



Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 05:04 pm BST

PDB ID : 9FAV / pdb_00009fav
EMDB ID : EMD-50283
Title : CryoEM structure of human full-length beta3gamma2 GABA(A) receptor in complex with GARLH4, the TMD of Neuroligin2 and Megabody25, in a closed state (StateC2)
Authors : Kasaragod, V.B.; Aricescu, A.R.
Deposited on : 2024-05-10
Resolution : 3.20 Å (reported)
Based on initial model : 7QNB

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.44

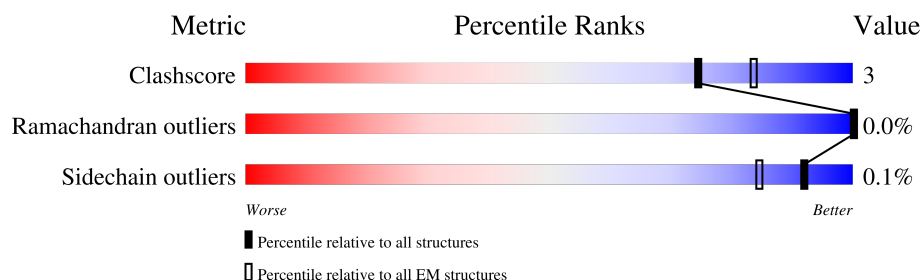
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.





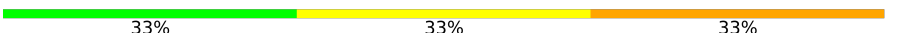
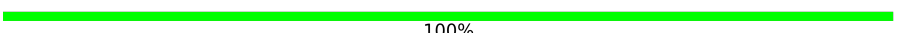
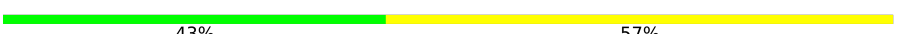
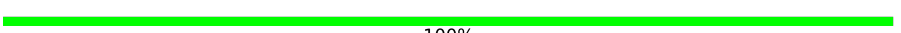




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	439	
1	B	439	
1	D	439	
1	E	439	
2	C	405	
3	H	33	
4	L	185	
5	F	522	

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Mol	Chain	Length	Quality of chain
5	K	522	 21% 78%
5	O	522	 20% 78%
6	G	3	 33% 33% 33%
6	N	3	 100%
7	I	7	 43% 57%
8	J	2	 100%
8	Q	2	 100%
9	M	6	 17% 83%
10	P	8	 38% 50% 12%
11	R	5	 20% 40% 60%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18975 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 Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	330	Total	C	N	O	S	0	0
			2712	1777	442	477	16		
1	E	331	Total	C	N	O	S	3	0
			2745	1805	444	480	16		
1	A	330	Total	C	N	O	S	2	0
			2731	1792	446	477	16		
1	D	330	Total	C	N	O	S	2	0
			2732	1795	443	478	16		

- Molecule 2 is a protein called Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	352	Total	C	N	O	S	2	0
			2951	1935	480	516	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	GLY	-	expression tag	UNP P18507

- Molecule 3 is a protein called Neuroligin-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	33	Total	C	N	O	0	0
			255	168	38	49		

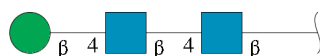
- Molecule 4 is a protein called LHFPL tetraspan subfamily member 4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	185	Total	C	N	O	S	1	0
			1432	953	226	238	15		

- Molecule 5 is a protein called Megabody25.

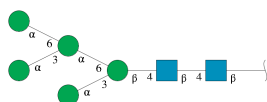
Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	117	Total	C	N	O	S	0	0
			912	575	156	177	4		
5	O	115	Total	C	N	O	S	0	0
			902	570	154	174	4		
5	F	117	Total	C	N	O	S	0	0
			912	575	156	177	4		

- Molecule 6 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
6	G	3	Total	C	N	O	0	0
			39	22	2	15		
6	N	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



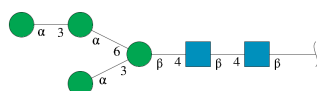
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



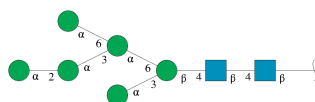
Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	2	Total	C	N	O	0	0
			28	16	2	10		
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



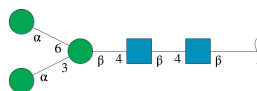
Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



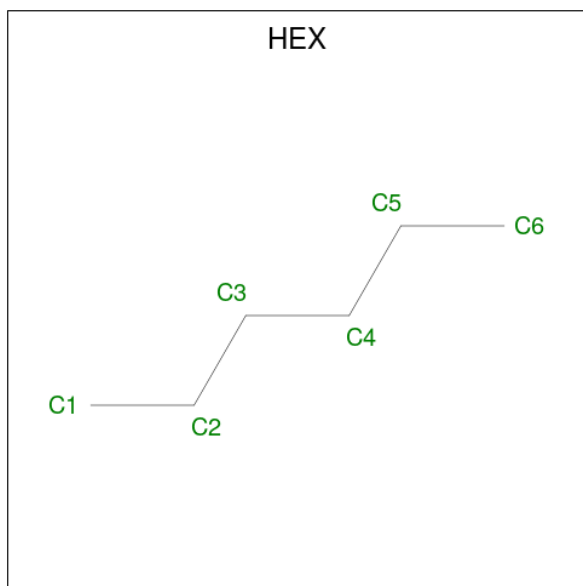
Mol	Chain	Residues	Atoms				AltConf	Trace
10	P	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 11 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.



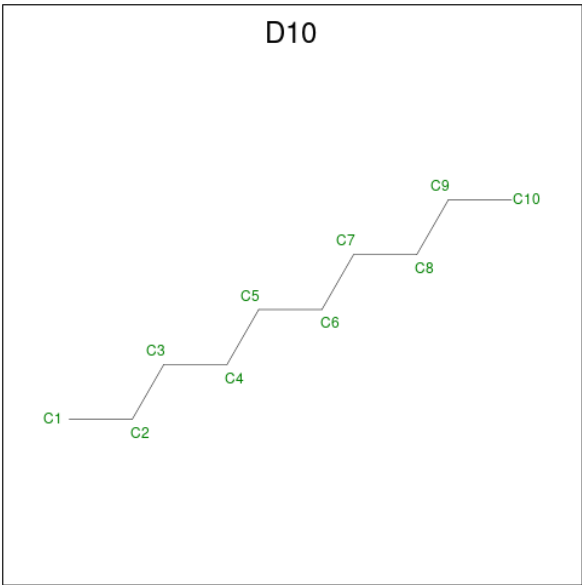
Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



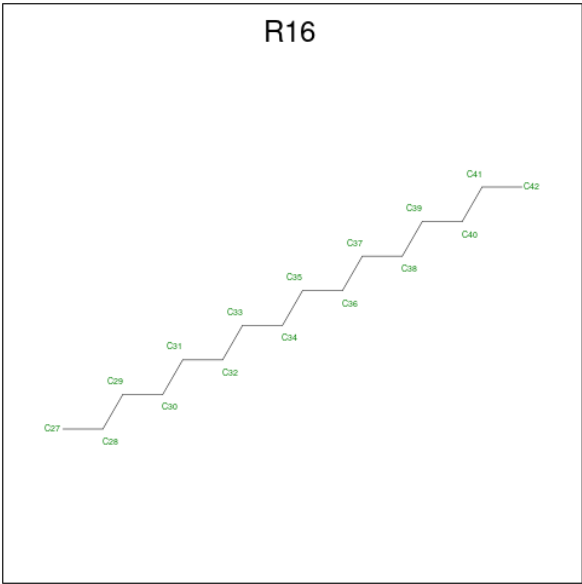
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	C	0
			6	6	
12	B	1	Total	C	0
			6	6	
12	E	1	Total	C	0
			6	6	
12	E	1	Total	C	0
			6	6	
12	A	1	Total	C	0
			6	6	

- Molecule 13 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



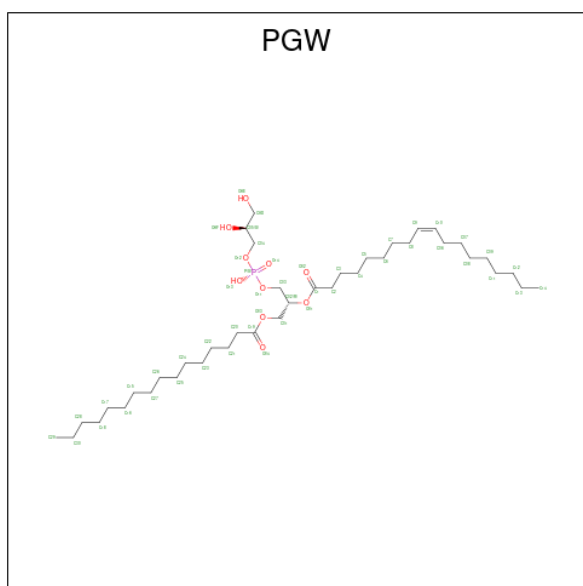
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total	C	0
			10	10	
13	E	1	Total	C	0
			10	10	
13	A	1	Total	C	0
			10	10	
13	C	1	Total	C	0
			10	10	

- Molecule 14 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



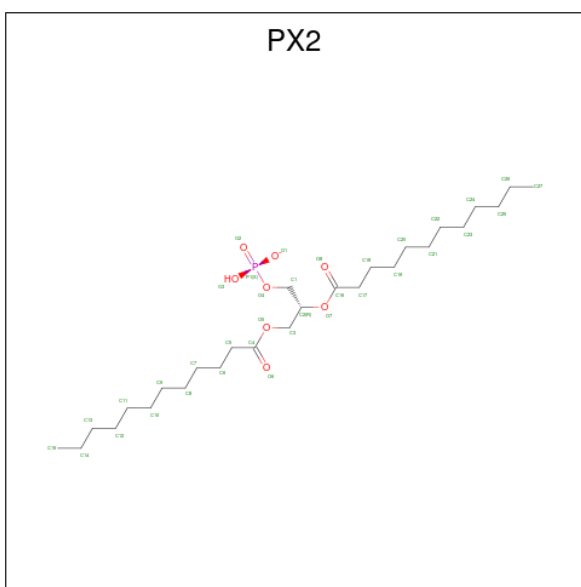
Mol	Chain	Residues	Atoms		AltConf
14	B	1	Total	C	0
			16	16	
14	C	1	Total	C	0
			16	16	
14	C	1	Total	C	0
			16	16	

- Molecule 15 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



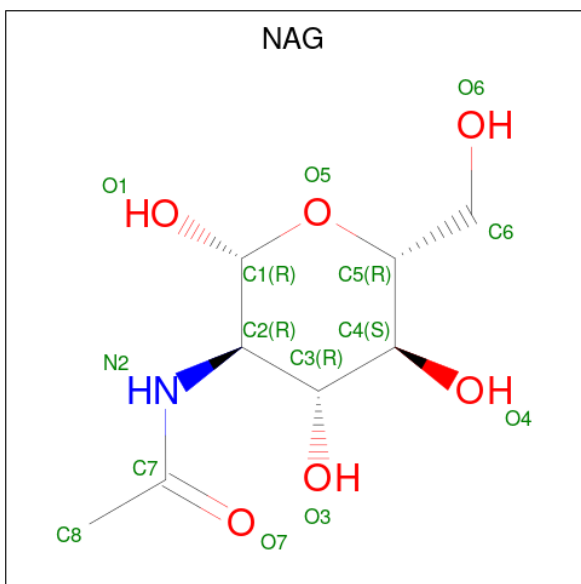
Mol	Chain	Residues	Atoms				AltConf
15	B	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 16 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: C₂₇H₅₂O₈P).



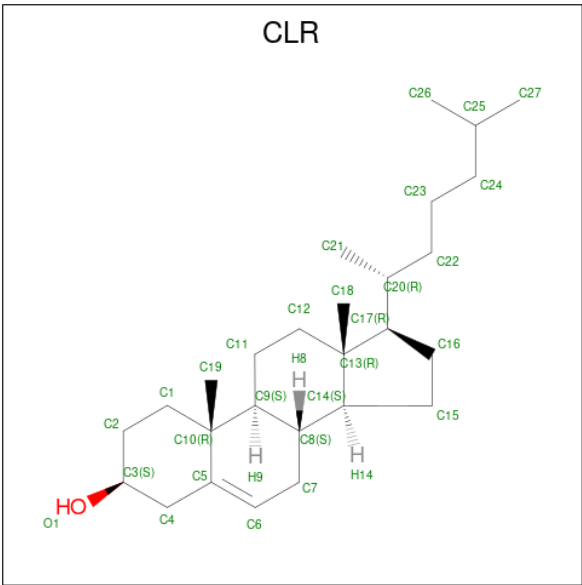
Mol	Chain	Residues	Atoms				AltConf
16	D	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 18 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			28	27	1	

GLY
ILE
GLY
ASP
THR
ARG
ASN
SER
ALA
ILE
SER
PHE
ASP
ASN
GLY
ILE
GLN
TVR
ARG
LYS
GLN
SER
MET
PRO
ARG
GLY
GLY
HIS
GLY
ARG
PHE
LEU
GLY
ASP
ARG
SER
LEU
PRO
HIS
LYS
LYS
THR
HIS
LEU
ARG
ARG
ARG
SER
SER
GLN
LEU
LYS
ILE
LYS
PRO
ASP
LEU
THR

D419
S427
V430
V447

- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3


Chain D:  70% 5% 25%

H9
L19
L27
Y62
Y74
D84
N85
R86
V87
S104
M115
D121
G122
T123
L128
D146
E147
Q148
E179
R180
I181
E182
I188
R192
A201
T202
L235
R269
E270
I275
L296
A300
R309
GLY
PRO
GLN
GLN
ARG
GLY
LYS
LYS

LEU
ALA
GLU
LYS
THR
ALA
LYS
ALA
ASN
ASP
ARG
ARG
SER
LYS
GLU
SER
ASN
ARG
VAL
ASP
ALA
HIS
HIS
ASN
TLE
LEU
LEU
THR
SER
LEU
GLU
VAL
HIS
ASN
GLU
MET
ASN
GLU
VAL
SER
GLY
GLY
TLE
GLY
ASP
THR
ASN
SER
ALA
ILE
SER
PHE
ASP
ASN
SER
GLY
GLN

TYR
ARG
LYS
GLN
MET
PRO
ARG
GLU
GLY
HIS
HIS
ARG
PHE
LEU
GLY
ASP
SER
ARG
SER
LEU
PRO
HIS
HIS
THR
HIS
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LEU
LYS
ILE
LYS
TLE
PRO
ASP
LEU
THR
D419
Y447

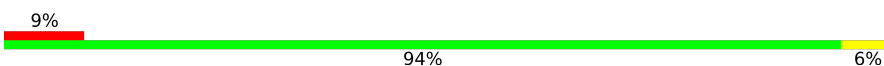
- Molecule 2: Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2

Chain C:  80% 7% 13%

G25
D26
V27
R43
P44
D45
G63
N66
N69
T73
I74
D75
S116
I124
T125
M135
D136
Y174
I179
R185
L250
V253
T305
L311
N323
K324
K325
PRO
LYS
LYS
ASP
LYS
ASP
LYS
LYS
LYS
LYS
ASN
PRO
ALA
PRO
THR
ILE
ASP

ILE
ARG
PRO
ARG
ALA
THR
ILE
GLN
MET
ASN
ASN
ALA
THR
HIS
HIS
LEU
GLN
GLU
ARG
ASP
GLU
GLU
GLU
TYR
TVR
GLU
C369
L370
D371
G372
K373
D374
C380
C381
C385
ARG
THR
GLY
ALA
TRP
ARG
HIS
GLY
ARG
ILE
E396
I408
S424
L428
Q429

- Molecule 3: Neuroligin-2

Chain H:  9% 94% 6%

D668
G683
F688
L689
N690
A695
Y699
K700

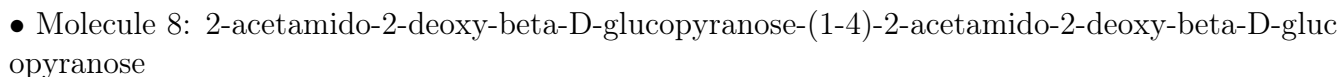
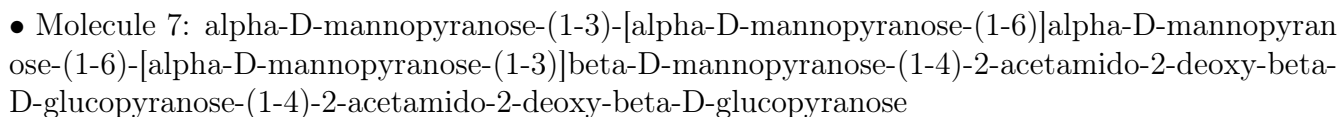
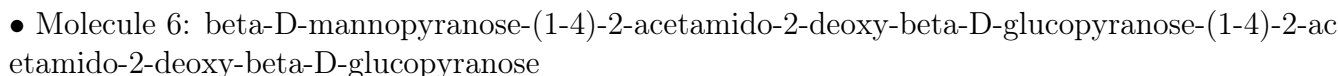
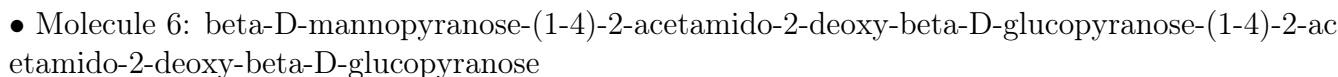
- Molecule 4: LHFPL tetraspan subfamily member 4 protein

Chain L:  90% 10%

R17
A21
L25
F29
A34
I42
S50
T53
G67
S68
G69
L70
A71
G72
R73
E74
L75
I87
A95
V99
I110
T111
S114
L133
L137
I182
L190
Q201

- Molecule 5: Megabody25

Chain K:  21% 78%



Chain J:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MAG1
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  17% 83%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  38% 50% 12%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 11: 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

Chain R:  20% 40% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26047	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 ($e^-/\text{\AA}^2$)	45.28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.591	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	338.25598, 338.25598, 338.25598	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, MAN, P1L, PGW, PX2, CLR, NAG, HEX, R16, BMA

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	0/2811	0.42	0/3824
1	B	0.17	0/2784	0.39	0/3787
1	D	0.16	0/2813	0.38	0/3828
1	E	0.17	0/2830	0.41	0/3851
2	C	0.30	0/2964	0.54	0/4024
3	H	0.17	0/259	0.36	0/352
4	L	0.17	0/1474	0.36	0/2003
5	F	0.16	0/935	0.38	0/1266
5	K	0.17	0/935	0.35	0/1266
5	O	0.18	0/925	0.39	0/1253
All	All	0.20	0/18730	0.42	0/25454

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2731	0	2728	30	0
1	B	2712	0	2705	19	0
1	D	2732	0	2724	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2745	0	2736	10	0
2	C	2951	0	2967	23	0
3	H	255	0	256	2	0
4	L	1432	0	1446	12	0
5	F	912	0	856	5	0
5	K	912	0	856	5	0
5	O	902	0	848	9	0
6	G	39	0	34	1	0
6	N	39	0	34	0	0
7	I	83	0	70	1	0
8	J	28	0	25	0	0
8	Q	28	0	25	0	0
9	M	72	0	61	1	0
10	P	94	0	79	1	0
11	R	61	0	52	1	0
12	A	6	0	14	0	0
12	B	12	0	28	0	0
12	E	12	0	28	0	0
13	A	10	0	22	1	0
13	B	10	0	22	0	0
13	C	10	0	22	2	0
13	E	10	0	22	0	0
14	B	16	0	34	0	0
14	C	32	0	68	0	0
15	B	51	0	76	0	0
16	D	36	0	52	0	0
17	C	14	0	13	0	0
18	C	28	0	46	0	0
All	All	18975	0	18949	114	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 3.

All (114) 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:225:THR:HG23	1:A:268:LEU:CD1	1.81	1.11
1:A:225:THR:HG21	1:A:281:ILE:HD11	1.38	1.00
1:A:225:THR:HG23	1:A:268:LEU:HD11	1.54	0.89
1:E:296:LEU:HD23	1:D:235:LEU:HD22	1.63	0.80
2:C:428:LEU:HD13	4:L:42:ILE:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HE	1:A:83:LEU:HD12	1.55	0.71
1:E:190:GLU:OE1	1:E:213:ARG:NH2	2.24	0.70
1:D:146:ASP:OD2	1:D:148:GLN:NE2	2.24	0.70
1:B:160:THR:OG1	1:B:204:ALA:O	2.13	0.67
1:D:62[B]:TYR:OH	1:D:115:MET:SD	2.50	0.67
1:A:146:ASP:OD2	1:A:148:GLN:NE2	2.28	0.66
1:A:225:THR:HG23	1:A:268:LEU:HD13	1.76	0.65
5:K:426:GLN:NE2	5:K:430:LYS:O	2.29	0.65
5:O:439:SER:O	5:O:459:ARG:NE	2.32	0.63
1:D:84:ASP:OD2	1:D:86:ARG:NH2	2.32	0.62
2:C:43:ARG:NH1	2:C:45:ASP:O	2.32	0.62
1:A:225:THR:CG2	1:A:268:LEU:CD1	2.71	0.62
1:A:87:VAL:HG13	1:A:91:LEU:HD13	1.81	0.61
1:B:26:ARG:NH1	1:A:85:ASN:OD1	2.34	0.61
1:E:44:ILE:HG21	1:E:181:ILE:HD11	1.83	0.61
1:D:128:LEU:CD1	2:C:125:THR:HG23	2.31	0.59
2:C:66:ASN:ND2	2:C:69:ASN:OD1	2.36	0.58
1:B:296:LEU:HD23	1:A:235:LEU:HD22	1.86	0.58
1:E:235:LEU:HD22	1:A:296:LEU:HD23	1.85	0.57
5:K:6:GLU:OE2	5:K:504:GLN:N	2.38	0.57
2:C:63:GLY:N	2:C:73:THR:O	2.39	0.56
1:D:104:SER:HB2	2:C:124:ILE:HD11	1.87	0.56
5:O:478:THR:HG22	5:O:510:VAL:H	1.71	0.54
1:A:87:VAL:HG11	1:A:116:ILE:HG21	1.90	0.53
5:F:6:GLU:OE2	5:F:483:CYS:N	2.41	0.53
1:B:26:ARG:NE	1:A:83:LEU:HD12	2.22	0.53
5:F:438:ILE:HD13	5:F:445:THR:HG22	1.90	0.52
2:C:408:ILE:HD11	13:C:504:D10:H52	1.92	0.51
1:D:104:SER:CB	2:C:124:ILE:HD11	2.41	0.51
1:D:270:GLU:N	1:D:270:GLU:OE2	2.45	0.50
1:B:104:SER:CB	1:B:132:THR:HG22	2.41	0.50
5:O:450:SER:O	5:O:454:ARG:NH2	2.43	0.50
1:A:190:GLU:OE1	1:A:213:ARG:NH2	2.44	0.50
1:A:101:ASP:OD1	1:A:102:LYS:N	2.45	0.50
1:B:235:LEU:HD22	2:C:311:LEU:HD23	1.93	0.49
1:A:245:ASP:OD1	1:A:246:ALA:N	2.46	0.49
1:A:258:VAL:O	1:A:262:THR:HG23	2.13	0.48
1:B:130:ILE:HG22	1:B:132:THR:HG23	1.95	0.48
1:B:155:GLU:OE1	1:B:207:ARG:NH2	2.46	0.48
1:D:300:ALA:HB2	2:C:253:VAL:HG13	1.96	0.48
1:B:84:ASP:O	1:B:87:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:SER:HB3	1:B:132:THR:HG22	1.96	0.48
1:B:227:MET:CE	2:C:305:ILE:HD11	2.44	0.48
1:A:301:PHE:CE1	13:A:501:D10:H22	2.49	0.47
1:A:47:ILE:HG22	1:A:47:ILE:O	2.13	0.47
2:C:408:ILE:HD11	13:C:504:D10:C5	2.44	0.47
1:B:142:ARG:O	1:B:145:LEU:N	2.47	0.47
4:L:67:GLY:HA2	4:L:75:LEU:HD23	1.96	0.47
5:F:438:ILE:HD13	5:F:445:THR:CG2	2.44	0.47
1:E:121:ASP:OD1	1:E:122:GLY:N	2.47	0.47
1:E:199:VAL:HG21	5:O:497:THR:HG21	1.97	0.47
1:A:64:GLN:OE1	1:A:169:ARG:NH2	2.46	0.47
1:A:155:GLU:OE1	1:A:207:ARG:NH2	2.44	0.47
1:D:182:GLU:OE1	1:D:182:GLU:N	2.47	0.47
5:F:504:GLN:OE1	5:F:504:GLN:N	2.45	0.47
2:C:135:ASN:OD1	2:C:136:ASP:N	2.49	0.46
2:C:424:SER:HA	2:C:428:LEU:HD11	1.97	0.46
4:L:111:THR:O	4:L:114:SER:OG	2.32	0.46
1:D:296:LEU:HD23	2:C:250:LEU:HD22	1.96	0.46
4:L:34:ALA:HB2	4:L:110:ILE:HD11	1.98	0.46
2:C:373:LYS:O	2:C:374:ASP:C	2.58	0.46
2:C:428:LEU:CD1	4:L:42:ILE:HD12	2.43	0.46
1:A:38:VAL:HG12	1:A:40:MET:HE2	1.97	0.46
1:A:47:ILE:HD12	1:A:181:ILE:HG12	1.98	0.46
5:O:500:ASP:N	5:O:500:ASP:OD1	2.49	0.46
1:A:40:MET:HG3	1:A:208:LEU:HD22	1.97	0.46
3:H:683:GLY:HA3	4:L:182:ILE:HD13	1.98	0.46
2:C:174:TYR:CG	2:C:179:ILE:HD12	2.50	0.45
4:L:133:LEU:O	4:L:137:LEU:HD23	2.16	0.45
6:G:2:NAG:H83	6:G:2:NAG:H3	1.99	0.45
1:D:19:LEU:HD21	1:D:74:TYR:HB3	1.98	0.45
1:B:243:ASN:OD1	2:C:323:ASN:ND2	2.50	0.45
1:E:139:ASP:OD1	1:E:141:ARG:NH1	2.50	0.45
5:F:431:GLU:N	5:F:431:GLU:OE1	2.49	0.45
1:A:225:THR:CG2	1:A:268:LEU:HD13	2.42	0.45
1:D:121:ASP:OD1	1:D:123:THR:HG22	2.17	0.44
5:K:470:MET:HB3	5:K:473:LEU:HD21	1.97	0.44
1:D:84:ASP:O	1:D:87:VAL:HG12	2.17	0.44
1:B:129:ARG:NH2	2:C:116:SER:O	2.48	0.44
1:B:146:ASP:OD1	1:B:146:ASP:N	2.51	0.44
1:B:286:MET:HE1	1:A:228:PRO:HG3	1.98	0.44
1:A:15:THR:HG21	1:A:77:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLY:O	1:B:257:THR:OG1	2.28	0.43
2:C:370:LEU:C	2:C:372:GLY:H	2.25	0.43
5:O:439:SER:OG	5:O:440:TRP:N	2.50	0.43
1:B:192:ARG:HG3	7:I:1:NAG:H83	1.99	0.43
5:O:421:MET:HE2	5:O:459:ARG:HH22	1.82	0.43
4:L:95:ALA:O	4:L:99:VAL:HG23	2.19	0.43
1:D:146:ASP:OD1	1:D:146:ASP:N	2.52	0.43
1:A:225:THR:HG21	1:A:281:ILE:CD1	2.28	0.43
1:A:266:THR:HG23	1:A:269:ARG:HH22	1.83	0.43
1:D:179:GLU:HG3	5:O:493:LEU:HD11	2.00	0.42
1:D:181:ILE:HG21	1:D:188:ILE:HD11	2.00	0.42
1:E:173:LYS:NZ	5:K:449:ASP:OD2	2.52	0.42
1:D:104:SER:OG	2:C:124:ILE:HD11	2.20	0.42
3:H:690:ASN:HD21	4:L:29:PHE:HB3	1.85	0.42
10:P:3:BMA:H62	10:P:4:MAN:H2	1.60	0.42
4:L:21:ALA:O	4:L:25:LEU:HD23	2.20	0.41
9:M:1:NAG:O3	9:M:2:NAG:O5	2.33	0.41
4:L:50:SER:N	4:L:53:THR:OG1	2.53	0.41
5:K:6:GLU:OE2	5:K:505:GLY:N	2.45	0.41
1:D:275:ILE:O	1:D:275:ILE:HG23	2.20	0.41
1:E:12:VAL:O	1:E:15:THR:HG22	2.20	0.41
1:A:427:SER:HA	1:A:430:VAL:HG12	2.03	0.41
1:D:192:ARG:NH2	11:R:1:NAG:O3	2.50	0.41
4:L:29:PHE:HB2	4:L:190:LEU:HD21	2.02	0.41
1:E:146:ASP:OD1	1:E:146:ASP:N	2.55	0.40
1:D:27:LEU:HD11	2:C:27:VAL:HG21	2.03	0.40
5:O:419:PRO:HG2	5:O:420:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/439 (75%)	315 (96%)	13 (4%)	0	100	100
1	B	326/439 (74%)	309 (95%)	17 (5%)	0	100	100
1	D	328/439 (75%)	313 (95%)	15 (5%)	0	100	100
1	E	330/439 (75%)	320 (97%)	10 (3%)	0	100	100
2	C	346/405 (85%)	326 (94%)	19 (6%)	1 (0%)	37	69
3	H	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
4	L	184/185 (100%)	179 (97%)	5 (3%)	0	100	100
5	F	113/522 (22%)	107 (95%)	6 (5%)	0	100	100
5	K	113/522 (22%)	109 (96%)	4 (4%)	0	100	100
5	O	111/522 (21%)	104 (94%)	7 (6%)	0	100	100
All	All	2210/3945 (56%)	2112 (96%)	97 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	63	GLY

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	299/392 (76%)	299 (100%)	0	100	100
1	B	297/392 (76%)	297 (100%)	0	100	100
1	D	299/392 (76%)	299 (100%)	0	100	100
1	E	300/392 (76%)	300 (100%)	0	100	100
2	C	322/366 (88%)	320 (99%)	2 (1%)	84	92
3	H	27/27 (100%)	27 (100%)	0	100	100
4	L	152/151 (101%)	152 (100%)	0	100	100
5	F	94/430 (22%)	94 (100%)	0	100	100
5	K	94/430 (22%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	O	93/430 (22%)	93 (100%)	0	100	100
All	All	1977/3402 (58%)	1975 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	75	ASP
2	C	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
2	C	318	HIS
3	H	690	ASN
5	F	414	HIS
5	F	426	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	P1L	C	380	2	21,22,23	1.07	1 (4%)	18,23,25	1.54	3 (16%)
2	P1L	C	381	2	21,22,23	0.60	0	18,23,25	1.93	3 (16%)
2	P1L	C	385	2	21,22,23	1.07	1 (4%)	18,23,25	1.45	2 (11%)

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	P1L	C	380	2	-	5/20/22/24	-
2	P1L	C	381	2	-	5/20/22/24	-
2	P1L	C	385	2	-	10/20/22/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	385	P1L	O-C	4.14	1.36	1.19
2	C	380	P1L	O-C	4.09	1.36	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	381	P1L	CB-SG-C7	6.61	110.08	100.84
2	C	385	P1L	CB-SG-C7	5.07	107.93	100.84
2	C	380	P1L	CB-SG-C7	4.29	106.84	100.84
2	C	380	P1L	C8-C7-SG	-3.82	109.01	113.46
2	C	381	P1L	C8-C7-SG	-3.29	109.63	113.46
2	C	381	P1L	O7-C7-SG	2.88	126.35	122.61
2	C	380	P1L	O7-C7-SG	2.61	126.00	122.61
2	C	385	P1L	O7-C7-SG	2.13	125.38	122.61

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	380	P1L	N-CA-CB-SG
2	C	380	P1L	C-CA-CB-SG
2	C	381	P1L	CA-CB-SG-C7
2	C	381	P1L	O7-C7-SG-CB
2	C	381	P1L	C8-C7-SG-CB
2	C	385	P1L	O7-C7-SG-CB
2	C	385	P1L	C8-C7-SG-CB
2	C	380	P1L	C16-C17-C18-C19
2	C	380	P1L	C14-C15-C16-C17
2	C	385	P1L	C11-C12-C13-C14
2	C	380	P1L	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	C	381	P1L	C11-C10-C9-C8
2	C	385	P1L	SG-C7-C8-C9
2	C	385	P1L	O7-C7-C8-C9
2	C	385	P1L	C19-C20-C21-C22
2	C	385	P1L	C11-C10-C9-C8
2	C	385	P1L	C9-C10-C11-C12
2	C	385	P1L	C12-C13-C14-C15
2	C	381	P1L	C18-C19-C20-C21
2	C	385	P1L	C7-C8-C9-C10

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

36 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	$\# Z > 2$
6	NAG	G	1	6	14,14,15	0.88	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	G	2	6	14,14,15	0.26	0	17,19,21	1.35	2 (11%)
6	BMA	G	3	6	11,11,12	0.60	0	15,15,17	0.76	0
7	NAG	I	1	1,7	14,14,15	0.27	0	17,19,21	0.39	0
7	NAG	I	2	7	14,14,15	0.23	0	17,19,21	0.39	0
7	BMA	I	3	7	11,11,12	0.59	0	15,15,17	0.80	0
7	MAN	I	4	7	11,11,12	0.42	0	15,15,17	0.82	1 (6%)
7	MAN	I	5	7	11,11,12	0.25	0	15,15,17	0.74	0
7	MAN	I	6	7	11,11,12	0.31	0	15,15,17	0.87	1 (6%)
7	MAN	I	7	7	11,11,12	0.67	0	15,15,17	1.09	2 (13%)
8	NAG	J	1	8	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	J	2	8	14,14,15	0.20	0	17,19,21	0.41	0
9	NAG	M	1	9	14,14,15	0.26	0	17,19,21	0.37	0
9	NAG	M	2	9	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	M	3	9	11,11,12	0.57	0	15,15,17	0.78	0
9	MAN	M	4	9	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
9	MAN	M	5	9	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
9	MAN	M	6	9	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	N	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	BMA	N	3	6	11,11,12	0.60	0	15,15,17	0.79	0
10	NAG	P	1	10,1	14,14,15	0.42	0	17,19,21	1.20	2 (11%)
10	NAG	P	2	10	14,14,15	0.44	0	17,19,21	0.54	0
10	BMA	P	3	10	11,11,12	0.60	0	15,15,17	0.56	0
10	MAN	P	4	10	11,11,12	0.47	0	15,15,17	1.18	1 (6%)
10	MAN	P	5	10	11,11,12	0.86	1 (9%)	15,15,17	1.10	1 (6%)
10	MAN	P	6	10	11,11,12	0.22	0	15,15,17	0.78	1 (6%)
10	MAN	P	7	10	11,11,12	0.41	0	15,15,17	0.78	0
10	MAN	P	8	10	11,11,12	0.36	0	15,15,17	0.56	0
8	NAG	Q	1	8,1	14,14,15	0.24	0	17,19,21	0.61	0
8	NAG	Q	2	8	14,14,15	0.22	0	17,19,21	0.46	0
11	NAG	R	1	11	14,14,15	0.23	0	17,19,21	0.40	0
11	NAG	R	2	11	14,14,15	0.18	0	17,19,21	0.41	0
11	BMA	R	3	11	11,11,12	0.60	0	15,15,17	0.77	0
11	MAN	R	4	11	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
11	MAN	R	5	11	11,11,12	0.65	0	15,15,17	1.03	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
6	NAG	G	1	6	-	4/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	1/2/19/22	0/1/1/1
7	MAN	I	7	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
9	NAG	M	1	9	-	1/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	2/2/19/22	0/1/1/1
9	MAN	M	5	9	-	1/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
10	NAG	P	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	1/2/19/22	0/1/1/1
10	MAN	P	4	10	-	0/2/19/22	0/1/1/1
10	MAN	P	5	10	-	1/2/19/22	0/1/1/1
10	MAN	P	6	10	-	1/2/19/22	0/1/1/1
10	MAN	P	7	10	-	1/2/19/22	0/1/1/1
10	MAN	P	8	10	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
11	NAG	R	1	11	-	0/6/23/26	0/1/1/1
11	NAG	R	2	11	-	0/6/23/26	0/1/1/1
11	BMA	R	3	11	-	0/2/19/22	0/1/1/1
11	MAN	R	4	11	-	0/2/19/22	0/1/1/1
11	MAN	R	5	11	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1	NAG	O5-C1	3.03	1.48	1.43
10	P	5	MAN	C1-C2	2.47	1.57	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	2	NAG	C2-N2-C7	4.49	129.30	122.90
6	G	1	NAG	C1-O5-C5	4.09	117.73	112.19
10	P	1	NAG	C1-C2-N2	3.55	116.55	110.49
10	P	4	MAN	C1-C2-C3	3.27	113.69	109.67
10	P	5	MAN	O2-C2-C1	3.19	115.68	109.15
7	I	7	MAN	C1-O5-C5	2.37	115.40	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	5	MAN	C1-O5-C5	2.32	115.34	112.19
7	I	6	MAN	C1-O5-C5	2.31	115.32	112.19
10	P	1	NAG	C2-N2-C7	2.30	126.18	122.90
11	R	4	MAN	C1-O5-C5	2.28	115.29	112.19
7	I	7	MAN	O2-C2-C3	-2.28	105.56	110.14
9	M	5	MAN	C1-O5-C5	2.27	115.27	112.19
9	M	4	MAN	O2-C2-C3	-2.27	105.60	110.14
11	R	4	MAN	O2-C2-C3	-2.25	105.62	110.14
9	M	5	MAN	O2-C2-C3	-2.24	105.64	110.14
9	M	6	MAN	C1-O5-C5	2.24	115.23	112.19
9	M	6	MAN	O2-C2-C3	-2.20	105.73	110.14
11	R	5	MAN	O2-C2-C3	-2.18	105.76	110.14
6	G	2	NAG	C1-C2-N2	2.17	114.19	110.49
7	I	4	MAN	C1-O5-C5	2.13	115.08	112.19
10	P	6	MAN	C1-C2-C3	2.10	112.25	109.67
9	M	4	MAN	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	P	1	NAG	C3-C2-N2-C7
9	M	2	NAG	O5-C5-C6-O6
9	M	4	MAN	O5-C5-C6-O6
9	M	4	MAN	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
6	G	1	NAG	C8-C7-N2-C2
6	G	1	NAG	O7-C7-N2-C2
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
8	Q	1	NAG	C4-C5-C6-O6
10	P	3	BMA	O5-C5-C6-O6
10	P	7	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
10	P	5	MAN	O5-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
9	M	5	MAN	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6

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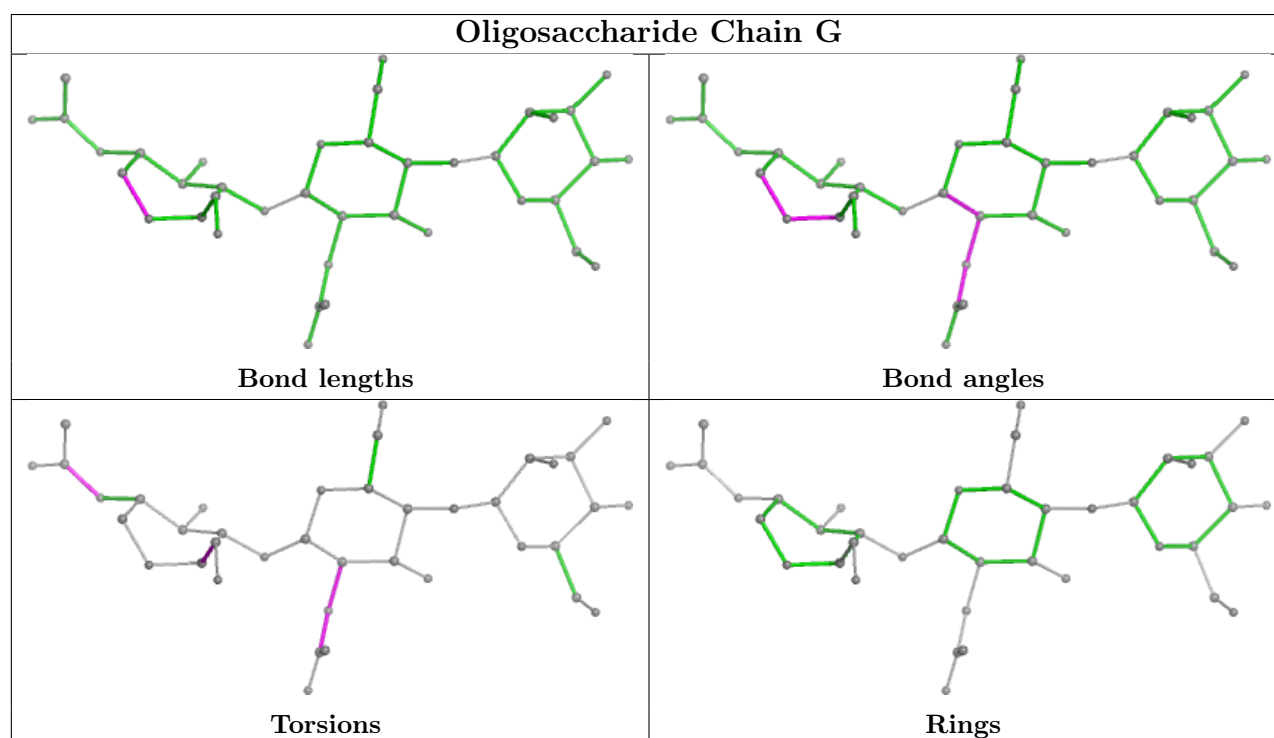
Mol	Chain	Res	Type	Atoms
9	M	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C3-C2-N2-C7
8	Q	2	NAG	C1-C2-N2-C7
6	G	1	NAG	O5-C5-C6-O6
6	G	2	NAG	C3-C2-N2-C7
6	G	2	NAG	C1-C2-N2-C7

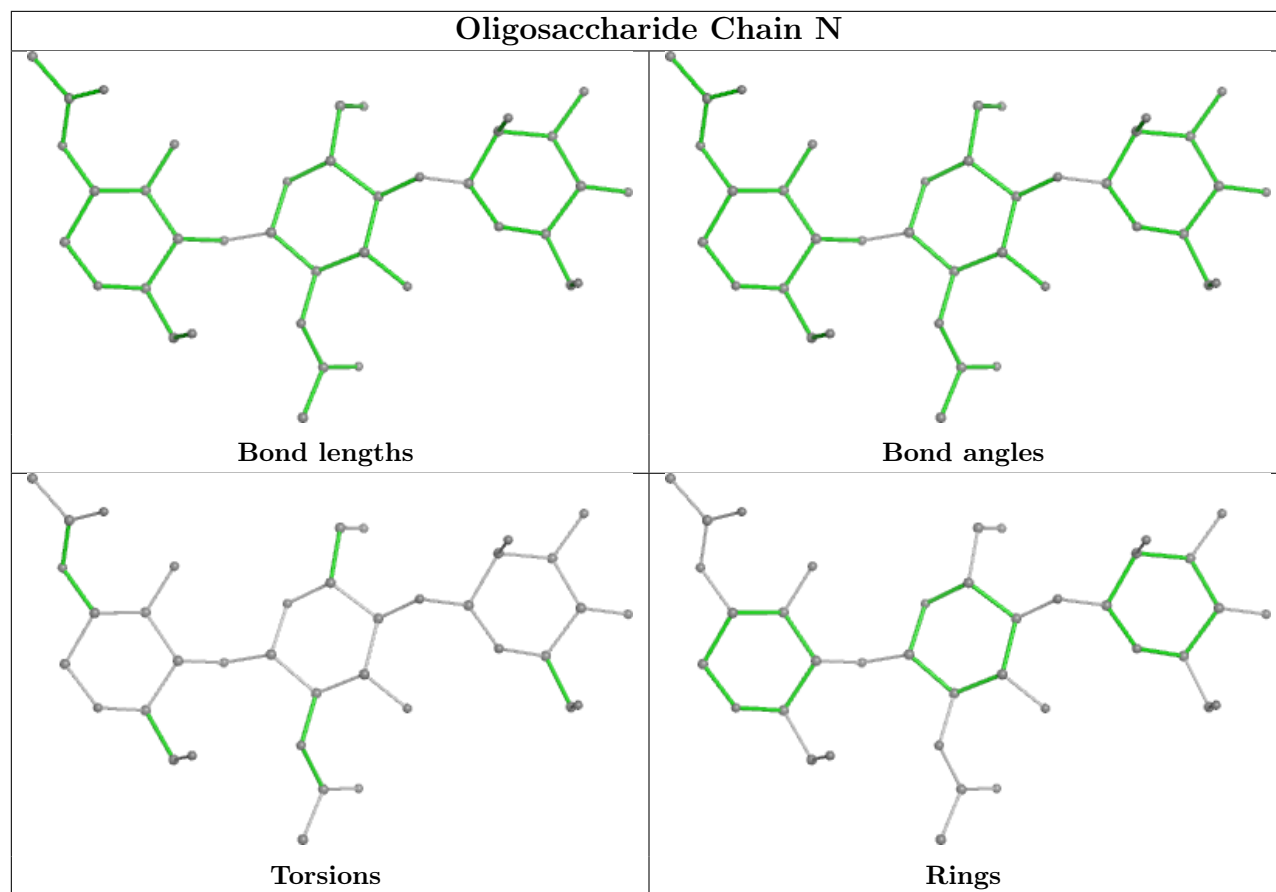
There are no ring outliers.

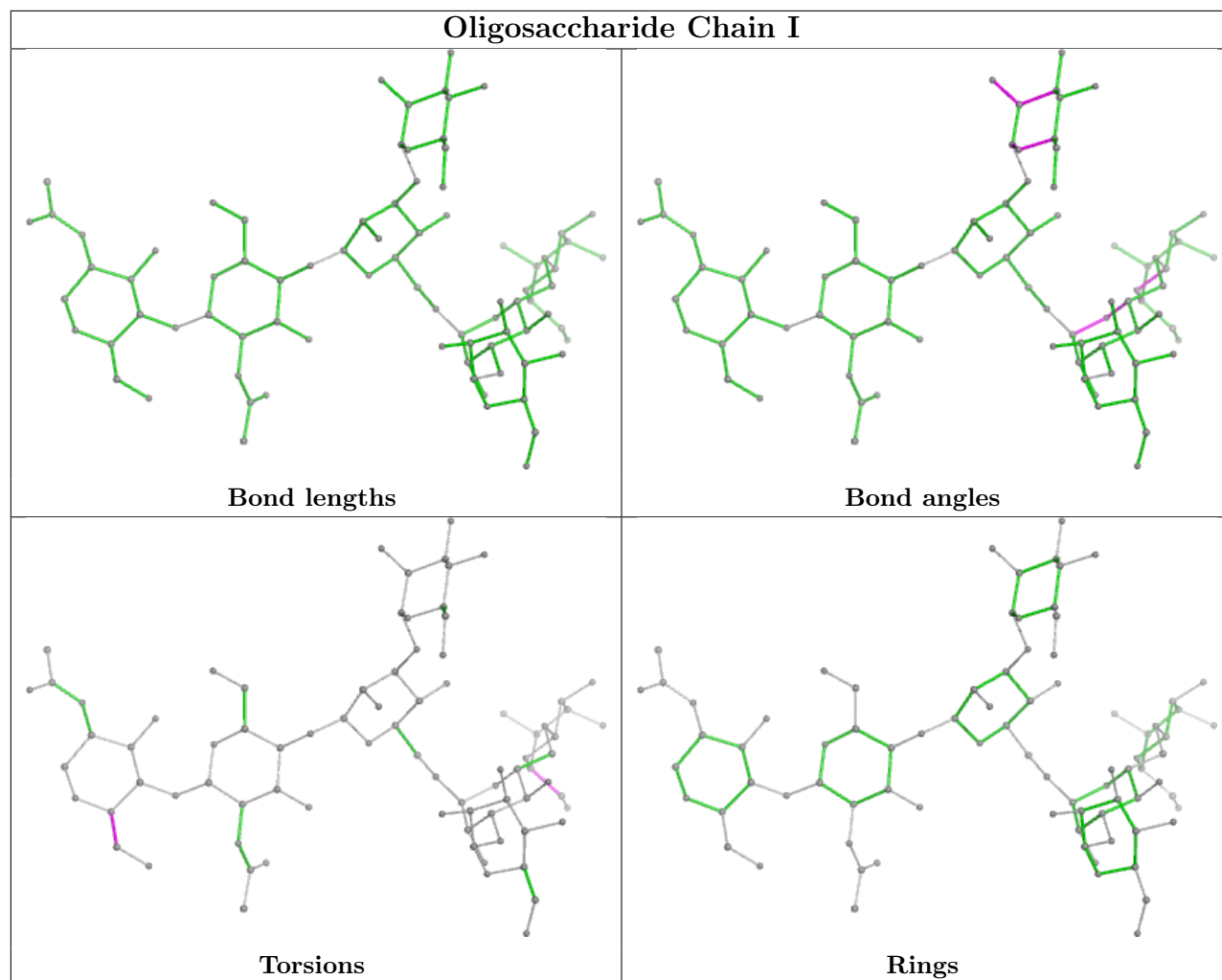
7 monomers are involved in 5 short contacts:

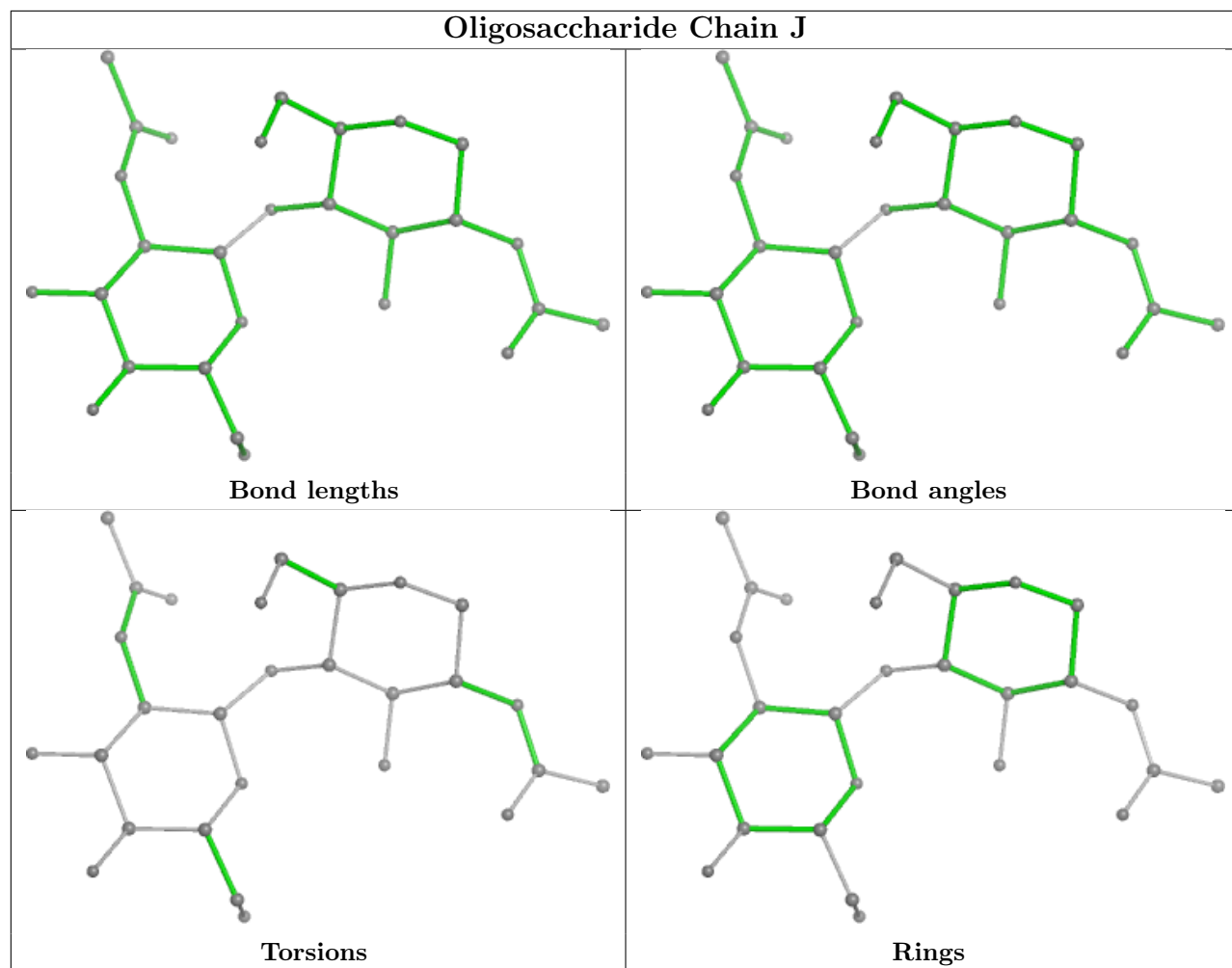
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	2	NAG	1	0
10	P	4	MAN	1	0
7	I	1	NAG	1	0
10	P	3	BMA	1	0
11	R	1	NAG	1	0
6	G	2	NAG	1	0
9	M	1	NAG	1	0

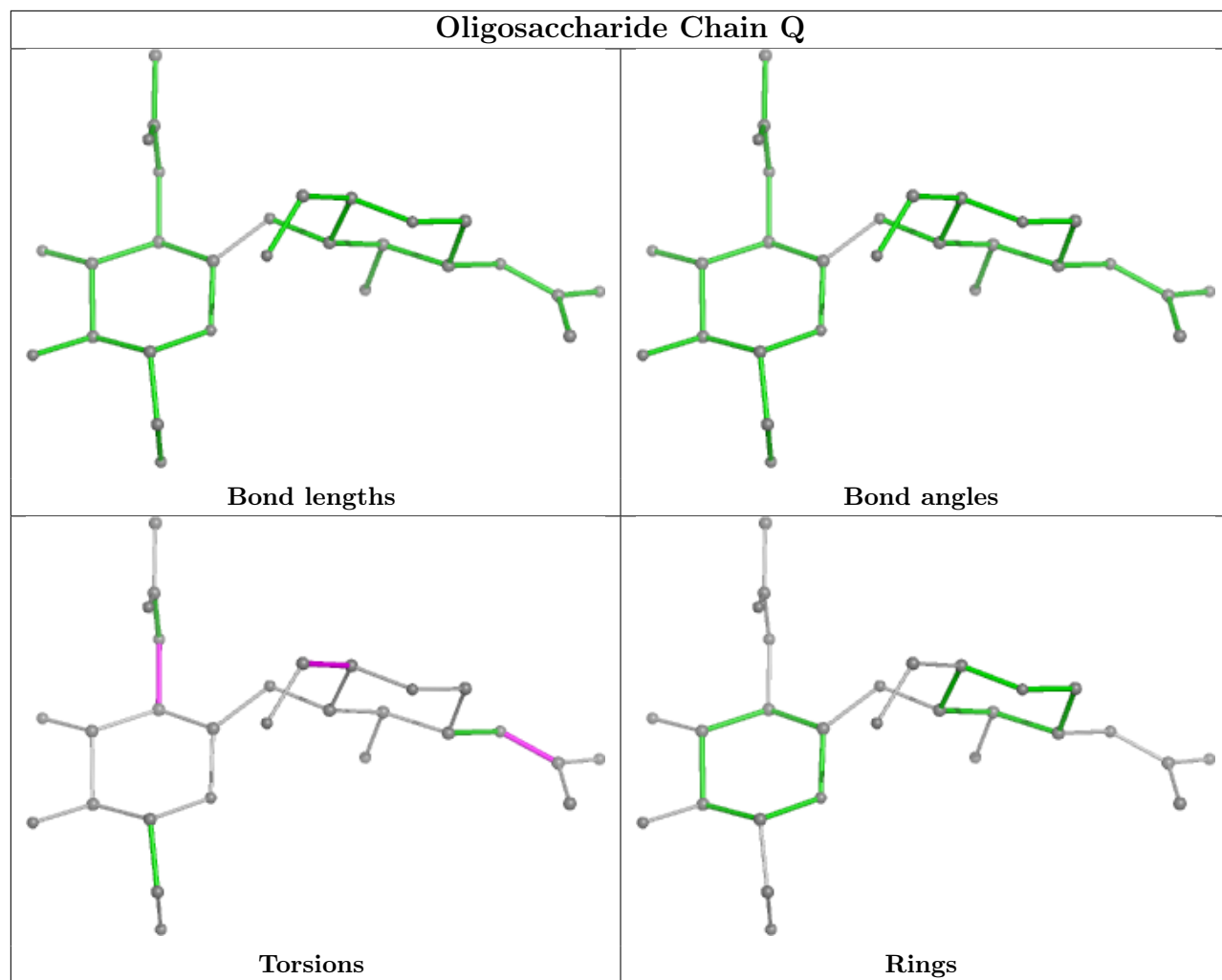
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

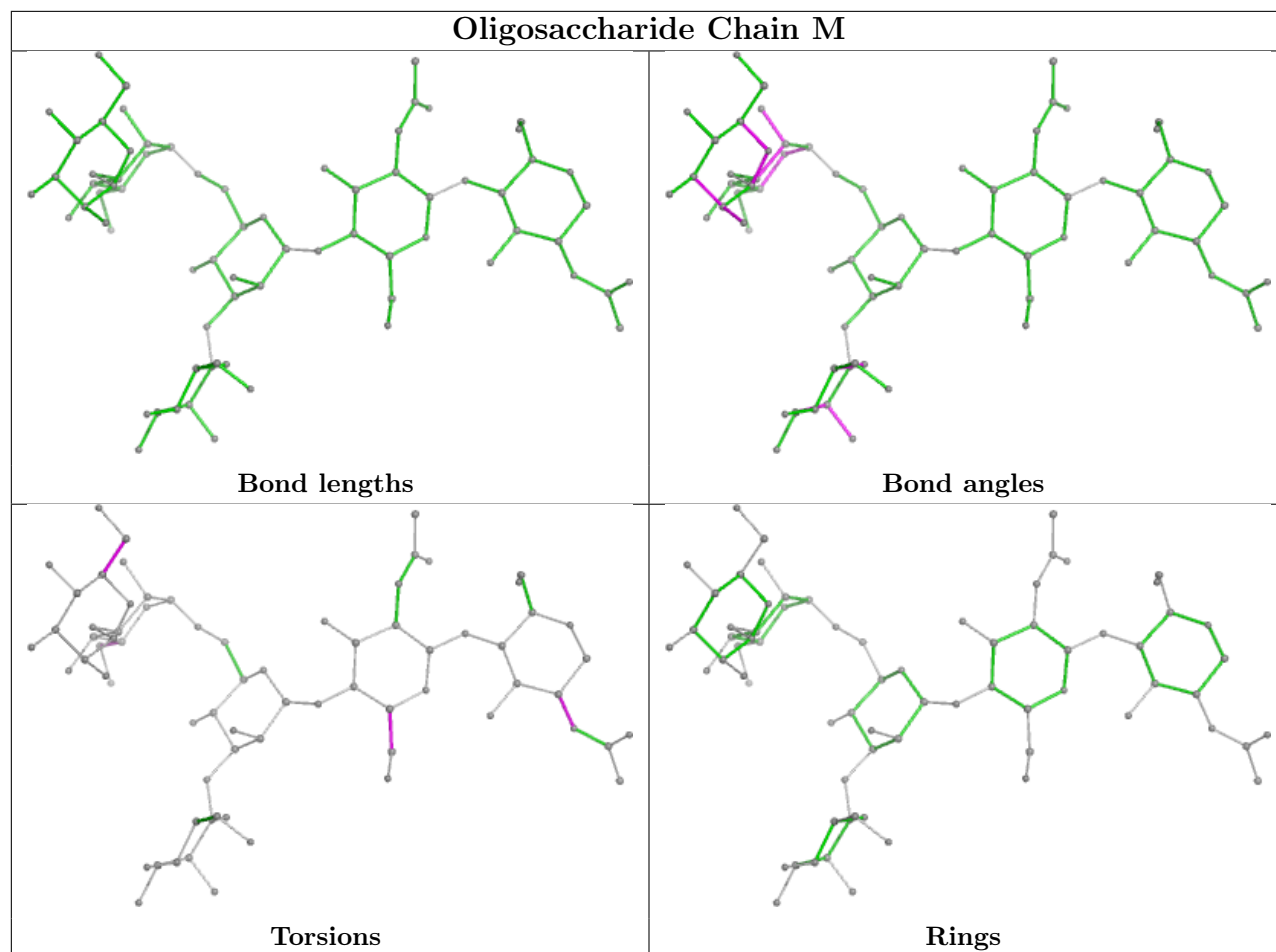


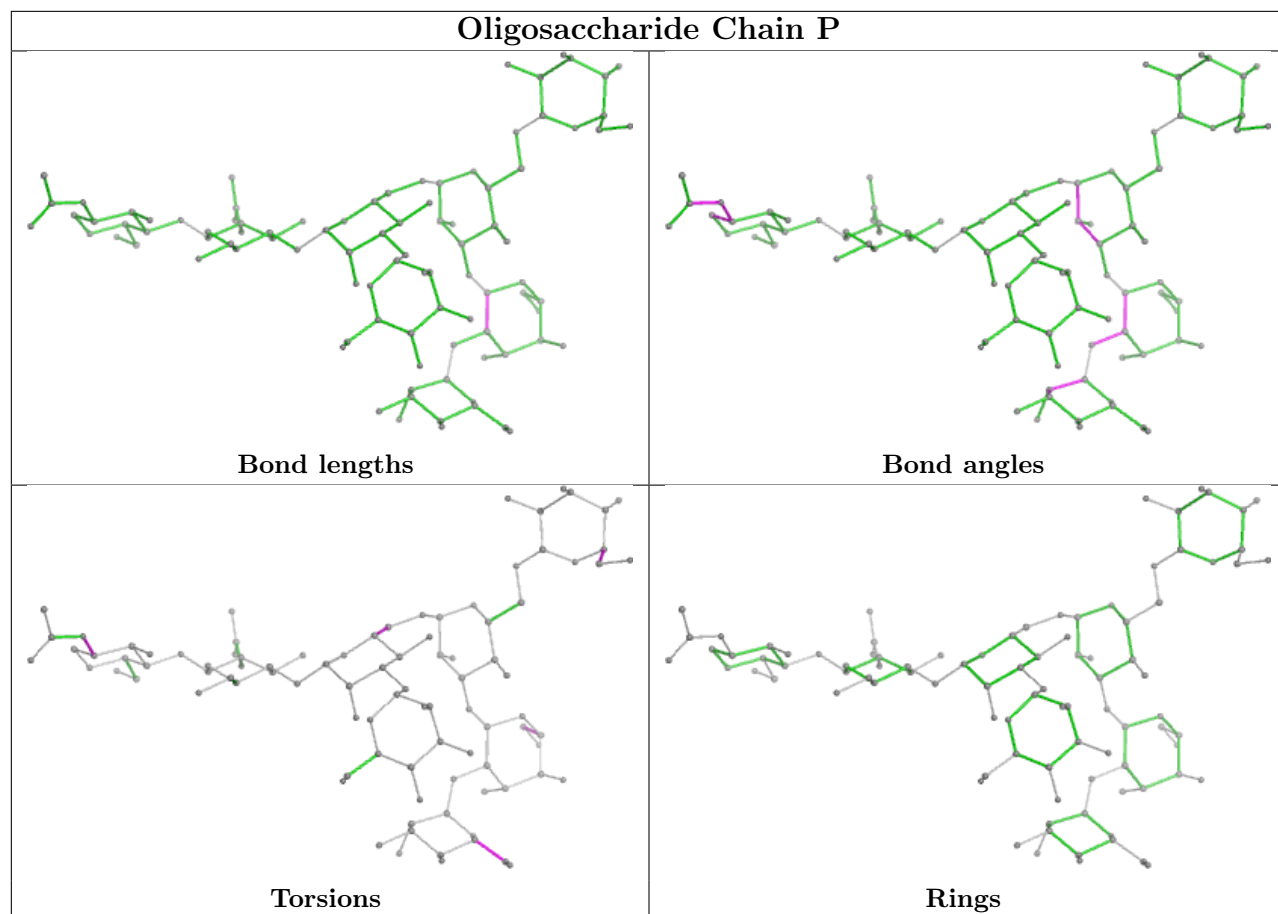


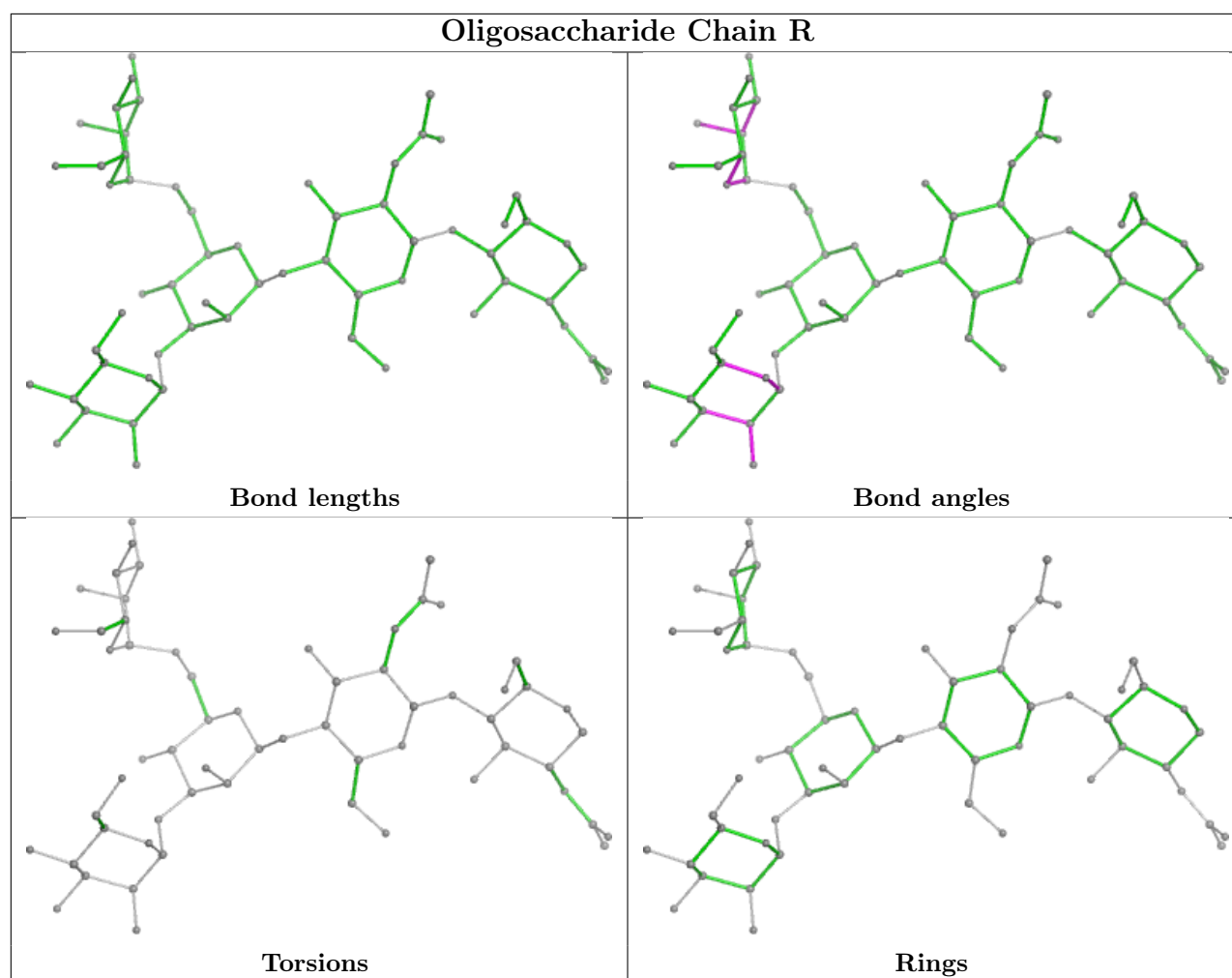












5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
12	HEX	E	501	-	5,5,5	0.30	0	4,4,4	0.58	0
13	D10	A	501	-	9,9,9	0.13	0	8,8,8	0.11	0
12	HEX	B	501	-	5,5,5	0.30	0	4,4,4	0.55	0
13	D10	C	504	-	9,9,9	0.15	0	8,8,8	0.11	0
14	R16	B	504	-	15,15,15	0.31	0	14,14,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	R16	C	502	-	15,15,15	0.32	0	14,14,14	0.72	0
18	CLR	C	505	-	31,31,31	0.17	0	48,48,48	0.34	0
13	D10	E	503	-	9,9,9	0.30	0	8,8,8	0.76	0
14	R16	C	503	-	15,15,15	0.33	0	14,14,14	0.68	0
13	D10	B	503	-	9,9,9	0.31	0	8,8,8	0.74	0
12	HEX	B	502	-	5,5,5	0.31	0	4,4,4	0.55	0
16	PX2	D	501	-	35,35,35	1.02	3 (8%)	39,40,40	1.23	2 (5%)
12	HEX	E	502	-	5,5,5	0.31	0	4,4,4	0.55	0
12	HEX	A	502	-	5,5,5	0.13	0	4,4,4	0.09	0
17	NAG	C	501	-	14,14,15	0.21	0	17,19,21	0.47	0
15	PGW	B	505	-	50,50,50	0.98	2 (4%)	53,56,56	0.93	2 (3%)

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
12	HEX	E	501	-	-	0/3/3/3	-
13	D10	A	501	-	-	0/7/7/7	-
12	HEX	B	501	-	-	0/3/3/3	-
13	D10	C	504	-	-	2/7/7/7	-
14	R16	B	504	-	-	6/13/13/13	-
14	R16	C	502	-	-	3/13/13/13	-
18	CLR	C	505	-	-	0/10/68/68	0/4/4/4
13	D10	E	503	-	-	3/7/7/7	-
14	R16	C	503	-	-	1/13/13/13	-
13	D10	B	503	-	-	2/7/7/7	-
12	HEX	B	502	-	-	0/3/3/3	-
16	PX2	D	501	-	-	19/37/37/37	-
12	HEX	E	502	-	-	0/3/3/3	-
12	HEX	A	502	-	-	0/3/3/3	-
17	NAG	C	501	-	-	4/6/23/26	0/1/1/1
15	PGW	B	505	-	-	20/55/55/55	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	505	PGW	O03-C19	2.91	1.41	1.33
15	B	505	PGW	O01-C1	2.82	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	PX2	O5-C4	2.81	1.41	1.33
16	D	501	PX2	O7-C16	2.43	1.41	1.34
16	D	501	PX2	O7-C2	-2.18	1.41	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	PX2	O7-C16-C17	4.79	121.82	111.50
15	B	505	PGW	O01-C1-C2	3.80	119.69	111.50
15	B	505	PGW	O03-C19-C20	2.77	120.60	111.91
16	D	501	PX2	O5-C4-C5	2.41	119.47	111.91

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	501	PX2	C1-O4-P1-O1
16	D	501	PX2	C1-O4-P1-O3
16	D	501	PX2	O8-C16-O7-C2
16	D	501	PX2	C17-C16-O7-C2
15	B	505	PGW	C20-C19-O03-C01
15	B	505	PGW	O04-C19-O03-C01
17	C	501	NAG	O5-C5-C6-O6
17	C	501	NAG	C4-C5-C6-O6
15	B	505	PGW	C04-O12-P-O11
14	C	503	R16	C34-C35-C36-C37
15	B	505	PGW	C24-C25-C26-C27
16	D	501	PX2	C5-C6-C7-C8
16	D	501	PX2	C22-C23-C24-C25
15	B	505	PGW	C5-C6-C7-C8
14	C	502	R16	C38-C39-C40-C41
14	C	502	R16	C31-C32-C33-C34
16	D	501	PX2	C18-C19-C20-C21
15	B	505	PGW	C2-C1-O01-C02
13	C	504	D10	C4-C5-C6-C7
13	E	503	D10	C4-C5-C6-C7
15	B	505	PGW	C23-C24-C25-C26
15	B	505	PGW	O02-C1-O01-C02
16	D	501	PX2	C4-C5-C6-C7
14	B	504	R16	C33-C34-C35-C36
15	B	505	PGW	C16-C15-C27-C26
16	D	501	PX2	C1-O4-P1-O2

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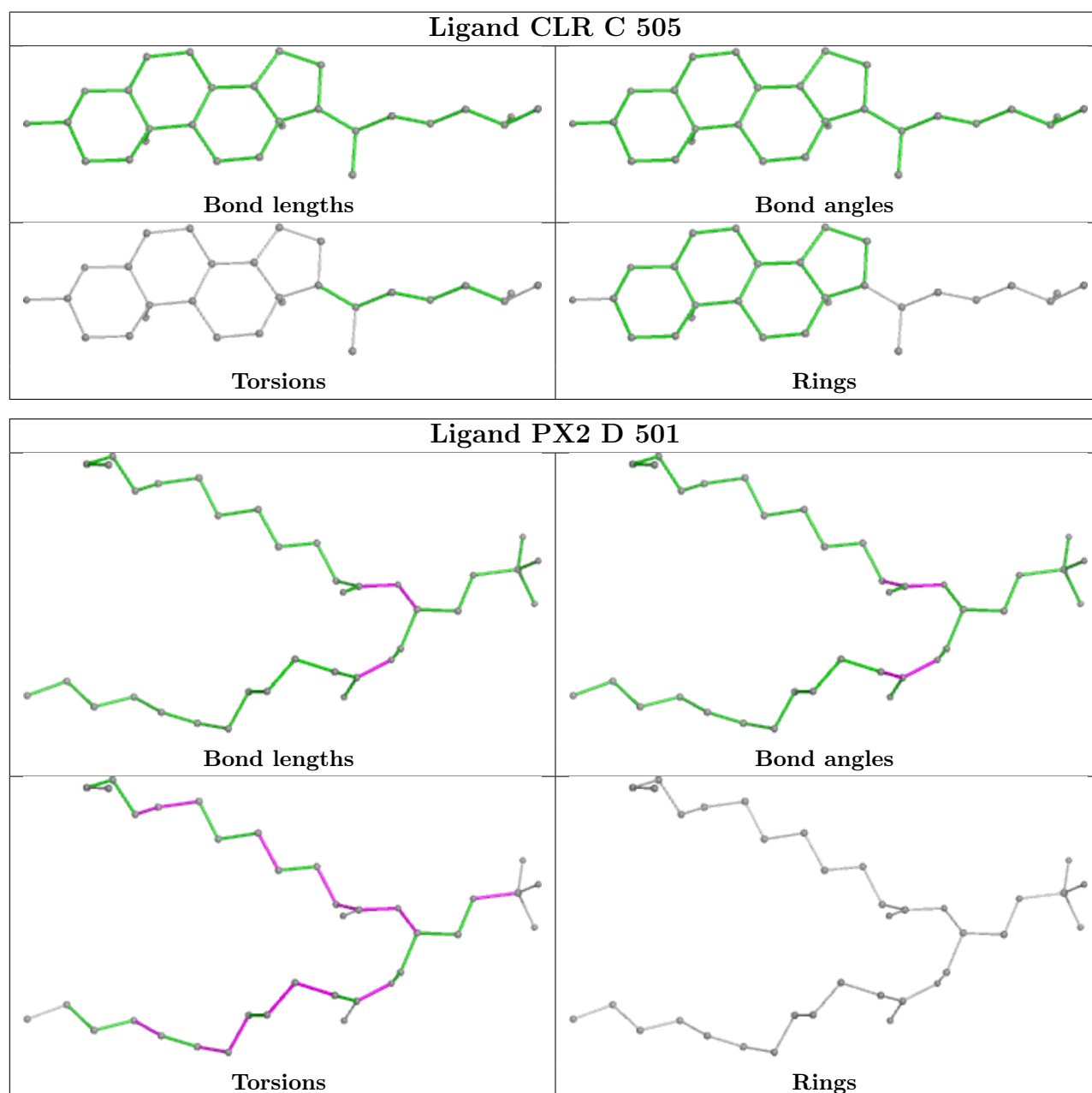
Mol	Chain	Res	Type	Atoms
15	B	505	PGW	C27-C15-C16-C17
16	D	501	PX2	C11-C10-C9-C8
16	D	501	PX2	C5-C4-O5-C3
14	B	504	R16	C37-C38-C39-C40
14	B	504	R16	C32-C33-C34-C35
14	B	504	R16	C28-C29-C30-C31
15	B	505	PGW	O01-C02-C03-O11
16	D	501	PX2	O6-C4-O5-C3
15	B	505	PGW	C02-C03-O11-P
14	B	504	R16	C35-C36-C37-C38
16	D	501	PX2	C10-C11-C12-C13
16	D	501	PX2	C16-C17-C18-C19
14	B	504	R16	C36-C37-C38-C39
15	B	505	PGW	C05-C04-O12-P
15	B	505	PGW	C04-O12-P-O13
15	B	505	PGW	C04-O12-P-O14
15	B	505	PGW	C01-C02-C03-O11
14	C	502	R16	C28-C29-C30-C31
16	D	501	PX2	C3-C2-O7-C16
16	D	501	PX2	C21-C22-C23-C24
15	B	505	PGW	C07-C06-C10-C9
15	B	505	PGW	C03-O11-P-O12
17	C	501	NAG	C3-C2-N2-C7
17	C	501	NAG	C1-C2-N2-C7
13	B	503	D10	C2-C3-C4-C5
15	B	505	PGW	C3-C4-C5-C6
13	E	503	D10	C1-C2-C3-C4
13	E	503	D10	C2-C3-C4-C5
13	C	504	D10	C2-C3-C4-C5
13	B	503	D10	C1-C2-C3-C4
16	D	501	PX2	O7-C16-C17-C18
15	B	505	PGW	C03-O11-P-O14
16	D	501	PX2	C7-C8-C9-C10
16	D	501	PX2	O8-C16-C17-C18

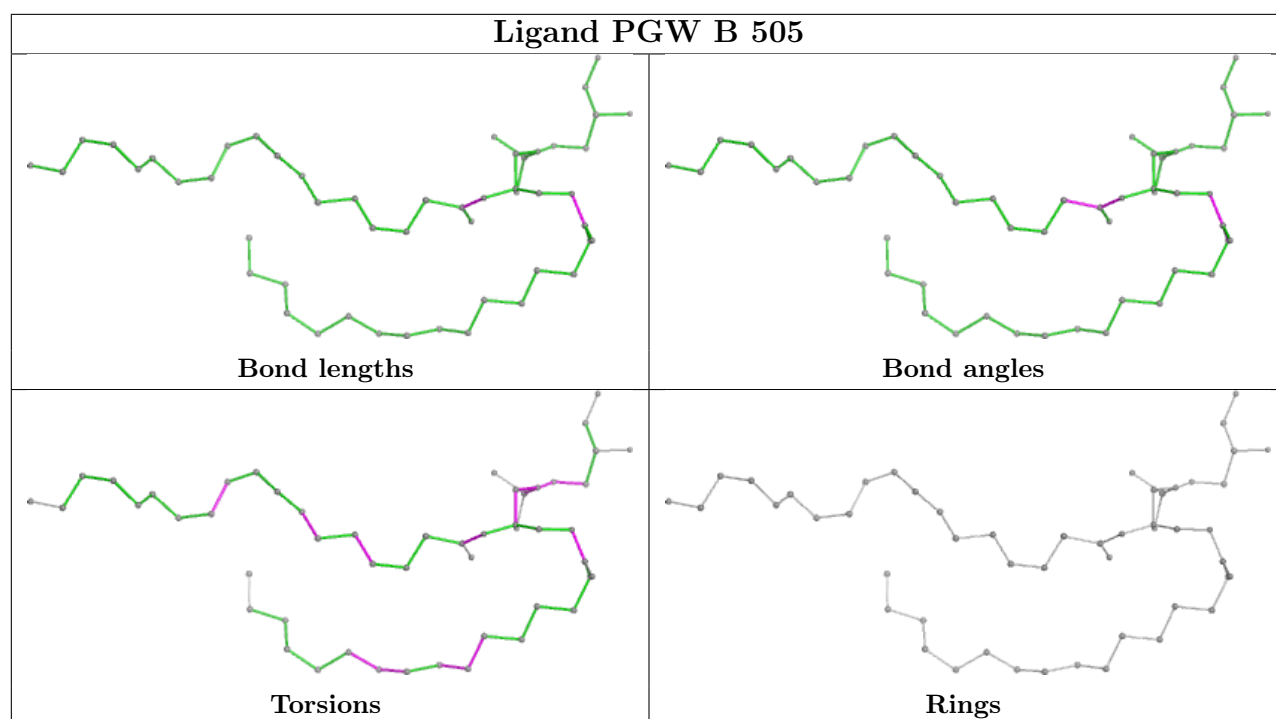
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	501	D10	1	0
13	C	504	D10	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

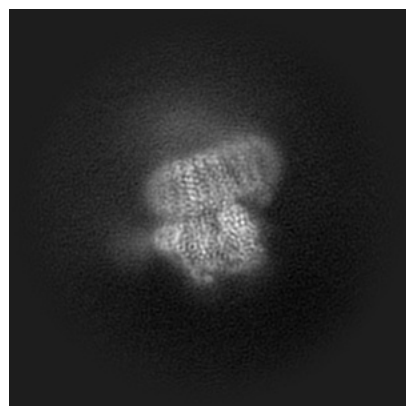
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50283. These allow visual inspection of the internal detail of the map and identification of artifacts.

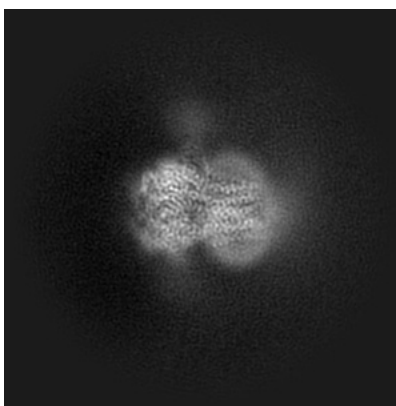
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

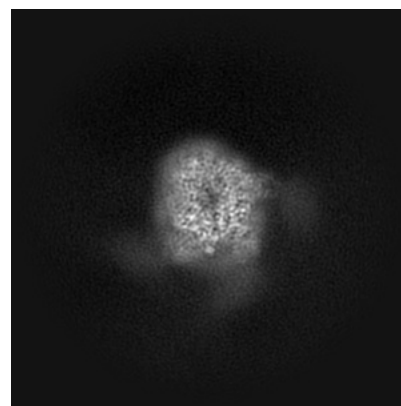
6.1.1 Primary map



X

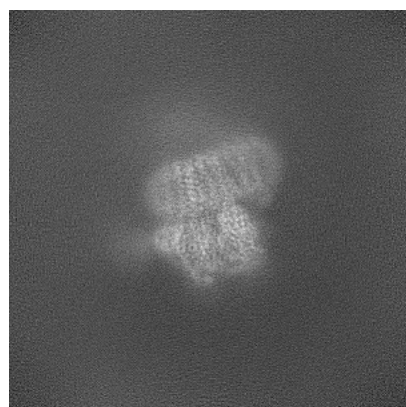


Y

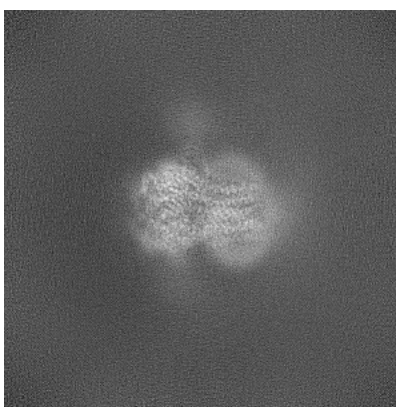


Z

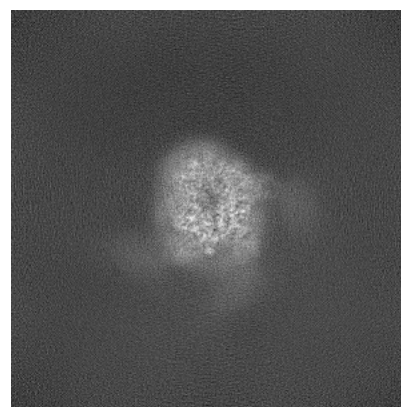
6.1.2 Raw map



X



Y

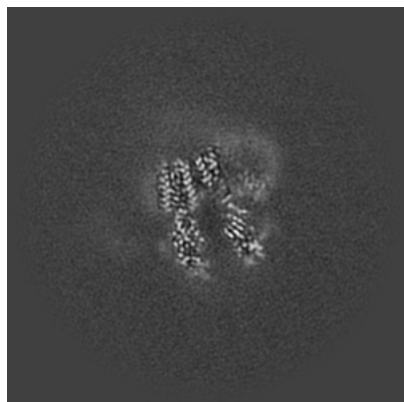


Z

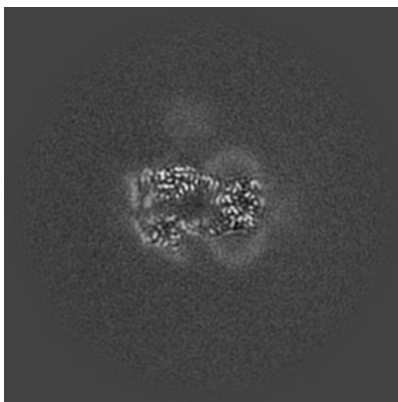
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

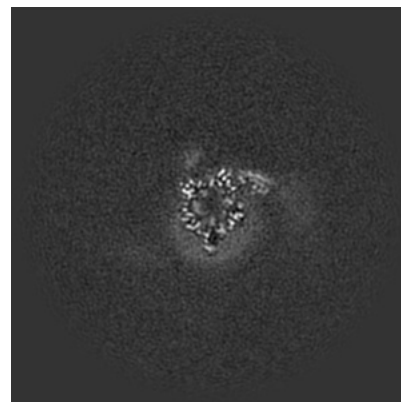
6.2.1 Primary map



X Index: 232

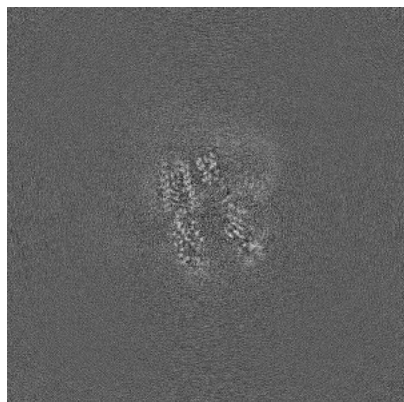


Y Index: 232

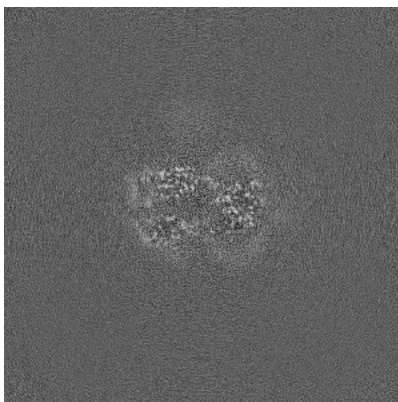


Z Index: 232

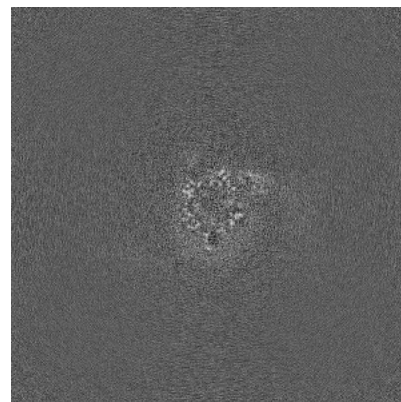
6.2.2 Raw map



X Index: 232



Y Index: 232

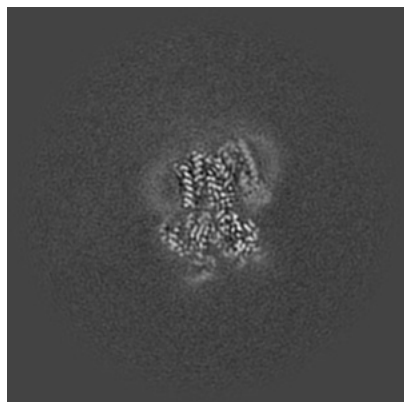


Z Index: 232

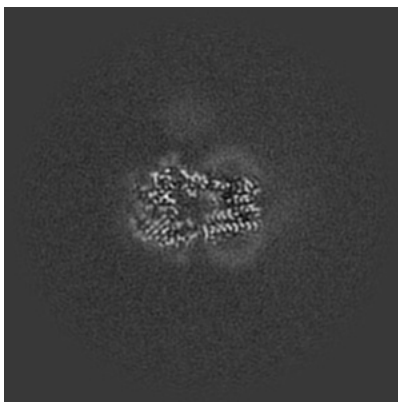
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

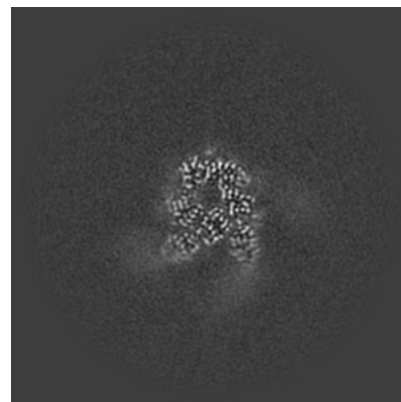
6.3.1 Primary map



X Index: 212

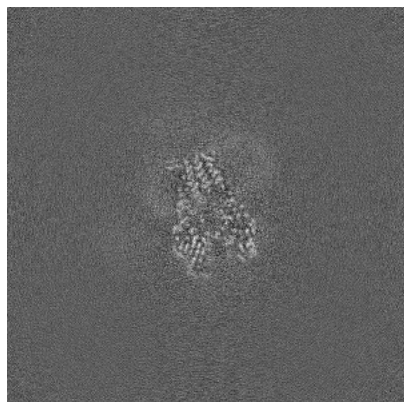


Y Index: 223

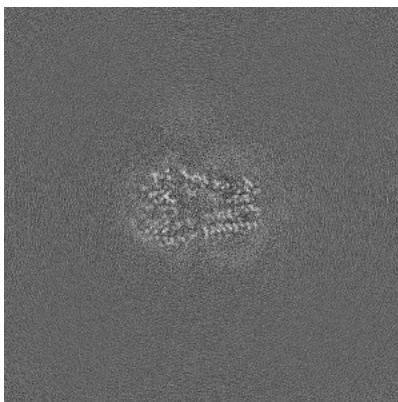


Z Index: 195

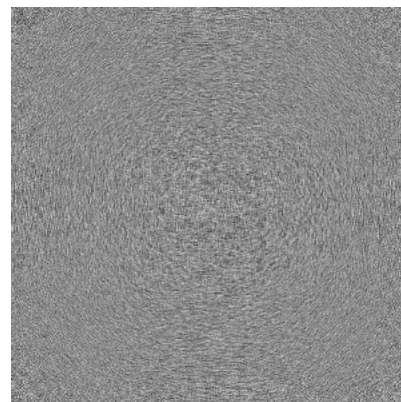
6.3.2 Raw map



X Index: 244



Y Index: 223

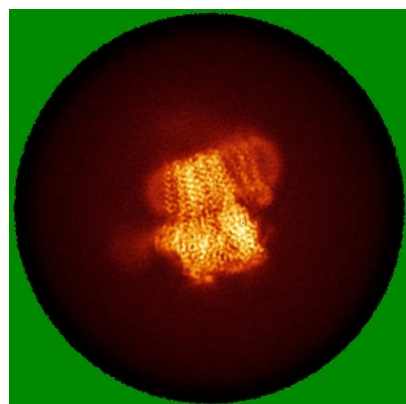


Z Index: 0

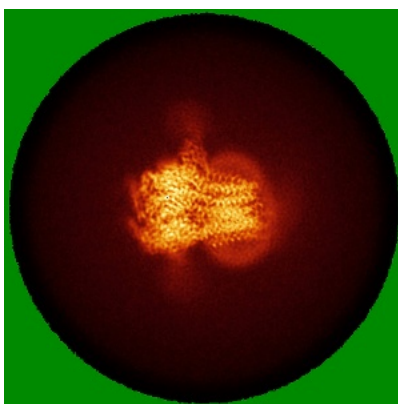
The images above show the largest variance slices of the map in three orthogonal directions.

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

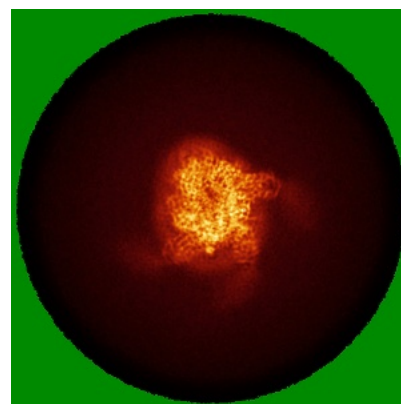
6.4.1 Primary map



X

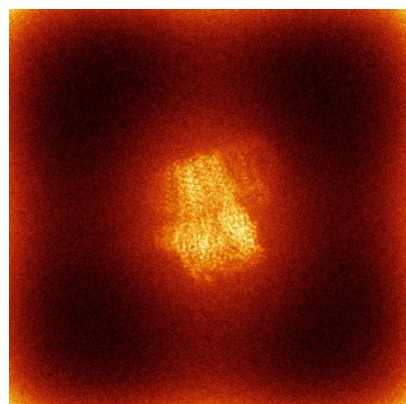


Y

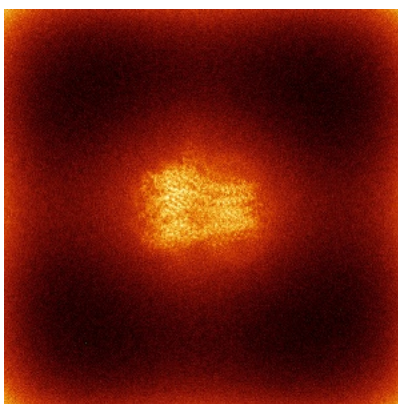


Z

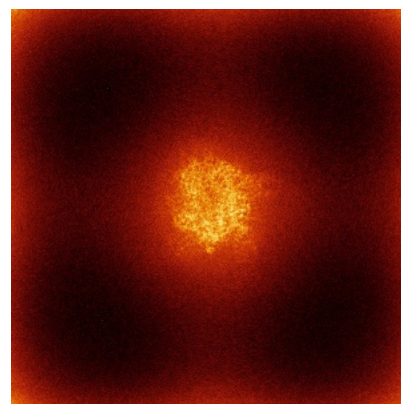
6.4.2 Raw map



X



Y

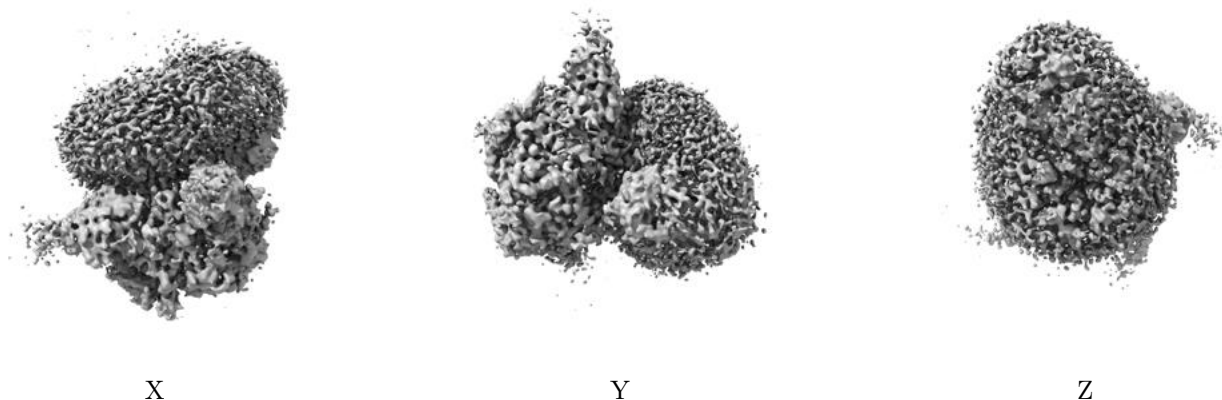


Z

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.

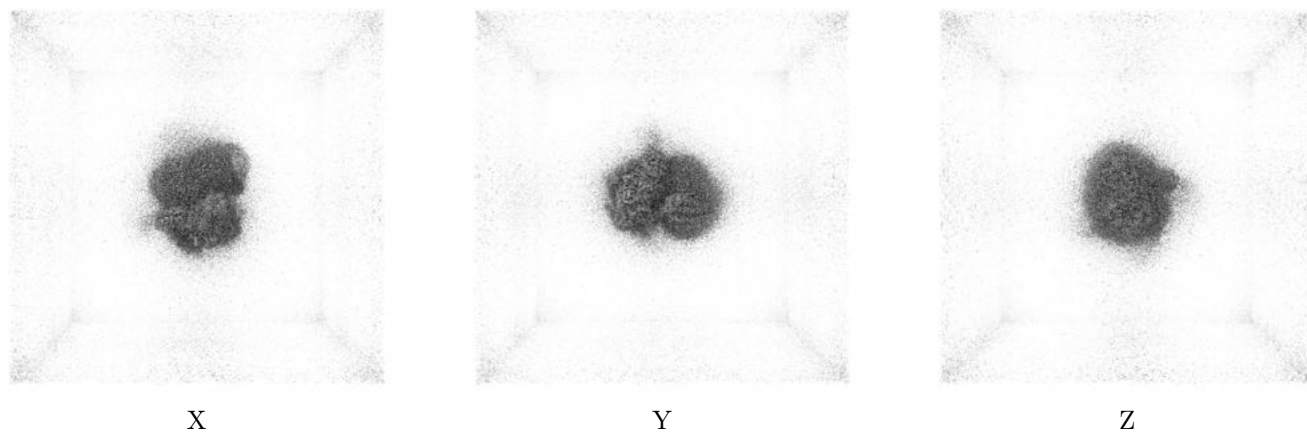
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

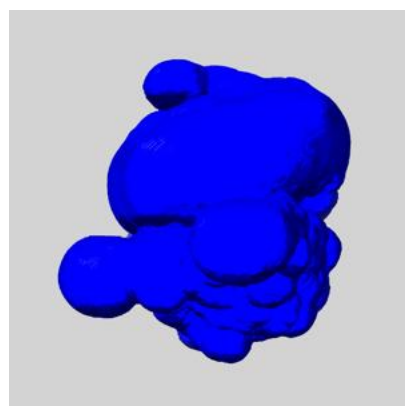
6.6 Mask visualisation [i](#)

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

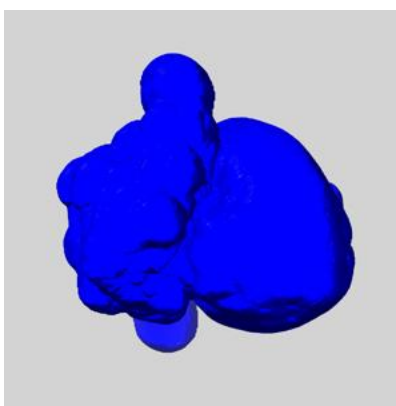
A mask typically either:

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

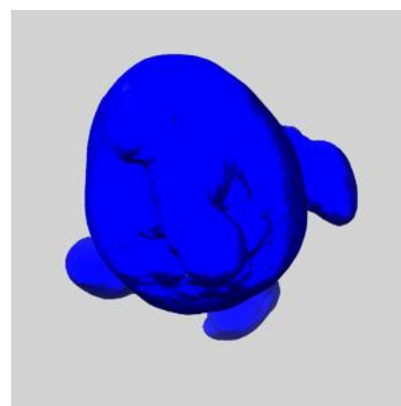
6.6.1 emd_50283_msk_1.map [i](#)



X



Y

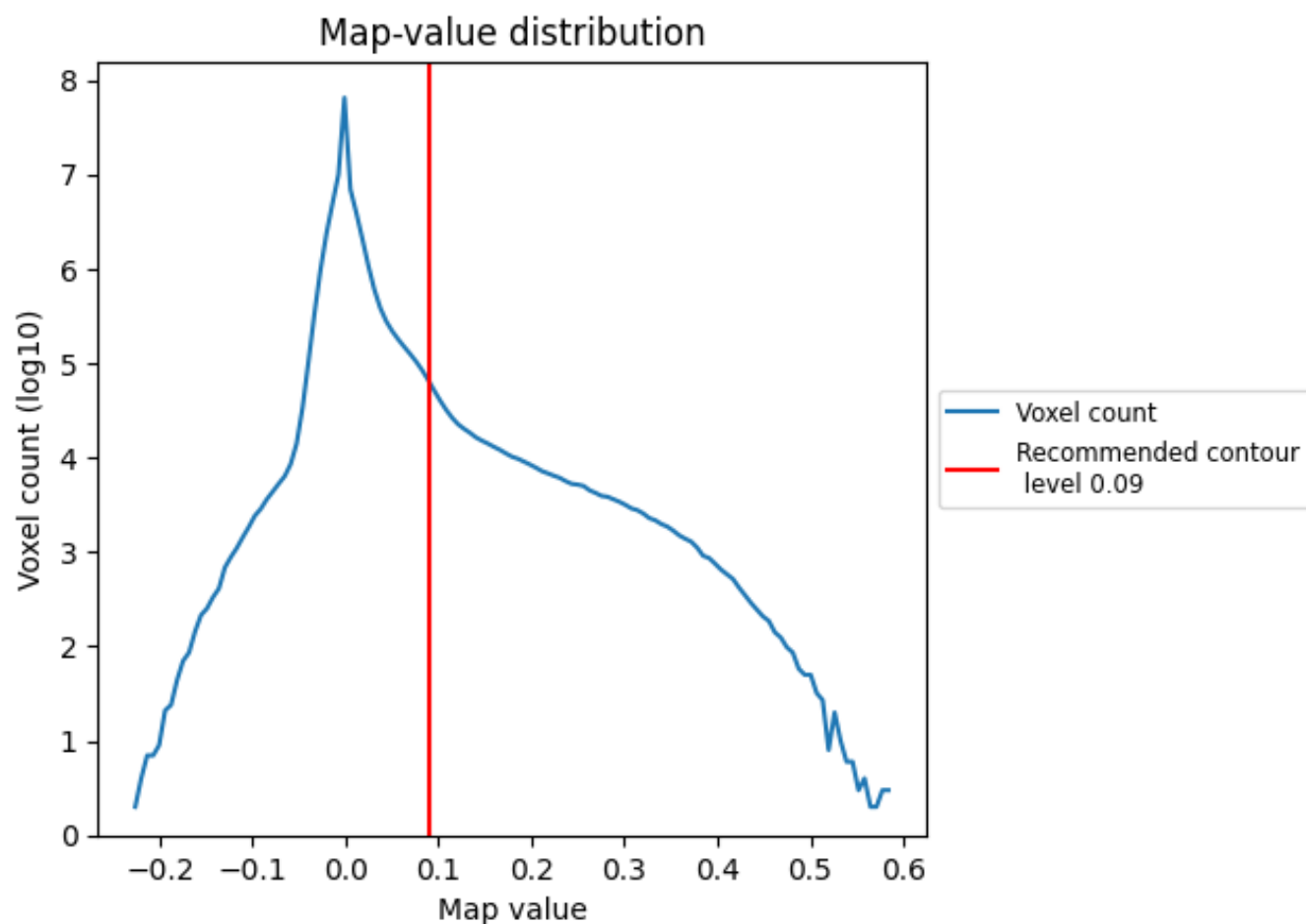


Z

7 Map analysis [i](#)

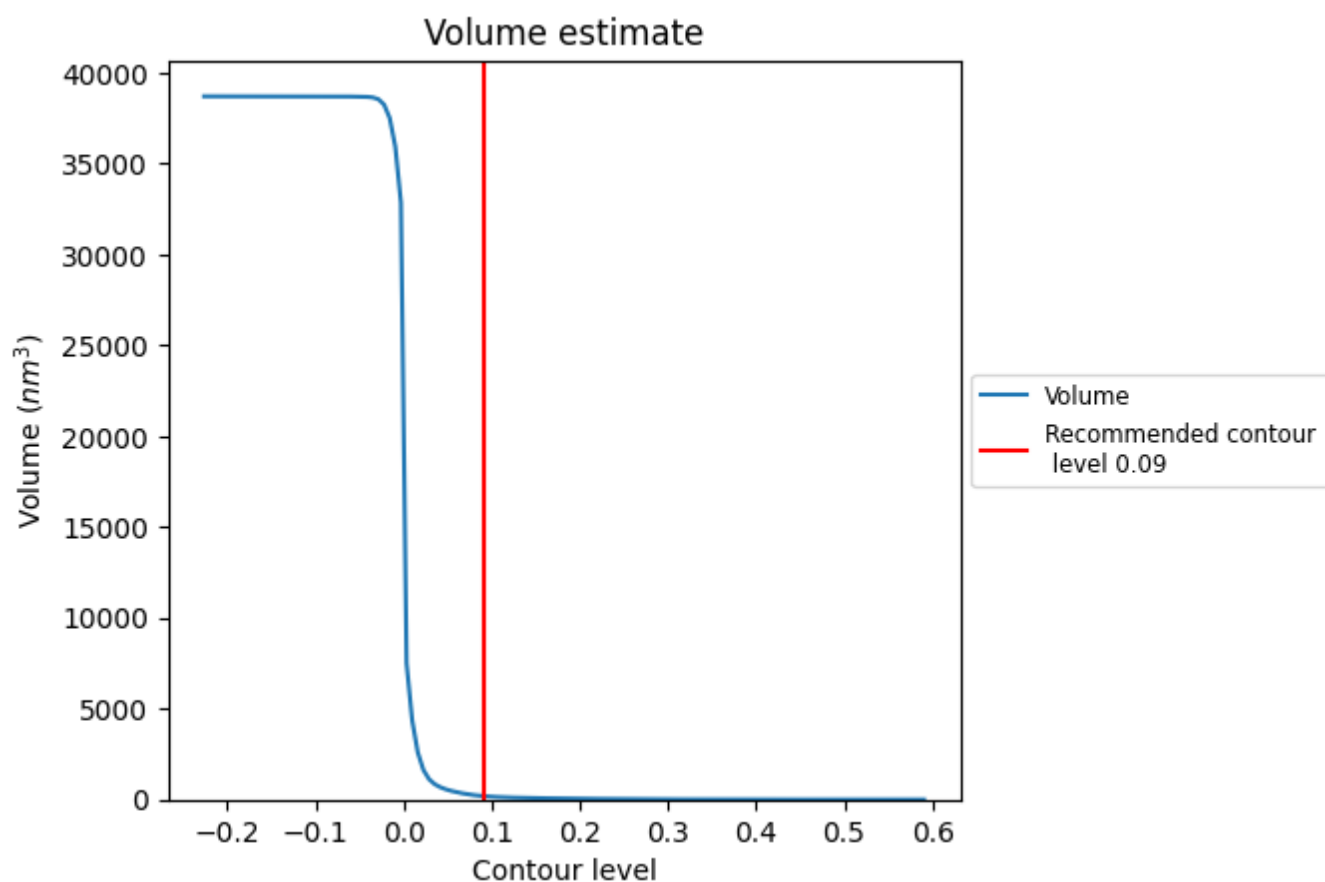
This section contains the results of statistical analysis of the map.

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.

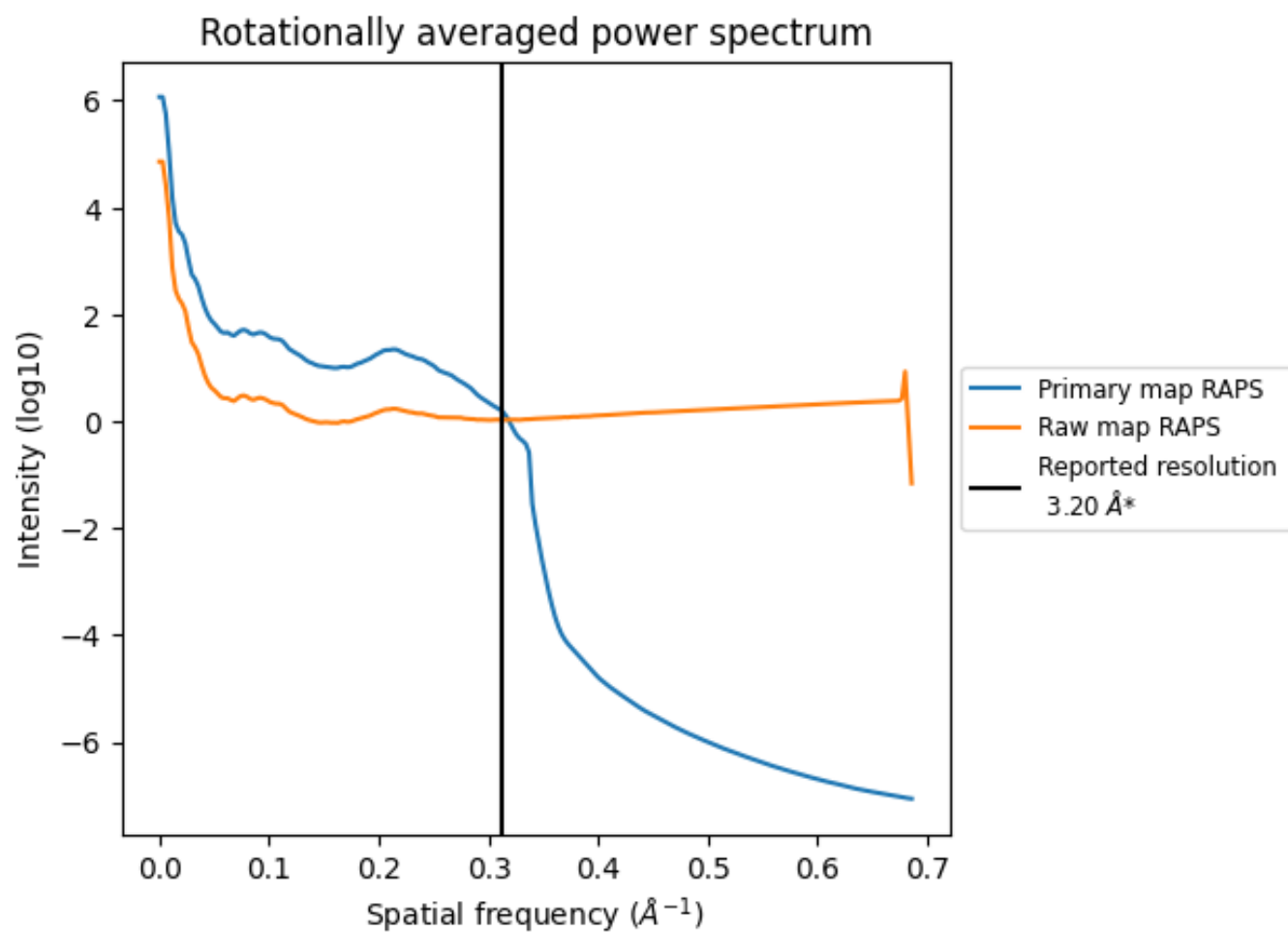
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 174 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 ⓘ

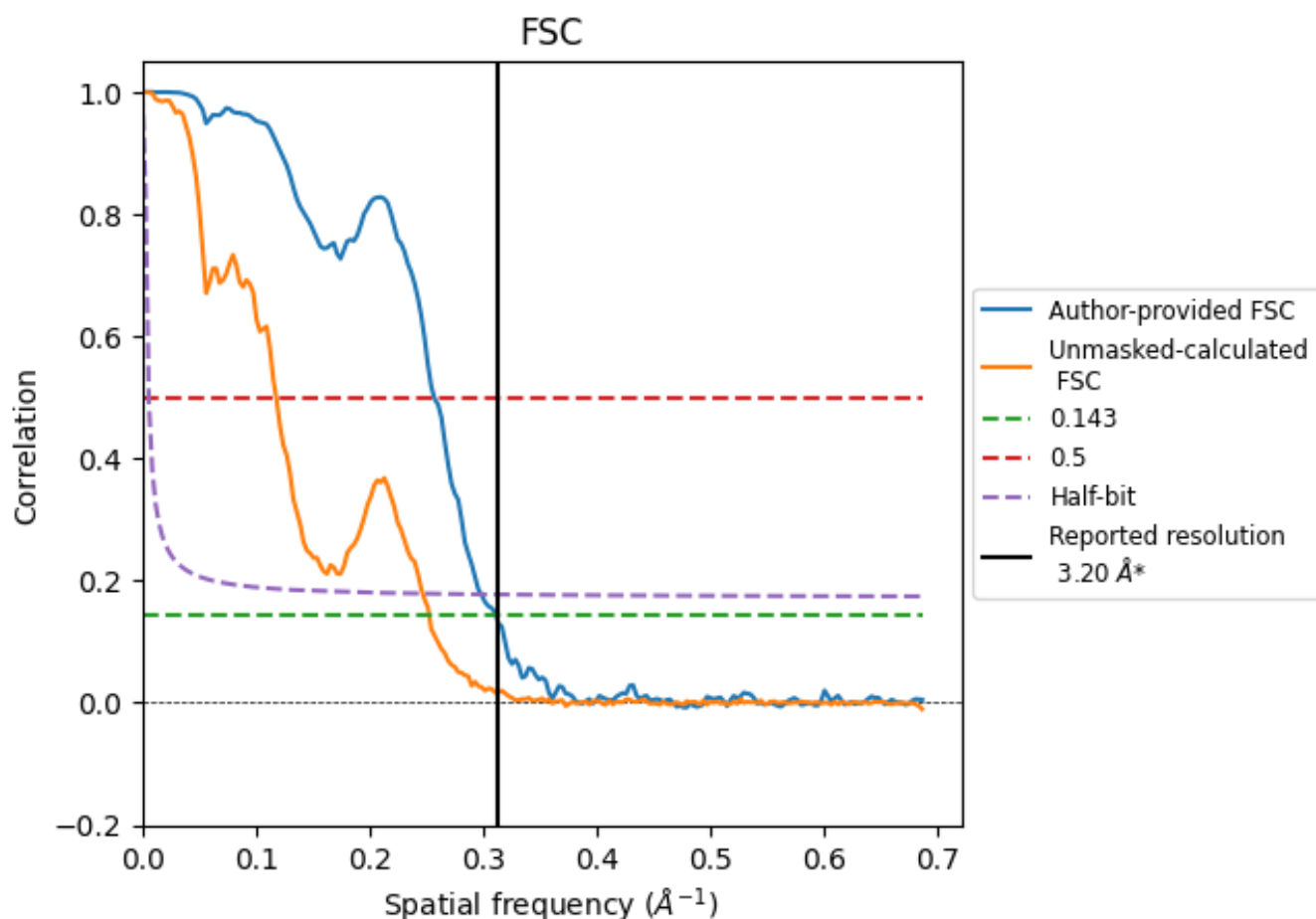


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

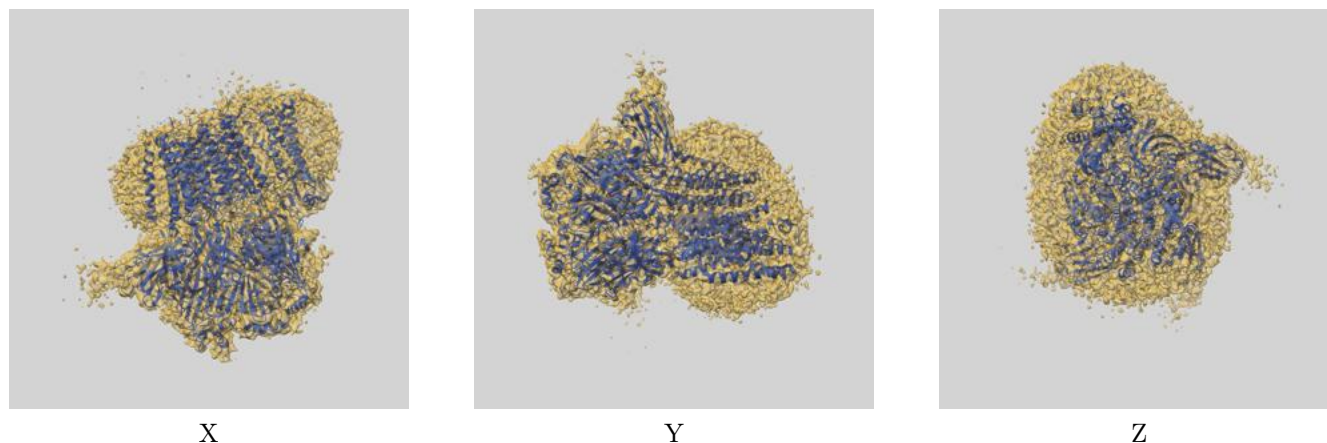
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.89	3.35
Unmasked-calculated*	3.96	8.50	4.05

*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 3.96 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

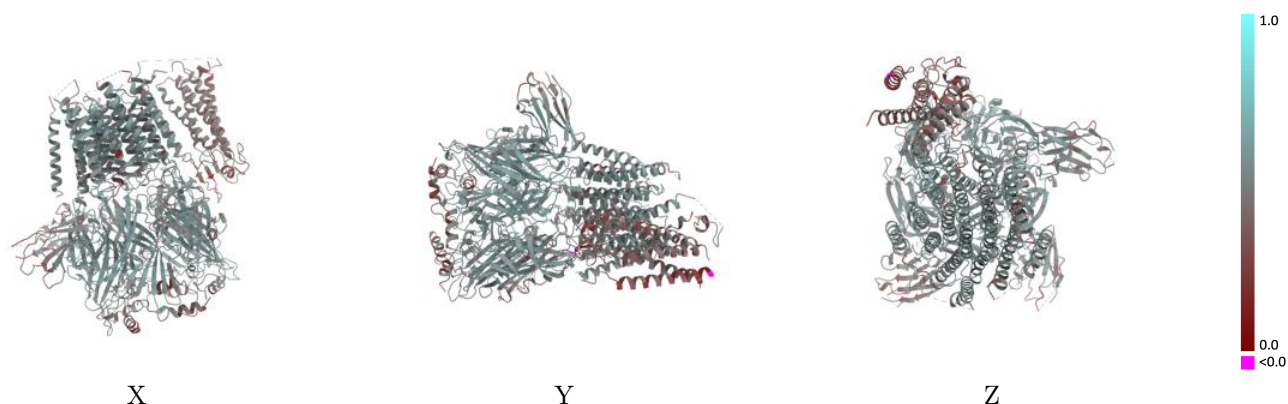
This section contains information regarding the fit between EMDB map EMD-50283 and PDB model 9FAV. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



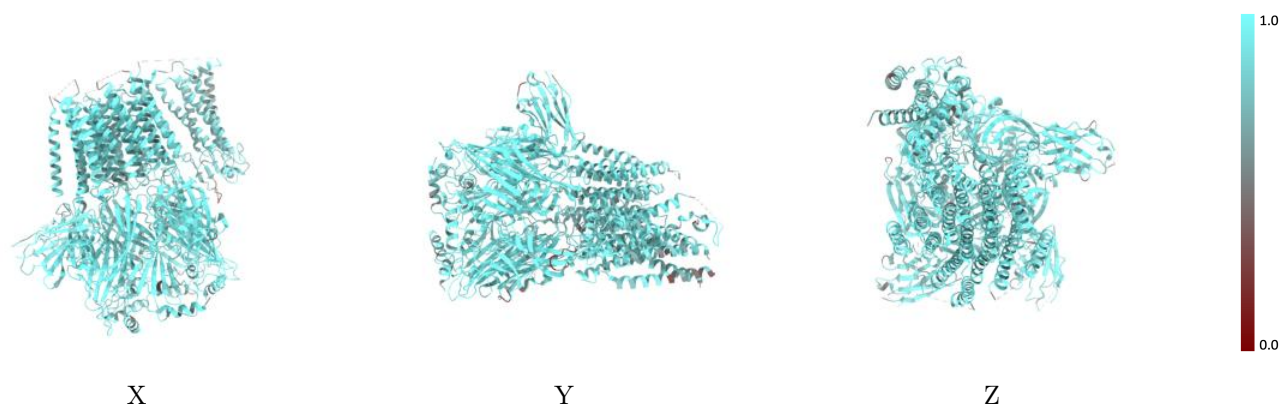
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



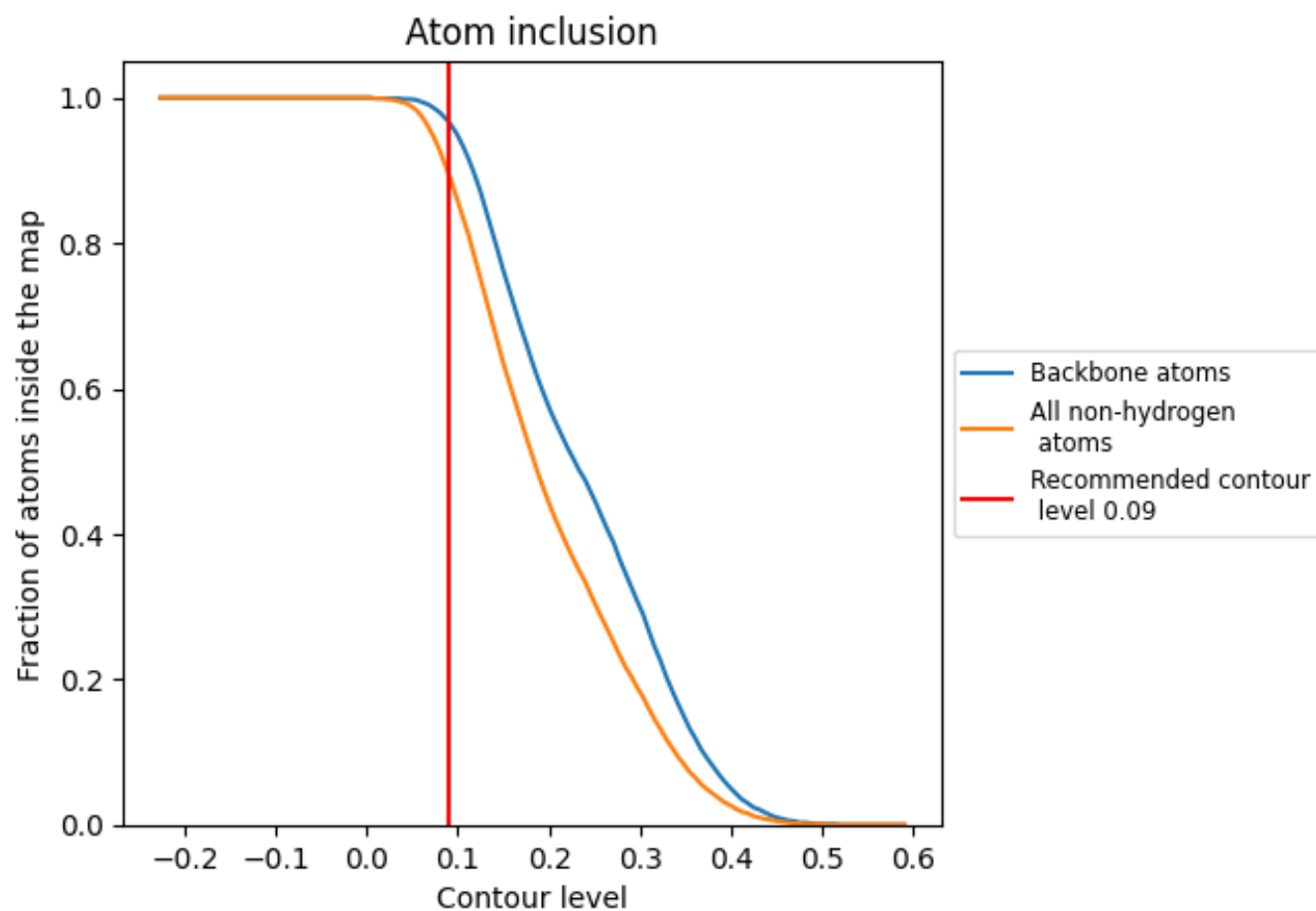
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.4980
A	 0.9190	 0.5200
B	 0.9270	 0.5360
C	 0.9010	 0.5170
D	 0.8990	 0.5080
E	 0.9200	 0.5180
F	 0.8850	 0.4970
G	 0.8720	 0.4550
H	 0.6960	 0.2720
I	 0.9520	 0.5040
J	 0.7860	 0.4190
K	 0.9010	 0.4830
L	 0.7980	 0.3800
M	 0.9720	 0.5010
N	 0.7690	 0.4140
O	 0.8530	 0.4360
P	 0.9250	 0.5000
Q	 0.7500	 0.3750
R	 0.6720	 0.3870

