



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 06:48 PM JST

PDB ID : 8KEV
EMDB ID : EMD-37168
Title : Cryo-EM structure of human complex C
Authors : Qian, H.W.; He, J.J.
Deposited on : 2023-08-13
Resolution : 3.50 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

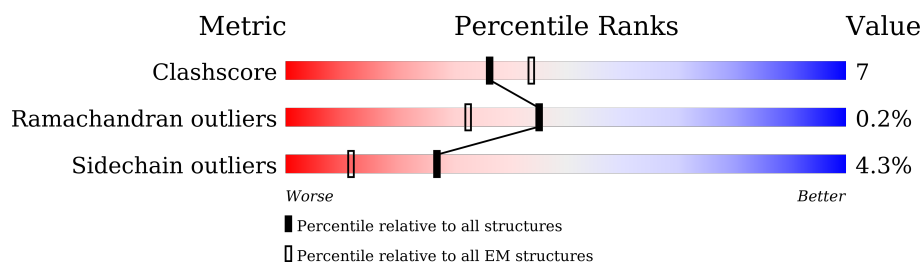
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	C	794	
1	D	794	
2	G	3	
2	H	3	
3	E	483	
3	F	483	
4	A	617	
4	B	617	

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Mol	Chain	Length	Quality of chain
5	I	7	<div><div></div><div>29%</div><div>71%</div><div>29%</div></div>
5	J	7	<div><div></div><div>29%</div><div>14%</div><div>57%</div><div>29%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12831 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 Protein sel-1 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	438	Total	C	N	O	S	1	0
			3267	2072	576	606	13		
1	C	436	Total	C	N	O	S	1	0
			3276	2085	574	603	14		

- Molecule 2 is a protein called Ala-Asn-Ala.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	3	Total	C	N	O	0	0
			18	10	4	4		
2	H	3	Total	C	N	O	0	0
			18	10	4	4		

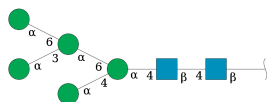
- Molecule 3 is a protein called Endoplasmic reticulum lectin 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	232	Total	C	N	O	S	0	0
			1745	1105	301	326	13		
3	F	231	Total	C	N	O	S	0	0
			1407	870	256	273	8		

- Molecule 4 is a protein called E3 ubiquitin-protein ligase synoviolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			1427	873	274	279	1		
4	B	266	Total	C	N	O	S	0	0
			1423	871	273	278	1		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



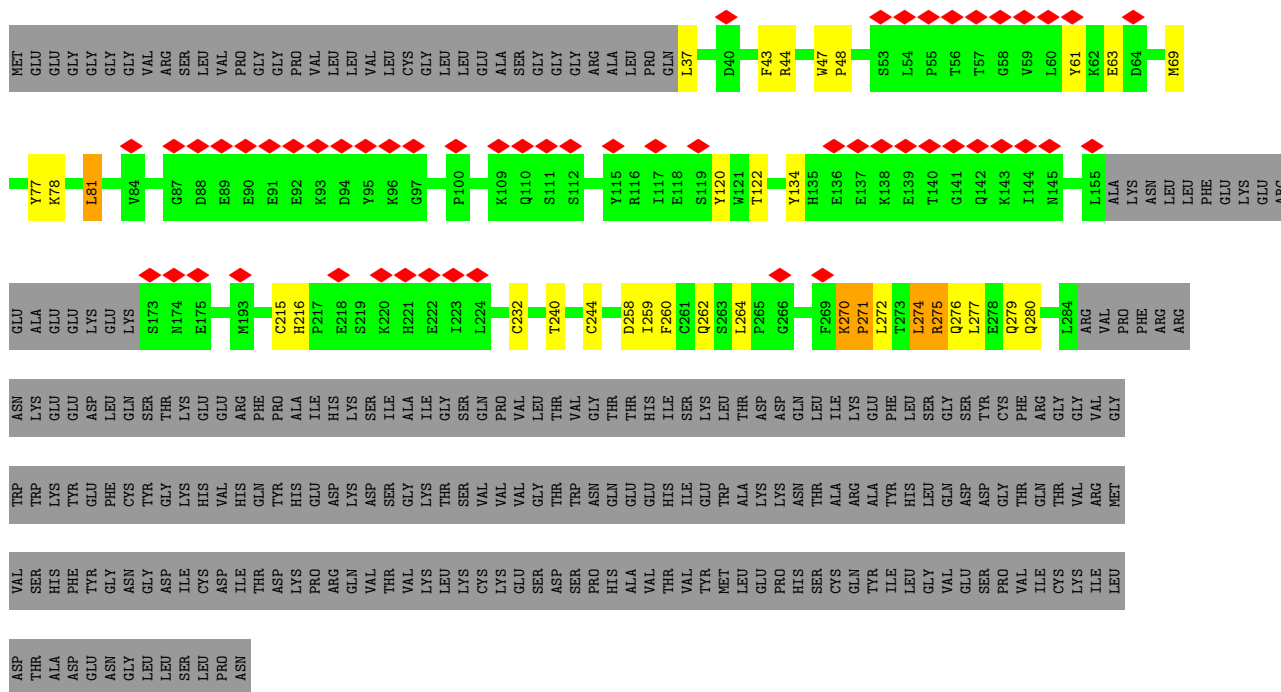
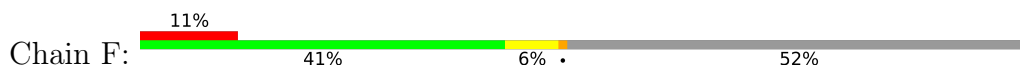
Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	7	Total	C	N	O	0	0
			83	46	2	35		
5	J	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

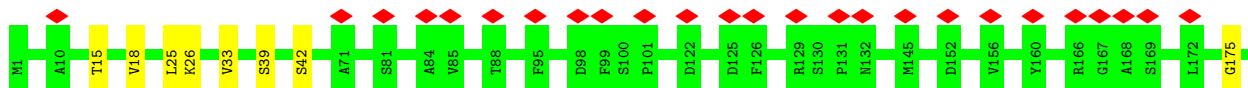


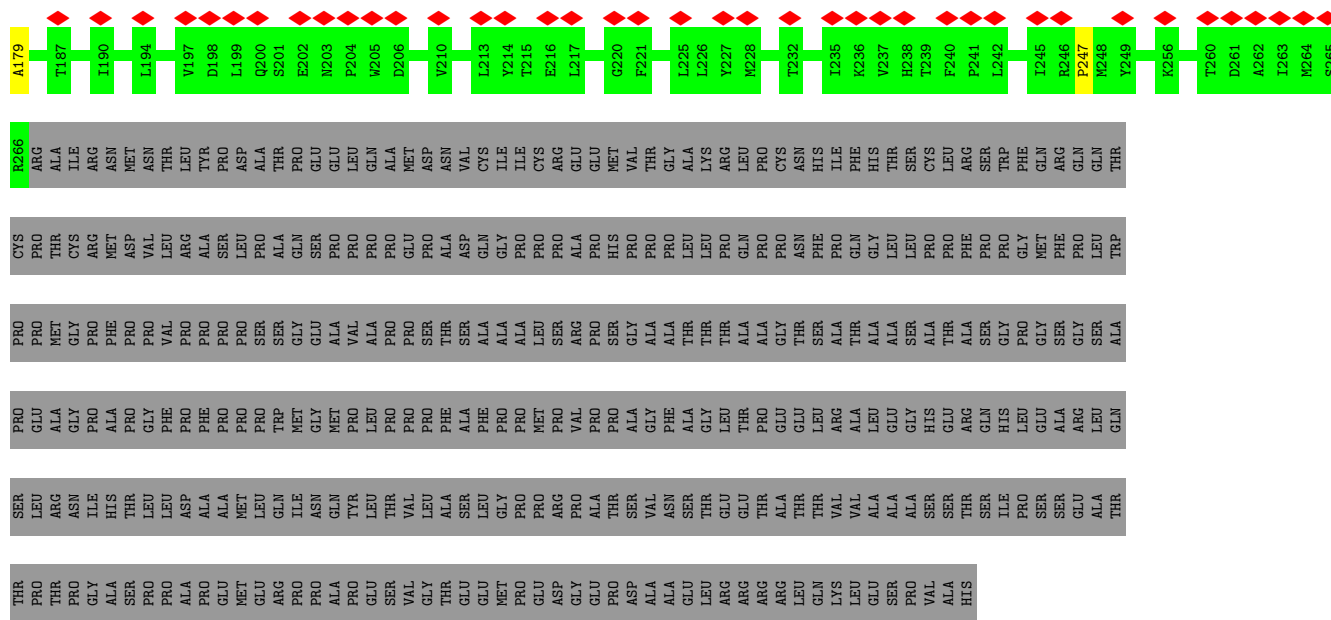
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3: Endoplasmic reticulum lectin 1

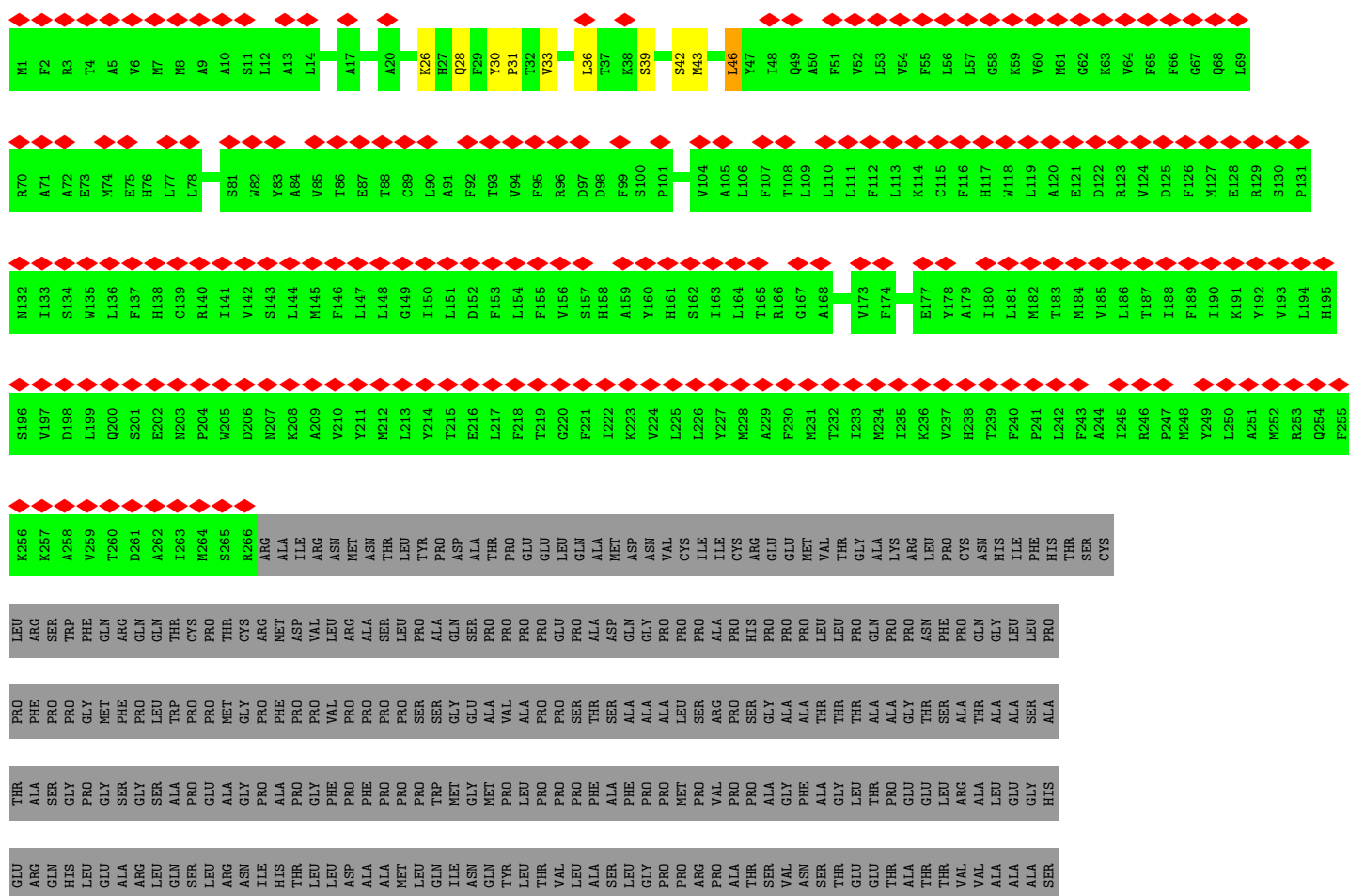


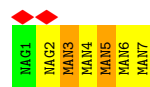
- Molecule 4: E3 ubiquitin-protein ligase synoviolin





• Molecule 4: E3 ubiquitin-protein ligase synoviolin



ALA
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.484	Depositor
Minimum map value	-0.991	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.109	Depositor
Map size (\AA)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.32	0/3349	0.71	7/4537 (0.2%)
1	D	0.31	0/3336	0.62	3/4518 (0.1%)
2	G	0.25	0/17	0.37	0/22
2	H	0.24	0/17	0.31	0/22
3	E	0.36	1/1788 (0.1%)	0.78	5/2437 (0.2%)
3	F	0.34	0/1425	0.81	5/1961 (0.3%)
4	A	0.25	0/1436	0.46	1/1997 (0.1%)
4	B	0.25	0/1432	0.48	1/1992 (0.1%)
All	All	0.31	1/12800 (0.0%)	0.66	22/17486 (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	D	0	2
3	E	0	1
4	A	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	198	PRO	CG-CD	-6.26	1.29	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	198	PRO	CA-N-CD	-12.33	94.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	271	PRO	CA-N-CD	-10.45	96.87	111.50
3	E	198	PRO	N-CD-CG	-8.80	90.00	103.20
1	C	469	LEU	CA-CB-CG	7.56	132.69	115.30
3	F	48	PRO	CA-N-CD	-7.56	100.92	111.50
3	F	274	LEU	CA-CB-CG	7.36	132.23	115.30
1	C	329	ILE	CG1-CB-CG2	-6.63	96.81	111.40
3	F	264	LEU	CA-CB-CG	6.39	129.99	115.30
4	B	46	LEU	CA-CB-CG	6.29	129.77	115.30
4	A	25	LEU	CA-CB-CG	6.26	129.71	115.30
1	C	233	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	692	ASP	CB-CG-OD1	5.91	123.62	118.30
3	E	185	MET	CB-CG-SD	5.66	129.39	112.40
1	C	670	LEU	CA-CB-CG	5.54	128.05	115.30
3	F	275	ARG	CA-CB-CG	5.52	125.55	113.40
3	E	244	CYS	CA-CB-SG	5.44	123.79	114.00
1	C	696	GLU	CA-CB-CG	5.39	125.25	113.40
1	D	311	CYS	CA-CB-SG	5.17	123.32	114.00
3	E	198	PRO	CA-CB-CG	-5.09	94.33	104.00
1	D	700	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	469	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	686	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	247	PRO	Peptide
1	D	544	GLU	Mainchain
1	D	590	GLN	Mainchain
3	E	244	CYS	Peptide

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	C	3276	0	3056	72	0
1	D	3267	0	3039	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	18	0	14	0	0
2	H	18	0	14	0	0
3	E	1745	0	1571	33	0
3	F	1407	0	953	22	0
4	A	1427	0	807	4	0
4	B	1423	0	801	6	0
5	I	83	0	70	3	0
5	J	83	0	70	3	0
6	C	42	0	39	0	0
6	D	42	0	39	0	0
All	All	12831	0	10473	174	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 7.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ILE:HD11	1:C:516:GLY:HA2	1.61	0.81
1:C:686:LEU:HD23	1:C:689:ARG:HH12	1.49	0.76
4:A:39:SER:HG	4:A:42:SER:HG	1.32	0.75
3:E:132:ARG:HH12	3:E:148:GLU:HB3	1.52	0.73
1:C:224:ARG:O	1:C:224:ARG:NH1	2.22	0.69
1:D:499:VAL:HG12	1:C:480:GLN:HE22	1.58	0.69
3:E:125:VAL:HG23	3:E:131:ILE:HG12	1.74	0.68
1:C:477:ALA:O	1:C:480:GLN:NE2	2.26	0.68
3:E:133:GLN:HB2	3:E:151:LEU:HD11	1.77	0.66
4:B:39:SER:HG	4:B:42:SER:HG	1.39	0.65
3:E:275:ARG:O	3:E:279:GLN:NE2	2.29	0.64
1:C:473:TYR:HA	1:C:476:LYS:HG2	1.80	0.64
1:D:223:GLU:OE2	1:D:254:SER:OG	2.16	0.63
3:E:78:LYS:O	3:E:262:GLN:N	2.31	0.63
1:C:339:ARG:HH22	1:C:552:ARG:HA	1.63	0.63
1:D:269:LEU:HD21	1:D:576:ILE:HD12	1.79	0.63
1:D:231:PHE:O	1:D:577:GLN:NE2	2.33	0.62
1:D:586:TYR:O	1:D:590:GLN:NE2	2.33	0.61
1:C:246:PHE:HB3	1:C:261:LEU:HD22	1.83	0.61
3:F:215:CYS:SG	3:F:216:HIS:N	2.74	0.60
3:E:45:VAL:HA	3:E:259:ILE:HG22	1.84	0.60
1:D:536:MET:SD	1:D:536:MET:N	2.74	0.59
3:F:120:TYR:HE2	5:J:3:MAN:H62	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:LEU:HD22	3:E:259:ILE:HD11	1.84	0.59
3:E:194:GLY:HA2	3:E:208:SER:HA	1.85	0.57
1:D:339:ARG:HB3	1:D:588:VAL:HG21	1.88	0.56
1:C:639:TYR:OH	4:B:28:GLN:OE1	2.23	0.56
1:D:684:ILE:HG23	1:D:712:LEU:HD11	1.87	0.56
3:E:79:CYS:HA	3:E:261:CYS:HA	1.87	0.56
1:C:519:ILE:HG23	1:C:549:VAL:HG22	1.87	0.56
3:F:270:LYS:HE3	3:F:275:ARG:NE	2.20	0.55
1:C:282:TYR:HB3	1:C:297:LEU:HD21	1.89	0.55
1:C:664:ALA:HA	1:C:667:MET:HG2	1.89	0.55
1:D:332:THR:OG1	1:D:554:ARG:NH2	2.39	0.55
1:D:526:ALA:HB2	1:D:545:LEU:HB2	1.88	0.55
1:C:231:PHE:HZ	1:C:580:LEU:HD22	1.71	0.55
1:D:704:PRO:HG3	4:A:33:VAL:HB	1.88	0.55
3:E:66:TYR:HB2	3:E:78:LYS:NZ	2.22	0.54
1:C:501:ARG:O	1:C:505:GLN:HG3	2.07	0.54
3:F:270:LYS:HE3	3:F:275:ARG:HE	1.72	0.54
1:C:686:LEU:HA	1:C:689:ARG:NH1	2.22	0.54
1:C:655:ARG:O	1:C:658:SER:N	2.40	0.54
1:C:214:ALA:HB1	1:C:222:LEU:HD23	1.90	0.54
1:C:337:VAL:HG23	1:C:560:MET:HG2	1.90	0.54
3:F:81:LEU:HB3	3:F:259:ILE:HD12	1.89	0.53
3:F:275:ARG:O	3:F:279:GLN:HG2	2.07	0.53
4:A:15:THR:HA	4:A:18:VAL:HG12	1.89	0.53
1:D:578:TYR:HB3	1:D:593:ALA:HB2	1.89	0.53
1:D:329:ILE:HD12	1:D:519:ILE:HD11	1.89	0.53
1:C:323:ASN:ND2	1:C:523:TYR:OH	2.40	0.53
3:F:78:LYS:HG2	3:F:262:GLN:HB3	1.90	0.53
1:D:498:GLY:HA2	1:D:501:ARG:HH22	1.74	0.53
1:D:515:GLN:HE21	1:D:552:ARG:HD3	1.74	0.53
1:C:497:ILE:HG22	1:C:501:ARG:HG3	1.90	0.52
3:E:62:LYS:HD3	3:E:64:ASP:HB3	1.91	0.52
4:B:26:LYS:HD2	4:B:31:PRO:HB2	1.91	0.52
1:D:248:LYS:HA	1:D:251:GLU:HG3	1.92	0.52
1:C:465:VAL:O	1:C:469:LEU:HD12	2.09	0.52
1:C:580:LEU:O	1:C:584:GLN:HB2	2.10	0.52
3:E:125:VAL:HA	3:E:131:ILE:HG23	1.91	0.51
1:C:286:ALA:HB1	1:C:294:HIS:CE1	2.45	0.51
1:C:341:ARG:NH2	1:C:587:GLU:OE1	2.39	0.51
1:C:568:ASP:N	1:C:568:ASP:OD1	2.43	0.51
3:E:205:ARG:HD2	3:E:206:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ALA:HB2	1:C:705:VAL:HG21	1.92	0.51
1:D:559:LEU:HD13	1:D:581:LEU:HD13	1.93	0.51
1:C:616:LEU:HD11	3:F:37:LEU:HB2	1.92	0.51
1:C:516:GLY:O	1:C:520:LEU:HD22	2.12	0.50
3:F:63:GLU:N	3:F:63:GLU:OE1	2.45	0.50
1:D:695:ALA:HB2	1:D:705:VAL:HG11	1.95	0.49
3:E:130:HIS:HE2	3:E:132:ARG:HB2	1.76	0.49
1:C:313:SER:HA	1:C:316:THR:HG22	1.93	0.49
1:C:644:ASP:OD1	1:C:644:ASP:N	2.40	0.49
1:D:217:ASN:N	1:D:217:ASN:OD1	2.45	0.49
1:D:246:PHE:O	1:D:250:THR:HG23	2.13	0.48
1:C:548:ASN:OD1	1:C:552:ARG:NH2	2.45	0.48
1:C:325:VAL:O	1:C:329:ILE:HG22	2.12	0.48
3:E:130:HIS:NE2	3:E:132:ARG:HB2	2.29	0.48
1:C:536:MET:SD	1:C:536:MET:N	2.81	0.48
1:C:295:MET:HG2	1:C:584:GLN:HG2	1.95	0.48
1:C:556:SER:O	1:C:556:SER:OG	2.26	0.48
3:E:49:GLY:HA2	3:E:269:PHE:HB2	1.96	0.48
1:C:630:ARG:HB3	1:C:657:ALA:HB2	1.96	0.48
1:D:461:ARG:O	1:D:465:VAL:HG13	2.14	0.47
1:D:337:VAL:HG11	1:D:556:SER:HB2	1.95	0.47
1:C:328:ASP:OD1	1:C:332:THR:OG1	2.26	0.47
1:D:219:THR:HA	1:D:222:LEU:HB2	1.95	0.47
1:C:686:LEU:HD23	1:C:689:ARG:NH1	2.24	0.47
3:E:62:LYS:NZ	3:E:65:ASN:HB3	2.30	0.47
1:C:245:MET:HA	1:C:248:LYS:HZ3	1.80	0.46
1:C:284:PHE:HE2	3:F:69:MET:HB3	1.80	0.46
1:C:337:VAL:HG11	1:C:556:SER:HG	1.80	0.46
3:E:246:HIS:CD2	3:E:247:PRO:HD2	2.51	0.46
3:F:215:CYS:HB3	3:F:244:CYS:HB3	1.77	0.46
1:C:276:ALA:O	1:C:280:VAL:HG13	2.16	0.46
1:C:689:ARG:HB3	5:J:5:MAN:H61	1.97	0.46
1:D:276:ALA:HB1	3:E:259:ILE:HD12	1.98	0.46
4:B:36:LEU:O	4:B:43:MET:HB3	2.16	0.46
3:E:60:LEU:HB3	3:E:83:LEU:HD12	1.97	0.45
1:D:476:LYS:HA	1:D:479:GLU:HG2	1.97	0.45
1:C:608:ASN:OD1	1:C:608:ASN:N	2.50	0.45
5:I:4:MAN:H3	5:I:5:MAN:H2	1.78	0.45
1:D:264:LEU:HD22	1:D:269:LEU:HB3	1.97	0.45
1:C:307:VAL:HG12	3:F:43:PHE:O	2.17	0.45
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:66:TYR:HB2	3:E:78:LYS:HZ1	1.79	0.45
3:E:176:ILE:HG12	3:E:249:TYR:HE1	1.82	0.44
1:C:282:TYR:CZ	1:C:296:VAL:HG11	2.51	0.44
1:C:500:LYS:HA	1:C:503:TYR:HB2	1.97	0.44
3:F:47:TRP:CG	3:F:270:LYS:HB2	2.52	0.44
1:D:635:ASP:OD1	1:D:654:TYR:OH	2.20	0.44
1:D:473:TYR:HB3	1:C:506:ALA:HB2	1.99	0.44
3:F:272:LEU:O	3:F:275:ARG:HG2	2.17	0.44
1:C:559:LEU:HG	1:C:581:LEU:HD13	1.98	0.44
1:D:467:TYR:O	1:D:471:LEU:HG	2.17	0.44
1:D:498:GLY:HA2	1:D:501:ARG:NH2	2.33	0.44
1:C:558:ARG:HB3	1:C:581:LEU:HD11	2.00	0.44
1:C:631:ILE:HD12	1:C:631:ILE:H	1.83	0.44
1:D:513:ALA:HB1	1:C:467:TYR:CD2	2.53	0.43
1:D:669:ASN:O	1:D:673:MET:HG3	2.18	0.43
3:E:68:ILE:HD12	3:E:68:ILE:HA	1.91	0.43
1:C:502:ASP:OD1	1:C:502:ASP:N	2.40	0.43
1:C:526:ALA:HB1	1:C:546:PHE:CD1	2.53	0.43
3:F:122:THR:OG1	3:F:134:TYR:O	2.32	0.43
1:D:282:TYR:CZ	1:D:296:VAL:HG11	2.53	0.43
3:F:120:TYR:CE2	5:J:3:MAN:H62	2.48	0.43
1:D:538:SER:O	1:D:540:HIS:N	2.47	0.42
1:C:544:GLU:OE1	1:C:544:GLU:N	2.44	0.42
1:C:660:GLN:HB2	1:C:661:GLN:OE1	2.20	0.42
1:D:254:SER:O	1:D:258:GLN:NE2	2.52	0.42
1:C:604:ILE:H	1:C:604:ILE:HD12	1.84	0.42
1:C:674:HIS:CE1	1:C:680:ILE:HD11	2.54	0.42
1:C:511:ASN:O	1:C:515:GLN:HG2	2.20	0.42
5:I:1:NAG:H4	5:I:2:NAG:C7	2.49	0.42
1:C:684:ILE:HG23	1:C:712:LEU:HD11	2.00	0.42
1:C:561:THR:O	1:C:565:SER:OG	2.35	0.42
1:C:652:ILE:O	1:C:656:LEU:HG	2.20	0.42
1:D:207:TYR:HA	1:D:210:LEU:HD12	2.01	0.42
1:D:640:GLY:HA3	1:D:645:VAL:HG22	2.02	0.41
3:E:65:ASN:O	3:E:81:LEU:HG	2.20	0.41
1:C:217:ASN:OD1	1:C:217:ASN:N	2.53	0.41
3:E:247:PRO:HA	3:E:250:ARG:NH1	2.35	0.41
3:E:263:SER:OG	3:E:268:PRO:O	2.32	0.41
1:C:340:ILE:HD12	1:C:340:ILE:HA	1.81	0.41
3:E:76:LYS:HB3	3:E:264:LEU:HD12	2.02	0.41
1:C:296:VAL:HG22	1:C:584:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:33:VAL:HA	4:B:36:LEU:HG	2.02	0.41
3:F:215:CYS:HA	3:F:240:THR:O	2.19	0.41
1:D:515:GLN:O	1:D:519:ILE:HG23	2.21	0.41
3:E:121:TRP:HZ2	5:I:4:MAN:H62	1.86	0.41
1:D:520:LEU:O	1:D:524:ASN:ND2	2.48	0.41
3:E:71:THR:OG1	3:E:72:ALA:N	2.54	0.41
4:A:175:GLY:O	4:A:179:ALA:N	2.49	0.41
1:C:319:ARG:O	1:C:323:ASN:OD1	2.38	0.41
1:C:665:GLN:HE21	4:B:30:TYR:HB3	1.86	0.41
1:D:243:ARG:HE	1:D:271:VAL:HG22	1.85	0.41
1:D:248:LYS:HE2	1:D:248:LYS:HB2	1.90	0.41
3:E:68:ILE:HD11	3:E:264:LEU:HD11	2.03	0.41
3:E:150:TYR:O	3:E:197:THR:HG22	2.21	0.41
3:E:209:SER:OG	3:E:234:TYR:HB2	2.21	0.41
1:C:596:ILE:HD13	1:C:596:ILE:HA	1.85	0.41
3:F:274:LEU:HA	3:F:277:LEU:HB3	2.02	0.41
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.94	0.41
1:C:245:MET:HA	1:C:248:LYS:NZ	2.35	0.41
1:C:693:MET:HA	1:C:696:GLU:OE1	2.20	0.41
3:F:61:TYR:OH	3:F:258:ASP:O	2.26	0.41
3:F:276:GLN:O	3:F:280:GLN:N	2.50	0.41
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.75	0.40
3:E:246:HIS:CE1	3:E:248:LYS:H	2.39	0.40
3:F:77:TYR:CZ	3:F:271:PRO:HD3	2.56	0.40
1:D:339:ARG:HH21	1:D:552:ARG:HA	1.86	0.40
1:D:667:MET:HB3	1:D:694:ALA:HB2	2.04	0.40
1:C:243:ARG:O	1:C:247:GLU:HG2	2.22	0.40
3:F:270:LYS:HZ3	3:F:274:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	433/794 (54%)	404 (93%)	29 (7%)	0	100	100
1	D	435/794 (55%)	412 (95%)	19 (4%)	4 (1%)	14	49
2	G	1/3 (33%)	1 (100%)	0	0	100	100
2	H	1/3 (33%)	1 (100%)	0	0	100	100
3	E	228/483 (47%)	217 (95%)	11 (5%)	0	100	100
3	F	227/483 (47%)	214 (94%)	13 (6%)	0	100	100
4	A	264/617 (43%)	255 (97%)	9 (3%)	0	100	100
4	B	264/617 (43%)	260 (98%)	4 (2%)	0	100	100
All	All	1853/3794 (49%)	1764 (95%)	85 (5%)	4 (0%)	45	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	552	ARG
1	D	539	CYS
1	D	483	VAL
1	D	492	MET

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	C	301/649 (46%)	284 (94%)	17 (6%)	17	45
1	D	299/649 (46%)	292 (98%)	7 (2%)	45	69
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
3	E	174/433 (40%)	166 (95%)	8 (5%)	23	52
3	F	79/433 (18%)	74 (94%)	5 (6%)	15	42
4	A	30/519 (6%)	29 (97%)	1 (3%)	33	61
4	B	29/519 (6%)	28 (97%)	1 (3%)	32	60
All	All	914/3204 (28%)	875 (96%)	39 (4%)	27	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	217	ASN
1	D	504	LYS
1	D	523	TYR
1	D	536	MET
1	D	568	ASP
1	D	578	TYR
1	D	587	GLU
3	E	62	LYS
3	E	118	GLU
3	E	150	TYR
3	E	154	MET
3	E	208	SER
3	E	212	MET
3	E	232	CYS
3	E	248	LYS
1	C	217	ASN
1	C	220	LYS
1	C	227	TYR
1	C	234	TYR
1	C	246	PHE
1	C	267	SER
1	C	282	TYR
1	C	330	SER
1	C	338	GLN
1	C	342	LEU
1	C	461	ARG
1	C	468	ASP
1	C	469	LEU
1	C	536	MET
1	C	556	SER
1	C	668	PHE
1	C	688	LYS
3	F	44	ARG
3	F	81	LEU
3	F	232	CYS
3	F	260	PHE
3	F	270	LYS
4	A	26	LYS
4	B	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	515	GLN
1	C	338	GLN
1	C	480	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	I	1	2,5	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	I	2	5	14,14,15	0.57	0	17,19,21	0.64	0
5	MAN	I	3	5	11,11,12	1.46	3 (27%)	15,15,17	1.77	5 (33%)
5	MAN	I	4	5	11,11,12	0.97	1 (9%)	15,15,17	1.32	3 (20%)
5	MAN	I	5	5	11,11,12	1.21	2 (18%)	15,15,17	1.44	2 (13%)
5	MAN	I	6	5	11,11,12	0.88	0	15,15,17	1.24	2 (13%)
5	MAN	I	7	5	11,11,12	0.78	0	15,15,17	0.96	2 (13%)
5	NAG	J	1	2,5	14,14,15	0.24	0	17,19,21	0.65	0
5	NAG	J	2	5	14,14,15	0.59	1 (7%)	17,19,21	0.63	0
5	MAN	J	3	5	11,11,12	1.34	1 (9%)	15,15,17	1.91	2 (13%)
5	MAN	J	4	5	11,11,12	0.80	0	15,15,17	1.46	2 (13%)
5	MAN	J	5	5	11,11,12	0.83	0	15,15,17	1.03	2 (13%)
5	MAN	J	6	5	11,11,12	1.07	1 (9%)	15,15,17	1.47	2 (13%)
5	MAN	J	7	5	11,11,12	0.67	0	15,15,17	0.92	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	MAN	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	1/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	0/1/1/1
5	MAN	I	6	5	-	1/2/19/22	1/1/1/1
5	MAN	I	7	5	-	1/2/19/22	0/1/1/1
5	NAG	J	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	MAN	J	3	5	-	1/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	1/1/1/1
5	MAN	J	6	5	-	1/2/19/22	1/1/1/1
5	MAN	J	7	5	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	3	MAN	O5-C5	4.06	1.51	1.43
5	I	3	MAN	C4-C5	2.96	1.59	1.53
5	I	5	MAN	C1-C2	2.74	1.58	1.52
5	I	4	MAN	C1-C2	2.65	1.58	1.52
5	I	3	MAN	O5-C5	2.64	1.48	1.43
5	J	6	MAN	C1-C2	2.12	1.57	1.52
5	I	3	MAN	C4-C3	2.10	1.57	1.52
5	I	5	MAN	C2-C3	2.09	1.55	1.52
5	J	2	NAG	C1-C2	2.01	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	MAN	C1-O5-C5	6.12	120.48	112.19
5	J	6	MAN	C1-O5-C5	4.50	118.28	112.19
5	I	5	MAN	C1-O5-C5	4.02	117.64	112.19
5	I	3	MAN	C1-O5-C5	3.99	117.60	112.19
5	J	4	MAN	C1-O5-C5	3.97	117.56	112.19
5	I	6	MAN	C1-O5-C5	3.58	117.05	112.19
5	I	3	MAN	C3-C4-C5	3.42	116.33	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	4	MAN	C1-O5-C5	2.94	116.17	112.19
5	J	5	MAN	C1-O5-C5	2.71	115.87	112.19
5	J	4	MAN	O2-C2-C3	-2.58	104.96	110.14
5	I	4	MAN	C1-C2-C3	2.49	112.72	109.67
5	J	3	MAN	O5-C5-C6	2.48	111.09	107.20
5	I	3	MAN	C2-C3-C4	2.36	114.98	110.89
5	I	3	MAN	O2-C2-C3	-2.29	105.54	110.14
5	J	7	MAN	O2-C2-C3	-2.29	105.56	110.14
5	J	6	MAN	O2-C2-C3	-2.28	105.56	110.14
5	I	7	MAN	O2-C2-C3	-2.28	105.58	110.14
5	I	6	MAN	O2-C2-C3	-2.25	105.62	110.14
5	I	3	MAN	O5-C5-C4	2.25	116.31	110.83
5	I	4	MAN	O2-C2-C3	-2.24	105.65	110.14
5	I	7	MAN	C1-O5-C5	2.11	115.05	112.19
5	J	7	MAN	C1-O5-C5	2.09	115.03	112.19
5	J	5	MAN	O2-C2-C3	-2.09	105.95	110.14
5	I	5	MAN	O2-C2-C3	-2.09	105.96	110.14

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	4	MAN	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	4	MAN	C4-C5-C6-O6
5	I	6	MAN	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	6	MAN	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
5	I	7	MAN	O5-C5-C6-O6
5	J	3	MAN	O5-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6

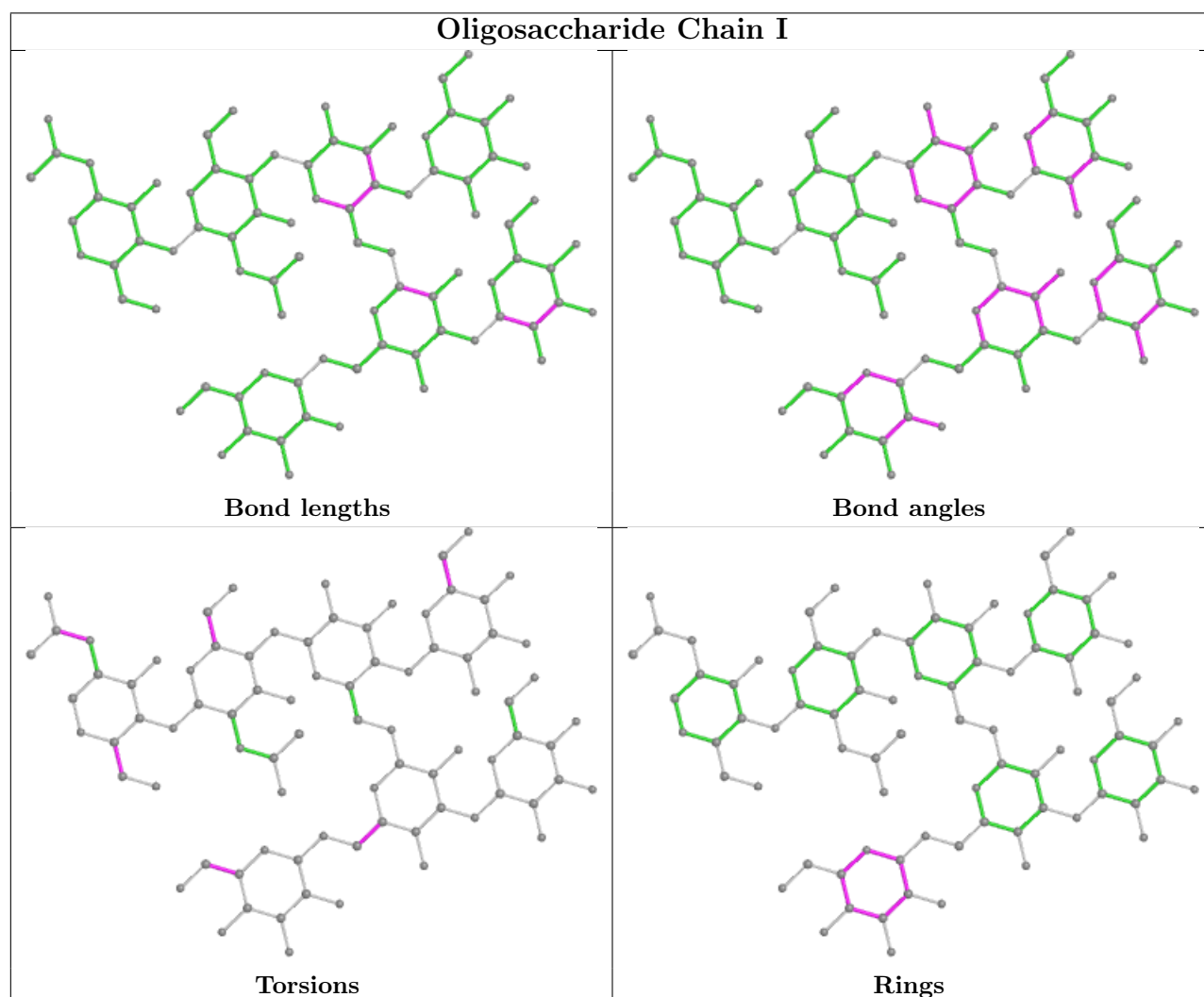
All (3) ring outliers are listed below:

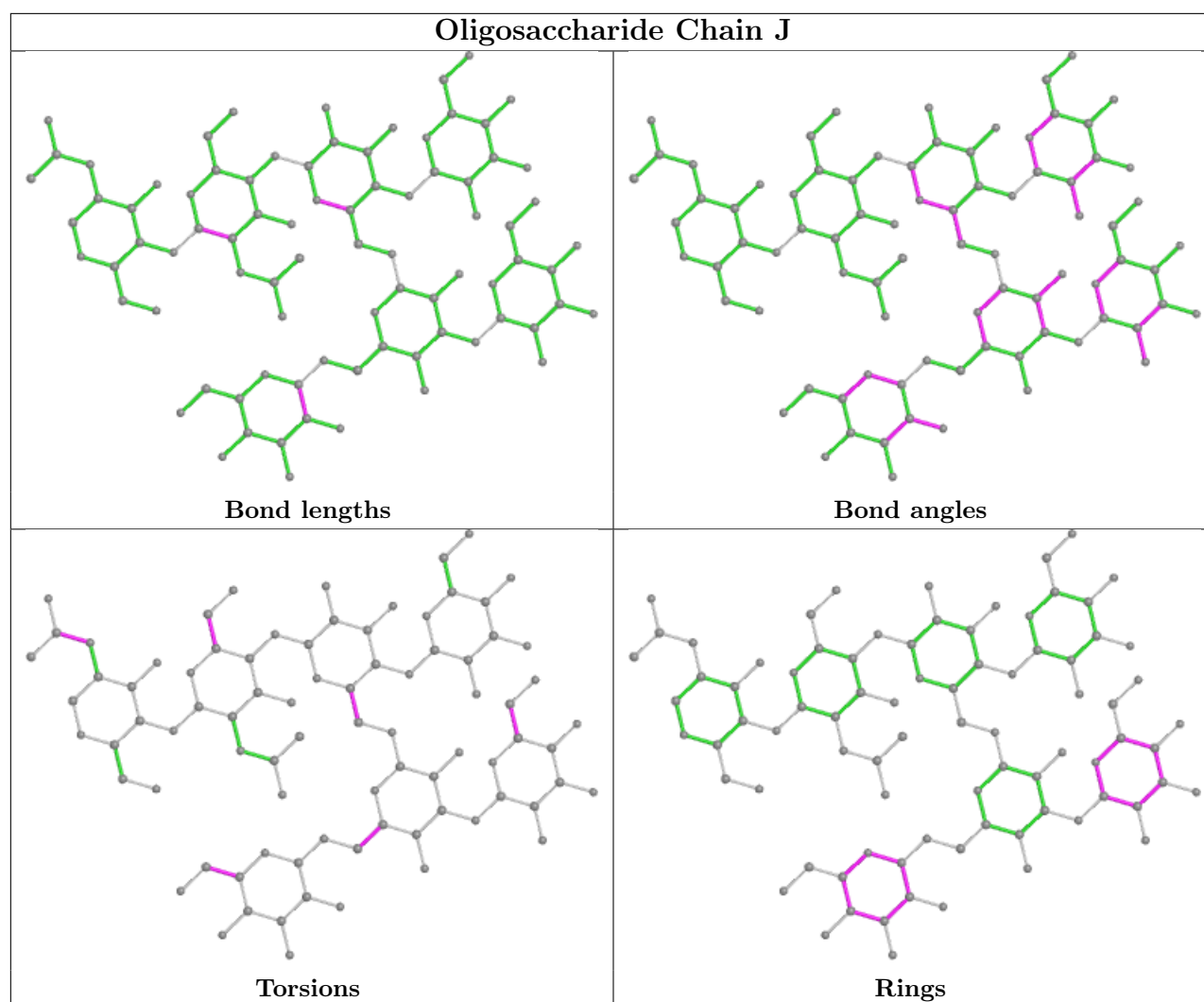
Mol	Chain	Res	Type	Atoms
5	J	6	MAN	C1-C2-C3-C4-C5-O5
5	J	5	MAN	C1-C2-C3-C4-C5-O5
5	I	6	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	5	MAN	1	0
5	I	4	MAN	2	0
5	J	3	MAN	2	0
5	I	2	NAG	1	0
5	I	1	NAG	1	0
5	I	5	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	803	1	14,14,15	0.61	0	17,19,21	1.17	2 (11%)
6	NAG	C	802	1	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	D	802	1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	D	803	1	14,14,15	0.55	0	17,19,21	0.63	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	801	1	14,14,15	0.28	0	17,19,21	0.42	0
6	NAG	D	801	1	14,14,15	0.43	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	803	1	-	2/6/23/26	0/1/1/1
6	NAG	C	802	1	-	2/6/23/26	0/1/1/1
6	NAG	D	802	1	-	2/6/23/26	0/1/1/1
6	NAG	D	803	1	-	2/6/23/26	0/1/1/1
6	NAG	C	801	1	-	2/6/23/26	0/1/1/1
6	NAG	D	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	803	NAG	C1-O5-C5	3.04	116.31	112.19
6	C	803	NAG	C3-C4-C5	2.76	115.16	110.24
6	D	803	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	802	NAG	C4-C5-C6-O6
6	D	803	NAG	C4-C5-C6-O6
6	D	802	NAG	O5-C5-C6-O6
6	D	801	NAG	C4-C5-C6-O6
6	C	803	NAG	C4-C5-C6-O6
6	C	802	NAG	O5-C5-C6-O6
6	D	801	NAG	O5-C5-C6-O6
6	D	803	NAG	O5-C5-C6-O6
6	C	803	NAG	O5-C5-C6-O6
6	C	802	NAG	C4-C5-C6-O6
6	C	801	NAG	O5-C5-C6-O6
6	C	801	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

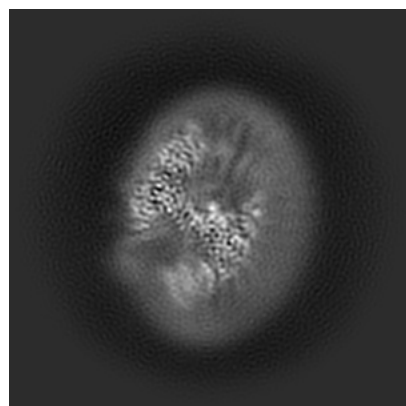
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37168. These allow visual inspection of the internal detail of the map and identification of artifacts.

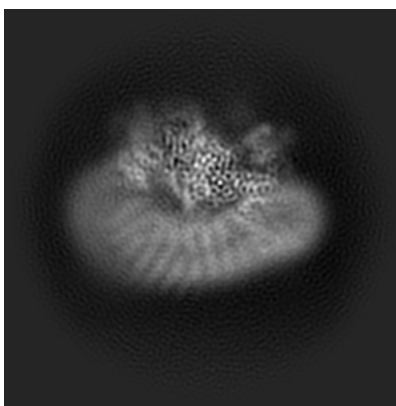
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

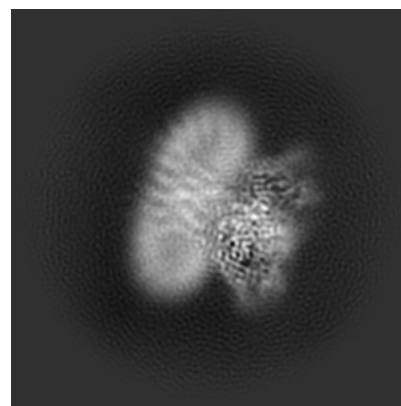
6.1.1 Primary map



X

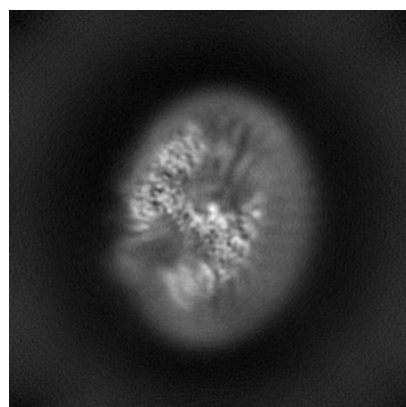


Y

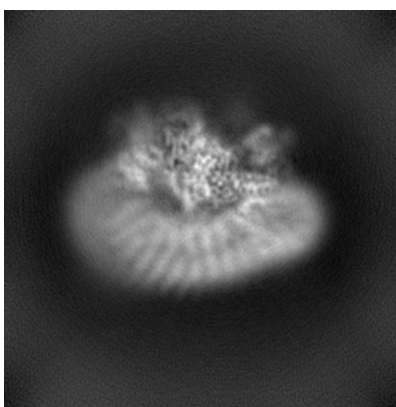


Z

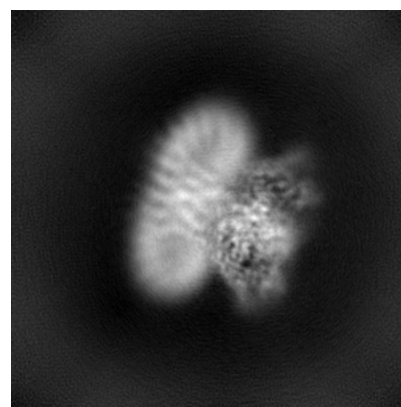
6.1.2 Raw map



X



Y

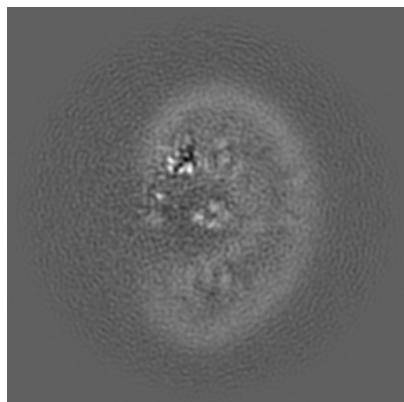


Z

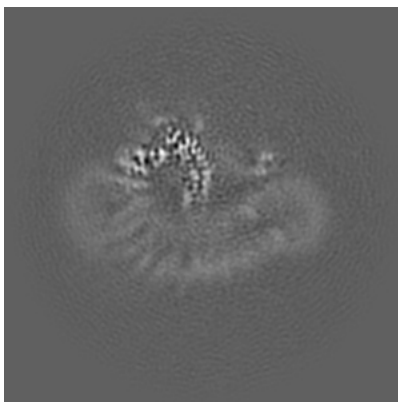
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

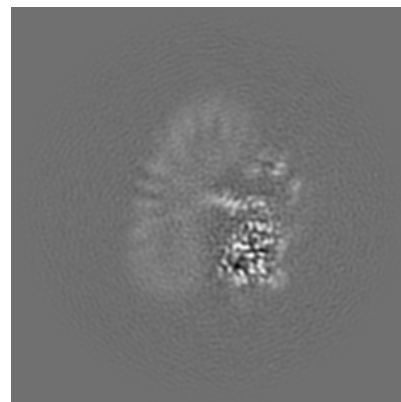
6.2.1 Primary map



X Index: 128

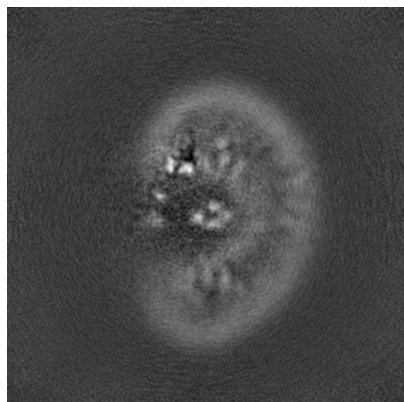


Y Index: 128

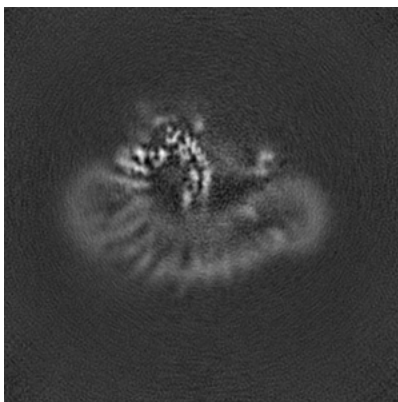


Z Index: 128

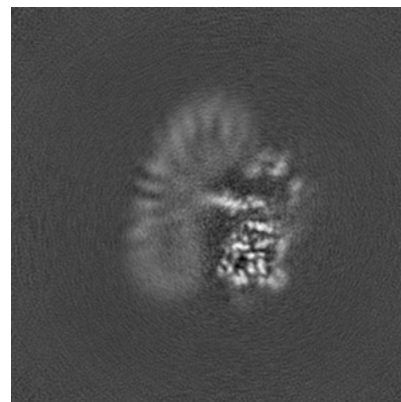
6.2.2 Raw map



X Index: 128



Y Index: 128

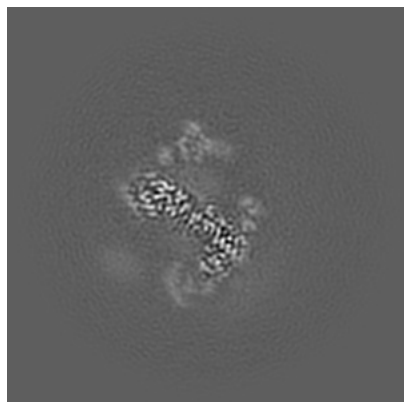


Z Index: 128

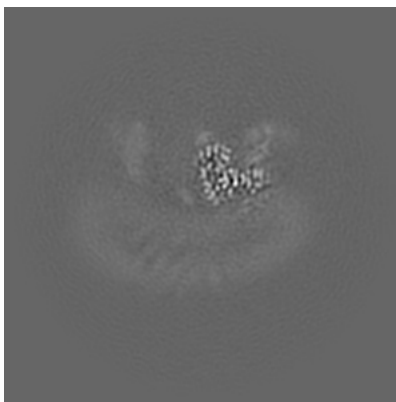
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

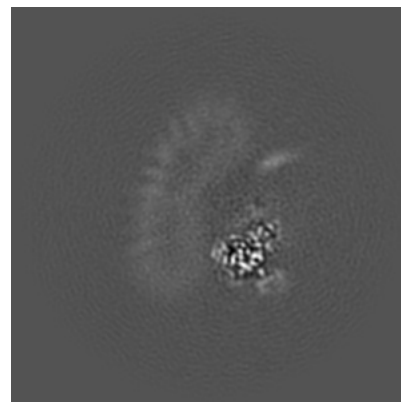
6.3.1 Primary map



X Index: 159

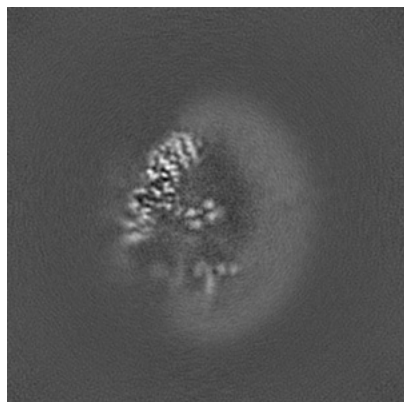


Y Index: 101

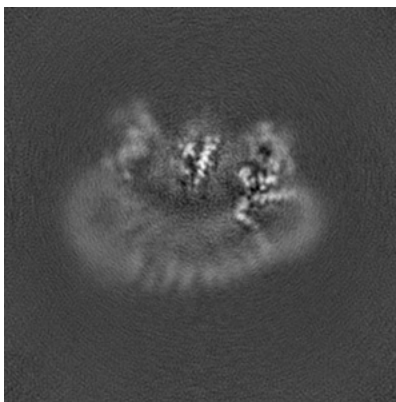


Z Index: 134

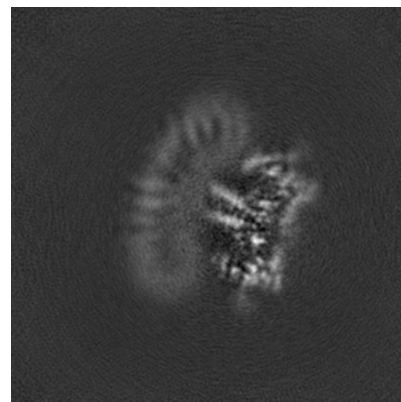
6.3.2 Raw map



X Index: 144



Y Index: 115

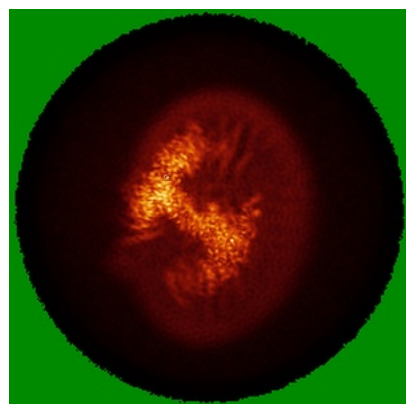


Z Index: 123

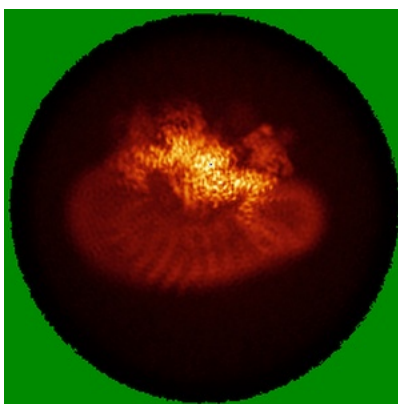
The images above show the largest variance slices of the map in three orthogonal directions.

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

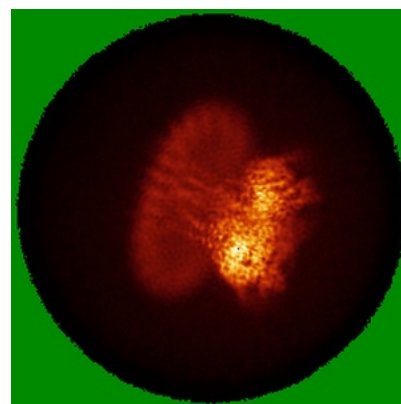
6.4.1 Primary map



X

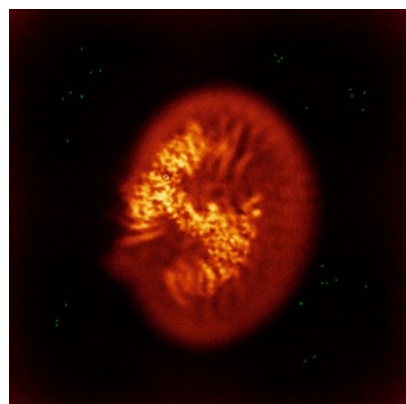


Y

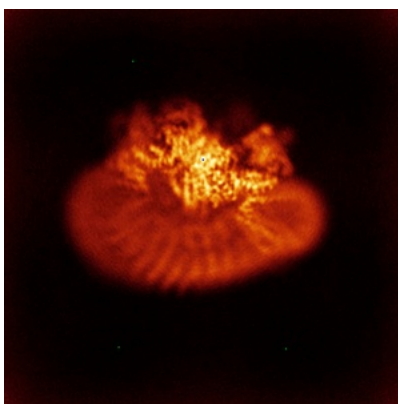


Z

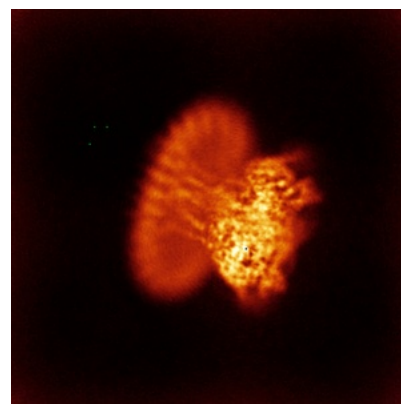
6.4.2 Raw map



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](#)

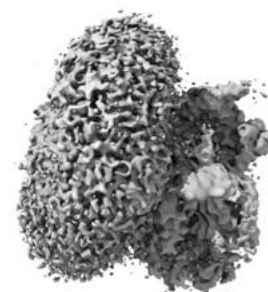
6.5.1 Primary map



X



Y



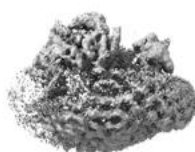
Z

The images above show the 3D surface view of the map at the recommended contour level 0.109. 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.

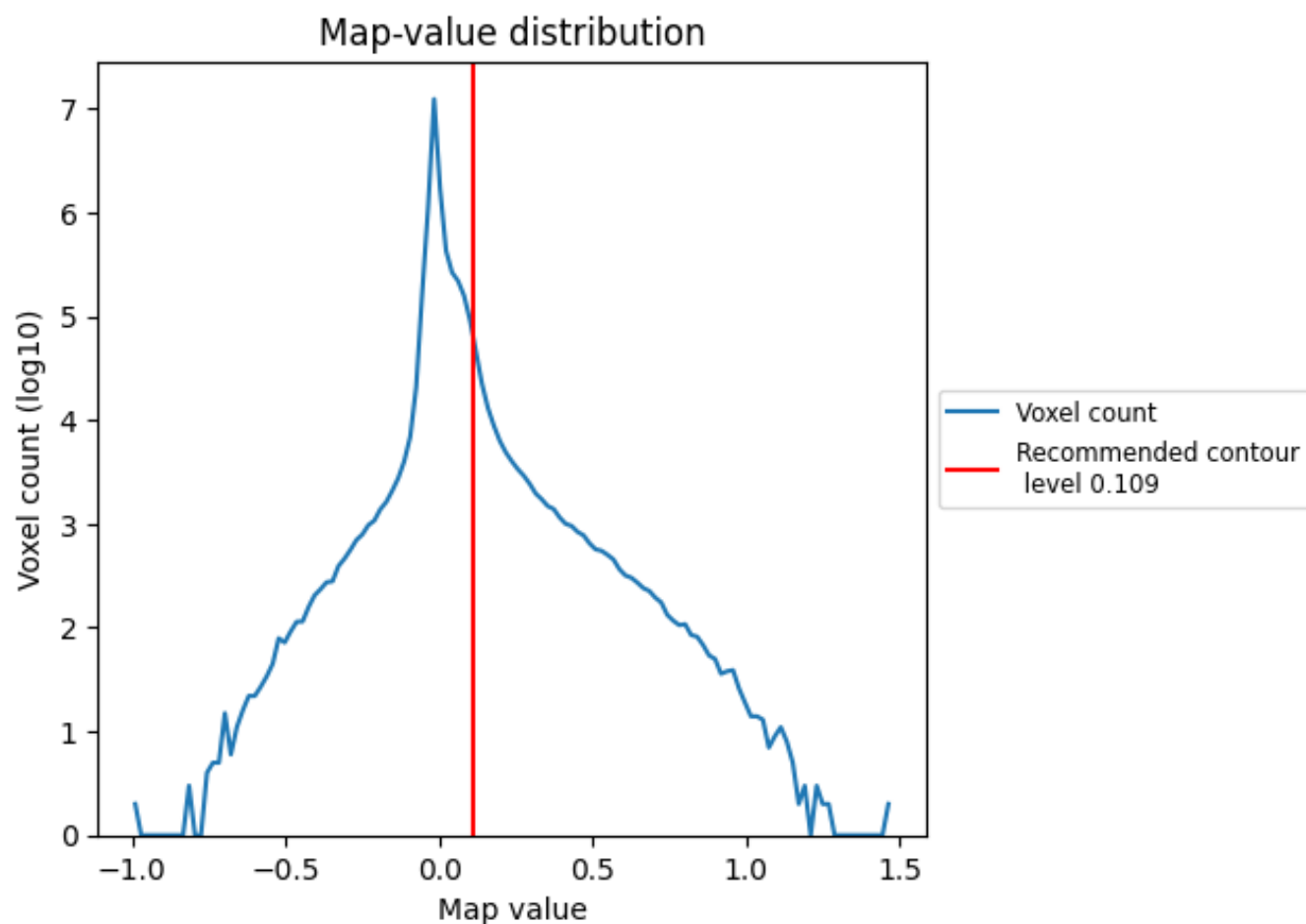
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

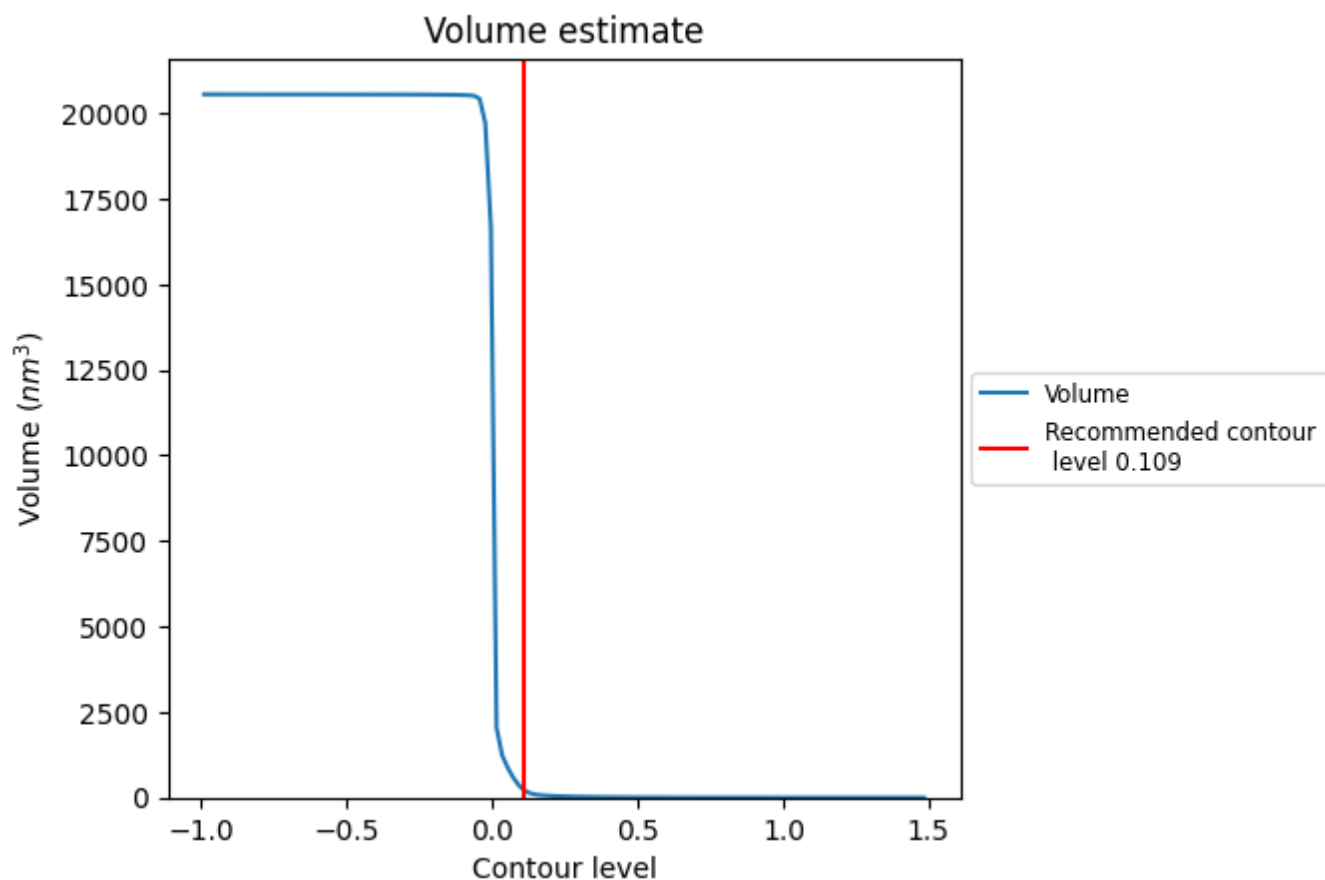
This section contains the results of statistical analysis of the map.

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.

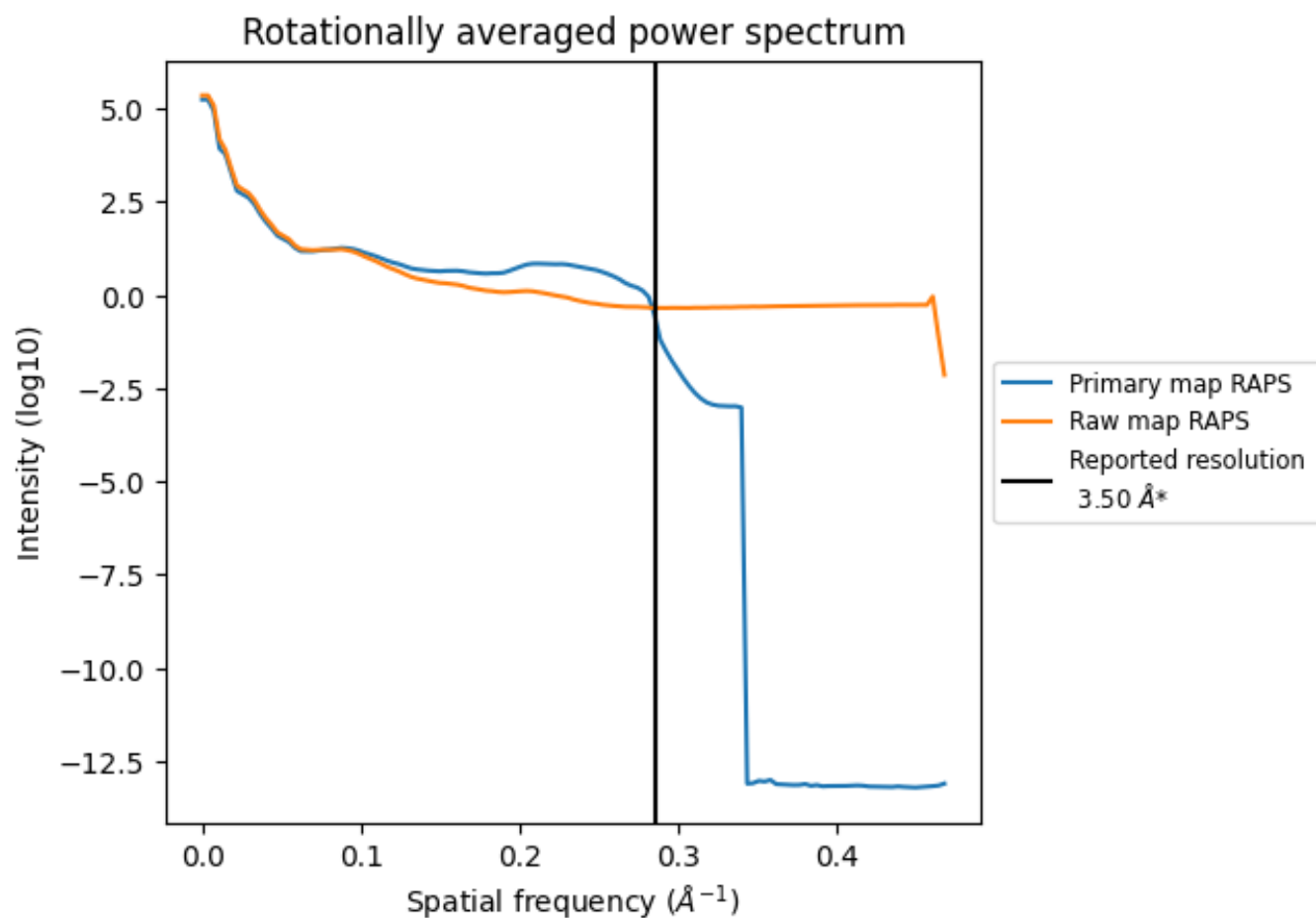
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm^3 ; this corresponds to an approximate mass of 197 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 ⓘ

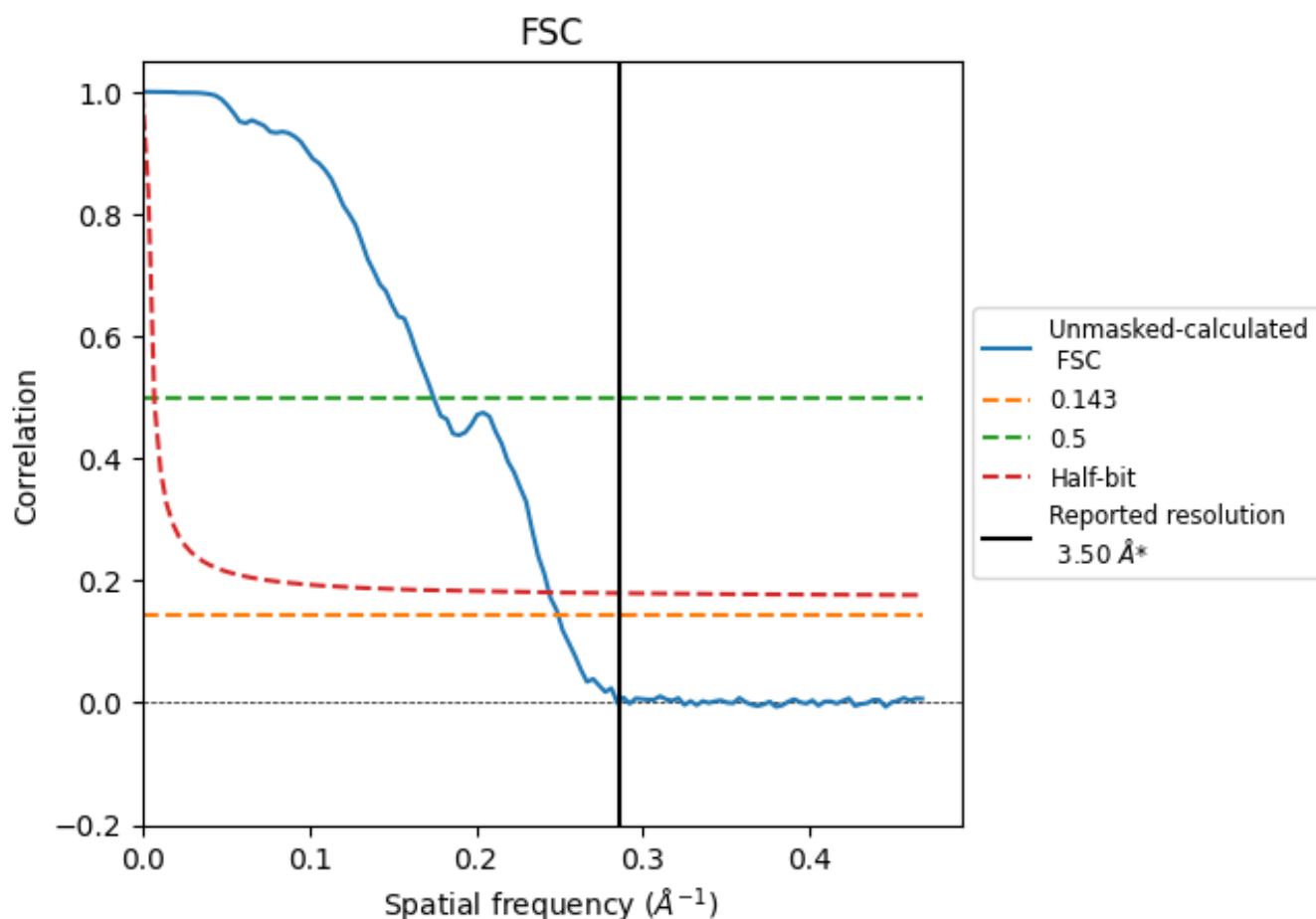


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

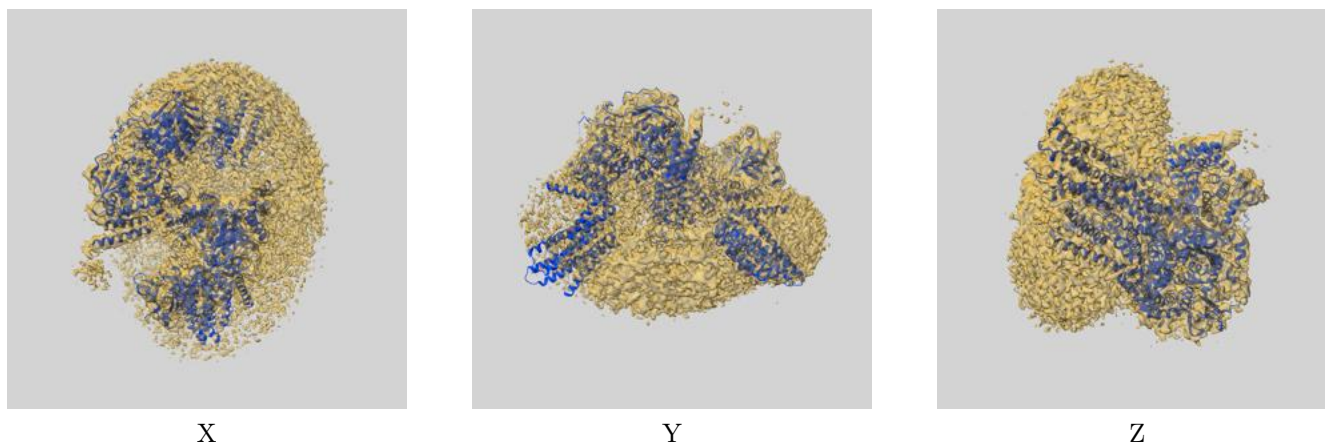
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	5.73	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

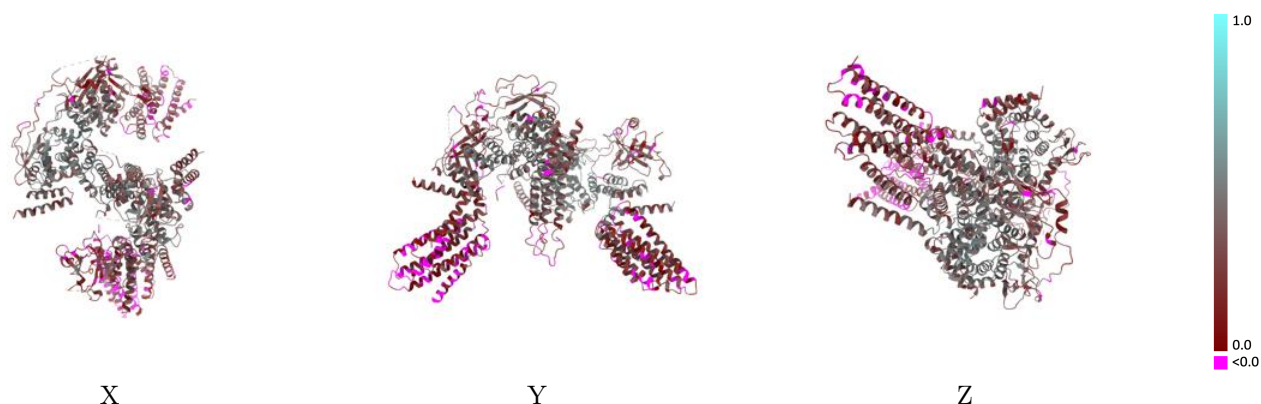
This section contains information regarding the fit between EMDB map EMD-37168 and PDB model 8KEV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



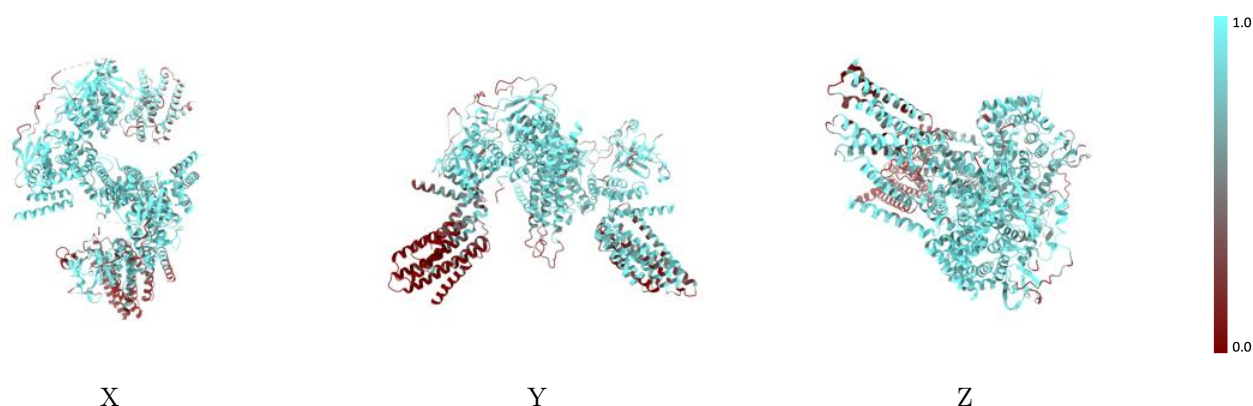
The images above show the 3D surface view of the map at the recommended contour level 0.109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



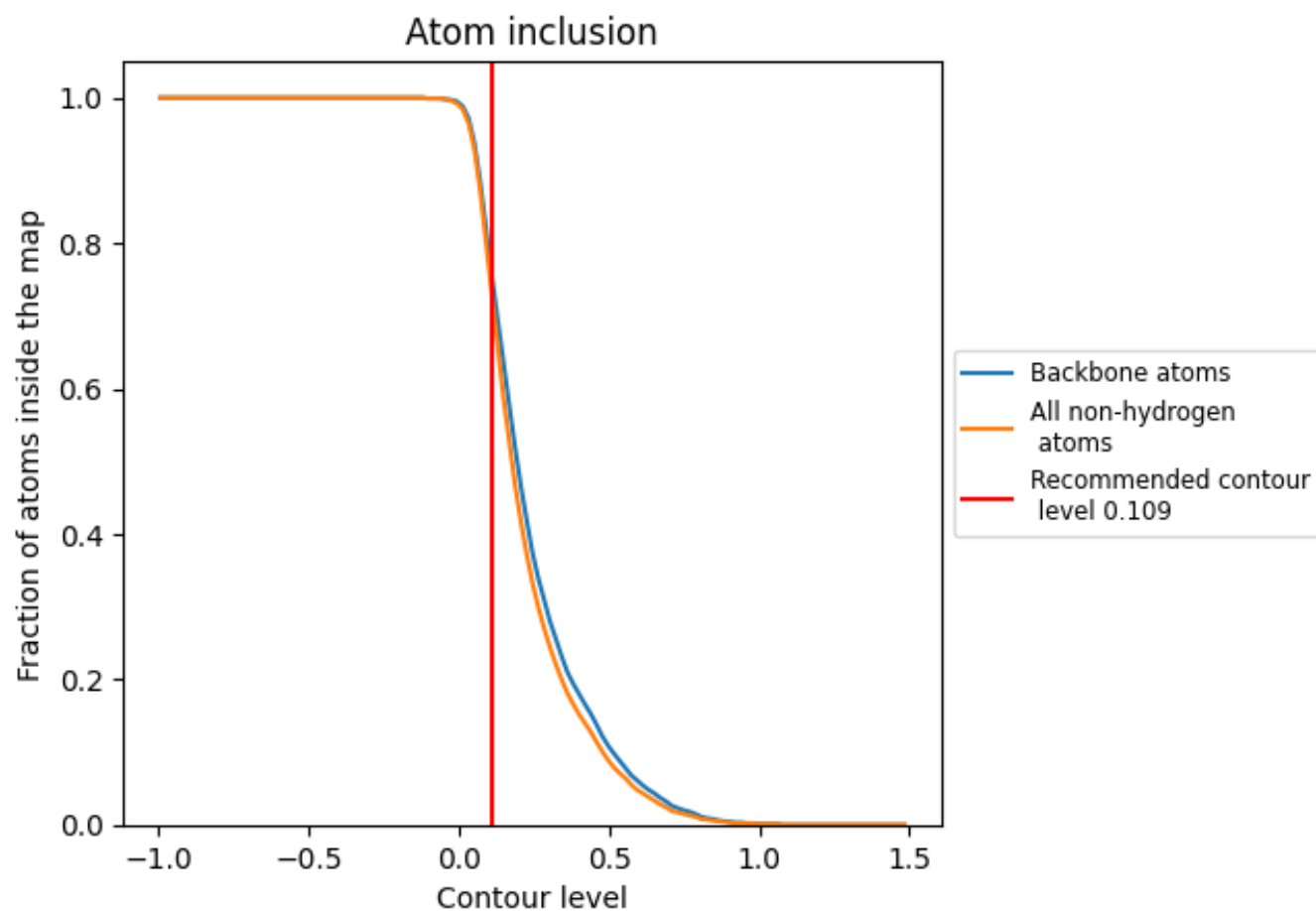
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.109).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7370	<div></div> 0.3170
A	<div></div> 0.7050	<div></div> 0.2080
B	<div></div> 0.2510	<div></div> 0.0930
C	<div></div> 0.8220	<div></div> 0.3850
D	<div></div> 0.8830	<div></div> 0.4330
E	<div></div> 0.8030	<div></div> 0.3150
F	<div></div> 0.6840	<div></div> 0.2450
G	<div></div> 0.0560	<div></div> 0.0560
H	<div></div> 0.0000	<div></div> -0.0360
I	<div></div> 0.6150	<div></div> 0.2240
J	<div></div> 0.5060	<div></div> 0.2120

1.0
0.0
<0.0