Full wwPDB EM Validation Report (i)

Mar 5, 2026 – 10:25 PM UTC

PDB ID	:	9LC1 / pdb_00009lc1
EMDB ID	:	EMD-62962
Title	:	portal of mature phage N4
Authors	:	Liu, H.; Chen, W.
Deposited on	:	2025-01-03
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

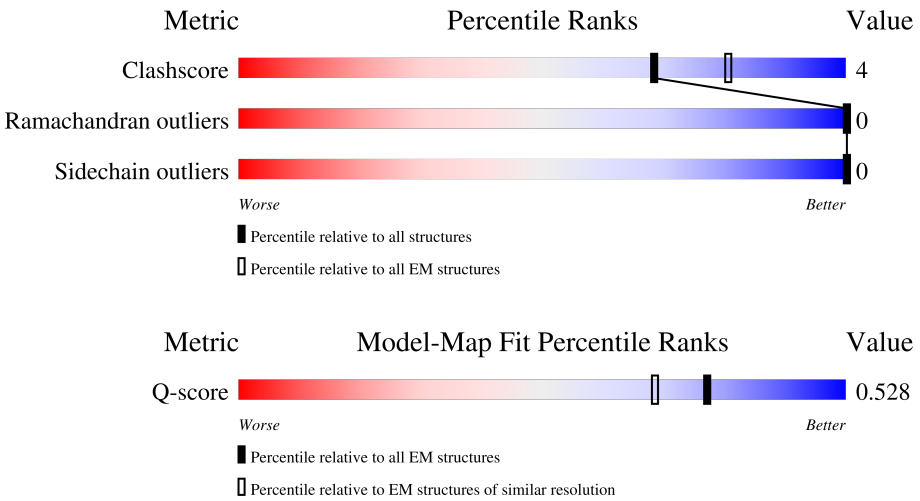
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 <=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	763	9% 79% 10% 12%
1	B	763	9% 78% 10% 12%
1	C	763	10% 79% 9% 12%
1	D	763	9% 80% 8% 12%

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Mol	Chain	Length	Quality of chain
1	E	763	9% 80% 9% 12%
1	F	763	10% 79% 9% 12%
1	G	763	9% 80% 8% 12%
1	H	763	9% 79% 9% 12%
1	I	763	10% 79% 9% 12%
1	J	763	9% 79% 9% 12%
1	K	763	9% 79% 9% 12%
1	L	763	10% 80% 9% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 64272 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 Probable portal protein.

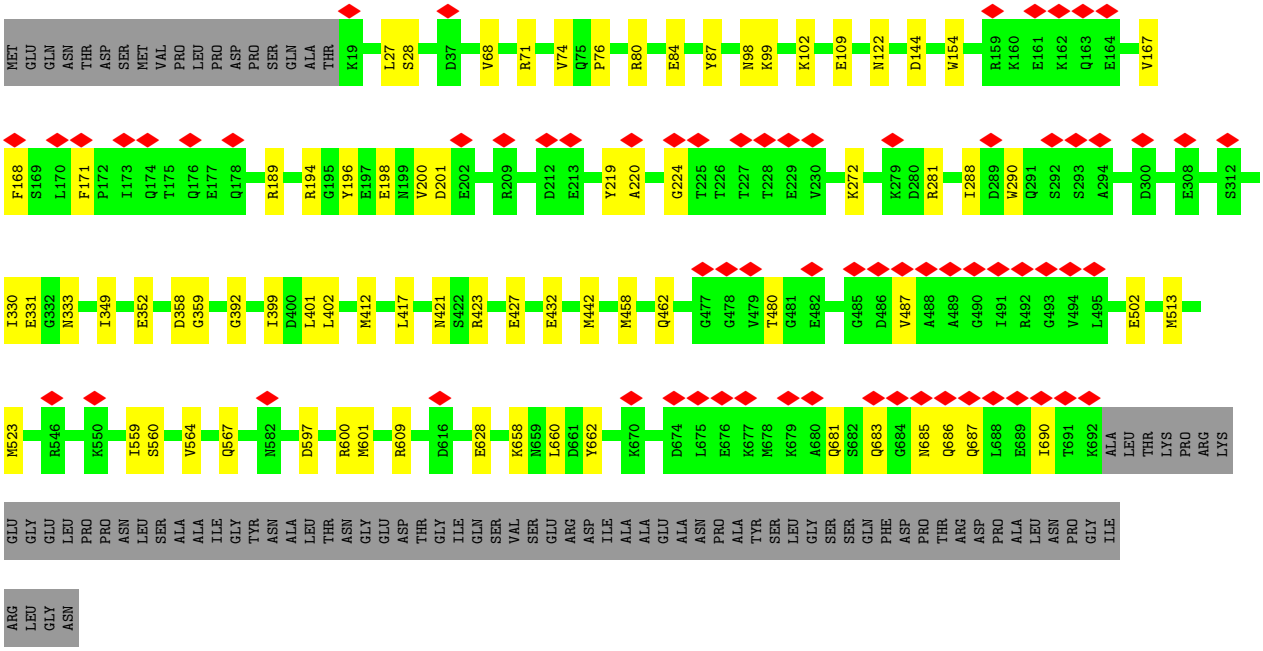
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	674	5356	3357	942	1034	23	0	0
1	B	674	5356	3357	942	1034	23	0	0
1	C	674	5356	3357	942	1034	23	0	0
1	D	674	5356	3357	942	1034	23	0	0
1	E	674	5356	3357	942	1034	23	0	0
1	F	674	5356	3357	942	1034	23	0	0
1	G	674	5356	3357	942	1034	23	0	0
1	H	674	5356	3357	942	1034	23	0	0
1	I	674	5356	3357	942	1034	23	0	0
1	J	674	5356	3357	942	1034	23	0	0
1	K	674	5356	3357	942	1034	23	0	0
1	L	674	5356	3357	942	1034	23	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

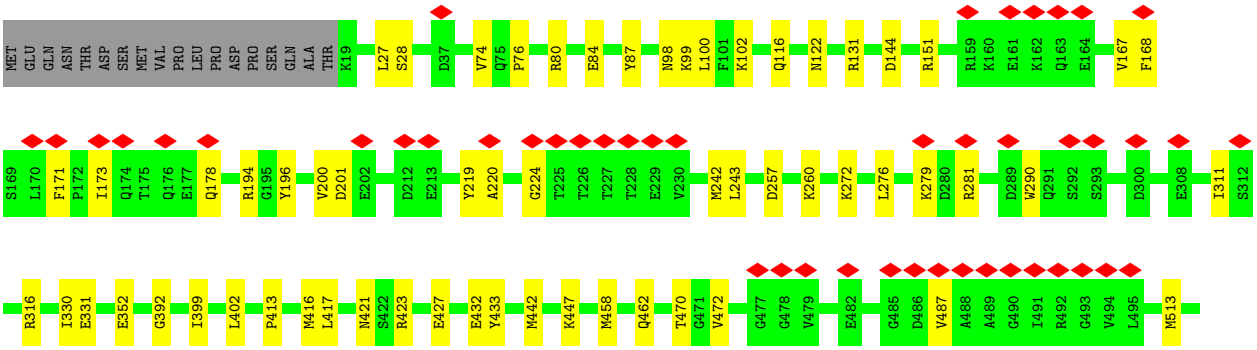
• Molecule 1: Probable portal protein

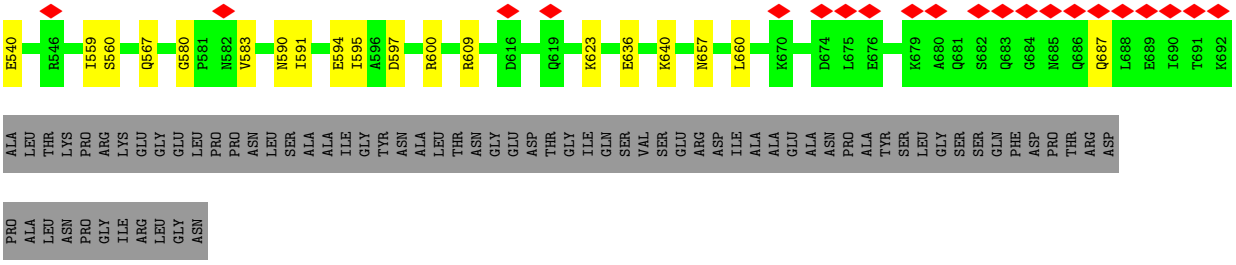
Chain A:



• Molecule 1: Probable portal protein

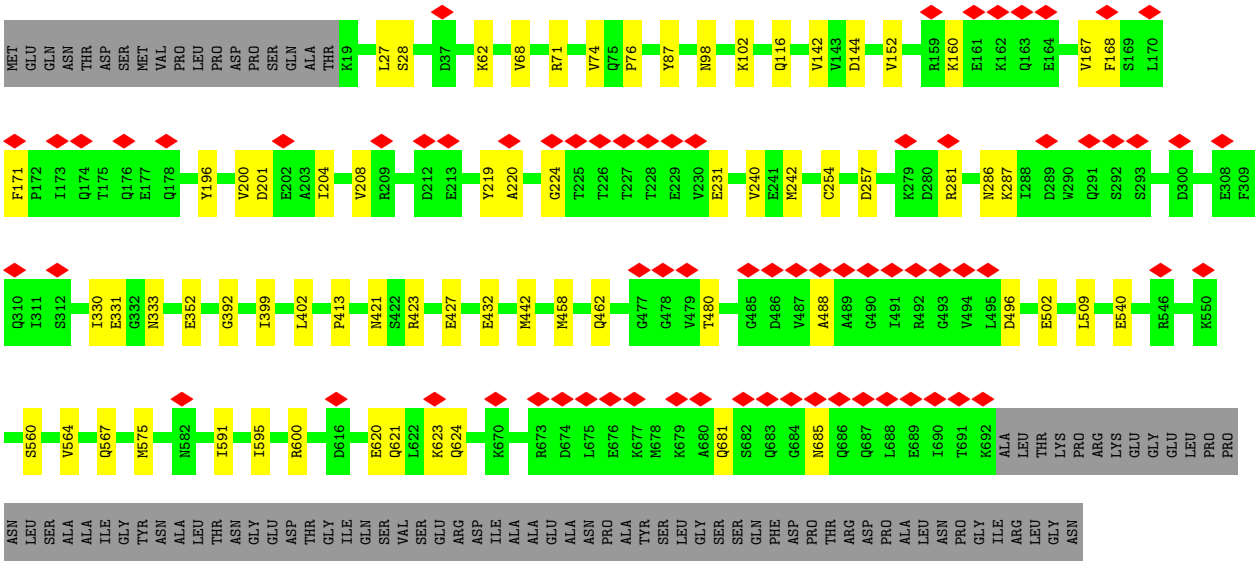
Chain B:





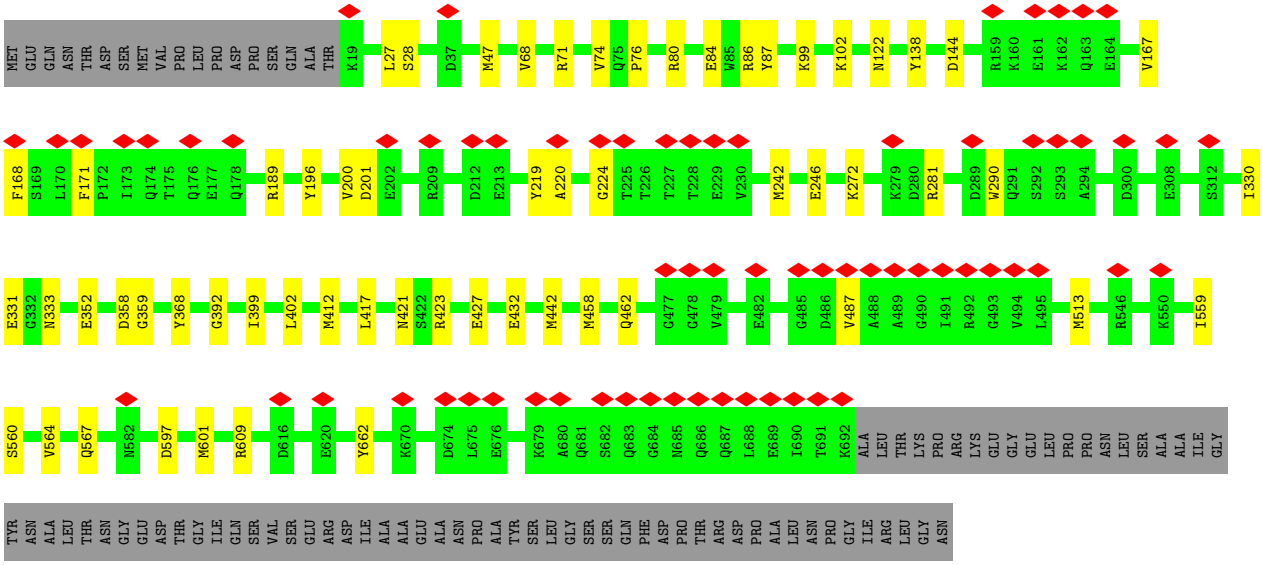
• Molecule 1: Probable portal protein

Chain C:



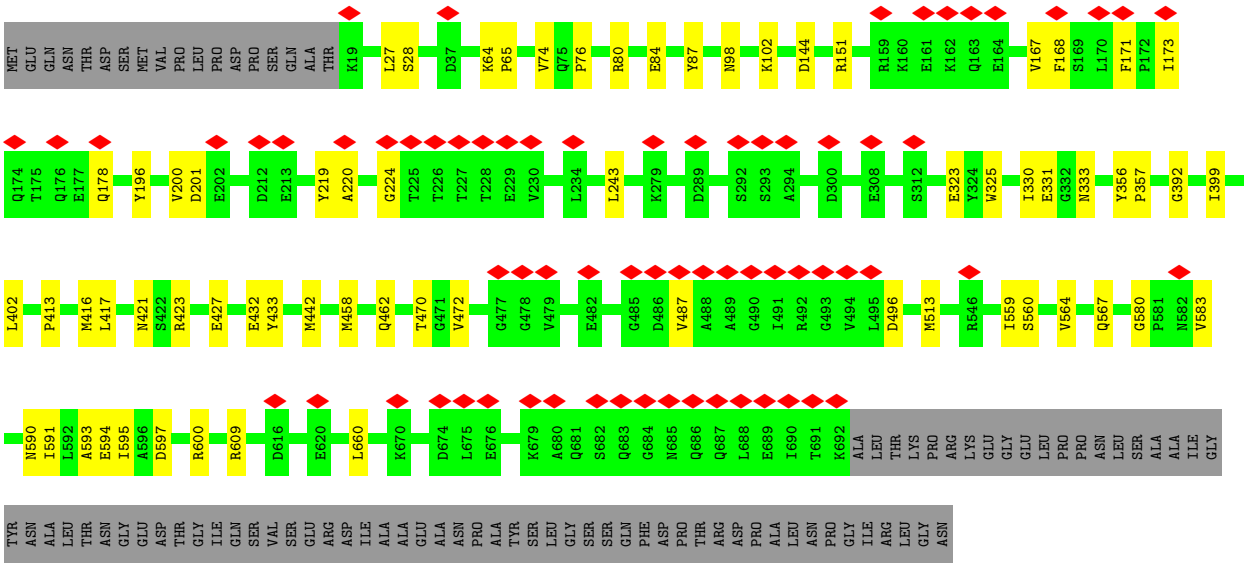
• Molecule 1: Probable portal protein

Chain D:



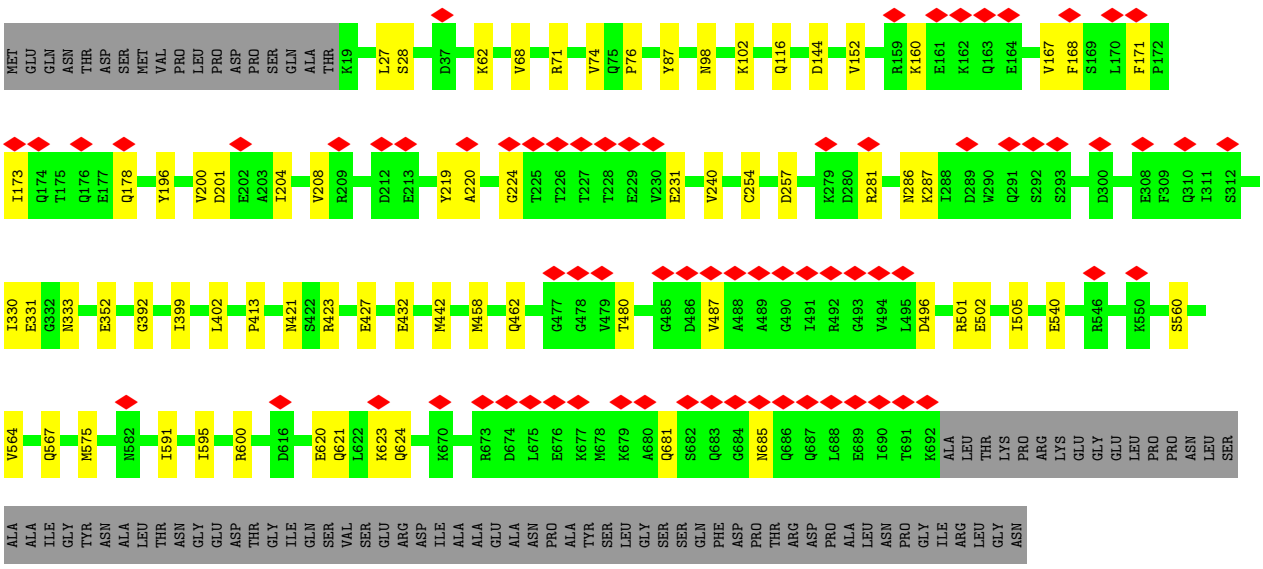
- Molecule 1: Probable portal protein

Chain E:



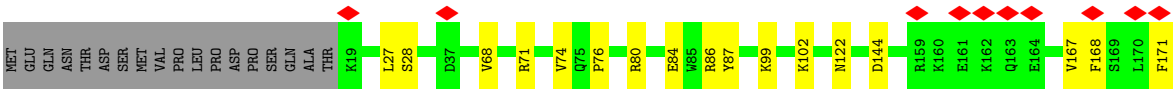
- Molecule 1: Probable portal protein

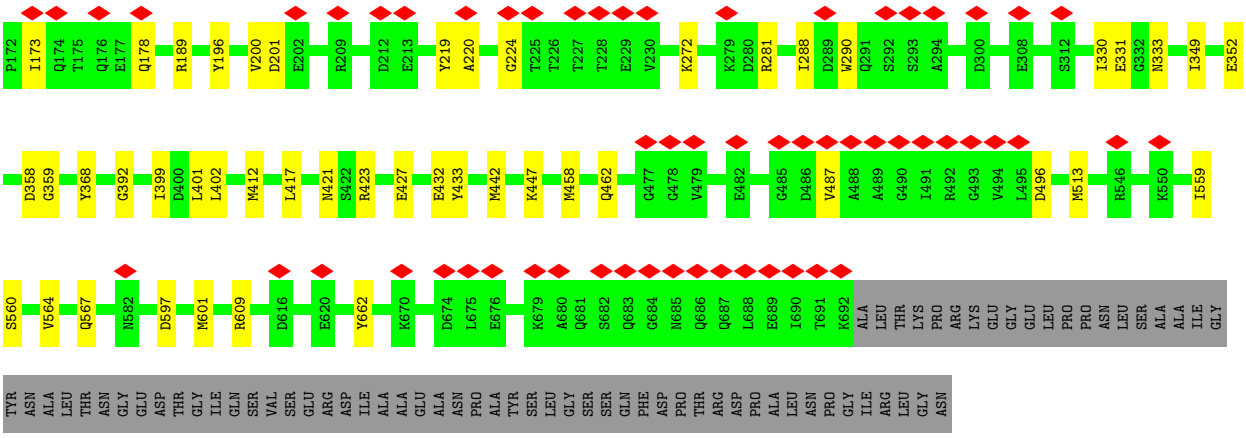
Chain F:



- Molecule 1: Probable portal protein

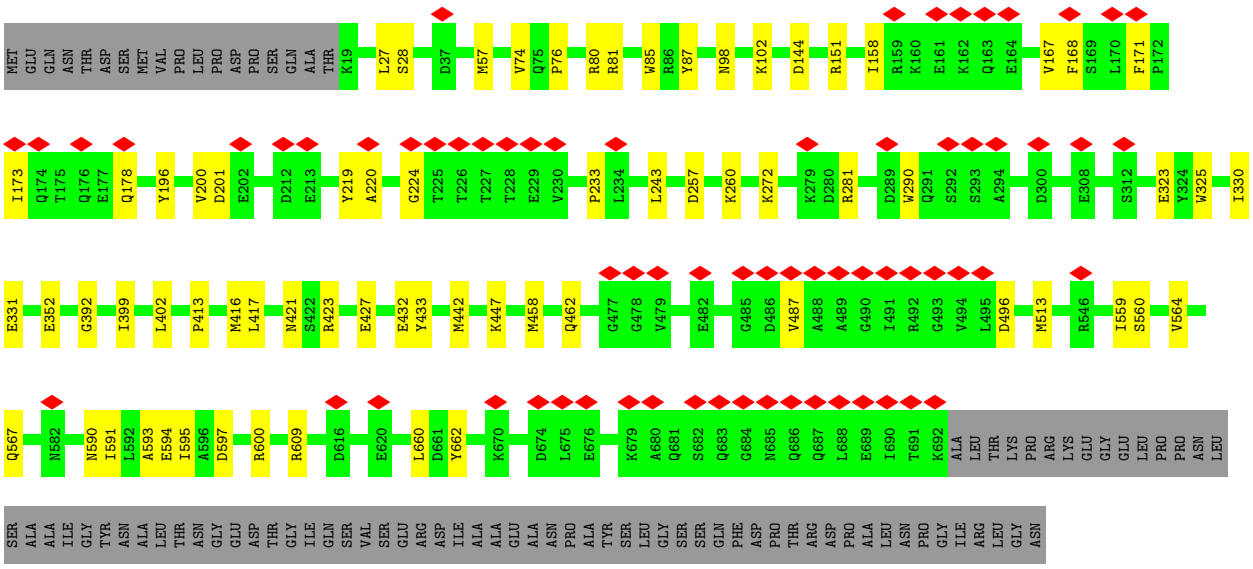
Chain G:





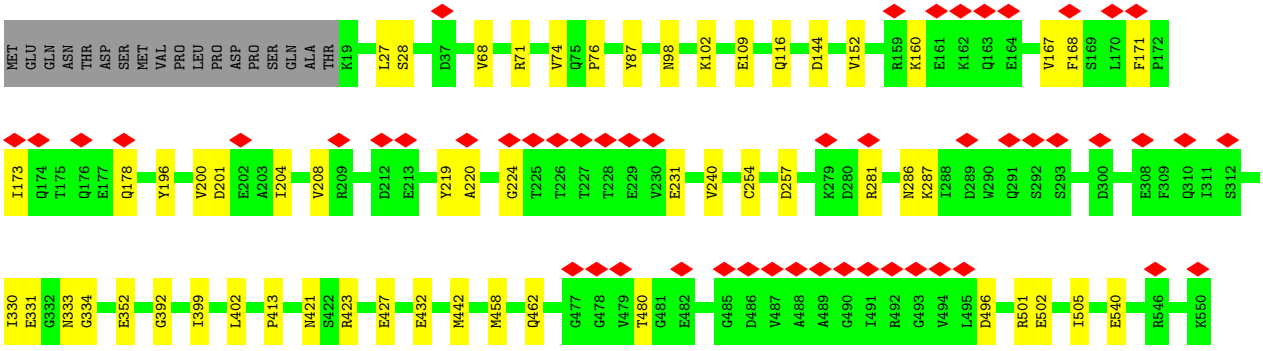
- Molecule 1: Probable portal protein

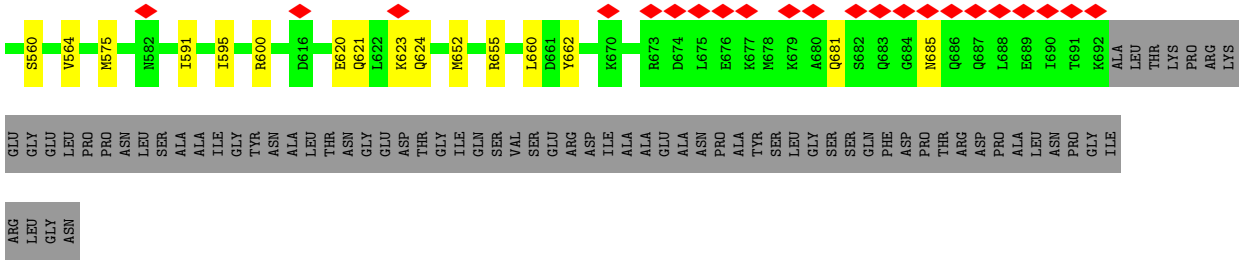
Chain H:



- Molecule 1: Probable portal protein

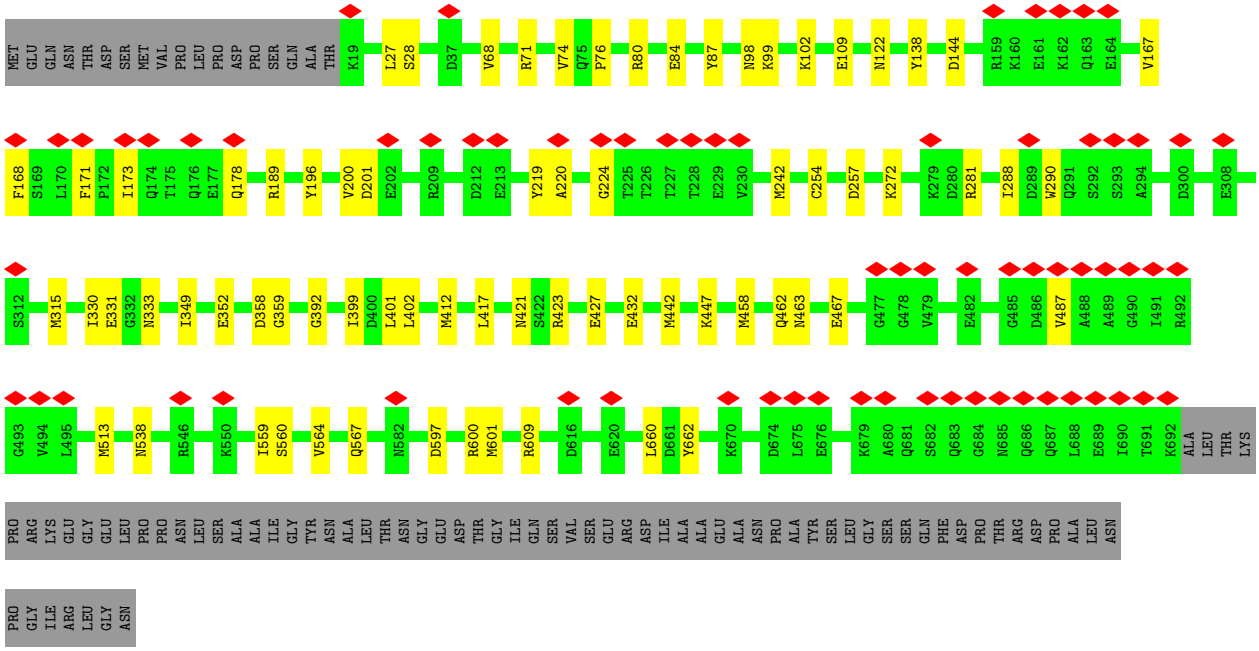
Chain I:





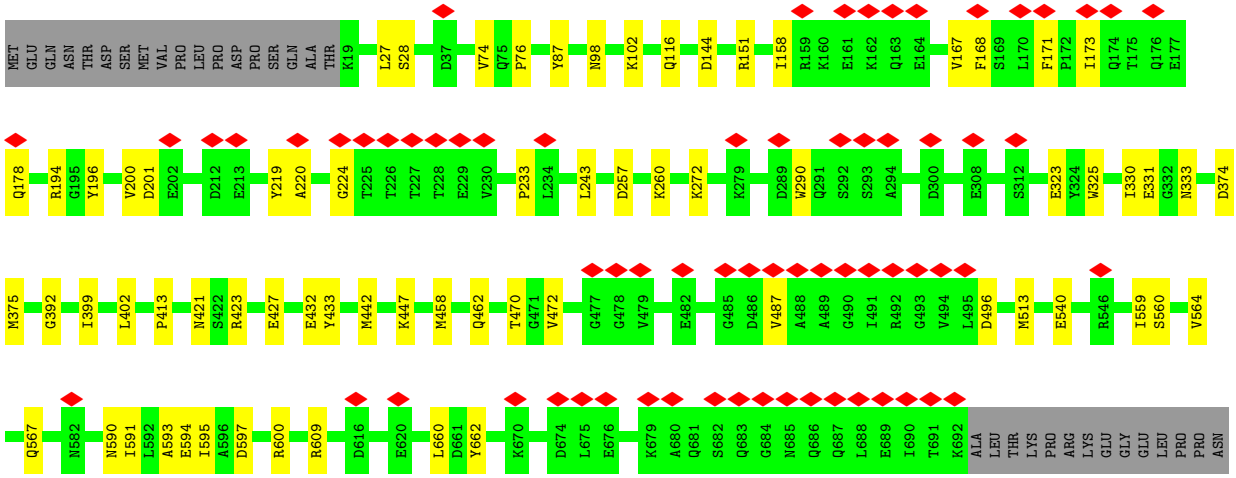
• Molecule 1: Probable portal protein

Chain J:



• Molecule 1: Probable portal protein

Chain K:



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

- Molecule 1: Probable portal protein

Chain L:

MET GLU GLN ASN THR ASP SER MET VAL PRO LEU PRO ASP PRO SER GLN ALA THR K19 L27 S28 D37 V68 R71 V74 Q75 P76 Y87 N98 K102 V142 V143 D144 V152 R159 K160 E161 K162 Q163 E164 V167 F168 S169 L170 F171 P172 I173 Q174

T175 Q176 E177 Q178 Y196 V200 D201 E202 A203 I204 V208 R209 D212 E213 Y219 A220 G224 T225 T226 T227 T228 E229 V230 E231 V240 E241 M242 C254 D257 K279 D280 R281 N286 K287 I288 D289 W290 Q291 S292 S293 D300 E308 F309 Q310 I311 S312

I330 E331 G332 N333 E352 G392 I399 L402 P413 N421 S422 R423 E427 E432 M442 M458 Q462 G477 G478 V479 T480 G485 D486 V487 A488 A489 G490 I491 R492 G493 V494 L495 D496 E502 L509 R546 K550 S560 V564 M575

N582 I591 I595 R600 D616 E620 N634 M652 R655 L660 D661 Y662 K670 R673 D674 L675 E676 K677 M678 K679 A680 Q681 S682 Q683 G684 N685 Q686 Q687 L688 E689 I690 T691 K692 ALA LEU THR LYS PRO ARG LYS GLU GLY GLU LEU PRO PRO ASN LEU

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.129	Depositor
Minimum map value	-5.827	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.626	Depositor
Recommended contour level	2	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.11	0/5452	0.28	0/7375
1	B	0.12	0/5452	0.29	0/7375
1	C	0.11	0/5452	0.29	0/7375
1	D	0.11	0/5452	0.28	0/7375
1	E	0.12	0/5452	0.29	0/7375
1	F	0.11	0/5452	0.29	0/7375
1	G	0.11	0/5452	0.28	0/7375
1	H	0.12	0/5452	0.30	0/7375
1	I	0.11	0/5452	0.29	0/7375
1	J	0.11	0/5452	0.28	0/7375
1	K	0.12	0/5452	0.29	0/7375
1	L	0.11	0/5452	0.28	0/7375
All	All	0.11	0/65424	0.29	0/88500

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5356	0	5338	47	0
1	B	5356	0	5338	48	0
1	C	5356	0	5338	41	0
1	D	5356	0	5338	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5356	0	5338	41	0
1	F	5356	0	5338	41	0
1	G	5356	0	5338	42	0
1	H	5356	0	5338	41	0
1	I	5356	0	5338	44	0
1	J	5356	0	5338	45	0
1	K	5356	0	5338	41	0
1	L	5356	0	5338	41	0
All	All	64272	0	64056	471	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 4.

All (471) 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:B:102:LYS:HB2	1:B:560:SER:HB2	1.70	0.73
1:E:102:LYS:HB2	1:E:560:SER:HB2	1.71	0.73
1:I:102:LYS:HB2	1:I:560:SER:HB2	1.71	0.72
1:J:102:LYS:HB2	1:J:560:SER:HB2	1.72	0.72
1:A:102:LYS:HB2	1:A:560:SER:HB2	1.72	0.71
1:G:102:LYS:HB2	1:G:560:SER:HB2	1.73	0.71
1:K:102:LYS:HB2	1:K:560:SER:HB2	1.72	0.71
1:L:102:LYS:HB2	1:L:560:SER:HB2	1.71	0.71
1:F:102:LYS:HB2	1:F:560:SER:HB2	1.72	0.71
1:H:102:LYS:HB2	1:H:560:SER:HB2	1.72	0.70
1:D:102:LYS:HB2	1:D:560:SER:HB2	1.73	0.70
1:C:102:LYS:HB2	1:C:560:SER:HB2	1.73	0.69
1:A:683:GLN:O	1:A:687:GLN:NE2	2.26	0.68
1:L:74:VAL:HG21	1:L:399:ILE:HD12	1.76	0.68
1:G:412:MET:HE3	1:G:417:LEU:HD12	1.77	0.67
1:A:628:GLU:OE1	1:L:634:ASN:ND2	2.28	0.67
1:C:74:VAL:HG21	1:C:399:ILE:HD12	1.76	0.67
1:J:412:MET:HE3	1:J:417:LEU:HD12	1.77	0.67
1:D:68:VAL:HG11	1:D:71:ARG:HD2	1.77	0.67
1:A:412:MET:HE3	1:A:417:LEU:HD12	1.77	0.66
1:J:68:VAL:HG11	1:J:71:ARG:HD2	1.78	0.66
1:F:74:VAL:HG21	1:F:399:ILE:HD12	1.76	0.66
1:G:68:VAL:HG11	1:G:71:ARG:HD2	1.77	0.66
1:A:68:VAL:HG11	1:A:71:ARG:HD2	1.77	0.66
1:L:413:PRO:HG3	1:L:442:MET:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:MET:HE3	1:D:417:LEU:HD12	1.78	0.66
1:I:74:VAL:HG21	1:I:399:ILE:HD12	1.78	0.65
1:K:116:GLN:NE2	1:K:540:GLU:O	2.29	0.65
1:D:138:TYR:HA	1:D:242:MET:HE2	1.79	0.65
1:I:116:GLN:NE2	1:I:540:GLU:O	2.30	0.65
1:K:74:VAL:HG21	1:K:399:ILE:HD12	1.80	0.64
1:J:138:TYR:HA	1:J:242:MET:HE2	1.79	0.63
1:B:74:VAL:HG21	1:B:399:ILE:HD12	1.80	0.63
1:B:281:ARG:NH2	1:B:352:GLU:OE2	2.32	0.63
1:D:281:ARG:NH1	1:D:352:GLU:OE2	2.32	0.63
1:J:281:ARG:NH1	1:J:352:GLU:OE2	2.32	0.62
1:G:281:ARG:NH1	1:G:352:GLU:OE2	2.32	0.62
1:A:281:ARG:NH1	1:A:352:GLU:OE2	2.32	0.62
1:B:116:GLN:NE2	1:B:540:GLU:O	2.30	0.61
1:E:74:VAL:HG21	1:E:399:ILE:HD12	1.81	0.61
1:H:74:VAL:HG21	1:H:399:ILE:HD12	1.82	0.61
1:D:421:ASN:ND2	1:D:432:GLU:O	2.34	0.61
1:C:116:GLN:NE2	1:C:540:GLU:O	2.33	0.61
1:H:168:PHE:HB3	1:H:220:ALA:HB1	1.83	0.60
1:L:281:ARG:NH1	1:L:352:GLU:OE2	2.34	0.60
1:F:116:GLN:NE2	1:F:540:GLU:O	2.32	0.60
1:A:74:VAL:HG21	1:A:399:ILE:HD12	1.82	0.60
1:F:281:ARG:NH1	1:F:352:GLU:OE2	2.34	0.60
1:C:281:ARG:NH1	1:C:352:GLU:OE2	2.34	0.60
1:G:74:VAL:HG21	1:G:399:ILE:HD12	1.83	0.60
1:I:281:ARG:NH1	1:I:352:GLU:OE2	2.34	0.60
1:C:168:PHE:HB3	1:C:220:ALA:HB1	1.84	0.60
1:J:74:VAL:HG21	1:J:399:ILE:HD12	1.83	0.60
1:B:168:PHE:HB3	1:B:220:ALA:HB1	1.83	0.59
1:E:168:PHE:HB3	1:E:220:ALA:HB1	1.83	0.59
1:I:168:PHE:HB3	1:I:220:ALA:HB1	1.84	0.59
1:D:74:VAL:HG21	1:D:399:ILE:HD12	1.84	0.59
1:G:168:PHE:HB3	1:G:220:ALA:HB1	1.85	0.59
1:D:168:PHE:HB3	1:D:220:ALA:HB1	1.85	0.59
1:F:168:PHE:HB3	1:F:220:ALA:HB1	1.84	0.59
1:J:330:ILE:HG13	1:J:331:GLU:HG2	1.85	0.59
1:L:87:TYR:OH	1:L:144:ASP:OD2	2.21	0.58
1:L:204:ILE:O	1:L:208:VAL:HG23	2.04	0.58
1:G:330:ILE:HG13	1:G:331:GLU:HG2	1.85	0.58
1:C:204:ILE:O	1:C:208:VAL:HG23	2.04	0.58
1:E:421:ASN:ND2	1:E:432:GLU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:GLU:OE1	1:H:325:TRP:NE1	2.34	0.58
1:K:168:PHE:HB3	1:K:220:ALA:HB1	1.83	0.58
1:H:57:MET:HE3	1:H:80:ARG:HD2	1.85	0.58
1:H:87:TYR:OH	1:H:144:ASP:OD2	2.21	0.58
1:K:323:GLU:OE1	1:K:325:TRP:NE1	2.34	0.58
1:B:421:ASN:ND2	1:B:432:GLU:O	2.36	0.58
1:K:421:ASN:ND2	1:K:432:GLU:O	2.36	0.58
1:D:330:ILE:HG13	1:D:331:GLU:HG2	1.84	0.58
1:F:204:ILE:O	1:F:208:VAL:HG23	2.04	0.57
1:F:413:PRO:HG3	1:F:442:MET:HB3	1.86	0.57
1:L:168:PHE:HB3	1:L:220:ALA:HB1	1.84	0.57
1:C:423:ARG:O	1:C:427:GLU:HG3	2.05	0.57
1:H:421:ASN:ND2	1:H:432:GLU:O	2.37	0.57
1:A:330:ILE:HG13	1:A:331:GLU:HG2	1.85	0.57
1:F:423:ARG:O	1:F:427:GLU:HG3	2.05	0.57
1:I:204:ILE:O	1:I:208:VAL:HG23	2.04	0.57
1:C:575:MET:HG3	1:D:601:MET:HE1	1.87	0.57
1:A:168:PHE:HB3	1:A:220:ALA:HB1	1.85	0.57
1:J:168:PHE:HB3	1:J:220:ALA:HB1	1.85	0.57
1:J:401:LEU:HD21	1:K:447:LYS:HG2	1.87	0.57
1:L:423:ARG:O	1:L:427:GLU:HG3	2.04	0.57
1:I:413:PRO:HG3	1:I:442:MET:HB3	1.86	0.56
1:C:87:TYR:OH	1:C:144:ASP:OD2	2.21	0.56
1:E:200:VAL:O	1:E:201:ASP:HB2	2.05	0.56
1:E:323:GLU:OE1	1:E:325:TRP:NE1	2.34	0.56
1:F:87:TYR:OH	1:F:144:ASP:OD2	2.22	0.56
1:F:575:MET:HG3	1:G:601:MET:HE1	1.87	0.56
1:G:401:LEU:HD21	1:H:447:LYS:HG2	1.87	0.56
1:I:423:ARG:O	1:I:427:GLU:HG3	2.05	0.56
1:A:200:VAL:O	1:A:201:ASP:HB2	2.05	0.56
1:B:458:MET:HG3	1:C:402:LEU:HD11	1.88	0.56
1:A:109:GLU:OE2	1:B:194:ARG:HD3	2.06	0.56
1:B:413:PRO:HG3	1:B:442:MET:HB3	1.88	0.56
1:D:423:ARG:O	1:D:427:GLU:HG3	2.06	0.56
1:H:423:ARG:O	1:H:427:GLU:HG3	2.06	0.56
1:J:109:GLU:OE2	1:K:194:ARG:HD3	2.06	0.56
1:K:423:ARG:O	1:K:427:GLU:HG3	2.06	0.56
1:L:200:VAL:O	1:L:201:ASP:HB2	2.06	0.56
1:A:401:LEU:HD21	1:B:447:LYS:HG2	1.87	0.55
1:H:81:ARG:HG2	1:H:85:TRP:CZ3	2.41	0.55
1:E:423:ARG:O	1:E:427:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:620:GLU:HA	1:I:623:LYS:HD2	1.88	0.55
1:F:620:GLU:HA	1:F:623:LYS:HD2	1.88	0.55
1:H:200:VAL:O	1:H:201:ASP:HB2	2.05	0.55
1:J:423:ARG:O	1:J:427:GLU:HG3	2.07	0.55
1:E:413:PRO:HG3	1:E:442:MET:HB3	1.88	0.55
1:H:413:PRO:HG3	1:H:442:MET:HB3	1.87	0.55
1:B:200:VAL:O	1:B:201:ASP:HB2	2.06	0.55
1:D:200:VAL:O	1:D:201:ASP:HB2	2.05	0.55
1:G:200:VAL:O	1:G:201:ASP:HB2	2.05	0.55
1:A:421:ASN:ND2	1:A:432:GLU:O	2.39	0.55
1:I:200:VAL:O	1:I:201:ASP:HB2	2.06	0.55
1:F:200:VAL:O	1:F:201:ASP:HB2	2.06	0.55
1:A:423:ARG:O	1:A:427:GLU:HG3	2.06	0.55
1:E:330:ILE:HG13	1:E:331:GLU:HG2	1.89	0.55
1:C:200:VAL:O	1:C:201:ASP:HB2	2.06	0.55
1:A:686:GLN:NE2	1:B:687:GLN:OE1	2.38	0.54
1:D:87:TYR:OH	1:D:144:ASP:OD1	2.22	0.54
1:I:87:TYR:OH	1:I:144:ASP:OD2	2.22	0.54
1:J:200:VAL:O	1:J:201:ASP:HB2	2.06	0.54
1:J:421:ASN:ND2	1:J:432:GLU:O	2.41	0.54
1:A:601:MET:HE1	1:L:575:MET:HG3	1.89	0.54
1:K:330:ILE:HG13	1:K:331:GLU:HG2	1.89	0.54
1:H:458:MET:HG3	1:I:402:LEU:HD11	1.88	0.54
1:K:200:VAL:O	1:K:201:ASP:HB2	2.06	0.54
1:D:47:MET:HG3	1:D:246:GLU:HG2	1.89	0.54
1:C:413:PRO:HG3	1:C:442:MET:HB3	1.89	0.54
1:B:330:ILE:HG13	1:B:331:GLU:HG2	1.90	0.53
1:E:458:MET:HG3	1:F:402:LEU:HD11	1.88	0.53
1:B:423:ARG:O	1:B:427:GLU:HG3	2.07	0.53
1:G:421:ASN:ND2	1:G:432:GLU:O	2.41	0.53
1:C:620:GLU:HA	1:C:623:LYS:HD2	1.89	0.53
1:B:87:TYR:OH	1:B:144:ASP:OD2	2.22	0.52
1:I:575:MET:HG3	1:J:601:MET:HE1	1.92	0.52
1:F:167:VAL:N	1:F:224:GLY:O	2.41	0.52
1:B:98:ASN:HD21	1:B:600:ARG:HD3	1.75	0.51
1:B:470:THR:HG22	1:B:472:VAL:HG23	1.92	0.51
1:C:102:LYS:HE2	1:C:564:VAL:HG11	1.92	0.51
1:B:257:ASP:HB3	1:B:260:LYS:HG3	1.91	0.51
1:G:423:ARG:O	1:G:427:GLU:HG3	2.11	0.51
1:B:276:LEU:HD22	1:B:279:LYS:HE2	1.93	0.51
1:G:87:TYR:OH	1:G:144:ASP:OD1	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ASP:OD2	1:A:609:ARG:NH2	2.43	0.51
1:I:68:VAL:HG11	1:I:71:ARG:HD2	1.92	0.51
1:J:288:ILE:HD11	1:J:349:ILE:HG21	1.93	0.51
1:K:257:ASP:HB3	1:K:260:LYS:HG3	1.92	0.51
1:L:286:ASN:OD1	1:L:287:LYS:N	2.44	0.51
1:A:288:ILE:HD11	1:A:349:ILE:HG21	1.93	0.50
1:A:687:GLN:HA	1:A:690:ILE:HG12	1.92	0.50
1:B:171:PHE:N	1:B:219:TYR:O	2.45	0.50
1:C:330:ILE:HG13	1:C:331:GLU:HG2	1.94	0.50
1:G:288:ILE:HD11	1:G:349:ILE:HG21	1.92	0.50
1:K:458:MET:HG3	1:L:402:LEU:HD11	1.93	0.50
1:E:167:VAL:N	1:E:224:GLY:O	2.41	0.50
1:J:597:ASP:OD2	1:J:609:ARG:NH2	2.44	0.50
1:E:470:THR:HG22	1:E:472:VAL:HG23	1.93	0.50
1:H:257:ASP:HB3	1:H:260:LYS:HG3	1.92	0.50
1:K:171:PHE:N	1:K:219:TYR:O	2.45	0.50
1:A:87:TYR:OH	1:A:144:ASP:OD1	2.23	0.50
1:E:171:PHE:N	1:E:219:TYR:O	2.45	0.50
1:C:68:VAL:HG11	1:C:71:ARG:HD2	1.94	0.50
1:E:591:ILE:O	1:E:595:ILE:HG13	2.12	0.50
1:G:171:PHE:N	1:G:219:TYR:O	2.45	0.50
1:D:171:PHE:N	1:D:219:TYR:O	2.45	0.49
1:J:171:PHE:N	1:J:219:TYR:O	2.45	0.49
1:K:470:THR:HG22	1:K:472:VAL:HG23	1.93	0.49
1:K:591:ILE:O	1:K:595:ILE:HG13	2.12	0.49
1:A:171:PHE:N	1:A:219:TYR:O	2.45	0.49
1:B:311:ILE:HG21	1:B:316:ARG:HB2	1.94	0.49
1:F:68:VAL:HG11	1:F:71:ARG:HD2	1.95	0.49
1:H:171:PHE:N	1:H:219:TYR:O	2.45	0.49
1:H:330:ILE:HG13	1:H:331:GLU:HG2	1.93	0.49
1:H:591:ILE:O	1:H:595:ILE:HG13	2.12	0.49
1:I:171:PHE:N	1:I:219:TYR:O	2.46	0.49
1:L:98:ASN:HD21	1:L:600:ARG:HD3	1.78	0.49
1:F:171:PHE:N	1:F:219:TYR:O	2.45	0.49
1:L:171:PHE:N	1:L:219:TYR:O	2.45	0.49
1:C:167:VAL:N	1:C:224:GLY:O	2.41	0.49
1:L:330:ILE:HG13	1:L:331:GLU:HG2	1.93	0.49
1:F:330:ILE:HG13	1:F:331:GLU:HG2	1.94	0.49
1:K:87:TYR:OH	1:K:144:ASP:OD2	2.22	0.49
1:G:597:ASP:OD2	1:G:609:ARG:NH2	2.46	0.48
1:L:167:VAL:N	1:L:224:GLY:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:600:ARG:HG3	1:E:600:ARG:HH11	1.77	0.48
1:F:98:ASN:HD21	1:F:600:ARG:HD3	1.78	0.48
1:H:597:ASP:OD2	1:H:609:ARG:NH2	2.46	0.48
1:K:167:VAL:N	1:K:224:GLY:O	2.41	0.48
1:I:330:ILE:HG13	1:I:331:GLU:HG2	1.94	0.48
1:C:171:PHE:N	1:C:219:TYR:O	2.46	0.48
1:J:442:MET:O	1:K:433:TYR:OH	2.30	0.48
1:B:167:VAL:N	1:B:224:GLY:O	2.42	0.48
1:F:681:GLN:HE22	1:F:685:ASN:HD21	1.62	0.48
1:I:681:GLN:HE22	1:I:685:ASN:HD21	1.62	0.48
1:K:102:LYS:HE2	1:K:564:VAL:HG11	1.96	0.48
1:I:76:PRO:HD2	1:I:392:GLY:HA2	1.96	0.48
1:I:167:VAL:N	1:I:224:GLY:O	2.41	0.48
1:J:167:VAL:N	1:J:224:GLY:O	2.42	0.48
1:H:102:LYS:HE2	1:H:564:VAL:HG11	1.96	0.48
1:A:102:LYS:HE2	1:A:564:VAL:HG11	1.96	0.48
1:C:681:GLN:HE22	1:C:685:ASN:HD21	1.62	0.48
1:K:597:ASP:OD2	1:K:609:ARG:NH2	2.46	0.48
1:A:98:ASN:HD21	1:A:600:ARG:HD3	1.79	0.47
1:C:98:ASN:HD21	1:C:600:ARG:HD3	1.79	0.47
1:D:167:VAL:N	1:D:224:GLY:O	2.42	0.47
1:K:513:MET:HB3	1:K:559:ILE:HD11	1.96	0.47
1:L:68:VAL:HG11	1:L:71:ARG:HD2	1.95	0.47
1:F:76:PRO:HD2	1:F:392:GLY:HA2	1.96	0.47
1:A:167:VAL:N	1:A:224:GLY:O	2.42	0.47
1:H:167:VAL:N	1:H:224:GLY:O	2.41	0.47
1:H:513:MET:HB3	1:H:559:ILE:HD11	1.97	0.47
1:L:681:GLN:HE22	1:L:685:ASN:HD21	1.62	0.47
1:A:487:VAL:C	1:A:567:GLN:HG2	2.40	0.47
1:J:358:ASP:OD1	1:J:359:GLY:N	2.48	0.47
1:J:458:MET:O	1:J:462:GLN:HG2	2.15	0.47
1:I:98:ASN:HD21	1:I:600:ARG:HD3	1.80	0.47
1:A:154:TRP:HE3	1:A:523:MET:HE3	1.81	0.46
1:D:597:ASP:OD2	1:D:609:ARG:NH2	2.46	0.46
1:L:591:ILE:O	1:L:595:ILE:HG13	2.15	0.46
1:A:458:MET:O	1:A:462:GLN:HG2	2.15	0.46
1:D:358:ASP:OD1	1:D:359:GLY:N	2.48	0.46
1:H:151:ARG:HB2	1:H:243:LEU:HD11	1.97	0.46
1:H:196:TYR:CD2	1:H:200:VAL:HG21	2.51	0.46
1:J:87:TYR:OH	1:J:144:ASP:OD1	2.22	0.46
1:L:102:LYS:HE2	1:L:564:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:MET:HG3	1:B:402:LEU:HD11	1.97	0.46
1:E:597:ASP:OD2	1:E:609:ARG:NH2	2.48	0.46
1:H:458:MET:O	1:H:462:GLN:HG2	2.15	0.46
1:I:591:ILE:O	1:I:595:ILE:HG13	2.16	0.46
1:K:27:LEU:HD12	1:K:28:SER:N	2.30	0.46
1:K:458:MET:O	1:K:462:GLN:HG2	2.15	0.46
1:A:681:GLN:HE22	1:A:685:ASN:HD21	1.62	0.46
1:E:196:TYR:CD2	1:E:200:VAL:HG21	2.51	0.46
1:F:591:ILE:O	1:F:595:ILE:HG13	2.16	0.46
1:F:621:GLN:HA	1:F:624:GLN:OE1	2.15	0.46
1:G:458:MET:HG3	1:H:402:LEU:HD11	1.96	0.46
1:B:196:TYR:CD2	1:B:200:VAL:HG21	2.51	0.46
1:F:102:LYS:HE2	1:F:564:VAL:HG11	1.96	0.46
1:B:27:LEU:HD12	1:B:28:SER:N	2.30	0.46
1:I:621:GLN:HA	1:I:624:GLN:OE1	2.15	0.46
1:A:658:LYS:HB3	1:B:657:ASN:HD21	1.81	0.46
1:C:591:ILE:O	1:C:595:ILE:HG13	2.16	0.46
1:C:621:GLN:HA	1:C:624:GLN:OE1	2.15	0.46
1:G:662:TYR:HE1	1:H:660:LEU:HB2	1.80	0.46
1:K:151:ARG:HB2	1:K:243:LEU:HD11	1.97	0.46
1:C:488:ALA:HA	1:C:567:GLN:HG2	1.97	0.46
1:D:80:ARG:NE	1:D:84:GLU:OE1	2.49	0.46
1:E:513:MET:HB3	1:E:559:ILE:HD11	1.96	0.46
1:C:76:PRO:HD2	1:C:392:GLY:HA2	1.96	0.46
1:D:27:LEU:HD12	1:D:28:SER:N	2.31	0.46
1:E:151:ARG:HB2	1:E:243:LEU:HD11	1.97	0.46
1:K:196:TYR:CD2	1:K:200:VAL:HG21	2.51	0.46
1:K:413:PRO:HG3	1:K:442:MET:HB3	1.96	0.46
1:A:194:ARG:O	1:A:198:GLU:HG3	2.16	0.46
1:B:513:MET:HB3	1:B:559:ILE:HD11	1.97	0.46
1:E:27:LEU:HD12	1:E:28:SER:N	2.30	0.46
1:F:458:MET:O	1:F:462:GLN:HG2	2.16	0.46
1:H:57:MET:HE1	1:H:87:TYR:OH	2.15	0.46
1:L:142:VAL:HG11	1:L:509:LEU:HD21	1.98	0.46
1:B:597:ASP:OD2	1:B:609:ARG:NH2	2.49	0.45
1:I:102:LYS:HE2	1:I:564:VAL:HG11	1.98	0.45
1:A:358:ASP:OD1	1:A:359:GLY:N	2.48	0.45
1:B:242:MET:HE3	1:B:242:MET:HB3	1.83	0.45
1:D:458:MET:O	1:D:462:GLN:HG2	2.15	0.45
1:E:458:MET:O	1:E:462:GLN:HG2	2.16	0.45
1:G:458:MET:O	1:G:462:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:LEU:HD12	1:H:28:SER:N	2.30	0.45
1:I:458:MET:O	1:I:462:GLN:HG2	2.16	0.45
1:L:76:PRO:HD2	1:L:392:GLY:HA2	1.97	0.45
1:J:102:LYS:HE2	1:J:564:VAL:HG11	1.99	0.45
1:J:662:TYR:HE1	1:K:660:LEU:HB2	1.82	0.45
1:C:458:MET:O	1:C:462:GLN:HG2	2.16	0.45
1:F:27:LEU:HD12	1:F:28:SER:N	2.31	0.45
1:G:102:LYS:HE2	1:G:564:VAL:HG11	1.98	0.45
1:A:402:LEU:HD11	1:L:458:MET:HG3	1.98	0.45
1:A:442:MET:O	1:B:433:TYR:OH	2.29	0.45
1:D:458:MET:HG3	1:E:402:LEU:HD11	1.97	0.45
1:B:458:MET:O	1:B:462:GLN:HG2	2.16	0.45
1:J:27:LEU:HD12	1:J:28:SER:N	2.31	0.45
1:G:27:LEU:HD12	1:G:28:SER:N	2.31	0.45
1:I:27:LEU:HD12	1:I:28:SER:N	2.31	0.45
1:I:109:GLU:OE1	1:J:538:ASN:ND2	2.50	0.45
1:J:458:MET:HG3	1:K:402:LEU:HD11	1.97	0.45
1:C:27:LEU:HD12	1:C:28:SER:N	2.31	0.45
1:E:580:GLY:O	1:E:583:VAL:HG12	2.17	0.45
1:F:458:MET:HG3	1:G:402:LEU:HD11	1.98	0.45
1:L:458:MET:O	1:L:462:GLN:HG2	2.16	0.45
1:A:27:LEU:HD12	1:A:28:SER:N	2.31	0.45
1:G:167:VAL:N	1:G:224:GLY:O	2.42	0.45
1:I:160:LYS:HG2	1:I:231:GLU:HG2	1.99	0.45
1:B:636:GLU:HG2	1:B:640:LYS:HE3	1.98	0.45
1:D:102:LYS:HE2	1:D:564:VAL:HG11	1.98	0.45
1:E:102:LYS:HE2	1:E:564:VAL:HG11	1.98	0.45
1:I:458:MET:HG3	1:J:402:LEU:HD11	1.98	0.45
1:C:152:VAL:HG22	1:C:240:VAL:HG12	2.00	0.44
1:G:80:ARG:NE	1:G:84:GLU:OE1	2.49	0.44
1:H:98:ASN:HD21	1:H:600:ARG:HD3	1.83	0.44
1:I:334:GLY:HA2	1:J:315:MET:HE3	1.99	0.44
1:L:27:LEU:HD12	1:L:28:SER:N	2.31	0.44
1:C:458:MET:HG3	1:D:402:LEU:HD11	1.99	0.44
1:F:152:VAL:HG22	1:F:240:VAL:HG12	1.99	0.44
1:K:98:ASN:HD21	1:K:600:ARG:HD3	1.83	0.44
1:C:160:LYS:HG2	1:C:231:GLU:HG2	1.99	0.44
1:I:421:ASN:ND2	1:I:432:GLU:O	2.51	0.44
1:L:152:VAL:HG22	1:L:240:VAL:HG12	1.99	0.44
1:C:142:VAL:HG11	1:C:509:LEU:HD21	1.99	0.44
1:F:487:VAL:C	1:F:567:GLN:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:PRO:HD2	1:H:392:GLY:HA2	2.00	0.44
1:K:487:VAL:C	1:K:567:GLN:HG2	2.43	0.44
1:L:458:MET:HE3	1:L:458:MET:HB3	1.94	0.44
1:D:513:MET:HB3	1:D:559:ILE:HD11	1.99	0.44
1:I:152:VAL:HG22	1:I:240:VAL:HG12	1.99	0.44
1:G:80:ARG:O	1:G:84:GLU:HB2	2.18	0.44
1:J:196:TYR:HA	1:J:200:VAL:HG23	2.00	0.44
1:B:623:LYS:HA	1:B:623:LYS:HD3	1.77	0.44
1:D:662:TYR:HE1	1:E:660:LEU:HB2	1.82	0.44
1:F:160:LYS:HG2	1:F:231:GLU:HG2	2.00	0.44
1:G:189:ARG:HB2	1:G:196:TYR:CD1	2.52	0.44
1:A:196:TYR:HA	1:A:200:VAL:HG23	1.99	0.43
1:E:496:ASP:OD2	1:E:496:ASP:N	2.51	0.43
1:J:98:ASN:HD21	1:J:600:ARG:HD3	1.83	0.43
1:L:160:LYS:HG2	1:L:231:GLU:HG2	2.00	0.43
1:B:580:GLY:O	1:B:583:VAL:HG12	2.19	0.43
1:E:458:MET:HE3	1:E:458:MET:HB3	1.93	0.43
1:F:421:ASN:ND2	1:F:432:GLU:O	2.51	0.43
1:G:358:ASP:OD1	1:G:359:GLY:N	2.52	0.43
1:B:591:ILE:O	1:B:595:ILE:HG13	2.19	0.43
1:G:196:TYR:CD1	1:G:200:VAL:HG21	2.53	0.43
1:G:442:MET:O	1:H:433:TYR:OH	2.30	0.43
1:G:458:MET:HE3	1:G:458:MET:HB3	1.92	0.43
1:G:513:MET:HB3	1:G:559:ILE:HD11	2.00	0.43
1:I:196:TYR:HA	1:I:200:VAL:HG23	2.01	0.43
1:J:513:MET:HB3	1:J:559:ILE:HD11	2.01	0.43
1:K:76:PRO:HD2	1:K:392:GLY:HA2	2.00	0.43
1:L:242:MET:HE3	1:L:242:MET:HB3	1.90	0.43
1:E:487:VAL:C	1:E:567:GLN:HG2	2.44	0.43
1:F:62:LYS:HB2	1:F:62:LYS:HE3	1.79	0.43
1:F:480:THR:HG21	1:F:502:GLU:HB3	2.01	0.43
1:I:496:ASP:OD1	1:I:496:ASP:N	2.52	0.43
1:H:496:ASP:OD2	1:H:496:ASP:N	2.52	0.43
1:J:99:LYS:HE2	1:J:122:ASN:ND2	2.34	0.43
1:B:487:VAL:C	1:B:567:GLN:HG2	2.44	0.43
1:C:496:ASP:OD1	1:C:496:ASP:N	2.52	0.43
1:G:196:TYR:HA	1:G:200:VAL:HG23	2.00	0.43
1:G:447:LYS:HE2	1:G:447:LYS:HB2	1.85	0.43
1:A:99:LYS:HE2	1:A:122:ASN:ND2	2.34	0.43
1:B:80:ARG:O	1:B:84:GLU:HB2	2.19	0.43
1:G:99:LYS:HE2	1:G:122:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:487:VAL:C	1:H:567:GLN:HG2	2.43	0.43
1:A:196:TYR:CD1	1:A:200:VAL:HG21	2.54	0.43
1:A:513:MET:HB3	1:A:559:ILE:HD11	2.01	0.43
1:B:151:ARG:HB2	1:B:243:LEU:HD11	1.99	0.43
1:D:196:TYR:CD1	1:D:200:VAL:HG21	2.54	0.43
1:E:76:PRO:HD2	1:E:392:GLY:HA2	2.01	0.43
1:B:458:MET:HE3	1:B:458:MET:HB3	1.93	0.42
1:D:80:ARG:O	1:D:84:GLU:HB2	2.18	0.42
1:D:331:GLU:HB2	1:D:333:ASN:OD1	2.19	0.42
1:H:416:MET:HG2	1:H:417:LEU:HG	2.01	0.42
1:K:496:ASP:OD2	1:K:496:ASP:N	2.51	0.42
1:A:331:GLU:HB2	1:A:333:ASN:OD1	2.20	0.42
1:D:196:TYR:HA	1:D:200:VAL:HG23	2.01	0.42
1:E:80:ARG:O	1:E:84:GLU:HB2	2.19	0.42
1:F:496:ASP:N	1:F:496:ASP:OD1	2.52	0.42
1:D:99:LYS:HE2	1:D:122:ASN:ND2	2.34	0.42
1:E:98:ASN:HD21	1:E:600:ARG:HD3	1.84	0.42
1:G:76:PRO:HD2	1:G:392:GLY:HA2	2.02	0.42
1:C:196:TYR:CD1	1:C:200:VAL:HG21	2.55	0.42
1:D:458:MET:HE3	1:D:458:MET:HB3	1.92	0.42
1:F:196:TYR:CD1	1:F:200:VAL:HG21	2.55	0.42
1:F:196:TYR:HA	1:F:200:VAL:HG23	2.01	0.42
1:I:480:THR:HG21	1:I:502:GLU:HB3	2.01	0.42
1:B:99:LYS:HE2	1:B:122:ASN:ND2	2.35	0.42
1:C:196:TYR:HA	1:C:200:VAL:HG23	2.01	0.42
1:D:86:ARG:NH1	1:D:368:TYR:OH	2.53	0.42
1:E:416:MET:HG2	1:E:417:LEU:HG	2.02	0.42
1:I:196:TYR:CD1	1:I:200:VAL:HG21	2.55	0.42
1:J:196:TYR:CD1	1:J:200:VAL:HG21	2.54	0.42
1:K:374:ASP:OD2	1:K:375:MET:N	2.53	0.42
1:L:196:TYR:CD1	1:L:200:VAL:HG21	2.55	0.42
1:A:80:ARG:O	1:A:84:GLU:HB2	2.20	0.42
1:B:76:PRO:HD2	1:B:392:GLY:HA2	2.00	0.42
1:I:286:ASN:OD1	1:I:287:LYS:N	2.53	0.42
1:F:442:MET:O	1:G:433:TYR:OH	2.33	0.42
1:G:272:LYS:HD2	1:G:290:TRP:CZ2	2.55	0.42
1:C:242:MET:HE3	1:C:242:MET:HB3	1.90	0.42
1:K:173:ILE:HD12	1:K:178:GLN:HB3	2.01	0.42
1:C:421:ASN:ND2	1:C:432:GLU:O	2.53	0.42
1:G:331:GLU:HB2	1:G:333:ASN:OD1	2.19	0.42
1:A:660:LEU:HB2	1:L:662:TYR:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASN:O	1:B:594:GLU:OE2	2.38	0.41
1:C:331:GLU:HB2	1:C:333:ASN:OD1	2.20	0.41
1:C:286:ASN:OD1	1:C:287:LYS:N	2.53	0.41
1:D:487:VAL:C	1:D:567:GLN:HG2	2.45	0.41
1:E:590:ASN:O	1:E:593:ALA:N	2.53	0.41
1:J:76:PRO:HD2	1:J:392:GLY:HA2	2.02	0.41
1:K:590:ASN:O	1:K:593:ALA:N	2.53	0.41
1:L:421:ASN:ND2	1:L:432:GLU:O	2.53	0.41
1:F:286:ASN:OD1	1:F:287:LYS:N	2.53	0.41
1:I:662:TYR:HE1	1:J:660:LEU:HB2	1.84	0.41
1:D:442:MET:O	1:E:433:TYR:OH	2.29	0.41
1:E:87:TYR:OH	1:E:144:ASP:OD2	2.23	0.41
1:I:458:MET:HE3	1:I:458:MET:HB3	1.93	0.41
1:K:590:ASN:O	1:K:594:GLU:OE2	2.38	0.41
1:L:196:TYR:HA	1:L:200:VAL:HG23	2.01	0.41
1:L:496:ASP:OD1	1:L:496:ASP:N	2.48	0.41
1:A:272:LYS:HD2	1:A:290:TRP:CZ2	2.56	0.41
1:B:100:LEU:HD22	1:B:131:ARG:HD2	2.03	0.41
1:H:173:ILE:HD12	1:H:178:GLN:HB3	2.01	0.41
1:B:416:MET:HG2	1:B:417:LEU:HG	2.01	0.41
1:C:62:LYS:HE3	1:C:62:LYS:HB2	1.79	0.41
1:H:281:ARG:NH1	1:H:352:GLU:OE2	2.54	0.41
1:H:590:ASN:O	1:H:593:ALA:N	2.53	0.41
1:H:590:ASN:O	1:H:594:GLU:OE2	2.38	0.41
1:I:331:GLU:HB2	1:I:333:ASN:OD1	2.20	0.41
1:J:487:VAL:C	1:J:567:GLN:HG2	2.45	0.41
1:B:272:LYS:HE3	1:B:276:LEU:HD11	2.03	0.41
1:C:480:THR:HG21	1:C:502:GLU:HB3	2.02	0.41
1:E:600:ARG:HG3	1:E:600:ARG:NH1	2.35	0.41
1:G:487:VAL:C	1:G:567:GLN:HG2	2.46	0.41
1:I:173:ILE:HD12	1:I:178:GLN:HB3	2.03	0.41
1:J:331:GLU:HB2	1:J:333:ASN:OD1	2.20	0.41
1:D:76:PRO:HD2	1:D:392:GLY:HA2	2.02	0.41
1:H:272:LYS:HD2	1:H:290:TRP:CZ2	2.56	0.41
1:K:272:LYS:HD2	1:K:290:TRP:CZ2	2.56	0.41
1:A:76:PRO:HD2	1:A:392:GLY:HA2	2.02	0.41
1:A:480:THR:HG21	1:A:502:GLU:HB3	2.03	0.41
1:A:662:TYR:HE1	1:B:660:LEU:HB2	1.85	0.41
1:F:173:ILE:HD12	1:F:178:GLN:HB3	2.03	0.41
1:F:254:CYS:HB2	1:F:257:ASP:O	2.21	0.41
1:F:331:GLU:HB2	1:F:333:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:ILE:HD12	1:G:178:GLN:HB3	2.03	0.41
1:G:496:ASP:OD1	1:G:496:ASP:N	2.52	0.41
1:H:662:TYR:HE1	1:I:660:LEU:HB2	1.86	0.41
1:J:80:ARG:O	1:J:84:GLU:HB2	2.21	0.41
1:J:189:ARG:HB2	1:J:196:TYR:CD1	2.56	0.41
1:L:173:ILE:HD12	1:L:178:GLN:HB3	2.03	0.41
1:L:254:CYS:HB2	1:L:257:ASP:O	2.21	0.41
1:F:501:ARG:O	1:F:505:ILE:HG13	2.21	0.41
1:H:158:ILE:HG22	1:H:233:PRO:HB3	2.03	0.41
1:J:173:ILE:HD12	1:J:178:GLN:HB3	2.03	0.41
1:L:331:GLU:HB2	1:L:333:ASN:OD1	2.21	0.41
1:A:189:ARG:HB2	1:A:196:TYR:CD1	2.56	0.40
1:E:173:ILE:HD12	1:E:178:GLN:HB3	2.01	0.40
1:E:331:GLU:HB2	1:E:333:ASN:OD1	2.21	0.40
1:B:173:ILE:HD12	1:B:178:GLN:HB3	2.01	0.40
1:B:272:LYS:HD2	1:B:290:TRP:CZ2	2.56	0.40
1:E:356:TYR:HA	1:E:357:PRO:HD3	1.97	0.40
1:I:254:CYS:HB2	1:I:257:ASP:O	2.21	0.40
1:I:501:ARG:O	1:I:505:ILE:HG13	2.21	0.40
1:J:272:LYS:HD2	1:J:290:TRP:CZ2	2.56	0.40
1:J:447:LYS:HB2	1:J:447:LYS:HE2	1.85	0.40
1:K:662:TYR:HE1	1:L:660:LEU:HB2	1.86	0.40
1:C:254:CYS:HB2	1:C:257:ASP:O	2.21	0.40
1:E:64:LYS:HA	1:E:65:PRO:HD3	1.98	0.40
1:E:590:ASN:O	1:E:594:GLU:OE2	2.38	0.40
1:J:254:CYS:HB2	1:J:257:ASP:O	2.22	0.40
1:K:331:GLU:HB2	1:K:333:ASN:OD1	2.21	0.40
1:C:458:MET:HG3	1:D:402:LEU:CD1	2.51	0.40
1:D:189:ARG:HB2	1:D:196:TYR:CD1	2.56	0.40
1:I:652:MET:HE3	1:I:655:ARG:HH21	1.86	0.40
1:L:480:THR:HG21	1:L:502:GLU:HB3	2.04	0.40
1:D:272:LYS:HD2	1:D:290:TRP:CZ2	2.57	0.40
1:G:86:ARG:NH1	1:G:368:TYR:OH	2.54	0.40
1:J:463:ASN:O	1:J:467:GLU:HG3	2.22	0.40
1:K:158:ILE:HG22	1:K:233:PRO:HB3	2.04	0.40
1:L:652:MET:HE3	1:L:655:ARG:HH21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	672/763 (88%)	663 (99%)	9 (1%)	0	100	100
1	B	672/763 (88%)	664 (99%)	8 (1%)	0	100	100
1	C	672/763 (88%)	662 (98%)	10 (2%)	0	100	100
1	D	672/763 (88%)	662 (98%)	10 (2%)	0	100	100
1	E	672/763 (88%)	663 (99%)	9 (1%)	0	100	100
1	F	672/763 (88%)	662 (98%)	10 (2%)	0	100	100
1	G	672/763 (88%)	661 (98%)	11 (2%)	0	100	100
1	H	672/763 (88%)	664 (99%)	8 (1%)	0	100	100
1	I	672/763 (88%)	661 (98%)	11 (2%)	0	100	100
1	J	672/763 (88%)	663 (99%)	9 (1%)	0	100	100
1	K	672/763 (88%)	663 (99%)	9 (1%)	0	100	100
1	L	672/763 (88%)	661 (98%)	11 (2%)	0	100	100
All	All	8064/9156 (88%)	7949 (99%)	115 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/652 (89%)	580 (100%)	0	100	100
1	B	580/652 (89%)	580 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	580/652 (89%)	580 (100%)	0	100	100
1	D	580/652 (89%)	580 (100%)	0	100	100
1	E	580/652 (89%)	580 (100%)	0	100	100
1	F	580/652 (89%)	580 (100%)	0	100	100
1	G	580/652 (89%)	580 (100%)	0	100	100
1	H	580/652 (89%)	580 (100%)	0	100	100
1	I	580/652 (89%)	580 (100%)	0	100	100
1	J	580/652 (89%)	580 (100%)	0	100	100
1	K	580/652 (89%)	580 (100%)	0	100	100
1	L	580/652 (89%)	580 (100%)	0	100	100
All	All	6960/7824 (89%)	6960 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	192	ASN
1	A	237	HIS
1	A	301	HIS
1	A	671	HIS
1	A	685	ASN
1	A	687	GLN
1	B	199	ASN
1	B	237	HIS
1	B	388	GLN
1	B	685	ASN
1	C	199	ASN
1	C	237	HIS
1	C	301	HIS
1	C	421	ASN
1	C	685	ASN
1	D	73	GLN
1	D	237	HIS
1	D	301	HIS
1	D	518	ASN
1	D	567	GLN

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Mol	Chain	Res	Type
1	D	685	ASN
1	E	124	GLN
1	E	199	ASN
1	E	259	ASN
1	E	388	GLN
1	E	524	ASN
1	F	117	ASN
1	F	199	ASN
1	F	301	HIS
1	F	407	ASN
1	F	421	ASN
1	F	438	ASN
1	F	685	ASN
1	G	73	GLN
1	G	237	HIS
1	G	301	HIS
1	G	552	ASN
1	G	567	GLN
1	H	124	GLN
1	H	199	ASN
1	H	237	HIS
1	H	524	ASN
1	H	685	ASN
1	I	124	GLN
1	I	199	ASN
1	I	301	HIS
1	I	407	ASN
1	I	438	ASN
1	I	524	ASN
1	I	685	ASN
1	J	73	GLN
1	J	199	ASN
1	J	301	HIS
1	J	685	ASN
1	K	124	GLN
1	K	199	ASN
1	K	283	HIS
1	K	388	GLN
1	K	524	ASN
1	L	73	GLN
1	L	124	GLN
1	L	199	ASN

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Mol	Chain	Res	Type
1	L	421	ASN
1	L	524	ASN
1	L	685	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

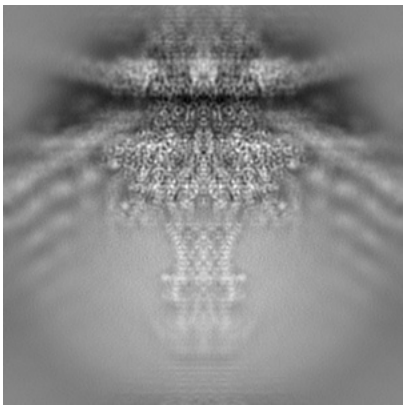
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-62962. These allow visual inspection of the internal detail of the map and identification of artifacts.

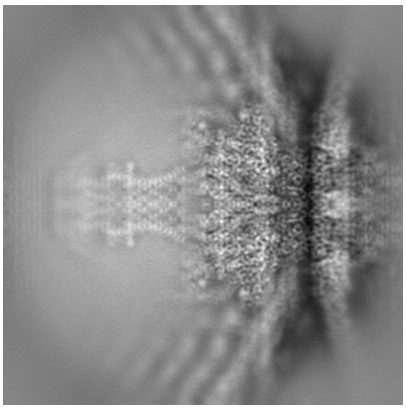
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

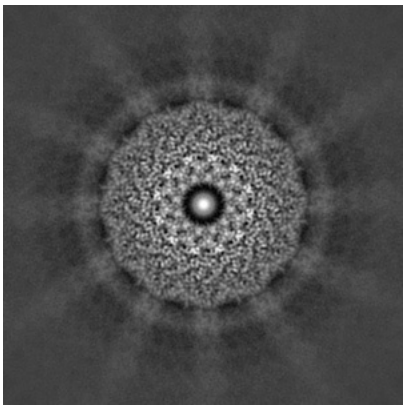
6.1.1 Primary map



X

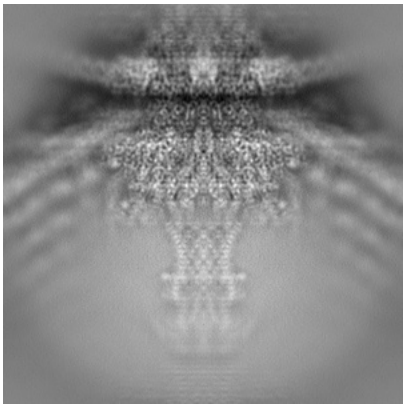


Y

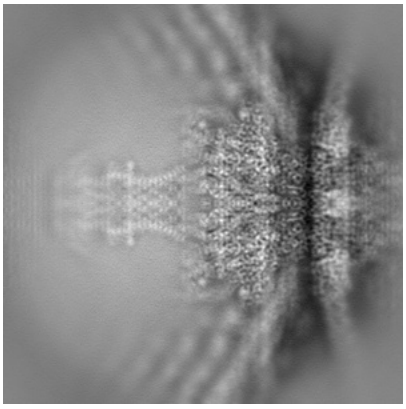


Z

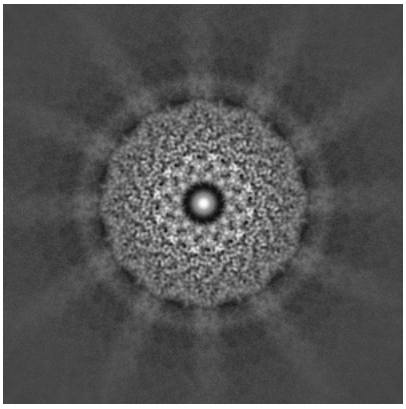
6.1.2 Raw map



X



Y

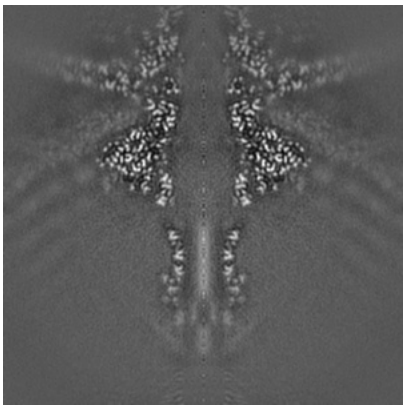


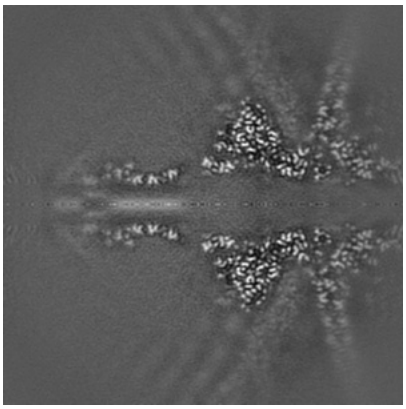
Z

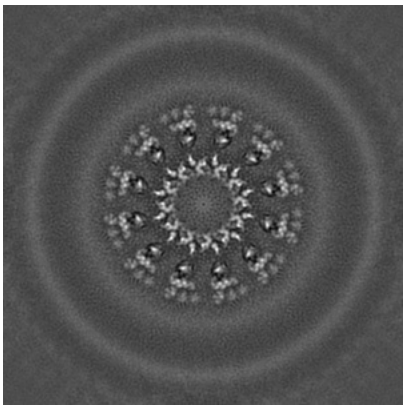
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

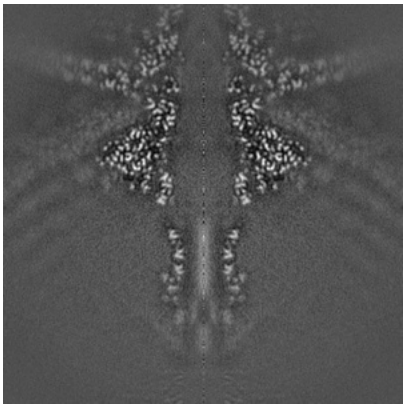
6.2.1 Primary map

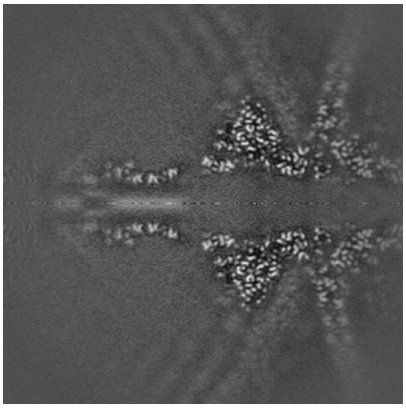

X Index: 160

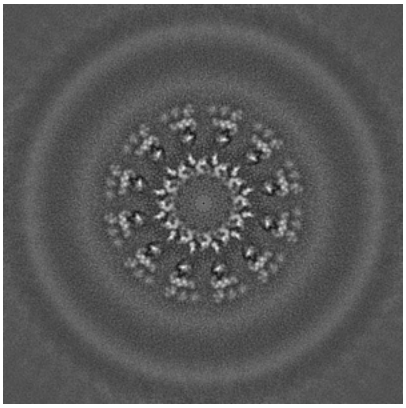

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

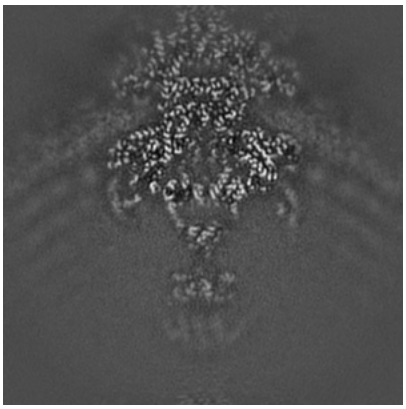

Y Index: 160

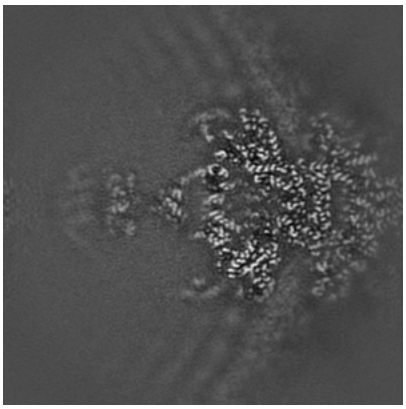

Z Index: 160

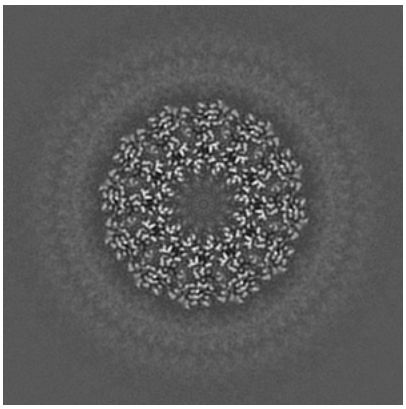
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

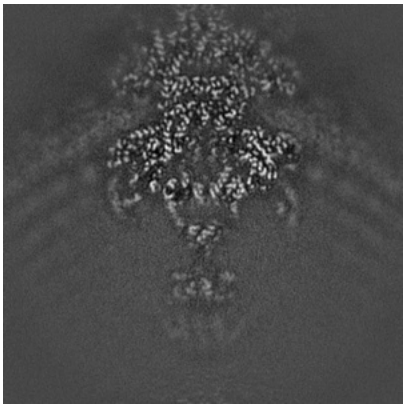
6.3.1 Primary map

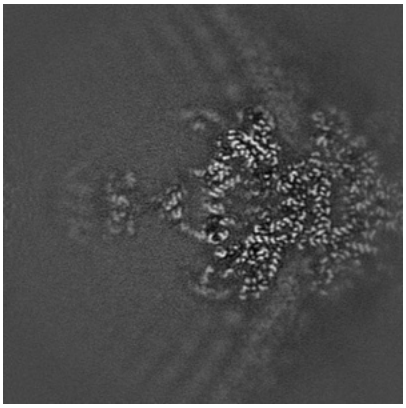

X Index: 135

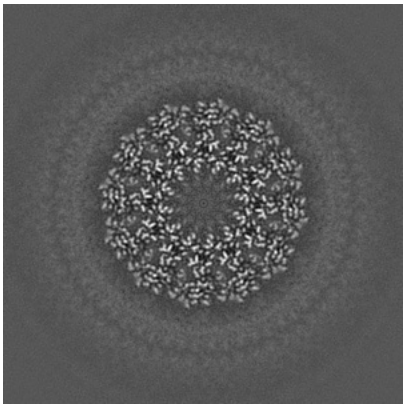

Y Index: 135


Z Index: 203

6.3.2 Raw map


X Index: 135

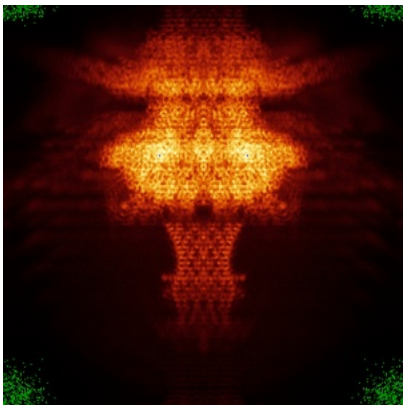

Y Index: 185

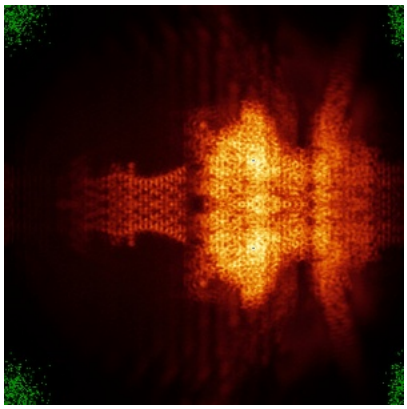

Z Index: 203

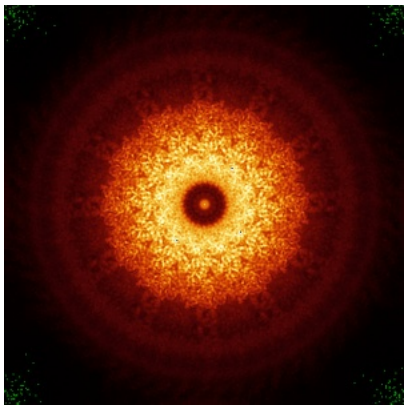
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

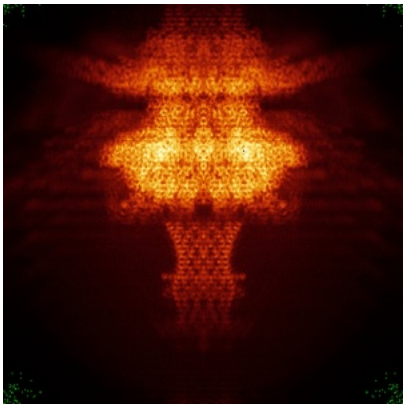
6.4.1 Primary map

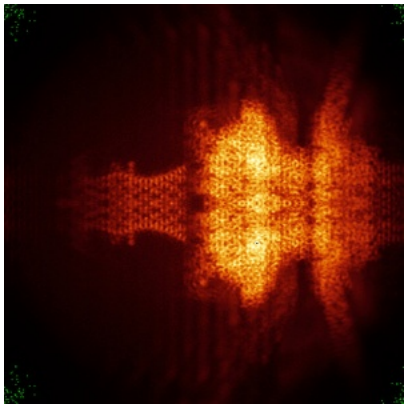

X

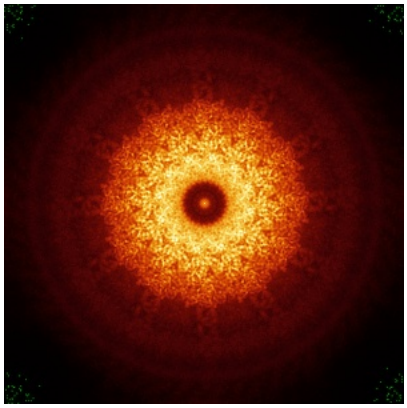

Y


Z

6.4.2 Raw map


X

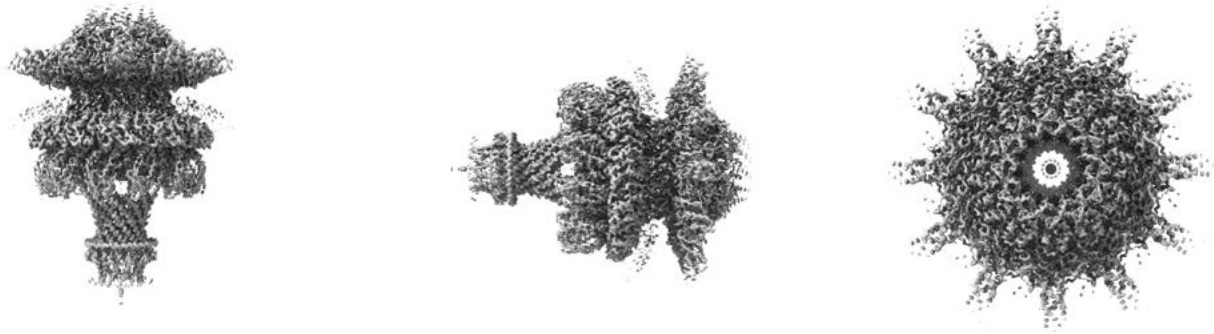

Y


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)

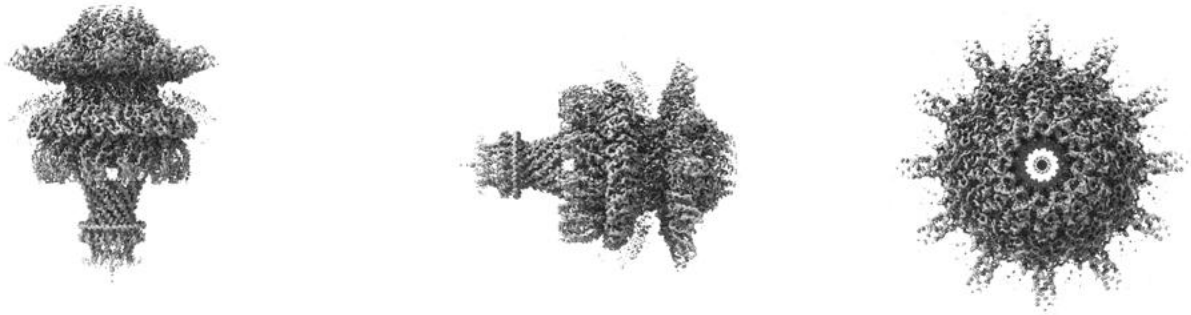
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. 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



X Y Z

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.

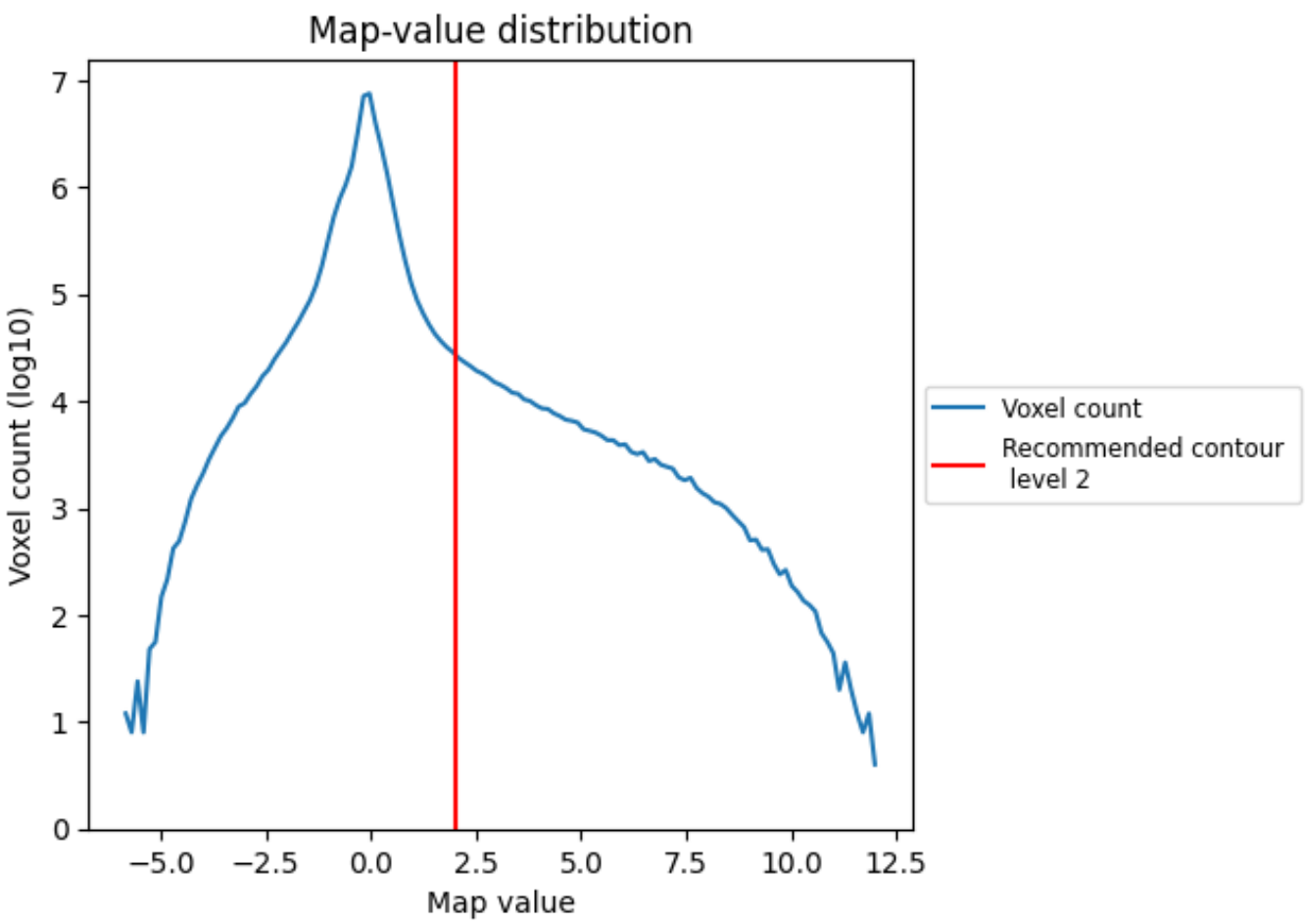
6.6 Mask visualisation (i)

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

7 Map analysis (i)

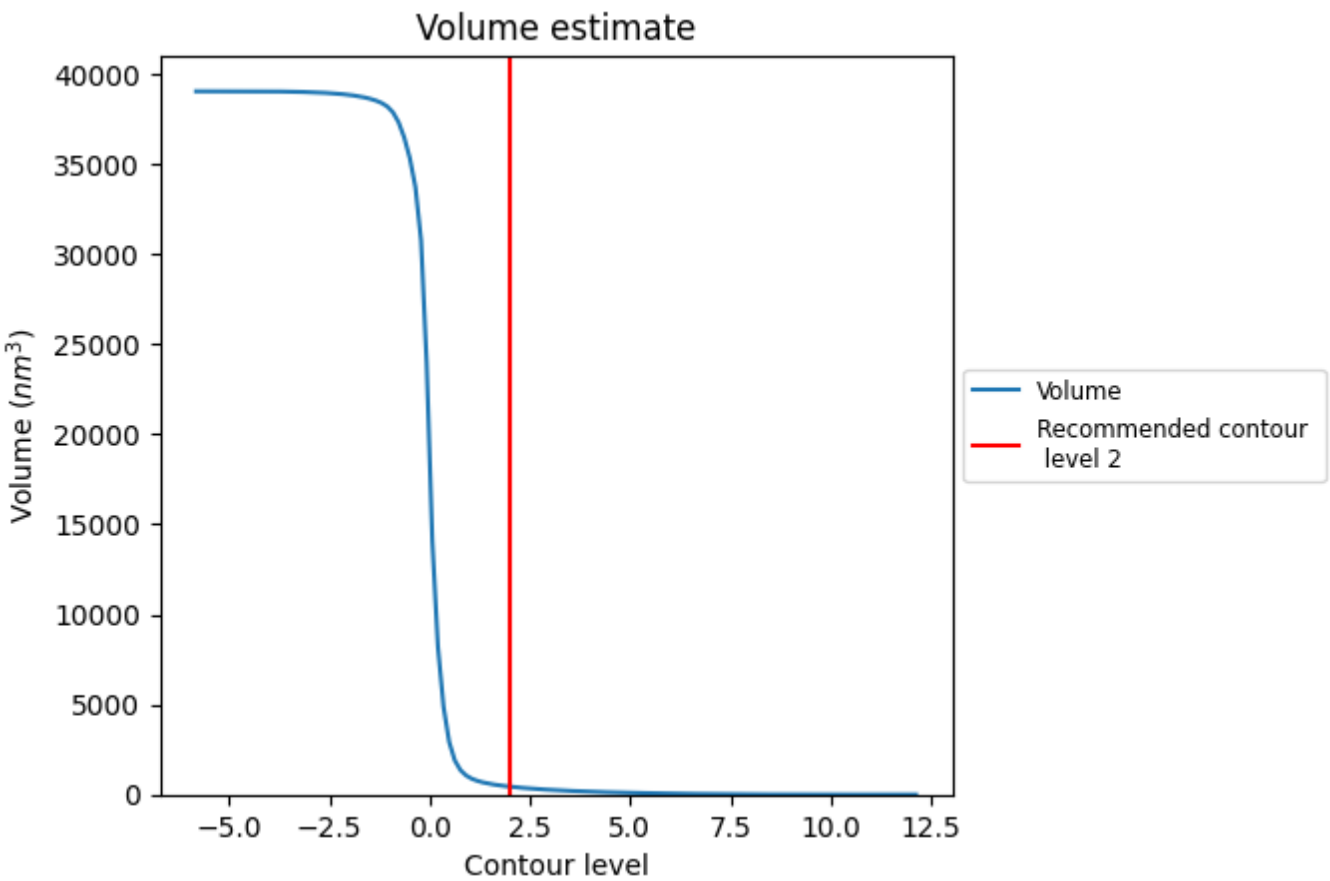
This section contains the results of statistical analysis of the map.

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.

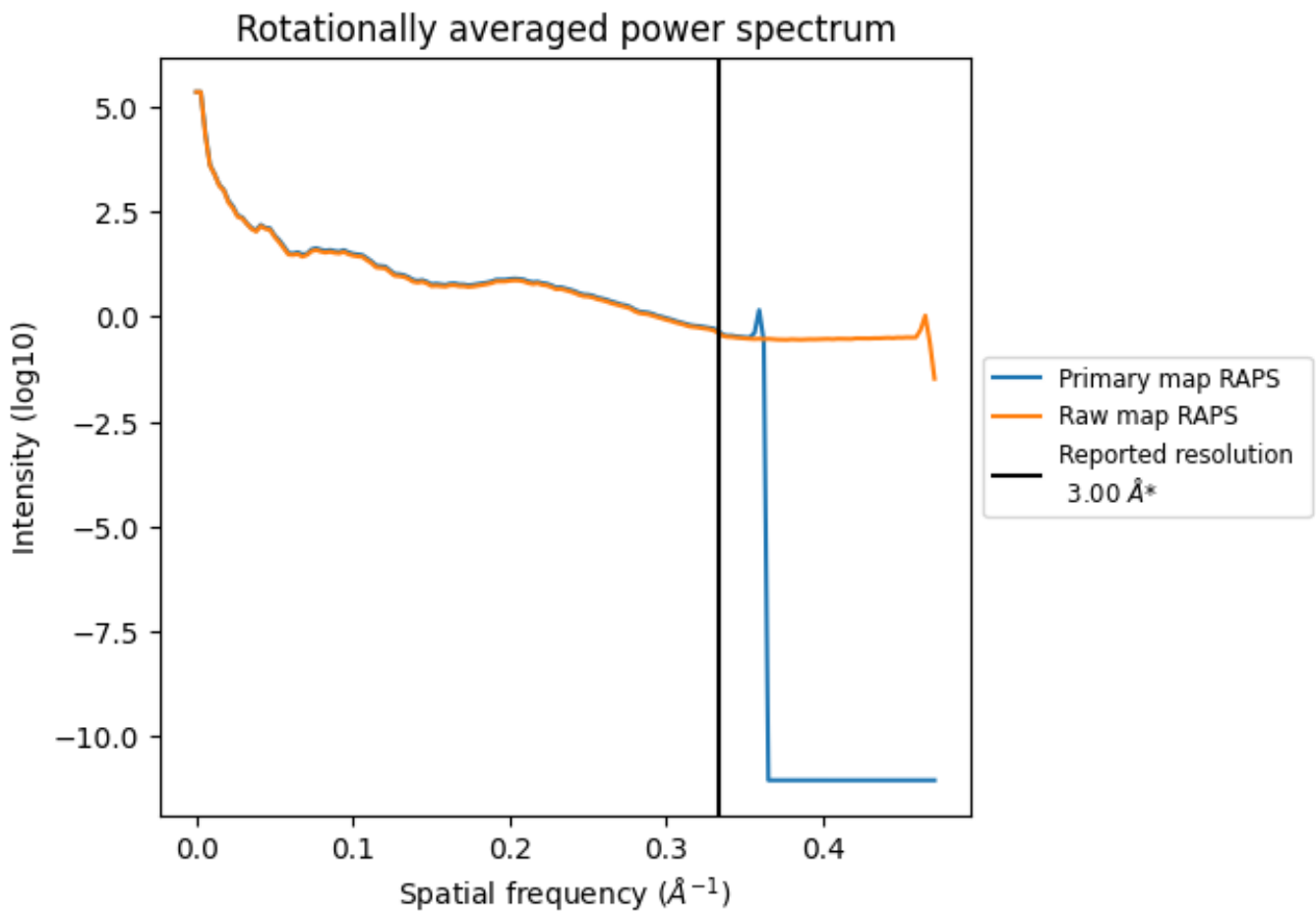
7.2 Volume estimate (i)



The volume at the recommended contour level is 439 nm^3; this corresponds to an approximate mass of 397 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

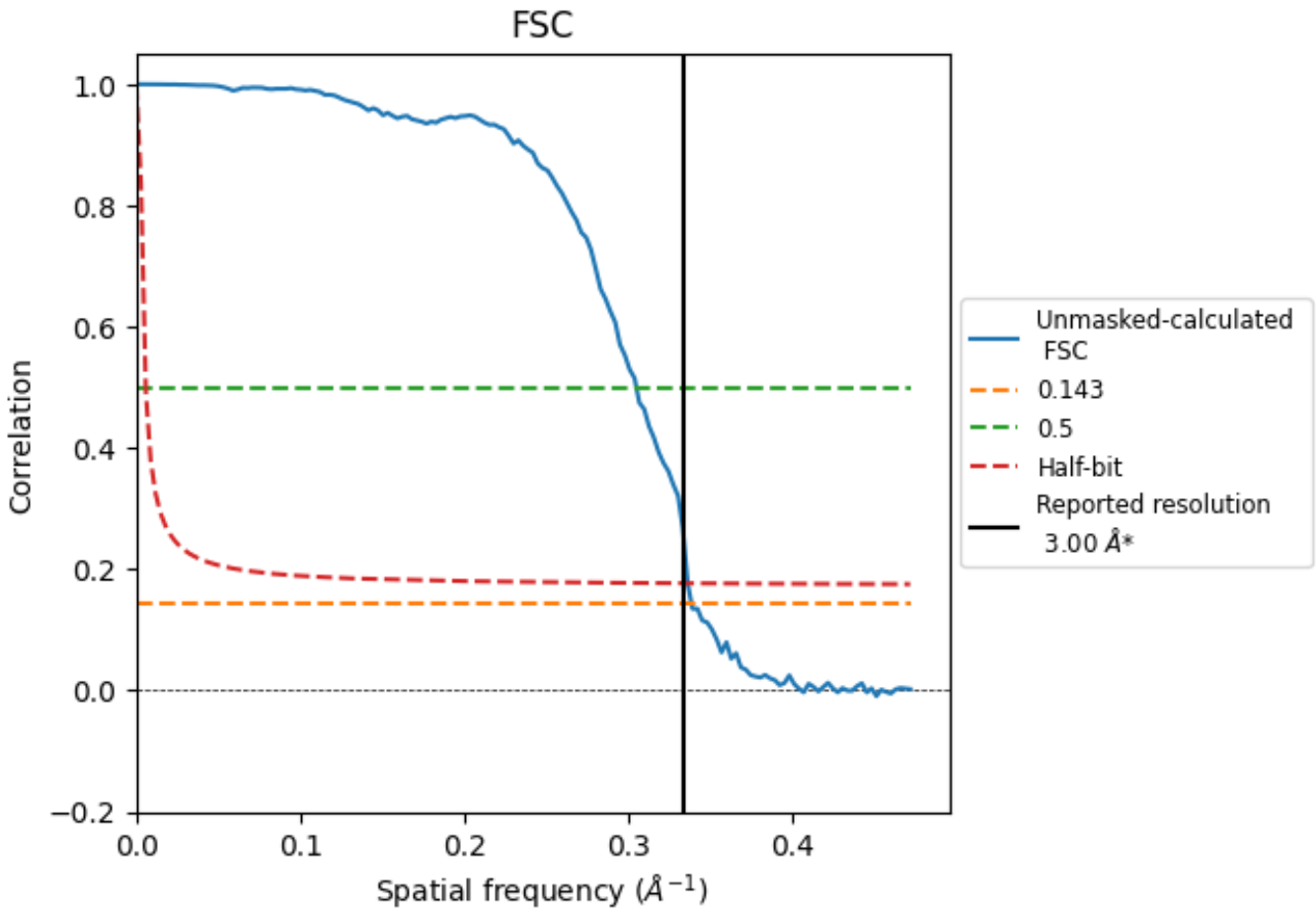


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.96	3.28	2.98

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

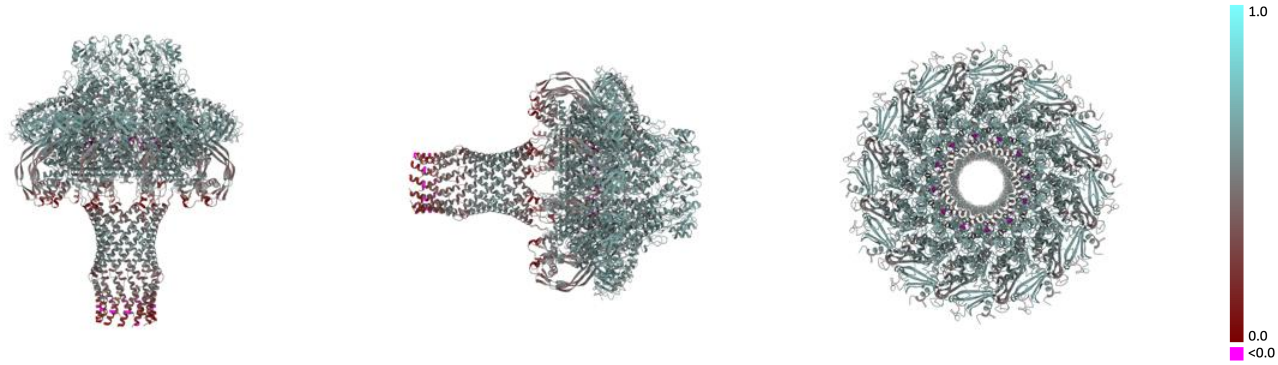
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62962 and PDB model 9LC1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

This section was not generated.

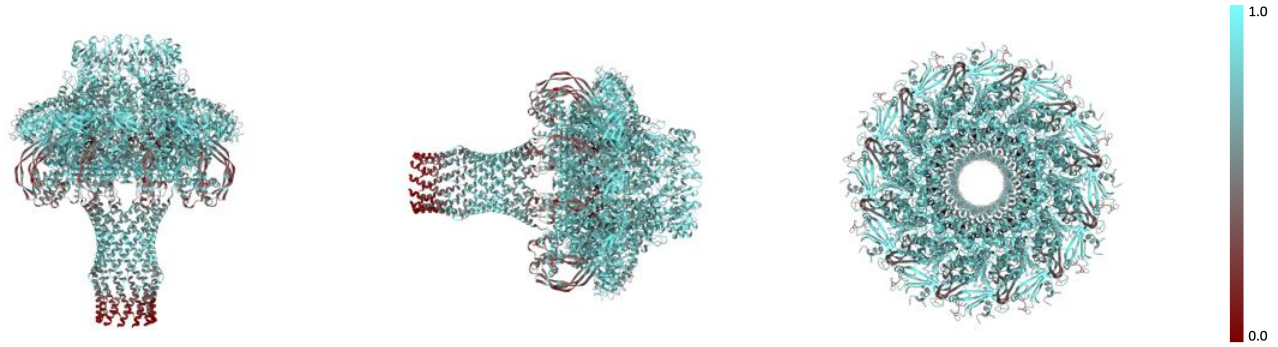
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

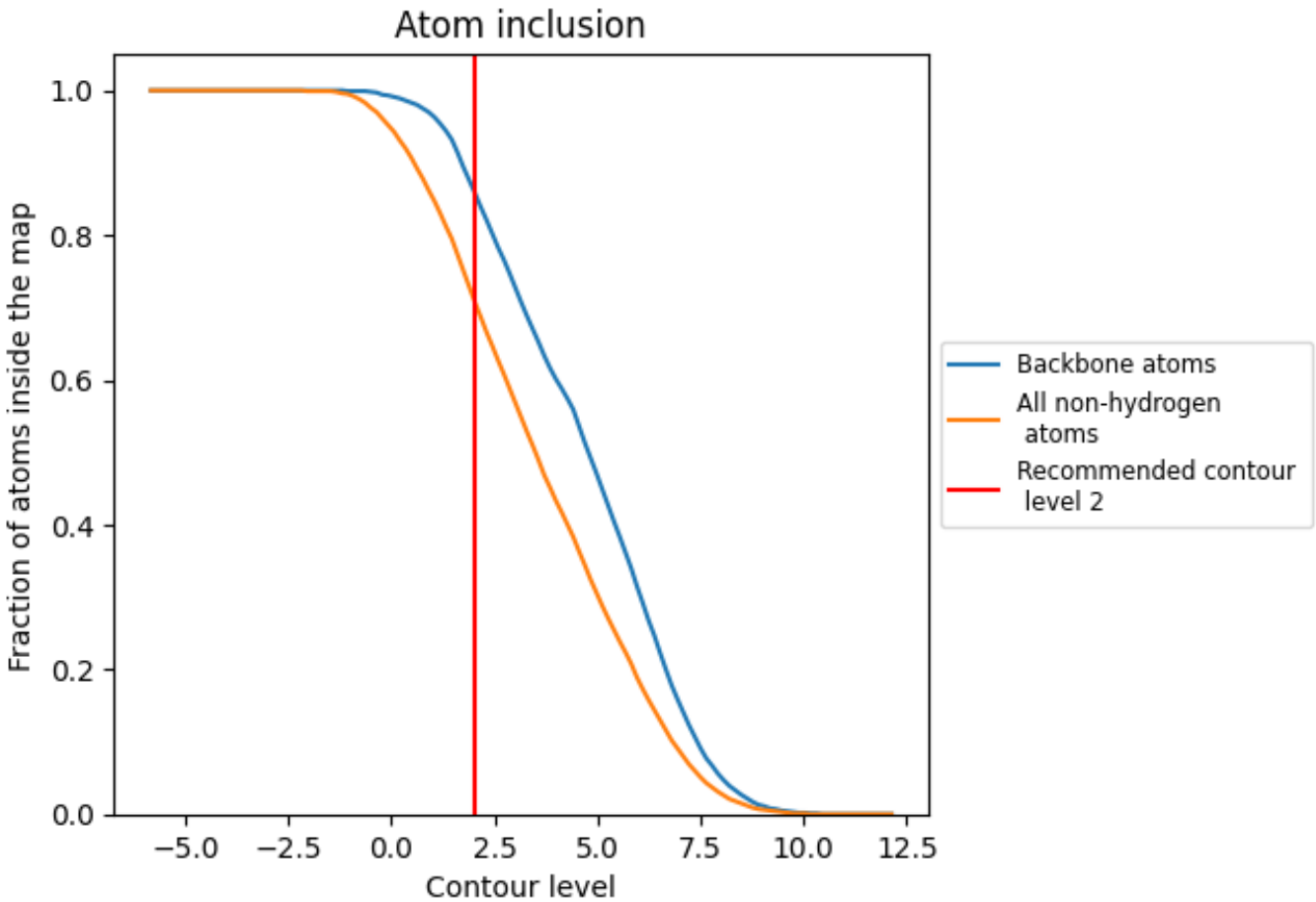
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.5280
A	0.7130	0.5290
B	0.7090	0.5250
C	0.7130	0.5270
D	0.7110	0.5270
E	0.7110	0.5260
F	0.7120	0.5270
G	0.7110	0.5290
H	0.7110	0.5270
I	0.7110	0.5280
J	0.7120	0.5300
K	0.7110	0.5270
L	0.7110	0.5270