



wwPDB EM Validation Summary Report ⓘ

Feb 28, 2024 – 02:16 PM JST

PDB ID : 8XMN
EMDB ID : EMD-38483
Title : Voltage-gated sodium channel Nav1.7 variant M2
Authors : Yan, N.; Li, Z.; Wu, Q.; Huang, G.
Deposited on : 2023-12-27
Resolution : 3.37 Å(reported)

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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:

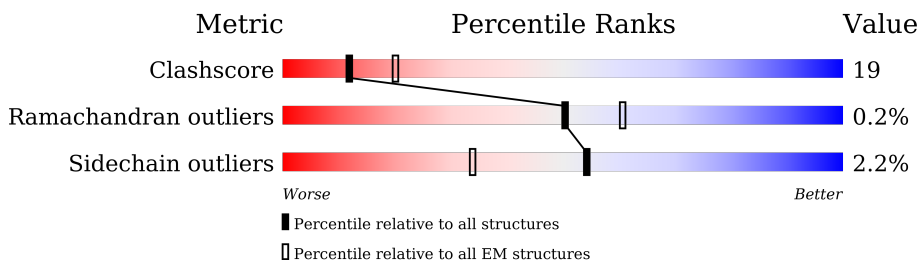
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.37 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2031	 5% 38% 24% 37%
2	B	230	 34% 41% 25%
3	C	227	 33% 28% 24% 48%
4	D	2	 50% 50%
4	E	2	 50% 50%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13110 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1277	10299	6825	1618	1778	78	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	866	PHE	LEU	variant	UNP Q15858
A	1454	CYS	GLY	variant	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	173	1416	902	232	272	10	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	LEU	-	expression tag	UNP Q07699
B	220	GLU	-	expression tag	UNP Q07699
B	221	HIS	-	expression tag	UNP Q07699
B	222	HIS	-	expression tag	UNP Q07699
B	223	HIS	-	expression tag	UNP Q07699
B	224	HIS	-	expression tag	UNP Q07699
B	225	HIS	-	expression tag	UNP Q07699
B	226	HIS	-	expression tag	UNP Q07699
B	227	HIS	-	expression tag	UNP Q07699
B	228	HIS	-	expression tag	UNP Q07699
B	229	HIS	-	expression tag	UNP Q07699
B	230	HIS	-	expression tag	UNP Q07699

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	119	980	615	172	183	10	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	216	LEU	-	expression tag	UNP O60939
C	217	GLU	-	expression tag	UNP O60939
C	218	HIS	-	expression tag	UNP O60939
C	219	HIS	-	expression tag	UNP O60939
C	220	HIS	-	expression tag	UNP O60939
C	221	HIS	-	expression tag	UNP O60939
C	222	HIS	-	expression tag	UNP O60939
C	223	HIS	-	expression tag	UNP O60939
C	224	HIS	-	expression tag	UNP O60939
C	225	HIS	-	expression tag	UNP O60939
C	226	HIS	-	expression tag	UNP O60939
C	227	HIS	-	expression tag	UNP O60939

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



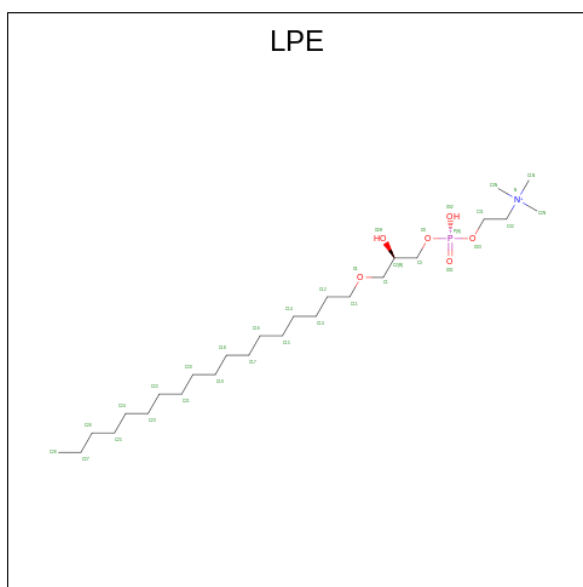
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



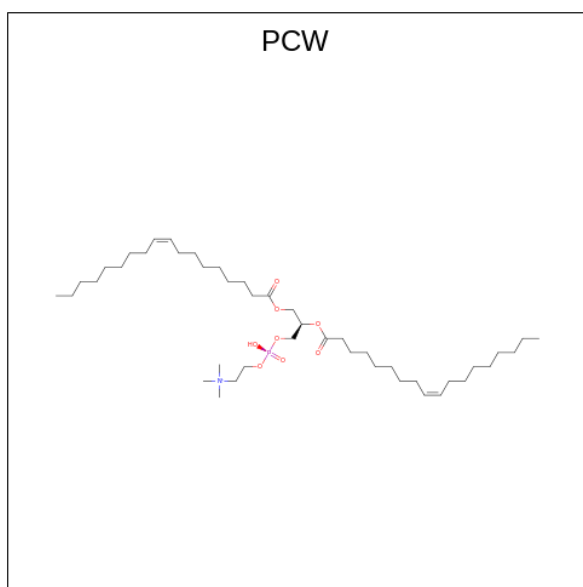
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C₂₆H₅₇NO₆P).

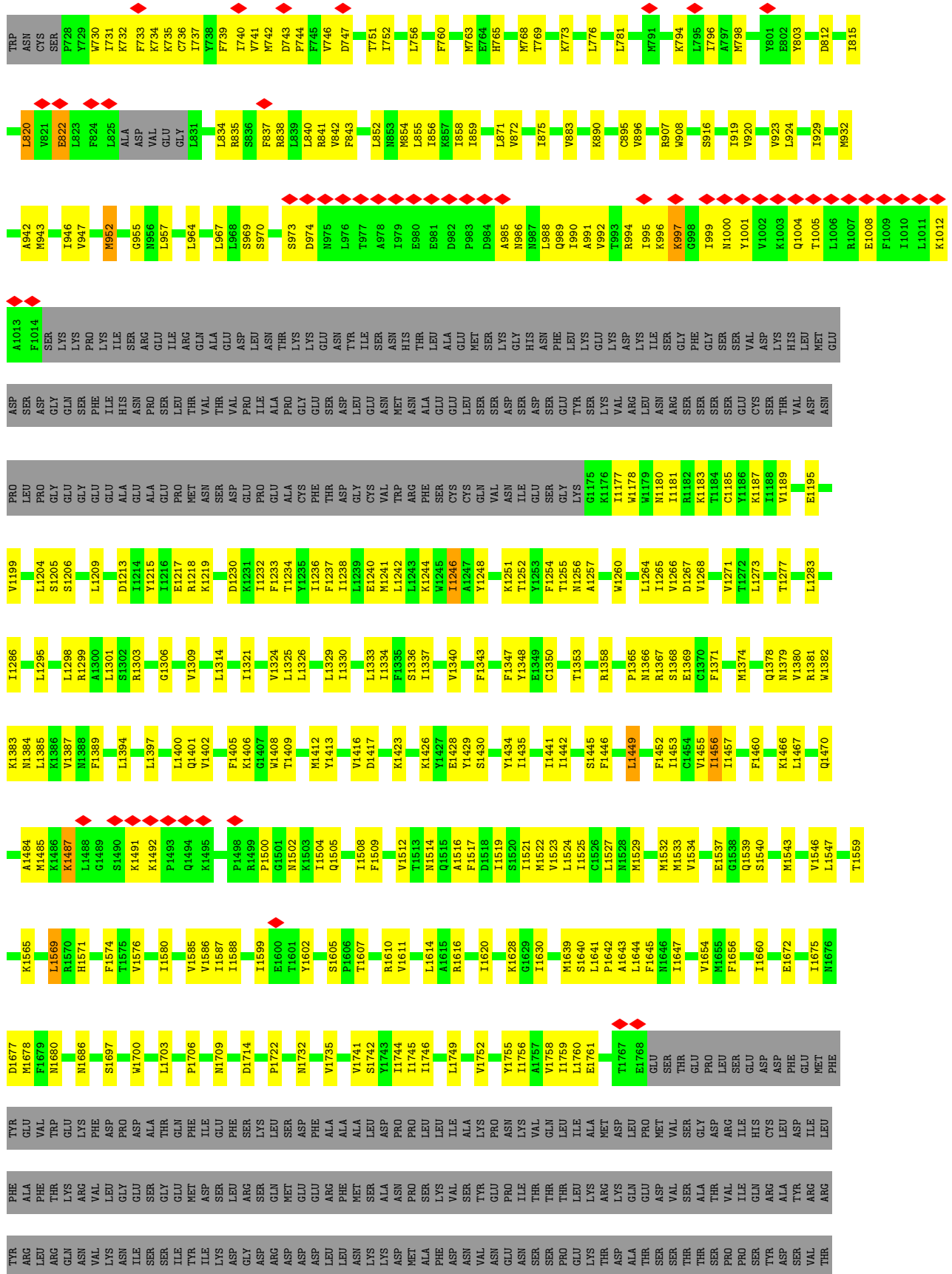


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	25	17	1	6	1	0
6	A	1	25	17	1	6	1	0
6	A	1	28	20	1	6	1	0
6	A	1	28	20	1	6	1	0
6	A	1	25	17	1	6	1	0

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	Total 53	43	1	8	1	0
7	A	1	Total 47	37	1	8	1	0
7	A	1	Total 44	34	1	8	1	0



LYS
PRO
ASP
LYS
LEU
GLU
LYS
TYR
GLU
GLN
GLY
ASP
ARG
THR
GLU
LYS
GLU
SER
LYS
LYS

- Molecule 2: Sodium channel subunit beta-1

Chain B:  34% 41% 25%


MET
GLY
ARG
LEU
LEU
ALA
LEU
VAL
VAL
GLY
GLY
ALA
THR
LEU
VAL
SER
SER
ALA
CYS
GLY
ASP
ASP
SER
GLU
LYS
LYS
LYS

V68
K69
I70
L71
S156
R72
Y73
E74
H75
E76
V77
L78
G79
L80
R85
F86
E87
Q88
R89
W92
N93
Q102
D103
L104
S105
V111
T112
Y113
M114
H115
E120
C121
H122
V123
Y124
R125
L126
L127
F128
F129
Y132
E133
H134
V139
K140
H143
I144
E145
V146
V147
D148
K149

D153
M154
A155
S156
V157
V158
I161
M162
M163
V164
V165
L166
I167
V168
V169
F170
L171
I172
W173
L174
V175
A176
E177
M178
I179
K183
A184
I185
A186
A187
E190
T191
A192
ALA
GLN
GLU
ASN
ALA
SER
GLU
TYR
LEU
ALA
ILE
THR
SER
SER
GLU
SER
LYS
GLU
ASN
CYS
THR
GLY
VAL
GLN
VAL

ALA
GLU
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 3: Sodium channel subunit beta-2

Chain C:  28% 33% 24% 48%

MET
HIS
ARG
ASP
ALA
TRP
LEU
PRO
ARG
PRO
ALA
PHE
SER
LEU
THR
GLY
LEU
SER
LEU
VAL
PRO
PRO
GLY
ARG
SER
R30
E31
V32
T33
V34
F35
A36
T37
L38
N39
V40
L41
M42
G43
S44
D45
A46
R47
L48
P49
F52
Y56
M59
H60
K61
Q62
F63
S64

L65
R66
W67
T68
Y69
Q70
E71
C72
H73
N74
C75
S76
E77
E78
M79
F80
L81
Q82
F83
R84
M85
K86
I87
L88
M89
L90
K91
L92
E93
R94
F95
Q96
D97
R98
V99
E100
F101
S102
S106
K107
V110
M113
L114
R115
M116
V117
Q118
P119
E120
D121
E122
G123
I124
Y125
M126
C127
Y128

I129
R135
H136
R137
G138
H139
G140
K141
I142
H143
L144
Q145
V146
L147
M148
GLU
GLU
PRO
PRO
GLU
GLU
ASP
ASP
SER
THR
VAL
ALA
VAL
ILE
VAL
GLY
ALA
SER
VAL
GLY
GLY
PHE
LEU
ALA
VAL
VAL
ILE
LEU
LEU
LEU
MET
VAL
VAL
VAL
CYS
VAL
ARG
ARG
LYS
LYS
GLU
GLN
LYS
LEU
SER

THR
ASP
ASP
LEU
LYS
THR
GLU
GLU
GLY
GLY
ASN
PRO
ASP
ASP
GLY
ALA
LYS
LEU
LEU
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77511	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.416	Depositor
Minimum map value	-0.821	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	241.1712, 241.1712, 241.1712	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8374, 0.8374, 0.8374	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: NAG, LPE, PCW

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	0.57	0/10549	0.66	0/14289
2	B	0.45	0/1442	0.56	0/1949
3	C	0.35	0/1011	0.60	0/1367
All	All	0.55	0/13002	0.65	0/17605

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 [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	10299	0	10525	396	0
2	B	1416	0	1380	77	0
3	C	980	0	945	47	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	28	0	26	1	0
5	B	56	0	52	2	0
6	A	131	0	184	7	0
7	A	144	0	203	6	0
All	All	13110	0	13365	515	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 19.

The worst 5 of 515 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:99:ARG:HD2	1:A:181:PHE:CZ	1.89	1.07
1:A:815:ILE:HG21	1:A:841:ARG:HD2	1.41	0.99
1:A:1599:ILE:HD11	1:A:1605:SER:HB2	1.52	0.91
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.59	0.85
1:A:1347:PHE:HB3	1:A:1385:LEU:HD23	1.60	0.83

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	1265/2031 (62%)	1180 (93%)	83 (7%)	2 (0%)	47 78
2	B	171/230 (74%)	158 (92%)	13 (8%)	0	100 100
3	C	120/227 (53%)	112 (93%)	7 (6%)	1 (1%)	19 53
All	All	1556/2488 (62%)	1450 (93%)	103 (7%)	3 (0%)	50 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PHE
1	A	183	PHE
3	C	97	ASP

5.3.2 Protein sidechains [i](#)

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	1140/1810 (63%)	1110 (97%)	30 (3%)	46	72
2	B	157/202 (78%)	157 (100%)	0	100	100
3	C	114/205 (56%)	113 (99%)	1 (1%)	78	89
All	All	1411/2217 (64%)	1380 (98%)	31 (2%)	54	76

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	820	LEU
1	A	1571	HIS
1	A	952	MET
1	A	1628	LYS
1	A	1466	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	102	GLN
2	B	115	HIS
3	C	139	HIS
1	A	1470	GLN
1	A	1505	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

4 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
4	NAG	D	1	1,4	14,14,15	0.53	0	17,19,21	0.93	1 (5%)
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	E	1	1,4	14,14,15	0.65	0	17,19,21	0.99	2 (11%)
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.55	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	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(°)
4	D	1	NAG	C1-O5-C5	2.92	116.15	112.19
4	E	1	NAG	O5-C5-C4	-2.24	105.39	110.83
4	E	1	NAG	C1-O5-C5	-2.10	109.34	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2

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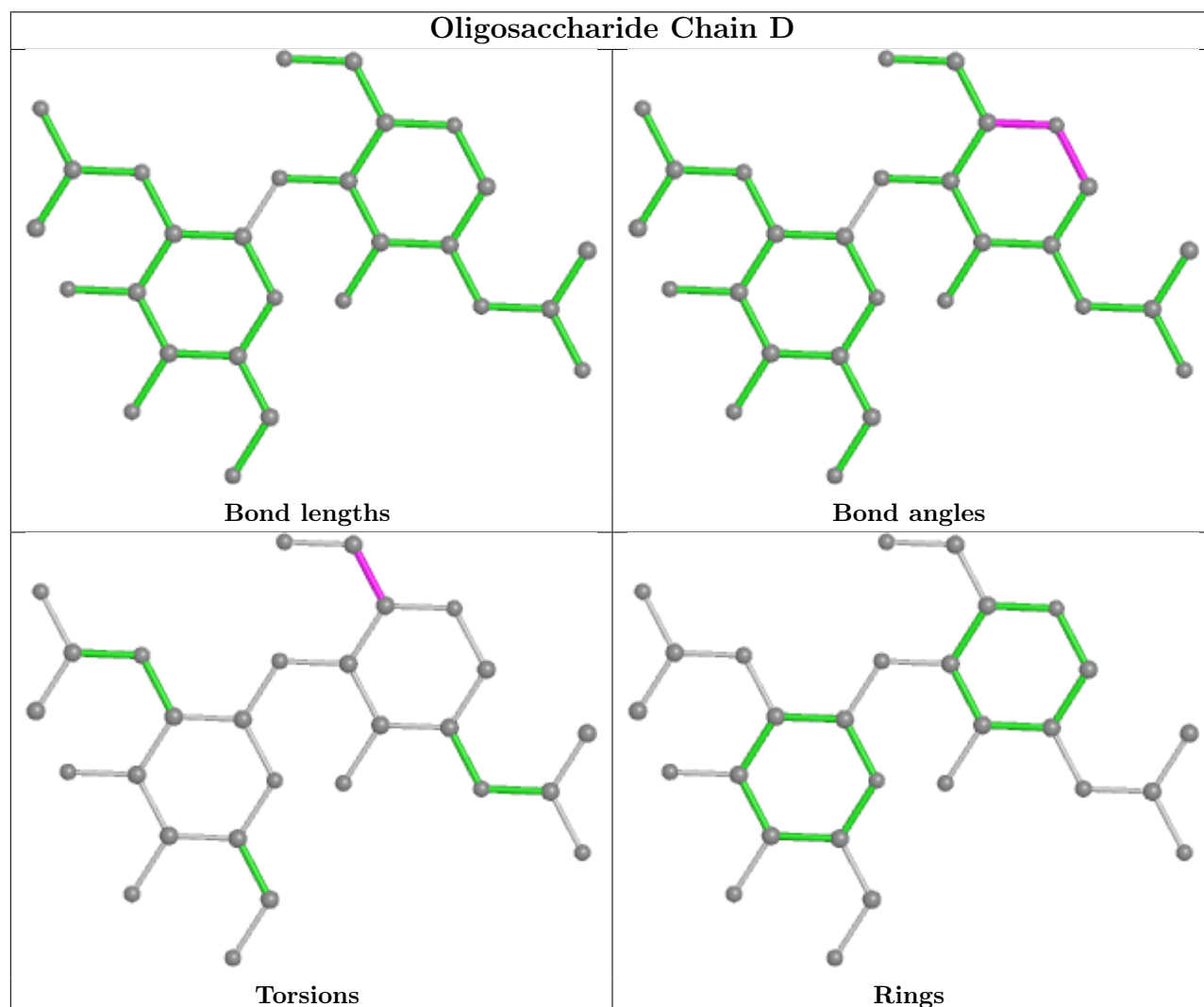
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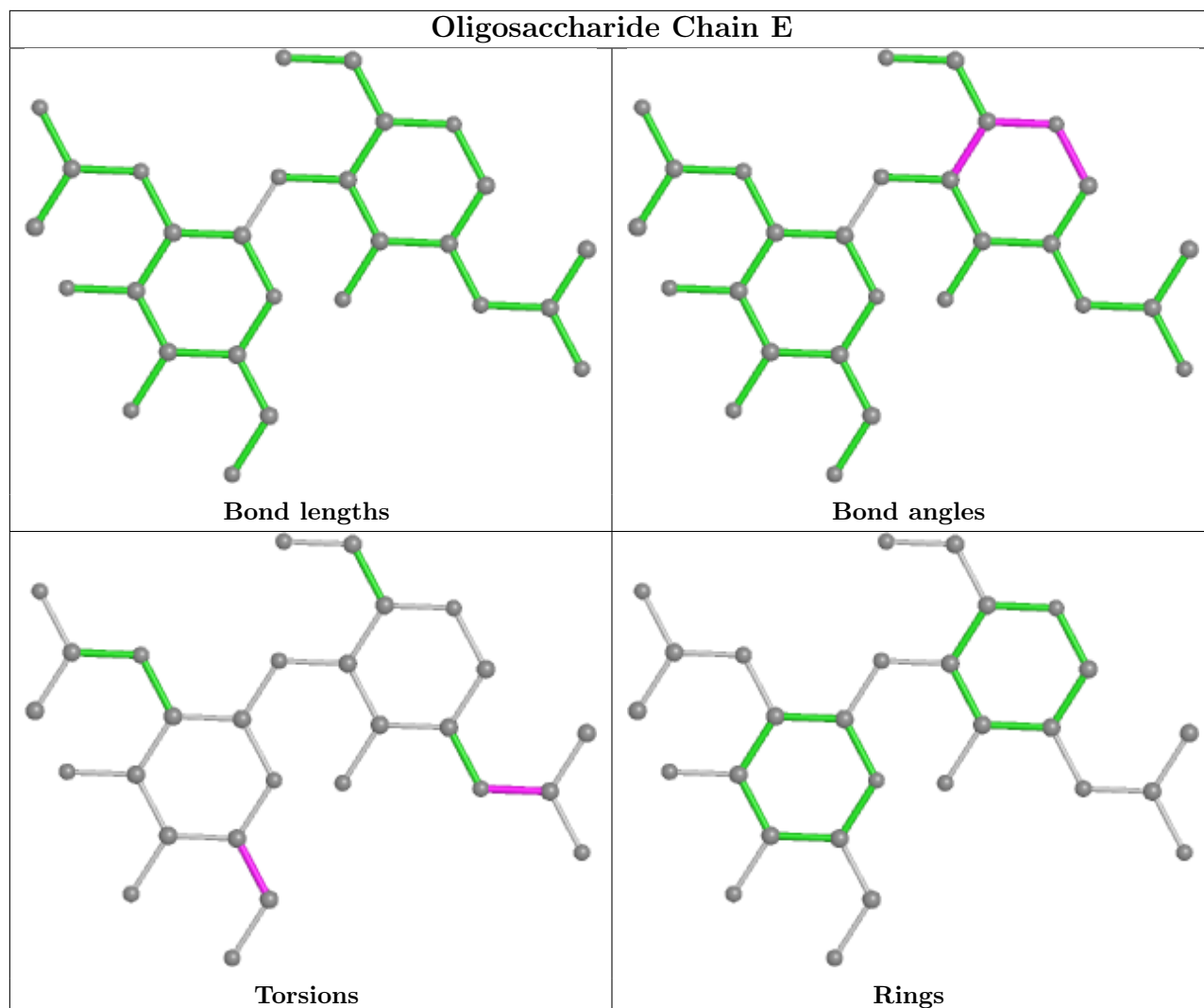
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

14 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	$\# Z > 2$
7	PCW	A	2005	-	52,52,53	0.92	2 (3%)	58,60,61	1.05	5 (8%)
6	LPE	A	2007	-	27,27,33	0.52	0	31,33,39	0.64	0
6	LPE	A	2006	-	27,27,33	0.53	0	31,33,39	0.74	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	0.37	0
5	NAG	A	2002	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	B	304	2	14,14,15	0.20	0	17,19,21	0.79	1 (5%)
5	NAG	B	303	2	14,14,15	0.32	0	17,19,21	0.55	0
5	NAG	B	301	2	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
6	LPE	A	2004	-	24,24,33	0.33	0	25,27,39	0.70	0
6	LPE	A	2010	-	24,24,33	0.55	0	28,30,39	0.60	1 (3%)
6	LPE	A	2003	-	24,24,33	0.54	0	28,30,39	0.72	0
7	PCW	A	2009	-	43,43,53	1.00	2 (4%)	49,51,61	1.19	3 (6%)
5	NAG	B	302	2	14,14,15	0.19	0	17,19,21	0.44	0
7	PCW	A	2008	-	46,46,53	0.98	2 (4%)	52,54,61	1.22	4 (7%)

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
7	PCW	A	2005	-	-	19/56/56/57	-
6	LPE	A	2007	-	-	11/28/28/34	-
6	LPE	A	2006	-	-	10/28/28/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	B	304	2	-	2/6/23/26	0/1/1/1
5	NAG	B	303	2	-	2/6/23/26	0/1/1/1
5	NAG	B	301	2	-	3/6/23/26	0/1/1/1
6	LPE	A	2004	-	-	10/25/25/34	-
6	LPE	A	2010	-	-	13/25/25/34	-
6	LPE	A	2003	-	-	10/25/25/34	-
7	PCW	A	2009	-	-	11/47/47/57	-
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
7	PCW	A	2008	-	-	19/50/50/57	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2008	PCW	O3-C11	4.17	1.45	1.33
7	A	2005	PCW	O3-C11	4.14	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2009	PCW	O3-C11	4.12	1.45	1.33
7	A	2009	PCW	O2-C31	3.98	1.45	1.34
7	A	2005	PCW	O2-C31	3.94	1.45	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2008	PCW	O2-C31-C32	4.97	122.22	111.50
7	A	2009	PCW	O2-C31-C32	4.41	121.00	111.50
7	A	2005	PCW	O2-C31-C32	3.84	119.77	111.50
7	A	2009	PCW	C2-O2-C31	-3.54	109.06	117.79
5	B	301	NAG	C1-O5-C5	3.35	116.73	112.19

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	LPE	C2-C3-O3-P
6	A	2003	LPE	C31-O33-P-O3
6	A	2003	LPE	C31-O33-P-O31
6	A	2004	LPE	O1-C1-C2-O2H
6	A	2004	LPE	C3-O3-P-O32

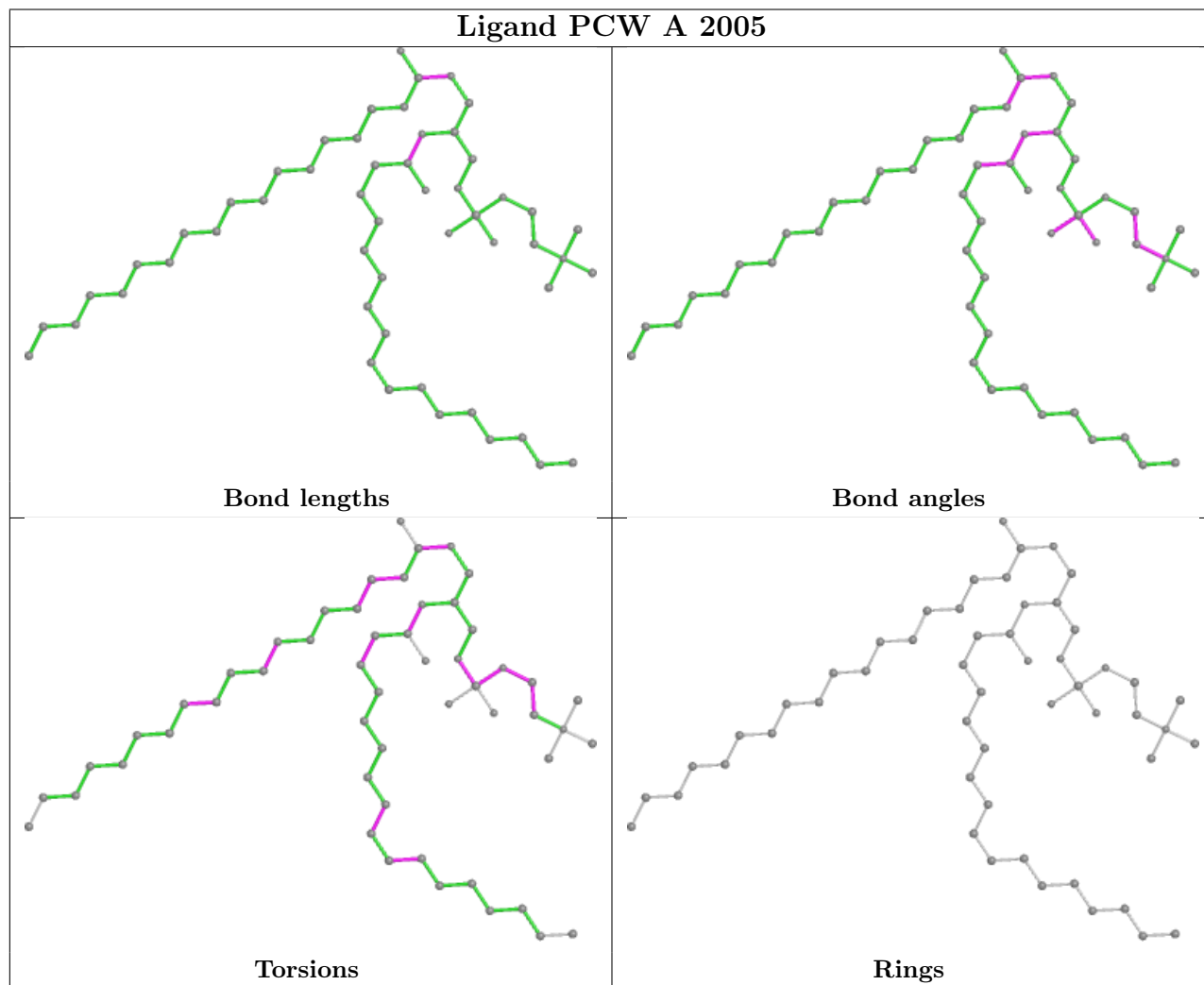
There are no ring outliers.

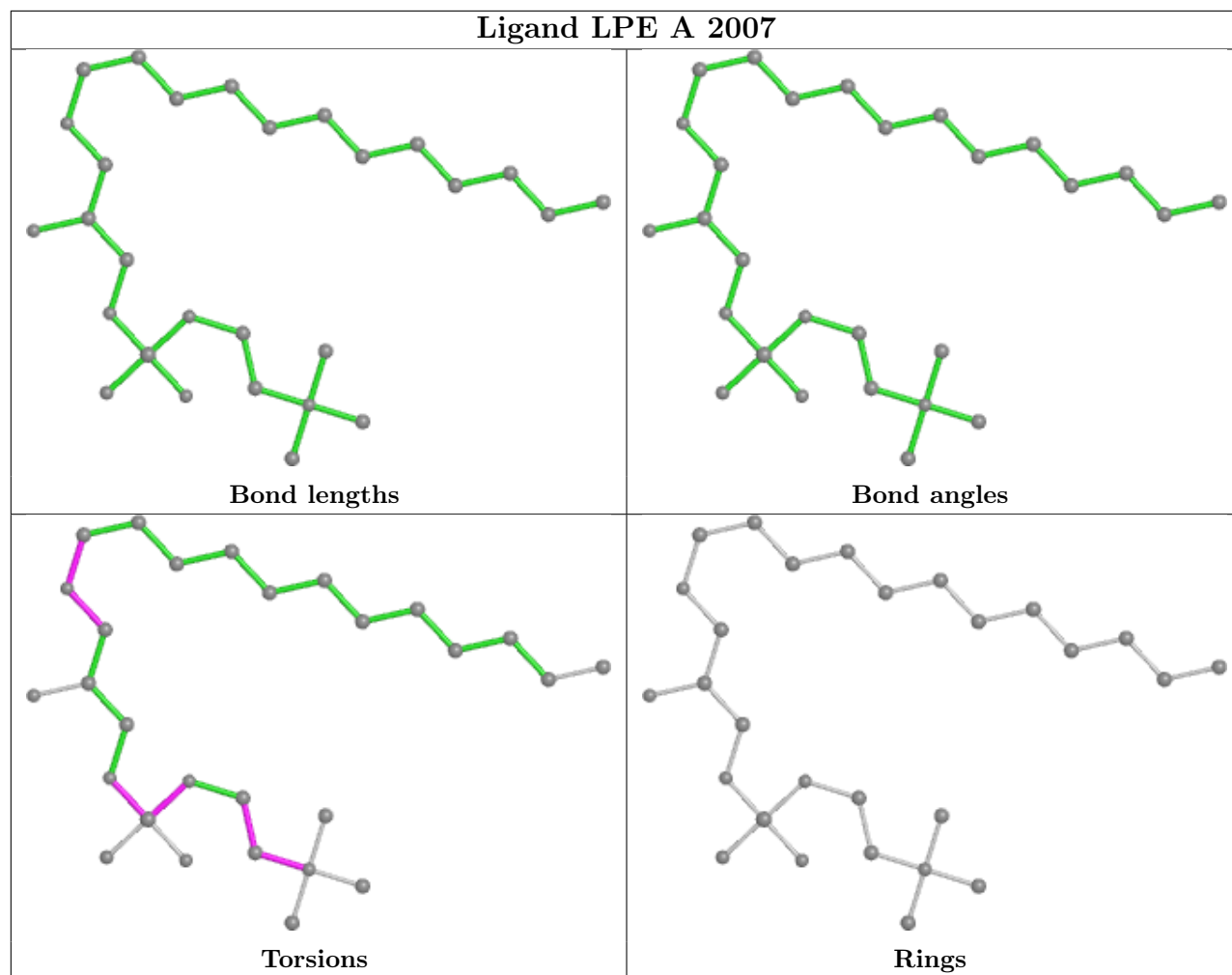
9 monomers are involved in 15 short contacts:

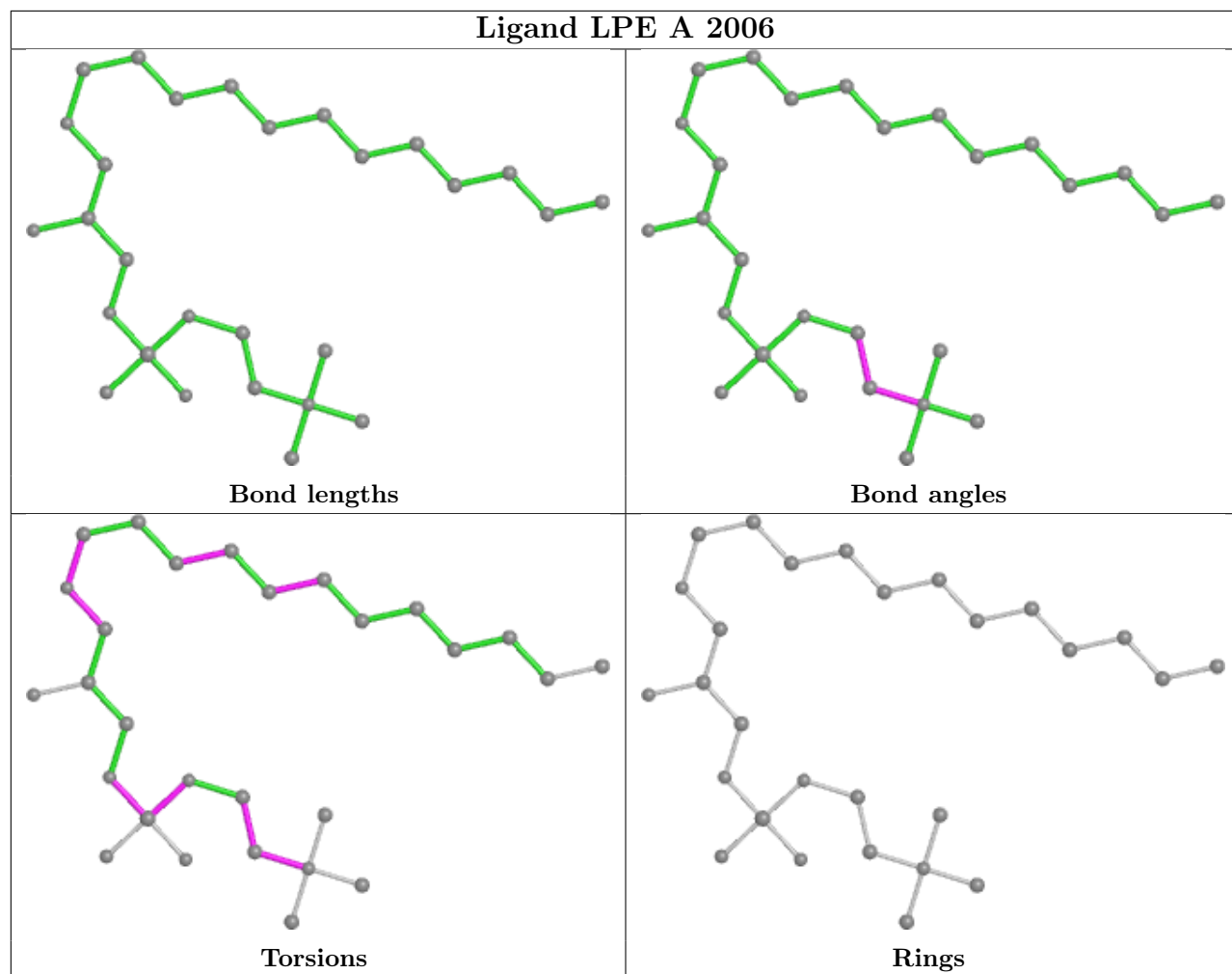
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2005	PCW	4	0
6	A	2006	LPE	1	0
5	A	2002	NAG	1	0
5	B	304	NAG	1	0
5	B	301	NAG	1	0
6	A	2004	LPE	1	0
6	A	2010	LPE	3	0
6	A	2003	LPE	2	0
7	A	2008	PCW	2	0

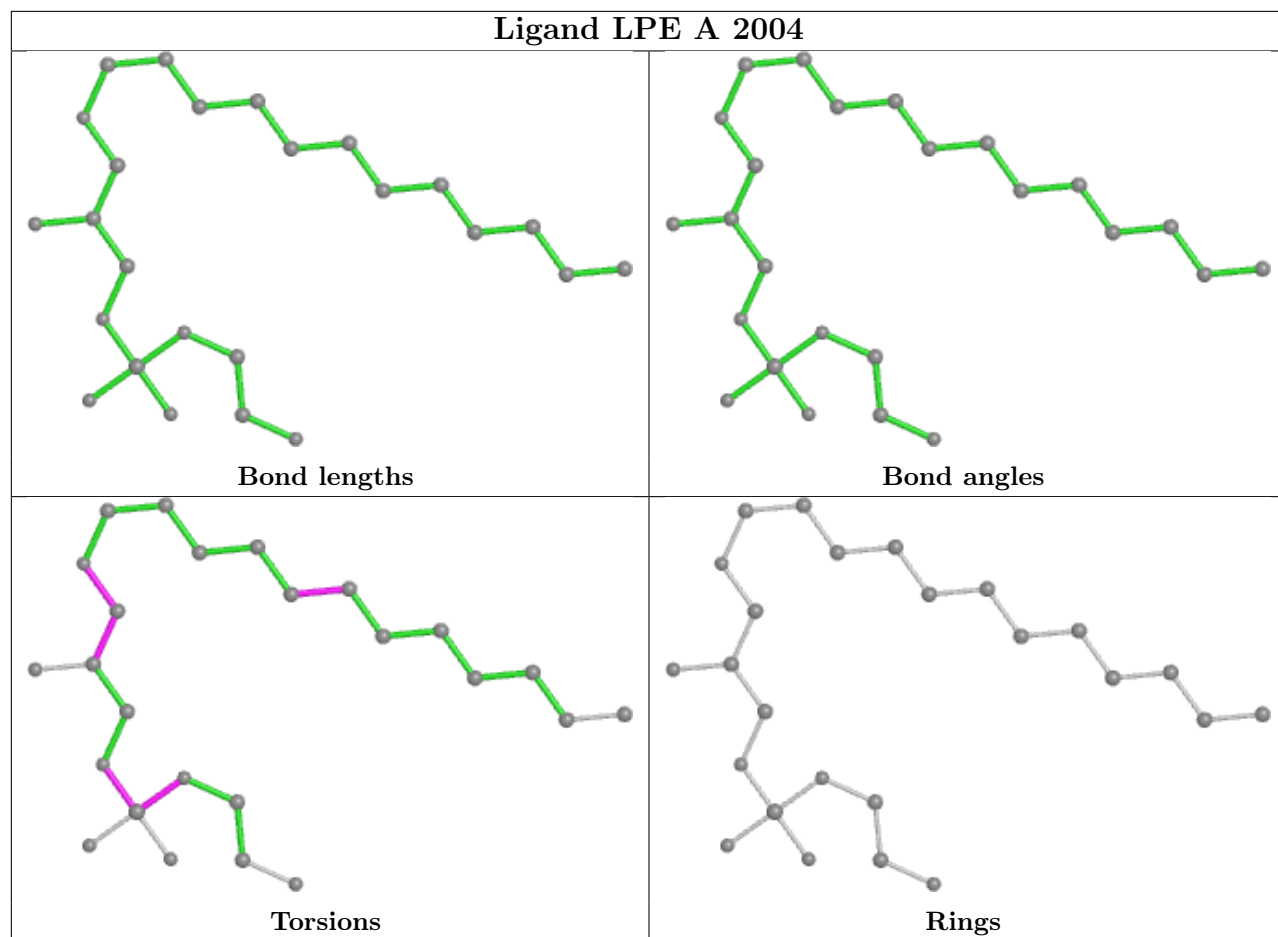
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

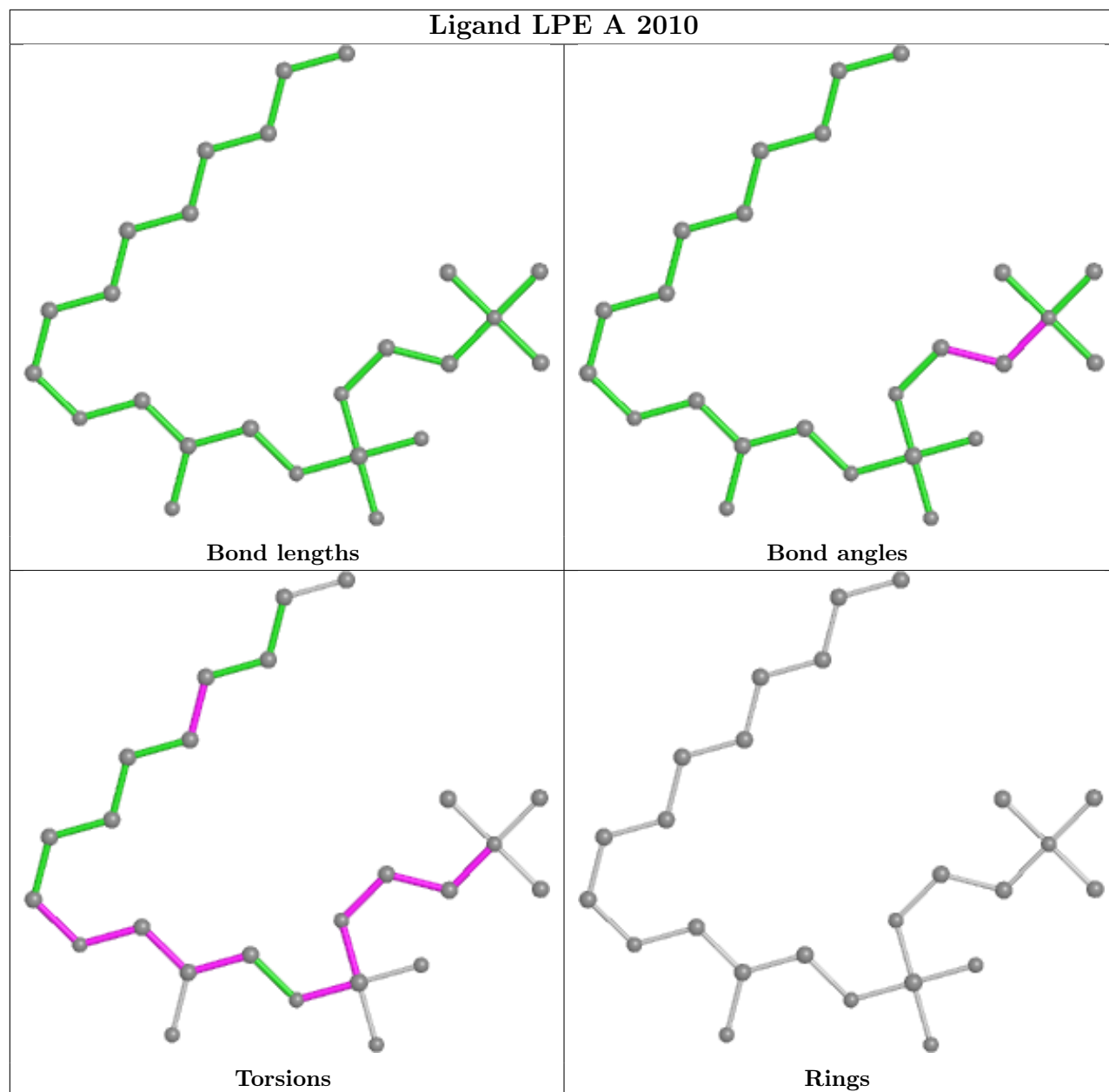
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

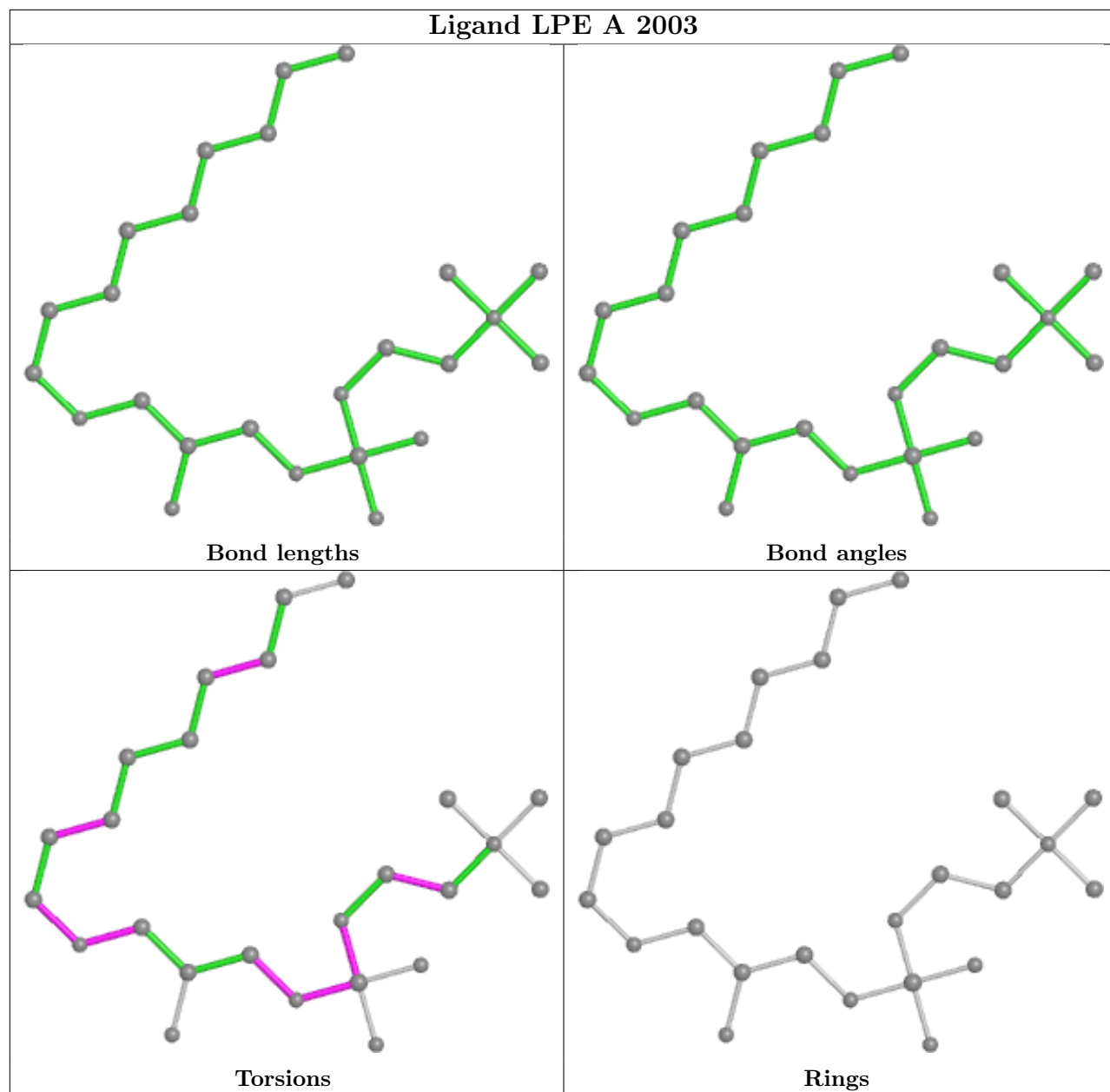


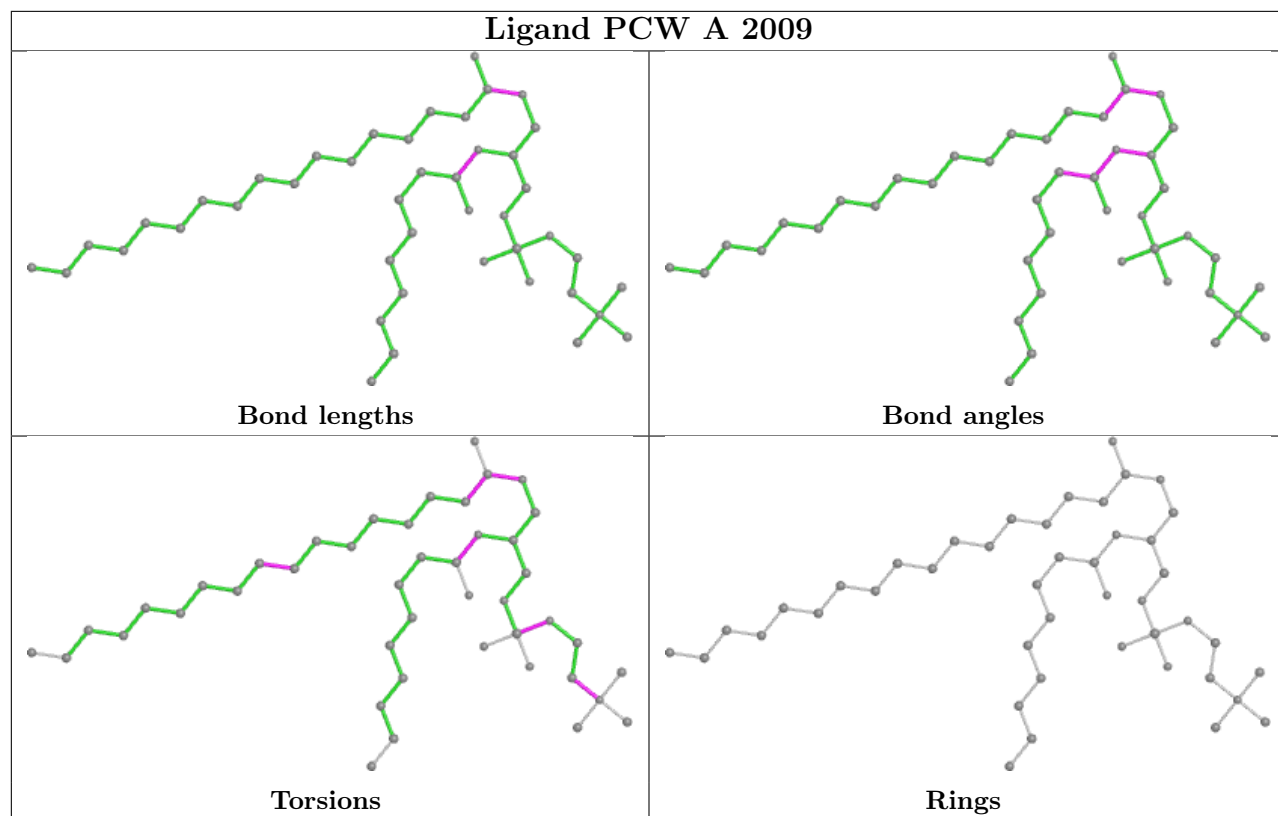


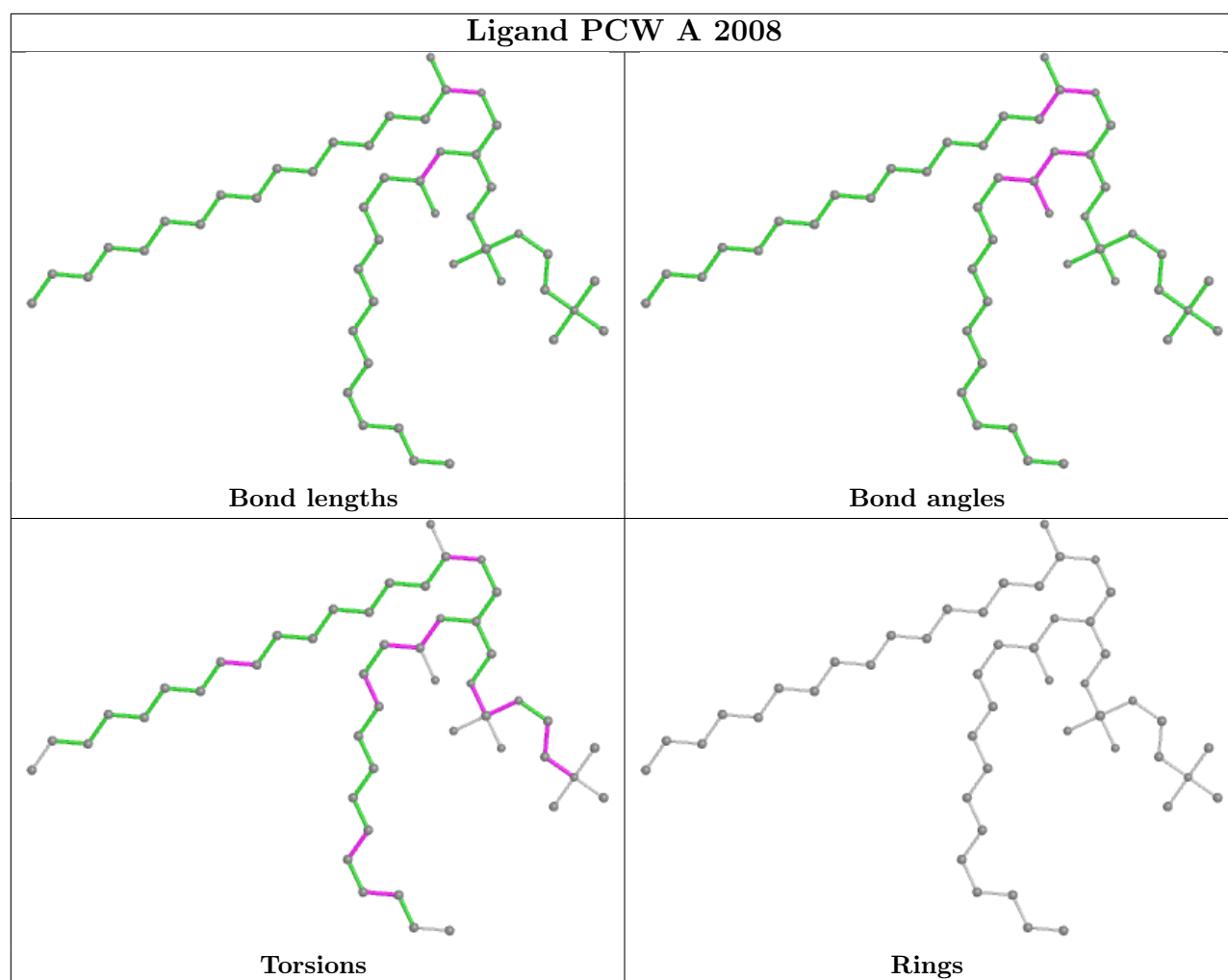












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

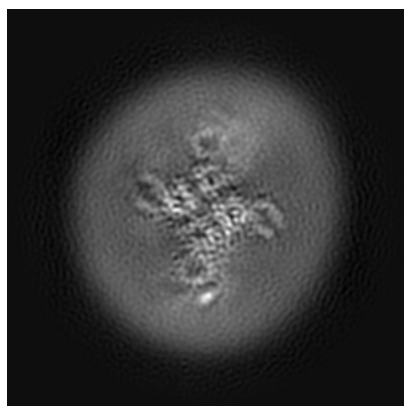
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38483. These allow visual inspection of the internal detail of the map and identification of artifacts.

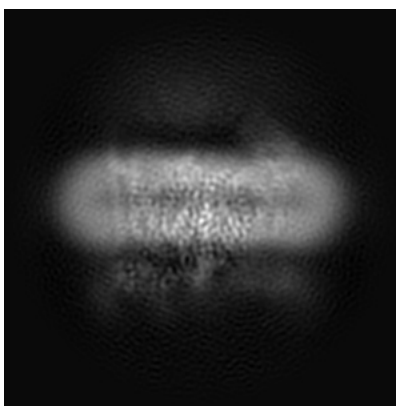
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

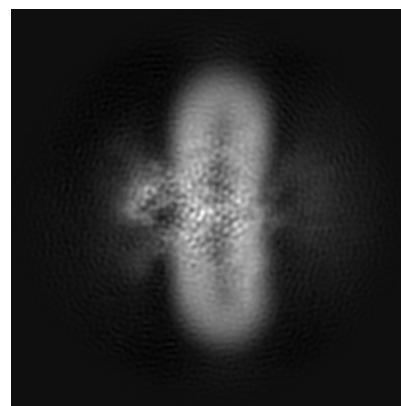
6.1.1 Primary map



X

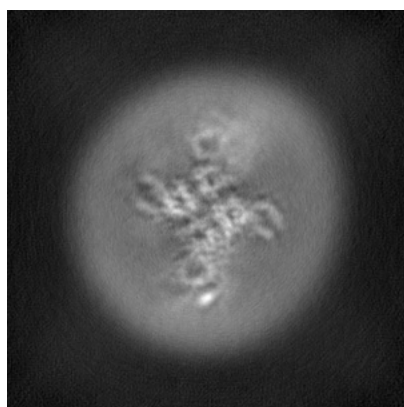


Y

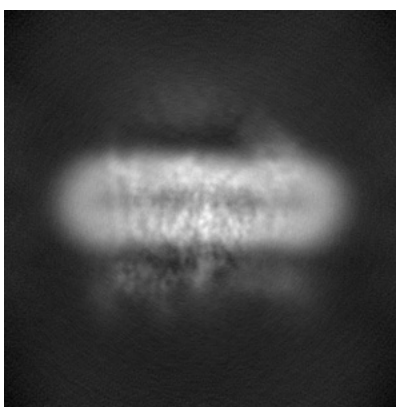


Z

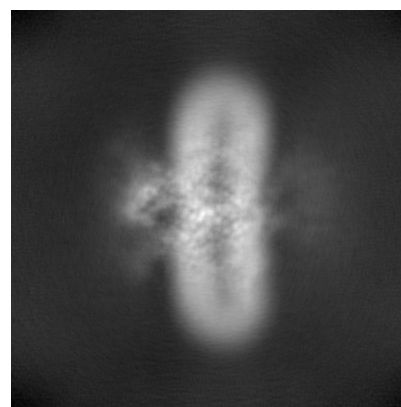
6.1.2 Raw map



X



Y

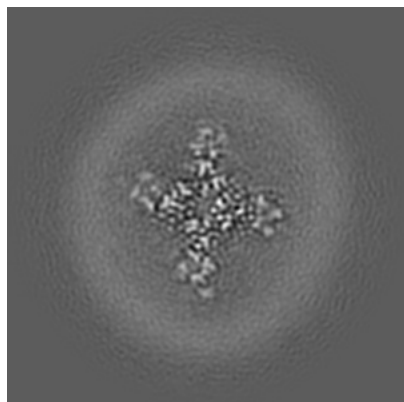


Z

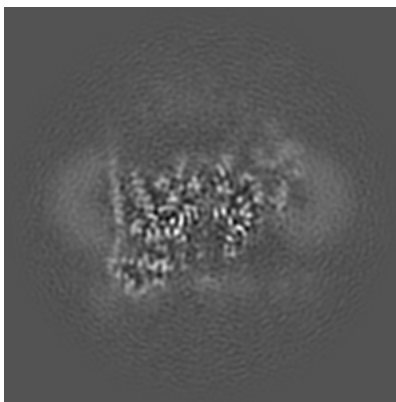
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

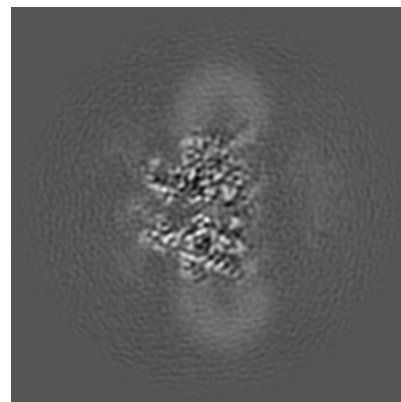
6.2.1 Primary map



X Index: 144

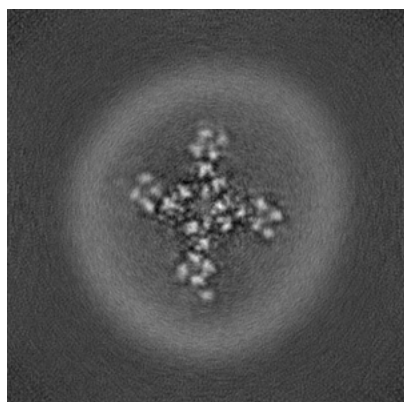


Y Index: 144

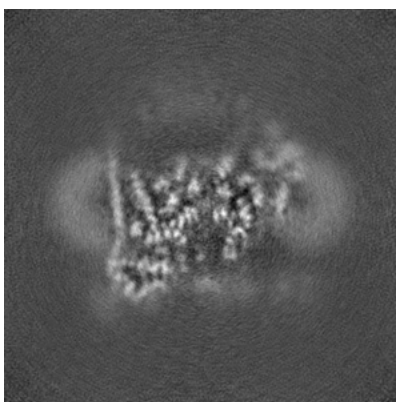


Z Index: 144

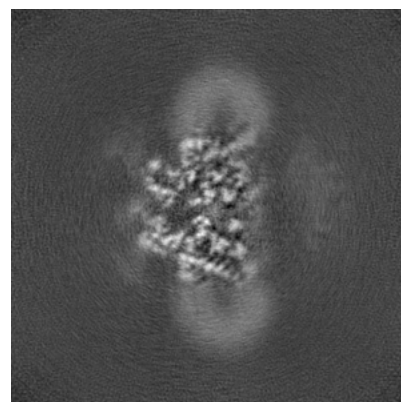
6.2.2 Raw map



X Index: 144



Y Index: 144

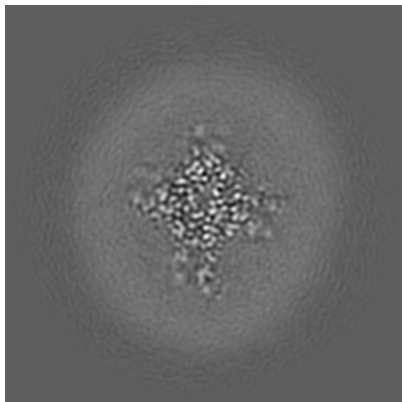


Z Index: 144

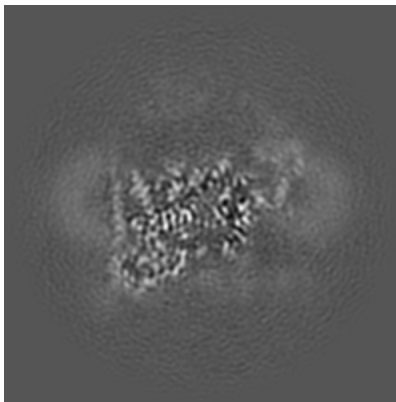
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

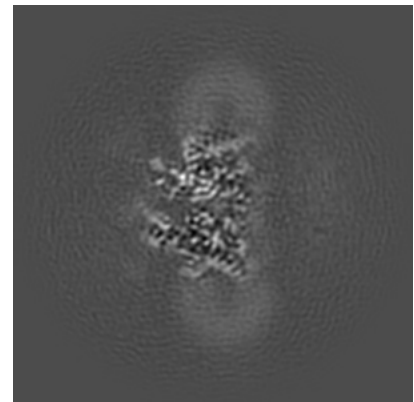
6.3.1 Primary map



X Index: 133

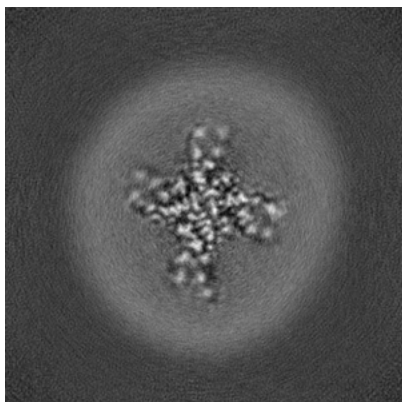


Y Index: 146

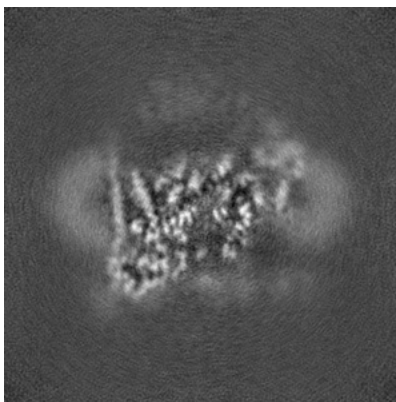


Z Index: 146

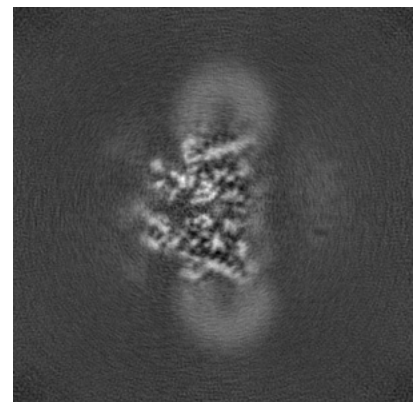
6.3.2 Raw map



X Index: 136



Y Index: 145

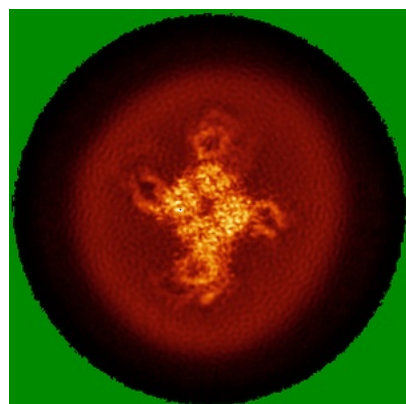


Z Index: 146

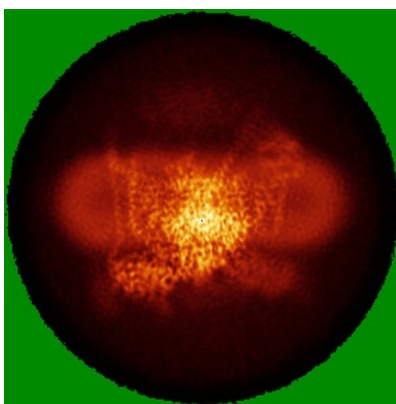
The images above show the largest variance slices of the map in three orthogonal directions.

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

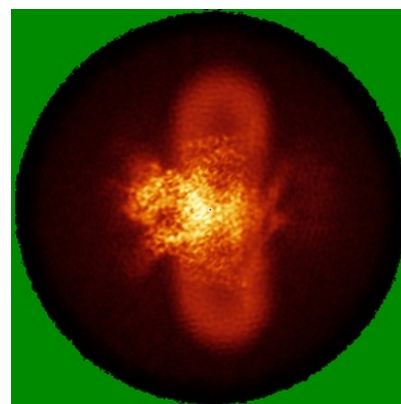
6.4.1 Primary map



X

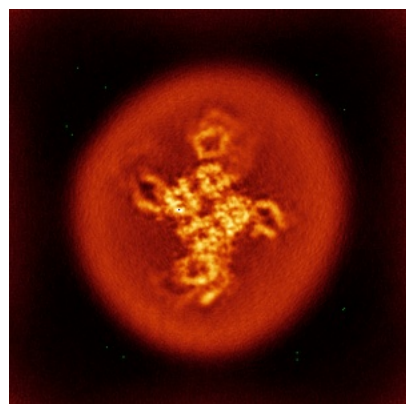


Y

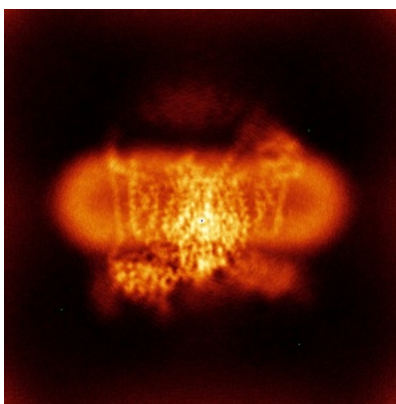


Z

6.4.2 Raw map



X



Y

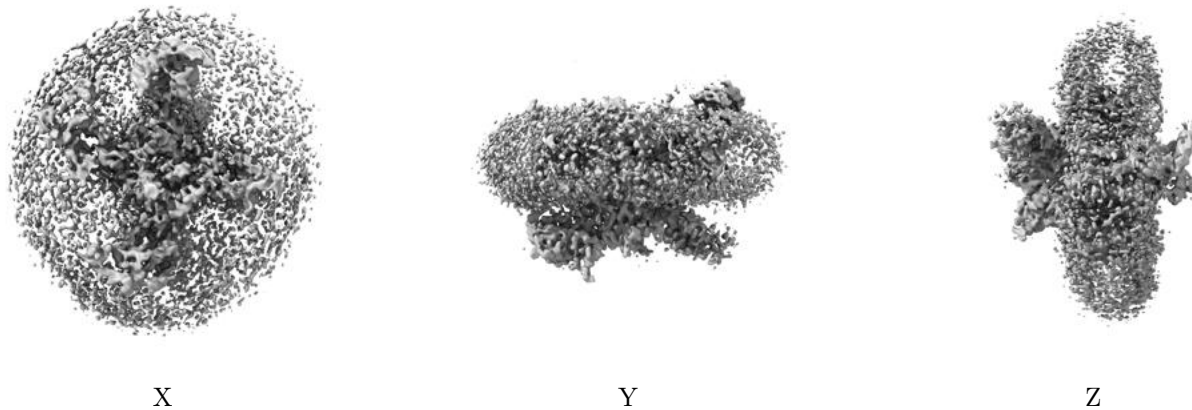


Z

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.

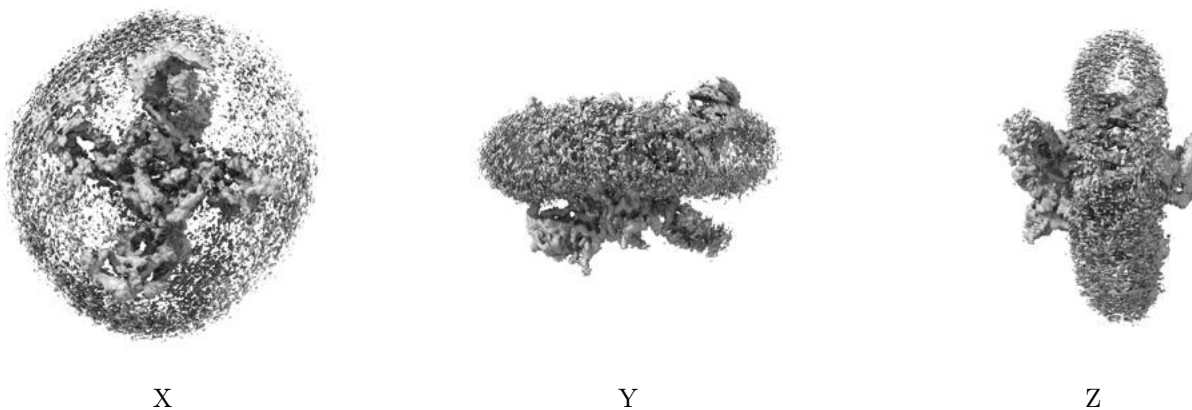
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

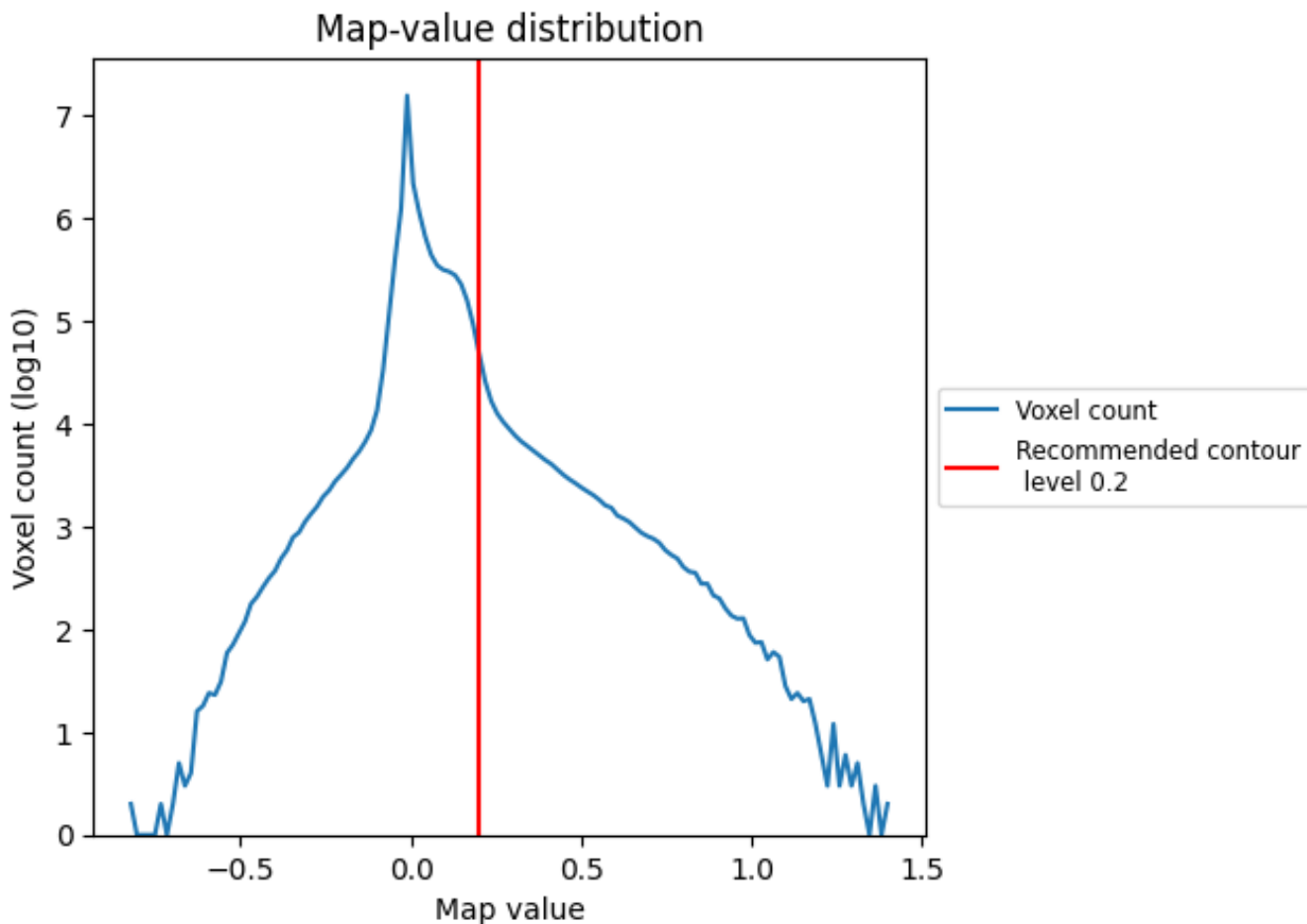
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

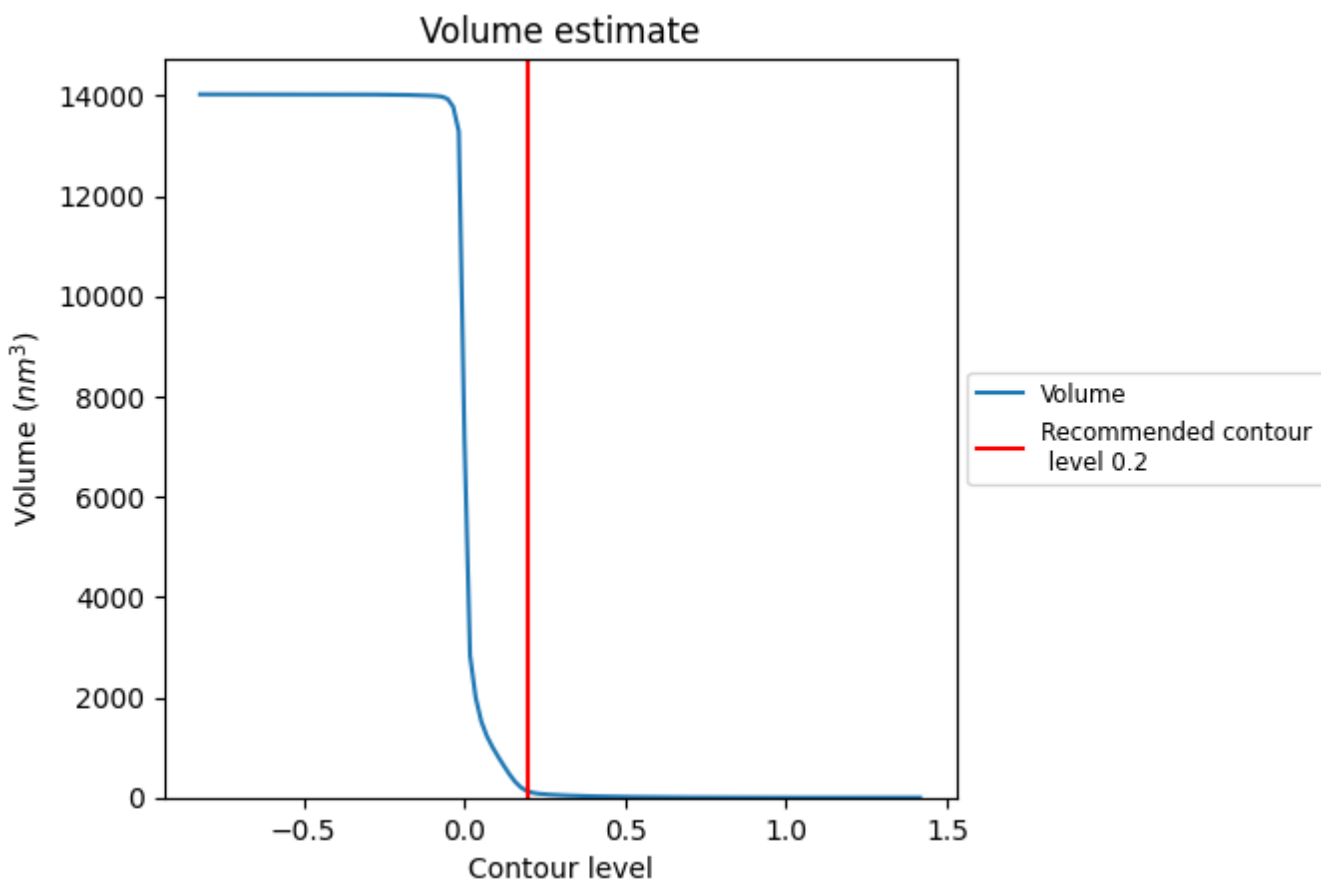
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

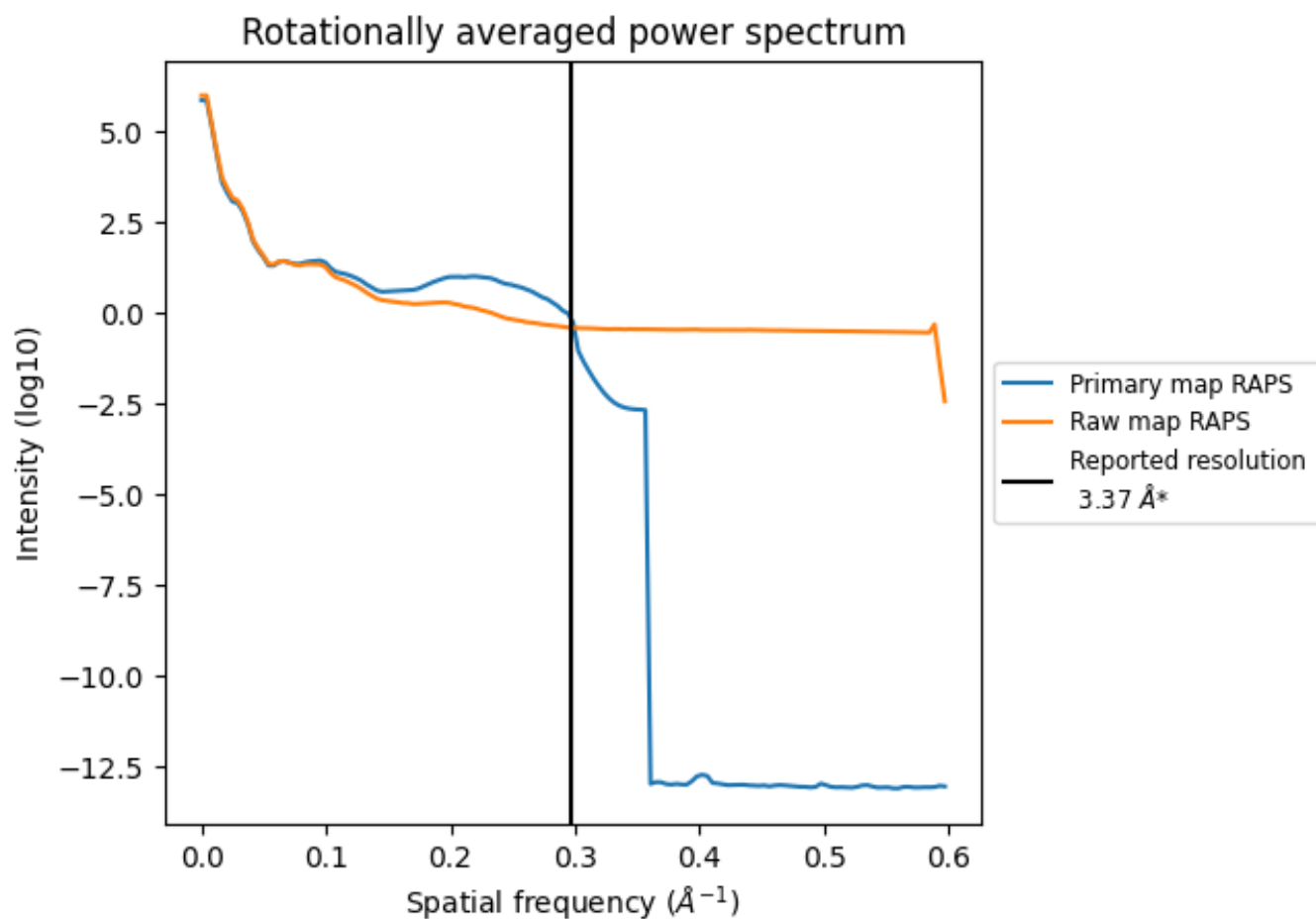
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

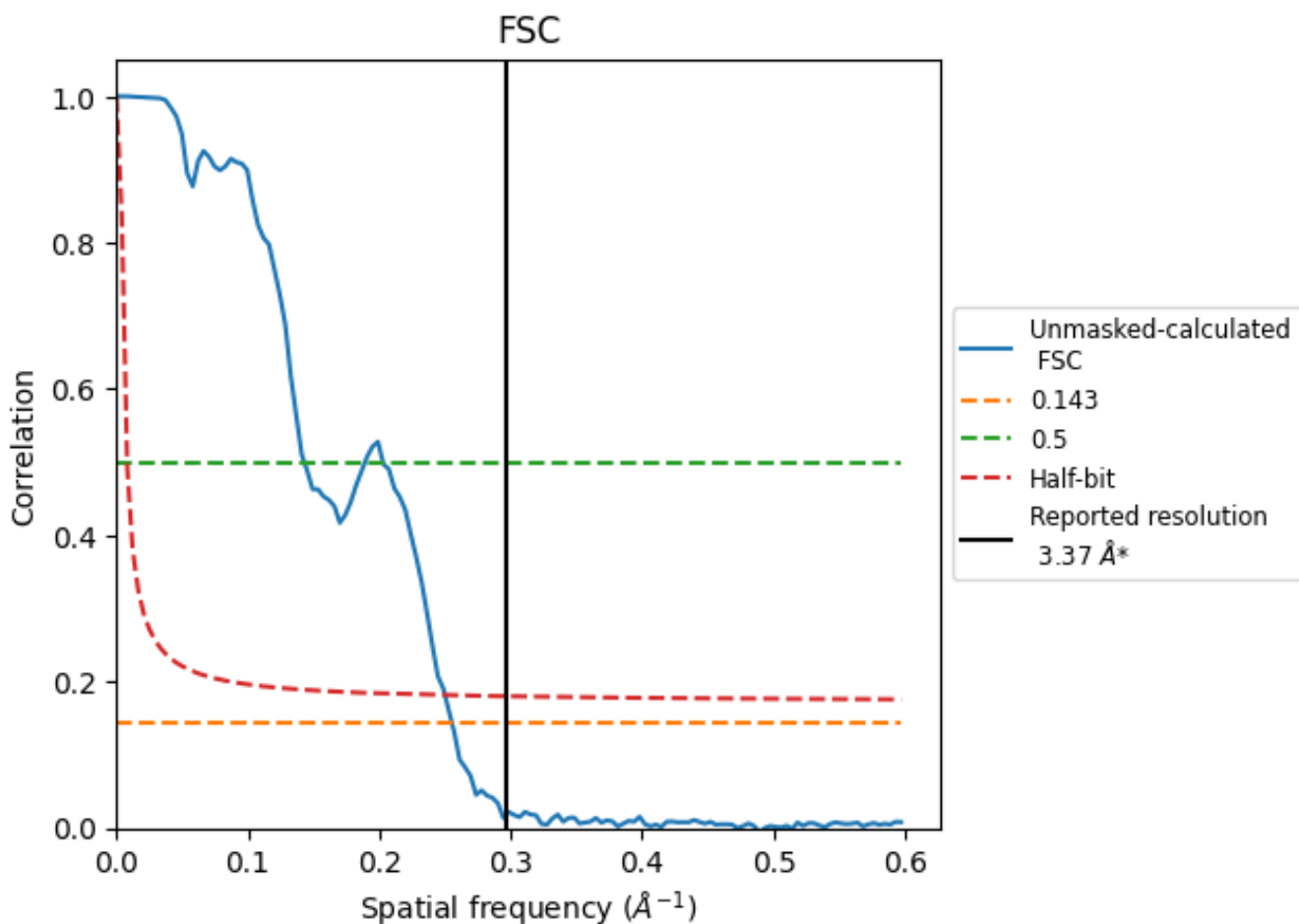


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 0.297 Å⁻¹

8.2 Resolution estimates [i](#)

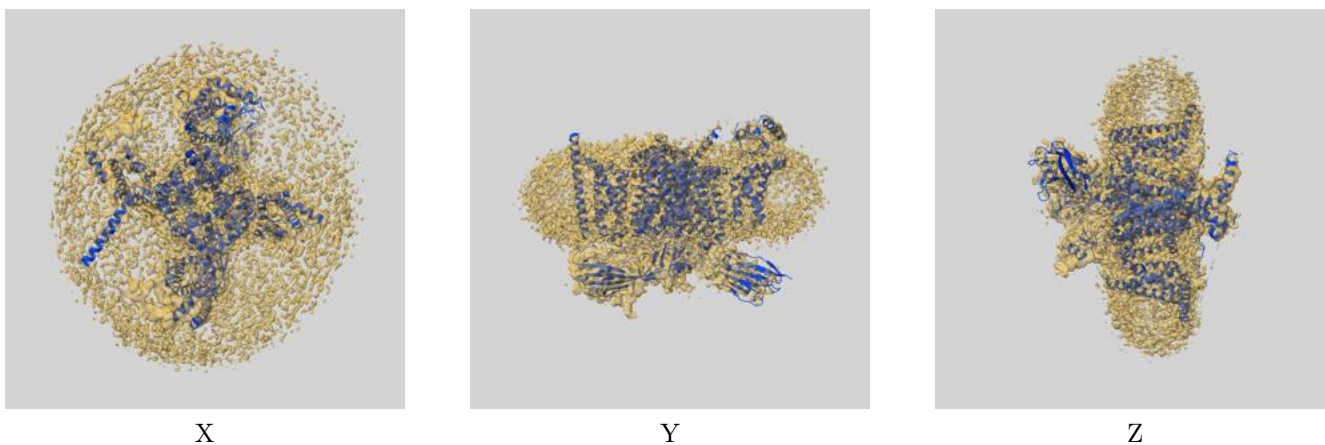
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	4.00

*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 3.92 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

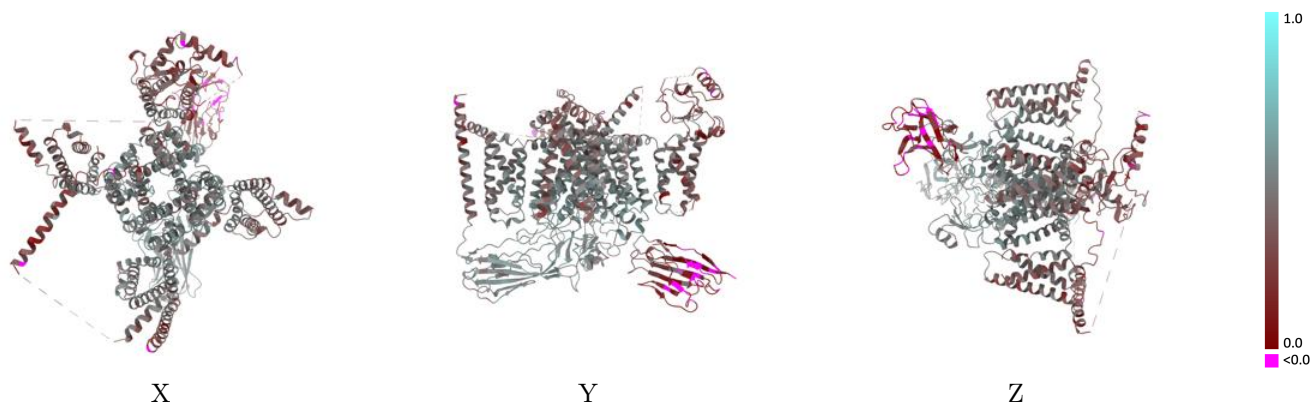
This section contains information regarding the fit between EMDB map EMD-38483 and PDB model 8XMN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



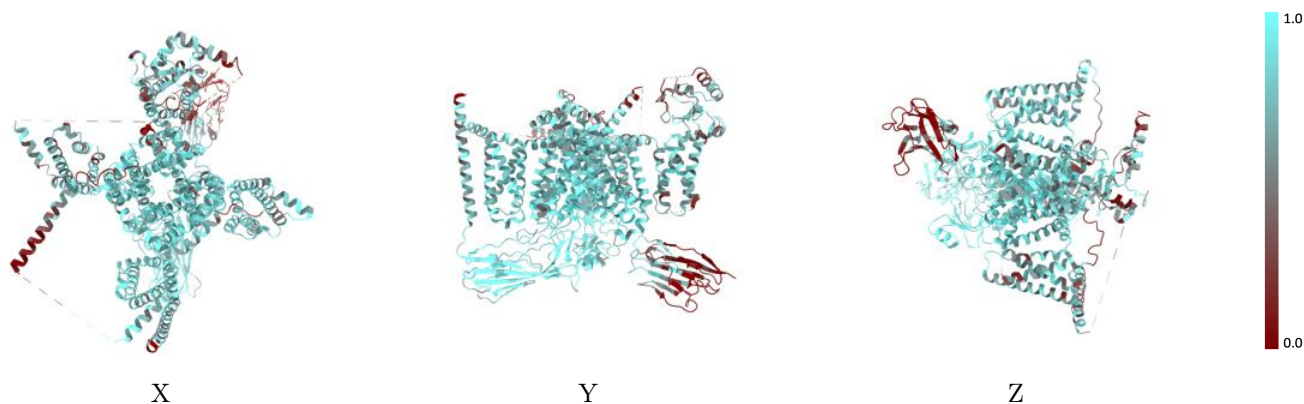
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



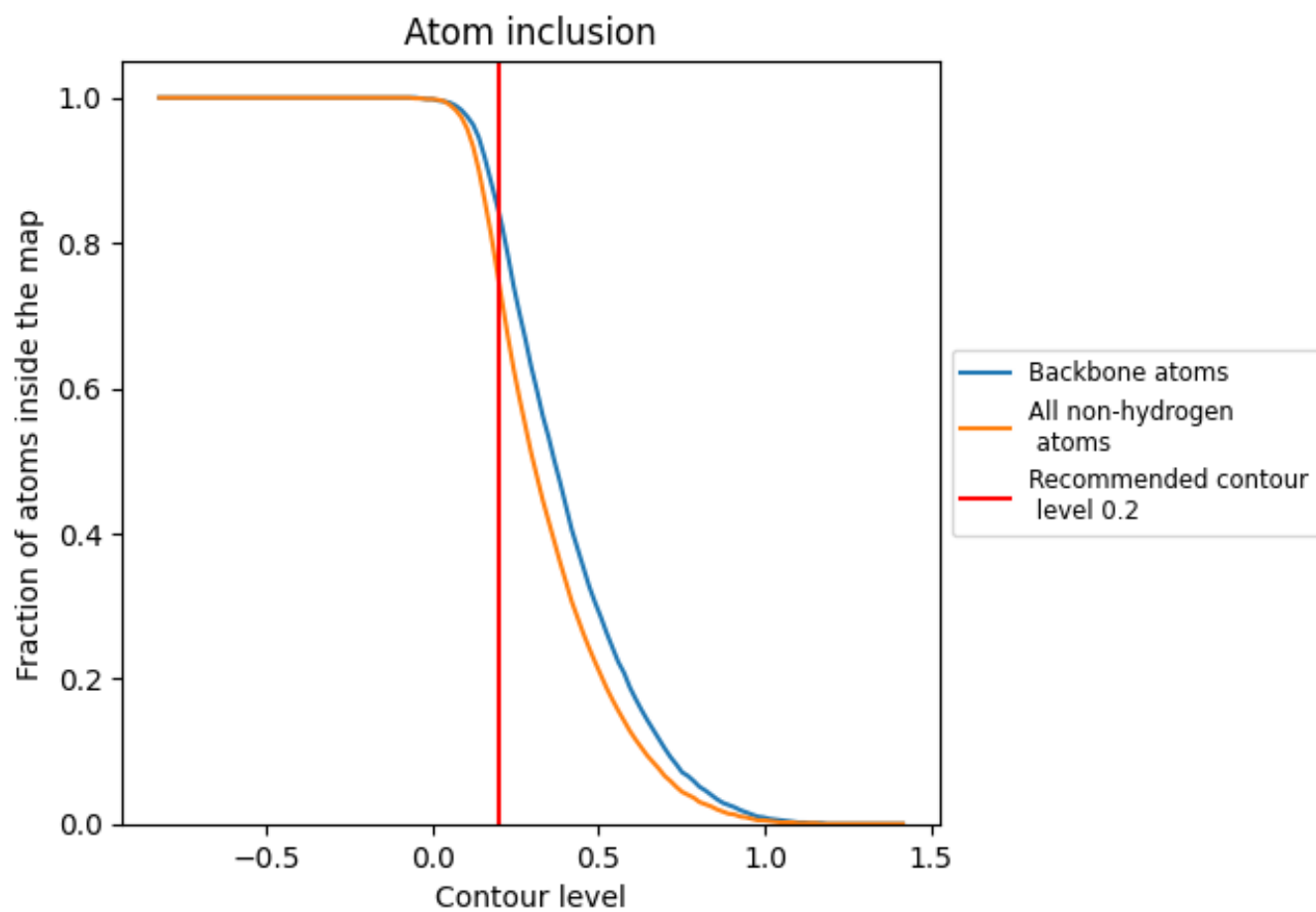
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).













9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.4310
A	 0.7730	 0.4510
B	 0.8320	 0.4690
C	 0.3080	 0.1480
D	 0.8570	 0.4480
E	 0.7860	 0.4950

