



Full wwPDB EM Validation Report ⓘ

Aug 24, 2025 – 07:15 am BST

PDB ID : 9RPD / pdb_00009rpd
EMDB ID : EMD-54161
Title : D. melanogaster Augmin TII N-clamp (GST-fusion) bound to a microtubule, well-defined subset of particles
Authors : Wuertz, M.; Vermeulen, B.J.A.; Tonon, G.; Pfeffer, S.
Deposited on : 2025-06-24
Resolution : 4.90 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

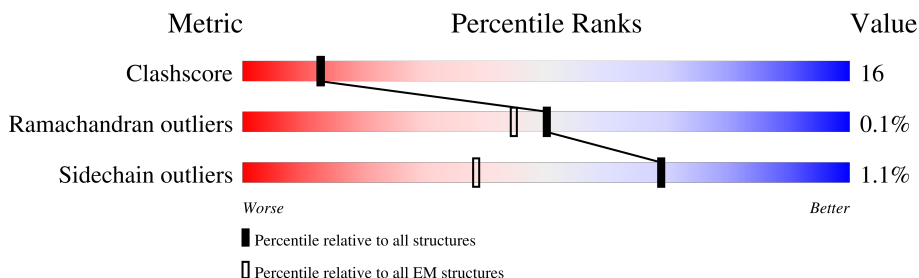
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	I	108	<div> <div>6%</div> <div>9%</div> <div>86%</div> </div>
2	J	280	<div> <div>20%</div> <div>29%</div> <div>19%</div> <div>48%</div> </div>
3	K	672	<div> <div>98%</div> </div>
4	B	445	<div> <div>45%</div> <div>86%</div> <div>9%</div> </div>
4	D	445	<div> <div>41%</div> <div>85%</div> <div>10%</div> </div>
5	A	451	<div> <div>46%</div> <div>88%</div> <div>8%</div> </div>
5	C	451	<div> <div>47%</div> <div>88%</div> <div>8%</div> </div>
5	E	451	<div> <div>48%</div> <div>87%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
5	G	451	<div><div></div><div>48%</div><div></div><div>86%</div><div></div><div>10%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41510 atoms, of which 19714 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 Augmin complex subunit dgt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	15	Total	C	N	O	S	0	0
			134	86	24	23	1		

- Molecule 2 is a protein called Augmin complex subunit dgt6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	146	Total	C	N	O	S	0	0
			1228	802	218	203	5		

- Molecule 3 is a protein called Augmin complex subunit msd5, Green fluorescent protein, Glutathione S-transferase class-mu 26 kDa isozyme.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	13	Total	C	N	O	0	0
			104	68	14	22		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	180	LEU	-	linker	UNP Q9W0G6
K	181	SER	-	linker	UNP Q9W0G6
K	182	GLY	-	linker	UNP Q9W0G6
K	183	GLU	-	linker	UNP Q9W0G6
K	184	ASN	-	linker	UNP Q9W0G6
K	185	LEU	-	linker	UNP Q9W0G6
K	186	TYR	-	linker	UNP Q9W0G6
K	187	PHE	-	linker	UNP Q9W0G6
K	188	GLN	-	linker	UNP Q9W0G6
K	189	GLY	-	linker	UNP Q9W0G6
K	190	GLY	-	linker	UNP Q9W0G6
K	191	SER	-	linker	UNP Q9W0G6
K	192	ALA	-	linker	UNP Q9W0G6
K	193	GLY	-	linker	UNP Q9W0G6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	194	SER	-	linker	UNP Q9W0G6
K	195	ALA	-	linker	UNP Q9W0G6
K	196	ALA	-	linker	UNP Q9W0G6
K	197	GLY	-	linker	UNP Q9W0G6
K	198	SER	-	linker	UNP Q9W0G6
K	199	GLY	-	linker	UNP Q9W0G6
K	200	GLU	-	linker	UNP Q9W0G6
K	201	PHE	-	linker	UNP Q9W0G6
K	202	MET	-	linker	UNP Q9W0G6
K	203	VAL	-	linker	UNP Q9W0G6
K	266	LEU	PHE	engineered mutation	UNP P42212
K	267	THR	SER	engineered mutation	UNP P42212
K	433	LEU	HIS	engineered mutation	UNP P42212
K	441	LEU	-	linker	UNP P42212
K	442	GLU	-	linker	UNP P42212
K	443	VAL	-	linker	UNP P42212
K	444	LEU	-	linker	UNP P42212
K	663	GLY	-	expression tag	UNP P08515
K	664	PRO	-	expression tag	UNP P08515
K	665	HIS	-	expression tag	UNP P08515
K	666	HIS	-	expression tag	UNP P08515
K	667	HIS	-	expression tag	UNP P08515
K	668	HIS	-	expression tag	UNP P08515
K	669	HIS	-	expression tag	UNP P08515
K	670	HIS	-	expression tag	UNP P08515
K	671	HIS	-	expression tag	UNP P08515
K	672	HIS	-	expression tag	UNP P08515

- Molecule 4 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	427	Total	C	H	N	O	S	0	0
			6600	2110	3241	576	647	26		
4	D	427	Total	C	H	N	O	S	0	0
			6600	2110	3241	576	647	26		

- Molecule 5 is a protein called Tubulin alpha-1A chain.

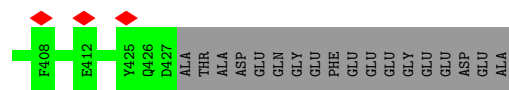
Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	436	Total	C	H	N	O	S	0	0
			6711	2152	3308	579	650	22		

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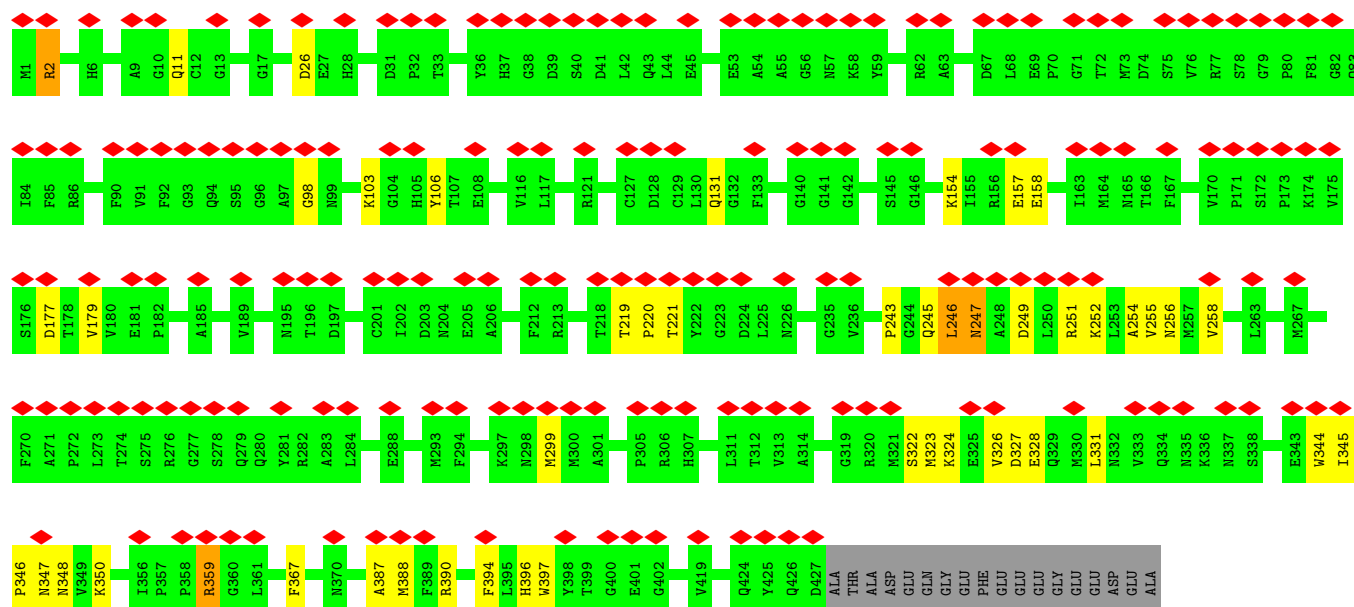
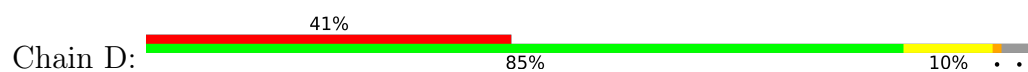
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Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	436	Total 6711	C 2152	H 3308	N 579	O 650	S 22	0	0
5	G	436	Total 6711	C 2152	H 3308	N 579	O 650	S 22	0	0
5	E	436	Total 6711	C 2152	H 3308	N 579	O 650	S 22	0	0

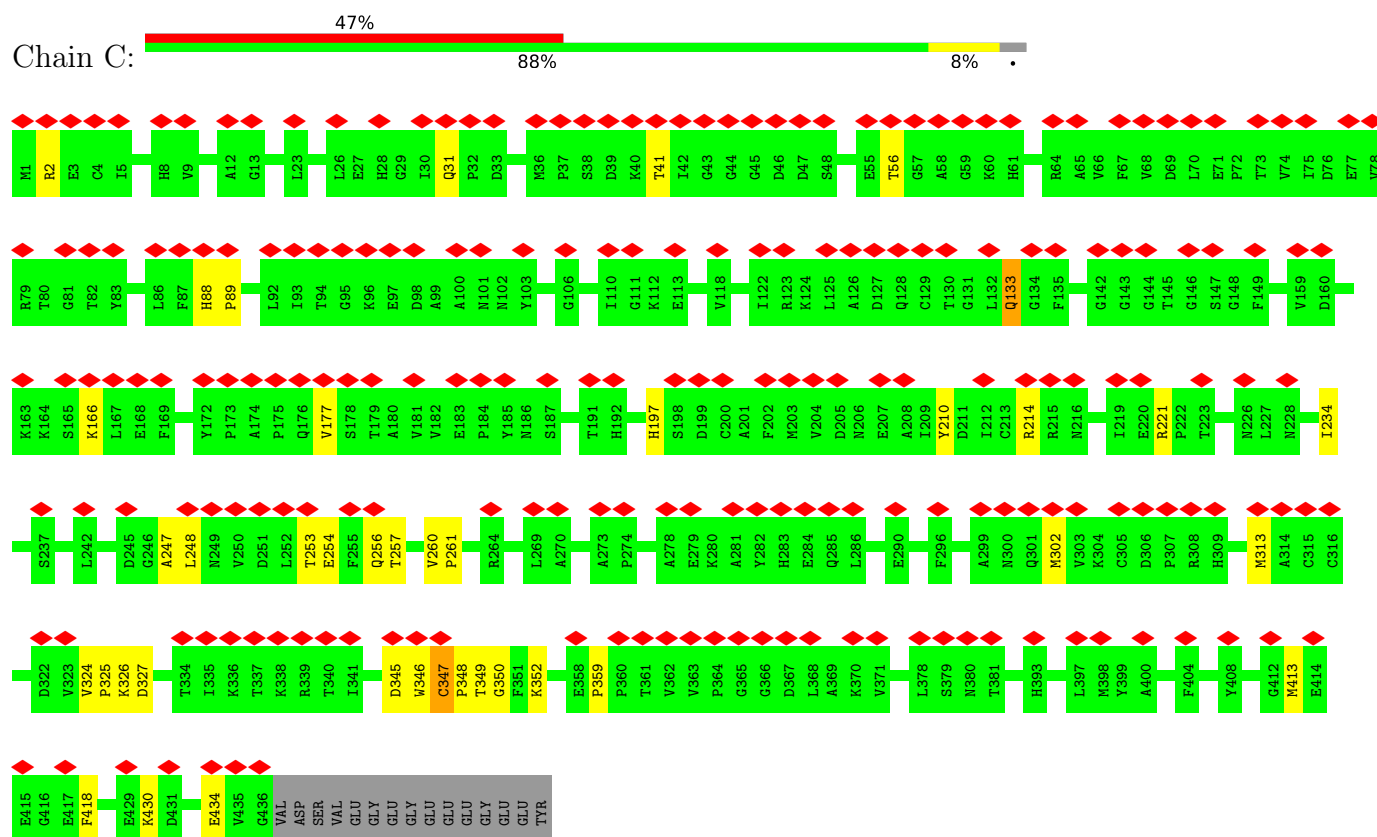




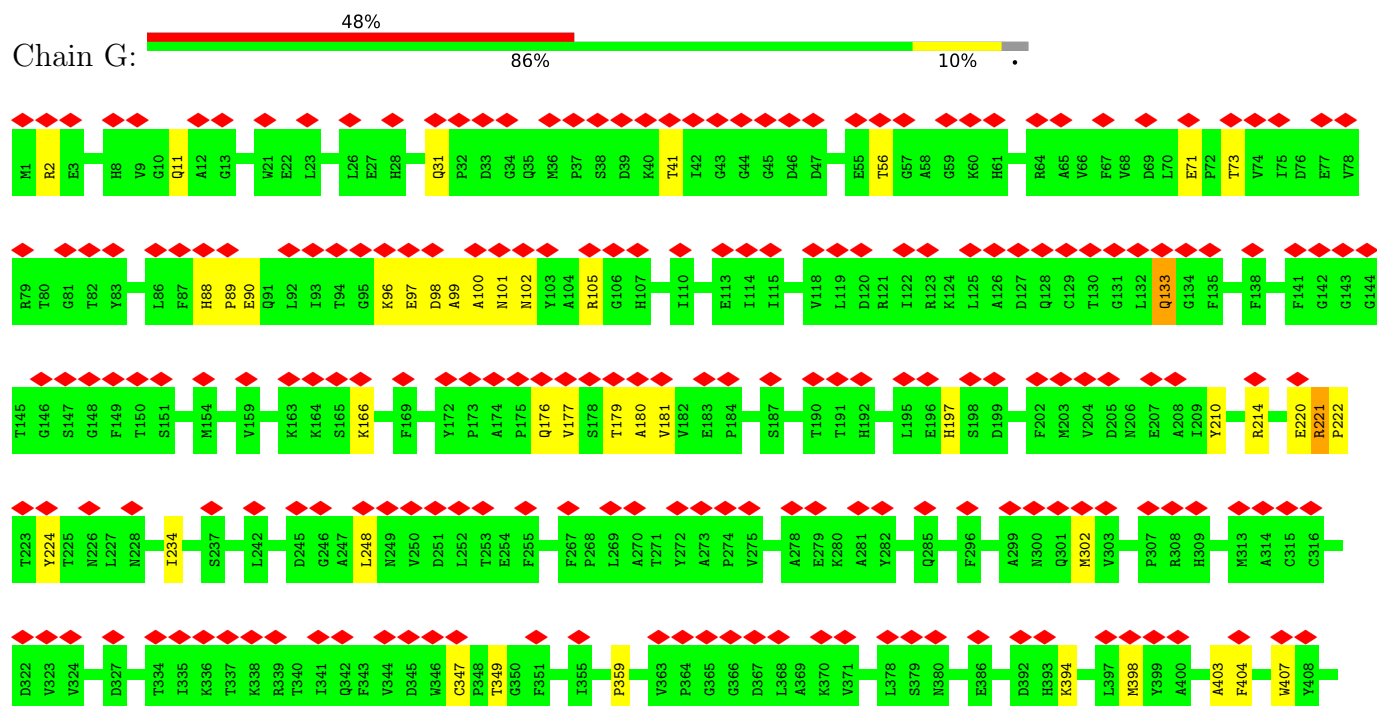
• Molecule 4: Tubulin beta chain

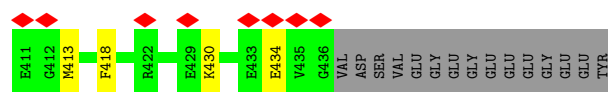


• Molecule 5: Tubulin alpha-1A chain



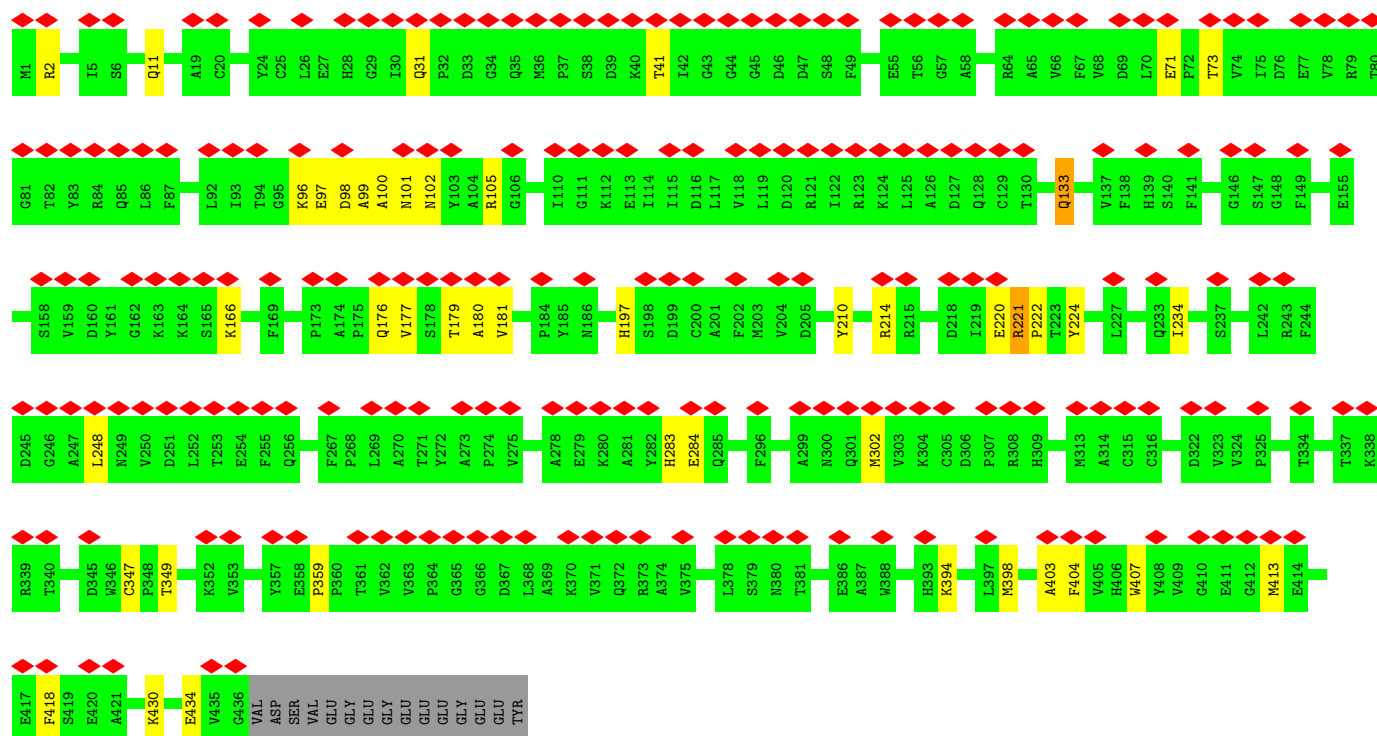
• Molecule 5: Tubulin alpha-1A chain





• Molecule 5: Tubulin alpha-1A chain

Chain E: 48% 87% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00846	Depositor
Map size (Å)	273.664, 273.664, 273.664	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	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	I	1.35	3/136 (2.2%)	0.82	0/181
2	J	1.23	20/1259 (1.6%)	1.10	14/1690 (0.8%)
3	K	0.74	0/105	0.59	0/141
4	B	0.73	0/3434	1.18	1/4652 (0.0%)
4	D	0.73	0/3434	1.18	1/4652 (0.0%)
5	A	0.74	0/3481	1.20	5/4725 (0.1%)
5	C	0.74	0/3481	1.20	5/4725 (0.1%)
5	E	0.74	0/3481	1.20	5/4725 (0.1%)
5	G	0.74	0/3481	1.20	5/4725 (0.1%)
All	All	0.78	23/22292 (0.1%)	1.19	36/30216 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
2	J	0	1
4	B	0	2
4	D	0	2
All	All	0	6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	107	ALA	C-N	-9.51	1.20	1.33
2	J	40	LEU	C-N	-8.61	1.24	1.33
2	J	54	PHE	C-N	-7.97	1.23	1.33
1	I	22	ASP	C-N	-7.74	1.22	1.33
2	J	31	HIS	C-N	-7.69	1.23	1.33
1	I	33	MET	C-N	-7.22	1.24	1.33
2	J	117	PRO	C-N	-6.96	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	100	GLU	C-N	-6.56	1.25	1.33
2	J	75	PHE	C-N	-6.39	1.25	1.33
2	J	81	LYS	C-N	-6.38	1.25	1.33
2	J	49	PRO	N-CD	6.23	1.56	1.47
1	I	32	ALA	C-N	-6.17	1.26	1.33
2	J	62	PHE	C-N	-6.16	1.25	1.34
2	J	128	GLU	C-N	-6.10	1.25	1.33
2	J	131	GLY	C-N	-5.91	1.26	1.33
2	J	35	ASP	C-N	-5.86	1.26	1.33
2	J	139	LYS	C-N	-5.81	1.26	1.33
2	J	93	GLU	C-N	-5.69	1.26	1.33
2	J	120	MET	C-N	-5.33	1.26	1.33
2	J	124	ASN	C-N	-5.22	1.27	1.33
2	J	138	ILE	C-N	-5.18	1.27	1.33
2	J	97	HIS	C-N	-5.13	1.27	1.33
2	J	55	VAL	C-N	-5.04	1.26	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	116	MET	O-C-N	9.29	129.60	121.34
2	J	113	LEU	CA-C-N	-7.92	112.19	122.16
2	J	113	LEU	C-N-CA	-7.92	112.19	122.16
4	D	131	GLN	OE1-CD-NE2	-6.87	115.73	122.60
4	B	131	GLN	OE1-CD-NE2	-6.86	115.74	122.60
5	E	221	ARG	NE-CZ-NH2	6.56	125.11	119.20
5	C	221	ARG	NE-CZ-NH2	6.53	125.08	119.20
5	A	221	ARG	NE-CZ-NH2	6.52	125.07	119.20
5	G	221	ARG	NE-CZ-NH2	6.51	125.06	119.20
5	C	133	GLN	OE1-CD-NE2	-6.26	116.33	122.60
5	E	133	GLN	OE1-CD-NE2	-6.20	116.40	122.60
5	G	133	GLN	OE1-CD-NE2	-6.20	116.40	122.60
5	A	133	GLN	OE1-CD-NE2	-6.19	116.41	122.60
2	J	108	ASN	CA-C-N	-5.77	111.58	121.97
2	J	108	ASN	C-N-CA	-5.77	111.58	121.97
5	G	221	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
5	E	221	ARG	NH1-CZ-NH2	-5.75	111.82	119.30
5	A	221	ARG	NH1-CZ-NH2	-5.74	111.84	119.30
5	C	221	ARG	NH1-CZ-NH2	-5.73	111.85	119.30
2	J	48	LYS	O-C-N	5.68	128.10	121.39
2	J	48	LYS	CA-C-N	-5.56	112.89	119.84
2	J	48	LYS	C-N-CA	-5.56	112.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	113	LEU	O-C-N	5.39	129.65	122.43
5	G	31	GLN	OE1-CD-NE2	-5.29	117.31	122.60
5	A	31	GLN	OE1-CD-NE2	-5.29	117.31	122.60
5	C	31	GLN	OE1-CD-NE2	-5.26	117.34	122.60
5	E	31	GLN	OE1-CD-NE2	-5.25	117.35	122.60
2	J	116	MET	CA-C-N	-5.21	113.33	119.84
2	J	116	MET	C-N-CA	-5.21	113.33	119.84
5	E	359	PRO	N-CA-CB	5.14	105.89	103.22
5	C	359	PRO	N-CA-CB	5.13	105.89	103.22
2	J	159	MET	O-C-N	5.07	127.50	122.12
2	J	107	ALA	CA-C-N	5.07	129.38	122.34
2	J	107	ALA	C-N-CA	5.07	129.38	122.34
5	G	359	PRO	N-CA-CB	5.07	105.86	103.22
5	A	359	PRO	N-CA-CB	5.04	105.84	103.22

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	2	ARG	Sidechain
4	B	359	ARG	Sidechain
4	D	2	ARG	Sidechain
4	D	359	ARG	Sidechain
1	I	22	ASP	Mainchain
2	J	109	ILE	Mainchain

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	I	134	0	130	3	0
2	J	1228	0	1256	64	0
3	K	104	0	99	1	0
4	B	3359	3241	3228	282	0
4	D	3359	3241	3228	294	0
5	A	3403	3308	3299	132	0
5	C	3403	3308	3299	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3403	3308	3302	207	0
5	G	3403	3308	3302	206	0
All	All	21796	19714	21143	701	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 16.

All (701) 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)
4:D:345:ILE:CG2	5:G:404:PHE:CE2	1.76	1.63
4:B:345:ILE:CG2	5:E:404:PHE:CE2	1.76	1.59
4:B:397:TRP:CH2	5:A:256:GLN:HG2	1.38	1.56
5:G:56:THR:HG22	5:E:284:GLU:CD	1.20	1.56
4:D:397:TRP:CH2	5:C:256:GLN:HG2	1.38	1.54
4:B:345:ILE:HG23	5:E:404:PHE:CE2	1.30	1.53
4:D:345:ILE:HG21	5:G:404:PHE:CZ	1.44	1.53
4:D:345:ILE:HG23	5:G:404:PHE:CE2	1.30	1.52
4:B:345:ILE:HG21	5:E:404:PHE:CZ	1.44	1.49
4:D:397:TRP:CH2	5:C:256:GLN:CG	1.95	1.49
4:B:397:TRP:CH2	5:A:256:GLN:CG	1.95	1.48
4:D:220:PRO:CD	5:C:326:LYS:HG3	1.21	1.48
4:D:324:LYS:HD2	5:G:222:PRO:CD	1.16	1.47
4:B:219:THR:CG2	5:A:327:ASP:H	1.29	1.46
4:B:220:PRO:CD	5:A:326:LYS:HG3	1.21	1.46
4:D:219:THR:CG2	5:C:327:ASP:H	1.29	1.46
4:D:220:PRO:CD	5:C:326:LYS:CG	1.78	1.45
4:D:219:THR:CG2	5:C:324:VAL:HG23	1.45	1.45
4:D:324:LYS:CD	5:G:222:PRO:HD3	1.44	1.44
4:B:324:LYS:CD	5:E:222:PRO:HD3	1.44	1.44
5:G:56:THR:CG2	5:E:284:GLU:CD	1.87	1.43
4:B:219:THR:CG2	5:A:324:VAL:HG23	1.45	1.43
4:D:220:PRO:HD3	5:C:326:LYS:CG	1.35	1.43
4:B:326:VAL:CB	5:E:221:ARG:NH1	1.77	1.42
4:B:220:PRO:HD3	5:A:326:LYS:CG	1.35	1.40
4:B:324:LYS:HD2	5:E:222:PRO:CD	1.16	1.39
4:B:397:TRP:CE2	5:A:257:THR:HA	1.31	1.39
4:B:252:LYS:CA	5:E:100:ALA:HB1	1.38	1.38
5:A:284:GLU:CD	5:C:56:THR:HG22	1.44	1.38
4:B:220:PRO:CD	5:A:326:LYS:CG	1.78	1.36
4:D:345:ILE:HG22	5:G:181:VAL:CG1	1.55	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:326:VAL:CB	5:G:221:ARG:NH1	1.77	1.36
4:B:252:LYS:HA	5:E:100:ALA:CB	1.55	1.35
4:B:345:ILE:HG22	5:E:181:VAL:CG1	1.55	1.35
2:J:81:LYS:CD	4:D:158:GLU:HA	1.42	1.35
4:B:331:LEU:CD1	5:E:176:GLN:HG3	1.57	1.35
4:D:252:LYS:HA	5:G:100:ALA:CB	1.55	1.34
4:D:397:TRP:CE2	5:C:257:THR:HA	1.31	1.34
4:D:219:THR:HG23	5:C:327:ASP:N	1.02	1.34
4:D:331:LEU:CD1	5:G:176:GLN:HG3	1.57	1.33
4:D:397:TRP:HH2	5:C:256:GLN:CB	1.21	1.33
4:B:397:TRP:HH2	5:A:256:GLN:CB	1.21	1.33
4:D:397:TRP:CD2	5:C:257:THR:HA	1.63	1.32
5:G:56:THR:HA	5:E:284:GLU:OE1	1.27	1.32
4:B:219:THR:HG23	5:A:327:ASP:N	1.02	1.31
4:D:252:LYS:CA	5:G:100:ALA:HB1	1.38	1.31
4:B:397:TRP:CD2	5:A:257:THR:HA	1.63	1.31
5:G:56:THR:CA	5:E:284:GLU:OE1	1.77	1.31
4:B:247:ASN:ND2	5:E:73:THR:HB	1.44	1.31
4:D:247:ASN:ND2	5:G:73:THR:HB	1.44	1.29
4:D:397:TRP:HH2	5:C:256:GLN:CG	1.35	1.29
4:B:397:TRP:HH2	5:A:256:GLN:CG	1.35	1.29
4:B:331:LEU:HD11	5:E:176:GLN:CB	1.63	1.28
4:D:397:TRP:CE2	5:C:257:THR:CA	2.16	1.28
5:G:56:THR:HB	5:E:284:GLU:CG	1.64	1.27
4:D:220:PRO:HD3	5:C:326:LYS:CD	1.65	1.27
4:D:331:LEU:HD11	5:G:176:GLN:CB	1.63	1.27
4:B:397:TRP:CE2	5:A:257:THR:CA	2.16	1.26
4:B:220:PRO:HD3	5:A:326:LYS:CD	1.65	1.25
4:B:219:THR:HG21	5:A:324:VAL:CG2	1.67	1.24
4:D:219:THR:HG21	5:C:324:VAL:CG2	1.67	1.24
4:B:251:ARG:HD2	5:E:105:ARG:CZ	1.66	1.24
4:D:387:ALA:O	5:C:346:TRP:HA	1.36	1.23
4:B:397:TRP:CH2	5:A:256:GLN:CB	2.07	1.23
4:B:387:ALA:O	5:A:346:TRP:HA	1.36	1.22
5:G:56:THR:CB	5:E:284:GLU:OE1	1.86	1.22
4:D:252:LYS:CA	5:G:100:ALA:CB	2.12	1.22
4:D:331:LEU:CD1	5:G:176:GLN:CG	2.18	1.22
4:D:251:ARG:HD2	5:G:105:ARG:CZ	1.66	1.22
4:D:345:ILE:HD13	5:G:404:PHE:CZ	1.74	1.22
4:B:331:LEU:CD1	5:E:176:GLN:CG	2.18	1.22
4:B:345:ILE:HD13	5:E:404:PHE:CZ	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:56:THR:CG2	5:E:284:GLU:OE1	1.86	1.21
4:D:397:TRP:CH2	5:C:256:GLN:CB	2.07	1.20
4:D:396:HIS:HE1	5:C:261:PRO:CA	1.55	1.19
5:G:56:THR:HG22	5:E:284:GLU:OE2	1.40	1.19
4:B:245:GLN:OE1	5:E:224:TYR:CE2	1.73	1.19
4:B:345:ILE:CG2	5:E:404:PHE:HE2	1.28	1.19
4:D:345:ILE:CG2	5:G:404:PHE:HE2	1.28	1.18
4:D:245:GLN:OE1	5:G:224:TYR:CE2	1.73	1.18
4:B:396:HIS:HE1	5:A:261:PRO:CA	1.55	1.18
4:D:396:HIS:ND1	5:C:261:PRO:O	1.76	1.18
4:D:345:ILE:CG2	5:G:181:VAL:HG11	1.74	1.18
4:B:396:HIS:ND1	5:A:261:PRO:O	1.76	1.18
4:B:345:ILE:CG2	5:E:181:VAL:HG11	1.74	1.17
4:B:331:LEU:HD11	5:E:176:GLN:CA	1.75	1.17
4:B:252:LYS:CE	5:E:100:ALA:H	1.51	1.16
4:D:396:HIS:CE1	5:C:261:PRO:HA	1.81	1.16
4:D:252:LYS:CE	5:G:100:ALA:H	1.51	1.15
4:D:331:LEU:HD11	5:G:176:GLN:CA	1.75	1.15
4:B:396:HIS:CE1	5:A:261:PRO:HA	1.81	1.15
4:B:252:LYS:HE2	5:E:100:ALA:H	0.99	1.13
4:D:252:LYS:HE2	5:G:100:ALA:H	0.99	1.13
5:G:56:THR:CB	5:E:284:GLU:CD	2.21	1.13
4:D:219:THR:HG23	5:C:326:LYS:C	1.74	1.13
4:B:219:THR:HG23	5:A:326:LYS:C	1.74	1.12
4:B:220:PRO:HD2	5:A:326:LYS:HG3	1.15	1.12
2:J:81:LYS:CD	4:D:158:GLU:CA	2.27	1.12
4:B:219:THR:CG2	5:A:327:ASP:N	1.96	1.12
4:D:258:VAL:HB	5:G:407:TRP:HZ2	1.03	1.11
4:D:219:THR:CG2	5:C:327:ASP:N	1.96	1.11
4:B:258:VAL:HB	5:E:407:TRP:HZ2	1.03	1.10
5:A:284:GLU:OE1	5:C:56:THR:HG22	1.50	1.10
5:G:56:THR:HG22	5:E:284:GLU:OE1	1.40	1.10
4:D:331:LEU:HD11	5:G:176:GLN:CG	1.79	1.10
4:D:331:LEU:HD13	5:G:176:GLN:HG3	1.16	1.10
4:B:331:LEU:HD13	5:E:176:GLN:HG3	1.16	1.10
5:A:284:GLU:HG3	5:C:56:THR:HB	1.26	1.09
4:D:220:PRO:HD2	5:C:326:LYS:HG3	1.15	1.09
4:B:396:HIS:HE1	5:A:261:PRO:HA	0.93	1.09
5:A:284:GLU:CD	5:C:56:THR:CG2	2.25	1.08
4:B:390:ARG:NH2	5:A:345:ASP:HB3	1.67	1.08
4:B:396:HIS:CE1	5:A:261:PRO:C	2.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:326:VAL:HB	5:E:221:ARG:NH1	0.99	1.07
4:B:331:LEU:HD11	5:E:176:GLN:CG	1.79	1.07
4:D:390:ARG:NH2	5:C:345:ASP:HB3	1.67	1.07
2:J:42:ALA:H	2:J:45:MET:HE2	0.96	1.06
4:D:396:HIS:HE1	5:C:261:PRO:HA	0.93	1.06
4:D:396:HIS:CE1	5:C:261:PRO:C	2.32	1.06
5:A:283:HIS:ND1	5:C:88:HIS:NE2	2.00	1.06
4:B:247:ASN:HD21	5:E:73:THR:HB	0.91	1.05
4:D:247:ASN:HD21	5:G:73:THR:HB	0.91	1.05
5:A:284:GLU:OE1	5:C:56:THR:HA	1.54	1.05
4:B:258:VAL:HB	5:E:407:TRP:CZ2	1.92	1.04
4:B:252:LYS:CA	5:E:100:ALA:CB	2.12	1.04
4:B:345:ILE:HG21	5:E:404:PHE:CE2	1.66	1.04
4:D:247:ASN:ND2	5:G:73:THR:CB	2.22	1.03
4:D:247:ASN:OD1	5:G:73:THR:CB	2.06	1.03
4:B:247:ASN:ND2	5:E:73:THR:CB	2.22	1.03
2:J:81:LYS:HD2	4:D:158:GLU:HA	1.07	1.03
4:B:247:ASN:OD1	5:E:73:THR:CB	2.06	1.02
4:B:258:VAL:O	5:E:407:TRP:NE1	1.92	1.02
4:B:396:HIS:CE1	5:A:261:PRO:O	2.12	1.02
4:D:258:VAL:HB	5:G:407:TRP:CZ2	1.92	1.02
4:D:326:VAL:HB	5:G:221:ARG:NH1	1.00	1.02
4:B:247:ASN:CG	5:E:73:THR:HB	1.83	1.02
4:D:247:ASN:HD21	5:G:73:THR:CB	1.72	1.02
4:D:396:HIS:CE1	5:C:261:PRO:O	2.12	1.02
2:J:42:ALA:H	2:J:45:MET:CE	1.72	1.02
4:D:247:ASN:CG	5:G:73:THR:HB	1.83	1.02
4:D:258:VAL:O	5:G:407:TRP:NE1	1.92	1.02
4:B:331:LEU:HD11	5:E:176:GLN:HA	1.38	1.01
4:D:345:ILE:CG2	5:G:404:PHE:CZ	2.21	1.01
4:D:388:MET:HG2	5:C:347:CYS:HA	1.42	1.01
4:B:252:LYS:HE2	5:E:100:ALA:N	1.75	1.01
4:B:396:HIS:CE1	5:A:261:PRO:CA	2.39	1.01
4:D:396:HIS:CE1	5:C:261:PRO:CA	2.39	1.01
4:B:247:ASN:HD21	5:E:73:THR:CB	1.73	1.01
4:D:331:LEU:HD11	5:G:176:GLN:HA	1.38	1.00
4:D:252:LYS:HE2	5:G:100:ALA:N	1.75	0.99
4:D:396:HIS:NE2	5:C:260:VAL:O	1.95	0.99
4:B:388:MET:HG2	5:A:347:CYS:HA	1.42	0.99
4:D:177:ASP:O	5:C:352:LYS:HB3	1.62	0.99
4:B:177:ASP:O	5:A:352:LYS:HB3	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:ASP:O	5:C:352:LYS:CB	2.11	0.99
4:B:324:LYS:CD	5:E:222:PRO:CD	2.06	0.99
4:B:326:VAL:CG1	5:E:221:ARG:HH12	1.76	0.99
4:B:396:HIS:NE2	5:A:260:VAL:O	1.95	0.99
4:B:177:ASP:O	5:A:352:LYS:CB	2.11	0.99
4:D:326:VAL:CG1	5:G:221:ARG:HH12	1.76	0.99
4:B:331:LEU:HD13	5:E:176:GLN:CG	1.86	0.98
2:J:42:ALA:N	2:J:45:MET:HE2	1.78	0.98
4:D:388:MET:HG2	5:C:347:CYS:CA	1.93	0.98
4:D:324:LYS:CD	5:G:222:PRO:CD	2.06	0.98
4:B:345:ILE:CG2	5:E:404:PHE:CZ	2.21	0.98
4:B:331:LEU:CD1	5:E:176:GLN:CB	2.43	0.97
4:B:388:MET:HG2	5:A:347:CYS:CA	1.93	0.97
4:D:331:LEU:HD13	5:G:176:GLN:CG	1.86	0.97
4:D:345:ILE:CB	5:G:404:PHE:HE2	1.77	0.97
4:B:256:ASN:HD21	5:E:101:ASN:HD22	0.97	0.97
4:D:345:ILE:HG22	5:G:181:VAL:HG11	0.97	0.97
4:B:345:ILE:HG22	5:E:181:VAL:HG11	0.97	0.97
4:D:256:ASN:HD21	5:G:101:ASN:HD22	0.97	0.96
4:D:331:LEU:CD1	5:G:176:GLN:CB	2.43	0.96
4:B:345:ILE:HG21	5:E:404:PHE:HZ	1.19	0.96
4:B:220:PRO:CD	5:A:326:LYS:CD	2.33	0.96
4:B:219:THR:CG2	5:A:324:VAL:CG2	2.35	0.96
4:B:345:ILE:CB	5:E:404:PHE:HE2	1.77	0.96
5:G:56:THR:HB	5:E:284:GLU:HG3	0.98	0.95
4:D:219:THR:CG2	5:C:324:VAL:CG2	2.35	0.95
4:D:345:ILE:HG21	5:G:404:PHE:CE2	1.66	0.95
5:G:56:THR:CB	5:E:284:GLU:HG3	1.95	0.95
4:D:247:ASN:CG	5:G:73:THR:CB	2.40	0.94
4:D:251:ARG:CD	5:G:105:ARG:CZ	2.44	0.94
5:A:283:HIS:HE1	5:C:89:PRO:HD2	1.31	0.94
4:B:251:ARG:CD	5:E:105:ARG:CZ	2.44	0.94
4:D:347:ASN:O	5:G:181:VAL:HA	1.68	0.94
4:B:347:ASN:O	5:E:181:VAL:HA	1.68	0.94
4:B:247:ASN:CG	5:E:73:THR:CB	2.40	0.93
4:D:220:PRO:CD	5:C:326:LYS:CD	2.33	0.93
4:D:397:TRP:CH2	5:C:256:GLN:HB3	2.03	0.93
4:B:322:SER:OG	5:E:221:ARG:HB3	1.68	0.93
4:B:397:TRP:CH2	5:A:256:GLN:HB3	2.03	0.93
5:G:56:THR:CB	5:E:284:GLU:CG	2.46	0.93
4:B:326:VAL:CB	5:E:221:ARG:HH12	1.55	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:350:LYS:HB3	5:G:179:THR:O	1.70	0.92
4:D:322:SER:OG	5:G:221:ARG:HB3	1.68	0.92
4:D:326:VAL:CB	5:G:221:ARG:HH12	1.55	0.92
4:D:345:ILE:HG21	5:G:404:PHE:HZ	1.19	0.92
4:B:245:GLN:OE1	5:E:224:TYR:HE2	0.98	0.92
2:J:88:ARG:HH12	4:D:154:LYS:NZ	1.67	0.91
4:B:350:LYS:HB3	5:E:179:THR:O	1.70	0.91
4:B:396:HIS:CE1	5:A:260:VAL:O	2.23	0.91
2:J:104:LEU:HD13	2:J:106:TRP:CZ2	2.05	0.91
4:D:396:HIS:CE1	5:C:260:VAL:O	2.23	0.91
2:J:81:LYS:HD2	4:D:158:GLU:CA	1.95	0.90
4:B:322:SER:O	5:E:221:ARG:HD3	1.72	0.89
5:A:284:GLU:OE1	5:C:56:THR:CA	2.20	0.89
4:D:344:TRP:O	5:G:398:MET:HG2	1.72	0.89
4:B:177:ASP:O	5:A:352:LYS:HD2	1.54	0.89
4:D:322:SER:O	5:G:221:ARG:HD3	1.72	0.89
4:D:345:ILE:HD13	5:G:404:PHE:CE2	2.09	0.88
4:B:345:ILE:HD13	5:E:404:PHE:CE2	2.09	0.88
5:A:284:GLU:OE1	5:C:56:THR:CG2	2.16	0.88
4:B:344:TRP:O	5:E:398:MET:HG2	1.72	0.87
4:D:256:ASN:ND2	5:G:101:ASN:HD22	1.73	0.87
4:B:256:ASN:ND2	5:E:101:ASN:HD22	1.73	0.87
4:B:345:ILE:CG1	5:E:404:PHE:CE2	2.56	0.86
4:D:345:ILE:CG1	5:G:404:PHE:CE2	2.56	0.86
5:A:284:GLU:CG	5:C:56:THR:HB	2.05	0.86
1:I:23:ASP:OD1	2:J:23:LYS:NZ	2.08	0.86
4:B:220:PRO:HD3	5:A:326:LYS:HG3	0.89	0.85
4:D:220:PRO:HD3	5:C:326:LYS:HG3	0.89	0.85
4:D:350:LYS:CB	5:G:179:THR:O	2.03	0.85
4:B:387:ALA:O	5:A:346:TRP:CA	2.22	0.84
4:B:252:LYS:CE	5:E:100:ALA:N	2.37	0.84
4:B:345:ILE:CG2	5:E:181:VAL:CG1	2.43	0.84
4:B:255:VAL:HA	5:E:407:TRP:CD2	2.14	0.83
4:B:256:ASN:HD21	5:E:101:ASN:ND2	1.75	0.83
4:D:252:LYS:CE	5:G:100:ALA:N	2.36	0.83
4:D:255:VAL:HA	5:G:407:TRP:CD2	2.14	0.83
4:D:256:ASN:HD21	5:G:101:ASN:ND2	1.75	0.83
4:B:179:VAL:O	5:A:348:PRO:HG3	1.76	0.83
4:B:220:PRO:CD	5:A:326:LYS:HD2	2.09	0.83
4:D:345:ILE:CG2	5:G:181:VAL:CG1	2.43	0.83
4:D:177:ASP:O	5:C:352:LYS:HD2	1.54	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:220:PRO:CD	5:C:326:LYS:HD2	2.09	0.83
4:B:255:VAL:HG22	5:E:407:TRP:CE3	2.14	0.83
4:D:179:VAL:O	5:C:348:PRO:HG3	1.76	0.83
4:B:347:ASN:C	5:E:181:VAL:HA	2.03	0.83
4:B:179:VAL:HB	5:A:348:PRO:HG2	1.61	0.82
4:D:255:VAL:HG22	5:G:407:TRP:CE3	2.14	0.82
4:B:220:PRO:N	5:A:326:LYS:HD2	1.94	0.82
4:B:345:ILE:CG1	5:E:404:PHE:HE2	1.91	0.82
4:D:345:ILE:CG1	5:G:404:PHE:HE2	1.91	0.82
4:D:347:ASN:C	5:G:181:VAL:HA	2.03	0.82
4:D:179:VAL:HB	5:C:348:PRO:HG2	1.61	0.82
4:D:387:ALA:O	5:C:346:TRP:CA	2.22	0.82
4:B:344:TRP:O	5:E:398:MET:HA	1.81	0.81
4:D:344:TRP:O	5:G:398:MET:HA	1.81	0.81
4:D:388:MET:HG2	5:C:347:CYS:C	2.05	0.81
4:B:397:TRP:CZ3	5:A:256:GLN:CG	2.62	0.81
4:D:397:TRP:CZ3	5:C:256:GLN:CG	2.62	0.81
4:B:2:ARG:NH2	5:E:98:ASP:N	2.29	0.81
4:D:2:ARG:NH2	5:G:98:ASP:N	2.29	0.81
4:D:220:PRO:N	5:C:326:LYS:HD2	1.94	0.80
4:B:251:ARG:CD	5:E:105:ARG:NH1	2.45	0.80
4:B:247:ASN:O	5:E:98:ASP:OD2	2.00	0.80
4:B:388:MET:HG2	5:A:347:CYS:C	2.05	0.80
4:D:247:ASN:O	5:G:98:ASP:OD2	2.00	0.80
2:J:81:LYS:HE2	4:D:157:GLU:HG2	1.65	0.79
4:B:397:TRP:CD2	5:A:257:THR:CA	2.55	0.79
4:D:98:GLY:HA2	5:C:254:GLU:OE1	1.82	0.79
4:D:251:ARG:CD	5:G:105:ARG:NH1	2.45	0.79
4:D:2:ARG:HH22	5:G:98:ASP:N	1.81	0.79
4:D:245:GLN:OE1	5:G:224:TYR:HE2	0.98	0.78
4:B:2:ARG:HH22	5:E:98:ASP:N	1.81	0.78
5:A:284:GLU:OE2	5:C:56:THR:HG22	1.82	0.78
4:B:98:GLY:HA2	5:A:254:GLU:OE1	1.82	0.78
4:B:345:ILE:HG23	5:E:404:PHE:CD2	2.16	0.78
4:D:397:TRP:CD2	5:C:257:THR:CA	2.55	0.78
5:G:56:THR:HB	5:E:284:GLU:CD	1.97	0.78
4:B:258:VAL:O	5:E:407:TRP:CE2	2.37	0.78
4:D:258:VAL:O	5:G:407:TRP:CE2	2.37	0.78
2:J:41:ILE:HA	2:J:45:MET:HE1	1.65	0.77
4:D:345:ILE:HG23	5:G:404:PHE:CD2	2.16	0.77
5:G:89:PRO:HD2	5:E:283:HIS:HE1	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:326:VAL:HG12	5:G:221:ARG:HH12	1.49	0.77
4:D:397:TRP:CZ2	5:C:256:GLN:HG2	2.17	0.77
4:D:324:LYS:HE3	5:G:214:ARG:HG2	1.66	0.77
4:D:219:THR:HG22	5:C:326:LYS:N	2.00	0.77
4:B:324:LYS:HG3	5:E:210:TYR:OH	1.85	0.77
4:B:326:VAL:HB	5:E:221:ARG:HH11	1.45	0.76
4:D:324:LYS:HG3	5:G:210:TYR:OH	1.85	0.76
4:B:326:VAL:HG12	5:E:221:ARG:HH12	1.49	0.76
4:B:245:GLN:CB	5:E:11:GLN:HE22	1.98	0.76
4:B:247:ASN:OD1	5:E:73:THR:HG21	1.86	0.76
4:B:345:ILE:HG22	5:E:181:VAL:HG12	1.65	0.76
4:D:245:GLN:CB	5:G:11:GLN:HE22	1.98	0.76
2:J:21:HIS:CE1	2:J:25:GLN:NE2	2.54	0.76
4:B:177:ASP:O	5:A:352:LYS:CD	2.03	0.76
4:B:324:LYS:HE3	5:E:214:ARG:HG2	1.66	0.76
4:D:247:ASN:OD1	5:G:73:THR:CG2	2.33	0.76
4:D:247:ASN:OD1	5:G:73:THR:HG21	1.86	0.76
4:B:247:ASN:OD1	5:E:73:THR:CG2	2.34	0.76
4:B:219:THR:HG22	5:A:326:LYS:N	2.00	0.75
4:D:247:ASN:OD1	5:G:73:THR:HB	1.81	0.75
4:D:326:VAL:HB	5:G:221:ARG:HH11	1.45	0.75
4:D:247:ASN:CG	5:G:73:THR:OG1	2.30	0.75
5:A:283:HIS:CE1	5:C:89:PRO:HD2	2.21	0.75
4:D:251:ARG:HD2	5:G:105:ARG:NH2	2.02	0.74
4:B:247:ASN:CG	5:E:73:THR:OG1	2.30	0.74
4:B:247:ASN:HD22	5:E:71:GLU:HG3	1.51	0.74
5:A:284:GLU:OE1	5:C:56:THR:CB	2.34	0.74
4:B:397:TRP:CZ2	5:A:256:GLN:HG2	2.17	0.74
4:D:346:PRO:O	5:G:181:VAL:HG13	1.86	0.74
4:B:346:PRO:O	5:E:181:VAL:HG13	1.86	0.74
2:J:64:LEU:HD23	2:J:137:LEU:HD11	1.70	0.74
4:D:387:ALA:O	5:C:345:ASP:O	2.06	0.74
2:J:41:ILE:HA	2:J:45:MET:CE	2.18	0.74
4:B:387:ALA:O	5:A:345:ASP:O	2.06	0.74
4:D:177:ASP:O	5:C:352:LYS:CD	2.03	0.74
4:D:345:ILE:CD1	5:G:404:PHE:CE2	2.71	0.73
4:B:219:THR:CG2	5:A:326:LYS:CA	2.66	0.73
4:D:219:THR:CG2	5:C:326:LYS:CA	2.66	0.73
2:J:55:VAL:HG11	2:J:78:ILE:HD12	1.70	0.73
4:D:247:ASN:HD22	5:G:71:GLU:HG3	1.51	0.73
4:B:345:ILE:CD1	5:E:404:PHE:CE2	2.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:345:ILE:CD1	5:E:404:PHE:CZ	2.65	0.73
4:B:251:ARG:HD2	5:E:105:ARG:NH2	2.02	0.73
4:B:219:THR:HG23	5:A:326:LYS:CA	2.19	0.72
4:B:331:LEU:CD1	5:E:176:GLN:HA	2.16	0.72
4:D:219:THR:HG23	5:C:326:LYS:CA	2.19	0.72
4:D:221:THR:HG22	5:C:325:PRO:HD2	1.71	0.72
4:D:331:LEU:CD1	5:G:176:GLN:HA	2.16	0.71
4:D:252:LYS:CA	5:G:100:ALA:HB2	2.16	0.71
4:B:2:ARG:NE	5:E:96:LYS:O	2.24	0.71
4:D:245:GLN:CA	5:G:11:GLN:HE22	2.03	0.71
4:D:345:ILE:CD1	5:G:404:PHE:CZ	2.65	0.71
2:J:88:ARG:HH12	4:D:154:LYS:HZ1	1.36	0.71
5:A:283:HIS:ND1	5:C:88:HIS:CD2	2.57	0.71
4:B:221:THR:HG22	5:A:325:PRO:HD2	1.71	0.71
4:D:247:ASN:OD1	5:G:73:THR:OG1	2.08	0.70
4:B:245:GLN:CA	5:E:11:GLN:HE22	2.03	0.70
4:D:345:ILE:HG22	5:G:181:VAL:HG12	1.65	0.70
4:B:98:GLY:HA2	5:A:254:GLU:CG	2.22	0.70
4:B:390:ARG:HH21	5:A:345:ASP:HB3	1.53	0.70
4:D:2:ARG:NE	5:G:96:LYS:O	2.24	0.70
5:A:283:HIS:CE1	5:C:88:HIS:NE2	2.59	0.70
4:B:252:LYS:HE3	5:E:98:ASP:C	2.15	0.70
4:D:98:GLY:HA2	5:C:254:GLU:CG	2.22	0.70
4:D:324:LYS:CE	5:G:222:PRO:HD3	2.22	0.70
4:D:331:LEU:HD11	5:G:176:GLN:HG3	1.42	0.70
2:J:69:GLU:OE1	2:J:73:ARG:NE	2.24	0.70
4:B:247:ASN:OD1	5:E:73:THR:OG1	2.08	0.70
4:D:252:LYS:HE3	5:G:98:ASP:C	2.15	0.70
4:D:390:ARG:HH21	5:C:345:ASP:HB3	1.53	0.70
4:D:220:PRO:HD2	5:C:326:LYS:CG	1.88	0.69
4:D:347:ASN:O	5:G:181:VAL:CA	2.38	0.69
4:B:324:LYS:CE	5:E:222:PRO:HD3	2.22	0.69
2:J:36:GLU:OE2	2:J:56:HIS:HE1	1.75	0.69
4:B:326:VAL:H	5:E:221:ARG:CD	2.06	0.69
4:B:347:ASN:O	5:E:181:VAL:CA	2.38	0.69
4:B:388:MET:CG	5:A:348:PRO:N	2.42	0.69
4:D:251:ARG:HD2	5:G:105:ARG:NH1	2.08	0.69
4:B:346:PRO:O	5:E:181:VAL:CG1	2.41	0.68
2:J:88:ARG:HB3	2:J:114:VAL:HG11	1.74	0.68
4:D:219:THR:HG22	5:C:326:LYS:H	1.57	0.68
2:J:88:ARG:HH12	4:D:154:LYS:HZ2	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:220:PRO:HD3	5:A:326:LYS:HD2	1.68	0.68
4:D:346:PRO:O	5:G:181:VAL:CG1	2.41	0.68
4:B:388:MET:HG2	5:A:348:PRO:N	2.06	0.68
4:D:219:THR:CB	5:C:324:VAL:HG23	2.24	0.68
4:D:388:MET:HG2	5:C:348:PRO:N	2.06	0.68
4:D:326:VAL:H	5:G:221:ARG:CD	2.06	0.68
4:B:397:TRP:NE1	5:A:257:THR:HA	2.03	0.68
4:B:220:PRO:HD3	5:A:326:LYS:CE	2.24	0.67
4:D:179:VAL:O	5:C:348:PRO:CG	2.42	0.67
4:D:245:GLN:HB3	5:G:11:GLN:HE22	1.58	0.67
2:J:81:LYS:HD3	4:D:158:GLU:CA	2.20	0.67
4:B:245:GLN:HB3	5:E:11:GLN:HE22	1.58	0.67
4:D:345:ILE:HG12	5:G:404:PHE:CE2	2.27	0.67
4:B:251:ARG:HD3	5:E:105:ARG:NH1	2.09	0.67
4:D:258:VAL:CB	5:G:407:TRP:HZ2	1.96	0.67
4:B:179:VAL:O	5:A:348:PRO:CG	2.42	0.67
4:B:219:THR:HG22	5:A:326:LYS:H	1.57	0.67
4:B:345:ILE:HG12	5:E:404:PHE:CE2	2.27	0.67
4:D:390:ARG:NH2	5:C:345:ASP:CB	2.53	0.67
4:B:258:VAL:CB	5:E:407:TRP:HZ2	1.96	0.67
2:J:17:SER:OG	2:J:43:TRP:O	2.13	0.66
4:D:220:PRO:HD3	5:C:326:LYS:CE	2.24	0.66
4:D:251:ARG:HD3	5:G:105:ARG:NH1	2.09	0.66
4:B:346:PRO:O	5:E:181:VAL:O	2.13	0.66
4:D:346:PRO:O	5:G:181:VAL:O	2.13	0.66
4:B:397:TRP:NE1	5:A:257:THR:O	2.28	0.66
4:D:397:TRP:NE1	5:C:257:THR:O	2.28	0.66
4:D:246:LEU:HD11	5:G:179:THR:CG2	2.26	0.66
4:D:255:VAL:HA	5:G:407:TRP:CE3	2.31	0.66
4:B:397:TRP:CZ3	5:A:256:GLN:CD	2.74	0.65
4:D:394:PHE:HZ	5:C:313:MET:O	1.78	0.65
5:G:88:HIS:NE2	5:E:283:HIS:ND1	2.41	0.65
4:B:394:PHE:HZ	5:A:313:MET:O	1.78	0.65
4:D:219:THR:HG21	5:C:324:VAL:HG23	0.71	0.65
4:B:177:ASP:O	5:A:352:LYS:CG	2.44	0.65
4:B:247:ASN:OD1	5:E:73:THR:HB	1.81	0.65
4:B:249:ASP:OD2	5:E:98:ASP:OD1	2.15	0.65
4:D:397:TRP:NE1	5:C:257:THR:HA	2.03	0.65
4:D:397:TRP:CZ3	5:C:256:GLN:CD	2.74	0.65
4:B:390:ARG:NH2	5:A:345:ASP:CB	2.53	0.65
5:A:284:GLU:CD	5:C:56:THR:CB	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:219:THR:HG21	5:A:324:VAL:HG23	0.71	0.65
4:B:246:LEU:HD11	5:E:179:THR:CG2	2.26	0.65
5:A:283:HIS:CE1	5:C:88:HIS:CD2	2.84	0.65
4:D:177:ASP:O	5:C:352:LYS:CG	2.44	0.65
4:D:249:ASP:OD2	5:G:98:ASP:OD1	2.15	0.65
4:D:251:ARG:CD	5:G:105:ARG:NH2	2.60	0.65
4:B:255:VAL:HA	5:E:407:TRP:CE3	2.31	0.64
4:B:219:THR:CB	5:A:324:VAL:HG23	2.24	0.64
4:B:390:ARG:CZ	5:A:345:ASP:HB3	2.27	0.64
4:B:251:ARG:CD	5:E:105:ARG:NH2	2.60	0.63
4:D:219:THR:CG2	5:C:326:LYS:N	2.60	0.63
4:B:331:LEU:HD11	5:E:176:GLN:HG3	1.42	0.63
4:B:350:LYS:CB	5:E:179:THR:O	2.03	0.63
4:D:390:ARG:CZ	5:C:345:ASP:HB3	2.27	0.63
4:B:346:PRO:HG2	5:E:394:LYS:O	1.99	0.63
4:B:397:TRP:CZ3	5:A:256:GLN:HB3	2.33	0.63
4:D:324:LYS:CG	5:G:222:PRO:CD	2.63	0.63
2:J:88:ARG:CB	2:J:114:VAL:HG11	2.29	0.63
4:D:327:ASP:N	5:G:221:ARG:NH1	2.32	0.63
4:B:219:THR:CG2	5:A:326:LYS:N	2.60	0.63
4:B:397:TRP:CG	5:A:257:THR:HG23	2.34	0.63
4:D:397:TRP:CG	5:C:257:THR:HG23	2.34	0.63
4:B:344:TRP:C	5:E:398:MET:HG2	2.23	0.63
4:D:344:TRP:C	5:G:398:MET:HG2	2.23	0.63
4:B:2:ARG:NH2	5:E:71:GLU:HB3	2.14	0.63
4:D:247:ASN:HD22	5:G:71:GLU:CG	2.03	0.62
4:D:397:TRP:CZ3	5:C:256:GLN:HB3	2.33	0.62
5:A:284:GLU:HG3	5:C:56:THR:CB	2.16	0.62
2:J:88:ARG:CG	2:J:114:VAL:HG12	2.29	0.62
4:D:324:LYS:CE	5:G:214:ARG:HG2	2.28	0.62
4:B:247:ASN:HD22	5:E:71:GLU:CG	2.03	0.62
4:B:344:TRP:CE3	5:E:403:ALA:HB2	2.35	0.62
4:D:254:ALA:O	5:G:407:TRP:CZ2	2.53	0.62
4:D:346:PRO:HG2	5:G:394:LYS:O	1.99	0.62
4:D:344:TRP:CE3	5:G:403:ALA:HB2	2.35	0.62
4:B:324:LYS:CE	5:E:214:ARG:HG2	2.28	0.61
4:B:397:TRP:CZ3	5:A:256:GLN:HG2	2.23	0.61
4:B:324:LYS:CG	5:E:222:PRO:CD	2.63	0.61
4:D:2:ARG:NH2	5:G:71:GLU:HB3	2.14	0.61
4:D:252:LYS:CE	5:G:98:ASP:C	2.72	0.61
4:B:345:ILE:CB	5:E:404:PHE:CE2	2.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:88:ARG:HB3	2:J:114:VAL:CG1	2.30	0.61
4:B:254:ALA:O	5:E:407:TRP:CZ2	2.53	0.61
4:D:251:ARG:NE	5:G:105:ARG:NH2	2.48	0.61
4:D:246:LEU:HD11	5:G:179:THR:HB	1.83	0.61
4:B:252:LYS:CE	5:E:98:ASP:C	2.72	0.61
4:B:251:ARG:NE	5:E:105:ARG:NH2	2.48	0.61
4:D:344:TRP:HE3	5:G:403:ALA:HB2	1.65	0.61
4:D:345:ILE:CB	5:G:404:PHE:CE2	2.62	0.61
4:D:350:LYS:CG	5:G:180:ALA:HA	2.13	0.61
5:G:56:THR:CG2	5:E:284:GLU:OE2	2.23	0.61
4:B:246:LEU:HD11	5:E:179:THR:HB	1.83	0.60
2:J:84:GLU:OE1	2:J:88:ARG:NH2	2.35	0.60
4:B:344:TRP:HE3	5:E:403:ALA:HB2	1.65	0.60
2:J:88:ARG:HG2	2:J:114:VAL:HG12	1.84	0.60
4:D:255:VAL:HA	5:G:407:TRP:CE2	2.36	0.60
4:B:388:MET:O	5:A:346:TRP:HB2	2.02	0.60
4:D:327:ASP:HB3	5:G:176:GLN:O	2.01	0.60
4:B:327:ASP:HB3	5:E:176:GLN:O	2.01	0.60
4:B:255:VAL:HA	5:E:407:TRP:CE2	2.36	0.60
2:J:20:LEU:HD21	2:J:126:LEU:HD23	1.84	0.60
4:D:388:MET:O	5:C:346:TRP:HB2	2.02	0.59
5:G:56:THR:CG2	5:E:284:GLU:CG	2.78	0.59
4:B:177:ASP:O	5:A:352:LYS:CA	2.50	0.59
4:B:220:PRO:HD2	5:A:326:LYS:CG	1.88	0.59
4:D:177:ASP:O	5:C:352:LYS:CA	2.50	0.59
4:B:219:THR:CB	5:A:324:VAL:CG2	2.79	0.59
4:B:350:LYS:HG3	5:E:180:ALA:HA	1.85	0.59
4:D:388:MET:CG	5:C:347:CYS:HA	2.24	0.59
4:B:388:MET:CG	5:A:347:CYS:HA	2.24	0.59
4:B:245:GLN:CA	5:E:11:GLN:NE2	2.66	0.58
4:B:219:THR:HG21	5:A:327:ASP:H	1.53	0.58
4:D:219:THR:CB	5:C:324:VAL:CG2	2.79	0.58
4:D:322:SER:O	5:G:221:ARG:CD	2.50	0.58
4:B:348:ASN:HB3	5:E:181:VAL:HG11	1.84	0.58
4:D:348:ASN:HB3	5:G:181:VAL:HG11	1.84	0.58
4:D:245:GLN:CA	5:G:11:GLN:NE2	2.66	0.58
2:J:36:GLU:OE2	2:J:56:HIS:CE1	2.56	0.58
4:D:219:THR:HG21	5:C:327:ASP:H	1.53	0.57
2:J:92:VAL:HG23	2:J:114:VAL:HG21	1.87	0.57
5:A:283:HIS:HE1	5:C:89:PRO:CD	2.13	0.57
4:D:350:LYS:HG3	5:G:180:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:348:ASN:N	5:G:181:VAL:HG13	2.20	0.57
5:A:284:GLU:CG	5:C:56:THR:CB	2.80	0.57
4:D:397:TRP:CZ3	5:C:256:GLN:CB	2.82	0.56
4:B:252:LYS:N	5:E:100:ALA:CB	2.68	0.56
4:B:252:LYS:CA	5:E:100:ALA:HB2	2.16	0.56
4:B:390:ARG:HH21	5:A:345:ASP:CB	2.18	0.56
4:D:252:LYS:N	5:G:100:ALA:CB	2.68	0.56
4:D:252:LYS:HA	5:G:100:ALA:HB1	0.61	0.56
4:B:348:ASN:N	5:E:181:VAL:HG13	2.20	0.56
4:D:397:TRP:CE2	5:C:257:THR:C	2.83	0.56
4:D:258:VAL:O	5:G:407:TRP:CZ2	2.59	0.56
2:J:59:HIS:HD2	2:J:70:PHE:CZ	2.24	0.55
4:B:322:SER:O	5:E:221:ARG:CD	2.50	0.55
4:D:388:MET:CG	5:C:348:PRO:N	2.42	0.55
4:B:326:VAL:CG1	5:E:221:ARG:NH1	2.46	0.55
4:D:390:ARG:HH21	5:C:345:ASP:C	2.15	0.55
4:D:397:TRP:CZ3	5:C:256:GLN:HG2	2.23	0.55
5:G:89:PRO:CD	5:E:283:HIS:HE1	2.16	0.55
4:B:390:ARG:HH21	5:A:345:ASP:C	2.15	0.55
5:G:88:HIS:CD2	5:E:283:HIS:HD1	2.25	0.55
2:J:95:LEU:HD13	2:J:125:PHE:HZ	1.70	0.55
4:B:331:LEU:CD1	5:E:176:GLN:HB3	2.32	0.55
4:B:397:TRP:CE2	5:A:257:THR:C	2.83	0.55
4:B:246:LEU:HD11	5:E:179:THR:CB	2.37	0.55
4:B:246:LEU:HD11	5:E:179:THR:HG21	1.88	0.55
5:G:2:ARG:HB3	5:G:133:GLN:HE21	1.72	0.55
5:C:2:ARG:HB3	5:C:133:GLN:HE21	1.72	0.55
4:B:258:VAL:O	5:E:407:TRP:CZ2	2.59	0.54
2:J:88:ARG:HG2	2:J:114:VAL:CG1	2.37	0.54
5:A:2:ARG:HB3	5:A:133:GLN:HE21	1.72	0.54
2:J:88:ARG:CB	2:J:114:VAL:CG1	2.86	0.54
4:B:98:GLY:HA2	5:A:254:GLU:CD	2.33	0.54
4:D:246:LEU:HD11	5:G:179:THR:CB	2.37	0.54
4:D:331:LEU:CD1	5:G:176:GLN:HB3	2.32	0.54
5:E:2:ARG:HB3	5:E:133:GLN:HE21	1.72	0.54
4:B:324:LYS:CG	5:E:222:PRO:HD2	2.38	0.54
4:D:390:ARG:HH21	5:C:345:ASP:CB	2.18	0.54
4:B:397:TRP:CZ3	5:A:256:GLN:CB	2.82	0.54
4:D:177:ASP:O	5:C:352:LYS:HA	2.08	0.54
4:D:246:LEU:HD11	5:G:179:THR:HG21	1.88	0.54
4:B:177:ASP:O	5:A:352:LYS:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:GLY:HA2	5:C:254:GLU:CD	2.33	0.54
4:D:324:LYS:CG	5:G:222:PRO:HD2	2.38	0.54
4:D:345:ILE:HA	5:G:398:MET:HG2	1.89	0.53
4:B:255:VAL:HG11	5:E:102:ASN:HB2	1.90	0.53
4:B:345:ILE:HA	5:E:398:MET:HG2	1.89	0.53
4:B:252:LYS:HA	5:E:100:ALA:HB1	0.61	0.53
4:D:251:ARG:HD2	5:G:105:ARG:NE	2.21	0.53
4:D:326:VAL:N	5:G:221:ARG:CD	2.51	0.53
4:B:327:ASP:N	5:E:221:ARG:NH1	2.32	0.53
4:D:326:VAL:CG1	5:G:221:ARG:NH1	2.46	0.53
4:D:324:LYS:HD2	5:G:222:PRO:HD3	0.54	0.52
2:J:76:TRP:CD2	2:J:77:PRO:HA	2.44	0.52
4:B:219:THR:HB	5:A:324:VAL:HG21	1.91	0.52
4:B:345:ILE:HA	5:E:398:MET:SD	2.49	0.52
4:D:219:THR:HB	5:C:324:VAL:HG21	1.91	0.52
4:D:324:LYS:HE3	5:G:214:ARG:CG	2.37	0.52
2:J:104:LEU:HD13	2:J:106:TRP:CH2	2.44	0.52
4:D:255:VAL:HG11	5:G:102:ASN:HB2	1.90	0.52
4:B:324:LYS:HE3	5:E:214:ARG:CG	2.37	0.52
4:B:245:GLN:HA	5:E:11:GLN:NE2	2.25	0.52
2:J:42:ALA:N	2:J:45:MET:CE	2.52	0.51
4:B:252:LYS:HE2	5:E:99:ALA:N	2.25	0.51
4:B:324:LYS:HD2	5:E:222:PRO:HD3	0.54	0.51
2:J:81:LYS:HD3	4:D:158:GLU:CB	2.40	0.51
4:D:345:ILE:HA	5:G:398:MET:SD	2.49	0.51
5:A:283:HIS:HD1	5:C:88:HIS:HE2	0.63	0.51
2:J:81:LYS:CD	4:D:158:GLU:CB	2.89	0.51
4:D:331:LEU:HD11	5:G:176:GLN:HB3	1.77	0.51
5:G:88:HIS:CD2	5:E:283:HIS:ND1	2.79	0.51
2:J:92:VAL:CG2	2:J:114:VAL:HG21	2.40	0.51
4:D:252:LYS:HE2	5:G:99:ALA:N	2.26	0.50
2:J:41:ILE:HD13	2:J:45:MET:HE1	1.92	0.50
4:B:2:ARG:NH2	5:E:97:GLU:C	2.70	0.50
4:D:255:VAL:HG22	5:G:407:TRP:HE3	1.73	0.50
4:B:348:ASN:HB3	5:E:181:VAL:CG1	2.42	0.50
4:D:245:GLN:HA	5:G:11:GLN:NE2	2.25	0.50
4:B:322:SER:C	5:E:221:ARG:HD3	2.34	0.50
4:B:350:LYS:CG	5:E:180:ALA:HA	2.13	0.50
4:D:2:ARG:NH2	5:G:98:ASP:H	2.09	0.50
4:D:348:ASN:HB3	5:G:181:VAL:CG1	2.42	0.50
4:D:345:ILE:HG12	5:G:404:PHE:HE2	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:120:MET:HE3	2:J:124:ASN:HD21	1.76	0.49
4:D:2:ARG:HH22	5:G:98:ASP:HB3	1.77	0.49
4:B:347:ASN:O	5:E:181:VAL:CG2	2.61	0.49
4:D:2:ARG:NH2	5:G:97:GLU:C	2.70	0.49
4:B:390:ARG:HH21	5:A:345:ASP:CA	2.24	0.49
2:J:95:LEU:HD13	2:J:125:PHE:CZ	2.48	0.49
4:B:251:ARG:HD2	5:E:105:ARG:NE	2.21	0.49
4:B:324:LYS:HG3	5:E:222:PRO:HD2	1.95	0.49
4:B:331:LEU:HD11	5:E:176:GLN:HB3	1.77	0.49
4:D:324:LYS:HG3	5:G:222:PRO:HD2	1.95	0.49
4:D:390:ARG:HH21	5:C:345:ASP:CA	2.24	0.49
4:D:322:SER:C	5:G:221:ARG:HD3	2.34	0.49
4:D:347:ASN:O	5:G:181:VAL:CG2	2.61	0.49
2:J:49:PRO:HA	2:J:117:PRO:O	2.14	0.48
4:B:255:VAL:HG22	5:E:407:TRP:HE3	1.73	0.48
4:B:2:ARG:HH22	5:E:98:ASP:HB3	1.77	0.48
4:B:345:ILE:HG12	5:E:403:ALA:HB1	1.94	0.48
4:D:345:ILE:HG12	5:G:403:ALA:HB1	1.95	0.48
4:D:344:TRP:O	5:G:398:MET:CG	2.55	0.48
2:J:88:ARG:CG	2:J:114:VAL:CG1	2.92	0.48
4:D:220:PRO:HD3	5:C:326:LYS:HD2	1.68	0.48
1:I:23:ASP:CG	2:J:23:LYS:NZ	2.71	0.48
5:A:210:TYR:CE1	5:A:214:ARG:HD2	2.49	0.47
5:E:210:TYR:CE1	5:E:214:ARG:HD2	2.49	0.47
2:J:76:TRP:CG	2:J:77:PRO:HA	2.49	0.47
4:D:252:LYS:N	5:G:100:ALA:HB2	2.29	0.47
4:B:252:LYS:N	5:E:100:ALA:HB2	2.29	0.47
4:D:388:MET:HG2	5:C:348:PRO:CD	2.08	0.47
5:C:210:TYR:CE1	5:C:214:ARG:HD2	2.49	0.47
5:G:210:TYR:CE1	5:G:214:ARG:HD2	2.49	0.47
2:J:88:ARG:NH1	4:D:154:LYS:HZ1	2.07	0.47
4:D:397:TRP:NE1	5:C:257:THR:C	2.73	0.47
4:B:397:TRP:NE1	5:A:257:THR:C	2.73	0.47
4:B:179:VAL:HG12	5:A:350:GLY:O	2.15	0.46
4:B:245:GLN:C	5:E:11:GLN:HE22	2.22	0.46
4:B:328:GLU:OE1	5:E:220:GLU:O	2.34	0.46
2:J:63:ARG:HE	2:J:63:ARG:HB3	1.53	0.46
4:D:179:VAL:HG12	5:C:350:GLY:O	2.16	0.46
4:D:328:GLU:OE1	5:G:220:GLU:O	2.34	0.46
5:A:234:ILE:HD13	5:A:302:MET:SD	2.56	0.46
5:C:234:ILE:HD13	5:C:302:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:347:ASN:O	5:E:181:VAL:HG22	2.01	0.46
5:G:234:ILE:HD13	5:G:302:MET:SD	2.56	0.46
5:E:234:ILE:HD13	5:E:302:MET:SD	2.56	0.46
4:D:245:GLN:C	5:G:11:GLN:HE22	2.22	0.46
4:B:2:ARG:NH2	5:E:98:ASP:H	2.09	0.46
2:J:111:SER:O	2:J:115:VAL:HG23	2.16	0.45
4:B:245:GLN:CB	5:E:11:GLN:NE2	2.75	0.45
4:B:251:ARG:HE	5:E:105:ARG:NH2	2.14	0.45
4:D:98:GLY:CA	5:C:254:GLU:CG	2.92	0.45
4:D:219:THR:HB	5:C:324:VAL:CG2	2.46	0.45
4:B:98:GLY:CA	5:A:254:GLU:CG	2.92	0.45
4:D:251:ARG:HE	5:G:105:ARG:NH2	2.14	0.45
2:J:81:LYS:HD2	4:D:158:GLU:HG3	1.99	0.45
4:B:26:ASP:OD2	4:B:359:ARG:HD2	2.17	0.45
4:D:26:ASP:OD2	4:D:359:ARG:HD2	2.17	0.45
4:D:397:TRP:CE3	5:C:257:THR:HA	2.39	0.44
4:B:247:ASN:HD21	5:E:73:THR:CA	2.30	0.44
4:B:345:ILE:HD13	5:E:404:PHE:HZ	1.64	0.44
4:B:346:PRO:C	5:E:181:VAL:HG13	2.41	0.44
4:B:326:VAL:N	5:E:221:ARG:CD	2.51	0.44
2:J:72:ARG:O	4:B:307:HIS:NE2	2.49	0.44
4:B:219:THR:HB	5:A:324:VAL:CG2	2.46	0.44
4:D:11:GLN:HE22	5:C:247:ALA:CB	2.30	0.44
4:B:344:TRP:O	5:E:398:MET:CA	2.60	0.44
5:A:166:LYS:HE2	5:A:197:HIS:O	2.18	0.44
5:E:166:LYS:HE2	5:E:197:HIS:O	2.18	0.44
2:J:108:ASN:O	2:J:110:LYS:N	2.50	0.44
4:B:252:LYS:CE	5:E:99:ALA:N	2.81	0.44
5:C:430:LYS:HE2	5:C:434:GLU:OE1	2.18	0.44
5:G:430:LYS:HE2	5:G:434:GLU:OE1	2.18	0.44
4:B:346:PRO:HG2	5:E:398:MET:HE2	1.65	0.44
4:D:98:GLY:HA2	5:C:254:GLU:HG2	1.99	0.44
4:D:252:LYS:CE	5:G:99:ALA:N	2.81	0.44
4:D:324:LYS:NZ	5:G:214:ARG:HG2	2.33	0.44
4:D:346:PRO:C	5:G:181:VAL:HG13	2.41	0.44
2:J:21:HIS:HE1	2:J:25:GLN:NE2	2.10	0.43
4:B:11:GLN:HE22	5:A:247:ALA:CB	2.31	0.43
2:J:59:HIS:CD2	2:J:70:PHE:CZ	3.06	0.43
4:D:255:VAL:HG13	5:G:407:TRP:HB3	1.99	0.43
4:D:258:VAL:C	5:G:407:TRP:HE1	2.22	0.43
4:B:98:GLY:HA2	5:A:254:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:251:ARG:NE	5:E:105:ARG:HH22	2.16	0.43
4:B:255:VAL:HG13	5:E:407:TRP:HB3	1.99	0.43
1:I:29:HIS:HB2	3:K:67:TYR:OH	2.18	0.43
4:B:397:TRP:CE3	5:A:257:THR:HA	2.39	0.43
5:A:430:LYS:HE2	5:A:434:GLU:OE1	2.18	0.43
5:C:166:LYS:HE2	5:C:197:HIS:O	2.18	0.43
4:D:243:PRO:HB3	5:G:73:THR:HG23	2.00	0.43
5:G:88:HIS:HD1	5:G:90:GLU:HB2	1.84	0.43
5:G:166:LYS:HE2	5:G:197:HIS:O	2.18	0.43
5:E:430:LYS:HE2	5:E:434:GLU:OE1	2.18	0.43
2:J:104:LEU:HD21	2:J:132:PHE:CD2	2.54	0.43
4:B:243:PRO:HB3	5:E:73:THR:HG23	2.00	0.43
4:B:324:LYS:NZ	5:E:214:ARG:HG2	2.33	0.43
4:B:177:ASP:C	5:A:352:LYS:HA	2.44	0.42
4:D:346:PRO:HG2	5:G:398:MET:HE2	1.65	0.42
4:B:324:LYS:CD	5:E:222:PRO:HD2	2.32	0.42
2:J:88:ARG:CA	2:J:114:VAL:HG11	2.49	0.42
4:B:397:TRP:NE1	5:A:257:THR:CA	2.75	0.42
2:J:12:GLU:HG2	2:J:120:MET:HE1	2.01	0.42
5:A:284:GLU:CG	5:C:56:THR:CG2	2.96	0.42
4:B:98:GLY:CA	5:A:254:GLU:HG2	2.50	0.41
4:B:344:TRP:O	5:E:398:MET:CG	2.55	0.41
4:D:177:ASP:C	5:C:352:LYS:HA	2.44	0.41
5:A:283:HIS:CE1	5:C:89:PRO:CD	2.95	0.41
2:J:116:MET:SD	4:D:106:TYR:HE1	2.43	0.41
4:D:397:TRP:NE1	5:C:257:THR:CA	2.75	0.41
4:B:331:LEU:CG	5:E:176:GLN:HA	2.51	0.41
4:D:299:MET:HE1	4:D:367:PHE:CE1	2.56	0.41
5:E:2:ARG:HB3	5:E:133:GLN:NE2	2.35	0.41
4:D:331:LEU:CG	5:G:176:GLN:HA	2.51	0.41
5:A:2:ARG:HB3	5:A:133:GLN:NE2	2.35	0.41
5:A:413:MET:HE2	5:A:418:PHE:CE2	2.56	0.41
5:G:2:ARG:HB3	5:G:133:GLN:NE2	2.35	0.41
2:J:42:ALA:O	2:J:45:MET:HE3	2.21	0.41
4:D:247:ASN:HD21	5:G:73:THR:CA	2.30	0.41
4:D:345:ILE:HA	5:G:398:MET:CG	2.51	0.41
5:C:2:ARG:HB3	5:C:133:GLN:NE2	2.35	0.41
5:E:413:MET:HE2	5:E:418:PHE:CE2	2.56	0.41
4:B:331:LEU:HD13	5:E:176:GLN:HG2	1.92	0.41
4:B:345:ILE:CA	5:E:398:MET:HG2	2.50	0.41
4:D:98:GLY:CA	5:C:254:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:413:MET:HE2	5:C:418:PHE:CE2	2.56	0.41
5:G:413:MET:HE2	5:G:418:PHE:CE2	2.56	0.41
2:J:58:MET:HE3	2:J:62:PHE:CZ	2.56	0.41
4:D:2:ARG:HH22	5:G:98:ASP:CB	2.34	0.41
4:D:345:ILE:CA	5:G:398:MET:HG2	2.50	0.41
4:B:299:MET:HE1	4:B:367:PHE:CE1	2.56	0.40
5:A:283:HIS:HD1	5:C:88:HIS:CD2	2.15	0.40
2:J:81:LYS:HD3	4:D:158:GLU:HB2	2.02	0.40
4:B:2:ARG:HH22	5:E:98:ASP:CB	2.34	0.40
5:G:88:HIS:CD2	5:E:283:HIS:CE1	3.10	0.40
4:B:103:LYS:NZ	5:A:253:THR:HG21	2.37	0.40
2:J:106:TRP:HB2	2:J:109:ILE:HD11	2.04	0.40
4:D:103:LYS:NZ	5:C:253:THR:HG21	2.37	0.40
5:G:413:MET:CE	5:G:418:PHE:CE2	3.05	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	I	13/108 (12%)	12 (92%)	1 (8%)	0	100	100
2	J	142/280 (51%)	139 (98%)	2 (1%)	1 (1%)	19	56
3	K	11/672 (2%)	11 (100%)	0	0	100	100
4	B	425/445 (96%)	416 (98%)	9 (2%)	0	100	100
4	D	425/445 (96%)	416 (98%)	8 (2%)	1 (0%)	44	78
5	A	434/451 (96%)	420 (97%)	14 (3%)	0	100	100
5	C	434/451 (96%)	420 (97%)	14 (3%)	0	100	100
5	E	434/451 (96%)	420 (97%)	14 (3%)	0	100	100
5	G	434/451 (96%)	420 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2752/3754 (73%)	2674 (97%)	76 (3%)	2 (0%)	50 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	247	ASN
2	J	109	ILE

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	I	14/94 (15%)	14 (100%)	0	100 100
2	J	132/244 (54%)	130 (98%)	2 (2%)	60 75
3	K	11/586 (2%)	11 (100%)	0	100 100
4	B	368/381 (97%)	366 (100%)	2 (0%)	86 89
4	D	368/381 (97%)	366 (100%)	2 (0%)	86 89
5	A	365/377 (97%)	360 (99%)	5 (1%)	62 76
5	C	365/377 (97%)	360 (99%)	5 (1%)	62 76
5	E	365/377 (97%)	360 (99%)	5 (1%)	62 76
5	G	365/377 (97%)	360 (99%)	5 (1%)	62 76
All	All	2353/3194 (74%)	2327 (99%)	26 (1%)	69 80

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	64	LEU
2	J	155	SER
4	B	246	LEU
4	B	323	MET
4	D	246	LEU
4	D	323	MET

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Mol	Chain	Res	Type
5	A	41	THR
5	A	177	VAL
5	A	248	LEU
5	A	347	CYS
5	A	349	THR
5	C	41	THR
5	C	177	VAL
5	C	248	LEU
5	C	347	CYS
5	C	349	THR
5	G	41	THR
5	G	177	VAL
5	G	248	LEU
5	G	347	CYS
5	G	349	THR
5	E	41	THR
5	E	177	VAL
5	E	248	LEU
5	E	347	CYS
5	E	349	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	25	GLN
2	J	21	HIS
2	J	25	GLN
2	J	31	HIS
2	J	56	HIS
2	J	59	HIS
2	J	124	ASN
4	B	11	GLN
4	B	190	HIS
4	B	292	GLN
4	B	414	ASN
4	D	11	GLN
4	D	190	HIS
4	D	280	GLN
4	D	292	GLN
4	D	414	ASN
5	A	61	HIS
5	A	216	ASN

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Mol	Chain	Res	Type
5	A	228	ASN
5	A	406	HIS
5	C	228	ASN
5	C	406	HIS
5	G	11	GLN
5	G	101	ASN
5	G	228	ASN
5	G	406	HIS
5	E	11	GLN
5	E	61	HIS
5	E	101	ASN
5	E	216	ASN
5	E	228	ASN
5	E	406	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	107:ALA	C	108:ASN	N	1.20

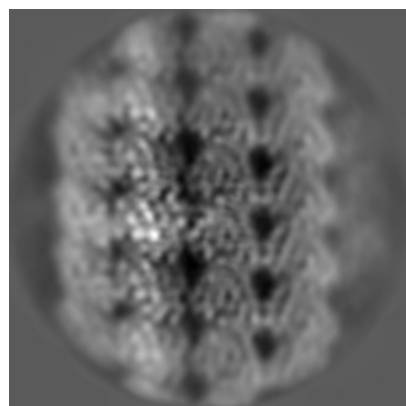
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54161. These allow visual inspection of the internal detail of the map and identification of artifacts.

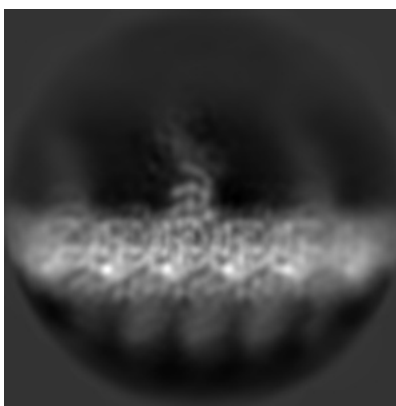
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

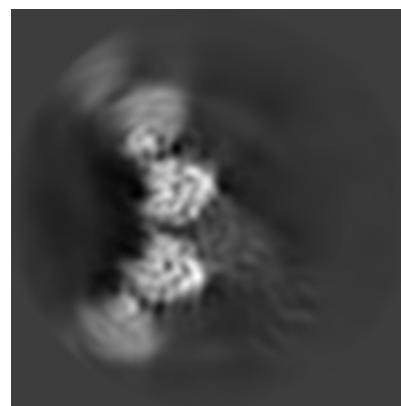
6.1.1 Primary map



X

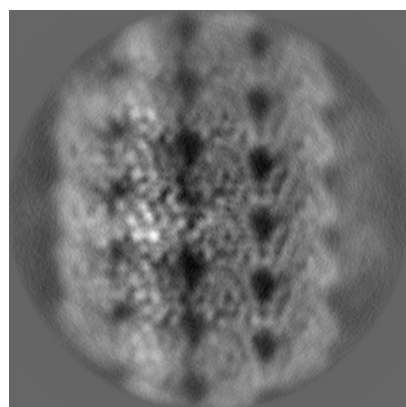


Y

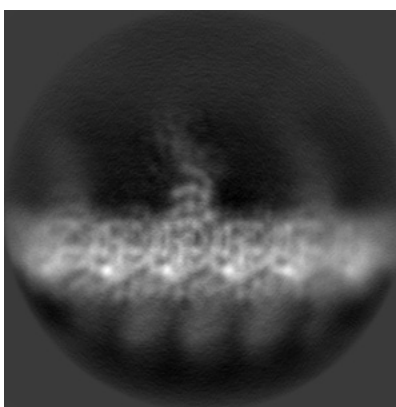


Z

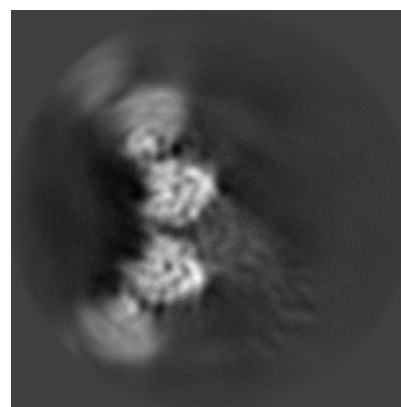
6.1.2 Raw map



X



Y

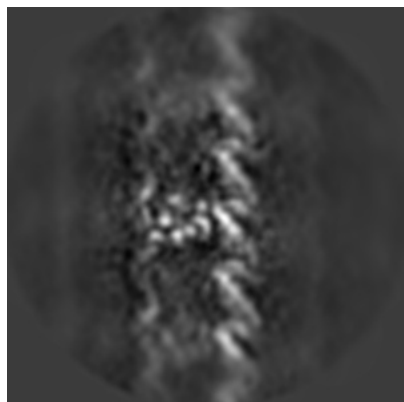


Z

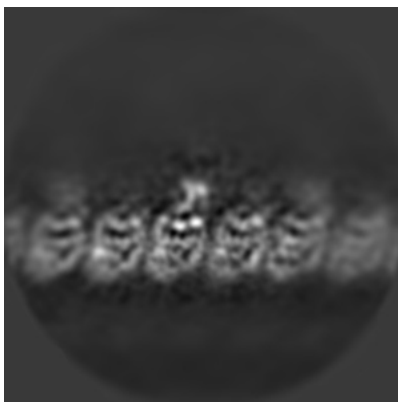
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

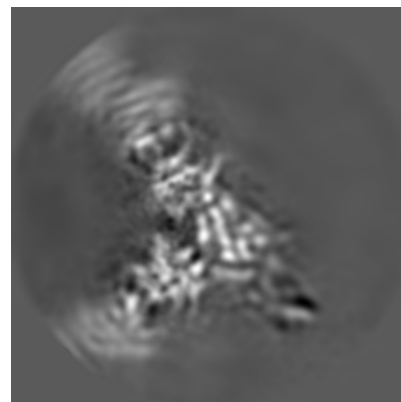
6.2.1 Primary map



X Index: 128

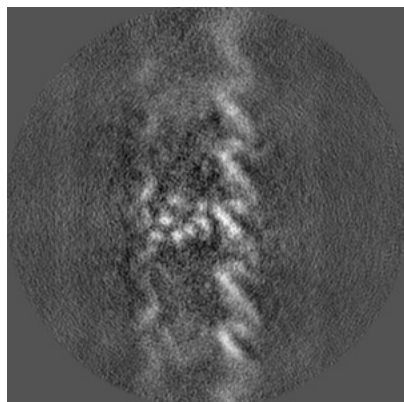


Y Index: 128

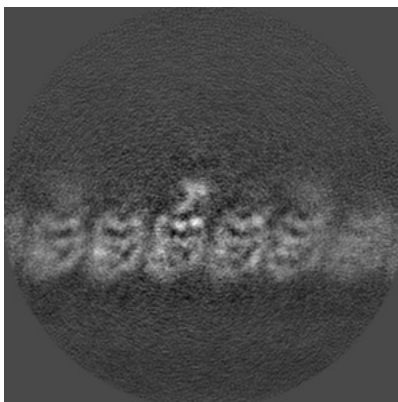


Z Index: 128

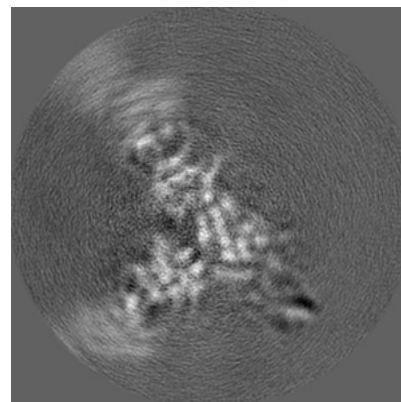
6.2.2 Raw map



X Index: 128



Y Index: 128

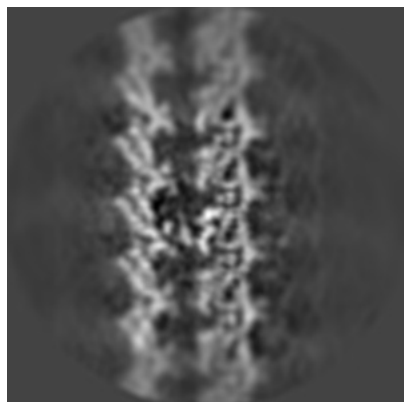


Z Index: 128

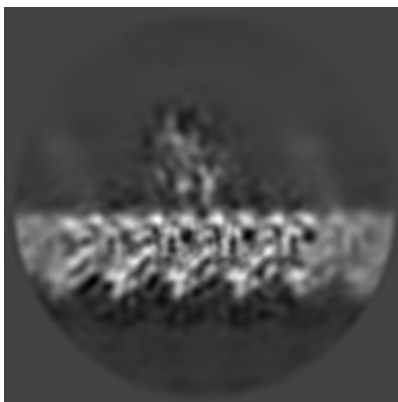
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

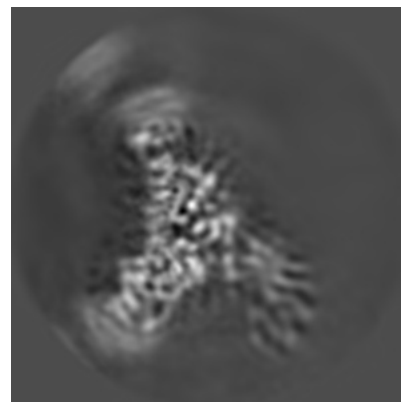
6.3.1 Primary map



X Index: 117

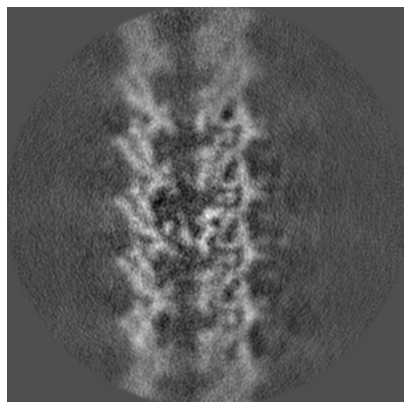


Y Index: 83

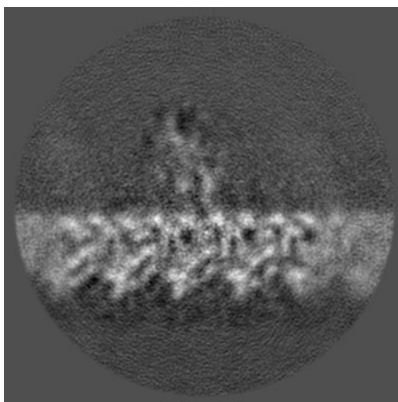


Z Index: 112

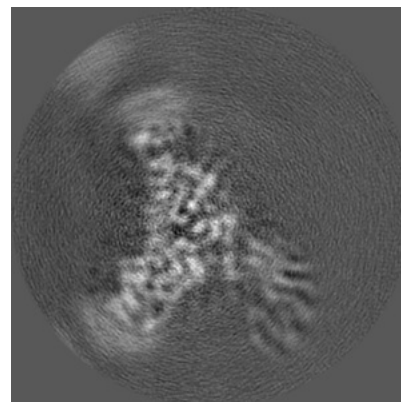
6.3.2 Raw map



X Index: 117



Y Index: 83

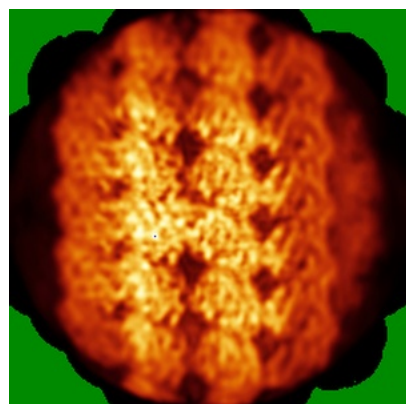


Z Index: 112

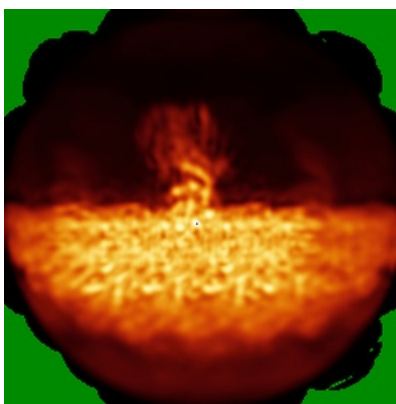
The images above show the largest variance slices of the map in three orthogonal directions.

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

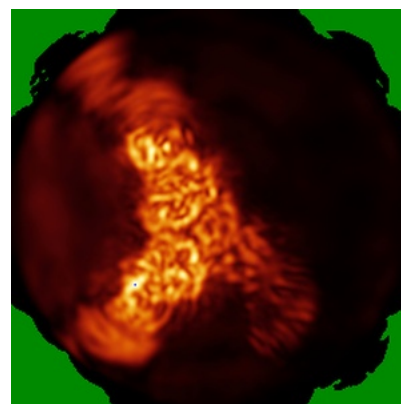
6.4.1 Primary map



X

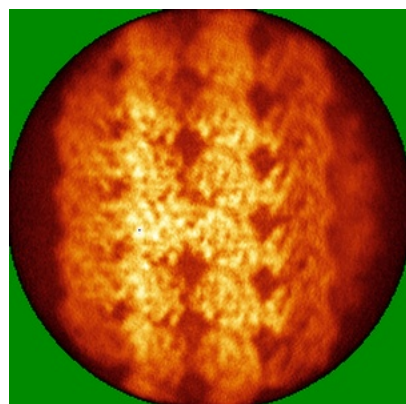


Y

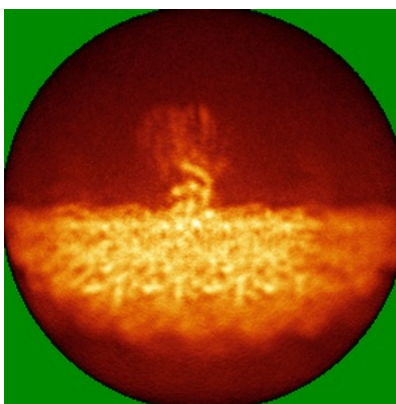


Z

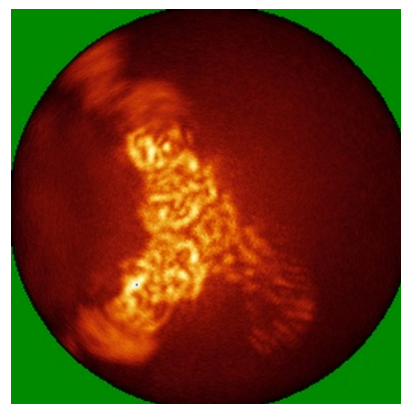
6.4.2 Raw map



X



Y



Z

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

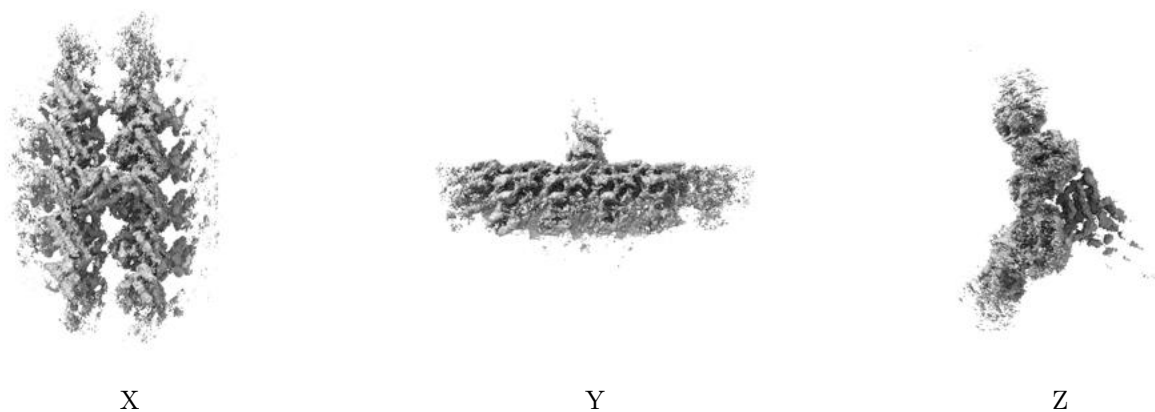
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00846. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

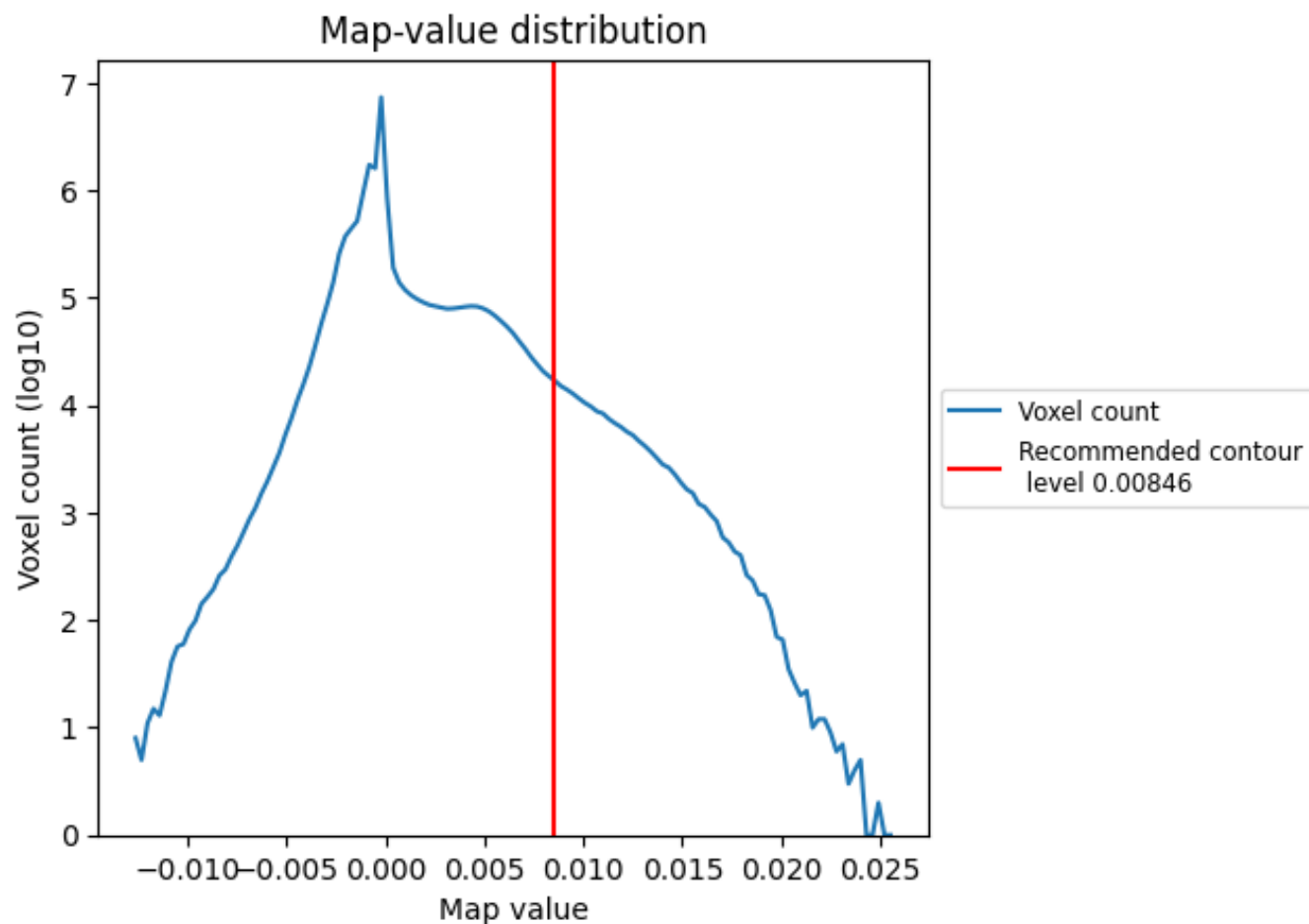
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

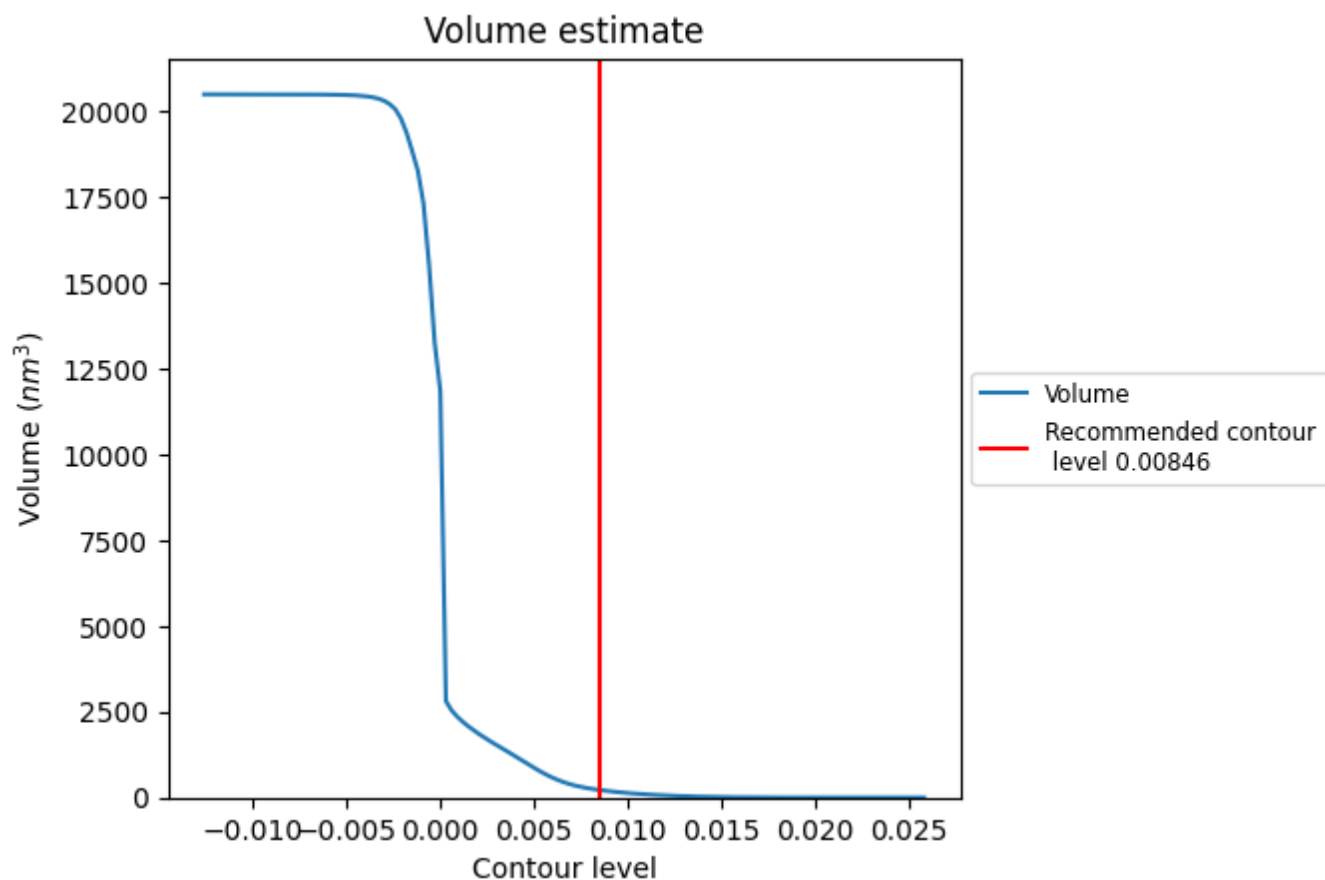
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

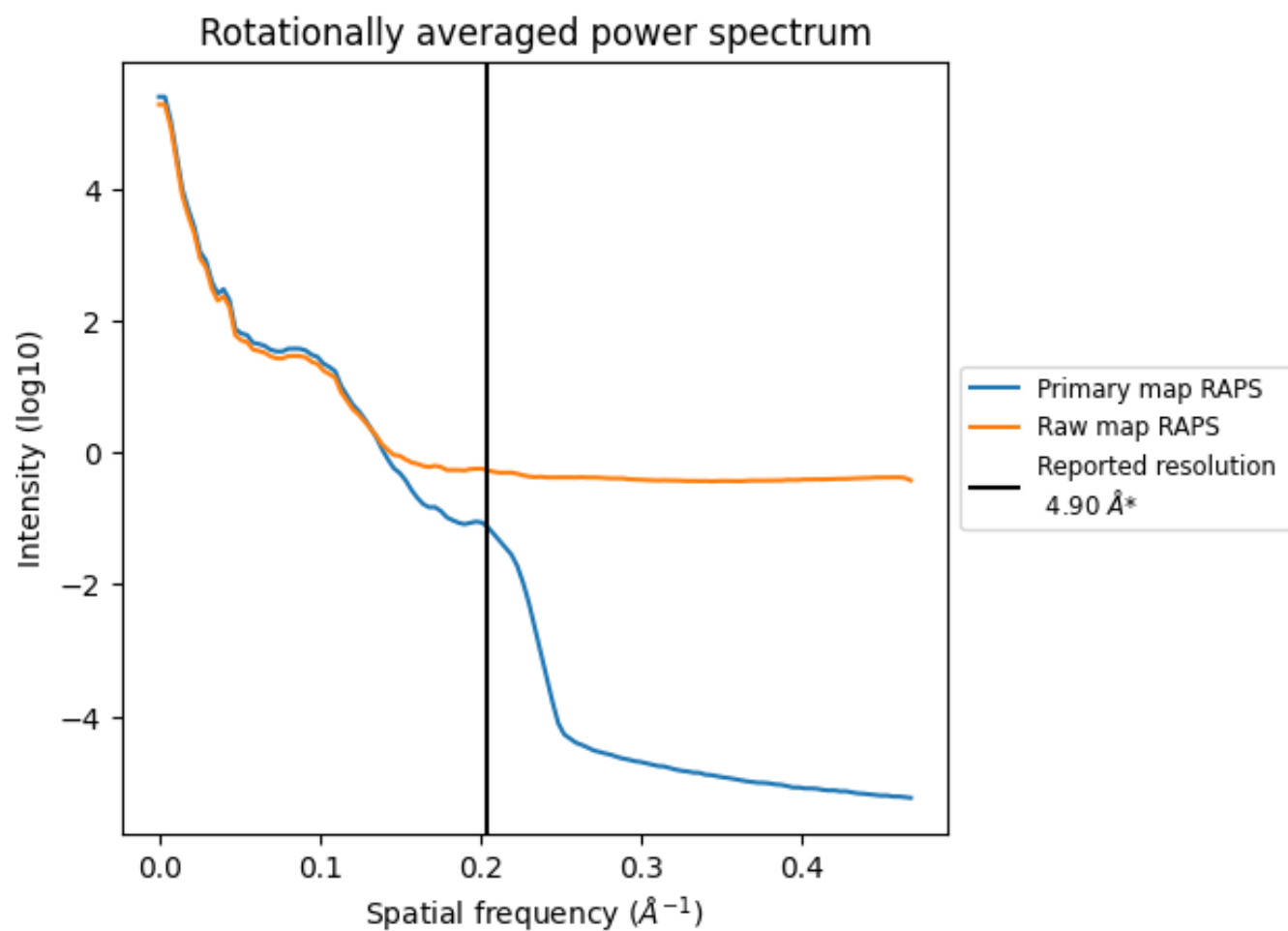
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 201 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](#)

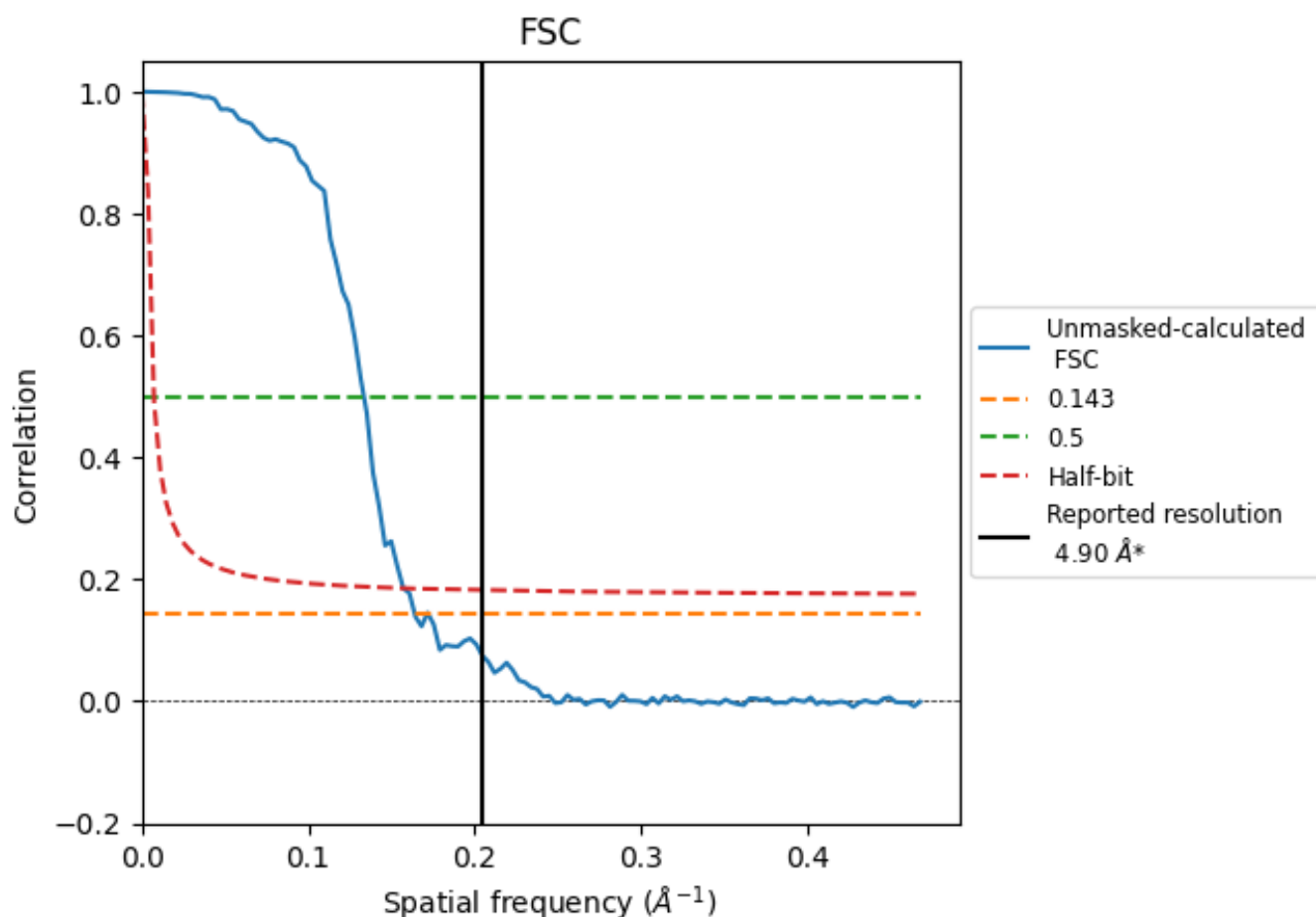


*Reported resolution corresponds to spatial frequency of 0.204 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.204 \AA^{-1}

8.2 Resolution estimates [i](#)

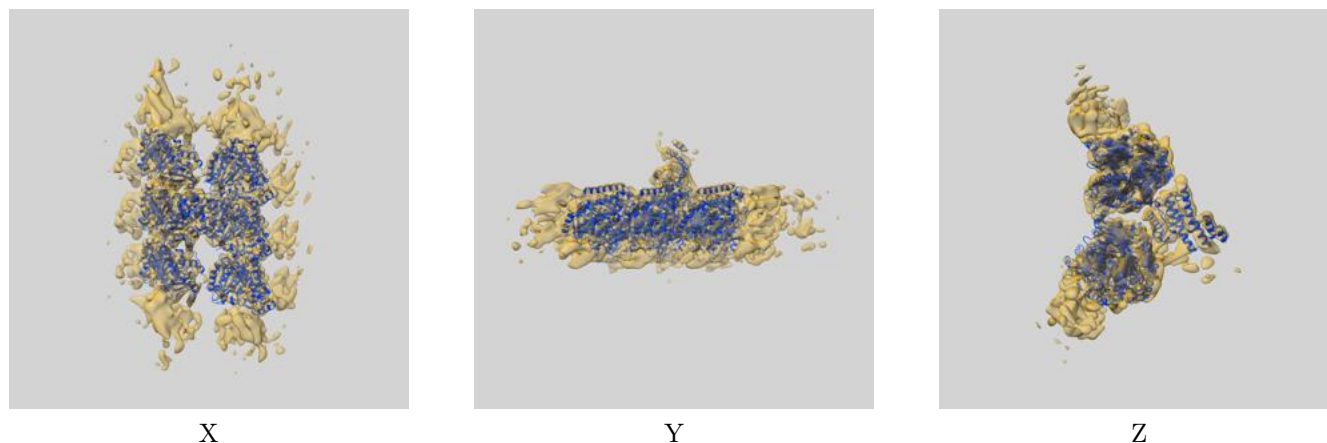
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.10	7.50	6.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.10 differs from the reported value 4.9 by more than 10 %

9 Map-model fit [i](#)

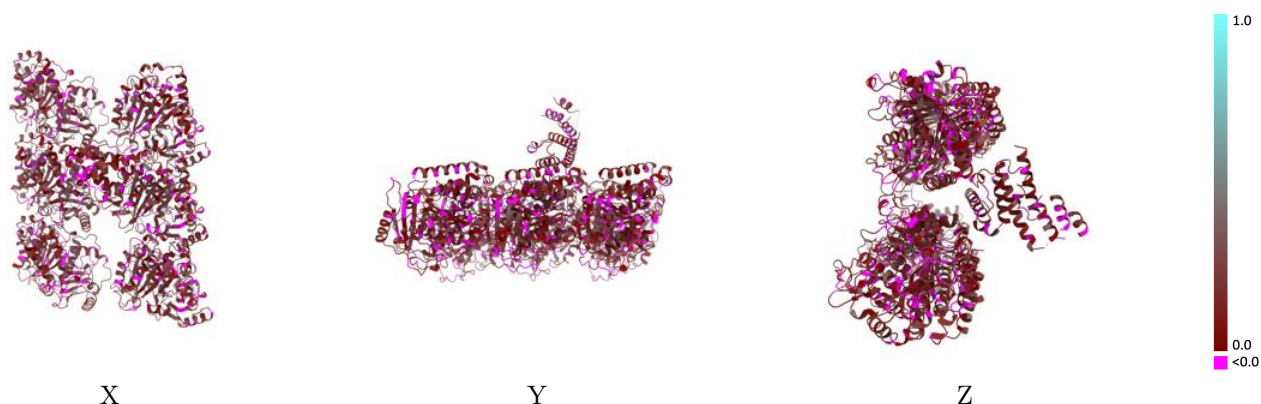
This section contains information regarding the fit between EMDB map EMD-54161 and PDB model 9RPD. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



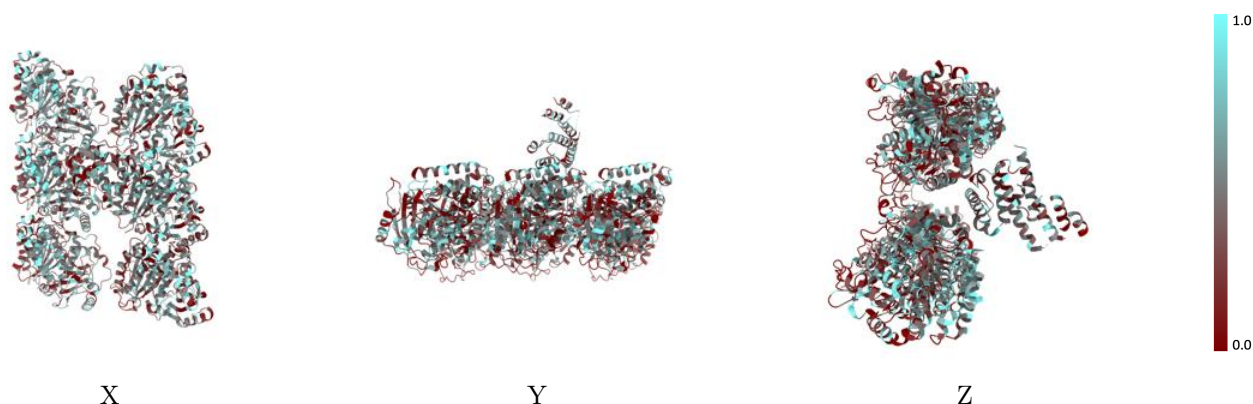
The images above show the 3D surface view of the map at the recommended contour level 0.00846 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



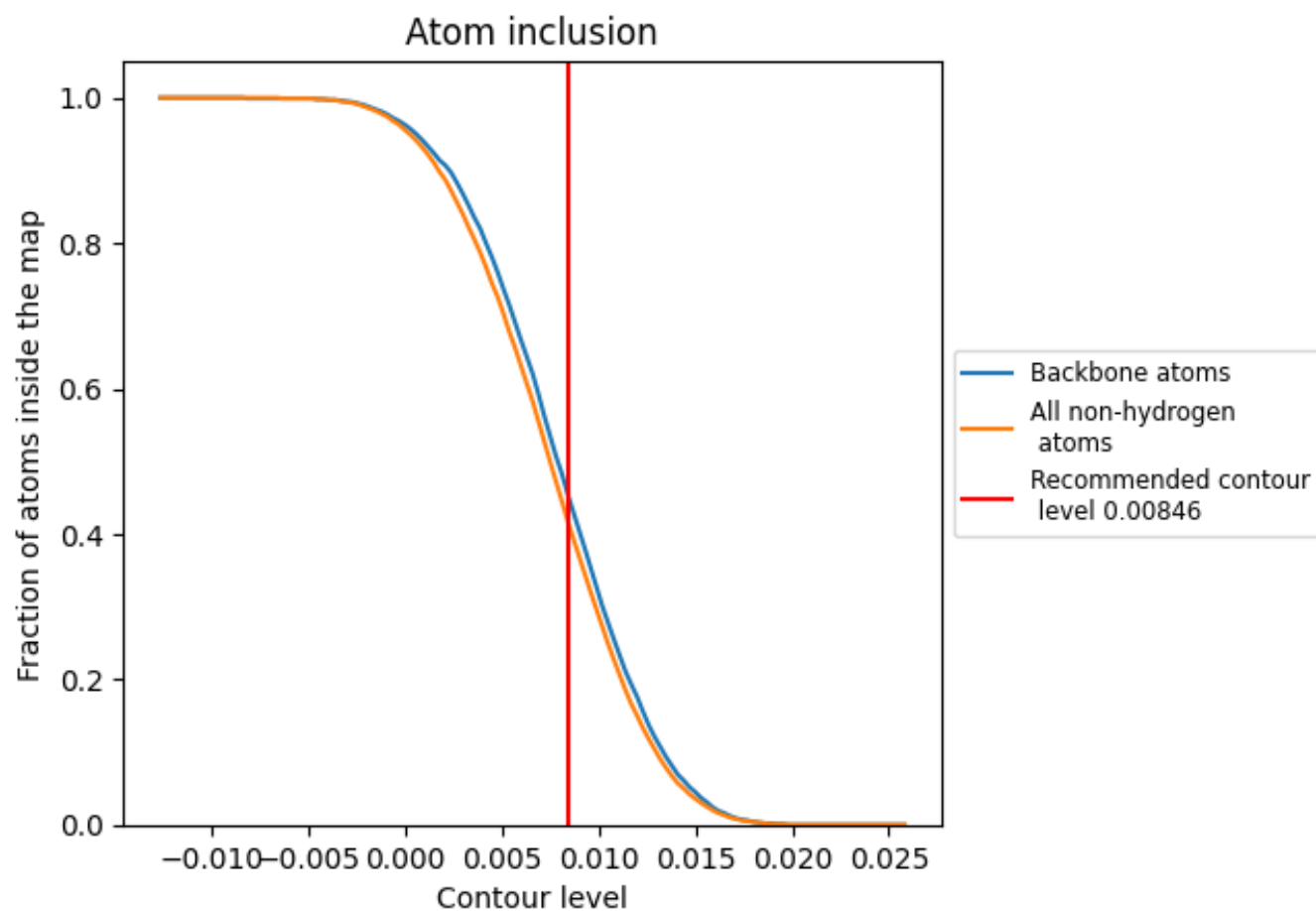
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00846).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 41% 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 (0.00846) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.4140</div>	<div><div></div>0.1260</div>
A	<div><div></div>0.4270</div>	<div><div></div>0.1300</div>
B	<div><div></div>0.4150</div>	<div><div></div>0.1300</div>
C	<div><div></div>0.4090</div>	<div><div></div>0.1320</div>
D	<div><div></div>0.4260</div>	<div><div></div>0.1340</div>
E	<div><div></div>0.4050</div>	<div><div></div>0.1080</div>
G	<div><div></div>0.3970</div>	<div><div></div>0.1250</div>
I	<div><div></div>0.4260</div>	<div><div></div>0.1030</div>
J	<div><div></div>0.4460</div>	<div><div></div>0.1210</div>
K	<div><div></div>0.3010</div>	<div><div></div>0.0510</div>

1.0

0.0

<0.0