



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:19 AM UTC

PDB ID : 8JAN / pdb_00008jan
EMDB ID : EMD-36130
Title : In situ structures of the ultra-long extended tail of Myoviridae phage P1
Authors : Zhou, J.Q.; Liu, H.R.
Deposited on : 2023-05-06
Resolution : 3.30 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:

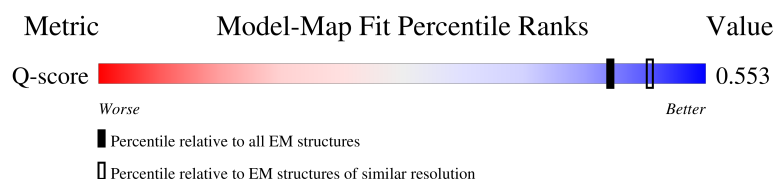
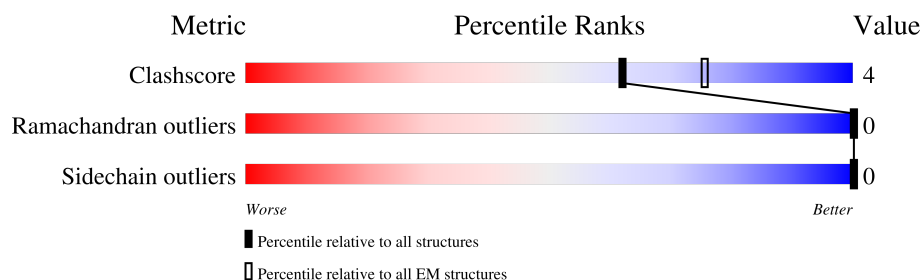
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

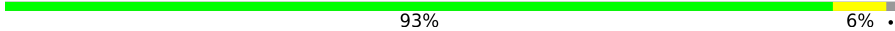
The reported resolution of this entry is 3.30 Å.

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.



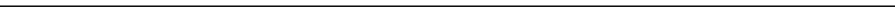
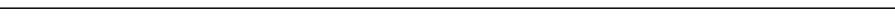
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	169	 88% 11% .
1	b	169	 91% 8% .
1	c	169	 93% 6% .
1	d	169	 89% 10% .

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Mol	Chain	Length	Quality of chain
1	e	169	 92% 7%
1	f	169	 87% 12%
1	g	169	 78% 17% 6%
1	h	169	 76% 18% 6%
1	i	169	 85% 9% 6%
1	j	169	 81% 13% 6%
1	k	169	 80% 14% 6%
1	l	169	 83% 11% 6%
2	m	529	 86% 13%
2	n	529	 89% 11%
2	o	529	 87% 13%
2	p	529	 87% 12%
2	q	529	 88% 12%
2	r	529	 86% 14%
2	s	529	 88% 12%
2	t	529	 88% 11%
2	u	529	 89% 10%
2	v	529	 89% 11%
2	w	529	 88% 12%
2	x	529	 88% 11%
3	A	261	 91% 8%
3	B	261	 92% 8%
3	C	261	 93% 6%
3	D	261	 92% 8%
3	y	261	 91% 9%

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Mol	Chain	Length	Quality of chain
3	z	261	 93% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 75114 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 BplB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	b	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	c	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	d	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	e	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	f	167	Total	C	N	O	S	0	0
			1304	815	226	258	5		
1	g	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		
1	h	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		
1	i	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		
1	j	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		
1	k	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		
1	l	159	Total	C	N	O	S	0	0
			1236	777	208	246	5		

- Molecule 2 is a protein called Gp22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		
2	n	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		
2	o	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	p	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		
2	q	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		
2	r	527	Total	C	N	O	S	0	0
			3984	2519	666	781	18		
2	s	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		
2	t	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		
2	u	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		
2	v	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		
2	w	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		
2	x	526	Total	C	N	O	S	0	0
			3975	2514	664	779	18		

- Molecule 3 is a protein called Gp24.

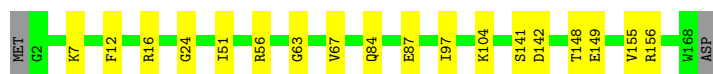
Mol	Chain	Residues	Atoms					AltConf	Trace
3	y	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		
3	z	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		
3	A	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		
3	B	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		
3	C	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		
3	D	260	Total	C	N	O	S	0	0
			2020	1286	335	393	6		

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: BplB

Chain a: 



- Molecule 1: BplB

Chain b: 



- Molecule 1: BplB

Chain c: 



- Molecule 1: BplB

Chain d: 



- Molecule 1: BplB

Chain e: 



- Molecule 1: BplB

Chain f:  87% 12% .



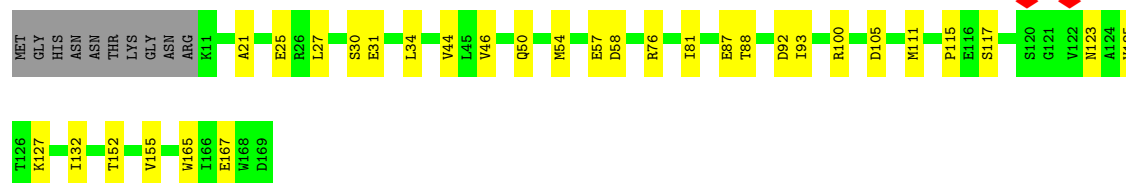
• Molecule 1: BplB

Chain g:  78% 17% 6%



• Molecule 1: BplB

Chain h:  76% 18% 6%



• Molecule 1: BplB

Chain i:  85% 9% 6%



• Molecule 1: BplB

Chain j:  81% 13% 6%



• Molecule 1: BplB

Chain k:  80% 14% 6%



W168
D169

• Molecule 1: BplB

Chain l:  83% 11% 6%

MET GLY HIS ASN THR LYS GLY ASN ARG K11 A21 L34 V44 L45 V46 Q50 D58 I81 E87 T88 I89 D92 I93 S117 K118 S119 S120 G121 V122 K127 T148 T152 V155 W156 E167 W168 D169

• Molecule 2: Gp22

Chain m:  86% 13%

MET S2 L10 D24 A25 R46 T56 F76 E77 R60 I86 D100 D141 S145 P146 L150 R164 L167 K168 T183 V186 S187 Y201 L202 P203 Y212 L213 V217 I222 K226 G241 D242 Q243 S244 V255 Y274

A281 V297 Y303 V310 T313 Y326 K333 D334 L345 H367 Y368 E374 R375 I378 A381 P392 K399 G400 R401 T423 Q424 D425 M426 H429 V433 P434 S435 L436 M437 A460 A479 V495 V498 D504 K505 W506 E507 V508 V509

C512 T515 R520 L526 L527 L528 LYS

• Molecule 2: Gp22

Chain n:  89% 11%

MET S2 L10 G11 D24 A25 R46 D100 D141 S145 P146 T147 T151 D158 D163 R164 T172 V178 S187 D194 D195 L202 P203 L206 A215 T224 S232 G241 V255 A281 K298 L301 T302 Y303 V310

T313 K333 H367 A381 P392 D393 M397 K398 K399 G400 R401 M413 T423 Q424 D425 H429 V433 P434 S435 L436 M437 H453 A460 A479 D504 K505 W506 V509 C512 T515 L526 L527 L528 LYS

• Molecule 2: Gp22

Chain o:  87% 13%

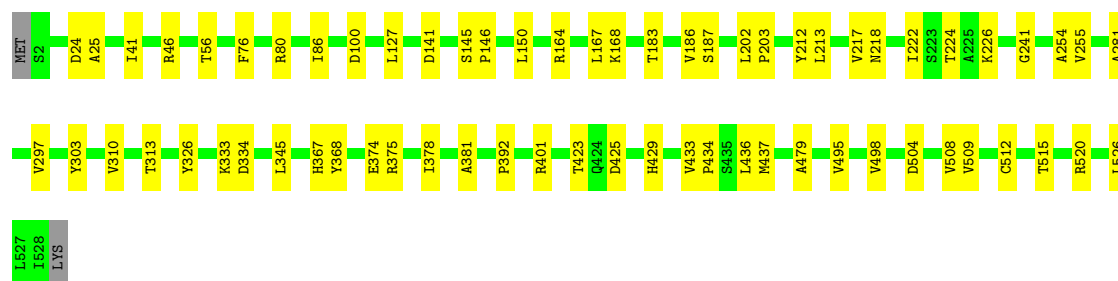
MET S2 L10 G11 A25 N34 I41 R46 Q75 F76 R80 D100 D109 L127 D128 S129 A132 D141 S145 P146 T151 R164 K168 T183 V186 S187 D194 D195 L202 Y212 L213 N218 T224 A225 K226 S232

G241 D242 Q243 S244 A254 V255 A281 Y303 V310 T313 K333 D334 L345 H367 Y368 R375 T378 A381 P392 K399 G400 R401 T423 Q424 D425 H429 V433 P434 S435 L436 M437 K465 A479 D504 V509 C512 T515

R520 T521 Q522 L526 L527 L528 LYS

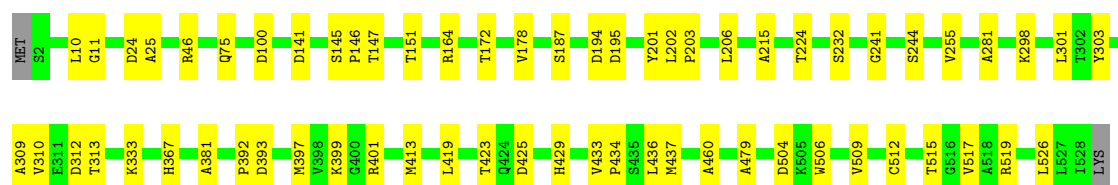
• Molecule 2: Gp22

Chain p:  87% 12%



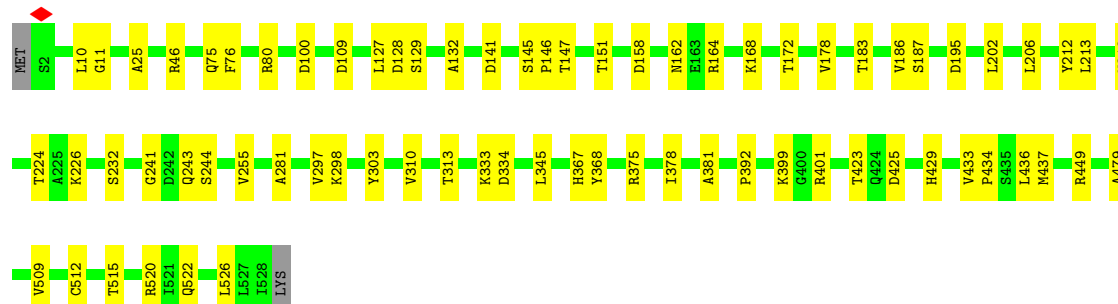
- Molecule 2: Gp22

Chain q:  88% 12%



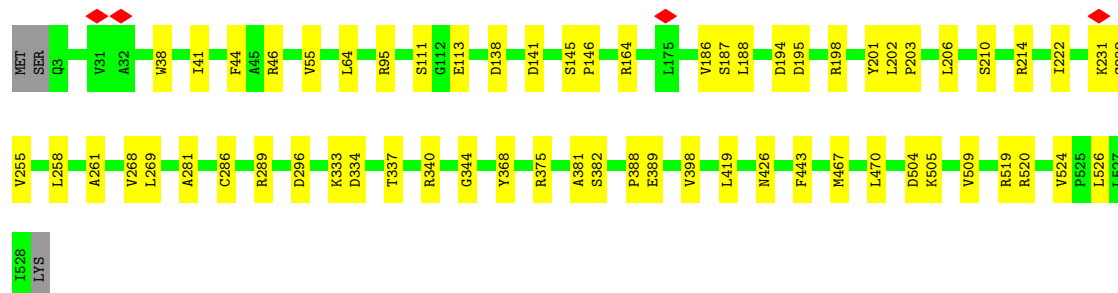
- Molecule 2: Gp22

Chain r:  86% 14%



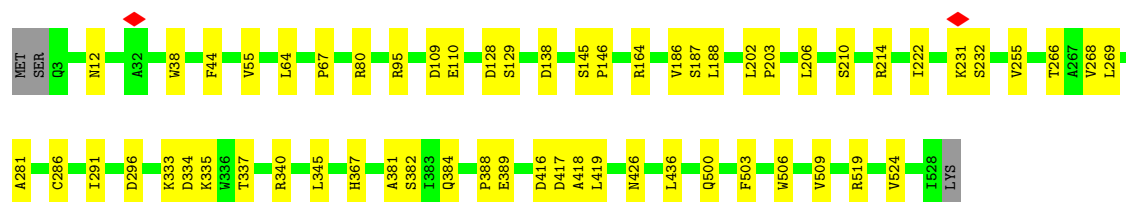
- Molecule 2: Gp22

Chain s:  88% 12%

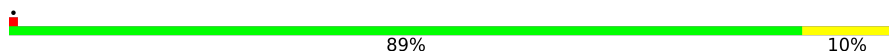


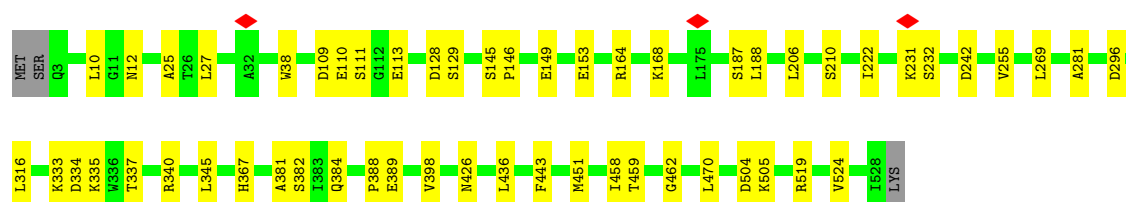
- Molecule 2: Gp22

Chain t:  88% 11% .

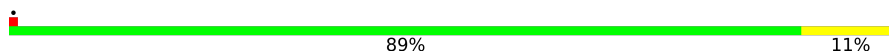


• Molecule 2: Gp22

Chain u:  89% 10% .

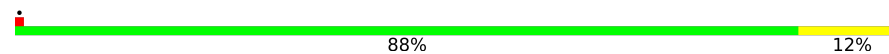


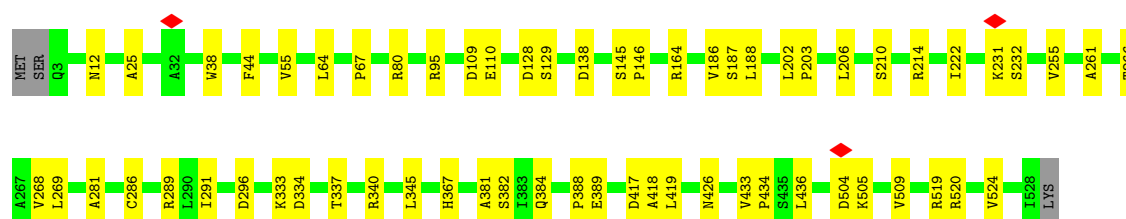
• Molecule 2: Gp22

Chain v:  89% 11% .



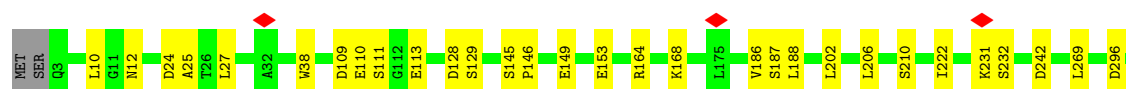
• Molecule 2: Gp22

Chain w:  88% 12% .



• Molecule 2: Gp22

Chain x:  88% 11% .





- Molecule 3: Gp24



- Molecule 3: Gp24



- Molecule 3: Gp24



- Molecule 3: Gp24



- Molecule 3: Gp24



- Molecule 3: Gp24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	32031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.15	0/1326	0.30	0/1795
1	b	0.15	0/1326	0.30	0/1795
1	c	0.15	0/1326	0.31	0/1795
1	d	0.15	0/1326	0.31	0/1795
1	e	0.15	0/1326	0.29	0/1795
1	f	0.15	0/1326	0.31	0/1795
1	g	0.15	0/1257	0.30	0/1705
1	h	0.15	0/1257	0.33	0/1705
1	i	0.15	0/1257	0.29	0/1705
1	j	0.15	0/1257	0.32	0/1705
1	k	0.15	0/1257	0.30	0/1705
1	l	0.15	0/1257	0.29	0/1705
2	m	0.14	0/4066	0.29	0/5537
2	n	0.15	0/4066	0.30	0/5537
2	o	0.15	0/4066	0.30	0/5537
2	p	0.15	0/4066	0.30	0/5537
2	q	0.15	0/4066	0.30	0/5537
2	r	0.15	0/4066	0.30	0/5537
2	s	0.13	0/4057	0.28	0/5525
2	t	0.13	0/4057	0.29	0/5525
2	u	0.13	0/4057	0.29	0/5525
2	v	0.13	0/4057	0.28	0/5525
2	w	0.13	0/4057	0.28	0/5525
2	x	0.13	0/4057	0.30	0/5525
3	A	0.13	0/2058	0.27	0/2794
3	B	0.12	0/2058	0.25	0/2794
3	C	0.21	0/2058	0.28	0/2794
3	D	0.13	0/2058	0.27	0/2794
3	y	0.12	0/2058	0.26	0/2794
3	z	0.21	0/2058	0.27	0/2794
All	All	0.14	0/76584	0.29	0/104136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1304	0	1282	12	0
1	b	1304	0	1282	10	0
1	c	1304	0	1282	8	0
1	d	1304	0	1282	11	0
1	e	1304	0	1282	10	0
1	f	1304	0	1282	14	0
1	g	1236	0	1209	21	0
1	h	1236	0	1209	20	0
1	i	1236	0	1209	11	0
1	j	1236	0	1209	15	0
1	k	1236	0	1209	15	0
1	l	1236	0	1209	14	0
2	m	3984	0	3935	47	0
2	n	3984	0	3935	38	0
2	o	3984	0	3935	45	0
2	p	3984	0	3935	43	0
2	q	3984	0	3935	41	0
2	r	3984	0	3935	49	0
2	s	3975	0	3927	39	0
2	t	3975	0	3927	39	0
2	u	3975	0	3927	35	0
2	v	3975	0	3927	37	0
2	w	3975	0	3927	39	0
2	x	3975	0	3927	39	0
3	A	2020	0	2000	17	0
3	B	2020	0	2000	17	0
3	C	2020	0	2000	16	0
3	D	2020	0	2000	16	0
3	y	2020	0	2000	17	0
3	z	2020	0	2000	15	0
All	All	75114	0	74118	641	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 (641) 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:r:509:VAL:HG12	2:x:524:VAL:HB	1.68	0.76
2:o:509:VAL:HG12	2:u:524:VAL:HB	1.69	0.75
2:n:194:ASP:OD1	2:n:195:ASP:N	2.22	0.73
2:u:443:PHE:HB3	2:u:470:LEU:HD21	1.71	0.73
2:p:367:HIS:HB3	2:p:436:LEU:HD21	1.71	0.73
3:B:179:ARG:NH1	3:C:128:ASP:OD2	2.22	0.72
2:m:367:HIS:HB3	2:m:436:LEU:HD21	1.71	0.72
2:q:509:VAL:HG12	2:w:524:VAL:HB	1.70	0.72
3:y:179:ARG:NH1	3:z:128:ASP:OD2	2.23	0.71
2:n:509:VAL:HG12	2:t:524:VAL:HB	1.70	0.71
3:A:179:ARG:NH1	3:B:128:ASP:OD2	2.24	0.71
2:t:509:VAL:HG12	3:z:255:LYS:HB2	1.73	0.70
2:w:509:VAL:HG12	3:C:255:LYS:HB2	1.72	0.70
3:y:128:ASP:OD2	3:D:179:ARG:NH1	2.24	0.70
2:w:426:ASN:O	3:C:6:GLN:NE2	2.26	0.69
2:m:509:VAL:HG12	2:s:524:VAL:HB	1.74	0.69
2:s:509:VAL:HG12	3:y:255:LYS:HB2	1.75	0.69
3:C:179:ARG:NH1	3:D:128:ASP:OD2	2.25	0.69
2:t:426:ASN:O	3:z:6:GLN:NE2	2.25	0.68
2:v:426:ASN:O	3:B:6:GLN:NE2	2.27	0.68
3:z:179:ARG:NH1	3:A:128:ASP:OD2	2.26	0.68
2:p:509:VAL:HG12	2:v:524:VAL:HB	1.76	0.67
2:v:509:VAL:HG12	3:B:255:LYS:HB2	1.74	0.67
2:r:367:HIS:HB3	2:r:436:LEU:HD21	1.77	0.66
1:a:87:GLU:HB3	1:a:155:VAL:HG13	1.78	0.66
2:o:368:TYR:HB3	2:o:375:ARG:HH12	1.60	0.66
2:x:509:VAL:HG12	3:D:255:LYS:HB2	1.78	0.66
2:u:426:ASN:O	3:A:6:GLN:NE2	2.30	0.65
1:d:87:GLU:HB3	1:d:155:VAL:HG13	1.78	0.65
2:x:426:ASN:O	3:D:6:GLN:NE2	2.30	0.65
1:h:34:LEU:HD23	1:h:46:VAL:HG11	1.77	0.65
1:k:87:GLU:HB3	1:k:155:VAL:HG13	1.79	0.64
2:p:46:ARG:HG3	2:p:141:ASP:HB2	1.78	0.64
1:k:34:LEU:HD23	1:k:46:VAL:HG11	1.78	0.64
2:r:145:SER:OG	2:r:146:PRO:HD3	1.98	0.64
2:s:164:ARG:HG2	2:s:187:SER:HB2	1.79	0.64
2:s:426:ASN:O	3:y:6:GLN:NE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:87:GLU:HB3	1:h:155:VAL:HG13	1.79	0.63
2:r:368:TYR:HB3	2:r:375:ARG:HH12	1.62	0.63
2:o:145:SER:OG	2:o:146:PRO:HD3	1.98	0.63
2:q:145:SER:OG	2:q:146:PRO:HD3	1.99	0.63
2:m:46:ARG:HG3	2:m:141:ASP:HB2	1.79	0.63
2:m:520:ARG:NH1	2:r:11:GLY:O	2.32	0.63
2:m:186:VAL:HG11	2:m:202:LEU:HD13	1.80	0.63
2:u:459:THR:HG23	2:u:462:GLY:H	1.63	0.63
1:j:87:GLU:HB3	1:j:155:VAL:HG13	1.81	0.62
2:r:425:ASP:HA	2:r:429:HIS:NE2	2.14	0.62
2:n:145:SER:OG	2:n:146:PRO:HD3	1.99	0.62
2:p:186:VAL:HG11	2:p:202:LEU:HD13	1.80	0.62
1:e:87:GLU:HB3	1:e:155:VAL:HG13	1.80	0.62
1:b:87:GLU:HB3	1:b:155:VAL:HG13	1.79	0.62
1:i:89:ILE:HD11	1:j:25:GLU:HB3	1.82	0.62
2:o:11:GLY:O	2:p:520:ARG:NH1	2.32	0.62
2:p:145:SER:OG	2:p:146:PRO:HD3	2.00	0.62
2:n:46:ARG:HG3	2:n:141:ASP:HB2	1.82	0.62
2:m:145:SER:OG	2:m:146:PRO:HD3	2.00	0.62
1:l:34:LEU:HD23	1:l:46:VAL:HG11	1.81	0.61
2:s:195:ASP:O	2:t:426:ASN:ND2	2.33	0.61
2:u:188:LEU:HD22	2:u:222:ILE:HD11	1.82	0.61
2:p:333:LYS:HB2	2:p:381:ALA:HB3	1.82	0.61
1:l:117:SER:HB2	1:l:127:LYS:HD3	1.81	0.61
2:o:194:ASP:OD1	2:o:195:ASP:N	2.33	0.61
2:o:367:HIS:HB3	2:o:436:LEU:HD21	1.82	0.61
2:q:46:ARG:HG3	2:q:141:ASP:HB2	1.82	0.61
2:p:100:ASP:HB2	2:p:241:GLY:HA3	1.83	0.61
2:s:188:LEU:HD22	2:s:222:ILE:HD11	1.83	0.61
1:c:97:ILE:HD13	1:c:141:SER:HB2	1.81	0.60
2:u:504:ASP:HB2	3:A:250:GLY:HA2	1.82	0.60
2:v:195:ASP:O	2:w:426:ASN:ND2	2.34	0.60
3:A:75:THR:HG22	3:A:113:SER:HB2	1.82	0.60
3:D:75:THR:HG22	3:D:113:SER:HB2	1.83	0.60
2:m:100:ASP:HB2	2:m:241:GLY:HA3	1.83	0.60
2:v:188:LEU:HD22	2:v:222:ILE:HD11	1.84	0.60
2:x:452:LYS:O	2:x:453:HIS:ND1	2.33	0.60
2:n:310:VAL:O	2:n:313:THR:OG1	2.20	0.60
2:p:164:ARG:HG2	2:p:187:SER:HB2	1.84	0.60
2:q:367:HIS:HB3	2:q:436:LEU:HD21	1.84	0.60
2:m:333:LYS:HB2	2:m:381:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:87:GLU:HB3	1:l:155:VAL:HG13	1.84	0.59
2:n:333:LYS:HB2	2:n:381:ALA:HB3	1.84	0.59
2:p:310:VAL:O	2:p:313:THR:OG1	2.20	0.59
2:o:34:ASN:O	2:o:34:ASN:ND2	2.36	0.59
2:m:164:ARG:HG2	2:m:187:SER:HB2	1.84	0.59
2:t:44:PHE:O	2:t:95:ARG:NH1	2.35	0.59
2:r:401:ARG:HH21	2:r:423:THR:HA	1.67	0.59
2:t:145:SER:OG	2:t:146:PRO:HD3	2.03	0.59
1:g:123:ASN:OD1	1:g:124:ALA:N	2.34	0.59
2:u:367:HIS:HB3	2:u:436:LEU:HD21	1.85	0.59
2:v:145:SER:OG	2:v:146:PRO:HD3	2.03	0.59
2:q:333:LYS:HB2	2:q:381:ALA:HB3	1.83	0.59
2:w:44:PHE:O	2:w:95:ARG:NH1	2.36	0.59
2:w:145:SER:OG	2:w:146:PRO:HD3	2.03	0.59
1:i:88:THR:OG1	1:i:92:ASP:OD1	2.21	0.59
2:r:425:ASP:HA	2:r:429:HIS:CE1	2.38	0.59
1:f:97:ILE:HD13	1:f:141:SER:HB2	1.85	0.58
2:q:194:ASP:OD1	2:q:195:ASP:N	2.36	0.58
2:o:310:VAL:O	2:o:313:THR:OG1	2.21	0.58
2:q:147:THR:OG1	2:q:172:THR:OG1	2.22	0.58
2:s:145:SER:OG	2:s:146:PRO:HD3	2.03	0.58
2:q:100:ASP:HB2	2:q:241:GLY:HA3	1.86	0.58
2:q:310:VAL:O	2:q:313:THR:OG1	2.21	0.58
2:x:188:LEU:HD22	2:x:222:ILE:HD11	1.83	0.58
1:l:88:THR:OG1	1:l:92:ASP:OD1	2.21	0.58
2:n:367:HIS:HB3	2:n:436:LEU:HD21	1.84	0.58
2:x:500:GLN:OE1	2:x:506:TRP:NE1	2.31	0.58
2:n:433:VAL:HB	2:n:434:PRO:HD3	1.86	0.58
2:p:368:TYR:HB3	2:p:375:ARG:HH12	1.69	0.58
1:b:97:ILE:HD13	1:b:141:SER:HB2	1.86	0.57
1:i:87:GLU:HB3	1:i:155:VAL:HG13	1.86	0.57
2:x:367:HIS:HB3	2:x:436:LEU:HD21	1.86	0.57
1:e:97:ILE:HD13	1:e:141:SER:HB2	1.86	0.57
2:m:310:VAL:O	2:m:313:THR:OG1	2.20	0.57
2:q:433:VAL:HB	2:q:434:PRO:HD3	1.86	0.57
2:x:145:SER:OG	2:x:146:PRO:HD3	2.04	0.57
1:f:87:GLU:HB3	1:f:155:VAL:HG13	1.87	0.57
2:x:504:ASP:HB3	3:D:250:GLY:HA3	1.86	0.57
3:y:53:ASP:OD1	3:y:54:ARG:N	2.38	0.57
2:m:368:TYR:HB3	2:m:375:ARG:HH12	1.69	0.57
2:r:186:VAL:HG11	2:r:202:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:333:LYS:HB2	2:o:381:ALA:HB3	1.87	0.57
2:q:425:ASP:HA	2:q:429:HIS:CE1	2.40	0.57
2:u:145:SER:OG	2:u:146:PRO:HD3	2.04	0.57
1:c:87:GLU:HB3	1:c:155:VAL:HG13	1.87	0.57
2:o:425:ASP:HA	2:o:429:HIS:NE2	2.20	0.57
2:o:433:VAL:HB	2:o:434:PRO:HD3	1.87	0.57
2:r:151:THR:HG22	2:r:232:SER:H	1.70	0.57
1:d:97:ILE:HD13	1:d:141:SER:HB2	1.87	0.56
1:f:84:GLN:OE1	1:f:156:ARG:NH2	2.27	0.56
2:n:100:ASP:HB2	2:n:241:GLY:HA3	1.87	0.56
2:n:433:VAL:O	2:n:437:MET:HG2	2.05	0.56
2:o:128:ASP:OD1	2:o:129:SER:N	2.39	0.56
2:w:80:ARG:NH2	2:w:334:ASP:OD2	2.39	0.56
2:m:425:ASP:HA	2:m:429:HIS:CE1	2.41	0.56
2:r:433:VAL:HB	2:r:434:PRO:HD3	1.87	0.56
2:r:128:ASP:OD1	2:r:129:SER:N	2.39	0.56
2:r:147:THR:OG1	2:r:172:THR:OG1	2.23	0.56
1:a:97:ILE:HD13	1:a:141:SER:HB2	1.88	0.56
2:o:186:VAL:HG11	2:o:202:LEU:HD13	1.87	0.56
1:e:104:LYS:HE2	1:f:56:ARG:NH1	2.21	0.56
2:m:433:VAL:HB	2:m:434:PRO:HD3	1.88	0.56
2:p:425:ASP:HA	2:p:429:HIS:CE1	2.41	0.56
2:t:255:VAL:HG11	2:t:281:ALA:HB1	1.88	0.56
2:w:255:VAL:HG11	2:w:281:ALA:HB1	1.88	0.56
2:q:479:ALA:O	2:q:515:THR:OG1	2.23	0.56
1:a:141:SER:OG	1:a:142:ASP:N	2.39	0.55
1:b:104:LYS:HE2	1:c:56:ARG:NH1	2.21	0.55
1:h:50:GLN:HB2	1:h:81:ILE:HG13	1.88	0.55
2:n:147:THR:OG1	2:n:172:THR:OG1	2.22	0.55
2:n:425:ASP:HA	2:n:429:HIS:NE2	2.22	0.55
2:p:425:ASP:HA	2:p:429:HIS:NE2	2.21	0.55
2:u:153:GLU:OE2	2:u:168:LYS:NZ	2.32	0.55
1:a:84:GLN:OE1	1:a:156:ARG:NH2	2.29	0.55
2:n:425:ASP:HA	2:n:429:HIS:CE1	2.42	0.55
1:d:141:SER:OG	1:d:142:ASP:N	2.39	0.55
2:o:436:LEU:HD22	2:o:479:ALA:HB1	1.88	0.55
2:v:186:VAL:HG11	2:v:202:LEU:HD13	1.89	0.55
2:r:333:LYS:HB2	2:r:381:ALA:HB3	1.87	0.55
2:t:80:ARG:NH2	2:t:334:ASP:OD2	2.38	0.55
2:q:433:VAL:O	2:q:437:MET:HG2	2.05	0.55
1:k:50:GLN:HB2	1:k:81:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:453:HIS:NE2	2:t:416:ASP:O	2.40	0.55
2:o:151:THR:HG22	2:o:232:SER:H	1.71	0.55
2:o:164:ARG:HG2	2:o:187:SER:HB2	1.89	0.55
2:m:425:ASP:HA	2:m:429:HIS:NE2	2.21	0.55
2:r:100:ASP:HB2	2:r:241:GLY:HA3	1.89	0.55
2:s:186:VAL:HG11	2:s:202:LEU:HD13	1.88	0.55
2:q:425:ASP:HA	2:q:429:HIS:NE2	2.22	0.54
2:n:25:ALA:HB3	2:o:526:LEU:HD22	1.89	0.54
1:f:141:SER:OG	1:f:142:ASP:N	2.38	0.54
1:g:88:THR:OG1	1:g:92:ASP:OD2	2.22	0.54
2:r:164:ARG:HG2	2:r:187:SER:HB2	1.88	0.54
1:h:152:THR:HG22	3:z:208:GLY:HA2	1.90	0.54
2:m:504:ASP:HB2	2:s:519:ARG:HG2	1.89	0.54
1:g:87:GLU:HG3	1:h:27:LEU:HD13	1.90	0.54
2:t:186:VAL:HG11	2:t:202:LEU:HD13	1.88	0.54
2:x:452:LYS:HD2	2:x:453:HIS:ND1	2.22	0.54
1:c:84:GLN:OE1	1:c:156:ARG:NH2	2.26	0.54
2:p:433:VAL:HB	2:p:434:PRO:HD3	1.88	0.54
2:t:340:ARG:NH2	2:t:382:SER:OG	2.41	0.54
2:q:25:ALA:HB3	2:r:526:LEU:HD22	1.89	0.54
2:w:186:VAL:HG11	2:w:202:LEU:HD13	1.88	0.54
2:p:479:ALA:O	2:p:515:THR:OG1	2.24	0.54
1:g:100:ARG:NH2	1:g:105:ASP:OD2	2.39	0.53
2:t:296:ASP:OD2	2:t:345:LEU:N	2.42	0.53
2:x:340:ARG:NH2	2:x:382:SER:OG	2.41	0.53
3:y:62:PHE:HA	3:y:65:ARG:HD3	1.91	0.53
2:r:479:ALA:O	2:r:515:THR:OG1	2.24	0.53
2:t:333:LYS:HB2	2:t:381:ALA:HB3	1.91	0.53
2:w:340:ARG:NH2	2:w:382:SER:OG	2.41	0.53
2:r:310:VAL:O	2:r:313:THR:OG1	2.22	0.53
2:w:296:ASP:OD2	2:w:345:LEU:N	2.42	0.53
2:o:100:ASP:HB2	2:o:241:GLY:HA3	1.89	0.53
1:d:63:GLY:N	1:d:67:VAL:O	2.36	0.53
2:p:504:ASP:HB2	2:v:519:ARG:HG2	1.90	0.53
3:z:62:PHE:HA	3:z:65:ARG:HD3	1.91	0.53
1:k:152:THR:HG22	3:C:208:GLY:HA2	1.90	0.53
2:r:46:ARG:HG3	2:r:141:ASP:HB2	1.91	0.53
1:b:104:LYS:HE2	1:c:56:ARG:HH12	1.74	0.52
2:u:504:ASP:OD1	2:u:505:LYS:HD2	2.08	0.52
2:t:334:ASP:HB3	2:t:337:THR:O	2.09	0.52
2:m:526:LEU:HD22	2:r:25:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:436:LEU:HD22	2:r:479:ALA:HB1	1.91	0.52
2:w:188:LEU:HD22	2:w:222:ILE:HD11	1.91	0.52
2:m:479:ALA:O	2:m:515:THR:OG1	2.24	0.52
2:n:504:ASP:HB2	2:t:519:ARG:HG2	1.91	0.52
2:u:340:ARG:NH2	2:u:382:SER:OG	2.42	0.52
2:w:333:LYS:HB2	2:w:381:ALA:HB3	1.91	0.52
2:w:334:ASP:HB3	2:w:337:THR:O	2.09	0.52
3:B:62:PHE:HA	3:B:65:ARG:HD3	1.91	0.52
2:o:25:ALA:HB3	2:p:526:LEU:HD22	1.91	0.52
2:p:168:LYS:HG2	2:p:183:THR:HG22	1.92	0.52
2:o:46:ARG:HG3	2:o:141:ASP:HB2	1.91	0.52
1:a:12:PHE:O	1:a:16:ARG:HG2	2.10	0.52
2:s:206:LEU:O	2:s:210:SER:OG	2.24	0.52
1:g:87:GLU:HB3	1:g:155:VAL:HG13	1.92	0.52
3:C:62:PHE:HA	3:C:65:ARG:HD3	1.91	0.52
2:o:345:LEU:HD11	2:o:378:ILE:HD13	1.92	0.51
2:x:186:VAL:HG11	2:x:202:LEU:HD13	1.91	0.51
1:j:100:ARG:NH2	1:j:105:ASP:OD2	2.40	0.51
2:p:41:ILE:HD11	2:p:254:ALA:HB3	1.92	0.51
3:z:179:ARG:HE	3:A:120:ILE:HG21	1.76	0.51
2:p:436:LEU:HD22	2:p:479:ALA:HB1	1.92	0.51
2:x:206:LEU:O	2:x:210:SER:OG	2.22	0.51
1:d:12:PHE:O	1:d:16:ARG:HG2	2.10	0.51
1:k:111:MET:HB3	1:k:132:ILE:HG22	1.93	0.51
2:q:504:ASP:HB2	2:w:519:ARG:HG2	1.91	0.51
1:g:25:GLU:HB3	1:l:89:ILE:HD11	1.92	0.51
1:i:152:THR:HG22	3:A:208:GLY:HA2	1.92	0.51
2:m:168:LYS:HG2	2:m:183:THR:HG22	1.92	0.51
1:l:152:THR:HG22	3:D:208:GLY:HA2	1.92	0.51
1:l:165:TRP:CD1	1:l:167:GLU:HG2	2.46	0.51
2:r:345:LEU:HD11	2:r:378:ILE:HD13	1.93	0.51
2:t:417:ASP:OD1	2:t:418:ALA:N	2.43	0.51
2:t:500:GLN:HE21	2:t:503:PHE:HA	1.76	0.51
2:x:153:GLU:OE2	2:x:168:LYS:NZ	2.32	0.51
3:B:145:LEU:HD12	3:B:245:MET:HE3	1.92	0.51
1:h:87:GLU:OE1	1:h:93:ILE:HB	2.11	0.51
2:s:467:MET:HE3	2:s:467:MET:HA	1.92	0.51
2:s:526:LEU:HD22	2:x:25:ALA:HB3	1.93	0.51
2:w:367:HIS:HB3	2:w:436:LEU:HD21	1.92	0.51
3:y:145:LEU:HD12	3:y:245:MET:HE3	1.93	0.51
2:m:426:ASN:ND2	2:r:195:ASP:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:436:LEU:HD22	2:m:479:ALA:HB1	1.93	0.50
2:t:506:TRP:HE1	3:z:15:LYS:NZ	2.09	0.50
1:i:165:TRP:CD1	1:i:167:GLU:HG2	2.46	0.50
2:q:164:ARG:HG2	2:q:187:SER:HB2	1.92	0.50
2:o:479:ALA:O	2:o:515:THR:OG1	2.24	0.50
2:v:467:MET:HA	2:v:467:MET:HE3	1.92	0.50
2:x:334:ASP:HB3	2:x:337:THR:O	2.12	0.50
3:C:179:ARG:HE	3:D:120:ILE:HG21	1.76	0.50
1:a:63:GLY:N	1:a:67:VAL:O	2.37	0.50
2:n:460:ALA:HB2	2:n:506:TRP:CH2	2.47	0.50
2:p:25:ALA:HB3	2:q:526:LEU:HD22	1.94	0.50
2:u:206:LEU:O	2:u:210:SER:OG	2.22	0.50
2:p:24:ASP:OD1	2:p:24:ASP:N	2.45	0.50
1:k:87:GLU:OE1	1:k:93:ILE:HB	2.12	0.49
2:m:25:ALA:HB3	2:n:526:LEU:HD22	1.93	0.49
1:c:104:LYS:HE2	1:d:56:ARG:NH1	2.28	0.49
2:m:150:LEU:HD23	2:m:167:LEU:HD11	1.94	0.49
2:n:479:ALA:O	2:n:515:THR:OG1	2.24	0.49
2:p:433:VAL:O	2:p:437:MET:HG2	2.11	0.49
2:v:334:ASP:HB3	2:v:337:THR:O	2.12	0.49
1:k:44:VAL:HG21	1:l:21:ALA:HB1	1.94	0.49
2:m:80:ARG:NH2	2:m:334:ASP:OD2	2.43	0.49
2:u:334:ASP:HB3	2:u:337:THR:O	2.12	0.49
2:m:24:ASP:OD1	2:m:24:ASP:N	2.45	0.49
2:r:433:VAL:O	2:r:437:MET:HG2	2.11	0.49
2:s:334:ASP:HB3	2:s:337:THR:O	2.12	0.49
1:j:58:ASP:OD1	1:j:58:ASP:N	2.45	0.49
1:l:50:GLN:HB2	1:l:81:ILE:HG13	1.93	0.49
2:m:433:VAL:O	2:m:437:MET:HG2	2.12	0.49
1:h:44:VAL:HG21	1:i:21:ALA:HB1	1.94	0.49
1:h:88:THR:OG1	1:h:92:ASP:OD2	2.26	0.49
2:o:425:ASP:HA	2:o:429:HIS:CE1	2.46	0.49
2:n:11:GLY:O	2:o:520:ARG:NH1	2.46	0.49
2:o:401:ARG:HH21	2:o:423:THR:HA	1.77	0.49
2:p:150:LEU:HD23	2:p:167:LEU:HD11	1.95	0.49
2:u:255:VAL:HG11	2:u:281:ALA:HB1	1.93	0.49
1:h:58:ASP:OD1	1:h:58:ASP:N	2.46	0.49
2:o:255:VAL:HG11	2:o:281:ALA:HB1	1.94	0.49
1:e:104:LYS:HE2	1:f:56:ARG:HH12	1.78	0.49
2:r:449:ARG:NH2	2:x:407:VAL:O	2.46	0.49
1:f:88:THR:OG1	1:f:92:ASP:OD1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:388:PRO:O	2:w:389:GLU:HG2	2.13	0.48
3:D:62:PHE:HA	3:D:65:ARG:HD3	1.95	0.48
2:q:460:ALA:HB2	2:q:506:TRP:CH2	2.48	0.48
2:t:388:PRO:O	2:t:389:GLU:HG2	2.13	0.48
1:a:24:GLY:HA3	1:b:5:ASN:ND2	2.29	0.48
1:g:117:SER:HB2	1:g:127:LYS:HD3	1.95	0.48
1:a:56:ARG:NH1	1:f:104:LYS:HE2	2.27	0.48
1:d:24:GLY:HA3	1:e:5:ASN:ND2	2.28	0.48
2:w:164:ARG:HB3	2:w:187:SER:HB2	1.96	0.48
3:A:62:PHE:HA	3:A:65:ARG:HD3	1.96	0.48
1:g:16:ARG:HH11	1:g:16:ARG:HG3	1.78	0.48
1:h:123:ASN:OD1	1:h:125:VAL:HG22	2.13	0.48
1:j:152:THR:HG22	3:B:208:GLY:HA2	1.95	0.48
2:t:206:LEU:O	2:t:210:SER:OG	2.23	0.48
1:d:84:GLN:OE1	1:d:156:ARG:NH2	2.29	0.48
2:m:217:VAL:HG13	2:m:222:ILE:HG21	1.95	0.48
2:p:401:ARG:HH21	2:p:423:THR:HA	1.78	0.48
2:r:255:VAL:HG11	2:r:281:ALA:HB1	1.95	0.48
2:q:206:LEU:HD12	2:q:215:ALA:HB2	1.96	0.48
2:v:138:ASP:HB2	2:v:214:ARG:HG2	1.96	0.48
1:g:44:VAL:HG21	1:h:21:ALA:HB1	1.96	0.47
1:j:44:VAL:HG21	1:k:21:ALA:HB1	1.96	0.47
2:w:138:ASP:HB2	2:w:214:ARG:HG2	1.96	0.47
2:o:437:MET:HE1	2:o:512:CYS:SG	2.54	0.47
2:p:80:ARG:NH2	2:p:334:ASP:OD2	2.43	0.47
2:u:10:LEU:HD13	2:v:520:ARG:HB3	1.96	0.47
2:v:55:VAL:HG11	2:v:64:LEU:HD13	1.96	0.47
2:v:368:TYR:HB3	2:v:375:ARG:HH12	1.80	0.47
2:x:388:PRO:O	2:x:389:GLU:HG2	2.14	0.47
2:v:41:ILE:HG23	2:v:258:LEU:HD11	1.96	0.47
2:x:505:LYS:HE3	2:x:505:LYS:HB2	1.68	0.47
2:v:333:LYS:HB2	2:v:381:ALA:HB3	1.96	0.47
2:w:12:ASN:HB3	2:x:398:VAL:HG11	1.96	0.47
2:m:401:ARG:HH21	2:m:423:THR:HA	1.79	0.47
2:s:388:PRO:O	2:s:389:GLU:HG2	2.15	0.47
2:t:164:ARG:HB3	2:t:187:SER:HB2	1.96	0.47
1:i:50:GLN:HB2	1:i:81:ILE:HG13	1.97	0.47
1:j:88:THR:OG1	1:j:92:ASP:OD2	2.27	0.47
1:l:58:ASP:OD1	1:l:58:ASP:N	2.48	0.47
2:n:10:LEU:HD11	2:o:522:GLN:HB2	1.97	0.47
2:o:303:TYR:CE1	2:o:392:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:138:ASP:HB2	2:t:214:ARG:HG2	1.97	0.47
2:x:164:ARG:HB3	2:x:187:SER:HB2	1.96	0.47
1:k:57:GLU:OE2	1:k:76:ARG:NE	2.40	0.47
2:n:172:THR:HG22	2:n:178:VAL:HG22	1.96	0.47
2:u:296:ASP:OD2	2:u:345:LEU:N	2.48	0.47
1:h:111:MET:HB3	1:h:132:ILE:HG22	1.97	0.47
2:v:388:PRO:O	2:v:389:GLU:HG2	2.15	0.47
3:z:179:ARG:NE	3:A:120:ILE:HG21	2.30	0.47
2:p:217:VAL:HG13	2:p:222:ILE:HG21	1.96	0.47
2:r:80:ARG:NH2	2:r:334:ASP:OD2	2.47	0.47
2:w:25:ALA:HB3	2:x:526:LEU:HD22	1.97	0.47
2:x:38:TRP:HB2	2:x:269:LEU:HD13	1.97	0.47
1:a:51:ILE:HB	1:f:144:ILE:HB	1.97	0.46
1:d:104:LYS:HE2	1:e:56:ARG:NH1	2.31	0.46
2:q:172:THR:HG22	2:q:178:VAL:HG22	1.96	0.46
2:r:399:LYS:HB3	2:r:399:LYS:HE2	1.70	0.46
3:y:107:MET:HB2	3:y:108:PRO:HD3	1.97	0.46
1:e:148:THR:O	1:e:149:GLU:HG3	2.15	0.46
2:s:41:ILE:HG23	2:s:258:LEU:HD11	1.97	0.46
2:s:138:ASP:HB2	2:s:214:ARG:HG2	1.96	0.46
2:s:520:ARG:HB3	2:x:10:LEU:HD13	1.97	0.46
1:f:63:GLY:N	1:f:67:VAL:O	2.40	0.46
2:r:158:ASP:OD1	2:r:162:ASN:N	2.48	0.46
2:t:12:ASN:HB3	2:u:398:VAL:HG11	1.98	0.46
2:t:109:ASP:OD1	2:t:110:GLU:N	2.49	0.46
2:u:388:PRO:O	2:u:389:GLU:HG2	2.14	0.46
2:w:206:LEU:O	2:w:210:SER:OG	2.23	0.46
2:x:296:ASP:OD2	2:x:345:LEU:N	2.49	0.46
2:x:333:LYS:HB2	2:x:381:ALA:HB3	1.98	0.46
1:h:100:ARG:NH2	1:h:105:ASP:OD2	2.47	0.46
2:n:206:LEU:HD12	2:n:215:ALA:HB2	1.97	0.46
2:s:55:VAL:HG11	2:s:64:LEU:HD13	1.96	0.46
3:y:179:ARG:NE	3:z:120:ILE:HG21	2.30	0.46
2:s:333:LYS:HB2	2:s:381:ALA:HB3	1.97	0.46
2:t:367:HIS:HB3	2:t:436:LEU:HD21	1.98	0.46
2:t:419:LEU:HD21	2:t:519:ARG:HH12	1.79	0.46
2:u:333:LYS:HB2	2:u:381:ALA:HB3	1.98	0.46
1:g:151:VAL:HA	1:h:30:SER:OG	2.15	0.46
2:s:368:TYR:HB3	2:s:375:ARG:HH12	1.80	0.46
2:v:206:LEU:O	2:v:210:SER:OG	2.24	0.46
3:A:179:ARG:NE	3:B:120:ILE:HG21	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:144:ILE:HB	1:d:51:ILE:HB	1.98	0.46
2:n:202:LEU:HB3	2:n:203:PRO:HD3	1.98	0.46
3:B:107:MET:HB2	3:B:108:PRO:HD3	1.97	0.46
2:u:242:ASP:N	2:u:242:ASP:OD1	2.49	0.46
2:v:111:SER:OG	2:v:113:GLU:OE1	2.32	0.46
3:B:39:ALA:O	3:B:42:GLU:HG2	2.16	0.46
1:i:58:ASP:OD1	1:i:58:ASP:N	2.47	0.45
2:o:168:LYS:HG2	2:o:183:THR:HG22	1.97	0.45
3:y:39:ALA:O	3:y:42:GLU:HG2	2.17	0.45
1:i:44:VAL:HG21	1:j:21:ALA:HB1	1.97	0.45
2:x:242:ASP:OD1	2:x:242:ASP:N	2.49	0.45
3:y:120:ILE:HG21	3:D:179:ARG:NE	2.31	0.45
3:C:39:ALA:O	3:C:42:GLU:HG2	2.17	0.45
3:C:107:MET:HB2	3:C:108:PRO:HD3	1.98	0.45
1:b:148:THR:O	1:b:149:GLU:HG3	2.15	0.45
1:g:50:GLN:HB2	1:g:81:ILE:HG13	1.98	0.45
1:k:100:ARG:NH2	1:k:105:ASP:OD2	2.48	0.45
2:p:345:LEU:HD11	2:p:378:ILE:HD13	1.98	0.45
2:q:11:GLY:O	2:r:520:ARG:NH1	2.50	0.45
2:r:172:THR:HG22	2:r:178:VAL:HG22	1.97	0.45
3:D:39:ALA:O	3:D:42:GLU:HG2	2.17	0.45
2:m:345:LEU:HD11	2:m:378:ILE:HD13	1.97	0.45
2:o:399:LYS:HB3	2:o:399:LYS:HE2	1.69	0.45
2:q:202:LEU:HB3	2:q:203:PRO:HD3	1.98	0.45
2:s:296:ASP:OD2	2:s:344:GLY:HA3	2.16	0.45
3:y:15:LYS:HE3	3:y:250:GLY:HA3	1.97	0.45
3:B:179:ARG:NE	3:C:120:ILE:HG21	2.31	0.45
3:C:179:ARG:NE	3:D:120:ILE:HG21	2.31	0.45
1:g:101:ILE:HG13	1:h:54:MET:HG3	1.98	0.45
1:l:87:GLU:OE1	1:l:93:ILE:HB	2.16	0.45
2:n:164:ARG:HG2	2:n:187:SER:HB2	1.97	0.45
3:z:112:LEU:HD12	3:z:157:LEU:HD21	1.99	0.45
1:j:165:TRP:CD1	1:j:167:GLU:HG2	2.51	0.45
2:p:303:TYR:CE1	2:p:392:PRO:HB3	2.52	0.45
2:q:309:ALA:HA	2:q:312:ASP:HB2	1.98	0.45
2:r:303:TYR:CE1	2:r:392:PRO:HB3	2.51	0.45
2:s:443:PHE:HB3	2:s:470:LEU:CD2	2.47	0.45
1:a:104:LYS:HE2	1:b:56:ARG:NH1	2.31	0.45
2:s:504:ASP:OD1	2:s:505:LYS:N	2.49	0.45
3:z:107:MET:HB2	3:z:108:PRO:HD3	1.98	0.45
1:g:165:TRP:CD1	1:g:167:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:57:GLU:OE2	1:h:76:ARG:NE	2.40	0.45
1:j:50:GLN:HB2	1:j:81:ILE:HG13	1.98	0.45
2:r:401:ARG:NH2	2:r:429:HIS:HE1	2.14	0.45
2:w:504:ASP:OD1	2:w:505:LYS:HG2	2.15	0.45
3:C:112:LEU:HD12	3:C:157:LEU:HD21	1.98	0.45
1:g:58:ASP:OD1	1:g:58:ASP:N	2.45	0.45
1:k:165:TRP:CD1	1:k:167:GLU:HG2	2.52	0.45
2:m:399:LYS:HB3	2:m:399:LYS:HE2	1.72	0.45
2:n:399:LYS:HB3	2:n:399:LYS:HE2	1.72	0.45
2:o:109:ASP:HA	2:o:132:ALA:H	1.82	0.45
2:o:433:VAL:O	2:o:437:MET:HG2	2.17	0.45
2:t:231:LYS:HG3	2:t:232:SER:H	1.82	0.45
2:v:443:PHE:HB3	2:v:470:LEU:HD23	1.99	0.45
2:q:413:MET:HE3	2:q:413:MET:HB3	1.83	0.45
2:t:266:THR:HA	2:t:291:ILE:HD12	1.99	0.45
2:u:340:ARG:NH1	2:u:384:GLN:OE1	2.50	0.45
2:v:38:TRP:HB2	2:v:269:LEU:HD13	1.98	0.45
2:x:111:SER:OG	2:x:113:GLU:OE1	2.31	0.45
2:x:340:ARG:NH1	2:x:384:GLN:OE1	2.50	0.45
1:g:152:THR:HG22	3:y:208:GLY:HA2	1.98	0.44
2:m:255:VAL:HG11	2:m:281:ALA:HB1	1.99	0.44
2:m:303:TYR:CE1	2:m:392:PRO:HB3	2.52	0.44
2:p:255:VAL:HG11	2:p:281:ALA:HB1	1.99	0.44
2:q:201:TYR:CD2	2:q:203:PRO:HD2	2.52	0.44
2:v:261:ALA:O	2:v:289:ARG:NH2	2.48	0.44
2:w:266:THR:HA	2:w:291:ILE:HD12	1.99	0.44
3:A:39:ALA:O	3:A:42:GLU:HG2	2.17	0.44
1:g:25:GLU:O	1:l:89:ILE:HG13	2.17	0.44
1:g:123:ASN:OD1	1:g:125:VAL:N	2.50	0.44
1:h:165:TRP:CD1	1:h:167:GLU:HG2	2.52	0.44
1:j:123:ASN:OD1	1:j:125:VAL:HG22	2.17	0.44
2:n:24:ASP:OD1	2:n:24:ASP:N	2.47	0.44
2:n:437:MET:HE1	2:n:512:CYS:SG	2.57	0.44
2:r:127:LEU:HD13	2:r:218:ASN:HB2	1.99	0.44
2:s:38:TRP:HB2	2:s:269:LEU:HD13	1.99	0.44
2:t:268:VAL:HG11	2:t:286:CYS:HB2	2.00	0.44
2:u:334:ASP:OD1	2:u:335:LYS:N	2.50	0.44
1:k:88:THR:OG1	1:k:92:ASP:OD2	2.27	0.44
2:t:38:TRP:HB2	2:t:269:LEU:HD13	1.99	0.44
2:w:38:TRP:HB2	2:w:269:LEU:HD13	2.00	0.44
2:w:109:ASP:OD1	2:w:110:GLU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:334:ASP:OD1	2:x:335:LYS:N	2.51	0.44
2:r:168:LYS:HG2	2:r:183:THR:HG22	1.99	0.44
2:x:109:ASP:OD1	2:x:110:GLU:N	2.48	0.44
2:o:127:LEU:HD13	2:o:218:ASN:HB2	2.00	0.44
2:q:151:THR:HG22	2:q:232:SER:H	1.82	0.44
3:z:39:ALA:O	3:z:42:GLU:HG2	2.17	0.44
2:n:255:VAL:HG11	2:n:281:ALA:HB1	2.00	0.44
2:q:437:MET:HE1	2:q:512:CYS:SG	2.57	0.44
2:v:231:LYS:HG3	2:v:232:SER:H	1.83	0.44
2:v:296:ASP:OD2	2:v:344:GLY:HA3	2.17	0.44
2:w:268:VAL:HG11	2:w:286:CYS:HB2	2.00	0.44
1:b:25:GLU:OE2	1:c:6:THR:HG22	2.18	0.44
2:m:76:PHE:HB2	2:m:80:ARG:NH1	2.33	0.44
2:n:151:THR:HG22	2:n:232:SER:H	1.82	0.44
2:s:261:ALA:O	2:s:289:ARG:NH2	2.48	0.43
2:u:109:ASP:OD1	2:u:110:GLU:N	2.49	0.43
2:v:201:TYR:CD2	2:v:203:PRO:HD2	2.53	0.43
2:w:231:LYS:HG3	2:w:232:SER:H	1.83	0.43
1:j:101:ILE:HG13	1:k:54:MET:HG3	1.99	0.43
2:r:212:TYR:HB2	2:r:213:LEU:HD12	2.00	0.43
2:s:368:TYR:HB3	2:s:375:ARG:NH1	2.33	0.43
2:w:417:ASP:OD1	2:w:418:ALA:N	2.49	0.43
3:y:111:ASN:OD1	3:y:112:LEU:N	2.51	0.43
1:g:89:ILE:HD13	1:h:25:GLU:HB3	1.99	0.43
1:h:117:SER:HB2	1:h:127:LYS:HD3	2.00	0.43
2:p:202:LEU:HB3	2:p:203:PRO:HD3	2.00	0.43
2:q:399:LYS:HE2	2:q:399:LYS:HB3	1.72	0.43
2:s:46:ARG:HG3	2:s:64:LEU:O	2.18	0.43
2:u:111:SER:OG	2:u:113:GLU:OE1	2.32	0.43
2:v:368:TYR:HB3	2:v:375:ARG:NH1	2.33	0.43
1:g:21:ALA:HB1	1:l:44:VAL:HG21	1.99	0.43
2:p:226:LYS:HB3	2:p:226:LYS:HE3	1.76	0.43
2:s:201:TYR:CD2	2:s:203:PRO:HD2	2.53	0.43
2:x:149:GLU:HB3	2:x:232:SER:HB2	2.01	0.43
1:a:148:THR:O	1:a:149:GLU:HG2	2.18	0.43
2:m:201:TYR:CD2	2:m:203:PRO:HD2	2.53	0.43
2:p:56:THR:C	2:p:86:ILE:HD11	2.43	0.43
1:h:31:GLU:HB3	1:h:115:PRO:HG3	2.01	0.43
2:m:202:LEU:HB3	2:m:203:PRO:HD3	1.99	0.43
2:o:80:ARG:NH2	2:o:334:ASP:OD2	2.49	0.43
2:o:212:TYR:HB2	2:o:213:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:231:LYS:HG3	2:s:232:SER:H	1.83	0.43
2:w:67:PRO:HB2	2:w:80:ARG:HH12	1.84	0.43
3:y:174:LEU:HD23	3:y:174:LEU:HA	1.89	0.43
2:o:10:LEU:HD23	2:o:10:LEU:HA	1.80	0.43
2:p:76:PHE:HB2	2:p:80:ARG:NH1	2.34	0.43
2:p:212:TYR:HB2	2:p:213:LEU:HD12	2.01	0.43
2:r:10:LEU:HD23	2:r:10:LEU:HA	1.80	0.43
1:d:148:THR:O	1:d:149:GLU:HG2	2.18	0.43
1:j:57:GLU:OE2	1:j:76:ARG:NE	2.40	0.43
2:n:413:MET:HE3	2:n:413:MET:HB3	1.83	0.43
2:p:495:VAL:HG23	2:u:27:LEU:HD13	2.00	0.43
3:y:14:LYS:HB3	3:y:14:LYS:HE2	1.71	0.43
3:A:18:LEU:HD23	3:A:245:MET:HG3	2.01	0.43
1:a:7:LYS:HE3	1:a:7:LYS:HB3	1.77	0.43
1:l:148:THR:HG21	3:y:127:ARG:HD2	2.01	0.43
2:u:451:MET:HG2	2:u:458:ILE:HD13	2.01	0.43
1:b:147:SER:OG	1:b:150:ASP:OD2	2.37	0.42
2:q:10:LEU:HD11	2:r:522:GLN:HB2	2.00	0.42
2:q:255:VAL:HG11	2:q:281:ALA:HB1	2.01	0.42
2:v:46:ARG:HG3	2:v:64:LEU:O	2.18	0.42
2:o:76:PHE:HB2	2:o:80:ARG:NH1	2.34	0.42
2:p:437:MET:HE1	2:p:512:CYS:SG	2.59	0.42
2:w:419:LEU:HD21	2:w:519:ARG:HH12	1.85	0.42
2:s:111:SER:OG	2:s:113:GLU:OE1	2.33	0.42
3:B:174:LEU:HD23	3:B:174:LEU:HA	1.89	0.42
2:m:56:THR:C	2:m:86:ILE:HD11	2.45	0.42
2:n:401:ARG:HH21	2:n:423:THR:HA	1.85	0.42
2:o:75:GLN:HE21	2:o:244:SER:N	2.18	0.42
2:s:44:PHE:O	2:s:95:ARG:NH1	2.52	0.42
2:v:44:PHE:O	2:v:95:ARG:NH1	2.52	0.42
2:m:437:MET:HE1	2:m:512:CYS:SG	2.60	0.42
2:r:333:LYS:HB3	2:r:333:LYS:HE2	1.76	0.42
2:s:340:ARG:NH2	2:s:382:SER:OG	2.52	0.42
2:t:67:PRO:HB2	2:t:80:ARG:HH12	1.84	0.42
2:u:164:ARG:HB3	2:u:187:SER:HB2	2.01	0.42
1:k:58:ASP:OD1	1:k:58:ASP:N	2.46	0.42
2:m:10:LEU:HD23	2:m:10:LEU:HA	1.85	0.42
2:t:188:LEU:HD22	2:t:222:ILE:HD11	2.00	0.42
3:A:23:LYS:HA	3:A:23:LYS:HD3	1.71	0.42
3:A:107:MET:HB2	3:A:108:PRO:HD3	2.01	0.42
2:m:242:ASP:OD1	2:m:244:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:333:LYS:HB3	2:p:333:LYS:HE2	1.77	0.42
2:s:194:ASP:N	2:s:198:ARG:O	2.44	0.42
3:z:111:ASN:OD1	3:z:112:LEU:N	2.53	0.42
2:m:212:TYR:HB2	2:m:213:LEU:HD12	2.01	0.42
2:m:374:GLU:HG3	2:m:375:ARG:HD3	2.02	0.42
2:m:495:VAL:HG23	2:x:27:LEU:HD13	2.01	0.42
2:s:195:ASP:HB3	2:t:426:ASN:HD21	1.85	0.42
3:A:112:LEU:HD12	3:A:157:LEU:HD21	2.00	0.42
3:B:111:ASN:OD1	3:B:112:LEU:N	2.52	0.42
3:D:23:LYS:HA	3:D:23:LYS:HD3	1.71	0.42
1:f:147:SER:OG	1:f:150:ASP:OD2	2.37	0.42
2:t:334:ASP:OD1	2:t:335:LYS:N	2.51	0.42
2:t:500:GLN:NE2	2:t:503:PHE:HA	2.35	0.42
2:x:24:ASP:OD1	2:x:24:ASP:N	2.53	0.42
3:D:16:LYS:HB3	3:D:247:GLN:HE21	1.85	0.42
2:n:158:ASP:OD1	2:n:162:ASN:N	2.52	0.42
2:u:12:ASN:HB3	2:v:398:VAL:HG11	2.02	0.42
2:u:128:ASP:OD1	2:u:129:SER:N	2.53	0.42
2:w:340:ARG:NH1	2:w:384:GLN:OE1	2.53	0.42
2:s:398:VAL:HG11	2:x:12:ASN:HB3	2.02	0.41
2:x:128:ASP:OD1	2:x:129:SER:N	2.53	0.41
1:e:147:SER:OG	1:e:150:ASP:OD2	2.37	0.41
1:i:87:GLU:OE1	1:i:93:ILE:HB	2.19	0.41
2:o:226:LYS:HE3	2:o:226:LYS:HB3	1.75	0.41
2:p:498:VAL:HG22	2:p:508:VAL:HG23	2.00	0.41
2:q:401:ARG:HH21	2:q:423:THR:HA	1.85	0.41
2:t:340:ARG:NH1	2:t:384:GLN:OE1	2.53	0.41
3:B:23:LYS:HA	3:B:23:LYS:HD3	1.83	0.41
3:B:112:LEU:HD12	3:B:157:LEU:HD21	2.01	0.41
2:r:76:PHE:HB2	2:r:80:ARG:NH1	2.35	0.41
2:t:128:ASP:OD1	2:t:129:SER:N	2.54	0.41
2:u:38:TRP:HB2	2:u:269:LEU:HD13	2.02	0.41
2:u:231:LYS:HG3	2:u:232:SER:H	1.85	0.41
2:u:316:LEU:HD12	2:u:316:LEU:HA	1.87	0.41
2:r:206:LEU:HD23	2:r:206:LEU:HA	1.90	0.41
2:r:226:LYS:HB3	2:r:226:LYS:HE3	1.75	0.41
2:v:419:LEU:HD21	2:v:519:ARG:HH12	1.86	0.41
1:j:123:ASN:OD1	1:j:124:ALA:N	2.53	0.41
2:n:393:ASP:O	2:n:397:MET:HG3	2.20	0.41
2:q:24:ASP:OD1	2:q:24:ASP:N	2.46	0.41
2:u:25:ALA:HB3	2:v:526:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:268:VAL:HG11	2:v:286:CYS:HB2	2.02	0.41
2:x:316:LEU:HD12	2:x:316:LEU:HA	1.86	0.41
3:z:3:LEU:HD13	3:z:8:TRP:CE2	2.55	0.41
1:i:148:THR:HG21	3:B:127:ARG:HD2	2.01	0.41
2:s:419:LEU:HD21	2:s:519:ARG:HH12	1.86	0.41
2:w:433:VAL:HB	2:w:434:PRO:HD3	2.03	0.41
1:g:31:GLU:HB3	1:g:115:PRO:HG3	2.02	0.41
2:m:498:VAL:HG22	2:m:508:VAL:HG23	2.02	0.41
2:o:504:ASP:HB2	2:u:519:ARG:HG2	2.02	0.41
2:q:419:LEU:HD22	2:q:429:HIS:HB3	2.02	0.41
2:r:75:GLN:HE21	2:r:244:SER:N	2.17	0.41
2:w:55:VAL:HG11	2:w:64:LEU:HD13	2.03	0.41
2:w:128:ASP:OD1	2:w:129:SER:N	2.54	0.41
2:w:202:LEU:HB3	2:w:203:PRO:HD3	2.03	0.41
2:n:298:LYS:HB3	2:n:301:LEU:HG	2.03	0.41
2:n:303:TYR:CE1	2:n:392:PRO:HB3	2.56	0.41
2:q:333:LYS:HB3	2:q:333:LYS:HE2	1.75	0.41
2:s:46:ARG:HE	2:s:141:ASP:CG	2.29	0.41
3:B:212:ILE:HD12	3:C:120:ILE:HG13	2.03	0.41
3:C:111:ASN:OD1	3:C:112:LEU:N	2.53	0.41
1:e:25:GLU:OE2	1:f:6:THR:HG22	2.20	0.41
1:f:148:THR:O	1:f:149:GLU:HG2	2.21	0.41
2:m:333:LYS:HB3	2:m:333:LYS:HE2	1.77	0.41
2:o:75:GLN:HE21	2:o:243:GLN:C	2.29	0.41
2:p:374:GLU:HG3	2:p:375:ARG:HD3	2.02	0.41
2:q:75:GLN:HE21	2:q:244:SER:N	2.19	0.41
2:q:303:TYR:CE1	2:q:392:PRO:HB3	2.56	0.41
2:r:75:GLN:HE21	2:r:243:GLN:C	2.29	0.41
2:t:55:VAL:HG11	2:t:64:LEU:HD13	2.03	0.41
2:v:80:ARG:NH2	2:v:334:ASP:OD2	2.34	0.41
2:v:202:LEU:HB3	2:v:203:PRO:HD3	2.03	0.41
2:w:261:ALA:O	2:w:289:ARG:NH2	2.49	0.41
3:A:135:VAL:HG11	3:A:198:TYR:CD2	2.56	0.41
1:k:37:ALA:HB2	1:k:108:ASP:O	2.21	0.41
2:m:226:LYS:HB3	2:m:226:LYS:HE3	1.76	0.41
2:n:333:LYS:HB3	2:n:333:LYS:HE2	1.75	0.41
2:o:224:THR:HG23	2:o:224:THR:O	2.21	0.41
2:t:202:LEU:HB3	2:t:203:PRO:HD3	2.03	0.41
2:w:426:ASN:HB3	3:C:6:GLN:HG3	2.03	0.41
2:x:231:LYS:HG3	2:x:232:SER:H	1.85	0.41
2:x:454:SER:HB2	2:x:455:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:MET:HB2	3:D:108:PRO:HD3	2.03	0.41
2:q:298:LYS:HB3	2:q:301:LEU:HG	2.03	0.40
2:q:517:VAL:HG13	2:q:519:ARG:HG3	2.03	0.40
2:u:149:GLU:HB3	2:u:232:SER:HB2	2.03	0.40
2:v:255:VAL:HG11	2:v:281:ALA:HB1	2.03	0.40
1:e:155:VAL:HG11	1:f:27:LEU:HD23	2.03	0.40
1:g:111:MET:HB3	1:g:132:ILE:HG22	2.03	0.40
2:m:297:VAL:HG12	2:m:326:TYR:O	2.22	0.40
2:n:224:THR:O	2:n:224:THR:HG23	2.21	0.40
2:o:41:ILE:HD11	2:o:254:ALA:HB3	2.02	0.40
2:p:297:VAL:HG12	2:p:326:TYR:O	2.21	0.40
2:q:224:THR:O	2:q:224:THR:HG23	2.21	0.40
2:q:393:ASP:O	2:q:397:MET:HG3	2.22	0.40
2:r:297:VAL:HG22	2:r:298:LYS:H	1.86	0.40
2:r:437:MET:HE1	2:r:512:CYS:SG	2.61	0.40
2:m:460:ALA:HB2	2:m:506:TRP:CH2	2.57	0.40
2:s:268:VAL:HG11	2:s:286:CYS:HB2	2.03	0.40
2:v:46:ARG:HE	2:v:141:ASP:CG	2.29	0.40
1:j:148:THR:HG21	3:C:127:ARG:HD2	2.04	0.40
2:m:77:GLU:OE2	2:m:274:TYR:OH	2.26	0.40
2:p:127:LEU:HD13	2:p:218:ASN:HB2	2.04	0.40
2:r:224:THR:HG23	2:r:224:THR:O	2.22	0.40
2:s:255:VAL:HG11	2:s:281:ALA:HB1	2.03	0.40
3:D:18:LEU:HD23	3:D:245:MET:HG3	2.03	0.40
1:b:49:SER:OG	1:b:50:GLN:N	2.55	0.40
2:o:465:LYS:HB3	2:o:465:LYS:HE2	1.93	0.40
2:p:224:THR:HG23	2:p:224:THR:O	2.22	0.40
2:r:109:ASP:HA	2:r:132:ALA:H	1.87	0.40
2:v:10:LEU:HD13	2:w:520:ARG:HB3	2.04	0.40
3:A:111:ASN:OD1	3:A:112:LEU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	b	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	c	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	d	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	e	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	f	165/169 (98%)	157 (95%)	8 (5%)	0	100	100
1	g	157/169 (93%)	145 (92%)	12 (8%)	0	100	100
1	h	157/169 (93%)	149 (95%)	8 (5%)	0	100	100
1	i	157/169 (93%)	144 (92%)	13 (8%)	0	100	100
1	j	157/169 (93%)	146 (93%)	11 (7%)	0	100	100
1	k	157/169 (93%)	148 (94%)	9 (6%)	0	100	100
1	l	157/169 (93%)	146 (93%)	11 (7%)	0	100	100
2	m	525/529 (99%)	509 (97%)	16 (3%)	0	100	100
2	n	525/529 (99%)	506 (96%)	19 (4%)	0	100	100
2	o	525/529 (99%)	504 (96%)	21 (4%)	0	100	100
2	p	525/529 (99%)	509 (97%)	16 (3%)	0	100	100
2	q	525/529 (99%)	507 (97%)	18 (3%)	0	100	100
2	r	525/529 (99%)	503 (96%)	22 (4%)	0	100	100
2	s	524/529 (99%)	500 (95%)	24 (5%)	0	100	100
2	t	524/529 (99%)	499 (95%)	25 (5%)	0	100	100
2	u	524/529 (99%)	502 (96%)	22 (4%)	0	100	100
2	v	524/529 (99%)	501 (96%)	23 (4%)	0	100	100
2	w	524/529 (99%)	500 (95%)	24 (5%)	0	100	100
2	x	524/529 (99%)	498 (95%)	26 (5%)	0	100	100
3	A	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
3	B	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
3	C	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
3	D	258/261 (99%)	249 (96%)	9 (4%)	0	100	100
3	y	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
3	z	258/261 (99%)	251 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9774/9942 (98%)	9359 (96%)	415 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	a	142/144 (99%)	142 (100%)	0	100	100
1	b	142/144 (99%)	142 (100%)	0	100	100
1	c	142/144 (99%)	142 (100%)	0	100	100
1	d	142/144 (99%)	142 (100%)	0	100	100
1	e	142/144 (99%)	142 (100%)	0	100	100
1	f	142/144 (99%)	142 (100%)	0	100	100
1	g	134/144 (93%)	134 (100%)	0	100	100
1	h	134/144 (93%)	134 (100%)	0	100	100
1	i	134/144 (93%)	134 (100%)	0	100	100
1	j	134/144 (93%)	134 (100%)	0	100	100
1	k	134/144 (93%)	134 (100%)	0	100	100
1	l	134/144 (93%)	134 (100%)	0	100	100
2	m	427/430 (99%)	427 (100%)	0	100	100
2	n	427/430 (99%)	427 (100%)	0	100	100
2	o	427/430 (99%)	427 (100%)	0	100	100
2	p	427/430 (99%)	427 (100%)	0	100	100
2	q	427/430 (99%)	427 (100%)	0	100	100
2	r	427/430 (99%)	427 (100%)	0	100	100
2	s	426/430 (99%)	426 (100%)	0	100	100
2	t	426/430 (99%)	426 (100%)	0	100	100
2	u	426/430 (99%)	426 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	v	426/430 (99%)	426 (100%)	0	100	100
2	w	426/430 (99%)	426 (100%)	0	100	100
2	x	426/430 (99%)	426 (100%)	0	100	100
3	A	217/220 (99%)	217 (100%)	0	100	100
3	B	217/220 (99%)	217 (100%)	0	100	100
3	C	217/220 (99%)	217 (100%)	0	100	100
3	D	217/220 (99%)	217 (100%)	0	100	100
3	y	217/220 (99%)	217 (100%)	0	100	100
3	z	217/220 (99%)	217 (100%)	0	100	100
All	All	8076/8208 (98%)	8076 (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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	20	ASN
1	b	95	GLN
1	c	20	ASN
1	c	95	GLN
1	e	5	ASN
1	e	20	ASN
1	e	77	ASN
1	e	95	GLN
1	f	95	GLN
1	g	95	GLN
1	i	65	ASN
1	l	65	ASN
1	l	82	GLN
2	m	22	ASN
2	m	184	HIS
2	m	426	ASN
2	m	429	HIS
2	n	22	ASN
2	n	184	HIS
2	o	22	ASN
2	p	22	ASN
2	p	184	HIS
2	p	429	HIS

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Mol	Chain	Res	Type
2	q	22	ASN
2	q	184	HIS
2	r	22	ASN
2	r	184	HIS
2	r	429	HIS
2	s	500	GLN
2	t	184	HIS
2	t	338	GLN
2	t	426	ASN
2	u	338	GLN
2	u	431	GLN
2	u	500	GLN
2	v	59	ASN
2	w	184	HIS
2	w	338	GLN
2	w	426	ASN
2	x	338	GLN
2	x	431	GLN
3	y	246	GLN
3	z	4	ASN
3	A	246	GLN
3	B	4	ASN
3	B	246	GLN
3	D	194	ASN
3	D	246	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

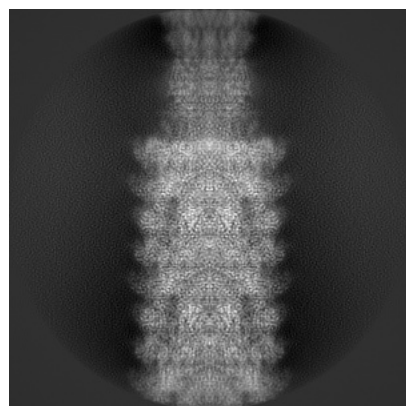
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36130. These allow visual inspection of the internal detail of the map and identification of artifacts.

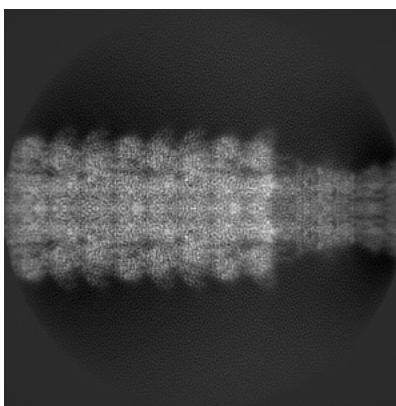
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

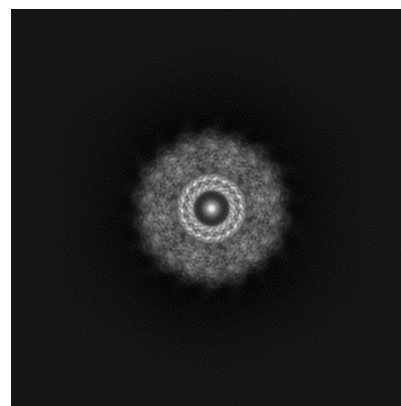
6.1.1 Primary map



X

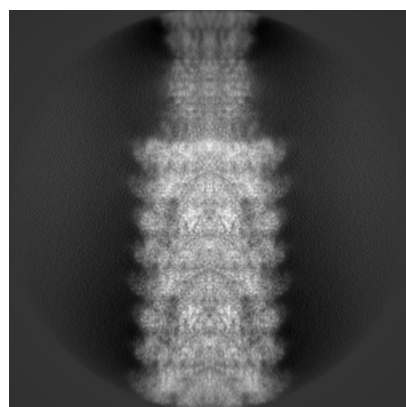


Y

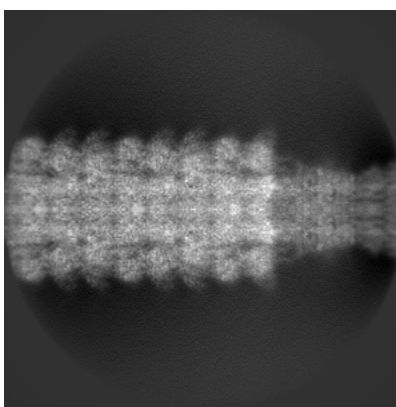


Z

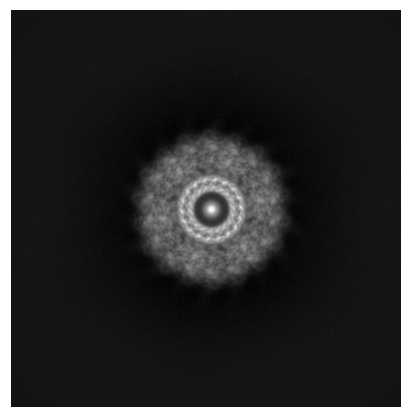
6.1.2 Raw map



X



Y

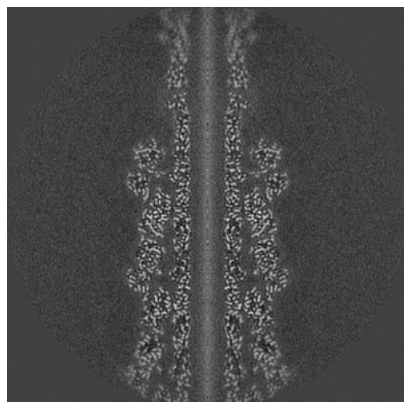


Z

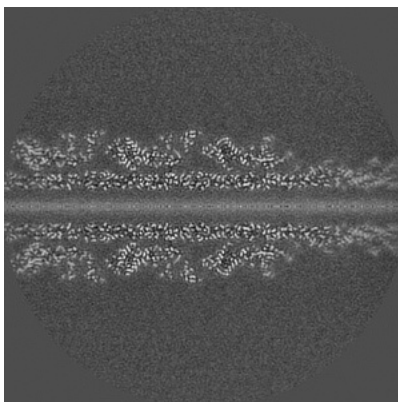
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

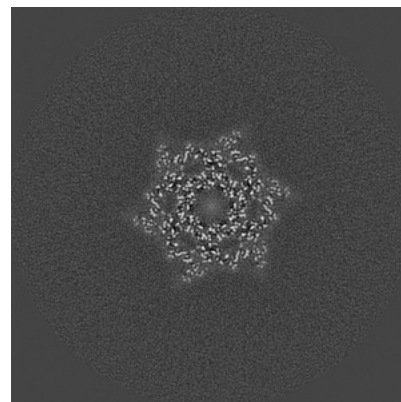
6.2.1 Primary map



X Index: 180

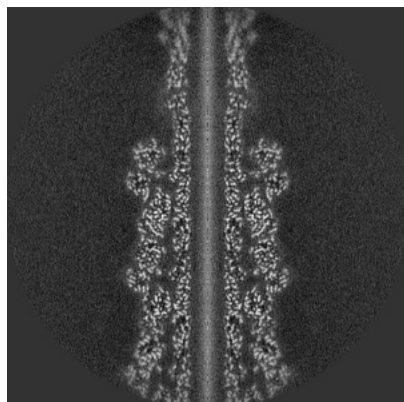


Y Index: 180

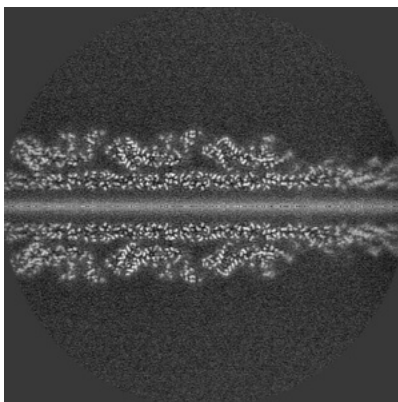


Z Index: 180

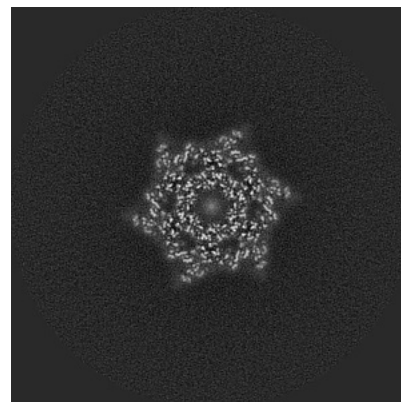
6.2.2 Raw map



X Index: 180



Y Index: 180

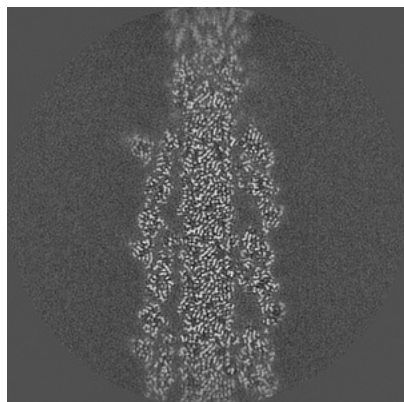


Z Index: 180

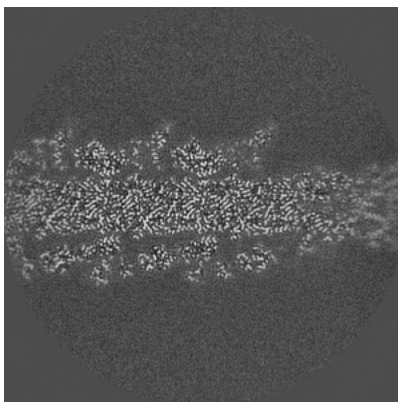
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

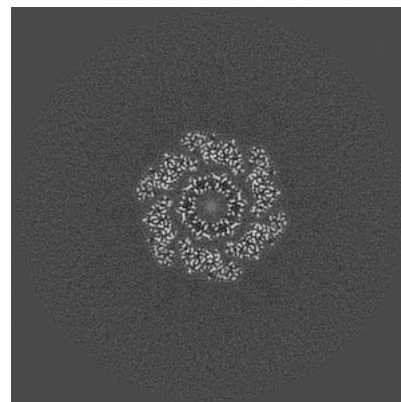
6.3.1 Primary map



X Index: 199

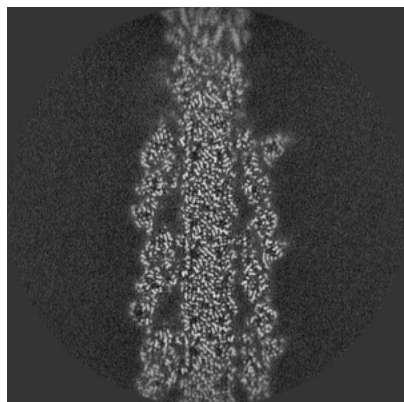


Y Index: 162

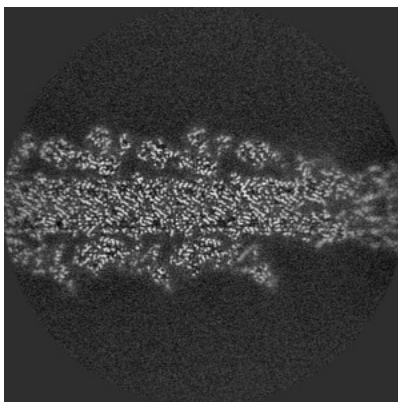


Z Index: 135

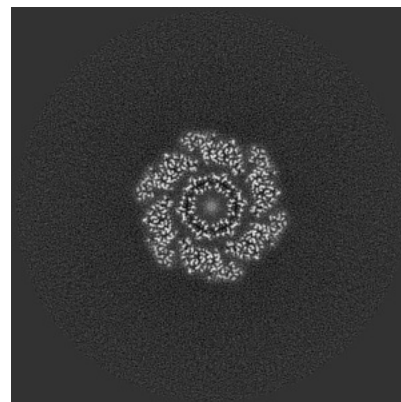
6.3.2 Raw map



X Index: 161



Y Index: 197

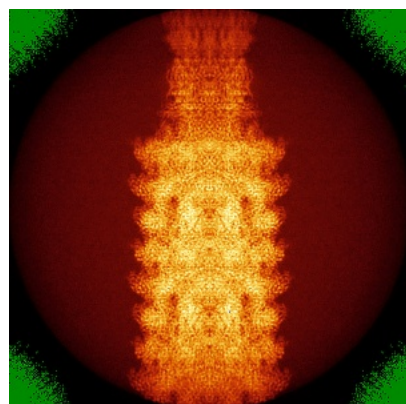


Z Index: 135

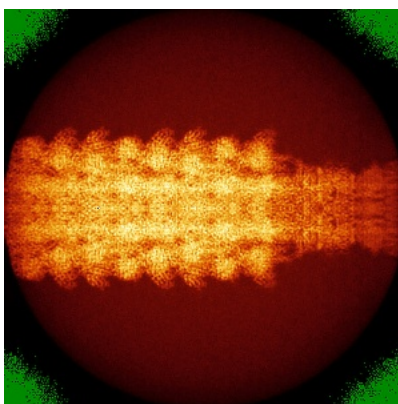
The images above show the largest variance slices of the map in three orthogonal directions.

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

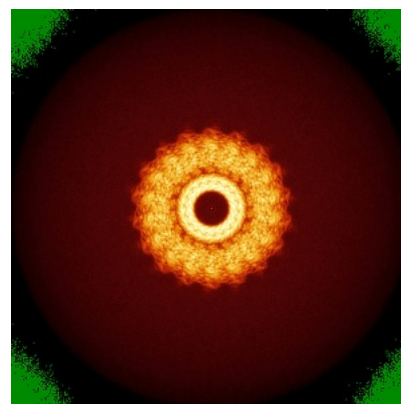
6.4.1 Primary map



X

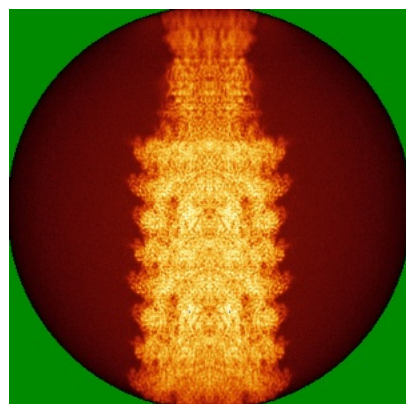


Y

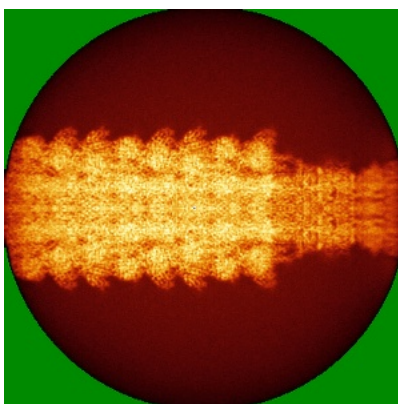


Z

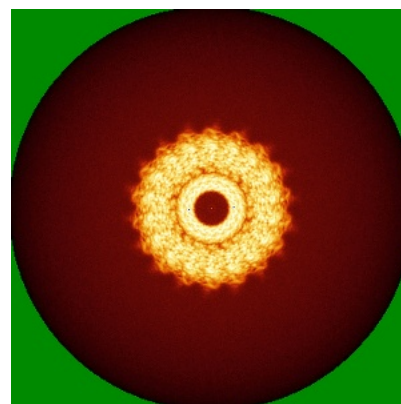
6.4.2 Raw map



X



Y

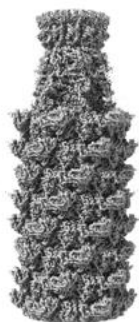


Z

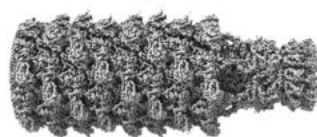
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

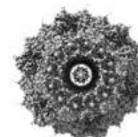
6.5.1 Primary map



X



Y



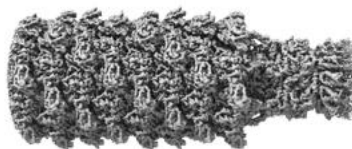
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

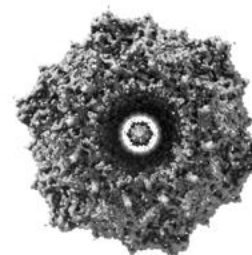
6.5.2 Raw map



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.

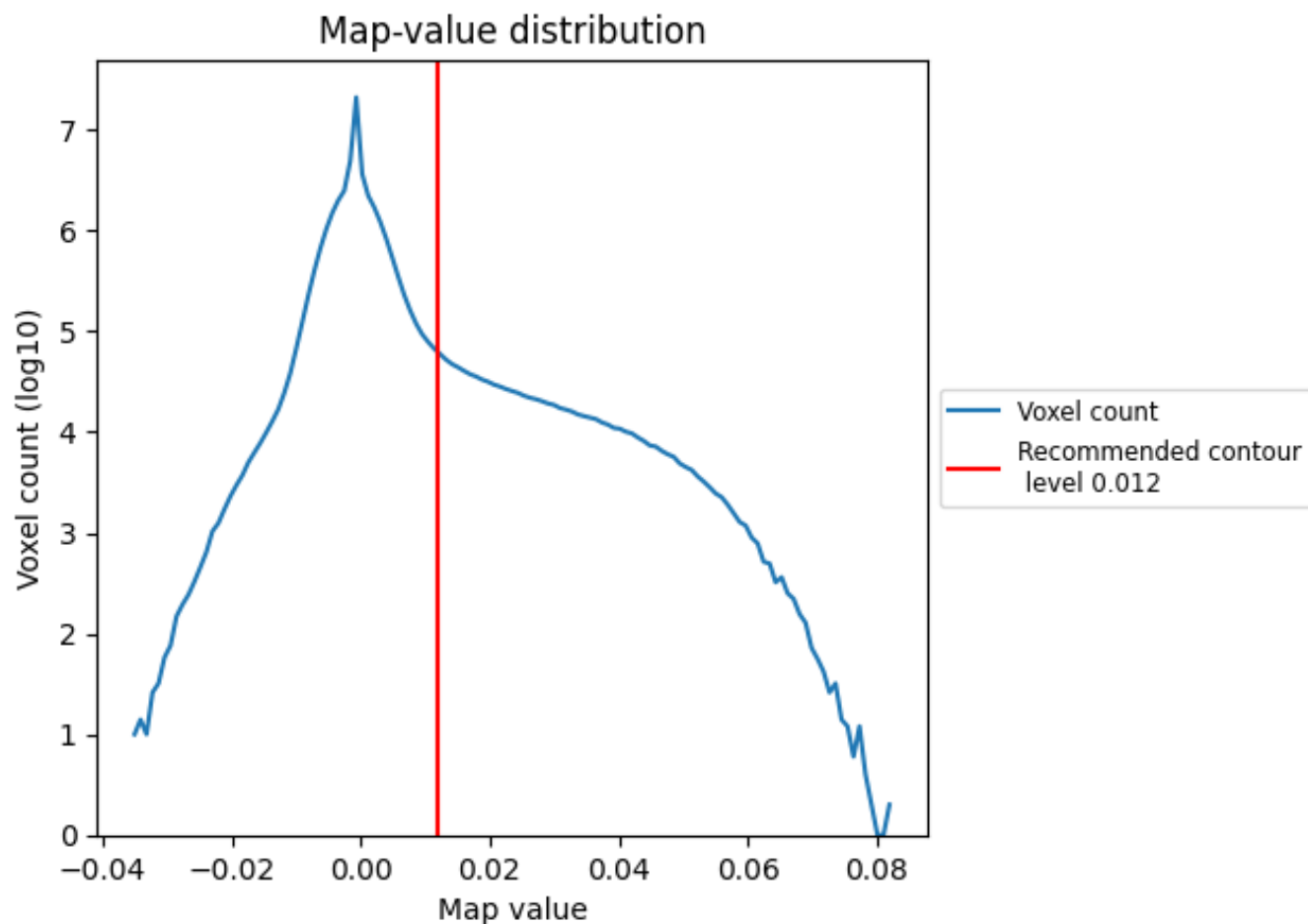
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

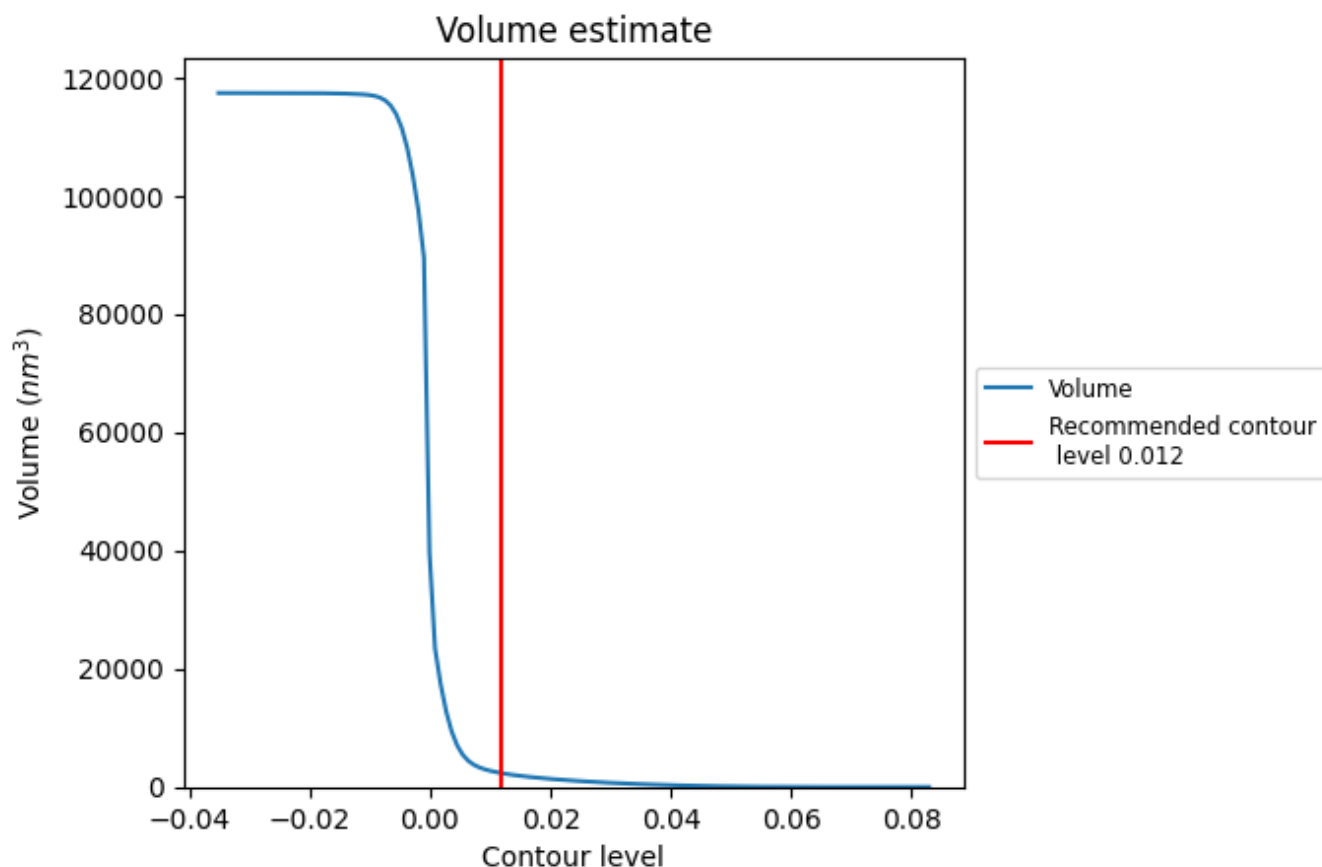
This section contains the results of statistical analysis of the map.

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.

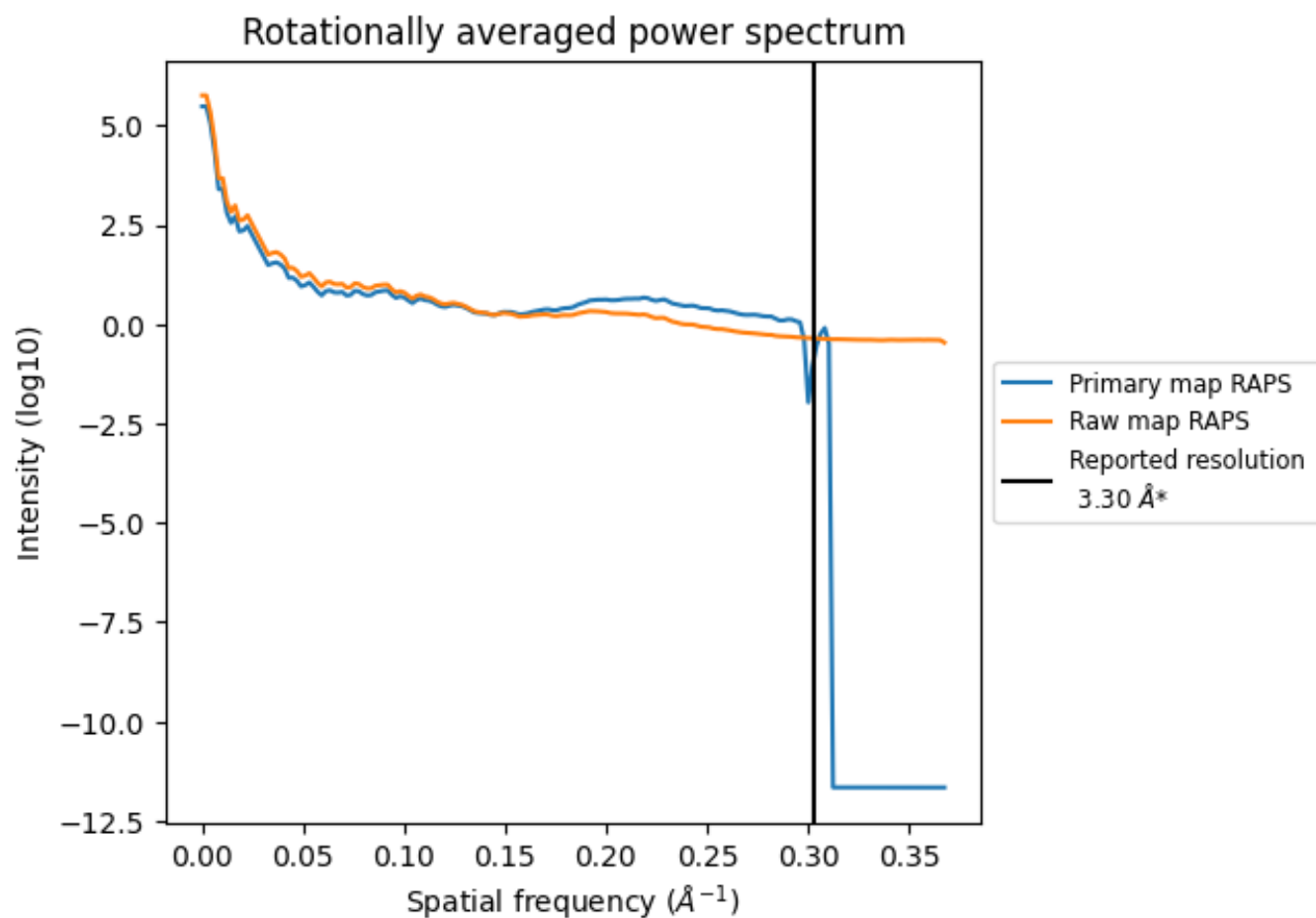
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2315 nm³; this corresponds to an approximate mass of 2091 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 ⓘ

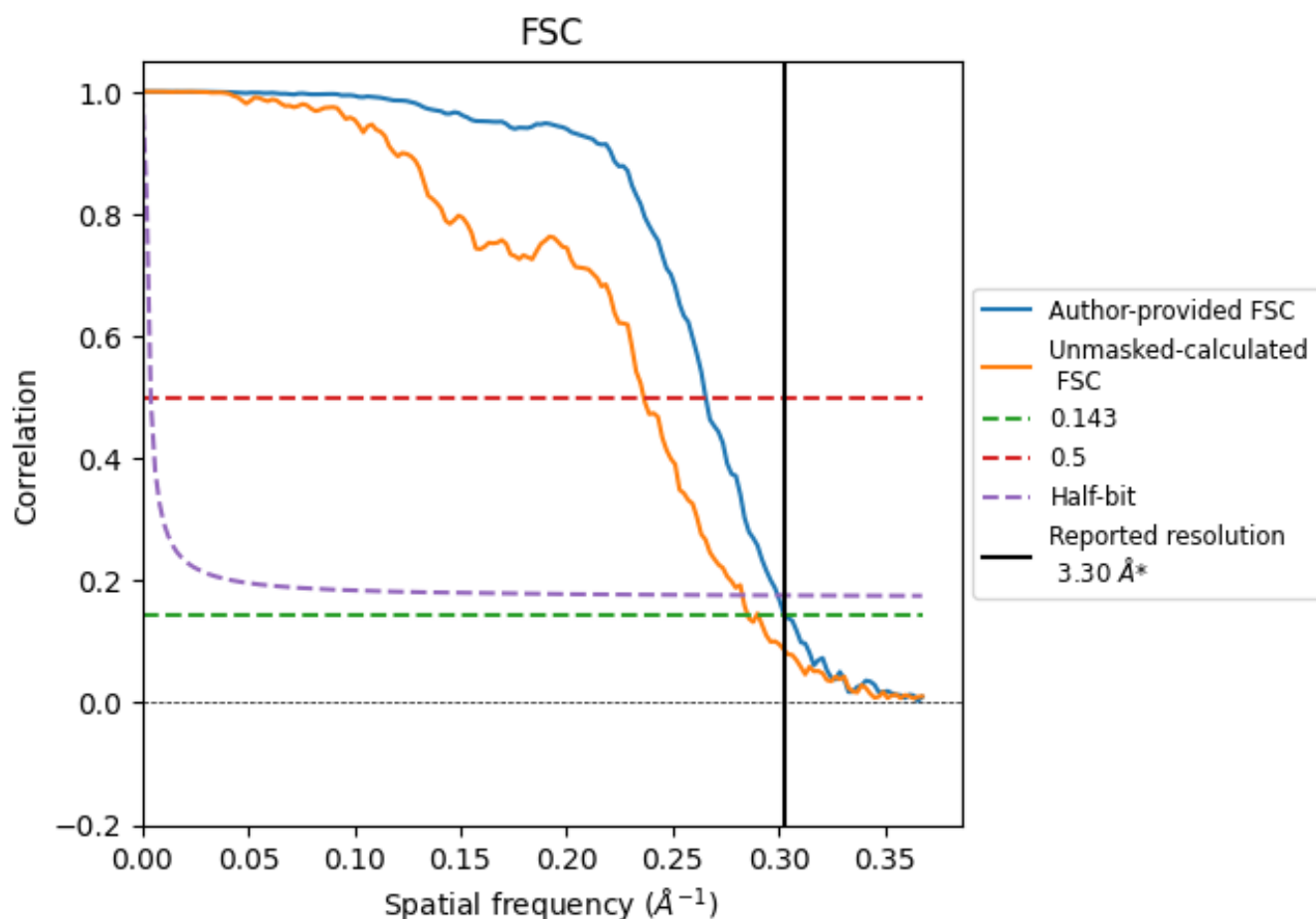


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

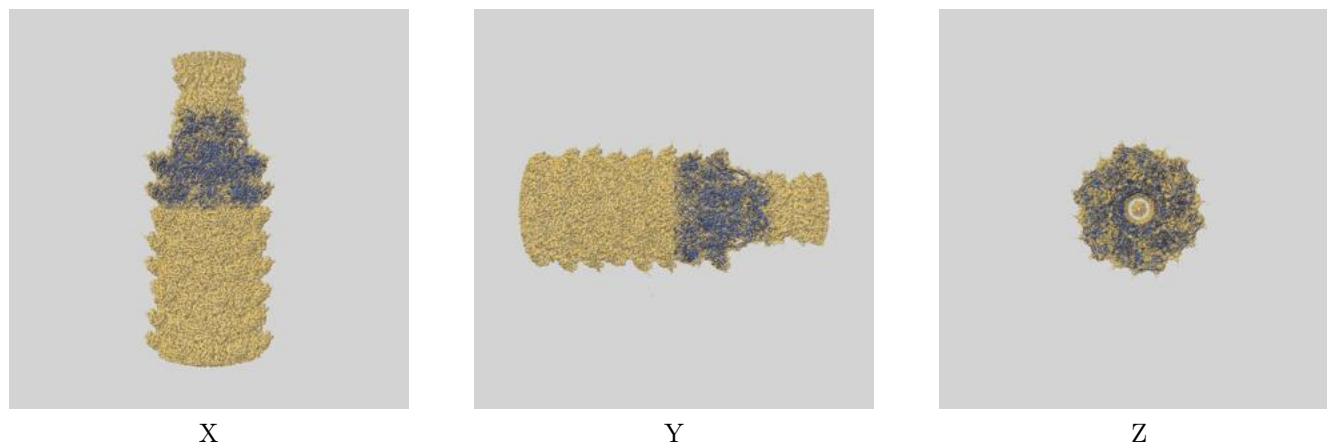
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.77	3.34
Unmasked-calculated*	3.50	4.23	3.53

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

9 Map-model fit [i](#)

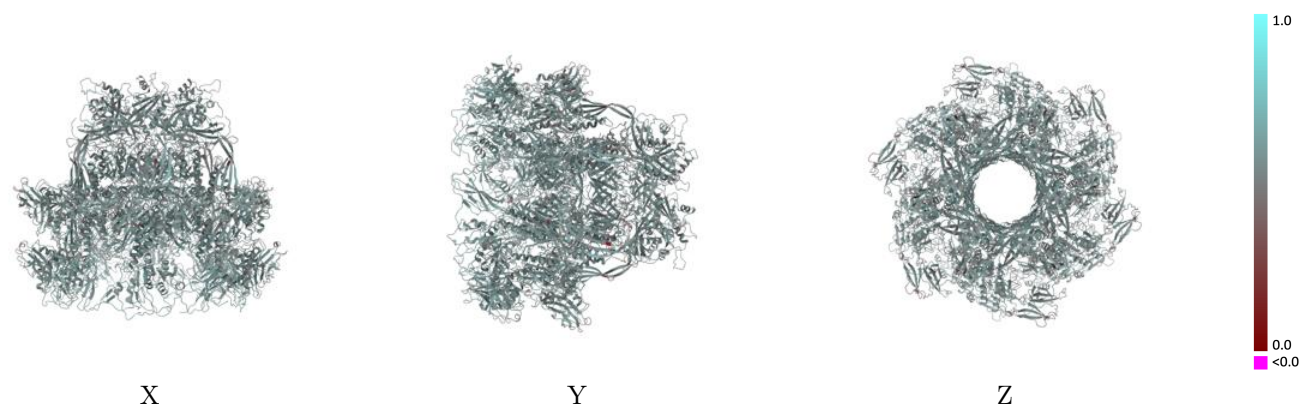
This section contains information regarding the fit between EMDB map EMD-36130 and PDB model 8JAN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



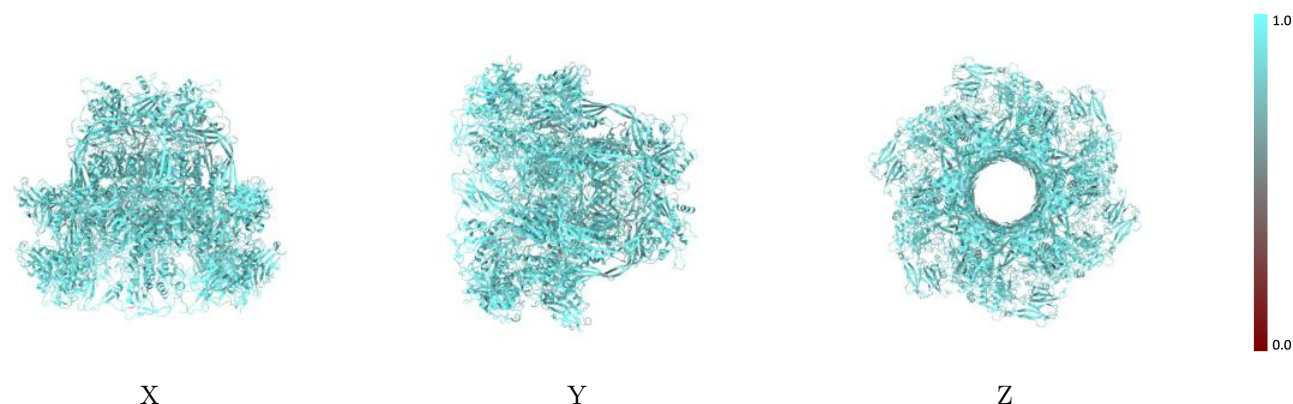
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



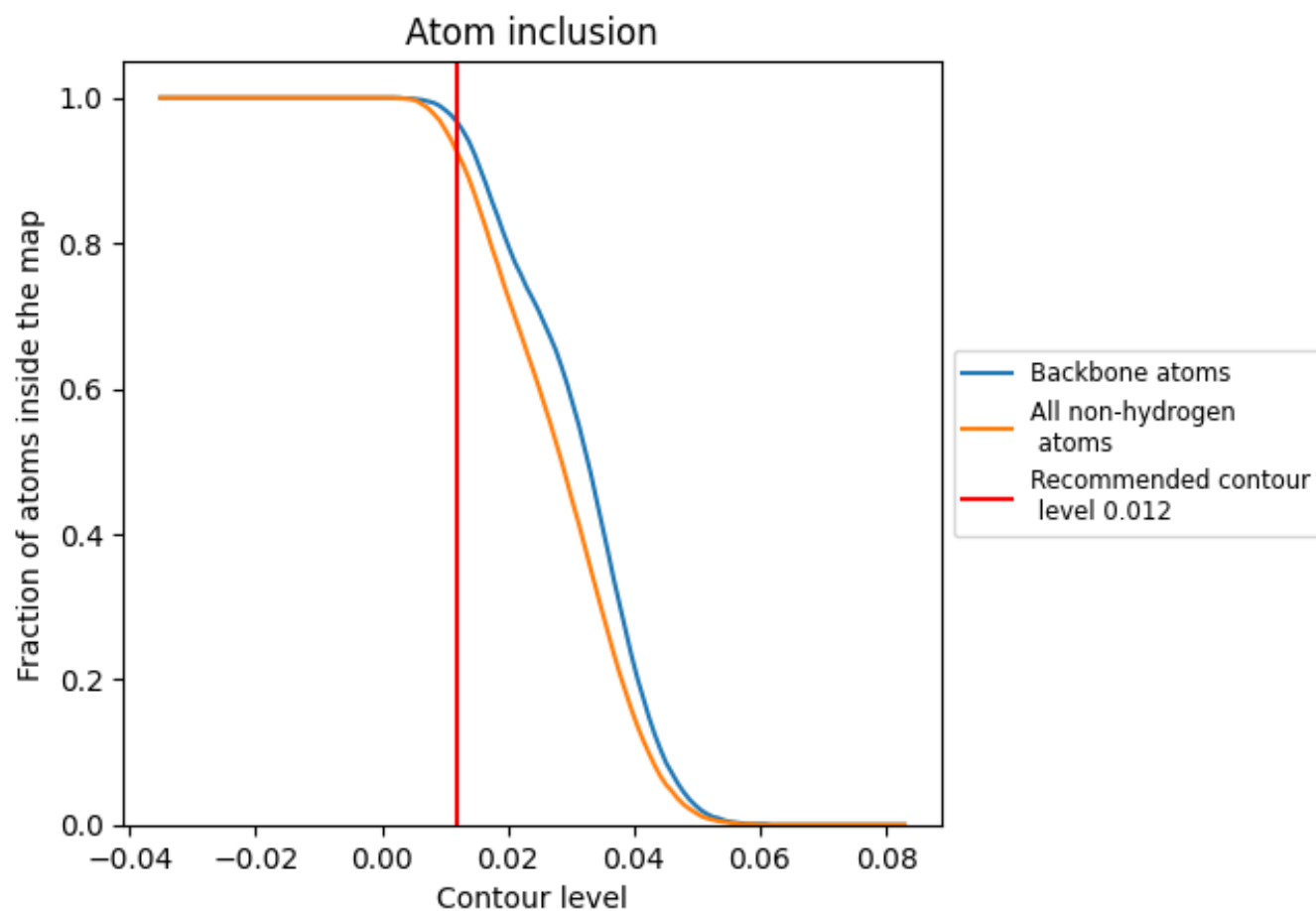
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.5530
A	 0.9090	 0.5400
B	 0.9070	 0.5420
C	 0.9080	 0.5420
D	 0.9080	 0.5400
a	 0.9570	 0.5760
b	 0.9600	 0.5730
c	 0.9570	 0.5750
d	 0.9550	 0.5730
e	 0.9590	 0.5740
f	 0.9570	 0.5740
g	 0.9130	 0.5540
h	 0.9110	 0.5500
i	 0.9180	 0.5560
j	 0.9170	 0.5500
k	 0.9120	 0.5530
l	 0.9150	 0.5500
m	 0.9390	 0.5630
n	 0.9400	 0.5640
o	 0.9380	 0.5640
p	 0.9380	 0.5630
q	 0.9390	 0.5630
r	 0.9380	 0.5620
s	 0.9120	 0.5420
t	 0.9080	 0.5410
u	 0.9140	 0.5420
v	 0.9120	 0.5420
w	 0.9100	 0.5410
x	 0.9080	 0.5380
y	 0.9080	 0.5420
z	 0.9090	 0.5410

