



Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 01:09 AM JST

PDB ID : 8JIF
EMDB ID : EMD-36311
Title : Cryo-EM Structure of 3-axis block of AAV9P31-Car4 complex
Authors : Zhang, R.; Liu, Y.; Lou, Z.
Deposited on : 2023-05-26
Resolution : 2.28 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

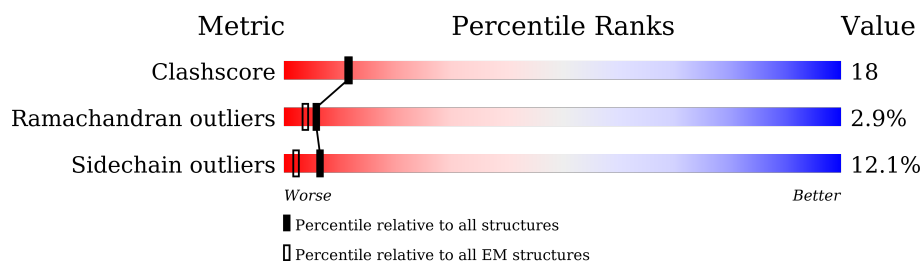
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.28 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	R	256	<div> <div>5%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	A	525	<div> <div>22%</div> <div>52%</div> <div>37%</div> <div>10%</div> <div>.</div> </div>
2	B	525	<div> <div>33%</div> <div>64%</div> <div>29%</div> <div>6%</div> </div>
2	C	525	<div> <div>25%</div> <div>64%</div> <div>28%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14630 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 Carbonic anhydrase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	256	Total	C	N	O	S	0	0
			2056	1302	359	383	12		

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		
2	B	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		
2	C	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	588A	TRP	-	insertion	UNP Q6JC40
A	588B	PRO	-	insertion	UNP Q6JC40
A	588C	THR	-	insertion	UNP Q6JC40
A	588D	SER	-	insertion	UNP Q6JC40
A	588E	TYR	-	insertion	UNP Q6JC40
A	588F	ASP	-	insertion	UNP Q6JC40
A	588G	ALA	-	insertion	UNP Q6JC40
B	588A	TRP	-	insertion	UNP Q6JC40
B	588B	PRO	-	insertion	UNP Q6JC40
B	588C	THR	-	insertion	UNP Q6JC40
B	588D	SER	-	insertion	UNP Q6JC40
B	588E	TYR	-	insertion	UNP Q6JC40
B	588F	ASP	-	insertion	UNP Q6JC40
B	588G	ALA	-	insertion	UNP Q6JC40
C	588A	TRP	-	insertion	UNP Q6JC40
C	588B	PRO	-	insertion	UNP Q6JC40
C	588C	THR	-	insertion	UNP Q6JC40

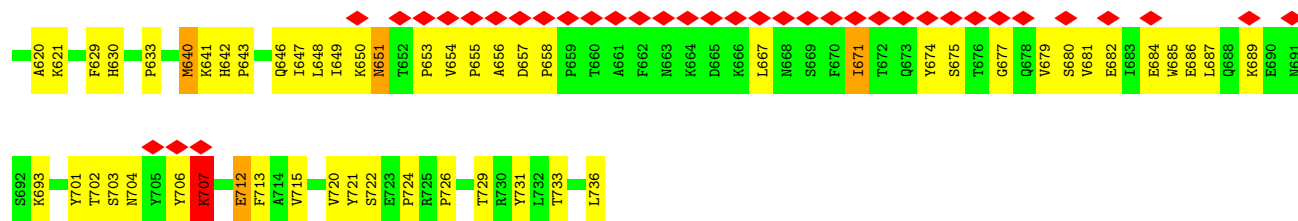
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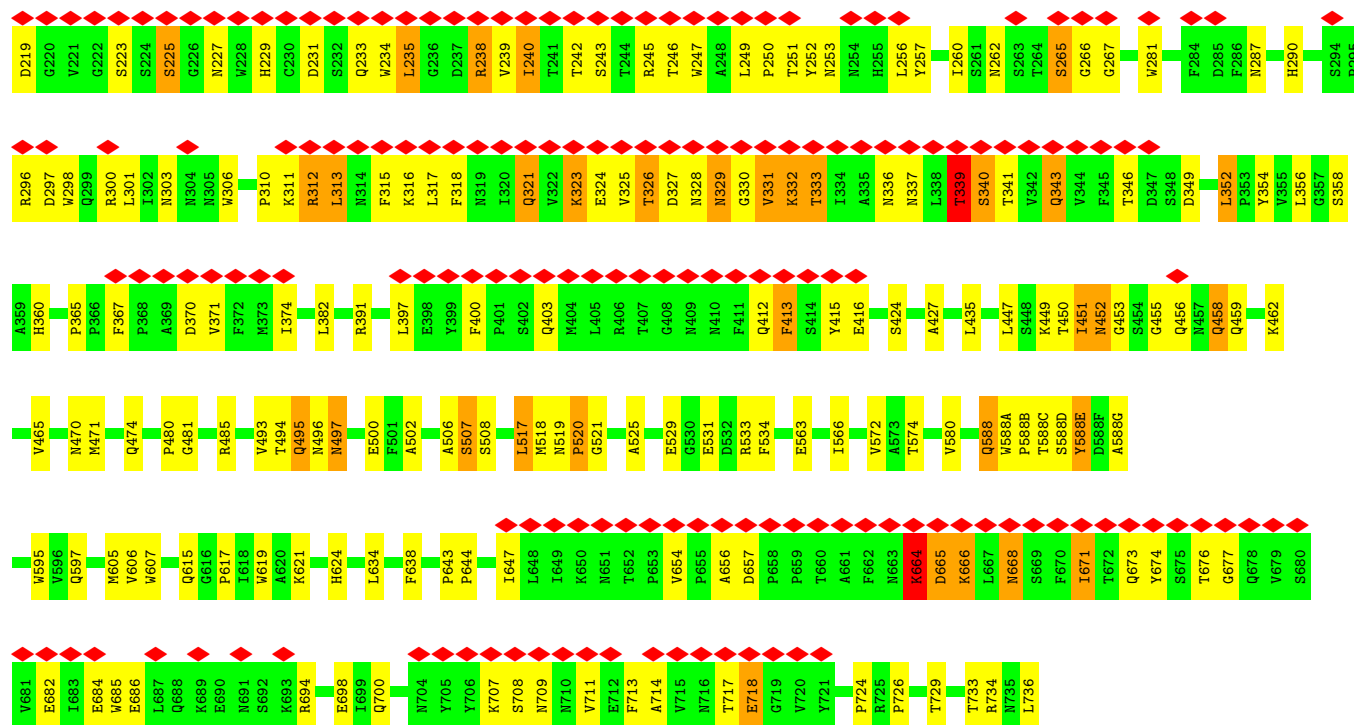
Chain	Residue	Modelled	Actual	Comment	Reference
C	588D	SER	-	insertion	UNP Q6JC40
C	588E	TYR	-	insertion	UNP Q6JC40
C	588F	ASP	-	insertion	UNP Q6JC40
C	588G	ALA	-	insertion	UNP Q6JC40

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

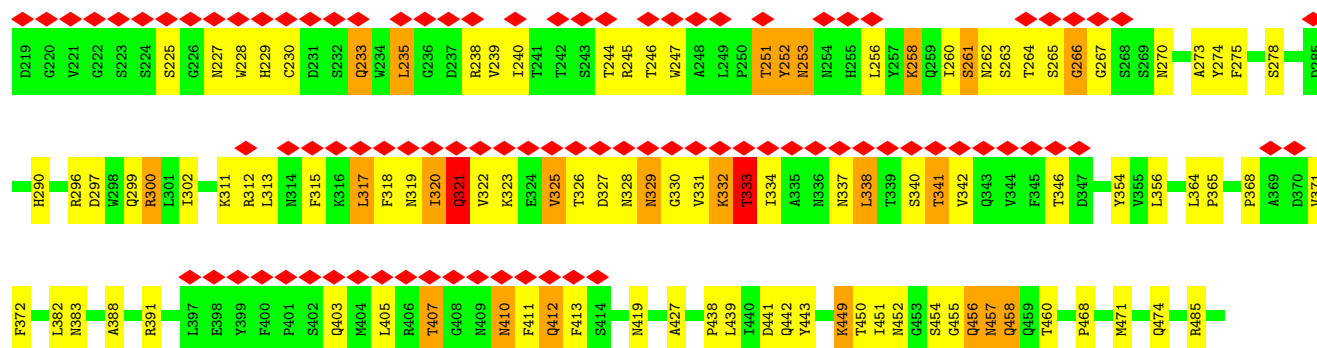
Mol	Chain	Residues	Atoms		AltConf
3	R	1	Total	Zn	0
			1	1	

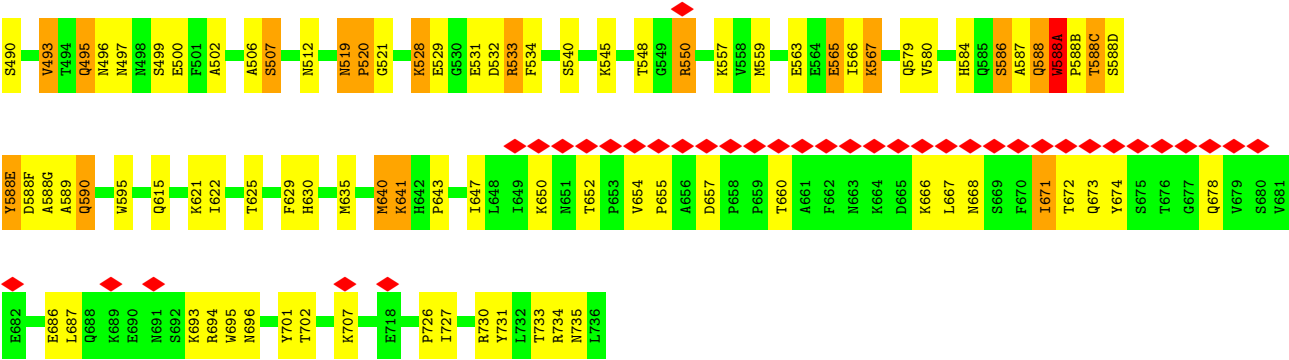


• Molecule 2: Capsid protein VP1



• Molecule 2: Capsid protein VP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13604676	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	134.928, 134.928, 134.928	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8433, 0.8433, 0.8433	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	R	0.25	0/2109	0.46	0/2855
2	A	0.31	0/4320	0.51	1/5889 (0.0%)
2	B	0.29	0/4320	0.51	0/5889
2	C	0.29	0/4320	0.49	0/5889
All	All	0.29	0/15069	0.50	1/20522 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	247	TRP	N-CA-C	5.49	125.83	111.00

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	R	2056	0	2027	58	0
2	A	4191	0	3932	194	0
2	B	4191	0	3932	149	0
2	C	4191	0	3932	146	0
3	R	1	0	0	0	0
All	All	14630	0	13823	499	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 18.

All (499) 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:A:327:ASP:HA	2:A:332:LYS:HA	1.29	1.12
1:R:51:SER:O	1:R:213:TYR:OH	1.68	1.10
2:B:327:ASP:HA	2:B:332:LYS:HA	1.32	1.08
2:C:519:ASN:HB3	2:C:520:PRO:HD2	1.35	1.08
1:R:51:SER:C	1:R:213:TYR:HH	1.61	1.04
2:C:327:ASP:HA	2:C:332:LYS:HA	1.41	0.98
2:C:403:GLN:HE22	2:C:411:PHE:HB2	1.33	0.93
2:C:588(A):TRP:HB2	2:C:588(B):PRO:HD2	1.53	0.90
1:R:51:SER:CA	1:R:213:TYR:OH	2.21	0.88
2:A:327:ASP:HA	2:A:332:LYS:CA	2.04	0.87
2:A:497:ASN:HD21	2:C:590:GLN:HE21	1.25	0.85
1:R:51:SER:C	1:R:213:TYR:OH	2.12	0.84
1:R:51:SER:HA	1:R:213:TYR:OH	1.76	0.84
2:A:260:ILE:HA	2:A:264:THR:HG21	1.59	0.82
2:C:519:ASN:HB3	2:C:520:PRO:CD	2.09	0.81
2:A:238:ARG:HG3	2:A:686:GLU:HA	1.63	0.81
2:B:225:SER:HB2	2:B:318:PHE:HB2	1.64	0.80
2:B:312:ARG:HD3	2:B:416:GLU:HG3	1.63	0.80
2:B:262:ASN:O	2:B:267:GLY:N	2.13	0.77
2:A:327:ASP:CA	2:A:332:LYS:HA	2.14	0.76
2:B:238:ARG:HH12	2:B:686:GLU:HG3	1.49	0.76
1:R:51:SER:O	1:R:213:TYR:CZ	2.38	0.76
2:A:588(A):TRP:CD1	2:A:588(B):PRO:HD3	2.20	0.75
2:A:284:PHE:HD2	2:A:647:ILE:HB	1.52	0.75
2:A:255:HIS:CG	2:A:653:PRO:HB3	2.22	0.74
2:B:413:PHE:HE1	2:B:647:ILE:HD11	1.53	0.74
2:C:322:VAL:HG12	2:C:323:LYS:H	1.54	0.72
2:A:372:PHE:HZ	2:A:375:PRO:HD3	1.54	0.72
2:A:296:ARG:HD3	2:A:300:ARG:HE	1.54	0.71
2:B:296:ARG:HG3	2:B:300:ARG:HH21	1.56	0.71
2:B:711:VAL:HG13	2:B:714:ALA:HB3	1.72	0.71
1:R:145:LEU:HD11	2:B:595:TRP:HZ2	1.55	0.71
2:B:327:ASP:HB2	2:B:332:LYS:HD2	1.71	0.71
2:A:588:GLN:HB3	2:A:588(D):SER:HA	1.71	0.70
2:B:327:ASP:CA	2:B:332:LYS:HA	2.18	0.70
2:A:262:ASN:HB2	2:A:273:ALA:HA	1.71	0.70
2:A:245:ARG:HH21	2:A:365:PRO:HB2	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:615:GLN:HE22	2:C:726:PRO:HA	1.57	0.70
2:B:718:GLU:N	2:B:718:GLU:OE1	2.24	0.69
2:A:255:HIS:CD2	2:A:653:PRO:HB3	2.28	0.69
2:A:527:HIS:HB2	2:A:531:GLU:HB3	1.76	0.68
2:A:588:GLN:HG2	2:A:588(G):ALA:HB2	1.75	0.68
2:C:262:ASN:HB3	2:C:273:ALA:HA	1.76	0.68
1:R:136:MET:HB3	1:R:163:ILE:HB	1.75	0.68
2:C:327:ASP:HB3	2:C:332:LYS:HE3	1.75	0.67
2:A:449:LYS:HB2	2:A:462:LYS:HB2	1.75	0.67
2:B:666:LYS:HZ1	2:B:668:ASN:HB2	1.60	0.66
2:A:237:ASP:HA	2:A:689:LYS:HE3	1.76	0.66
2:A:235:LEU:HD12	2:A:238:ARG:HB3	1.77	0.66
2:A:471:MET:HA	2:A:474:GLN:HG3	1.78	0.66
2:C:654:VAL:O	2:C:671:ILE:HG12	1.95	0.66
2:B:519:ASN:O	2:B:520:PRO:C	2.34	0.65
2:C:519:ASN:O	2:C:520:PRO:C	2.33	0.65
2:B:452:ASN:HD21	2:B:458:GLN:HB2	1.61	0.65
2:B:471:MET:HA	2:B:474:GLN:HG3	1.78	0.65
2:A:226:GLY:HA3	2:A:318:PHE:CD2	2.32	0.65
2:A:397:LEU:HD13	2:A:648:LEU:HD13	1.77	0.65
2:C:640:MET:HG3	2:C:643:PRO:HB3	1.79	0.64
2:B:323:LYS:HG3	2:B:674:TYR:CZ	2.32	0.64
1:R:206:LYS:HB3	1:R:233:GLN:HG2	1.79	0.63
2:A:313:LEU:HA	2:A:682:GLU:O	1.98	0.63
2:C:382:LEU:HD12	2:C:391:ARG:HB3	1.80	0.63
1:R:156:PHE:HB2	1:R:226:VAL:HG22	1.81	0.63
2:C:263:SER:HA	2:C:267:GLY:H	1.64	0.63
1:R:162:MET:HB2	1:R:234:PRO:HB3	1.80	0.62
1:R:98:CYS:SG	1:R:107:ARG:NH2	2.72	0.62
1:R:153:LYS:HA	1:R:225:THR:HG22	1.80	0.62
2:A:306:TRP:HD1	2:A:426:TYR:HB3	1.65	0.62
2:A:296:ARG:O	2:A:300:ARG:HG3	2.00	0.62
2:A:342:VAL:HA	2:A:651:ASN:HA	1.80	0.62
2:B:312:ARG:HG3	2:B:416:GLU:HA	1.80	0.62
1:R:66:LEU:HD21	1:R:212:ARG:HG3	1.81	0.62
2:A:299:GLN:HG3	2:A:701:TYR:HD2	1.65	0.61
2:C:588(A):TRP:HB2	2:C:588(B):PRO:CD	2.29	0.61
2:B:227:ASN:HB2	2:B:229:HIS:CE1	2.36	0.61
2:B:235:LEU:HD23	2:B:238:ARG:HB2	1.83	0.61
2:B:382:LEU:HD12	2:B:391:ARG:HB3	1.83	0.61
2:B:588(B):PRO:HG3	2:C:495:GLN:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:554:ASP:HB2	2:A:557:LYS:HZ2	1.65	0.60
1:R:86:GLN:HE21	1:R:186:PRO:HB2	1.67	0.60
2:A:588(A):TRP:CG	2:A:588(B):PRO:HD3	2.37	0.59
2:A:418:GLU:HG3	2:A:640:MET:HE2	1.83	0.59
2:A:528:LYS:HG2	2:A:572:VAL:HG21	1.83	0.59
1:R:187:HIS:CD2	2:A:456:GLN:N	2.71	0.59
1:R:187:HIS:CD2	2:A:456:GLN:H	2.20	0.59
2:A:249:LEU:HD12	2:A:250:PRO:HD2	1.85	0.59
2:B:588:GLN:HG2	2:B:588(G):ALA:HB2	1.85	0.59
2:C:337:ASN:OD1	2:C:340:SER:HB3	2.03	0.59
2:A:281:TRP:HA	2:A:650:LYS:HB2	1.85	0.59
2:A:588(A):TRP:CD2	2:B:495:GLN:HB3	2.37	0.59
2:A:562:ASN:HD21	2:A:564:GLU:HG3	1.68	0.58
2:B:297:ASP:HA	2:B:300:ARG:NH1	2.19	0.58
2:A:588(A):TRP:CE2	2:B:495:GLN:HB3	2.38	0.58
1:R:93:LEU:HD23	1:R:110:ALA:HB1	1.85	0.58
2:A:656:ALA:HB2	2:A:671:ILE:HG12	1.86	0.57
2:B:315:PHE:CE2	2:B:647:ILE:HD13	2.38	0.57
1:R:83:LYS:HG2	1:R:84:ASN:N	2.19	0.57
2:B:297:ASP:HA	2:B:300:ARG:HH12	1.70	0.57
2:A:281:TRP:CG	2:A:397:LEU:HD12	2.40	0.57
2:C:239:VAL:HG12	2:C:687:LEU:HD21	1.85	0.57
2:A:315:PHE:CE2	2:A:679:VAL:HG23	2.40	0.57
1:R:66:LEU:HG	1:R:212:ARG:HE	1.69	0.56
1:R:82:ILE:HG12	1:R:183:ILE:HD13	1.87	0.56
2:B:711:VAL:HG13	2:B:714:ALA:CB	2.35	0.56
2:C:354:TYR:CE2	2:C:356:LEU:HB2	2.41	0.56
2:A:245:ARG:NH2	2:A:365:PRO:HB2	2.20	0.56
2:A:343:GLN:HE22	2:A:650:LYS:HE3	1.70	0.56
2:A:615:GLN:HE22	2:A:726:PRO:HA	1.70	0.56
2:B:328:ASN:O	2:B:329:ASN:C	2.43	0.56
2:C:403:GLN:NE2	2:C:411:PHE:HB2	2.13	0.56
2:A:493:VAL:HA	2:A:496:ASN:HD22	1.70	0.56
2:C:588(C):THR:HA	2:C:588(E):TYR:CZ	2.40	0.56
2:B:249:LEU:HD12	2:B:250:PRO:HD2	1.87	0.56
2:A:313:LEU:HD13	2:A:681:VAL:HG23	1.87	0.56
2:B:413:PHE:CE1	2:B:647:ILE:HD11	2.37	0.56
2:C:311:LYS:HD3	2:C:686:GLU:HB2	1.88	0.56
2:A:372:PHE:CZ	2:A:375:PRO:HD3	2.38	0.55
2:A:503:TRP:CZ3	2:A:517:LEU:HB2	2.40	0.55
2:B:240:ILE:HD13	2:B:684:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:427:ALA:O	2:A:733:THR:HA	2.06	0.55
1:R:98:CYS:HA	1:R:109:GLU:HA	1.87	0.55
1:R:219:THR:HG21	2:A:588(D):SER:CB	2.37	0.55
2:B:346:THR:HG22	2:B:647:ILE:HG12	1.88	0.55
2:A:453:GLY:O	2:A:454:SER:C	2.45	0.55
2:A:230:CYS:SG	2:A:243:SER:HA	2.47	0.55
2:B:324:GLU:OE1	2:B:671:ILE:HG22	2.07	0.54
2:A:299:GLN:O	2:A:302:ILE:HG12	2.05	0.54
2:A:621:LYS:HZ3	2:A:643:PRO:HD2	1.73	0.54
2:C:325:VAL:HA	2:C:334:ILE:HA	1.89	0.54
2:B:231:ASP:H	2:B:242:THR:HB	1.71	0.54
2:A:315:PHE:HA	2:A:680:SER:O	2.07	0.54
2:A:509:TRP:HD1	2:A:518:MET:HG2	1.73	0.54
2:C:471:MET:HA	2:C:474:GLN:HG3	1.88	0.54
2:B:219:ASP:HB2	2:B:223:SER:HB3	1.90	0.54
2:B:452:ASN:HD21	2:B:458:GLN:CB	2.20	0.54
2:B:327:ASP:H	2:B:333:THR:H	1.55	0.54
2:C:245:ARG:CZ	2:C:368:PRO:HA	2.38	0.54
2:A:250:PRO:HG2	2:A:252:TYR:CE1	2.43	0.54
2:B:459:GLN:HB2	2:C:493:VAL:O	2.07	0.54
1:R:165:VAL:HG11	1:R:236:LYS:HB3	1.90	0.54
2:A:360:HIS:HA	2:C:442:GLN:HA	1.90	0.54
2:B:452:ASN:ND2	2:B:458:GLN:HB2	2.22	0.54
2:A:289:PHE:HE2	2:A:612:VAL:HB	1.73	0.53
2:B:450:THR:OG1	2:C:500:GLU:HA	2.08	0.53
2:C:227:ASN:HB2	2:C:229:HIS:NE2	2.22	0.53
1:R:203:PRO:HD2	1:R:206:LYS:HD2	1.89	0.53
2:A:265:SER:HB3	2:A:274:TYR:OH	2.08	0.53
1:R:39:GLU:N	1:R:39:GLU:OE1	2.41	0.53
2:A:452:ASN:HB2	2:A:458:GLN:NE2	2.24	0.53
2:C:468:PRO:O	2:C:471:MET:HG3	2.08	0.53
2:A:232:SER:HA	2:A:240:ILE:O	2.08	0.53
2:A:306:TRP:CD1	2:A:426:TYR:HB3	2.44	0.53
2:A:322:VAL:HG13	2:A:675:SER:HB3	1.91	0.53
2:C:325:VAL:HG13	2:C:334:ILE:HG12	1.89	0.53
2:B:427:ALA:O	2:B:733:THR:HA	2.09	0.53
2:B:451:ILE:HG12	2:C:499:SER:C	2.29	0.53
2:C:233:GLN:HG2	2:C:240:ILE:HB	1.91	0.53
2:A:227:ASN:O	2:A:228:TRP:C	2.46	0.52
2:C:519:ASN:O	2:C:521:GLY:N	2.42	0.52
2:B:451:ILE:HG21	2:C:499:SER:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:PHE:CD2	2:B:647:ILE:HD13	2.45	0.52
1:R:216:SER:HA	1:R:224:GLU:HA	1.92	0.52
2:C:341:THR:HG22	2:C:652:THR:OG1	2.09	0.52
2:C:496:ASN:O	2:C:497:ASN:HB2	2.10	0.52
2:C:529:GLU:N	2:C:567:LYS:NZ	2.58	0.52
2:B:621:LYS:HB2	2:B:643:PRO:HG3	1.90	0.52
2:A:667:LEU:N	2:A:667:LEU:HD12	2.24	0.52
2:B:502:ALA:O	2:B:506:ALA:HB2	2.10	0.52
1:R:105:PRO:HD2	1:R:108:TYR:HE1	1.74	0.52
2:C:531:GLU:HB3	2:C:534:PHE:HD2	1.75	0.52
2:C:672:THR:O	2:C:673:GLN:HG2	2.10	0.52
2:B:240:ILE:HG23	2:B:684:GLU:HB2	1.91	0.52
2:B:506:ALA:HB3	2:B:517:LEU:HD11	1.92	0.52
2:A:235:LEU:N	2:A:238:ARG:O	2.41	0.51
2:B:563:GLU:O	2:B:566:ILE:HG12	2.10	0.51
2:C:326:THR:N	2:C:333:THR:O	2.38	0.51
2:A:311:LYS:N	2:A:684:GLU:O	2.40	0.51
2:B:265:SER:OG	2:B:266:GLY:N	2.43	0.51
2:C:315:PHE:HB3	2:C:413:PHE:CE1	2.45	0.51
2:C:302:ILE:HD12	2:C:731:TYR:CE1	2.45	0.51
2:C:328:ASN:O	2:C:329:ASN:C	2.49	0.51
2:A:296:ARG:CZ	2:A:300:ARG:HG2	2.40	0.51
2:B:496:ASN:O	2:B:497:ASN:HB2	2.10	0.51
1:R:127:HIS:HE1	1:R:213:TYR:CE1	2.29	0.51
2:B:313:LEU:HD22	2:B:415:TYR:HB3	1.93	0.51
2:C:233:GLN:CG	2:C:240:ILE:HB	2.41	0.51
2:B:325:VAL:HG13	2:B:332:LYS:HE2	1.93	0.51
1:R:193:ARG:HG3	1:R:194:GLU:H	1.76	0.51
1:R:145:LEU:HD11	2:B:595:TRP:CZ2	2.43	0.51
2:A:312:ARG:HD2	2:A:684:GLU:OE1	2.10	0.51
2:A:693:LYS:HG3	2:B:400:PHE:CZ	2.46	0.51
2:B:328:ASN:O	2:B:330:GLY:N	2.43	0.51
2:A:309:ARG:O	2:A:309:ARG:HG2	2.10	0.51
2:C:323:LYS:HG3	2:C:674:TYR:CZ	2.45	0.51
2:C:328:ASN:HB2	2:C:331:VAL:HG13	1.92	0.50
1:R:121:ASN:HB3	1:R:135:ALA:HB2	1.94	0.50
2:A:655:PRO:HB3	2:A:667:LEU:CD2	2.42	0.50
2:B:580:VAL:HG22	2:C:485:ARG:HB3	1.93	0.50
2:A:519:ASN:HB2	2:A:520:PRO:HD3	1.92	0.50
2:B:253:ASN:HB3	2:B:256:LEU:O	2.11	0.50
2:A:344:VAL:HG13	2:A:649:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:LYS:HD3	2:B:412:GLN:HB2	1.94	0.50
2:A:271:ASP:HA	2:A:514:ARG:HG2	1.92	0.50
2:C:247:TRP:HB3	2:C:372:PHE:CZ	2.47	0.50
2:A:263:SER:H	2:A:386:SER:HB2	1.77	0.50
2:A:298:TRP:O	2:A:299:GLN:C	2.49	0.50
2:C:531:GLU:HB3	2:C:534:PHE:CD2	2.46	0.50
2:C:296:ARG:NH1	2:C:299:GLN:HB3	2.27	0.50
1:R:251:TYR:CE1	1:R:259:MET:HG3	2.46	0.50
2:A:261:SER:HA	2:A:275:PHE:HA	1.93	0.49
2:A:456:GLN:O	2:A:457:ASN:C	2.50	0.49
2:B:337:ASN:ND2	2:B:340:SER:HB3	2.27	0.49
2:C:615:GLN:NE2	2:C:726:PRO:HA	2.25	0.49
2:A:288:ARG:HB2	2:A:291:CYS:SG	2.52	0.49
2:A:546:GLN:HG2	2:A:721:TYR:O	2.12	0.49
2:B:588(B):PRO:HG3	2:C:495:GLN:CB	2.41	0.49
2:C:588(C):THR:HB	2:C:588(E):TYR:CE2	2.47	0.49
2:A:588(A):TRP:CG	2:B:495:GLN:HB3	2.47	0.49
2:A:361:GLU:HG2	2:C:441:ASP:O	2.12	0.49
2:C:329:ASN:HD22	2:C:330:GLY:H	1.59	0.49
2:A:503:TRP:HZ3	2:A:517:LEU:HB2	1.78	0.49
2:B:451:ILE:O	2:B:452:ASN:C	2.51	0.49
2:B:296:ARG:HD2	2:B:296:ARG:HA	1.56	0.49
2:B:315:PHE:HB3	2:B:413:PHE:CE1	2.47	0.49
2:B:323:LYS:HE3	2:B:336:ASN:HD22	1.78	0.49
2:B:597:GLN:OE1	2:B:597:GLN:HA	2.13	0.49
2:C:256:LEU:HB2	2:C:258:LYS:HE3	1.95	0.49
2:B:246:THR:HB	2:B:371:VAL:HG22	1.95	0.49
2:C:261:SER:H	2:C:264:THR:HB	1.77	0.49
2:C:621:LYS:HB2	2:C:643:PRO:HG3	1.94	0.49
1:R:163:ILE:HG12	1:R:235:ILE:HG22	1.95	0.48
2:A:251:THR:O	2:A:252:TYR:HB2	2.12	0.48
2:A:287:ASN:O	2:A:617:PRO:HA	2.13	0.48
2:A:288:ARG:HD3	2:C:443:TYR:CZ	2.48	0.48
2:A:296:ARG:HB3	2:A:300:ARG:HH21	1.77	0.48
2:B:324:GLU:HG2	2:B:673:GLN:HG2	1.95	0.48
2:C:529:GLU:CA	2:C:567:LYS:NZ	2.76	0.48
2:A:234:TRP:HE1	2:A:687:LEU:CD2	2.26	0.48
2:A:296:ARG:HH21	2:A:299:GLN:HB3	1.78	0.48
2:C:262:ASN:CB	2:C:273:ALA:HA	2.42	0.48
2:C:296:ARG:HG3	2:C:300:ARG:NH1	2.28	0.48
2:B:287:ASN:O	2:B:617:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:588:GLN:HA	2:C:588(D):SER:HA	1.96	0.48
2:C:629:PHE:O	2:C:630:HIS:C	2.52	0.48
2:A:418:GLU:HG3	2:A:640:MET:CE	2.43	0.48
2:C:641:LYS:HE2	2:C:641:LYS:HB3	1.52	0.48
1:R:81:PRO:HG2	1:R:92:THR:HB	1.96	0.48
2:B:354:TYR:CE2	2:B:356:LEU:HB2	2.49	0.48
2:C:297:ASP:HA	2:C:300:ARG:HH11	1.78	0.48
2:C:548:THR:HG23	2:C:557:LYS:HB3	1.96	0.48
1:R:202:PRO:HG3	1:R:235:ILE:HG12	1.96	0.47
2:A:527:HIS:HB2	2:A:531:GLU:CB	2.43	0.47
2:C:410:ASN:ND2	2:C:412:GLN:HE22	2.11	0.47
2:B:452:ASN:OD1	2:B:458:GLN:HB2	2.13	0.47
1:R:144:LYS:HD3	1:R:147:SER:HB2	1.97	0.47
2:B:517:LEU:HA	2:B:517:LEU:HD12	1.59	0.47
2:B:519:ASN:O	2:B:521:GLY:N	2.47	0.47
2:A:228:TRP:CZ3	2:A:230:CYS:HB2	2.49	0.47
2:B:219:ASP:HB2	2:B:223:SER:CB	2.43	0.47
2:B:588(E):TYR:O	2:B:588(E):TYR:CD1	2.67	0.47
2:B:249:LEU:HD13	2:B:374:ILE:HB	1.95	0.47
2:B:456:GLN:N	2:B:458:GLN:HE22	2.13	0.47
2:A:452:ASN:OD1	2:A:460:THR:HB	2.14	0.47
2:A:519:ASN:CB	2:A:520:PRO:HD3	2.44	0.47
2:B:358:SER:HB2	2:B:360:HIS:CD2	2.49	0.47
2:C:671:ILE:HG12	2:C:671:ILE:H	1.47	0.47
1:R:63:ASN:HB3	1:R:66:LEU:HD13	1.96	0.47
2:A:343:GLN:HE21	2:A:343:GLN:HB2	1.49	0.47
2:B:654:VAL:O	2:B:671:ILE:HG12	2.14	0.47
1:R:165:VAL:HG12	1:R:237:ILE:O	2.15	0.47
2:A:621:LYS:NZ	2:A:643:PRO:HD2	2.28	0.47
2:A:701:TYR:HB2	2:A:731:TYR:CZ	2.50	0.47
2:B:245:ARG:HD2	2:B:365:PRO:HG2	1.96	0.47
2:C:225:SER:OG	2:C:319:ASN:N	2.35	0.47
1:R:232:LYS:HG2	1:R:233:GLN:H	1.80	0.47
2:B:310:PRO:C	2:B:311:LYS:HD2	2.35	0.47
2:A:315:PHE:HE1	2:A:411:PHE:CD2	2.33	0.47
2:A:586:SER:HA	2:B:496:ASN:O	2.15	0.47
2:C:502:ALA:O	2:C:506:ALA:HB2	2.15	0.47
2:A:485:ARG:HB3	2:C:580:VAL:HG22	1.97	0.46
2:C:520:PRO:HG2	2:C:635:MET:HG2	1.96	0.46
2:A:245:ARG:HD3	2:A:365:PRO:HD2	1.98	0.46
2:A:656:ALA:CB	2:A:671:ILE:HG12	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:667:LEU:N	2:A:667:LEU:CD1	2.79	0.46
2:B:281:TRP:CG	2:B:397:LEU:HD22	2.50	0.46
2:C:495:GLN:OE1	2:C:533:ARG:HD2	2.15	0.46
1:R:156:PHE:HE2	2:A:588(C):THR:HG21	1.79	0.46
2:B:326:THR:O	2:B:327:ASP:C	2.53	0.46
2:A:495:GLN:HB2	2:C:588(A):TRP:CE3	2.50	0.46
2:A:245:ARG:NE	2:A:365:PRO:HD2	2.29	0.46
2:A:650:LYS:NZ	2:A:651:ASN:O	2.48	0.46
2:A:736:LEU:OXT	2:B:624:HIS:N	2.35	0.46
2:A:328:ASN:O	2:A:329:ASN:C	2.54	0.46
1:R:81:PRO:HD3	2:A:592:GLN:NE2	2.31	0.46
2:B:324:GLU:HG2	2:B:673:GLN:CG	2.46	0.46
2:B:321:GLN:OE1	2:B:677:GLY:HA2	2.16	0.46
2:C:251:THR:O	2:C:252:TYR:HB2	2.15	0.46
2:B:447:LEU:HD12	2:B:462:LYS:O	2.16	0.46
2:C:329:ASN:HD21	2:C:331:VAL:HG12	1.80	0.46
1:R:135:ALA:H	1:R:164:GLU:HB2	1.81	0.45
2:A:307:GLY:HA2	2:A:423:HIS:O	2.16	0.45
2:A:435:LEU:HD21	2:A:736:LEU:HD12	1.98	0.45
2:B:459:GLN:HG3	2:C:497:ASN:O	2.17	0.45
2:A:261:SER:H	2:A:264:THR:HG1	1.64	0.45
2:A:403:GLN:HG2	2:A:405:LEU:HD13	1.98	0.45
2:A:693:LYS:HG3	2:B:400:PHE:CE2	2.51	0.45
2:B:717:THR:OG1	2:B:718:GLU:OE1	2.15	0.45
2:C:318:PHE:CZ	2:C:678:GLN:HB3	2.50	0.45
2:A:261:SER:O	2:A:262:ASN:C	2.55	0.45
2:A:309:ARG:O	2:A:685:TRP:HA	2.16	0.45
2:A:351:GLN:HB3	2:C:693:LYS:HG2	1.98	0.45
2:A:641:LYS:NZ	2:A:641:LYS:H	2.15	0.45
2:C:322:VAL:O	2:C:323:LYS:HG2	2.16	0.45
2:A:445:TYR:CZ	2:A:465:VAL:HG23	2.51	0.45
2:A:300:ARG:O	2:A:301:LEU:C	2.55	0.45
2:A:327:ASP:HA	2:A:332:LYS:N	2.32	0.45
2:A:363:CYS:O	2:A:365:PRO:HD3	2.16	0.45
2:C:338:LEU:HD11	2:C:407:THR:HG21	1.99	0.45
2:C:622:ILE:HD12	2:C:641:LYS:HD2	1.97	0.45
2:A:488:ARG:HB2	2:C:584:HIS:CD2	2.52	0.45
2:A:488:ARG:HG3	2:A:574:THR:HG21	1.97	0.45
2:B:247:TRP:HE1	2:B:317:LEU:HD11	1.81	0.45
2:C:579:GLN:HG2	2:C:595:TRP:CE3	2.52	0.45
2:B:325:VAL:HG13	2:B:332:LYS:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:696:ASN:OD1	2:C:696:ASN:N	2.50	0.45
1:R:22:TRP:HE3	1:R:36:LEU:HD13	1.82	0.45
1:R:156:PHE:CE2	2:A:588(C):THR:HG21	2.51	0.45
2:A:323:LYS:HG3	2:A:674:TYR:CZ	2.51	0.45
1:R:124:GLY:HA2	1:R:133:HIS:HB3	1.98	0.45
2:A:246:THR:HA	2:A:677:GLY:O	2.17	0.45
2:A:475:GLY:HA2	2:B:519:ASN:HB3	1.98	0.45
2:A:528:LYS:O	2:A:531:GLU:HB2	2.16	0.45
2:A:562:ASN:HD21	2:A:564:GLU:CG	2.30	0.45
2:B:367:PHE:HB3	2:B:370:ASP:OD2	2.17	0.45
2:B:449:LYS:HB2	2:B:449:LYS:HE2	1.83	0.45
2:C:275:PHE:HB3	2:C:383:ASN:HB3	1.98	0.45
2:C:329:ASN:ND2	2:C:330:GLY:H	2.15	0.45
2:C:456:GLN:O	2:C:458:GLN:N	2.50	0.45
2:B:247:TRP:NE1	2:B:317:LEU:HD11	2.32	0.45
2:A:267:GLY:O	2:A:268:SER:C	2.56	0.44
2:B:531:GLU:HB3	2:B:534:PHE:HD2	1.81	0.44
2:B:480:PRO:O	2:B:605:MET:HG2	2.17	0.44
2:B:713:PHE:CE2	2:B:724:PRO:HD2	2.52	0.44
2:C:329:ASN:ND2	2:C:331:VAL:HG12	2.31	0.44
2:C:346:THR:HG22	2:C:647:ILE:HD12	1.98	0.44
2:A:258:LYS:HB2	2:A:278:SER:OG	2.16	0.44
2:A:565:GLU:CD	2:A:565:GLU:H	2.20	0.44
2:B:619:TRP:CZ2	2:B:644:PRO:HG2	2.52	0.44
2:A:588(A):TRP:CD1	2:B:495:GLN:HB3	2.52	0.44
2:A:279:THR:HG21	2:A:377:TYR:CD2	2.53	0.44
2:A:316:LYS:HE2	2:A:316:LYS:HB3	1.49	0.44
2:B:465:VAL:HG12	2:C:550:ARG:HH21	1.83	0.44
2:C:528:LYS:O	2:C:529:GLU:C	2.55	0.44
2:A:654:VAL:HG12	2:A:656:ALA:H	1.81	0.44
2:A:311:LYS:HB3	2:A:311:LYS:HE3	1.88	0.44
2:B:257:TYR:OH	2:B:397:LEU:HB2	2.18	0.44
2:B:352:LEU:HD12	2:B:352:LEU:HA	1.87	0.44
2:C:427:ALA:O	2:C:733:THR:HA	2.18	0.44
2:A:707:LYS:HE2	2:A:707:LYS:HB3	1.43	0.43
2:B:310:PRO:HD3	2:B:638:PHE:CE2	2.53	0.43
2:B:327:ASP:HA	2:B:332:LYS:CA	2.24	0.43
2:B:708:SER:O	2:B:709:ASN:C	2.55	0.43
2:C:245:ARG:HD2	2:C:365:PRO:HG2	2.00	0.43
2:C:263:SER:HA	2:C:267:GLY:N	2.30	0.43
2:C:317:LEU:HD22	2:C:317:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:85:ASN:HB2	1:R:90:GLU:HG2	2.00	0.43
1:R:126:GLU:HG3	1:R:139:HIS:CE1	2.53	0.43
2:A:219:ASP:HB2	2:A:408:GLY:O	2.18	0.43
2:C:327:ASP:HA	2:C:332:LYS:CA	2.30	0.43
1:R:127:HIS:CE1	1:R:213:TYR:CE1	3.06	0.43
2:A:245:ARG:CD	2:A:365:PRO:HD2	2.48	0.43
2:A:382:LEU:HD12	2:A:391:ARG:HB3	2.00	0.43
2:A:612:VAL:HG23	2:A:729:THR:HG21	1.99	0.43
2:C:545:LYS:HG3	2:C:557:LYS:O	2.18	0.43
2:A:271:ASP:OD1	2:A:515:ASN:N	2.50	0.43
2:B:508:SER:HB3	2:B:517:LEU:HD12	2.00	0.43
2:C:506:ALA:O	2:C:507:SER:HB2	2.18	0.43
1:R:108:TYR:OH	1:R:154:ASP:O	2.30	0.43
2:C:247:TRP:HA	2:C:372:PHE:O	2.18	0.43
2:C:253:ASN:HB3	2:C:258:LYS:NZ	2.34	0.43
1:R:51:SER:OG	1:R:52:PRO:HD3	2.17	0.43
1:R:187:HIS:HD2	2:A:456:GLN:N	2.16	0.43
2:A:629:PHE:O	2:A:630:HIS:C	2.57	0.43
2:B:306:TRP:CZ2	2:B:734:ARG:HB3	2.53	0.43
2:B:435:LEU:HD21	2:B:736:LEU:HD12	1.99	0.43
2:C:587:ALA:HB1	2:C:588:GLN:HE21	1.84	0.43
2:C:655:PRO:HB3	2:C:667:LEU:HD12	1.99	0.43
2:A:531:GLU:O	2:A:532:ASP:C	2.57	0.43
2:B:311:LYS:HD3	2:B:686:GLU:CB	2.49	0.43
1:R:107:ARG:HD3	1:R:145:LEU:HD22	2.01	0.43
1:R:189:THR:HG23	2:A:590:GLN:HE22	1.83	0.43
2:A:500:GLU:HB2	2:C:451:ILE:HD11	2.01	0.43
2:A:641:LYS:HE2	2:A:641:LYS:HB2	1.78	0.43
2:C:405:LEU:N	2:C:405:LEU:HD12	2.34	0.43
2:A:245:ARG:NH2	2:A:367:PHE:O	2.51	0.43
2:A:572:VAL:HG12	2:A:574:THR:H	1.84	0.43
2:A:579:GLN:HG2	2:A:595:TRP:CE3	2.54	0.43
2:B:296:ARG:HH12	2:B:300:ARG:HG3	1.84	0.43
2:C:238:ARG:NH2	2:C:240:ILE:HD11	2.34	0.43
2:C:452:ASN:HD22	2:C:458:GLN:HB2	1.84	0.43
2:C:693:LYS:NZ	2:C:693:LYS:HB3	2.34	0.43
1:R:79:GLN:HG2	1:R:193:ARG:O	2.19	0.42
2:B:238:ARG:NH2	2:B:684:GLU:OE2	2.52	0.42
2:B:713:PHE:CZ	2:B:724:PRO:HD2	2.54	0.42
2:C:246:THR:HB	2:C:371:VAL:HG22	2.00	0.42
2:C:641:LYS:H	2:C:641:LYS:HG2	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:TYR:CE2	2:A:642:HIS:HB3	2.55	0.42
2:B:588(E):TYR:O	2:B:588(E):TYR:CG	2.72	0.42
2:A:712:GLU:HB2	2:A:724:PRO:HG2	2.02	0.42
2:B:239:VAL:HG13	2:B:685:TRP:HB2	2.00	0.42
2:C:320:ILE:HG22	2:C:321:GLN:N	2.34	0.42
2:C:490:SER:HB2	2:C:534:PHE:HE1	1.85	0.42
2:A:221:VAL:HG22	2:A:407:THR:HG21	2.01	0.42
2:C:228:TRP:O	2:C:244:THR:OG1	2.36	0.42
2:C:565:GLU:CD	2:C:565:GLU:H	2.23	0.42
2:A:233:GLN:OE1	2:A:235:LEU:HD23	2.19	0.42
2:A:233:GLN:HB3	2:A:240:ILE:HG22	2.01	0.42
2:C:235:LEU:HD21	2:C:240:ILE:HD12	2.02	0.42
2:C:266:GLY:O	2:C:267:GLY:C	2.58	0.42
2:A:275:PHE:CD1	2:A:275:PHE:C	2.93	0.42
2:A:689:LYS:HA	2:A:689:LYS:HD3	1.63	0.42
2:B:234:TRP:HH2	2:B:301:LEU:HB2	1.85	0.42
2:C:338:LEU:HD13	2:C:338:LEU:HA	1.66	0.42
2:A:380:LEU:HD21	2:C:438:PRO:HB3	2.01	0.42
2:C:275:PHE:CZ	2:C:388:ALA:HB2	2.55	0.42
1:R:69:PHE:HA	1:R:101:GLY:HA3	2.01	0.42
2:A:245:ARG:HH11	2:A:245:ARG:HB2	1.85	0.42
2:A:328:ASN:HB2	2:A:331:VAL:HB	2.01	0.42
2:A:654:VAL:HG12	2:A:656:ALA:N	2.34	0.42
2:B:312:ARG:CD	2:B:416:GLU:HG3	2.41	0.42
2:B:606:VAL:CG1	2:C:625:THR:HG21	2.50	0.42
2:C:322:VAL:C	2:C:323:LYS:HG2	2.40	0.42
2:C:322:VAL:HG12	2:C:323:LYS:N	2.29	0.42
2:A:354:TYR:CE2	2:A:356:LEU:HB2	2.54	0.41
2:A:507:SER:O	2:A:517:LEU:HD12	2.19	0.41
2:B:481:GLY:HA3	2:B:607:TRP:HB3	2.02	0.41
2:A:327:ASP:HB2	2:A:332:LYS:HE3	2.02	0.41
2:A:576:SER:HB2	2:A:595:TRP:CE3	2.55	0.41
2:B:615:GLN:HE22	2:B:726:PRO:HA	1.85	0.41
2:C:586:SER:N	2:C:589:ALA:HB3	2.34	0.41
2:A:346:THR:HA	2:A:646:GLN:O	2.20	0.41
2:B:296:ARG:HH22	2:B:300:ARG:CB	2.33	0.41
2:C:563:GLU:O	2:C:566:ILE:HG12	2.19	0.41
2:B:296:ARG:HG3	2:B:300:ARG:NH2	2.30	0.41
2:B:332:LYS:HZ3	2:B:332:LYS:HG3	1.63	0.41
2:B:520:PRO:O	2:B:634:LEU:HB3	2.21	0.41
2:C:449:LYS:HB2	2:C:449:LYS:HE3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:519:ASN:C	2:C:521:GLY:N	2.74	0.41
2:C:650:LYS:HE2	2:C:650:LYS:HB3	1.80	0.41
2:A:271:ASP:HA	2:A:514:ARG:CD	2.51	0.41
2:A:279:THR:HG21	2:A:377:TYR:HD2	1.85	0.41
2:A:447:LEU:HD12	2:A:462:LYS:O	2.19	0.41
2:A:563:GLU:O	2:A:566:ILE:HG12	2.20	0.41
2:B:296:ARG:O	2:B:297:ASP:C	2.56	0.41
2:B:619:TRP:CE2	2:B:644:PRO:HG2	2.55	0.41
2:A:399:TYR:HB2	2:C:695:TRP:HZ3	1.85	0.41
2:A:574:THR:O	2:C:584:HIS:NE2	2.53	0.41
2:C:262:ASN:HA	2:C:274:TYR:CE1	2.56	0.41
2:A:268:SER:HB2	2:A:269:SER:H	1.63	0.41
2:A:713:PHE:HA	2:A:722:SER:O	2.20	0.41
2:B:328:ASN:N	2:B:331:VAL:O	2.53	0.41
2:B:694:ARG:HD3	2:B:698:GLU:HG2	2.03	0.41
2:C:734:ARG:HG3	2:C:735:ASN:O	2.20	0.41
2:A:581:ALA:HA	2:A:593:THR:HG22	2.02	0.41
2:A:588(A):TRP:CE2	2:A:588(B):PRO:HG3	2.56	0.41
2:A:620:ALA:HB3	2:A:633:PRO:HG3	2.02	0.41
2:A:715:VAL:HA	2:A:720:VAL:O	2.20	0.41
2:B:310:PRO:O	2:B:311:LYS:HD2	2.21	0.41
2:B:317:LEU:HD12	2:B:317:LEU:HA	1.90	0.41
2:B:606:VAL:HG13	2:C:625:THR:OG1	2.21	0.41
2:B:664:LYS:HG3	2:B:665:ASP:N	2.34	0.41
2:A:495:GLN:HB2	2:C:588(A):TRP:CZ3	2.56	0.41
2:C:364:LEU:HD22	2:C:372:PHE:CZ	2.56	0.41
2:B:303:ASN:HB3	2:B:700:GLN:NE2	2.36	0.40
2:B:339:THR:HB	2:B:340:SER:H	1.71	0.40
2:A:559:MET:HE2	2:A:559:MET:HB2	1.91	0.40
2:B:529:GLU:HB2	2:C:512:ASN:HD21	1.85	0.40
2:C:328:ASN:ND2	2:C:333:THR:OG1	2.54	0.40
1:R:22:TRP:HE3	1:R:36:LEU:CD1	2.35	0.40
1:R:41:TRP:CE2	1:R:220:PRO:HG3	2.57	0.40
2:A:246:THR:OG1	2:A:371:VAL:HG13	2.22	0.40
2:A:450:THR:HG23	2:B:500:GLU:OE1	2.21	0.40
2:A:584:HIS:NE2	2:B:574:THR:O	2.55	0.40
2:C:258:LYS:HG3	2:C:278:SER:OG	2.22	0.40
2:C:450:THR:HA	2:C:460:THR:O	2.22	0.40
2:A:393:SER:HB2	2:C:694:ARG:HG3	2.03	0.40
2:A:485:ARG:HG3	2:A:486:GLN:N	2.37	0.40
2:A:588(E):TYR:C	2:A:588(G):ALA:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ILE:H	2:B:240:ILE:HG12	1.61	0.40
2:B:343:GLN:HA	2:B:403:GLN:O	2.21	0.40
2:B:506:ALA:CB	2:B:517:LEU:HD11	2.51	0.40
2:B:525:ALA:HB3	2:B:572:VAL:HA	2.03	0.40
2:C:297:ASP:HA	2:C:300:ARG:HD2	2.02	0.40
2:C:454:SER:O	2:C:455:GLY:C	2.59	0.40
2:C:490:SER:HB2	2:C:534:PHE:CE1	2.56	0.40
2:A:584:HIS:HE2	2:B:574:THR:HB	1.86	0.40
2:B:298:TRP:CZ2	2:B:729:THR:HG22	2.57	0.40
2:B:506:ALA:O	2:B:507:SER:HB2	2.21	0.40
2:C:701:TYR:HB2	2:C:731:TYR:CZ	2.56	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	R	254/256 (99%)	226 (89%)	27 (11%)	1 (0%)	30	36
2	A	523/525 (100%)	454 (87%)	49 (9%)	20 (4%)	2	1
2	B	523/525 (100%)	469 (90%)	40 (8%)	14 (3%)	4	2
2	C	523/525 (100%)	464 (89%)	42 (8%)	17 (3%)	3	1
All	All	1823/1831 (100%)	1613 (88%)	158 (9%)	52 (3%)	6	2

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	51	SER
2	A	248	ALA
2	A	588(B)	PRO
2	B	329	ASN

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Mol	Chain	Res	Type
2	B	497	ASN
2	B	520	PRO
2	B	664	LYS
2	C	320	ILE
2	C	333	THR
2	C	457	ASN
2	C	519	ASN
2	C	588(A)	TRP
2	A	328	ASN
2	A	454	SER
2	A	496	ASN
2	B	339	THR
2	B	588(D)	SER
2	B	656	ALA
2	C	252	TYR
2	A	228	TRP
2	A	671	ILE
2	B	340	SER
2	B	452	ASN
2	B	455	GLY
2	C	329	ASN
2	A	231	ASP
2	A	252	TYR
2	A	299	GLN
2	A	374	ILE
2	A	588(E)	TYR
2	A	658	PRO
2	A	706	TYR
2	A	707	LYS
2	B	252	TYR
2	B	453	GLY
2	B	507	SER
2	C	588(F)	ASP
2	C	588(G)	ALA
2	A	456	GLN
2	C	253	ASN
2	C	321	GLN
2	C	507	SER
2	C	588(C)	THR
2	A	232	SER
2	B	588(C)	THR
2	C	493	VAL

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Mol	Chain	Res	Type
2	C	266	GLY
2	C	325	VAL
2	A	236	GLY
2	A	519	ASN
2	C	520	PRO
2	A	493	VAL

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	R	232/232 (100%)	219 (94%)	13 (6%)	17	23
2	A	459/459 (100%)	379 (83%)	80 (17%)	1	1
2	B	459/459 (100%)	411 (90%)	48 (10%)	5	5
2	C	459/459 (100%)	405 (88%)	54 (12%)	4	4
All	All	1609/1609 (100%)	1414 (88%)	195 (12%)	6	4

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	26	ILE
1	R	72	VAL
1	R	83	LYS
1	R	85	ASN
1	R	93	LEU
1	R	115	LEU
1	R	137	GLU
1	R	141	VAL
1	R	209	THR
1	R	219	THR
1	R	229	THR
1	R	230	VAL
1	R	235	ILE
2	A	223	SER
2	A	225	SER

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Mol	Chain	Res	Type
2	A	228	TRP
2	A	229	HIS
2	A	232	SER
2	A	233	GLN
2	A	234	TRP
2	A	235	LEU
2	A	238	ARG
2	A	243	SER
2	A	246	THR
2	A	253	ASN
2	A	254	ASN
2	A	256	LEU
2	A	258	LYS
2	A	261	SER
2	A	262	ASN
2	A	268	SER
2	A	269	SER
2	A	270	ASN
2	A	278	SER
2	A	296	ARG
2	A	302	ILE
2	A	309	ARG
2	A	312	ARG
2	A	313	LEU
2	A	315	PHE
2	A	316	LYS
2	A	321	GLN
2	A	323	LYS
2	A	324	GLU
2	A	326	THR
2	A	328	ASN
2	A	332	LYS
2	A	333	THR
2	A	334	ILE
2	A	341	THR
2	A	342	VAL
2	A	343	GLN
2	A	344	VAL
2	A	346	THR
2	A	349	ASP
2	A	361	GLU
2	A	373	MET

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Mol	Chain	Res	Type
2	A	404	MET
2	A	405	LEU
2	A	406	ARG
2	A	412	GLN
2	A	418	GLU
2	A	419	ASN
2	A	425	SER
2	A	449	LYS
2	A	452	ASN
2	A	457	ASN
2	A	462	LYS
2	A	470	ASN
2	A	493	VAL
2	A	495	GLN
2	A	507	SER
2	A	514	ARG
2	A	518	MET
2	A	526	SER
2	A	528	LYS
2	A	532	ASP
2	A	550	ARG
2	A	559	MET
2	A	562	ASN
2	A	565	GLU
2	A	567	LYS
2	A	579	GLN
2	A	580	VAL
2	A	588(F)	ASP
2	A	640	MET
2	A	651	ASN
2	A	657	ASP
2	A	702	THR
2	A	703	SER
2	A	704	ASN
2	A	707	LYS
2	A	712	GLU
2	B	225	SER
2	B	233	GLN
2	B	235	LEU
2	B	238	ARG
2	B	240	ILE
2	B	243	SER

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Mol	Chain	Res	Type
2	B	251	THR
2	B	260	ILE
2	B	265	SER
2	B	290	HIS
2	B	312	ARG
2	B	313	LEU
2	B	321	GLN
2	B	323	LYS
2	B	326	THR
2	B	331	VAL
2	B	332	LYS
2	B	333	THR
2	B	339	THR
2	B	341	THR
2	B	343	GLN
2	B	349	ASP
2	B	352	LEU
2	B	413	PHE
2	B	424	SER
2	B	451	ILE
2	B	458	GLN
2	B	470	ASN
2	B	485	ARG
2	B	493	VAL
2	B	494	THR
2	B	495	GLN
2	B	517	LEU
2	B	518	MET
2	B	533	ARG
2	B	588	GLN
2	B	588(A)	TRP
2	B	588(E)	TYR
2	B	657	ASP
2	B	664	LYS
2	B	665	ASP
2	B	666	LYS
2	B	668	ASN
2	B	671	ILE
2	B	676	THR
2	B	682	GLU
2	B	707	LYS
2	B	718	GLU

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Mol	Chain	Res	Type
2	C	230	CYS
2	C	233	GLN
2	C	235	LEU
2	C	251	THR
2	C	258	LYS
2	C	260	ILE
2	C	261	SER
2	C	265	SER
2	C	270	ASN
2	C	290	HIS
2	C	300	ARG
2	C	312	ARG
2	C	313	LEU
2	C	317	LEU
2	C	321	GLN
2	C	332	LYS
2	C	333	THR
2	C	338	LEU
2	C	341	THR
2	C	342	VAL
2	C	407	THR
2	C	410	ASN
2	C	412	GLN
2	C	419	ASN
2	C	439	LEU
2	C	449	LYS
2	C	456	GLN
2	C	457	ASN
2	C	458	GLN
2	C	495	GLN
2	C	528	LYS
2	C	532	ASP
2	C	533	ARG
2	C	540	SER
2	C	550	ARG
2	C	559	MET
2	C	565	GLU
2	C	567	LYS
2	C	586	SER
2	C	588	GLN
2	C	588(A)	TRP
2	C	588(E)	TYR

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Mol	Chain	Res	Type
2	C	590	GLN
2	C	640	MET
2	C	641	LYS
2	C	657	ASP
2	C	660	THR
2	C	666	LYS
2	C	668	ASN
2	C	671	ILE
2	C	702	THR
2	C	707	LYS
2	C	727	ILE
2	C	730	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	85	ASN
1	R	127	HIS
2	A	229	HIS
2	A	254	ASN
2	A	255	HIS
2	A	314	ASN
2	A	321	GLN
2	A	412	GLN
2	A	458	GLN
2	A	470	ASN
2	A	497	ASN
2	A	590	GLN
2	A	646	GLN
2	A	678	GLN
2	A	735	ASN
2	B	229	HIS
2	B	233	GLN
2	B	255	HIS
2	B	419	ASN
2	B	470	ASN
2	B	496	ASN
2	B	519	ASN
2	B	663	ASN
2	B	678	GLN
2	B	688	GLN
2	B	700	GLN

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Mol	Chain	Res	Type
2	C	227	ASN
2	C	321	GLN
2	C	329	ASN
2	C	403	GLN
2	C	410	ASN
2	C	452	ASN
2	C	579	GLN
2	C	588	GLN
2	C	678	GLN
2	C	735	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

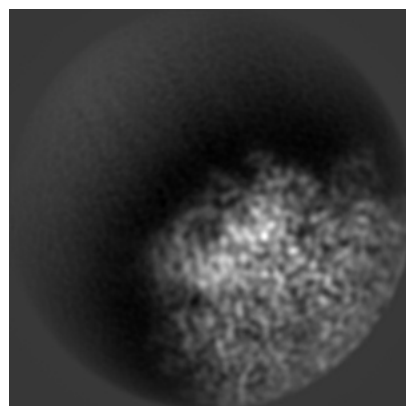
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36311. These allow visual inspection of the internal detail of the map and identification of artifacts.

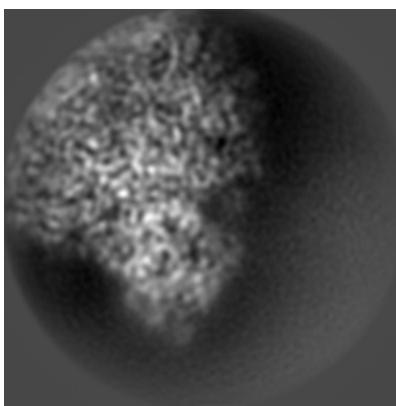
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

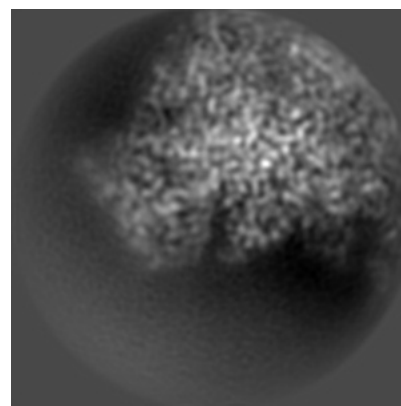
6.1.1 Primary map



X

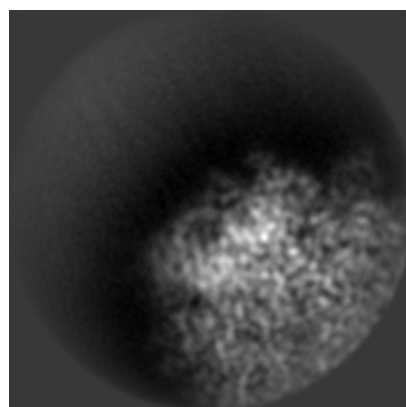


Y

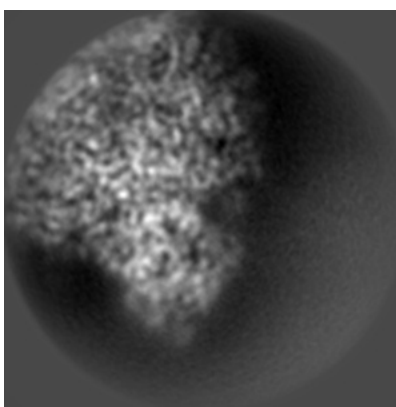


Z

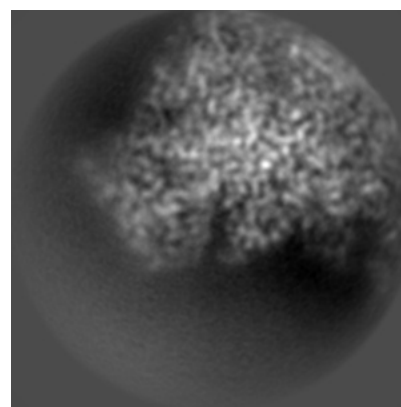
6.1.2 Raw map



X



Y

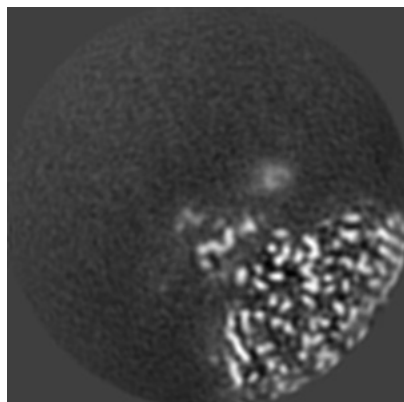


Z

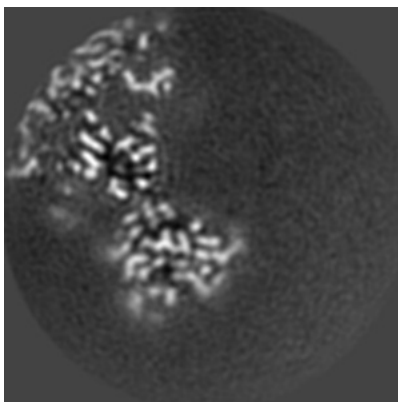
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

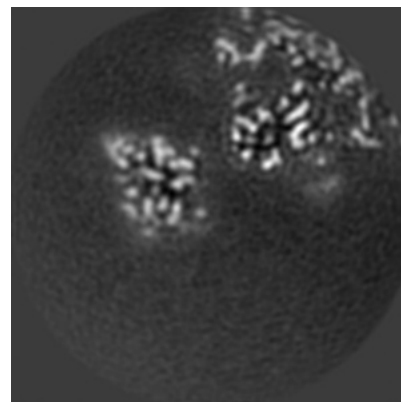
6.2.1 Primary map



X Index: 80

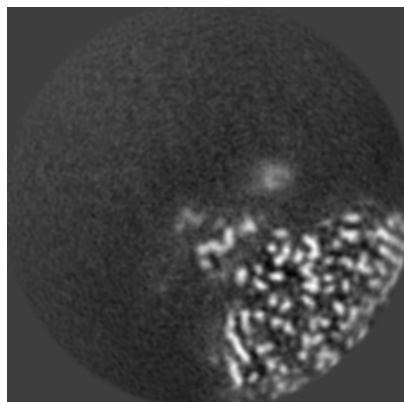


Y Index: 80

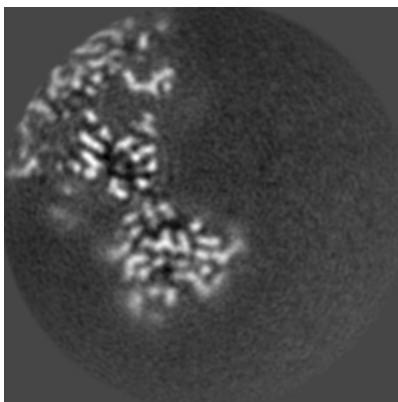


Z Index: 80

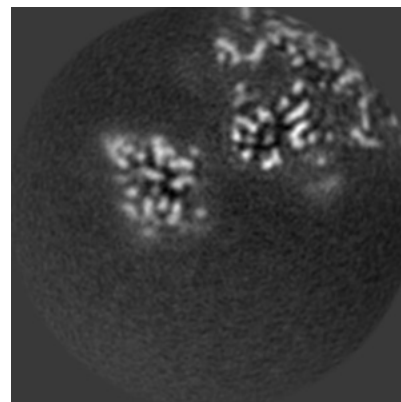
6.2.2 Raw map



X Index: 80



Y Index: 80

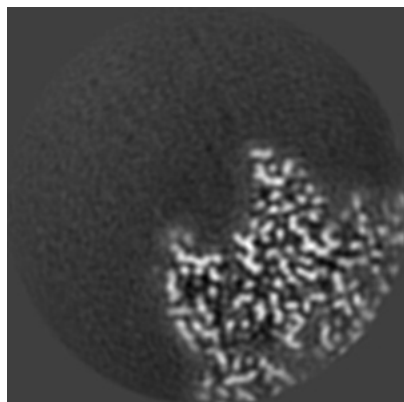


Z Index: 80

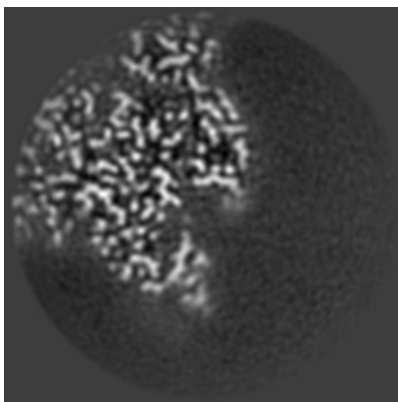
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

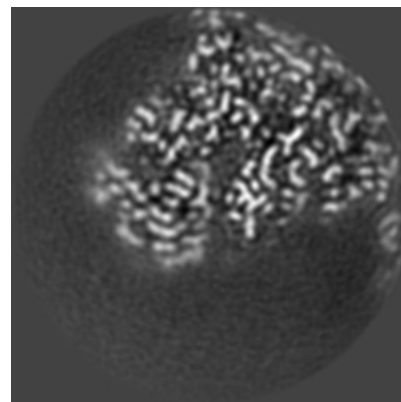
6.3.1 Primary map



X Index: 95

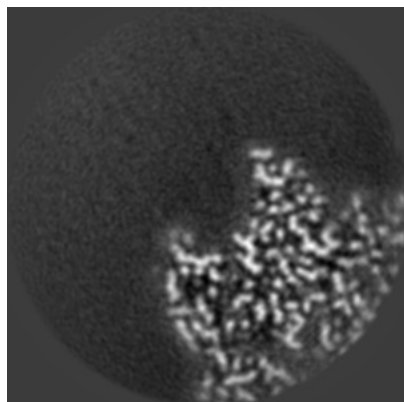


Y Index: 107

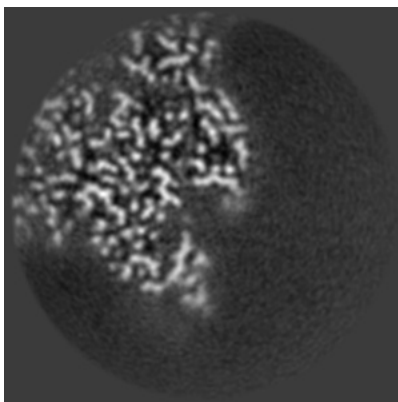


Z Index: 59

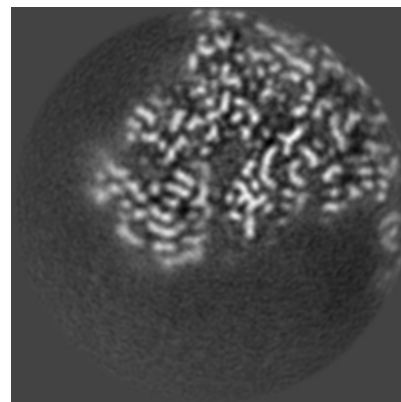
6.3.2 Raw map



X Index: 95



Y Index: 107

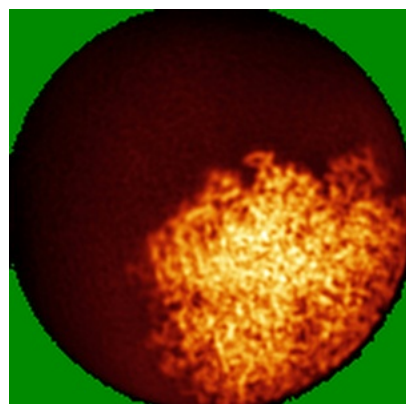


Z Index: 59

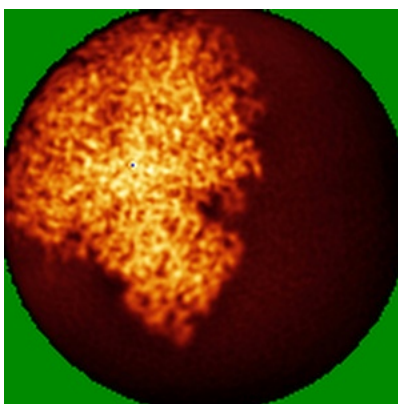
The images above show the largest variance slices of the map in three orthogonal directions.

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

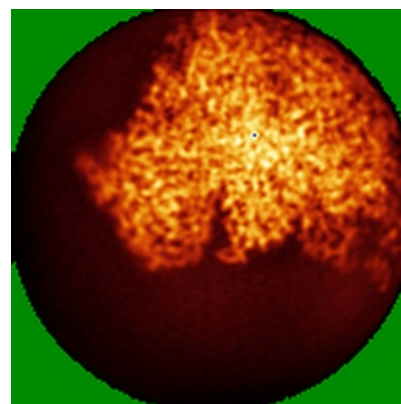
6.4.1 Primary map



X

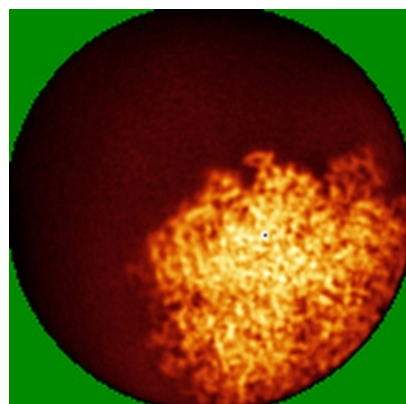


Y

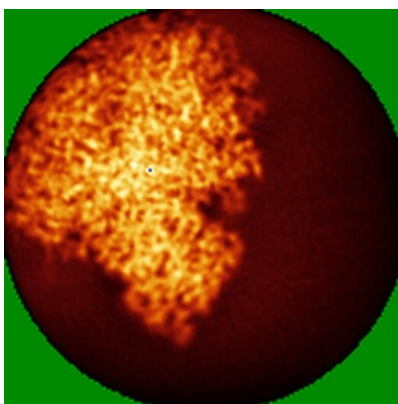


Z

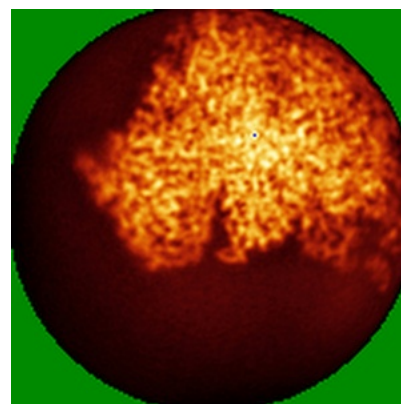
6.4.2 Raw map



X



Y

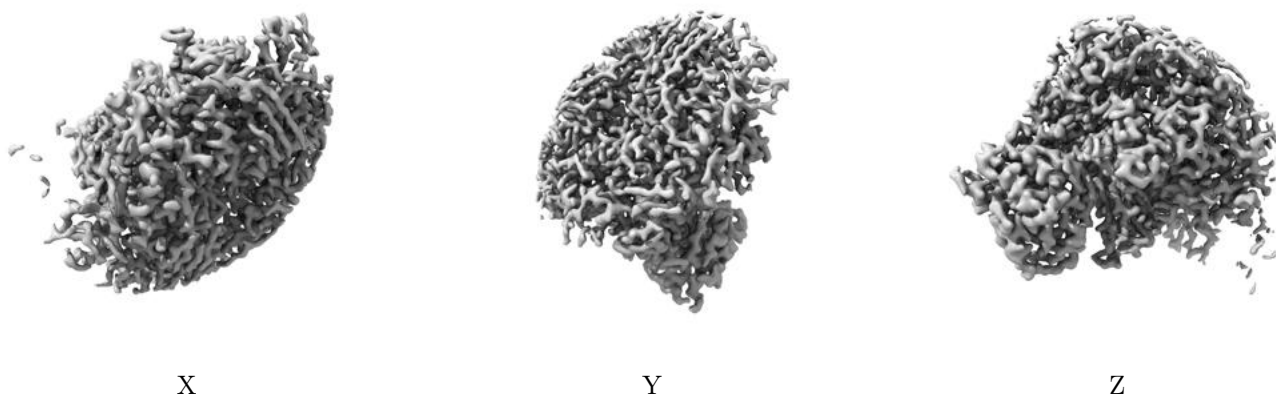


Z

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 0.01. 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.

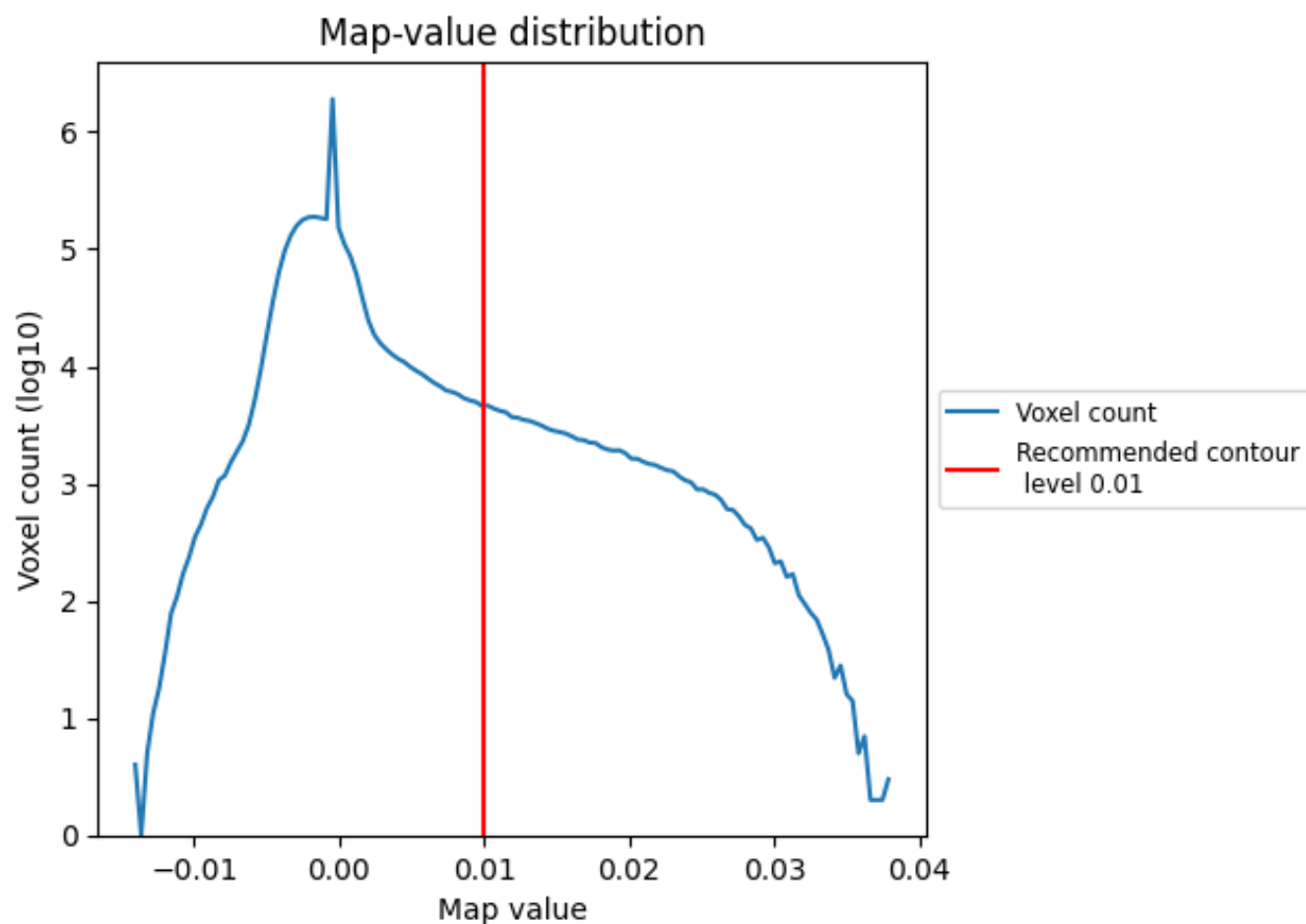
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

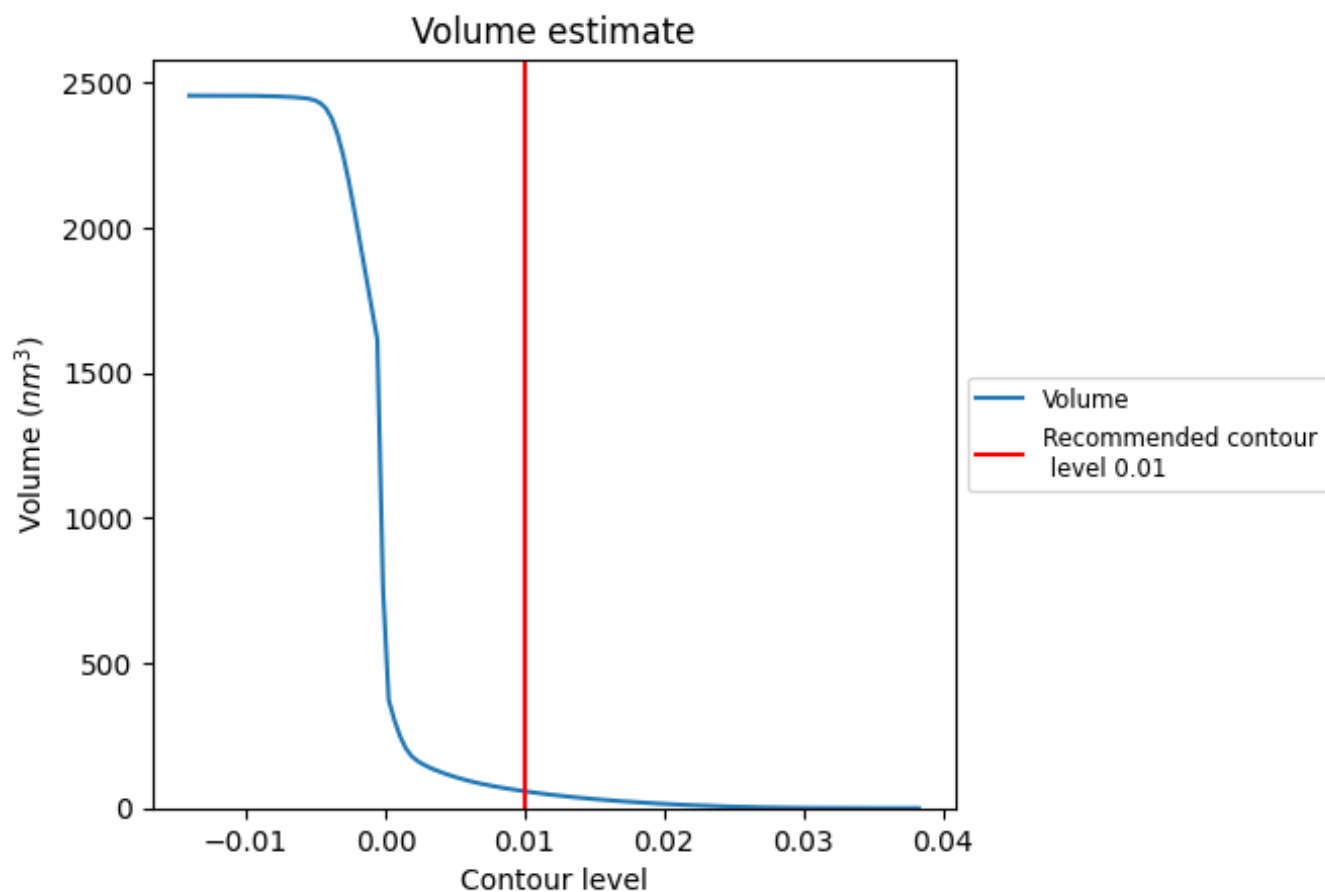
This section contains the results of statistical analysis of the map.

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.

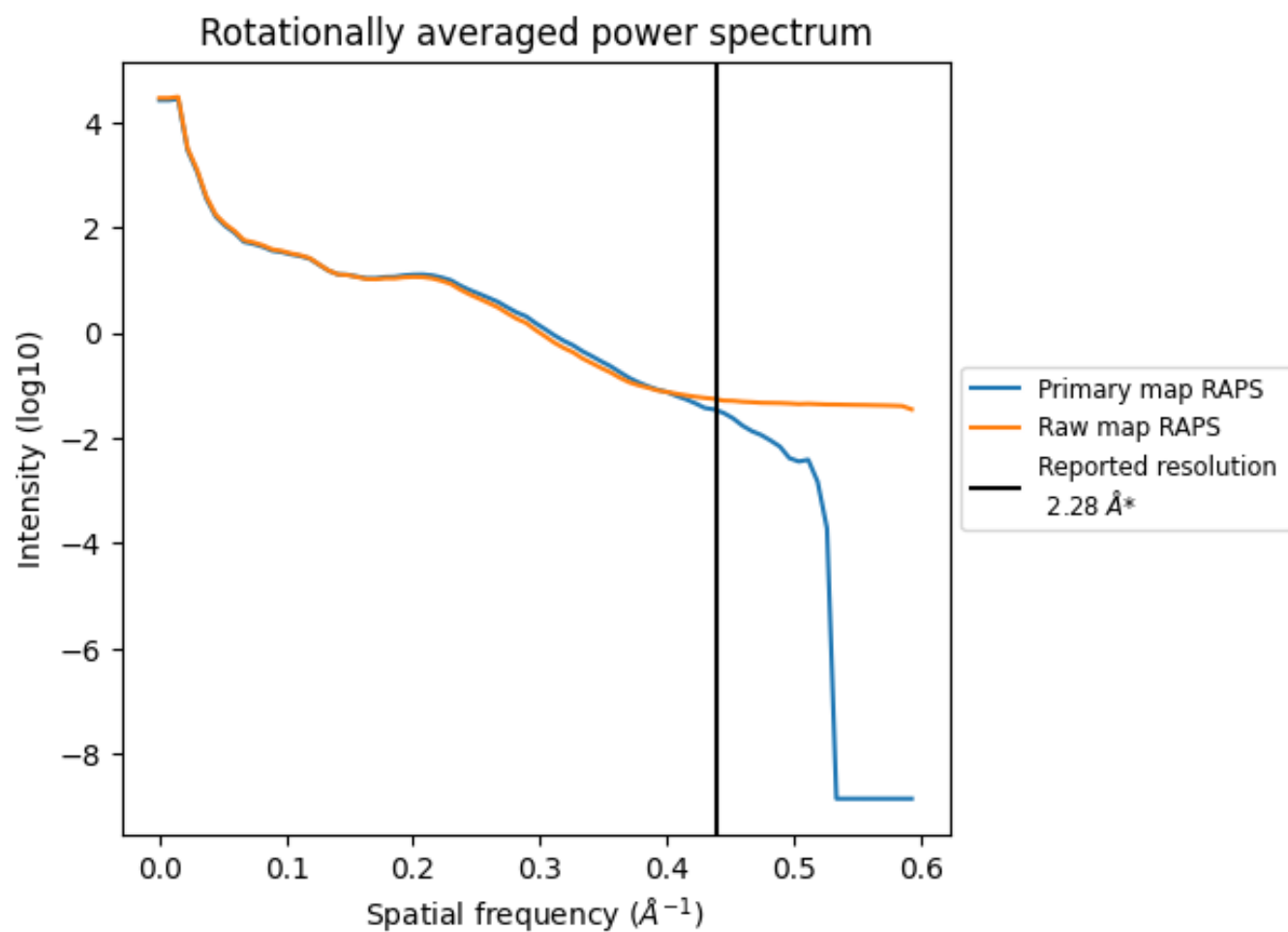
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm^3 ; this corresponds to an approximate mass of 53 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 ⓘ

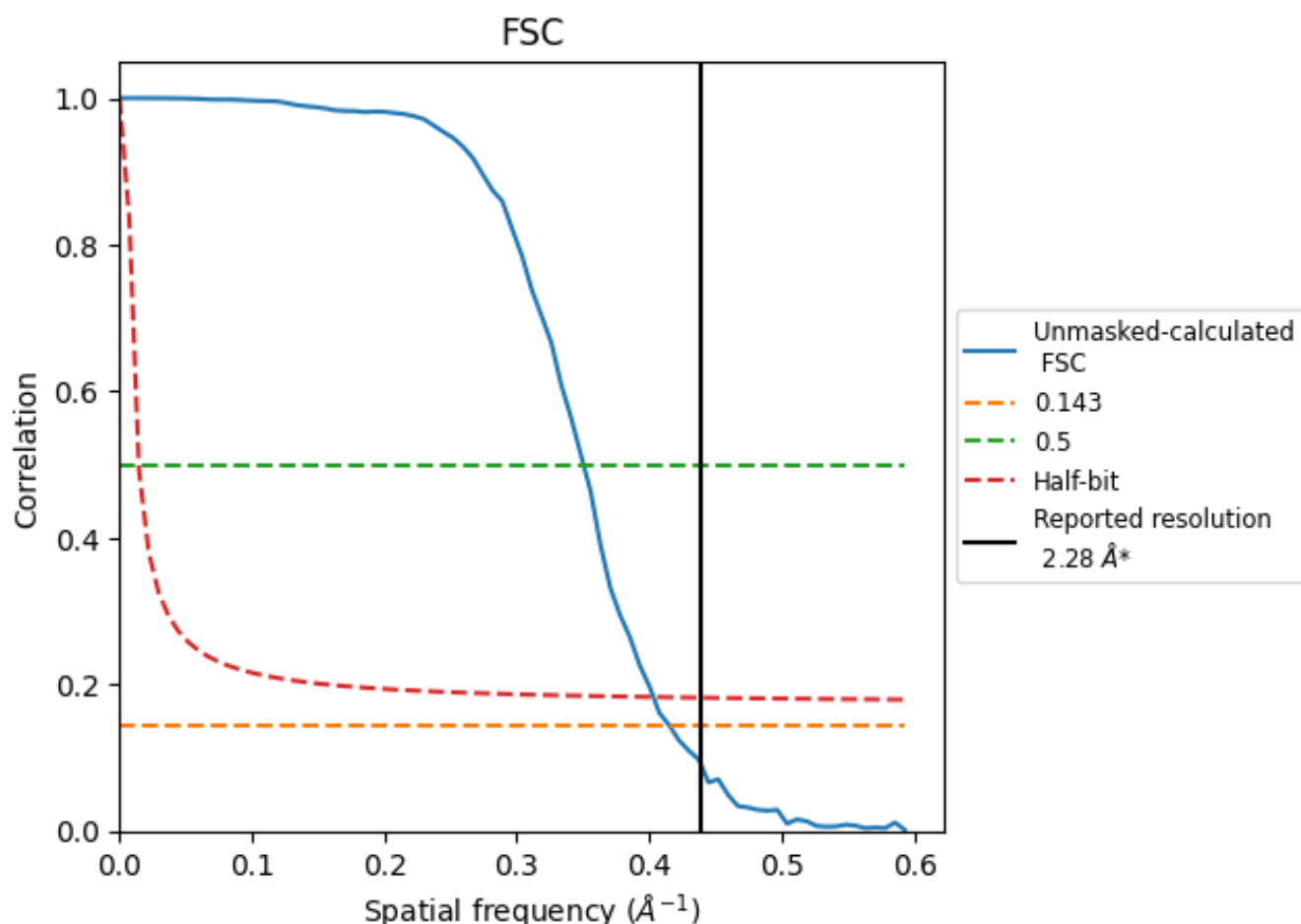


*Reported resolution corresponds to spatial frequency of 0.439 Å⁻¹

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 0.439 \AA^{-1}

8.2 Resolution estimates [i](#)

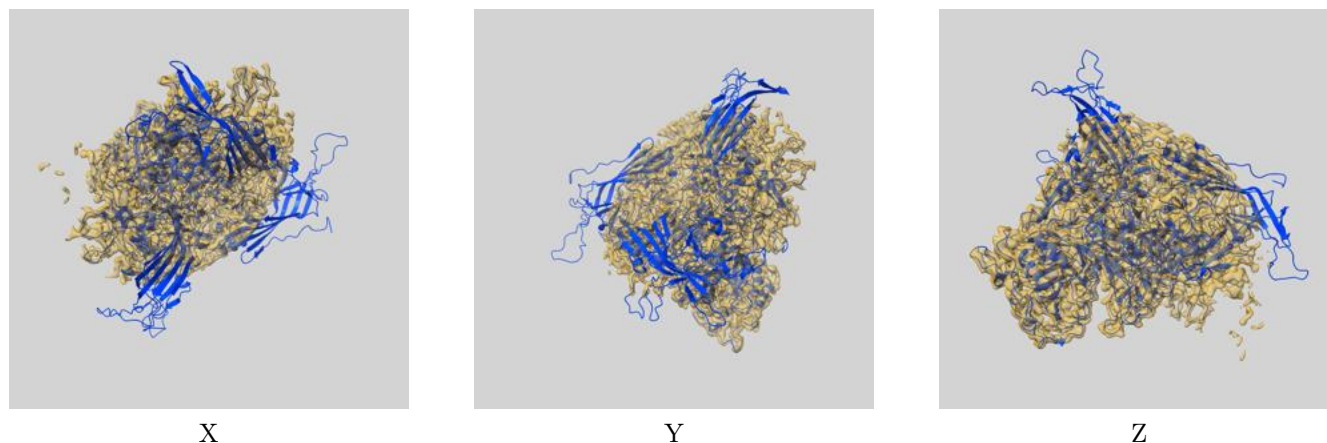
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.41	2.85	2.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

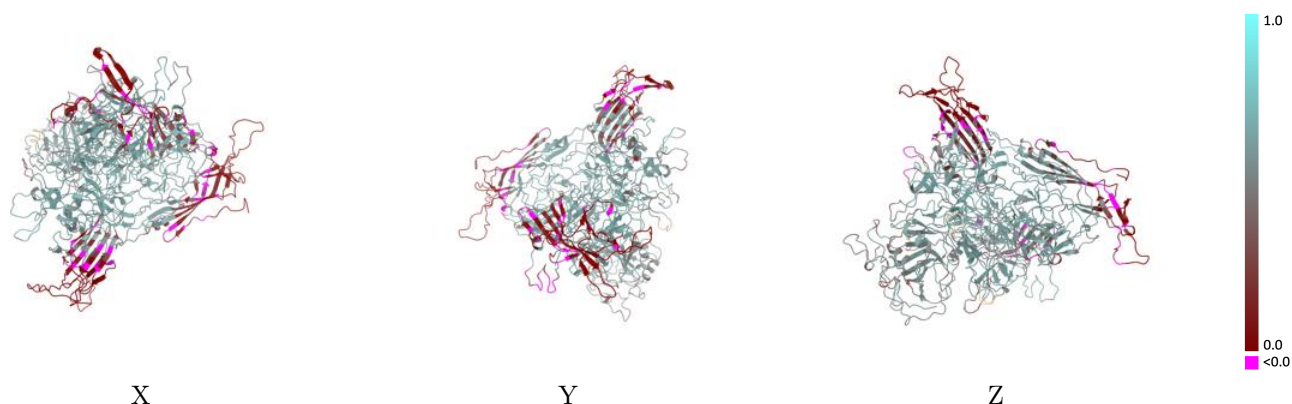
This section contains information regarding the fit between EMDB map EMD-36311 and PDB model 8JIF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



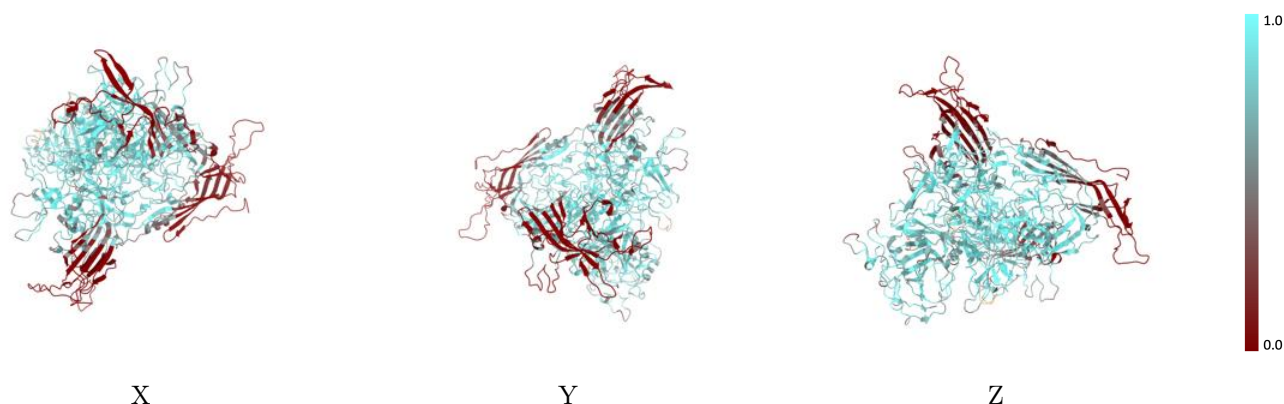
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



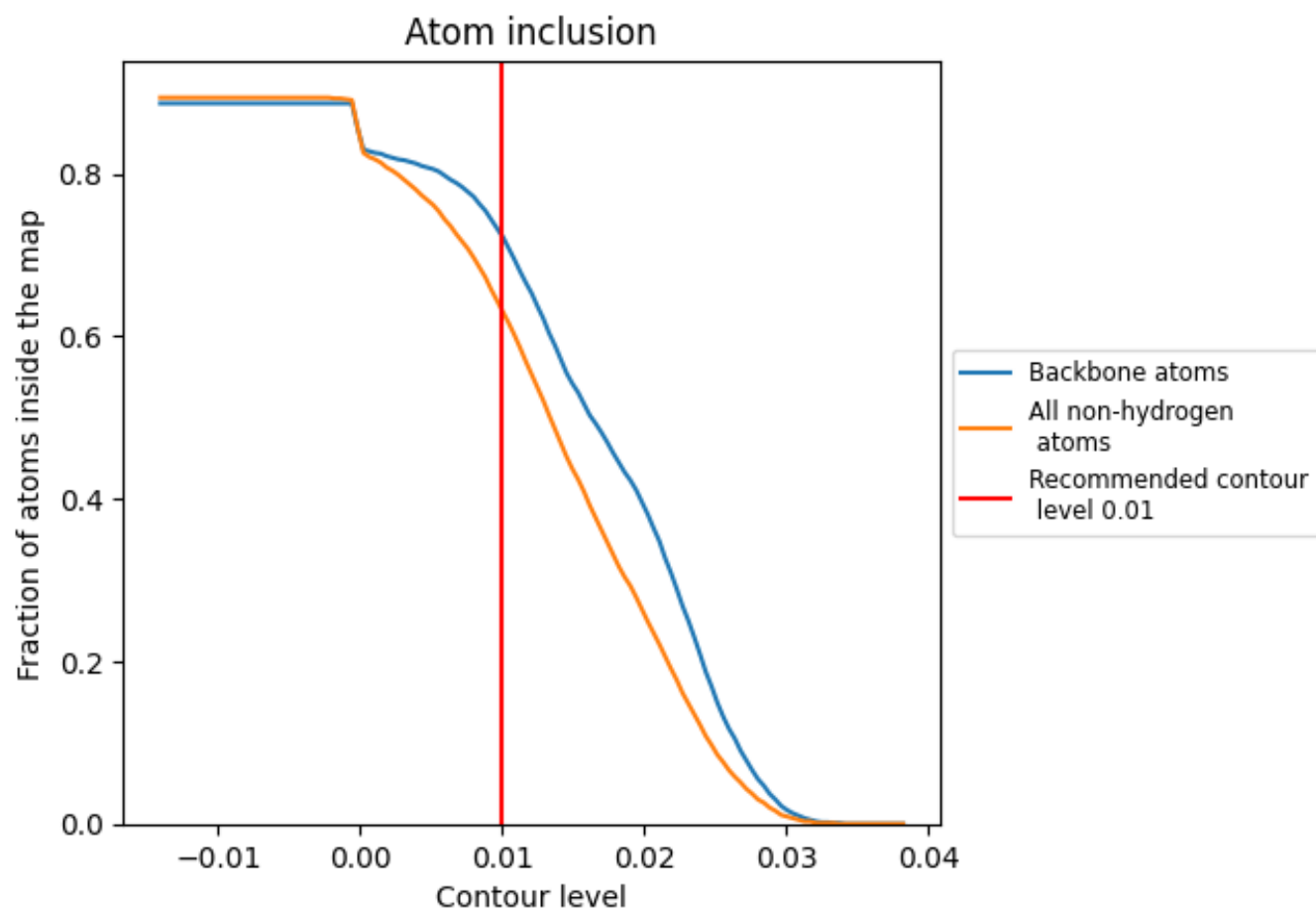
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 63% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6330	<div></div> 0.4730
A	<div></div> 0.6570	<div></div> 0.4910
B	<div></div> 0.5600	<div></div> 0.4320
C	<div></div> 0.6300	<div></div> 0.4770
R	<div></div> 0.7360	<div></div> 0.5090

