



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:25 AM UTC

PDB ID : 8JXJ / pdb_00008jxj
EMDB ID : EMD-36703
Title : rat megalin RAP complex leg
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-30
Resolution : 3.90 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

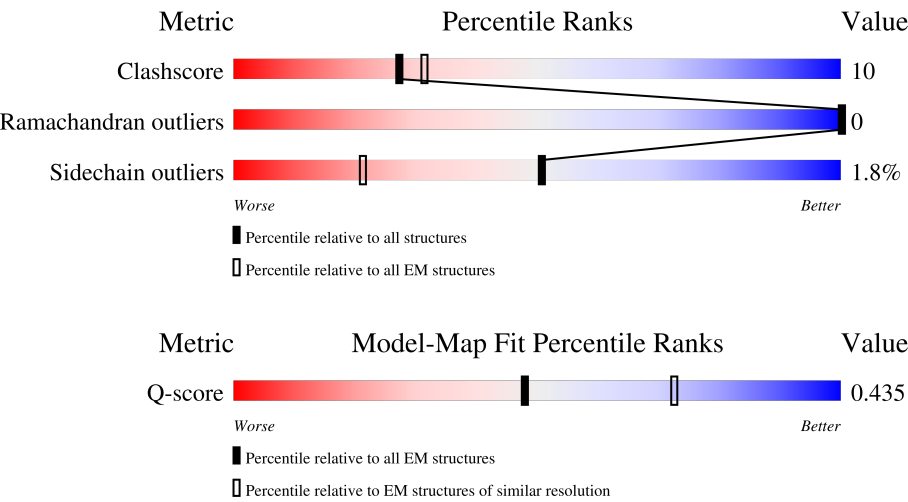
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	4660	10% . 88%
1	B	4660	9% . 88%
2	C	5	20% 60% 80%
3	D	3	33% 67%

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Mol	Chain	Length	Quality of chain
4	E	5	80% 20%40%40%
5	F	3	33% 100%

2 Entry composition [i](#)

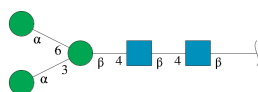
There are 7 unique types of molecules in this entry. The entry contains 9158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LDL receptor related protein 2.

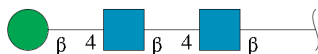
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	570	Total	C	N	O	S	0	0
			4461	2761	763	888	49		
1	B	570	Total	C	N	O	S	0	0
			4461	2761	763	888	49		

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



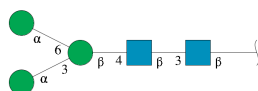
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



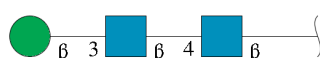
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

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



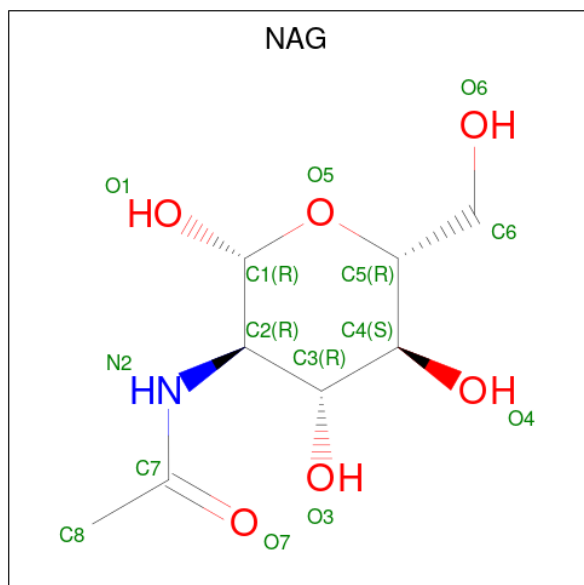
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total 4	Ca 4	0
7	B	4	Total 4	Ca 4	0







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

- Molecule 1: LDL receptor related protein 2

Chain B: 9% 88%

ALA	LEU	GLN	GLY	LEU	LYS	ASN	VAL	HIS	MET	GLN	PHE	ASP	E68
LYS	THR	GLU	CYS	PHE	ASP	ARG	PHE	GLN	GLY	ASP	CYS	HIS	S69
ILE	THR	ASP	ALA	GLU	LEU	ILE	THR	LEU	VAL	VAL	CYS	VAL	ARG
MET	ASP	VAL	GLN	HIS	VAL	THR	THR	LEU	THR	GLY	GLY	SER	GLY
ARG	TRP	MET	VAL	GLU	THR	VAL	THR	GLU	VAL	VAL	CYS	ASP	L71
ALA	ILE	VAL	CYS	VAL	LYS	ASN	GLN	GLU	ASN	GLY	GLY	CYS	F72
TRP	SER	PRO	VAL	PHE	VAL	LEU	LYS	GLU	ASN	ASP	PRO	ASP	L73
SER	ARG	VAL	LEU	THR	VAL	GLU	HIS	GLY	ASN	GLY	CYS	ASP	C74
ASP	ASN	THR	SER	THR	GLY	GLY	ARG	TYR	GLU	CYS	ILE	GLY	P75
GLY	LEU	GLY	HIS	ASP	VAL	ILE	VAL	ILE	GLU	GLU	SER	SER	A76
SER	TRP	SER	THR	THR	ALA	GLN	PHE	LEU	TYR	ASN	ARG	GLU	E77
HIS	TRP	PRO	THR	ALA	VAL	GLU	THR	LEU	CYS	GLN	TYR	ARG	G78
LEU	THR	SER	ASN	MET	ILE	VAL	ASP	GLY	HIS	SER	VAL	ASN	T79
MET	ASP	PHE	ASP	ALA	THR	THR	PRO	GLN	GLN	HIS	CYS	CYS	C80
PRO	GLY	VAL	GLY	LEU	THR	LEU	MET	HIS	THR	ASP	TYR	HIS	I81
ILE	GLY	VAL	LEU	MET	ASP	ILE	GLN	CYS	PRO	ARG	TYR	ASP	P82
VAL	LEU	ASP	GLY	LYS	LEU	THR	GLY	LYS	PHE	GLY	THR	THR	S83
THR	SER	THR	TYR	ALA	VAL	GLU	VAL	SER	GLY	PRO	ASP	CYS	S84
VAL	THR	ASP	ARG	LYS	ARG	ASN	PHE	ASP	GLY	ARG	GLN	GLN	V85
GLY	VAL	ALA	LYS	PHE	ARG	GLY	SER	SER	CYS	ALA	LEU	THR	V86
THR	THR	HIS	CYS	THR	THR	HIS	THR	PHE	CYS	PRO	ASP	CYS	C87
ALA	THR	GLN	THR	THR	VAL	ILE	ILE	ALA	PRO	ALA	ASP	ALA	D88
LYS	VAL	THR	PHE	GLU	ASP	ILE	GLY	SER	GLY	GLY	GLU	ASN	F89
ASP	GLN	TYR	LEU	VAL	ARG	LEU	ASN	ILE	GLY	ALA	ALA	GLY	D90
ILE	SER	SER	ASP	ARG	TYR	LEU	THR	PHE	ILE	ARG	CYS	ASP	K91
THR	ARG	SER	ASP	THR	ASP	PRO	GLN	ASN	CYS	TYR	TYR	ASN	D92
GLN	THR	LEU	ASP	THR	TYR	THR	GLU	ASN	SER	ILE	THR	ASN	C93
ALA	THR	GLU	GLY	VAL	ILE	VAL	ILE	GLY	ASN	SER	THR	ASN	S94
LYS	GLN	GLU	PHE	SER	GLU	GLY	LEU	VAL	ARG	ASN	GLN	SER	D95
THR	VAL	THR	GLY	THR	THR	ILE	VAL	LEU	ARG	GLY	ARG	CYS	G96
ASP	ARG	ILE	VAL	THR	TYR	PHE	SER	VAL	THR	THR	CYS	ASP	D96
VAL	THR	LYS	VAL	ASP	ASP	THR	VAL	GLY	ILE	GLN	GLN	ASP	N97
ALA	ARG	GLN	LYS	VAL	GLY	ASP	THR	ASP	PHE	GLY	LYS	VAL	G98
PHE	SER	ILE	PHE	VAL	ILE	TRP	PRO	LEU	THR	THR	VAL	VAL	E99
THR	ILE	ASP	LEU	THR	ARG	GLY	ASN	HIS	ASP	CYS	ASP	ASP	Q100
ASP	GLY	ASP	LEU	THR	ARG	SER	ASN	GLY	ASP	CYS	CYS	CYS	Q101
VAL	VAL	THR	LEU	THR	LYS	LEU	LEU	ARG	CYS	ARG	ARG	ARG	N102
LYS	VAL	THR	PHE	ALA	THR	SER	ALA	ASN	CYS	ASP	GLY	ASP	C103
ILE	HIS	GLY	SER	ILE	VAL	GLY	VAL	PHE	ILE	SER	GLN	SER	D48
GLU	PRO	LYS	SER	GLU	ALA	GLN	VAL	ARG	THR	CYS	THR	THR	A104
THR	ALA	GLU	LYS	THR	ARG	PRO	TRP	ILE	GLY	ASP	ILE	ASP	G49
ALA	VAL	VAL	THR	THR	GLY	LYS	ILE	LEU	ILE	GLY	GLY	GLY	L94
THR	GLY	ILE	ALA	VAL	GLY	VAL	ASN	ALA	CYS	GLU	GLN	ALA	D55
TYR	TYR	THR	VAL	ALA	SER	GLU	ASN	GLU	ASP	ASN	ASN	ASN	D56
ASP	MET	ALA	ARG	THR	LEU	ARG	LYS	SER	GLM	CYS	THR	CYS	T57
PHE	PHE	ASN	GLY	THR	VAL	ALA	VAL	VAL	GLN	THR	THR	ALA	D58
LEU	ARG	ARG	ILE	PRO	PRO	PHE	PRO	CYS	THR	CYS	THR	GLN	E59
SER	SER	LEU	PRO	CYS	HIS	MET	THR	ARG	GLY	GLY	LEU	CYS	I60
GLY	ASP	GLY	PHE	PRO	THR	ASP	VAL	GLY	ASN	GLY	CYS	THR	G61
LYS	LYS	SER	THR	PHE	THR	GLY	GLU	MET	ARG	ASP	SER	GLN	C62
LEU	VAL	LEU	THR	GLY	GLY	ILE	THR	VAL	GLM	THR	GLN	LYS	ASN
GLU	GLU	ARG	SER	ILE	ASN	ASN	LYS	MET	GLY	ASP	ASP	ASP	P63
CYS	CYS	THR	THR	THR	THR	THR	VAL	GLY	GLY	GLU	GLY	GLU	P64
													R65
													S66
													C67

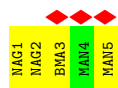






PRO ILE TYR ALA GLU MET ASP SER GLU VAL LYS ASP ALA VAL ALA VAL ALA PRO PRO PRO PRO SER SER LEU PRO ALA LYS ALA LYS SER LYS ARG ASN LEU THR PRO PRO GLY TYR THR ALA THR THR GLU ASP THR PHE LYS ASP THR ALA ASN LEU VAL LYS GLU ASP SER ASP VAL

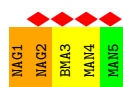
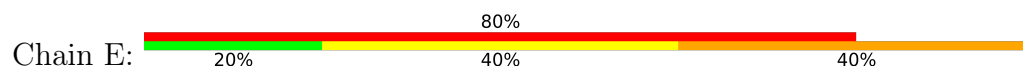
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.029	Depositor
Map size ($\text{\AA}$)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.411, 1.411, 1.411	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/4566	0.44	1/6189 (0.0%)
1	B	0.20	0/4566	0.44	1/6189 (0.0%)
All	All	0.19	0/9132	0.44	2/12378 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4124	ASN	N-CA-C	-5.25	106.83	113.18
1	A	3937	CYS	CB-CA-C	-5.18	110.18	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4461	0	4140	70	0
1	B	4461	0	4140	99	0
2	C	61	0	52	2	0
3	D	39	0	34	1	0
4	E	61	0	52	2	0
5	F	39	0	34	0	0
6	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
All	All	9158	0	8478	173	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 10.

All (173) 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:A:3963:GLY:HA2	1:A:4004:LYS:HE2	1.66	0.78
1:A:3937:CYS:SG	1:A:3938:SER:N	2.61	0.73
1:A:4313:VAL:O	1:A:4314:ASN:ND2	2.22	0.71
1:B:3983:GLN:NE2	1:B:3988:GLY:O	2.23	0.71
1:B:4269:ILE:HG22	1:B:4270:ILE:HG12	1.72	0.71
1:A:4056:PRO:HB2	1:A:4322:ILE:HD11	1.72	0.70
1:B:3943:ILE:HG13	1:B:3955:CYS:HB3	1.73	0.70
1:B:4295:GLU:HG2	1:B:4309:LYS:HE2	1.73	0.69
1:A:4131:ASN:HD21	1:A:4385:CYS:HB2	1.59	0.68
1:A:4398:LEU:O	1:A:4400:LYS:NZ	2.23	0.68
1:B:4100:LEU:HD11	1:B:4384:ARG:HG2	1.75	0.68
1:A:4386:MET:HG2	1:A:4412:CYS:HB2	1.76	0.67
1:B:4282:PHE:O	1:B:4283:GLU:HG3	1.94	0.67
2:C:1:NAG:H61	2:C:2:NAG:C7	2.25	0.66
1:A:4119:ARG:NH1	1:A:4173:LEU:O	2.29	0.65
1:B:4125:PHE:CD1	1:B:4127:SER:HB2	2.31	0.65
1:B:4204:THR:HG22	1:B:4212:ILE:HG12	1.79	0.64
1:B:4299:GLN:HE21	1:B:4307:LYS:HG3	1.63	0.63
1:B:4043:THR:HG22	1:B:4044:HIS:H	1.63	0.62
1:A:4274:MET:HE1	1:A:4297:TRP:CE2	2.36	0.61
1:B:4123:PRO:HB3	1:B:4125:PHE:CE1	2.35	0.60
1:A:3982:THR:HB	1:A:3990:ILE:HG23	1.84	0.60
4:E:1:NAG:O4	4:E:2:NAG:N2	2.36	0.59
1:B:4390:ASN:O	1:B:4401:CYS:HB2	2.03	0.59
1:A:4100:LEU:HD11	1:A:4384:ARG:HG2	1.84	0.59
1:B:3976:ILE:HG12	1:B:3989:PHE:HE2	1.67	0.58
1:A:3984:LEU:HD13	1:A:3987:GLY:HA3	1.84	0.58
1:B:4299:GLN:NE2	1:B:4307:LYS:HG3	2.19	0.57
1:B:4149:LEU:HD11	1:B:4158:ILE:HD11	1.85	0.57
1:B:4204:THR:HG23	1:B:4236:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4234:ASN:ND2	1:A:4251:SER:OG	2.38	0.57
1:B:4256:ILE:HB	1:B:4270:ILE:HB	1.86	0.57
1:A:4078:GLU:HG3	1:A:4079:TYR:N	2.20	0.56
1:B:3978:GLU:N	1:B:3978:GLU:OE1	2.38	0.56
1:B:4098:ILE:O	1:B:4384:ARG:NH2	2.38	0.56
1:B:36:ASP:HB2	1:B:57:THR:HG21	1.87	0.55
1:B:4073:SER:O	1:B:4075:LYS:NZ	2.40	0.55
1:B:4282:PHE:C	1:B:4283:GLU:HG3	2.32	0.55
1:A:4131:ASN:ND2	1:A:4385:CYS:HB2	2.22	0.55
1:B:4073:SER:HB3	1:B:4075:LYS:HG2	1.89	0.54
1:A:4254:ASP:HB2	1:A:4275:LYS:H	1.73	0.54
1:B:4284:ASP:O	1:B:4301:LYS:N	2.36	0.54
1:B:4234:ASN:HD21	1:B:4251:SER:HB3	1.74	0.53
1:A:4394:ASP:N	1:A:4400:LYS:HZ1	2.07	0.53
1:B:3981:CYS:SG	1:B:3982:THR:N	2.81	0.53
1:B:4125:PHE:HD1	1:B:4127:SER:HB2	1.72	0.53
1:A:4024:ARG:N	1:A:4031:GLU:O	2.41	0.52
1:B:4384:ARG:HD3	1:B:4411:TYR:CE2	2.44	0.52
1:B:4070:ASN:HD22	1:B:4073:SER:HB2	1.74	0.52
1:A:4068:LYS:HB2	1:A:4077:SER:HB2	1.91	0.52
1:B:4295:GLU:HG3	1:B:4312:VAL:HG13	1.91	0.51
1:A:4079:TYR:HD1	1:A:4080:LEU:H	1.56	0.51
1:A:4337:LYS:NZ	1:B:48:ASP:OD2	2.32	0.51
1:B:4125:PHE:CE1	1:B:4127:SER:HB2	2.46	0.51
1:B:4314:ASN:ND2	1:B:4316:TRP:HB2	2.26	0.51
1:B:4391:CYS:HA	1:B:4401:CYS:HB2	1.93	0.51
1:A:3930:CYS:N	1:A:3942:CYS:SG	2.85	0.50
1:B:4314:ASN:OD1	1:B:4314:ASN:N	2.44	0.50
1:A:4121:TYR:CD2	1:A:4382:PRO:HB3	2.46	0.50
1:A:4144:MET:SD	1:A:4144:MET:N	2.84	0.50
1:A:3950:ASP:OD1	1:A:3950:ASP:N	2.36	0.50
1:B:4100:LEU:HD21	1:B:4125:PHE:CZ	2.47	0.50
1:B:33:PHE:CD2	1:B:46:ARG:HG3	2.47	0.49
1:B:3930:CYS:HB2	1:B:3934:GLU:HB2	1.94	0.49
1:A:4218:ASN:HA	1:A:4345:LEU:HD13	1.94	0.49
1:B:3934:GLU:HA	1:B:3944:SER:HA	1.94	0.49
1:A:3949:CYS:SG	1:A:3990:ILE:HB	2.53	0.49
1:A:3949:CYS:HA	1:A:3961:GLU:HG3	1.95	0.48
1:A:4276:PRO:HB3	1:A:4288:TRP:CD1	2.48	0.48
1:B:3981:CYS:HA	1:B:3991:CYS:HA	1.94	0.48
1:B:4079:TYR:CG	1:B:4080:LEU:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4018:ILE:HG22	1:B:4019:CYS:SG	2.53	0.48
1:A:4394:ASP:H	1:A:4400:LYS:HZ1	1.61	0.48
1:B:4100:LEU:HD23	1:B:4123:PRO:HA	1.96	0.48
1:A:4273:ALA:C	1:A:4274:MET:HG3	2.39	0.47
1:A:89:GLU:N	1:A:99:GLU:OE1	2.47	0.47
1:A:3966:LEU:O	1:A:3970:ARG:NH2	2.48	0.47
1:B:4068:LYS:HB2	1:B:4077:SER:OG	2.15	0.47
1:B:4119:ARG:HH21	1:B:4173:LEU:C	2.22	0.47
1:B:4247:TYR:CD2	1:B:4258:ALA:HB2	2.50	0.47
1:B:4038:PHE:HB3	1:B:4049:CYS:SG	2.56	0.46
1:B:4125:PHE:C	1:B:4127:SER:H	2.24	0.46
1:A:4022:SER:OG	1:A:4033:PHE:O	2.29	0.46
1:A:4198:LEU:HD12	1:A:4198:LEU:O	2.15	0.46
1:B:4119:ARG:HD3	1:B:4379:MET:SD	2.56	0.46
1:A:3980:ASN:OD1	6:A:4701:NAG:N2	2.49	0.46
1:B:34:ARG:NE	1:B:38:GLY:HA2	2.30	0.46
1:A:4141:LYS:O	1:A:4178:ARG:NH2	2.42	0.46
1:B:4116:ALA:HA	1:B:4143:LEU:HD12	1.97	0.46
1:B:4065:ARG:HD2	1:B:4067:ARG:HD3	1.97	0.46
1:B:4065:ARG:HD3	1:B:4081:GLU:OE2	2.16	0.45
1:A:33:PHE:N	1:A:41:ILE:O	2.49	0.45
1:A:4269:ILE:HG22	1:A:4270:ILE:HG13	1.97	0.45
1:B:3941:ASN:N	1:B:3941:ASN:OD1	2.48	0.45
1:A:98:ASP:HA	1:A:102:ASN:ND2	2.31	0.45
1:A:4079:TYR:CD1	1:A:4080:LEU:N	2.85	0.45
1:B:4277:PHE:HB2	1:B:4291:LYS:HB3	1.99	0.45
1:B:4085:HIS:HB3	1:B:4108:LEU:HB2	1.99	0.45
1:A:4394:ASP:CG	1:A:4400:LYS:HZ2	2.25	0.45
1:A:4078:GLU:HG3	1:A:4079:TYR:H	1.82	0.45
1:B:4163:ALA:HA	1:B:4189:PRO:HD2	1.99	0.45
1:B:4398:LEU:HD12	1:B:4399:PRO:HD2	1.99	0.45
1:B:3962:THR:N	1:B:3990:ILE:HD11	2.31	0.44
1:B:3970:ARG:CZ	1:B:3976:ILE:HD13	2.47	0.44
1:B:4098:ILE:HG23	1:B:4384:ARG:HH21	1.81	0.44
1:B:4392:TYR:CZ	1:B:4400:LYS:HB2	2.51	0.44
1:A:4262:ASP:OD1	1:A:4262:ASP:C	2.60	0.44
1:B:4232:TRP:N	1:B:4232:TRP:CD1	2.85	0.44
3:D:1:NAG:H62	3:D:2:NAG:N2	2.32	0.44
1:B:4121:TYR:CD2	1:B:4382:PRO:HG3	2.52	0.44
1:A:4228:GLU:O	1:A:4266:ARG:NH1	2.28	0.44
1:B:73:LEU:HA	1:B:79:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4048:ARG:C	1:B:4048:ARG:HD3	2.42	0.44
1:A:3997:PHE:HB3	1:A:4007:CYS:HB3	2.00	0.44
1:A:4022:SER:O	1:A:4032:CYS:HB2	2.18	0.44
1:B:4061:PRO:HD2	1:B:4319:GLN:O	2.17	0.44
1:B:4234:ASN:HD21	1:B:4251:SER:CB	2.30	0.44
1:A:88:ASP:N	1:A:99:GLU:OE1	2.47	0.44
1:A:4079:TYR:HE2	1:A:4122:ILE:HG13	1.82	0.44
1:A:4274:MET:HE1	1:A:4297:TRP:NE1	2.32	0.43
1:A:3984:LEU:HB3	1:A:3988:GLY:N	2.34	0.43
1:B:4019:CYS:HB3	1:B:4032:CYS:HB3	1.78	0.43
1:B:4413:GLU:N	1:B:4413:GLU:OE1	2.51	0.43
1:A:4068:LYS:HD2	1:A:4079:TYR:HD2	1.84	0.43
1:B:4130:ASN:N	1:B:4130:ASN:OD1	2.51	0.43
2:C:2:NAG:O3	2:C:5:MAN:H5	2.18	0.43
1:A:4340:CYS:HB3	1:A:4353:CYS:HB3	1.80	0.43
1:A:83:SER:HA	1:A:86:VAL:HB	2.01	0.43
1:A:4023:CYS:SG	1:A:4024:ARG:N	2.92	0.43
1:B:4314:ASN:HD22	1:B:4316:TRP:HB2	1.83	0.43
1:B:4106:THR:HG22	1:B:4117:ILE:HG13	2.00	0.43
1:A:4256:ILE:HB	1:A:4270:ILE:HB	2.01	0.43
1:B:4413:GLU:HG2	1:B:4414:VAL:HG13	2.01	0.43
1:B:88:ASP:OD1	1:B:90:ASP:HB2	2.19	0.42
1:B:3935:TYR:N	1:B:3943:ILE:O	2.47	0.42
1:B:3949:CYS:N	1:B:3961:GLU:OE2	2.52	0.42
1:B:4191:ALA:HB3	1:B:4235:GLY:HA2	2.00	0.42
1:B:4242:ASN:OD1	1:B:4245:ARG:NH1	2.48	0.42
1:B:3998:LYS:O	1:B:4008:GLN:HG3	2.18	0.42
4:E:2:NAG:O3	4:E:2:NAG:C7	2.67	0.42
1:A:4149:LEU:HD11	1:A:4158:ILE:HD11	2.01	0.42
1:B:4293:LYS:HE3	1:B:4293:LYS:HB3	1.91	0.42
1:A:4087:GLN:HG3	1:A:4108:LEU:HD21	2.00	0.42
1:B:4036:ASP:OD1	1:B:4037:GLY:N	2.53	0.42
1:B:4119:ARG:HE	1:B:4138:LEU:HD21	1.85	0.42
1:B:3965:ASN:HB2	1:B:3989:PHE:CZ	2.55	0.41
1:B:4087:GLN:HG3	1:B:4108:LEU:HD11	2.02	0.41
1:A:41:ILE:O	1:A:41:ILE:HD12	2.20	0.41
1:B:4393:PHE:CE1	1:B:4399:PRO:HB3	2.55	0.41
1:A:4105:TYR:CZ	1:A:4118:LYS:HB2	2.56	0.41
1:B:3976:ILE:HG23	1:B:3991:CYS:SG	2.60	0.41
1:A:88:ASP:O	1:A:89:GLU:HB2	2.20	0.41
1:A:4027:LYS:HE2	1:A:4027:LYS:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4122:ILE:HD13	1:A:4323:PHE:CZ	2.56	0.41
1:B:4012:GLU:O	1:B:4018:ILE:HG13	2.20	0.41
1:A:4095:PRO:HB2	1:A:4096:GLU:OE2	2.21	0.41
1:A:4274:MET:HE1	1:A:4297:TRP:CD1	2.56	0.41
1:B:4203:TRP:CE2	1:B:4213:GLU:HB2	2.55	0.41
1:B:4391:CYS:HA	1:B:4401:CYS:CB	2.51	0.41
1:A:4401:CYS:HB2	1:A:4411:TYR:HA	2.03	0.41
1:B:100:GLN:H	1:B:100:GLN:HG3	1.69	0.41
1:B:3968:ASP:N	1:B:3968:ASP:OD1	2.54	0.41
1:B:4218:ASN:HA	1:B:4345:LEU:HD13	2.02	0.41
1:B:4127:SER:C	1:B:4129:SER:H	2.28	0.40
1:B:4284:ASP:OD1	1:B:4284:ASP:C	2.64	0.40
1:A:4386:MET:SD	1:A:4386:MET:N	2.93	0.40
1:B:4402:LYS:H	1:B:4402:LYS:HD2	1.87	0.40
1:A:4012:GLU:OE2	1:A:4030:TYR:HD1	2.05	0.40
1:A:97:ALA:O	1:A:101:GLN:HG3	2.22	0.40
1:A:4319:GLN:NE2	1:A:4321:ARG:HH21	2.20	0.40
1:B:63:PRO:HA	1:B:64:PRO:HD3	1.95	0.40
1:B:4009:ASP:CG	1:B:4028:GLY:H	2.29	0.40
1:B:4237:SER:HB3	1:B:4281:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/4660 (12%)	514 (91%)	52 (9%)	0	100	100
1	B	566/4660 (12%)	526 (93%)	40 (7%)	0	100	100
All	All	1132/9320 (12%)	1040 (92%)	92 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	502/4089 (12%)	493 (98%)	9 (2%)	51 67
1	B	502/4089 (12%)	493 (98%)	9 (2%)	51 67
All	All	1004/8178 (12%)	986 (98%)	18 (2%)	51 67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	98	ASP
1	A	4032	CYS
1	A	4047	GLU
1	A	4174	ASP
1	A	4236	LEU
1	A	4339	VAL
1	A	4377	VAL
1	A	4378	THR
1	B	58	ASP
1	B	103	CYS
1	B	3958	LEU
1	B	3962	THR
1	B	3971	THR
1	B	4130	ASN
1	B	4154	VAL
1	B	4284	ASP
1	B	4339	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	102	ASN
1	A	3946	HIS
1	A	4110	GLN

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Mol	Chain	Res	Type
1	A	4131	ASN
1	A	4206	GLN
1	A	4221	HIS
1	A	4234	ASN
1	A	4314	ASN
1	A	4342	HIS
1	B	102	ASN
1	B	3951	ASN
1	B	4008	GLN
1	B	4131	ASN
1	B	4234	ASN

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 ⓘ

16 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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.37	0	17,19,21	0.69	0
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	1.06	1 (6%)
2	MAN	C	4	2	11,11,12	0.20	0	15,15,17	0.62	0
2	MAN	C	5	2	11,11,12	0.20	0	15,15,17	0.69	0
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.84	1 (5%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.60	0
4	NAG	E	1	4,1	14,14,15	0.50	0	17,19,21	1.20	3 (17%)
4	NAG	E	2	4	14,14,15	0.37	0	17,19,21	1.05	2 (11%)
4	BMA	E	3	4	11,11,12	0.44	0	15,15,17	1.24	2 (13%)
4	MAN	E	4	4	11,11,12	0.38	0	15,15,17	1.07	2 (13%)
4	MAN	E	5	4	11,11,12	0.26	0	15,15,17	0.59	0
5	NAG	F	1	5,1	14,14,15	0.36	0	17,19,21	0.66	0
5	NAG	F	2	5	14,14,15	0.33	0	17,19,21	0.51	0
5	BMA	F	3	5	11,11,12	0.22	0	15,15,17	0.77	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
2	NAG	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	MAN	E	5	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	E	1	NAG	C4-C3-C2	-2.48	107.38	111.02
4	E	3	BMA	C3-C4-C5	-2.47	105.76	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O5-C1-C2	-2.41	107.56	111.29
3	D	1	NAG	C1-O5-C5	2.37	115.36	112.19
4	E	2	NAG	C1-O5-C5	2.37	115.36	112.19
4	E	2	NAG	O5-C1-C2	-2.31	107.71	111.29
4	E	3	BMA	O5-C5-C6	2.31	112.15	107.66
4	E	1	NAG	O3-C3-C4	2.26	115.71	110.38
4	E	4	MAN	C1-C2-C3	2.19	112.83	109.64
4	E	1	NAG	C2-N2-C7	-2.05	120.15	122.90
2	C	3	BMA	C6-C5-C4	-2.02	108.06	113.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C1-C2-N2-C7
5	F	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
4	E	4	MAN	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 5 short contacts:

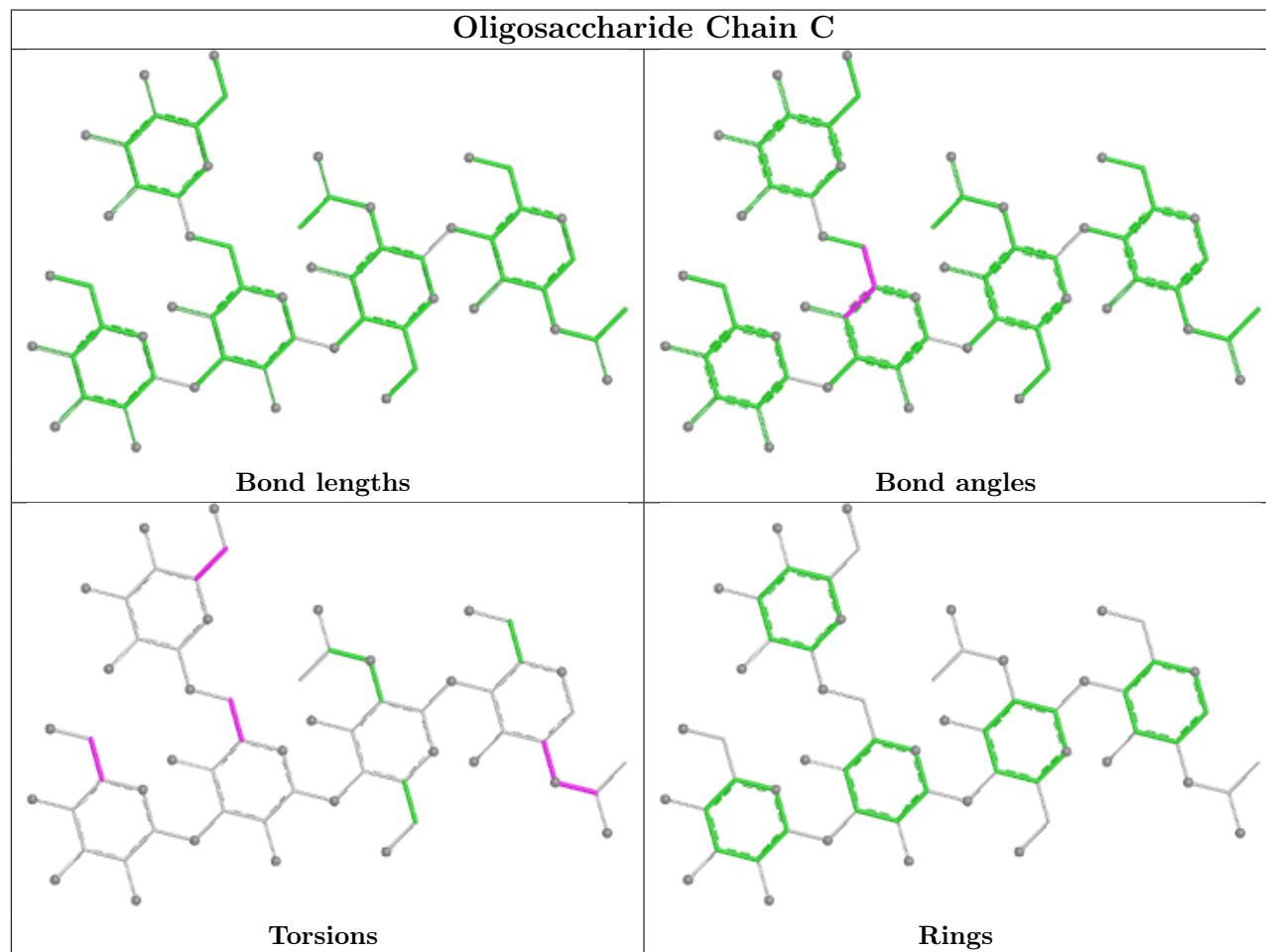
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
4	E	2	NAG	2	0
2	C	2	NAG	2	0
4	E	1	NAG	1	0
3	D	2	NAG	1	0

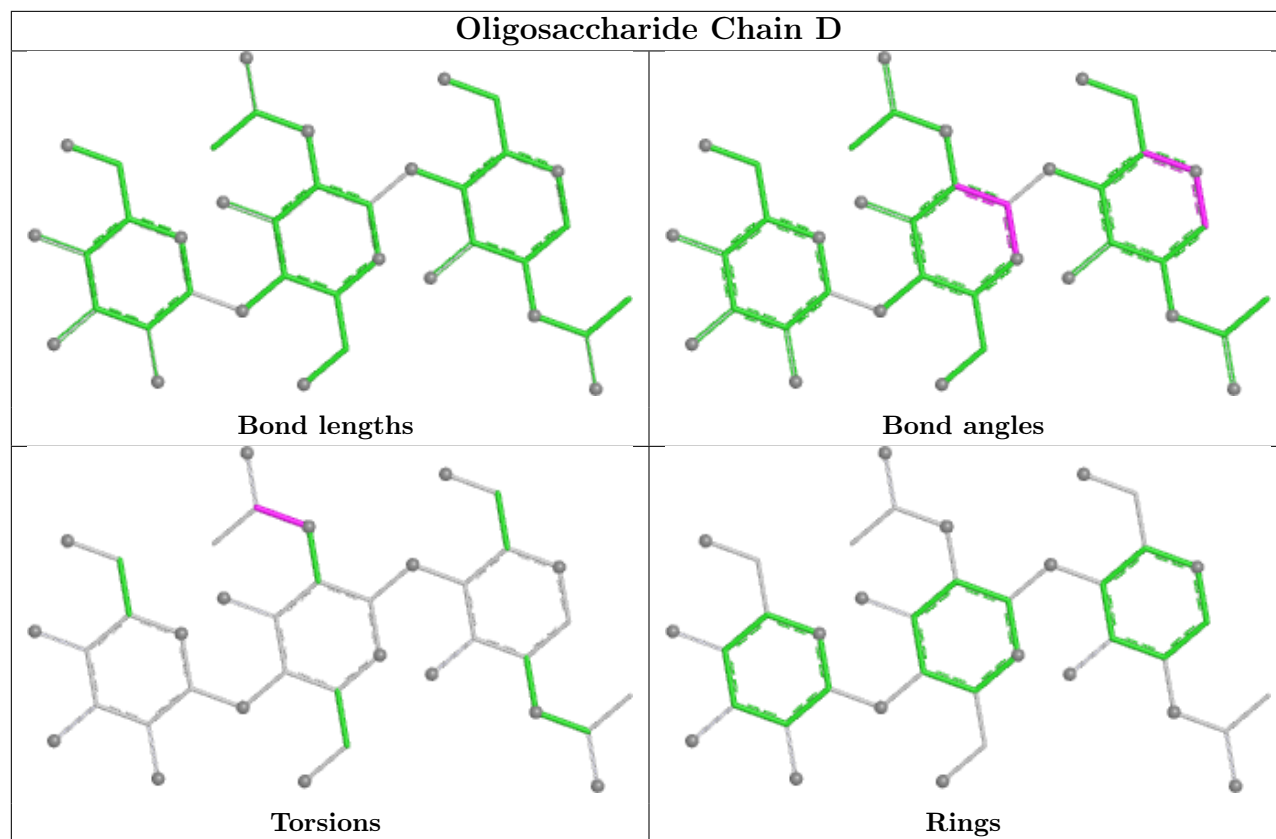
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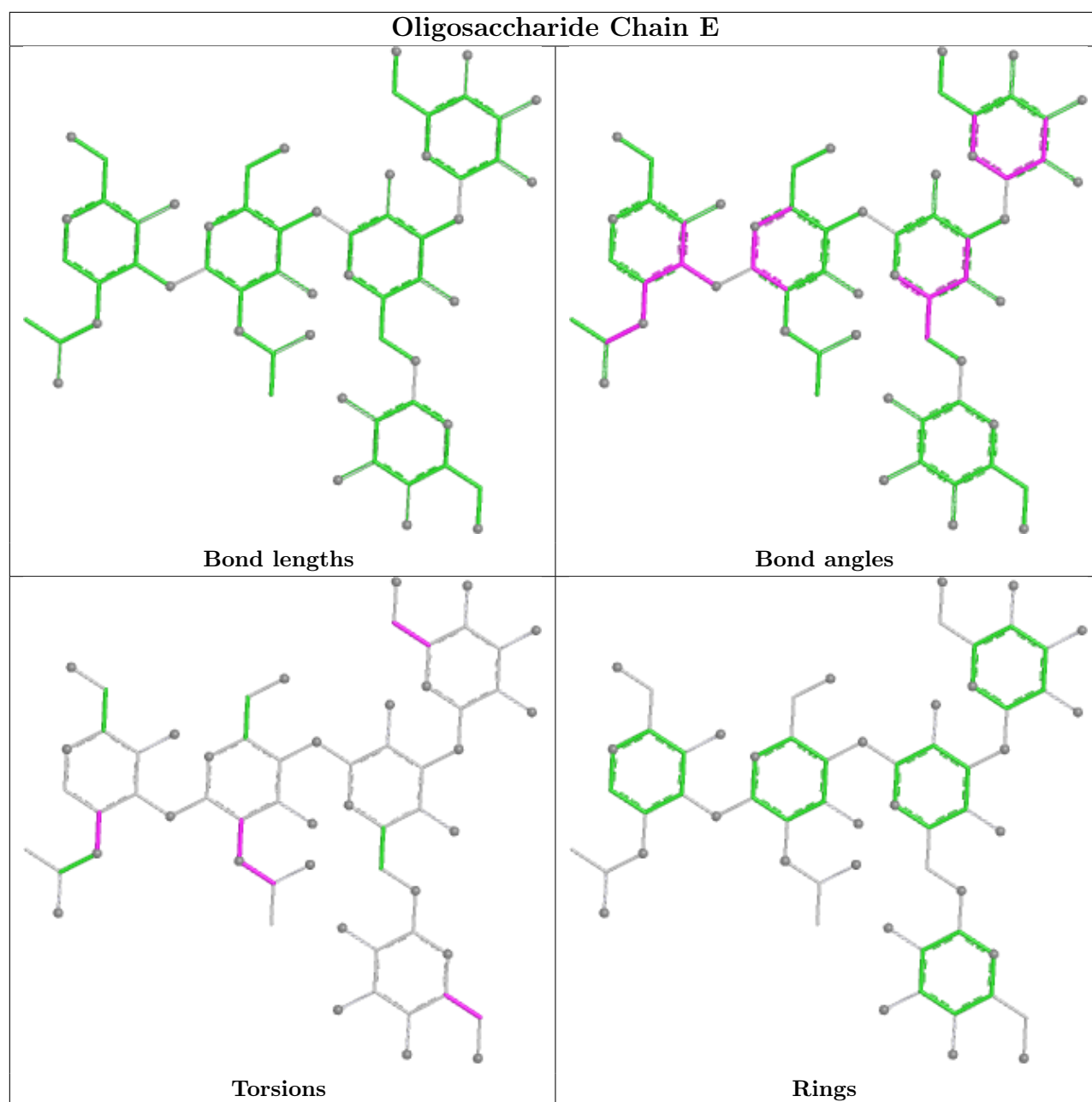
Continued from previous page...

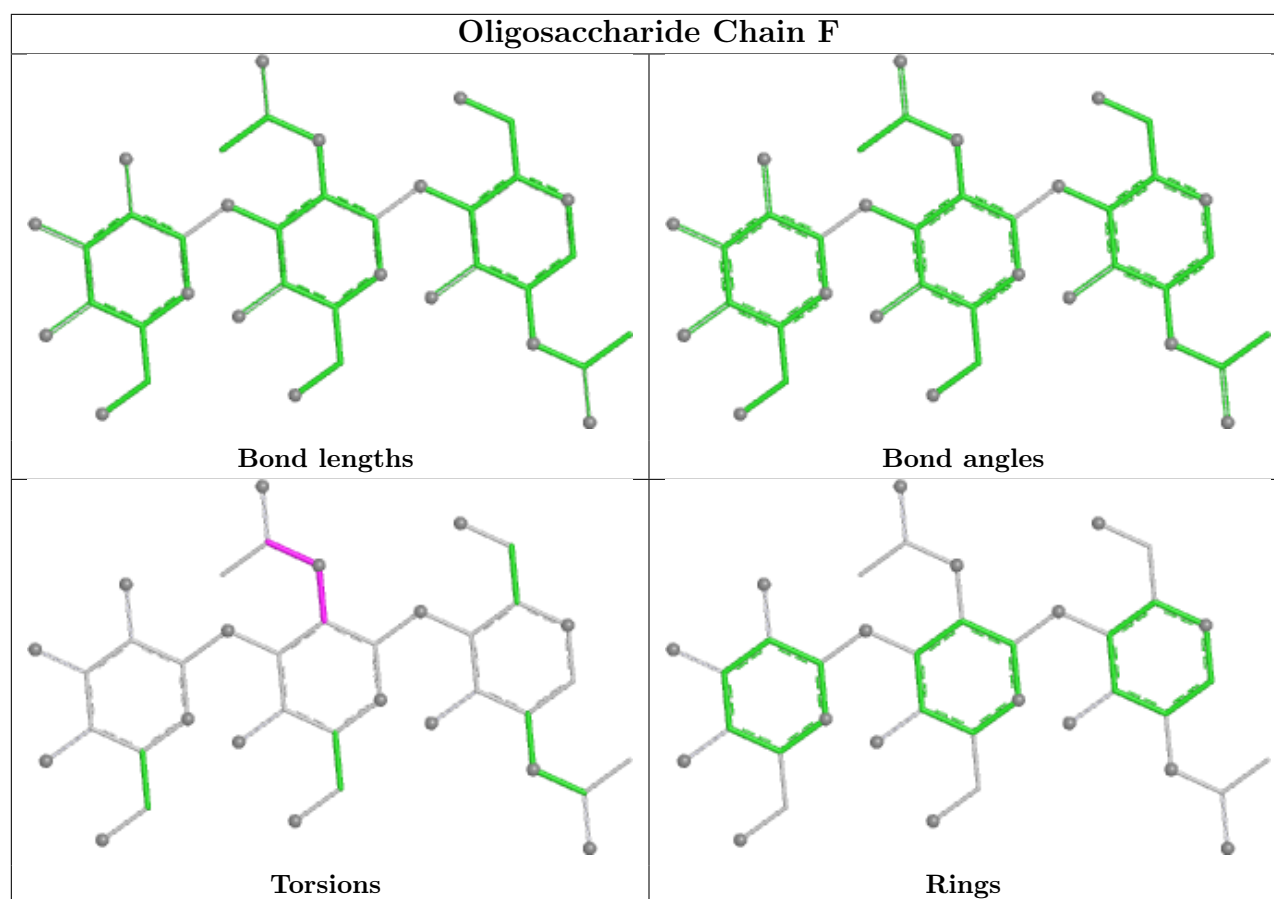
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	C	5	MAN	1	0

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](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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	A	4701	1	14,14,15	0.40	0	17,19,21	0.69	0
6	NAG	B	4701	1	14,14,15	0.59	0	17,19,21	1.34	3 (17%)

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	A	4701	1	-	0/6/23/26	0/1/1/1
6	NAG	B	4701	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	B	4701	NAG	O5-C5-C6	3.72	114.90	107.66
6	B	4701	NAG	C1-O5-C5	-2.18	109.26	112.19
6	B	4701	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	4701	NAG	C4-C5-C6-O6
6	B	4701	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

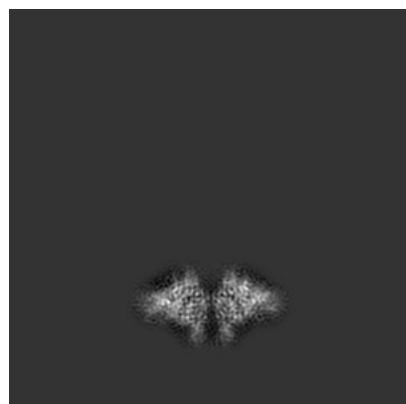
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36703. These allow visual inspection of the internal detail of the map and identification of artifacts.

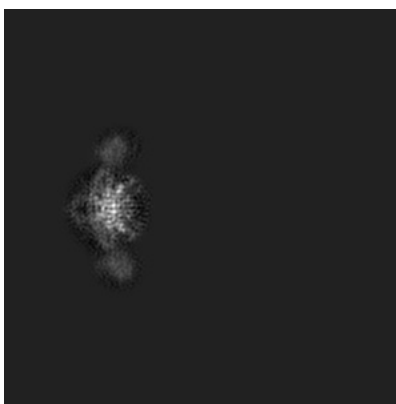
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

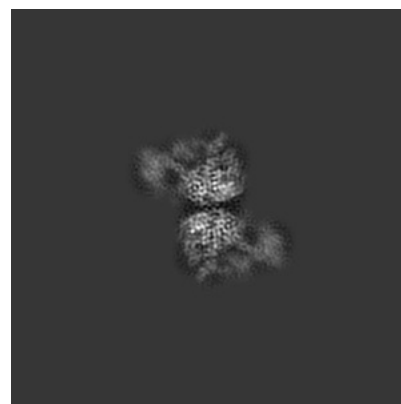
6.1.1 Primary map



X

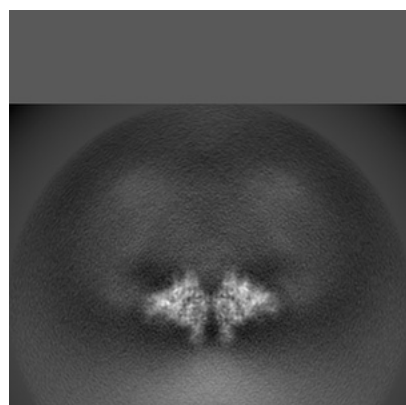


Y

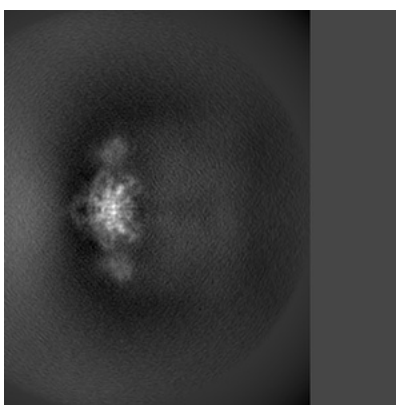


Z

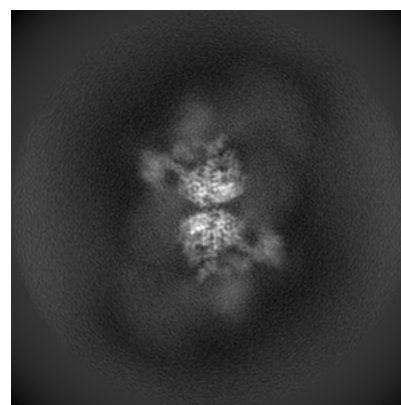
6.1.2 Raw map



X



Y

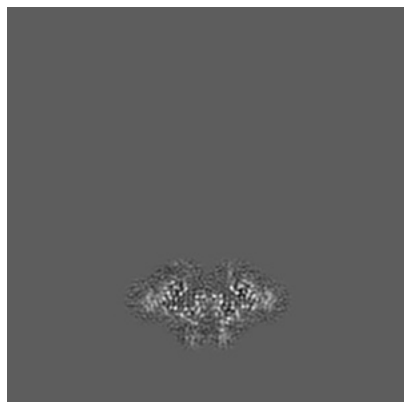


Z

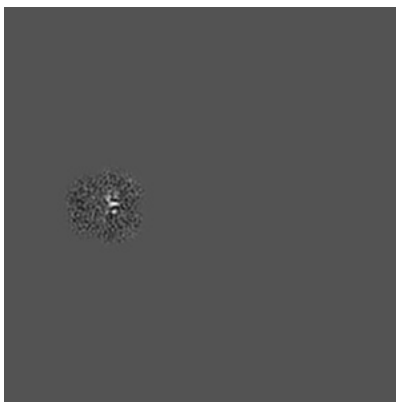
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

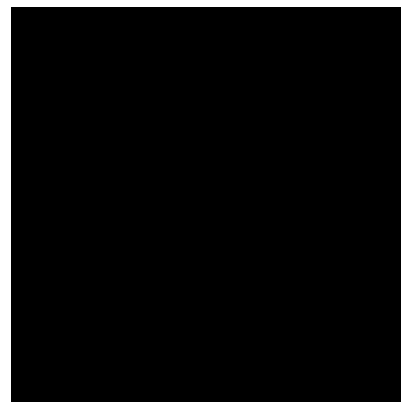
6.2.1 Primary map



X Index: 130

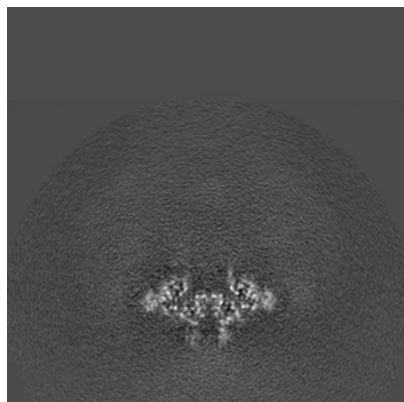


Y Index: 130

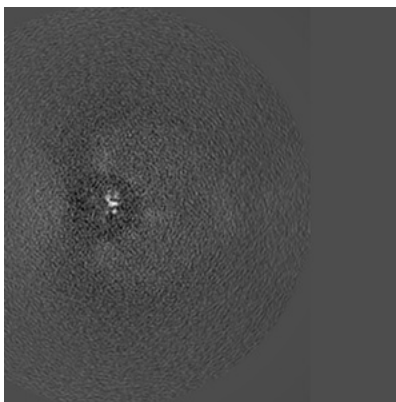


Z Index: 130

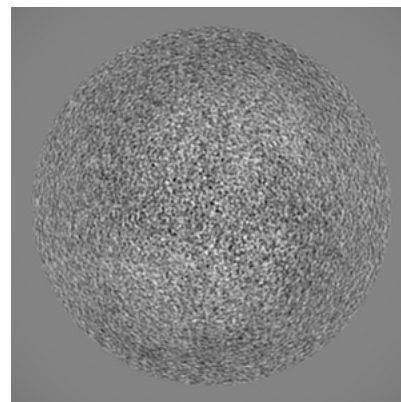
6.2.2 Raw map



X Index: 130



Y Index: 130



Z Index: 130

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

6.3 Largest variance slices [i](#)

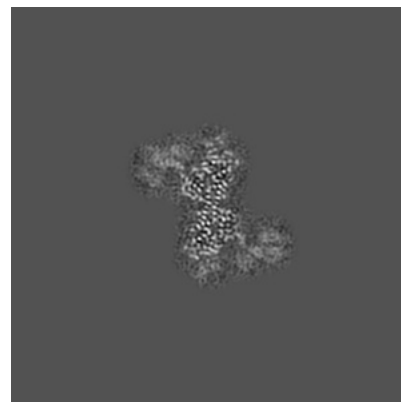
6.3.1 Primary map



X Index: 125

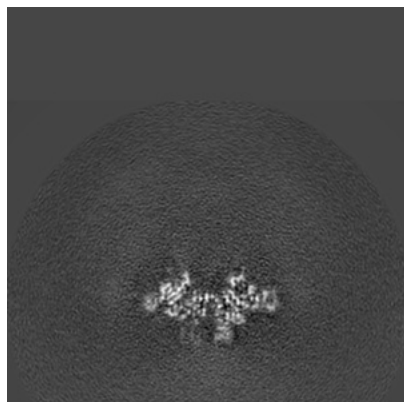


Y Index: 146

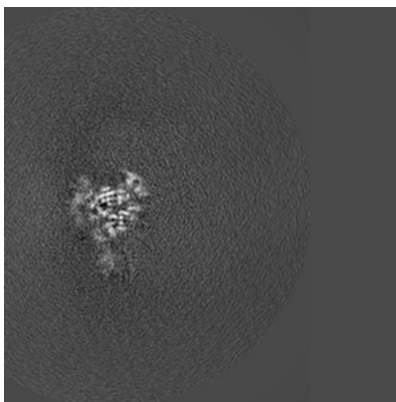


Z Index: 70

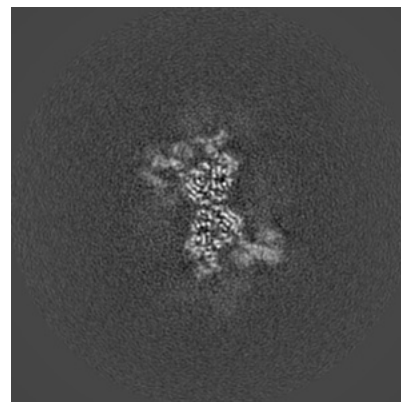
6.3.2 Raw map



X Index: 132



Y Index: 144

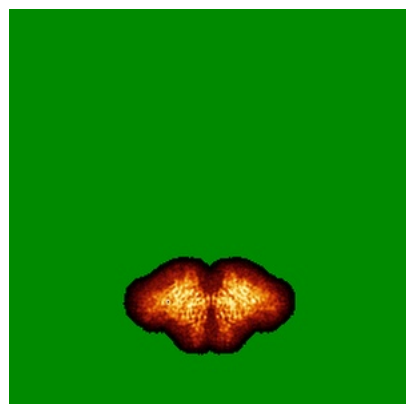


Z Index: 68

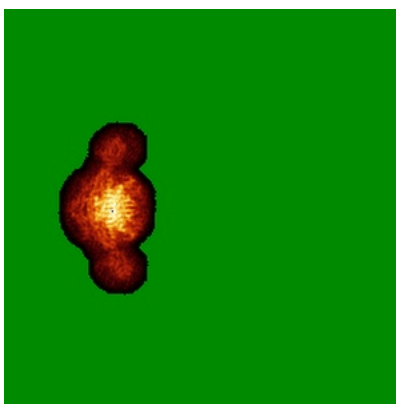
The images above show the largest variance slices of the map in three orthogonal directions.

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

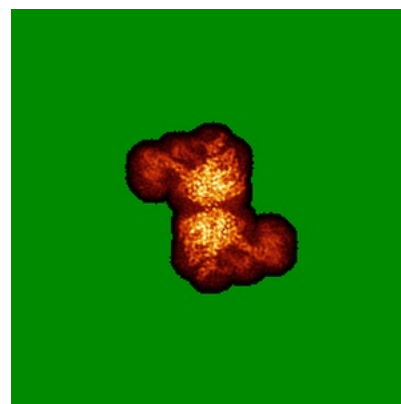
6.4.1 Primary map



X

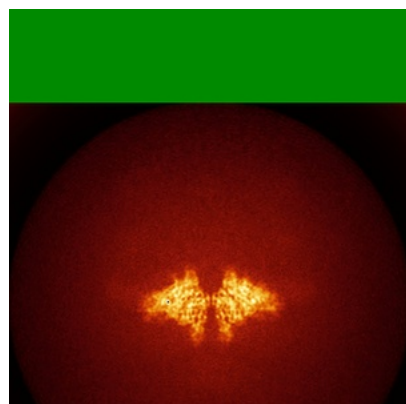


Y

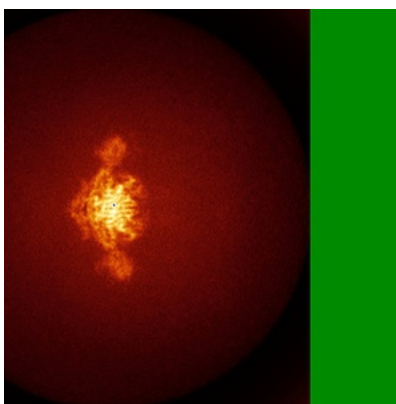


Z

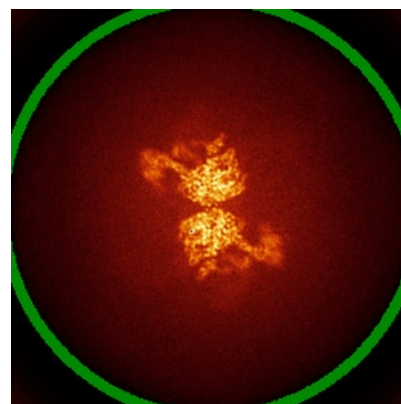
6.4.2 Raw map



X



Y

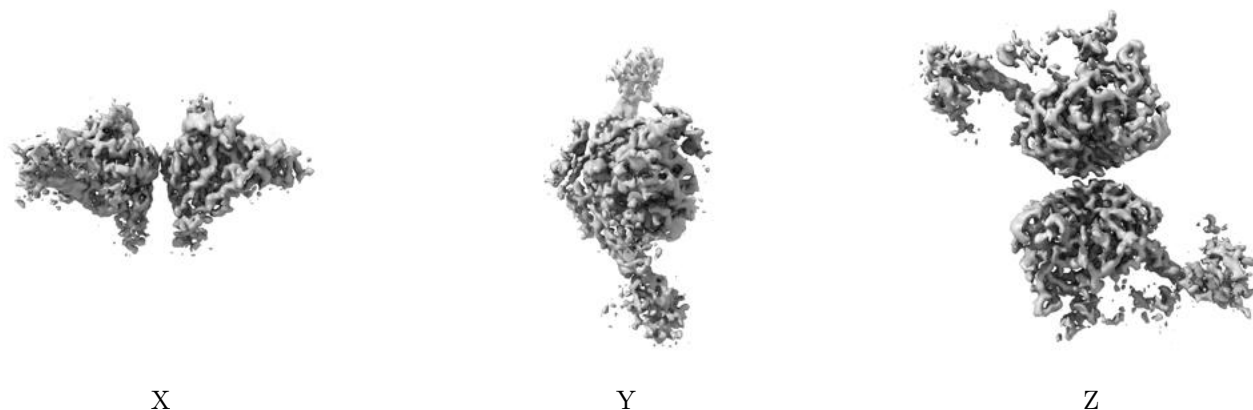


Z

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.

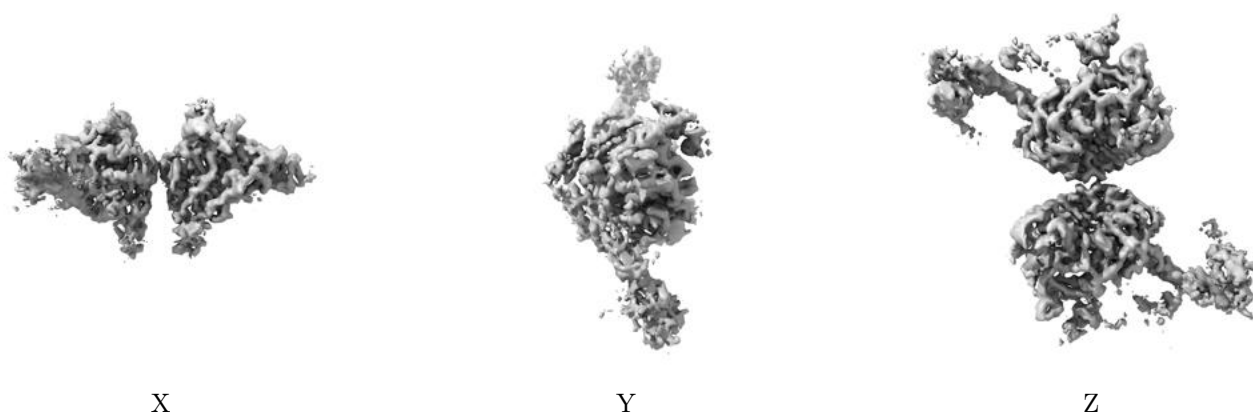
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. 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.

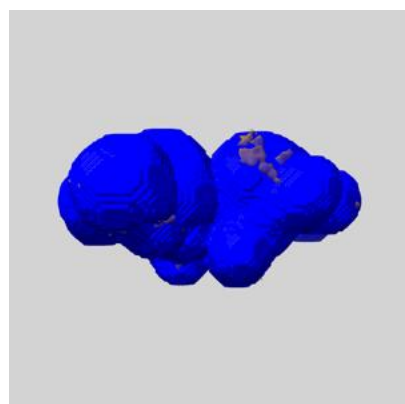
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

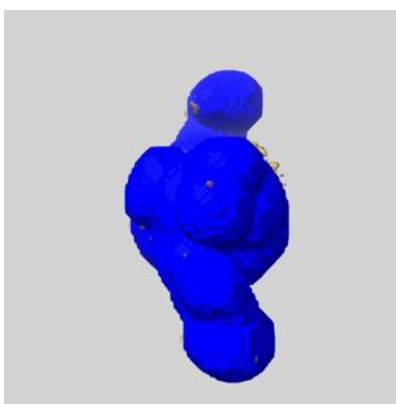
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

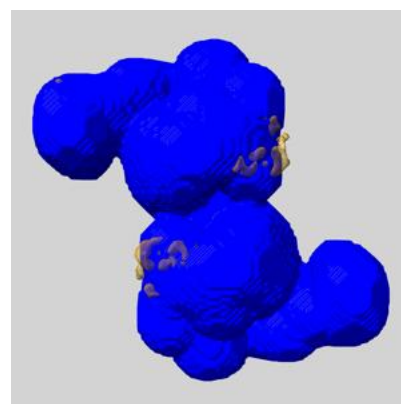
6.6.1 emd_36703_msk_1.map [i](#)



X



Y

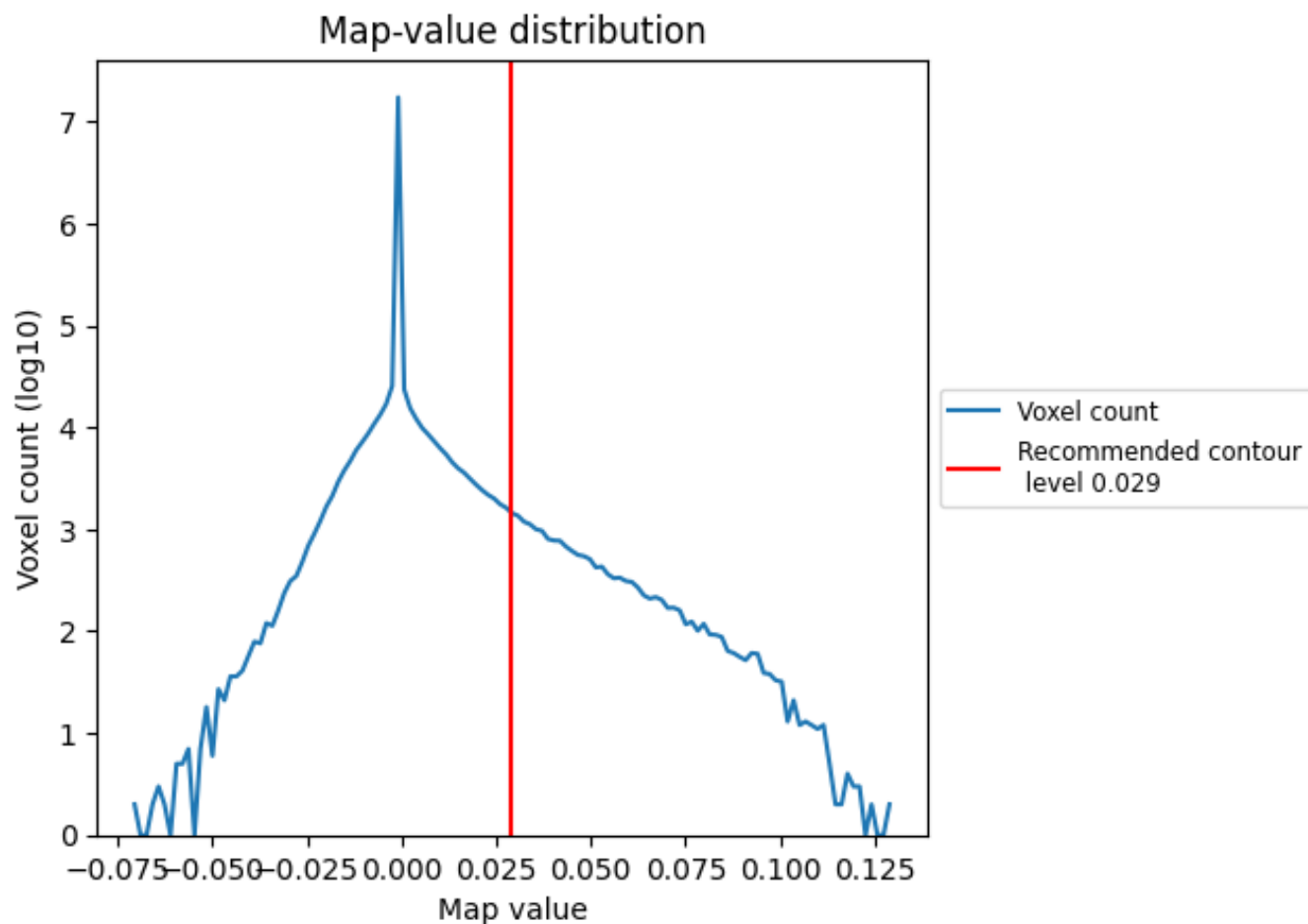


Z

7 Map analysis [i](#)

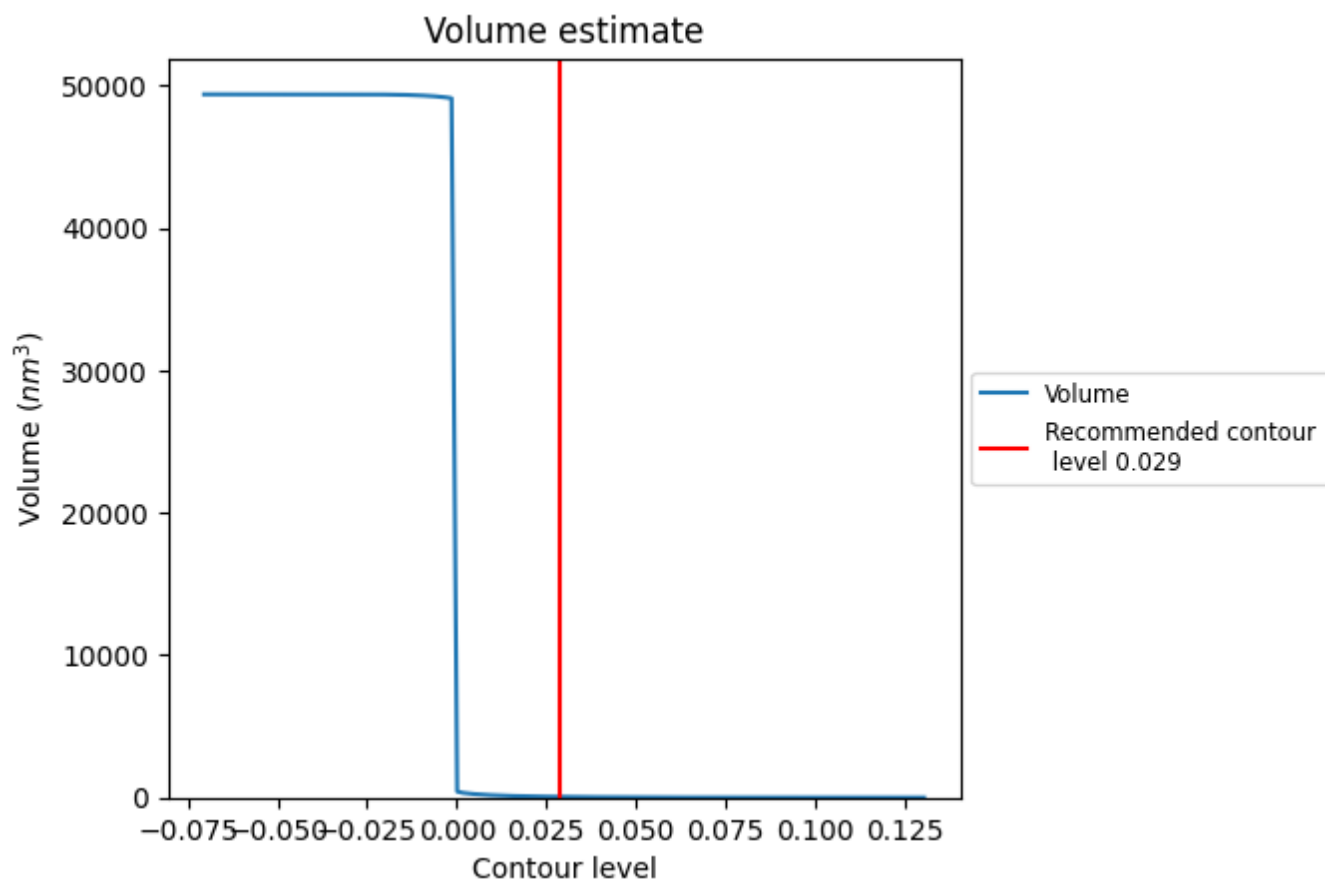
This section contains the results of statistical analysis of the map.

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.

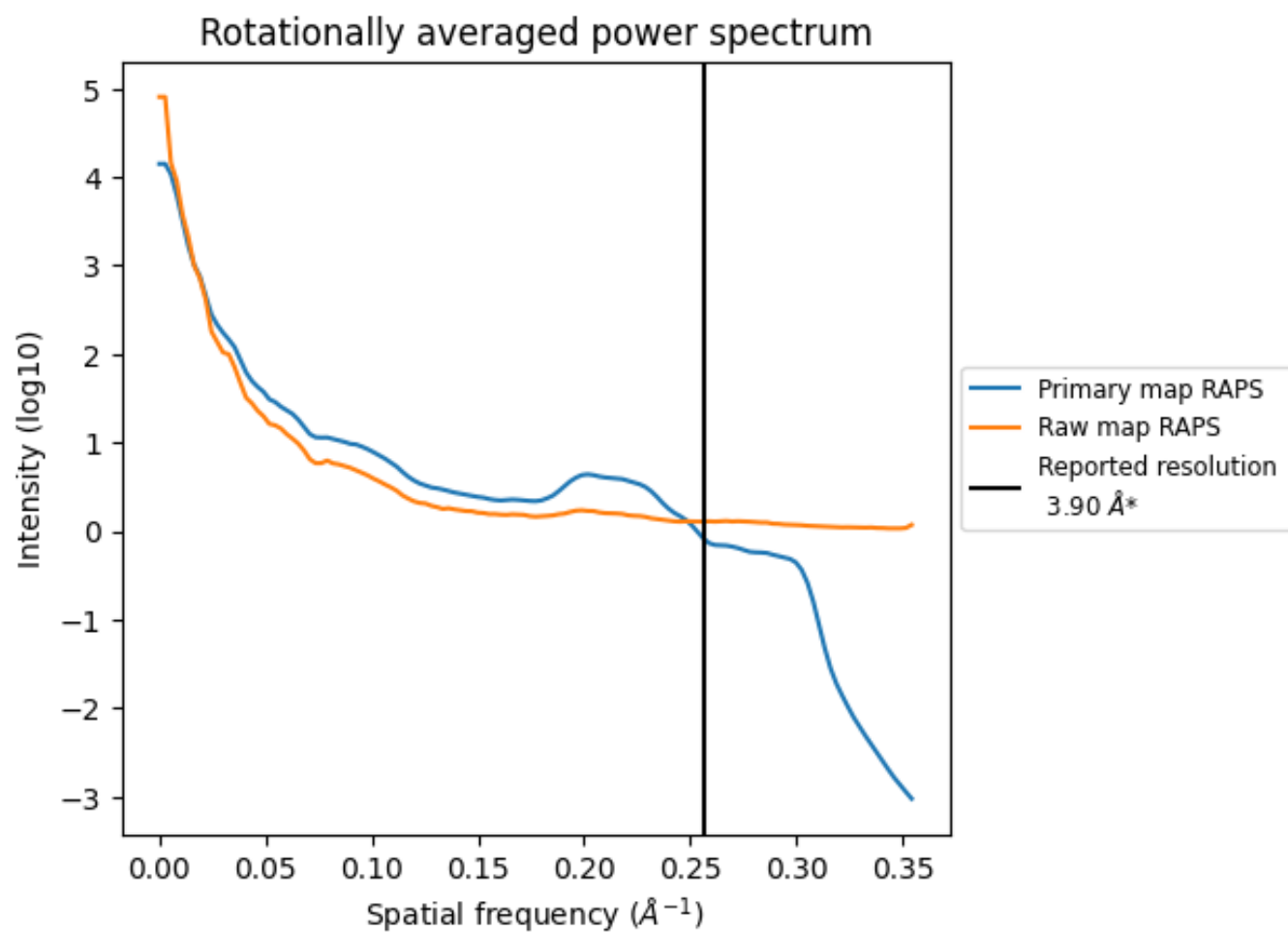
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm^3 ; this corresponds to an approximate mass of 46 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 ⓘ

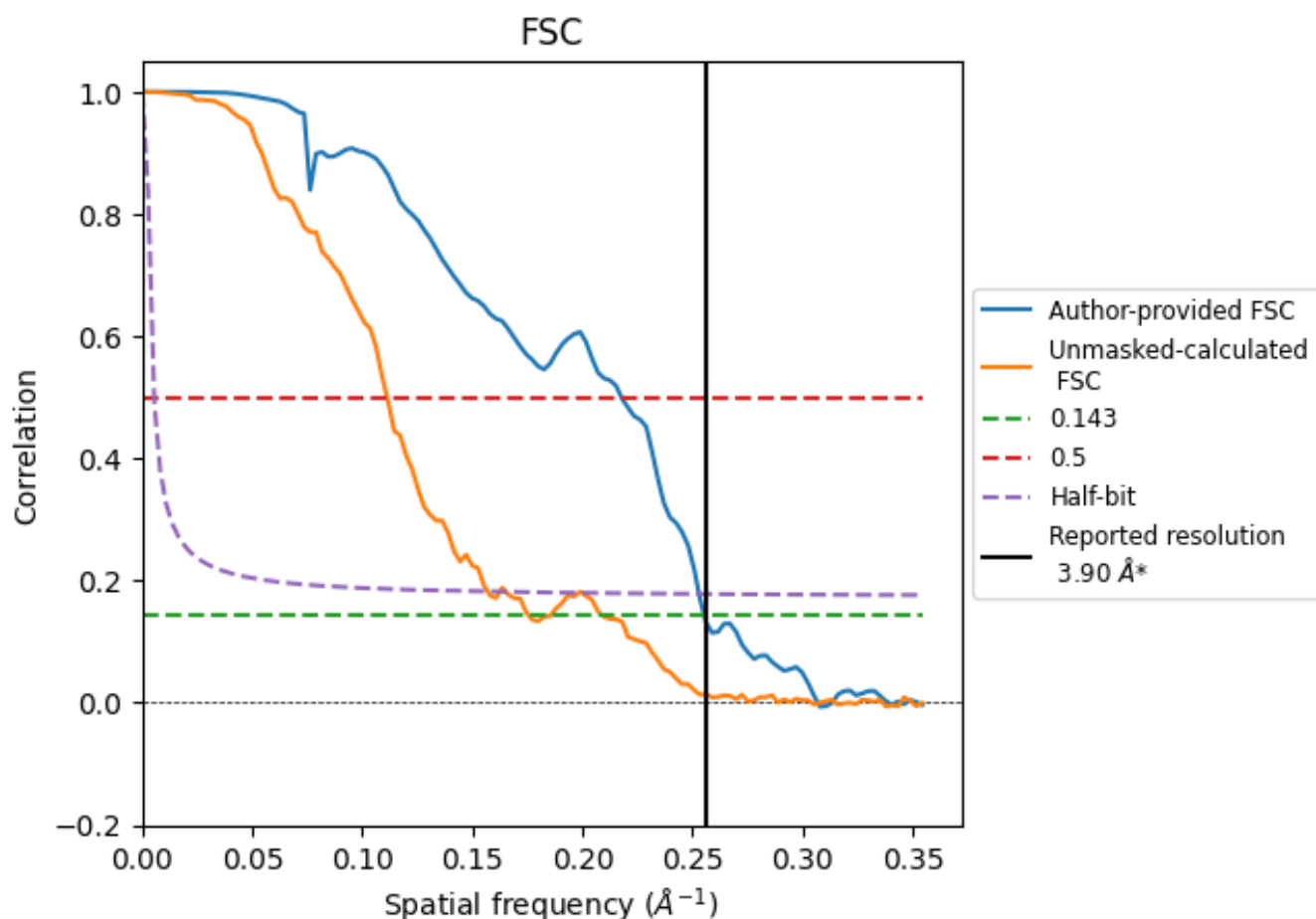


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

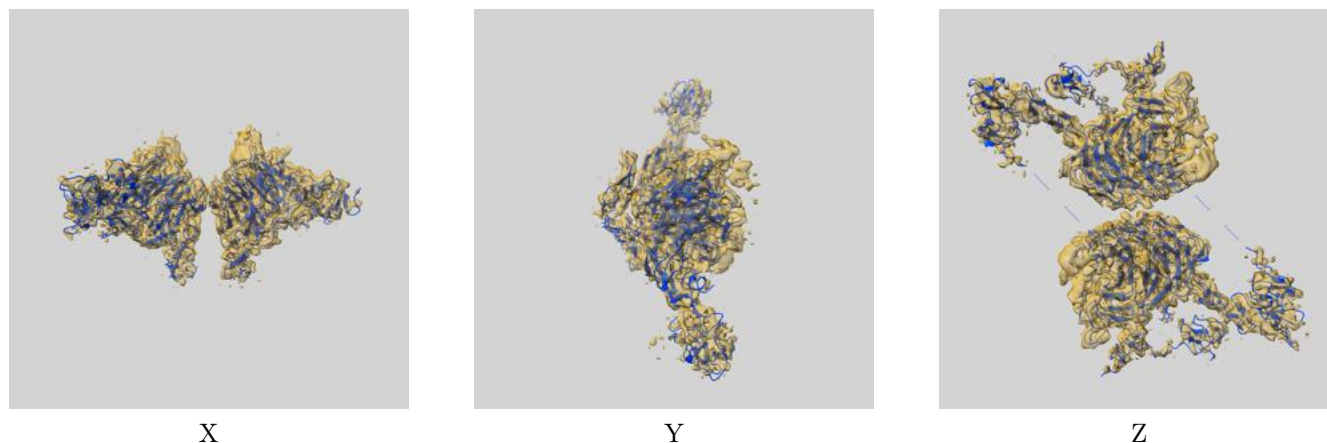
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.92	4.59	3.95
Unmasked-calculated*	5.70	8.99	6.37

*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 5.70 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

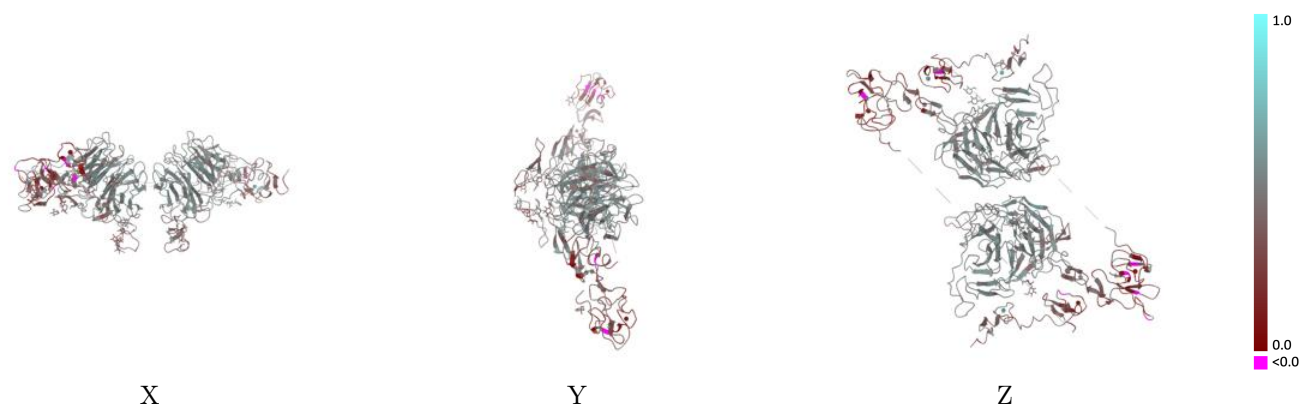
This section contains information regarding the fit between EMDB map EMD-36703 and PDB model 8JXJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



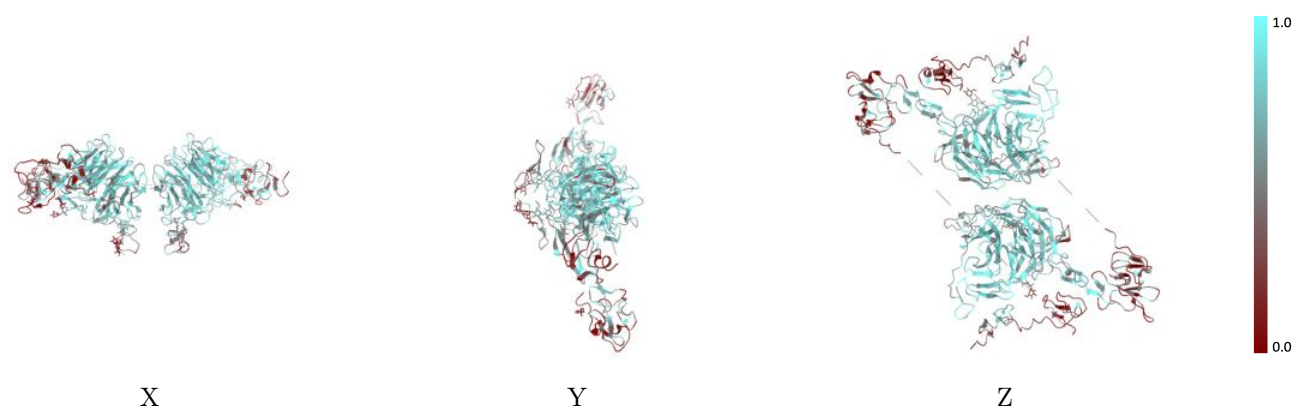
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



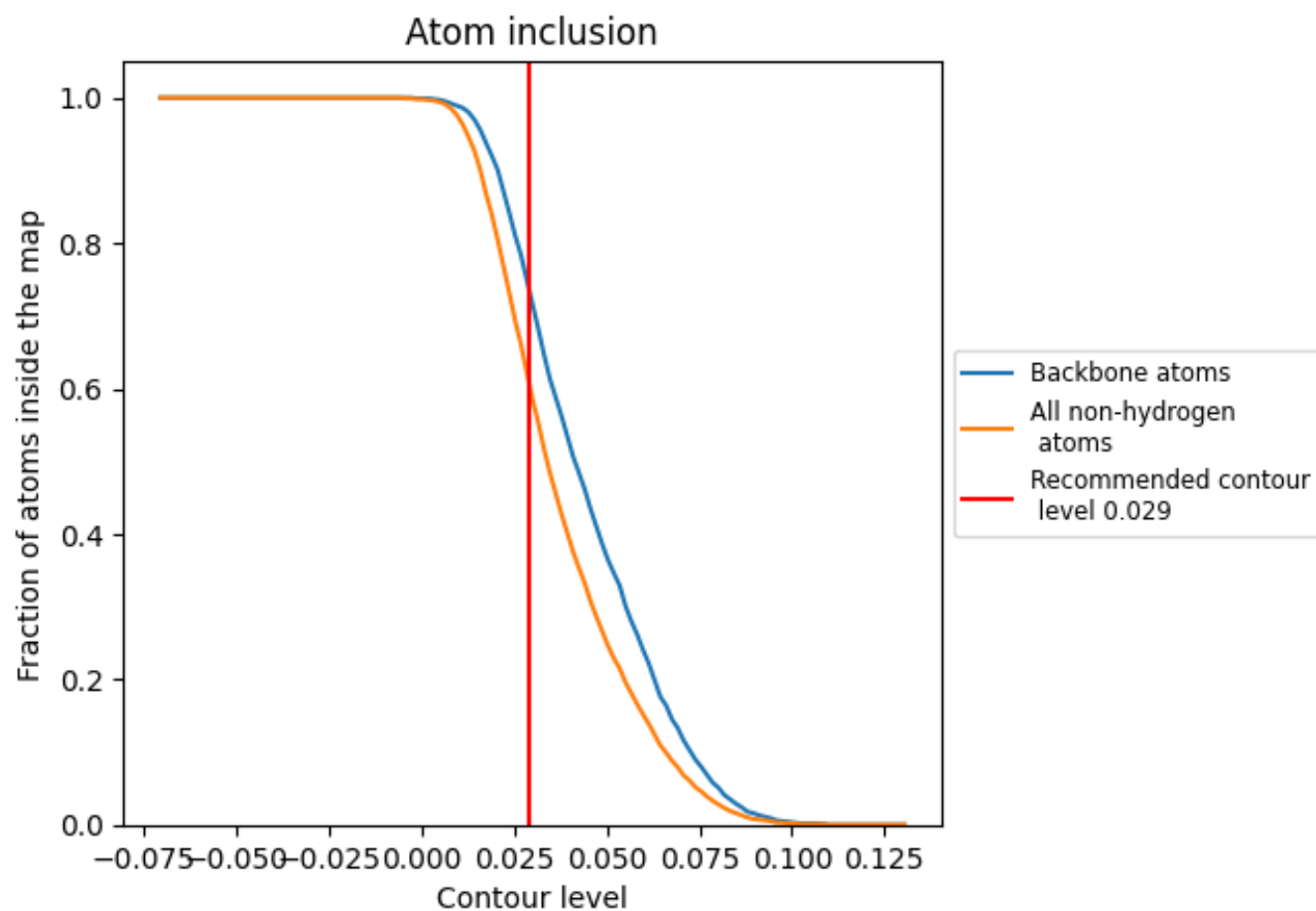
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 61% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6080	0.4350
A	0.6160	0.4360
B	0.6120	0.4370
C	0.2620	0.3610
D	0.5640	0.5250
E	0.2950	0.3590
F	0.5130	0.4320

1.0

0.0

<0.0