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 0.122 Å⁻¹

8.2 Resolution estimates [i](#)

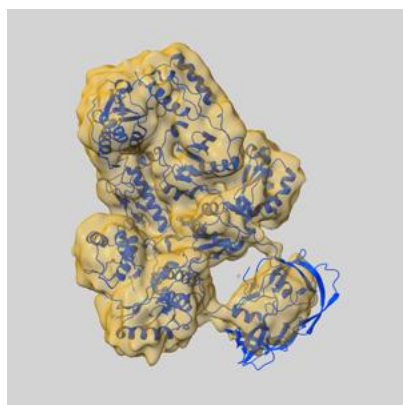
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	6.95	4.37

*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 4.28 differs from the reported value 8.2 by more than 10 %

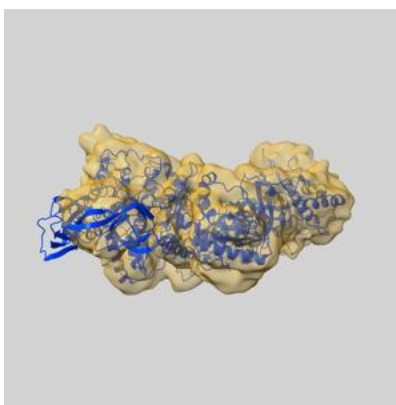
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25165 and PDB model 7SJX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

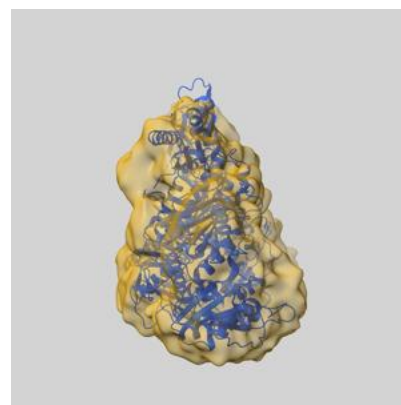
9.1 Map-model overlay [i](#)



X



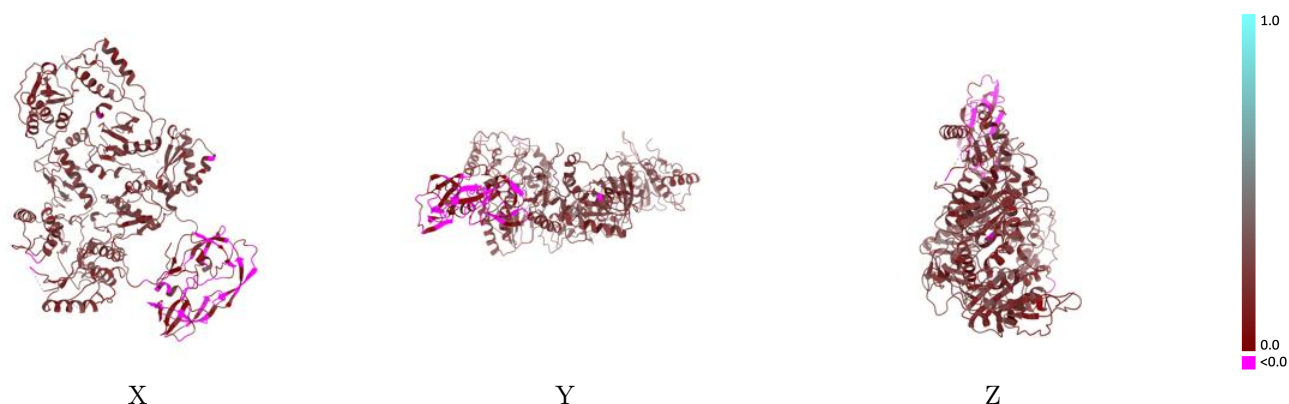
Y



Z

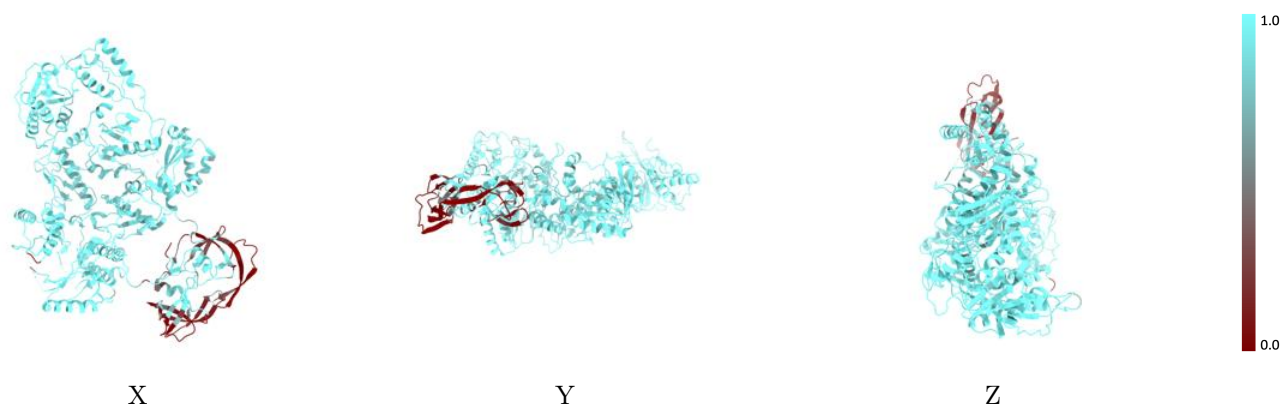
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



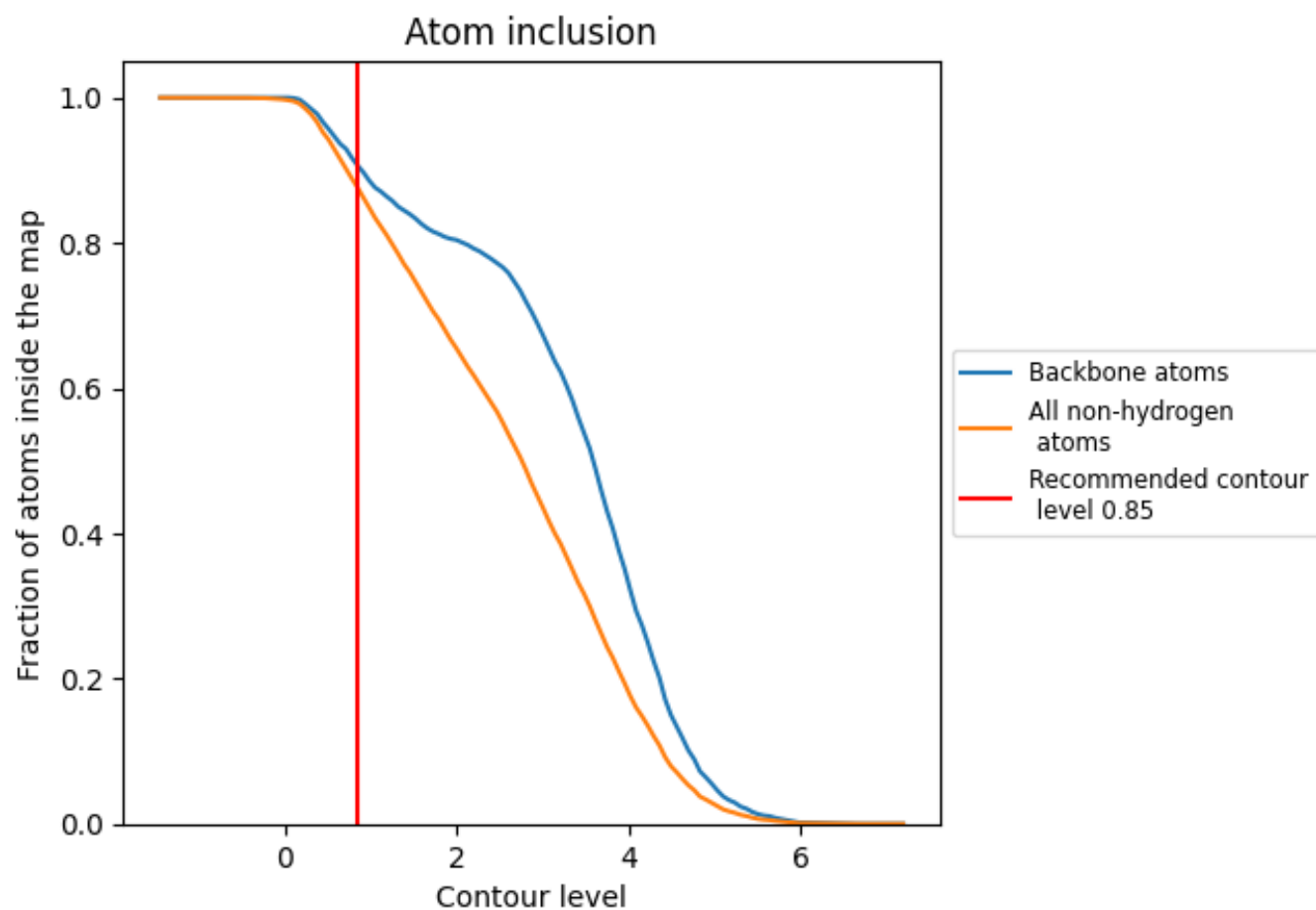
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8756	<div></div> 0.1880
A	<div></div> 0.8975	<div></div> 0.1880
B	<div></div> 0.8481	<div></div> 0.1890

