



Full wwPDB EM Validation Report ⓘ

Aug 26, 2021 – 12:15 pm BST

PDB ID : 7006
EMDB ID : EMD-13006
Title : Mechanosensitive channel MscS solubilized with DDM in closed conformation
with added lipid
Authors : Rasmussen, T.; Flegler, V.J.; Boettcher, B.
Deposited on : 2021-05-26
Resolution : 3.10 Å(reported)
Based on initial model : 6RLD

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

EMDB validation analysis : 0.0.0.dev97
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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

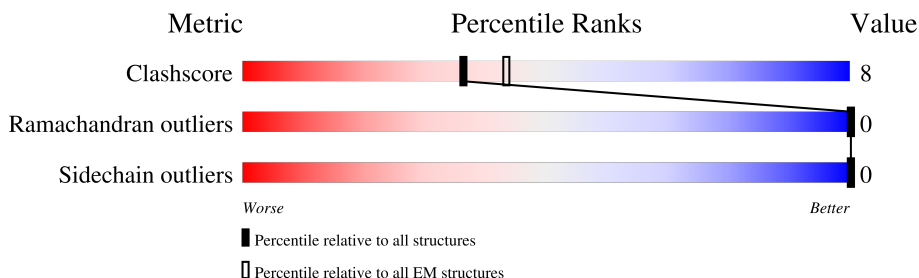
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	294	
1	B	294	
1	C	294	
1	D	294	
1	E	294	
1	F	294	
1	G	294	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14546 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 Mechanosensitive channel of small conductance (MscS).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	261	1989	1276	348	359	6	0	0
1	B	261	1989	1276	348	359	6	0	0
1	C	261	1989	1276	348	359	6	0	0
1	D	261	1989	1276	348	359	6	0	0
1	E	261	1989	1276	348	359	6	0	0
1	F	261	1989	1276	348	359	6	0	0
1	G	261	1989	1276	348	359	6	0	0

There are 56 discrepancies between the modelled and reference sequences:

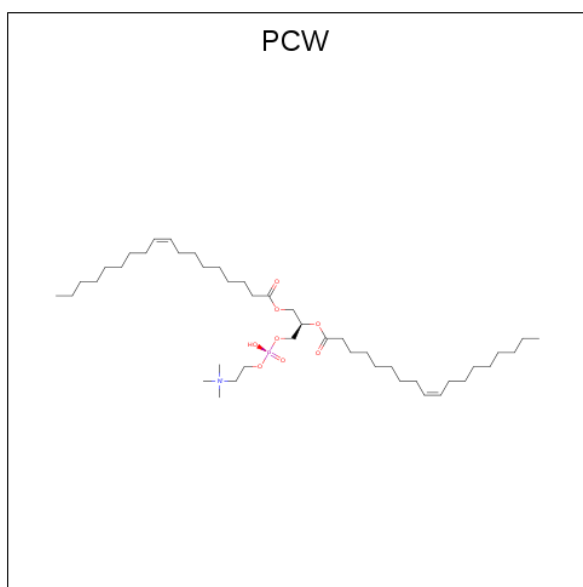
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	LEU	-	expression tag	UNP B6I756
A	288	GLU	-	expression tag	UNP B6I756
A	289	HIS	-	expression tag	UNP B6I756
A	290	HIS	-	expression tag	UNP B6I756
A	291	HIS	-	expression tag	UNP B6I756
A	292	HIS	-	expression tag	UNP B6I756
A	293	HIS	-	expression tag	UNP B6I756
A	294	HIS	-	expression tag	UNP B6I756
B	287	LEU	-	expression tag	UNP B6I756
B	288	GLU	-	expression tag	UNP B6I756
B	289	HIS	-	expression tag	UNP B6I756
B	290	HIS	-	expression tag	UNP B6I756
B	291	HIS	-	expression tag	UNP B6I756
B	292	HIS	-	expression tag	UNP B6I756
B	293	HIS	-	expression tag	UNP B6I756
B	294	HIS	-	expression tag	UNP B6I756

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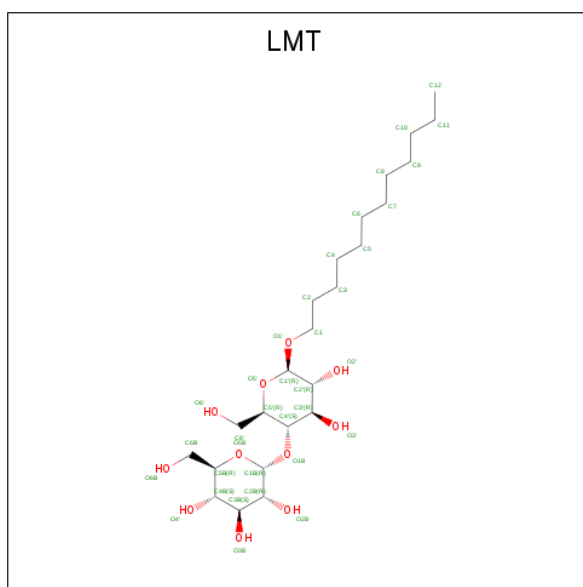
Chain	Residue	Modelled	Actual	Comment	Reference
C	287	LEU	-	expression tag	UNP B6I756
C	288	GLU	-	expression tag	UNP B6I756
C	289	HIS	-	expression tag	UNP B6I756
C	290	HIS	-	expression tag	UNP B6I756
C	291	HIS	-	expression tag	UNP B6I756
C	292	HIS	-	expression tag	UNP B6I756
C	293	HIS	-	expression tag	UNP B6I756
C	294	HIS	-	expression tag	UNP B6I756
D	287	LEU	-	expression tag	UNP B6I756
D	288	GLU	-	expression tag	UNP B6I756
D	289	HIS	-	expression tag	UNP B6I756
D	290	HIS	-	expression tag	UNP B6I756
D	291	HIS	-	expression tag	UNP B6I756
D	292	HIS	-	expression tag	UNP B6I756
D	293	HIS	-	expression tag	UNP B6I756
D	294	HIS	-	expression tag	UNP B6I756
E	287	LEU	-	expression tag	UNP B6I756
E	288	GLU	-	expression tag	UNP B6I756
E	289	HIS	-	expression tag	UNP B6I756
E	290	HIS	-	expression tag	UNP B6I756
E	291	HIS	-	expression tag	UNP B6I756
E	292	HIS	-	expression tag	UNP B6I756
E	293	HIS	-	expression tag	UNP B6I756
E	294	HIS	-	expression tag	UNP B6I756
F	287	LEU	-	expression tag	UNP B6I756
F	288	GLU	-	expression tag	UNP B6I756
F	289	HIS	-	expression tag	UNP B6I756
F	290	HIS	-	expression tag	UNP B6I756
F	291	HIS	-	expression tag	UNP B6I756
F	292	HIS	-	expression tag	UNP B6I756
F	293	HIS	-	expression tag	UNP B6I756
F	294	HIS	-	expression tag	UNP B6I756
G	287	LEU	-	expression tag	UNP B6I756
G	288	GLU	-	expression tag	UNP B6I756
G	289	HIS	-	expression tag	UNP B6I756
G	290	HIS	-	expression tag	UNP B6I756
G	291	HIS	-	expression tag	UNP B6I756
G	292	HIS	-	expression tag	UNP B6I756
G	293	HIS	-	expression tag	UNP B6I756
G	294	HIS	-	expression tag	UNP B6I756

- Molecule 2 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total 54	44	1	8	1	0
2	B	1	Total 54	44	1	8	1	0
2	C	1	Total 54	44	1	8	1	0
2	D	1	Total 54	44	1	8	1	0
2	E	1	Total 54	44	1	8	1	0
2	F	1	Total 54	44	1	8	1	0
2	G	1	Total 54	44	1	8	1	0

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

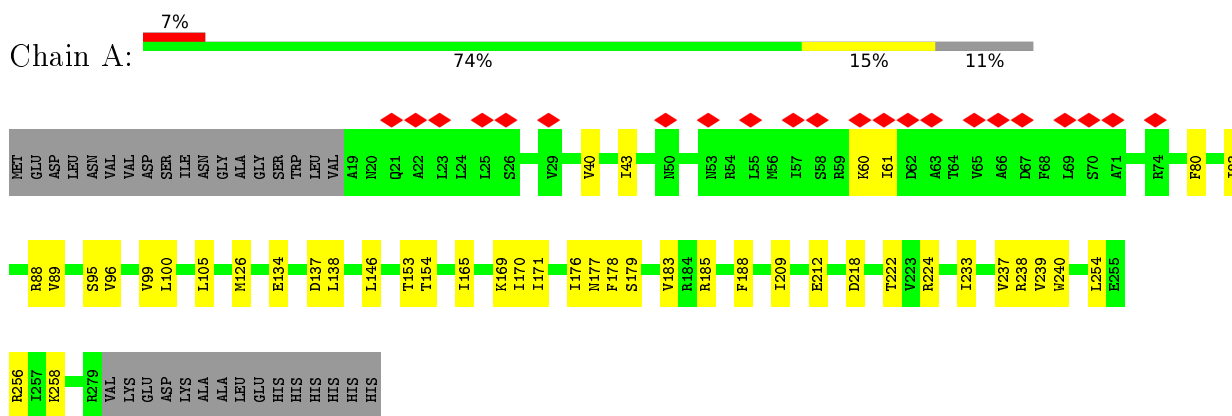


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	35	24	11	0
3	B	1	35	24	11	0
3	C	1	35	24	11	0
3	D	1	35	24	11	0
3	E	1	35	24	11	0
3	F	1	35	24	11	0
3	G	1	35	24	11	0

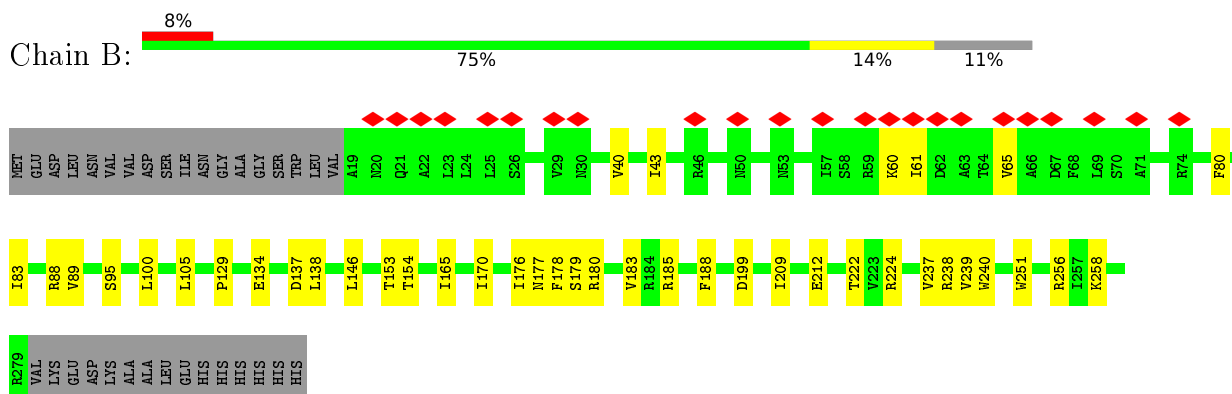
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

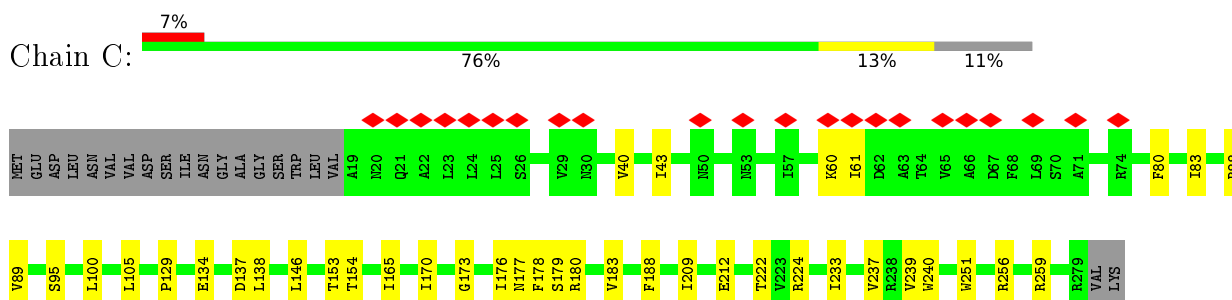
- Molecule 1: Mechanosensitive channel of small conductance (MscS)



- Molecule 1: Mechanosensitive channel of small conductance (MscS)



- Molecule 1: Mechanosensitive channel of small conductance (MscS)



GLU
ASP
LYS
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Mechanosensitive channel of small conductance (MscS)

Chain D: 7% 76% 13% 11%

MET
GLU
ASP
LYS
LEU
LEU
ASN
ASN
VAL
VAL
ASP
SER
SER
ILE
ASN
ASN
GLY
ALA
GLY
SER
TRP
TRP
LEU
VAL
A19
N20
Q21
A22
L23
L24
L25
S26
V29
N30
V40
I43
N50
N53
N56
I57
K60
I61
D62
A63
T64
V65
A66
D67
F68
L69
R74
F80
I83
R88
V89

S95
L100
L105
E134
D137
L138
L146
T153
T154
T165
K169
I170
I171
A172
G173
I176
M177
F178
S179
V183
F188
I209
E212
T222
V223
R224
E227
I233
V237
R238
V239
W240
R256
I257
K258
R279
VAL
LYS
GLU
ASP

LYS
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS

- Molecule 1: Mechanosensitive channel of small conductance (MscS)

Chain E: 8% 74% 14% 11%

MET
GLU
ASP
LYS
LEU
LEU
ASN
ASN
VAL
VAL
ASP
SER
SER
ILE
ASN
ASN
GLY
ALA
GLY
SER
TRP
TRP
LEU
VAL
A19
N20
Q21
A22
L23
L24
L25
S26
V29
N30
V40
I43
R46
N50
N53
N56
I57
K60
I61
D62
A63
T64
V65
A66
D67
F68
L69
R74
F80
I83

R88
V89
S95
L100
L105
E134
D137
L138
L146
T153
T154
T165
K169
I170
I171
G173
I176
M177
F178
S179
V183
R184
R185
F188
I209
E212
T222
V223
R224
E227
I233
V237
R238
V239
W240
V251
L254
E256
R256
I257

K258
R279
VAL
LYS
GLU
ASP
LYS
ALA
ALA
LEU
LEU
GLU
HIS
HIS
HIS
HIS

- Molecule 1: Mechanosensitive channel of small conductance (MscS)

Chain F: 7% 74% 15% 11%

MET
GLU
ASP
LYS
LEU
LEU
ASN
ASN
VAL
VAL
ASP
SER
SER
ILE
ASN
ASN
GLY
ALA
GLY
SER
TRP
TRP
LEU
VAL
A19
N20
Q21
A22
L23
L24
L25
S26
V29
N30
V40
I43
N50
I57
K60
I61
D62
A63
T64
V65
A66
D67
F68
L69
R74
F80
I83
R88
V89
S95
V96

V99
L100
L105
P129
E134
D137
L138
L146
T153
T154
T165
K169
I170
G173
I176
M177
F178
R180
V183
R184
R185
F188
I209
E212
T222
V223
R224
I233
V237
R238
V239
W240
L254
E256
R256
I257
R279
VAL

LYS
GLU
ASP
LYS
LEU
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Mechanosensitive channel of small conductance (MscS)

Chain G: 8% 74% 15% 11%

MET
GLU
ASP
LYS
LEU
LEU
ASN
ASN
VAL
VAL
ASP
SER
SER
ILE
ASN
ASN
GLY
ALA
GLY
SER
TRP
TRP
LEU
VAL
A19
N20
Q21
A22
L23
L24
L25
S26
V29
N30
V40
I43
R46
N50
N53
I57
S58
R59
K60
I61
D62
A63
T64
V65
A66
D67
F68
L69
R74
F80
I83

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	399384	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.409	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	272.256, 272.256, 272.256	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0635, 1.0635, 1.0635	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: LMT, 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	0.25	0/2014	0.47	0/2731
1	B	0.25	0/2014	0.47	0/2731
1	C	0.25	0/2014	0.47	0/2731
1	D	0.25	0/2014	0.48	0/2731
1	E	0.25	0/2014	0.47	0/2731
1	F	0.25	0/2014	0.47	0/2731
1	G	0.25	0/2014	0.48	0/2731
All	All	0.25	0/14098	0.47	0/19117

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	1989	0	2085	43	0
1	B	1989	0	2085	36	0
1	C	1989	0	2085	35	0
1	D	1989	0	2085	37	0
1	E	1989	0	2085	38	0
1	F	1989	0	2085	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1989	0	2085	41	0
2	A	54	0	84	6	0
2	B	54	0	84	6	0
2	C	54	0	84	6	0
2	D	54	0	84	6	0
2	E	54	0	84	7	0
2	F	54	0	84	6	0
2	G	54	0	84	7	0
3	A	35	0	46	3	0
3	B	35	0	46	4	0
3	C	35	0	46	3	0
3	D	35	0	46	4	0
3	E	35	0	46	5	0
3	F	35	0	46	3	0
3	G	35	0	46	4	0
All	All	14546	0	15505	251	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 8.

All (251) 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:95:SER:HB3	1:G:83:ILE:HD11	1.57	0.86
1:A:89:VAL:HG21	2:G:801:PCW:H212	1.57	0.86
1:E:83:ILE:HD11	1:F:95:SER:HB3	1.66	0.75
1:F:83:ILE:HD11	1:G:95:SER:HB3	1.68	0.74
1:C:83:ILE:HD11	1:D:95:SER:HB3	1.68	0.73
1:D:83:ILE:HD11	1:E:95:SER:HB3	1.71	0.72
3:D:802:LMT:H81	3:E:802:LMT:H82	1.72	0.71
3:C:802:LMT:H81	3:D:802:LMT:H82	1.75	0.69
1:E:83:ILE:HD11	1:F:95:SER:CB	2.22	0.69
1:A:95:SER:CB	1:G:83:ILE:HD11	2.22	0.69
3:E:802:LMT:H81	3:F:802:LMT:H82	1.75	0.68
1:C:83:ILE:HD11	1:D:95:SER:CB	2.23	0.68
1:B:83:ILE:HD11	1:C:95:SER:HB3	1.75	0.68
1:D:83:ILE:HD11	1:E:95:SER:CB	2.24	0.68
3:F:802:LMT:H81	3:G:802:LMT:H82	1.76	0.68
1:F:83:ILE:HD11	1:G:95:SER:CB	2.24	0.67
2:B:801:PCW:H212	1:C:89:VAL:HG21	1.77	0.66
1:G:137:ASP:HB2	1:G:178:PHE:HE1	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:HB2	1:C:178:PHE:HE1	1.63	0.64
1:D:137:ASP:HB2	1:D:178:PHE:HE1	1.63	0.64
1:A:137:ASP:HB2	1:A:178:PHE:HE1	1.63	0.63
1:F:137:ASP:HB2	1:F:178:PHE:HE1	1.63	0.63
1:B:137:ASP:HB2	1:B:178:PHE:HE1	1.63	0.63
1:B:212:GLU:OE1	1:B:256:ARG:NH2	2.33	0.62
1:F:212:GLU:OE1	1:F:256:ARG:NH2	2.33	0.62
1:E:137:ASP:HB2	1:E:178:PHE:HE1	1.63	0.62
1:G:137:ASP:HB3	1:G:176:ILE:HB	1.82	0.62
1:A:137:ASP:HB3	1:A:176:ILE:HB	1.82	0.62
1:E:212:GLU:OE1	1:E:256:ARG:NH2	2.33	0.62
1:G:212:GLU:OE1	1:G:256:ARG:NH2	2.33	0.62
1:A:212:GLU:OE1	1:A:256:ARG:NH2	2.33	0.61
1:D:212:GLU:OE1	1:D:256:ARG:NH2	2.33	0.61
1:C:212:GLU:OE1	1:C:256:ARG:NH2	2.33	0.61
1:F:137:ASP:HB3	1:F:176:ILE:HB	1.82	0.61
1:B:137:ASP:HB3	1:B:176:ILE:HB	1.82	0.61
1:B:83:ILE:HD11	1:C:95:SER:CB	2.30	0.61
1:C:137:ASP:HB3	1:C:176:ILE:HB	1.82	0.60
1:D:137:ASP:HB3	1:D:176:ILE:HB	1.82	0.60
1:E:137:ASP:HB3	1:E:176:ILE:HB	1.82	0.60
3:A:802:LMT:H81	3:B:802:LMT:H82	1.84	0.60
2:C:801:PCW:H39	2:C:801:PCW:H182	1.84	0.59
2:B:801:PCW:H182	2:B:801:PCW:H39	1.85	0.59
1:E:83:ILE:CD1	1:F:95:SER:HB3	2.33	0.59
2:D:801:PCW:H39	2:D:801:PCW:H182	1.85	0.59
2:G:801:PCW:H182	2:G:801:PCW:H39	1.84	0.58
1:A:95:SER:HB3	1:G:83:ILE:CD1	2.31	0.58
2:E:801:PCW:H182	2:E:801:PCW:H39	1.84	0.58
2:F:801:PCW:H39	2:F:801:PCW:H182	1.84	0.58
1:D:105:LEU:HD21	1:E:105:LEU:HD13	1.85	0.58
2:A:801:PCW:H39	2:A:801:PCW:H182	1.84	0.58
2:E:801:PCW:H212	1:F:89:VAL:HG21	1.85	0.58
1:A:99:VAL:HG21	1:G:80:PHE:HZ	1.68	0.58
1:E:105:LEU:HD21	1:F:105:LEU:HD13	1.85	0.58
2:F:801:PCW:H212	1:G:89:VAL:HG21	1.85	0.57
1:A:83:ILE:HD11	1:B:95:SER:HB3	1.85	0.57
1:C:83:ILE:CD1	1:D:95:SER:HB3	2.34	0.57
1:A:105:LEU:HD13	1:G:105:LEU:HD21	1.86	0.57
2:C:801:PCW:H212	1:D:89:VAL:HG21	1.85	0.57
1:A:88:ARG:HH22	2:A:801:PCW:H62	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:ARG:HH22	2:G:801:PCW:H62	1.69	0.57
1:B:88:ARG:HH22	2:B:801:PCW:H62	1.69	0.57
1:C:88:ARG:HH22	2:C:801:PCW:H62	1.69	0.57
1:F:105:LEU:HD21	1:G:105:LEU:HD13	1.85	0.57
1:F:88:ARG:HH22	2:F:801:PCW:H62	1.69	0.56
1:D:83:ILE:CD1	1:E:95:SER:HB3	2.35	0.56
1:D:88:ARG:HH22	2:D:801:PCW:H62	1.69	0.56
1:E:88:ARG:HH22	2:E:801:PCW:H62	1.69	0.56
1:F:153:THR:HG22	1:F:170:ILE:HD11	1.88	0.56
1:G:153:THR:HG22	1:G:170:ILE:HD11	1.88	0.55
1:F:83:ILE:CD1	1:G:95:SER:HB3	2.34	0.55
1:A:153:THR:HG22	1:A:170:ILE:HD11	1.88	0.55
1:E:153:THR:HG22	1:E:170:ILE:HD11	1.88	0.55
3:B:802:LMT:H81	3:C:802:LMT:H82	1.88	0.54
1:C:105:LEU:HD21	1:D:105:LEU:HD13	1.87	0.54
1:C:153:THR:HG22	1:C:170:ILE:HD11	1.88	0.54
1:B:153:THR:HG22	1:B:170:ILE:HD11	1.88	0.54
1:B:80:PHE:HB3	2:B:801:PCW:H471	1.90	0.54
1:D:153:THR:HG22	1:D:170:ILE:HD11	1.88	0.54
1:C:80:PHE:HB3	2:C:801:PCW:H471	1.90	0.54
1:D:80:PHE:HB3	2:D:801:PCW:H471	1.90	0.53
1:A:80:PHE:HB3	2:A:801:PCW:H471	1.90	0.53
1:D:233:ILE:HD13	1:E:258:LYS:HE3	1.91	0.53
1:B:80:PHE:HE1	1:B:100:LEU:HD21	1.74	0.53
1:D:80:PHE:HE1	1:D:100:LEU:HD21	1.74	0.53
3:A:802:LMT:H82	3:G:802:LMT:H81	1.91	0.53
1:E:80:PHE:HB3	2:E:801:PCW:H471	1.90	0.52
1:G:80:PHE:HE1	1:G:100:LEU:HD21	1.74	0.52
1:F:80:PHE:HB3	2:F:801:PCW:H471	1.90	0.52
1:E:80:PHE:HE1	1:E:100:LEU:HD21	1.74	0.52
1:G:80:PHE:HB3	2:G:801:PCW:H471	1.90	0.52
1:C:80:PHE:HE1	1:C:100:LEU:HD21	1.74	0.52
1:F:80:PHE:HE1	1:F:100:LEU:HD21	1.74	0.51
1:A:80:PHE:HE1	1:A:100:LEU:HD21	1.74	0.51
1:A:169:LYS:HE2	1:G:173:GLY:HA2	1.93	0.51
1:B:83:ILE:CD1	1:C:95:SER:HB3	2.41	0.51
1:A:153:THR:HG22	1:A:170:ILE:CD1	2.41	0.51
1:B:153:THR:HG22	1:B:170:ILE:CD1	2.41	0.51
1:D:153:THR:HG22	1:D:170:ILE:CD1	2.41	0.50
1:E:153:THR:HG22	1:E:170:ILE:CD1	2.41	0.50
1:G:153:THR:HG22	1:G:170:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:801:PCW:H212	1:E:89:VAL:HG21	1.92	0.50
1:C:153:THR:HG22	1:C:170:ILE:CD1	2.41	0.50
1:F:153:THR:HG22	1:F:170:ILE:CD1	2.41	0.50
1:A:138:LEU:HD12	1:A:165:ILE:HD12	1.94	0.50
1:B:209:ILE:HD12	1:B:239:VAL:HG11	1.94	0.50
1:B:138:LEU:HD12	1:B:165:ILE:HD12	1.94	0.49
1:C:88:ARG:NH2	2:C:801:PCW:O31	2.45	0.49
1:D:88:ARG:NH2	2:D:801:PCW:O31	2.45	0.49
1:E:209:ILE:HD12	1:E:239:VAL:HG11	1.93	0.49
1:F:209:ILE:HD12	1:F:239:VAL:HG11	1.93	0.49
2:A:801:PCW:H212	1:B:89:VAL:HG21	1.94	0.49
1:B:88:ARG:NH2	2:B:801:PCW:O31	2.45	0.49
1:A:209:ILE:HD12	1:A:239:VAL:HG11	1.94	0.49
1:G:138:LEU:HD12	1:G:165:ILE:HD12	1.94	0.49
1:C:138:LEU:HD12	1:C:165:ILE:HD12	1.94	0.49
1:A:88:ARG:NH2	2:A:801:PCW:O31	2.45	0.49
1:A:105:LEU:HD21	1:B:105:LEU:HD13	1.94	0.49
1:C:209:ILE:HD12	1:C:239:VAL:HG11	1.93	0.49
1:G:88:ARG:NH2	2:G:801:PCW:O31	2.45	0.49
1:G:209:ILE:HD12	1:G:239:VAL:HG11	1.93	0.49
1:E:88:ARG:NH2	2:E:801:PCW:O31	2.45	0.49
1:E:138:LEU:HD12	1:E:165:ILE:HD12	1.94	0.48
1:D:138:LEU:HD12	1:D:165:ILE:HD12	1.94	0.48
1:D:209:ILE:HD12	1:D:239:VAL:HG11	1.93	0.48
1:F:88:ARG:NH2	2:F:801:PCW:O31	2.45	0.48
1:F:138:LEU:HD12	1:F:165:ILE:HD12	1.94	0.48
1:A:96:VAL:HG23	2:G:801:PCW:H483	1.95	0.48
1:A:126:MET:SD	1:B:65:VAL:HG11	2.54	0.48
1:F:40:VAL:HA	1:F:43:ILE:HG12	1.96	0.48
1:G:40:VAL:HA	1:G:43:ILE:HG12	1.96	0.48
1:A:188:PHE:HB2	1:A:237:VAL:HB	1.96	0.47
1:C:183:VAL:HG12	1:C:240:TRP:HE3	1.79	0.47
1:B:183:VAL:HG12	1:B:240:TRP:HE3	1.79	0.47
1:B:188:PHE:HB2	1:B:237:VAL:HB	1.96	0.47
1:E:40:VAL:HA	1:E:43:ILE:HG12	1.96	0.47
1:E:188:PHE:HB2	1:E:237:VAL:HB	1.96	0.47
1:A:40:VAL:HA	1:A:43:ILE:HG12	1.96	0.47
1:A:99:VAL:HG21	1:G:80:PHE:CZ	2.48	0.47
1:D:227:GLU:HA	1:E:254:LEU:HD21	1.96	0.47
1:A:183:VAL:HG12	1:A:240:TRP:HE3	1.79	0.47
1:D:188:PHE:HB2	1:D:237:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:PHE:HB2	1:G:237:VAL:HB	1.96	0.47
1:D:40:VAL:HA	1:D:43:ILE:HG12	1.96	0.46
1:D:183:VAL:HG12	1:D:240:TRP:HE3	1.79	0.46
1:A:105:LEU:HG	3:B:802:LMT:H123	1.97	0.46
1:E:183:VAL:HG12	1:E:240:TRP:HE3	1.79	0.46
1:B:40:VAL:HA	1:B:43:ILE:HG12	1.96	0.46
1:C:188:PHE:HB2	1:C:237:VAL:HB	1.96	0.46
1:A:83:ILE:HD11	1:B:95:SER:CB	2.45	0.46
1:C:40:VAL:HA	1:C:43:ILE:HG12	1.96	0.46
1:F:183:VAL:HG12	1:F:240:TRP:HE3	1.79	0.46
1:F:188:PHE:HB2	1:F:237:VAL:HB	1.96	0.46
1:E:233:ILE:HD13	1:F:258:LYS:HE3	1.97	0.46
1:G:183:VAL:HG12	1:G:240:TRP:HE3	1.79	0.46
1:G:88:ARG:HA	1:G:88:ARG:HD2	1.79	0.46
2:D:801:PCW:H372	2:D:801:PCW:H171	1.99	0.45
2:F:801:PCW:H171	2:F:801:PCW:H372	1.99	0.45
3:C:802:LMT:H5'	3:C:802:LMT:H1B	1.80	0.45
2:E:801:PCW:H372	2:E:801:PCW:H171	1.99	0.45
2:G:801:PCW:H372	2:G:801:PCW:H171	1.99	0.45
2:A:801:PCW:H171	2:A:801:PCW:H372	1.99	0.45
1:D:173:GLY:HA2	1:E:169:LYS:HE2	1.98	0.45
2:C:801:PCW:H171	2:C:801:PCW:H372	1.99	0.44
1:B:134:GLU:OE2	1:B:177:ASN:ND2	2.46	0.44
2:B:801:PCW:H372	2:B:801:PCW:H171	1.99	0.44
1:D:224:ARG:HG3	1:E:251:TRP:CE3	2.53	0.44
3:B:802:LMT:H1B	3:B:802:LMT:H5'	1.80	0.44
1:D:105:LEU:HG	3:E:802:LMT:H123	1.99	0.44
1:D:88:ARG:HA	1:D:88:ARG:HD2	1.79	0.44
1:C:134:GLU:CD	1:C:177:ASN:HD21	2.21	0.43
3:A:802:LMT:H5'	3:A:802:LMT:H1B	1.80	0.43
1:E:173:GLY:HA2	1:F:169:LYS:HE2	1.98	0.43
1:A:88:ARG:HD2	1:A:88:ARG:HA	1.79	0.43
3:F:802:LMT:H1B	3:F:802:LMT:H5'	1.80	0.43
1:E:227:GLU:HA	1:F:254:LEU:HD21	2.00	0.43
3:E:802:LMT:H1B	3:E:802:LMT:H5'	1.80	0.43
1:F:233:ILE:HD13	1:G:258:LYS:HE3	2.00	0.43
1:A:134:GLU:OE2	1:A:177:ASN:ND2	2.46	0.43
1:D:134:GLU:CD	1:D:177:ASN:HD21	2.21	0.43
1:A:134:GLU:CD	1:A:177:ASN:HD21	2.21	0.42
1:E:88:ARG:HD2	1:E:88:ARG:HA	1.79	0.42
1:F:173:GLY:HA2	1:G:169:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:OD1	1:C:259:ARG:NH2	2.53	0.42
1:E:134:GLU:CD	1:E:177:ASN:HD21	2.21	0.42
1:G:134:GLU:CD	1:G:177:ASN:HD21	2.21	0.42
1:F:134:GLU:CD	1:F:177:ASN:HD21	2.21	0.42
1:B:105:LEU:HD21	1:C:105:LEU:HD13	2.02	0.42
1:B:224:ARG:HG3	1:C:251:TRP:CE3	2.54	0.42
1:C:60:LYS:HD3	1:C:61:ILE:N	2.35	0.42
1:C:233:ILE:HD13	1:D:258:LYS:HE3	2.02	0.42
1:E:146:LEU:HB2	1:E:154:THR:HG23	2.02	0.42
1:F:222:THR:HG23	1:F:224:ARG:HG2	2.02	0.42
1:A:222:THR:HG23	1:A:224:ARG:HG2	2.02	0.42
1:E:60:LYS:HD3	1:E:61:ILE:N	2.35	0.42
1:D:134:GLU:HG3	1:D:179:SER:OG	2.20	0.41
1:E:134:GLU:HG3	1:E:179:SER:OG	2.20	0.41
1:F:60:LYS:HD3	1:F:61:ILE:N	2.35	0.41
1:G:222:THR:HG23	1:G:224:ARG:HG2	2.02	0.41
1:B:146:LEU:HB2	1:B:154:THR:HG23	2.01	0.41
1:C:134:GLU:HG3	1:C:179:SER:OG	2.20	0.41
1:F:134:GLU:HG3	1:F:179:SER:OG	2.20	0.41
1:F:146:LEU:HB2	1:F:154:THR:HG23	2.02	0.41
1:G:60:LYS:HD3	1:G:61:ILE:N	2.35	0.41
1:A:218:ASP:OD1	1:A:218:ASP:N	2.52	0.41
3:D:802:LMT:H5'	3:D:802:LMT:H1B	1.80	0.41
3:D:802:LMT:H91	3:E:802:LMT:H101	2.01	0.41
1:E:80:PHE:HZ	1:F:99:VAL:HG21	1.86	0.41
1:E:222:THR:HG23	1:E:224:ARG:HG2	2.02	0.41
1:A:60:LYS:HD3	1:A:61:ILE:N	2.35	0.41
1:A:146:LEU:HB2	1:A:154:THR:HG23	2.02	0.41
1:B:134:GLU:CD	1:B:177:ASN:HD21	2.21	0.41
1:B:222:THR:HG23	1:B:224:ARG:HG2	2.02	0.41
1:C:88:ARG:HD2	1:C:88:ARG:HA	1.79	0.41
1:F:185:ARG:HD2	1:F:238:ARG:HB3	2.03	0.41
3:G:802:LMT:H5'	3:G:802:LMT:H1B	1.80	0.41
1:A:185:ARG:HD2	1:A:238:ARG:HB3	2.03	0.41
1:B:129:PRO:O	1:B:180:ARG:NH2	2.53	0.41
1:D:146:LEU:HB2	1:D:154:THR:HG23	2.02	0.41
1:G:218:ASP:OD1	1:G:218:ASP:N	2.52	0.41
1:B:60:LYS:HD3	1:B:61:ILE:N	2.35	0.41
1:D:171:ILE:HD13	1:D:171:ILE:HA	1.98	0.41
1:B:134:GLU:HG3	1:B:179:SER:OG	2.20	0.41
1:A:171:ILE:HD13	1:A:171:ILE:HA	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HD13	1:B:258:LYS:HE3	2.03	0.41
1:A:254:LEU:HD21	1:G:227:GLU:HA	2.03	0.41
1:A:258:LYS:HE3	1:G:233:ILE:HD13	2.03	0.41
1:B:185:ARG:HD2	1:B:238:ARG:HB3	2.03	0.41
1:B:222:THR:O	1:B:237:VAL:HA	2.21	0.41
1:C:173:GLY:HA2	1:D:169:LYS:HE2	2.01	0.41
1:C:222:THR:O	1:C:237:VAL:HA	2.21	0.41
1:C:222:THR:HG23	1:C:224:ARG:HG2	2.02	0.41
1:D:222:THR:HG23	1:D:224:ARG:HG2	2.02	0.41
1:E:185:ARG:HD2	1:E:238:ARG:HB3	2.03	0.41
1:F:80:PHE:HZ	1:G:99:VAL:HG21	1.86	0.41
1:F:134:GLU:OE2	1:F:177:ASN:ND2	2.46	0.41
1:F:222:THR:O	1:F:237:VAL:HA	2.21	0.41
1:A:222:THR:O	1:A:237:VAL:HA	2.21	0.41
1:A:224:ARG:HG3	1:B:251:TRP:CE3	2.55	0.41
1:A:134:GLU:HG3	1:A:179:SER:OG	2.20	0.40
1:C:146:LEU:HB2	1:C:154:THR:HG23	2.02	0.40
1:D:60:LYS:HD3	1:D:61:ILE:N	2.35	0.40
1:F:61:ILE:HD12	1:F:61:ILE:HA	1.97	0.40
1:C:129:PRO:O	1:C:180:ARG:NH2	2.53	0.40
2:E:801:PCW:H483	1:F:96:VAL:HG23	2.03	0.40
1:G:146:LEU:HB2	1:G:154:THR:HG23	2.02	0.40
1:G:171:ILE:HD13	1:G:171:ILE:HA	1.98	0.40
1:F:105:LEU:HG	3:G:802:LMT:H123	2.03	0.40
1:F:129:PRO:O	1:F:180:ARG:NH2	2.53	0.40
1:G:134:GLU:HG3	1:G:179:SER:OG	2.20	0.40
1:G:185:ARG:HD2	1:G:238:ARG:HB3	2.03	0.40
1:G:222:THR:O	1:G:237:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	B	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	C	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	D	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	E	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	F	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
1	G	259/294 (88%)	255 (98%)	4 (2%)	0	100	100
All	All	1813/2058 (88%)	1785 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	211/239 (88%)	211 (100%)	0	100	100
1	B	211/239 (88%)	211 (100%)	0	100	100
1	C	211/239 (88%)	211 (100%)	0	100	100
1	D	211/239 (88%)	211 (100%)	0	100	100
1	E	211/239 (88%)	211 (100%)	0	100	100
1	F	211/239 (88%)	211 (100%)	0	100	100
1	G	211/239 (88%)	211 (100%)	0	100	100
All	All	1477/1673 (88%)	1477 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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	$\# Z > 2$
3	LMT	D	802	-	36,36,36	0.09	0	47,47,47	0.20	0
3	LMT	C	802	-	36,36,36	0.08	0	47,47,47	0.19	0
2	PCW	C	801	-	53,53,53	0.25	0	59,61,61	0.22	0
2	PCW	D	801	-	53,53,53	0.25	0	59,61,61	0.23	0
2	PCW	B	801	-	53,53,53	0.25	0	59,61,61	0.22	0
3	LMT	B	802	-	36,36,36	0.09	0	47,47,47	0.20	0
3	LMT	G	802	-	36,36,36	0.09	0	47,47,47	0.20	0
3	LMT	F	802	-	36,36,36	0.08	0	47,47,47	0.20	0
2	PCW	G	801	-	53,53,53	0.25	0	59,61,61	0.23	0
3	LMT	E	802	-	36,36,36	0.09	0	47,47,47	0.20	0
3	LMT	A	802	-	36,36,36	0.09	0	47,47,47	0.20	0
2	PCW	A	801	-	53,53,53	0.25	0	59,61,61	0.23	0
2	PCW	F	801	-	53,53,53	0.25	0	59,61,61	0.23	0
2	PCW	E	801	-	53,53,53	0.25	0	59,61,61	0.23	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
3	LMT	D	802	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	C	802	-	-	5/21/61/61	0/2/2/2
2	PCW	C	801	-	-	12/57/57/57	-
2	PCW	D	801	-	-	12/57/57/57	-
2	PCW	B	801	-	-	12/57/57/57	-
3	LMT	B	802	-	-	5/21/61/61	0/2/2/2
3	LMT	G	802	-	-	5/21/61/61	0/2/2/2
3	LMT	F	802	-	-	5/21/61/61	0/2/2/2
2	PCW	G	801	-	-	12/57/57/57	-
3	LMT	E	802	-	-	5/21/61/61	0/2/2/2
3	LMT	A	802	-	-	5/21/61/61	0/2/2/2
2	PCW	A	801	-	-	12/57/57/57	-
2	PCW	F	801	-	-	12/57/57/57	-
2	PCW	E	801	-	-	12/57/57/57	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PCW	C1-O3P-P-O2P
2	A	801	PCW	C4-O4P-P-O1P
2	A	801	PCW	C4-O4P-P-O2P
2	B	801	PCW	C1-O3P-P-O2P
2	B	801	PCW	C4-O4P-P-O1P
2	B	801	PCW	C4-O4P-P-O2P
2	C	801	PCW	C1-O3P-P-O2P
2	C	801	PCW	C4-O4P-P-O1P
2	C	801	PCW	C4-O4P-P-O2P
2	D	801	PCW	C1-O3P-P-O2P
2	D	801	PCW	C4-O4P-P-O1P
2	D	801	PCW	C4-O4P-P-O2P
2	E	801	PCW	C1-O3P-P-O2P
2	E	801	PCW	C4-O4P-P-O1P
2	E	801	PCW	C4-O4P-P-O2P
2	F	801	PCW	C1-O3P-P-O2P
2	F	801	PCW	C4-O4P-P-O1P
2	F	801	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	G	801	PCW	C1-O3P-P-O2P
2	G	801	PCW	C4-O4P-P-O1P
2	G	801	PCW	C4-O4P-P-O2P
3	A	802	LMT	O5'-C1'-O1'-C1
3	B	802	LMT	O5'-C1'-O1'-C1
3	C	802	LMT	O5'-C1'-O1'-C1
3	D	802	LMT	O5'-C1'-O1'-C1
3	E	802	LMT	O5'-C1'-O1'-C1
3	F	802	LMT	O5'-C1'-O1'-C1
3	G	802	LMT	O5'-C1'-O1'-C1
3	A	802	LMT	C5'-C4'-O1B-C1B
3	B	802	LMT	C5'-C4'-O1B-C1B
3	C	802	LMT	C5'-C4'-O1B-C1B
3	D	802	LMT	C5'-C4'-O1B-C1B
3	E	802	LMT	C5'-C4'-O1B-C1B
3	F	802	LMT	C5'-C4'-O1B-C1B
3	G	802	LMT	C5'-C4'-O1B-C1B
2	A	801	PCW	C4-O4P-P-O3P
2	B	801	PCW	C4-O4P-P-O3P
2	C	801	PCW	C4-O4P-P-O3P
2	D	801	PCW	C4-O4P-P-O3P
2	E	801	PCW	C4-O4P-P-O3P
2	F	801	PCW	C4-O4P-P-O3P
2	G	801	PCW	C4-O4P-P-O3P
3	A	802	LMT	C3'-C4'-O1B-C1B
3	B	802	LMT	C3'-C4'-O1B-C1B
3	C	802	LMT	C3'-C4'-O1B-C1B
3	D	802	LMT	C3'-C4'-O1B-C1B
3	E	802	LMT	C3'-C4'-O1B-C1B
3	F	802	LMT	C3'-C4'-O1B-C1B
3	G	802	LMT	C3'-C4'-O1B-C1B
3	A	802	LMT	O5B-C5B-C6B-O6B
3	B	802	LMT	O5B-C5B-C6B-O6B
3	C	802	LMT	O5B-C5B-C6B-O6B
3	D	802	LMT	O5B-C5B-C6B-O6B
3	E	802	LMT	O5B-C5B-C6B-O6B
3	F	802	LMT	O5B-C5B-C6B-O6B
3	G	802	LMT	O5B-C5B-C6B-O6B
2	A	801	PCW	C1-O3P-P-O4P
2	B	801	PCW	C1-O3P-P-O4P
2	C	801	PCW	C1-O3P-P-O4P
2	D	801	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
2	E	801	PCW	C1-O3P-P-O4P
2	F	801	PCW	C1-O3P-P-O4P
2	G	801	PCW	C1-O3P-P-O4P
2	G	801	PCW	C14-C15-C16-C17
2	A	801	PCW	C14-C15-C16-C17
2	B	801	PCW	C14-C15-C16-C17
2	C	801	PCW	C14-C15-C16-C17
2	F	801	PCW	C14-C15-C16-C17
2	D	801	PCW	C14-C15-C16-C17
2	E	801	PCW	C14-C15-C16-C17
3	A	802	LMT	C2-C1-O1'-C1'
3	B	802	LMT	C2-C1-O1'-C1'
3	C	802	LMT	C2-C1-O1'-C1'
3	D	802	LMT	C2-C1-O1'-C1'
3	E	802	LMT	C2-C1-O1'-C1'
3	F	802	LMT	C2-C1-O1'-C1'
3	G	802	LMT	C2-C1-O1'-C1'
2	A	801	PCW	O4P-C4-C5-N
2	B	801	PCW	O4P-C4-C5-N
2	C	801	PCW	O4P-C4-C5-N
2	D	801	PCW	O4P-C4-C5-N
2	E	801	PCW	O4P-C4-C5-N
2	F	801	PCW	O4P-C4-C5-N
2	G	801	PCW	O4P-C4-C5-N
2	A	801	PCW	O3P-C1-C2-C3
2	B	801	PCW	O3P-C1-C2-C3
2	C	801	PCW	O3P-C1-C2-C3
2	D	801	PCW	O3P-C1-C2-C3
2	E	801	PCW	O3P-C1-C2-C3
2	F	801	PCW	O3P-C1-C2-C3
2	G	801	PCW	O3P-C1-C2-C3
2	B	801	PCW	O2-C31-C32-C33
2	A	801	PCW	O2-C31-C32-C33
2	E	801	PCW	O2-C31-C32-C33
2	F	801	PCW	O2-C31-C32-C33
2	G	801	PCW	O2-C31-C32-C33
2	C	801	PCW	O2-C31-C32-C33
2	D	801	PCW	O2-C31-C32-C33
2	A	801	PCW	O3P-C1-C2-O2
2	D	801	PCW	O3P-C1-C2-O2
2	G	801	PCW	O3P-C1-C2-O2
2	A	801	PCW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	B	801	PCW	C19-C20-C21-C22
2	C	801	PCW	C19-C20-C21-C22
2	D	801	PCW	C19-C20-C21-C22
2	E	801	PCW	C19-C20-C21-C22
2	F	801	PCW	C19-C20-C21-C22
2	G	801	PCW	C19-C20-C21-C22
2	B	801	PCW	O31-C31-C32-C33
2	C	801	PCW	O31-C31-C32-C33
2	D	801	PCW	O31-C31-C32-C33
2	F	801	PCW	O31-C31-C32-C33
2	G	801	PCW	O31-C31-C32-C33
2	A	801	PCW	O31-C31-C32-C33
2	E	801	PCW	O31-C31-C32-C33
2	B	801	PCW	O3P-C1-C2-O2
2	C	801	PCW	O3P-C1-C2-O2
2	E	801	PCW	O3P-C1-C2-O2
2	F	801	PCW	O3P-C1-C2-O2

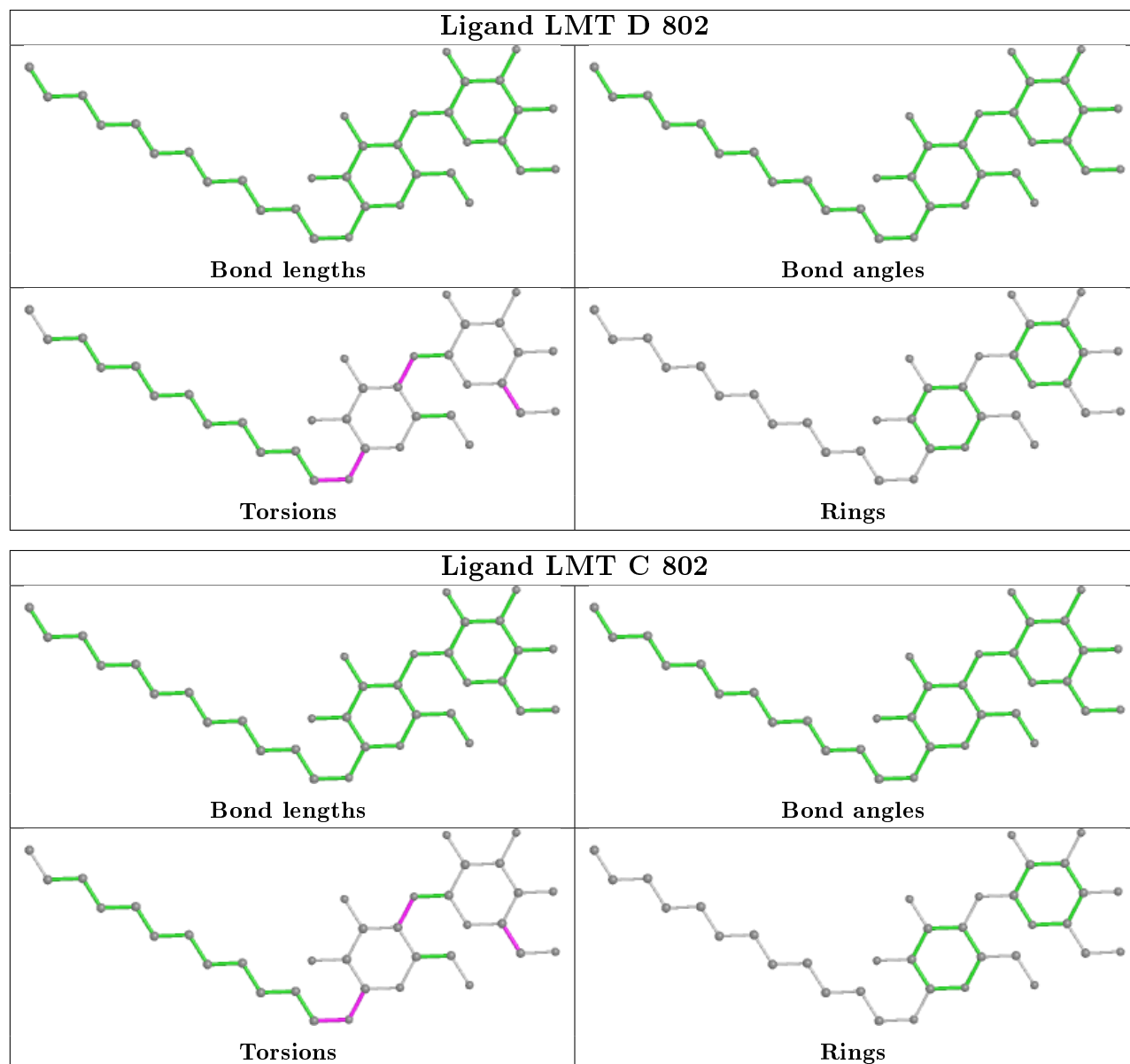
There are no ring outliers.

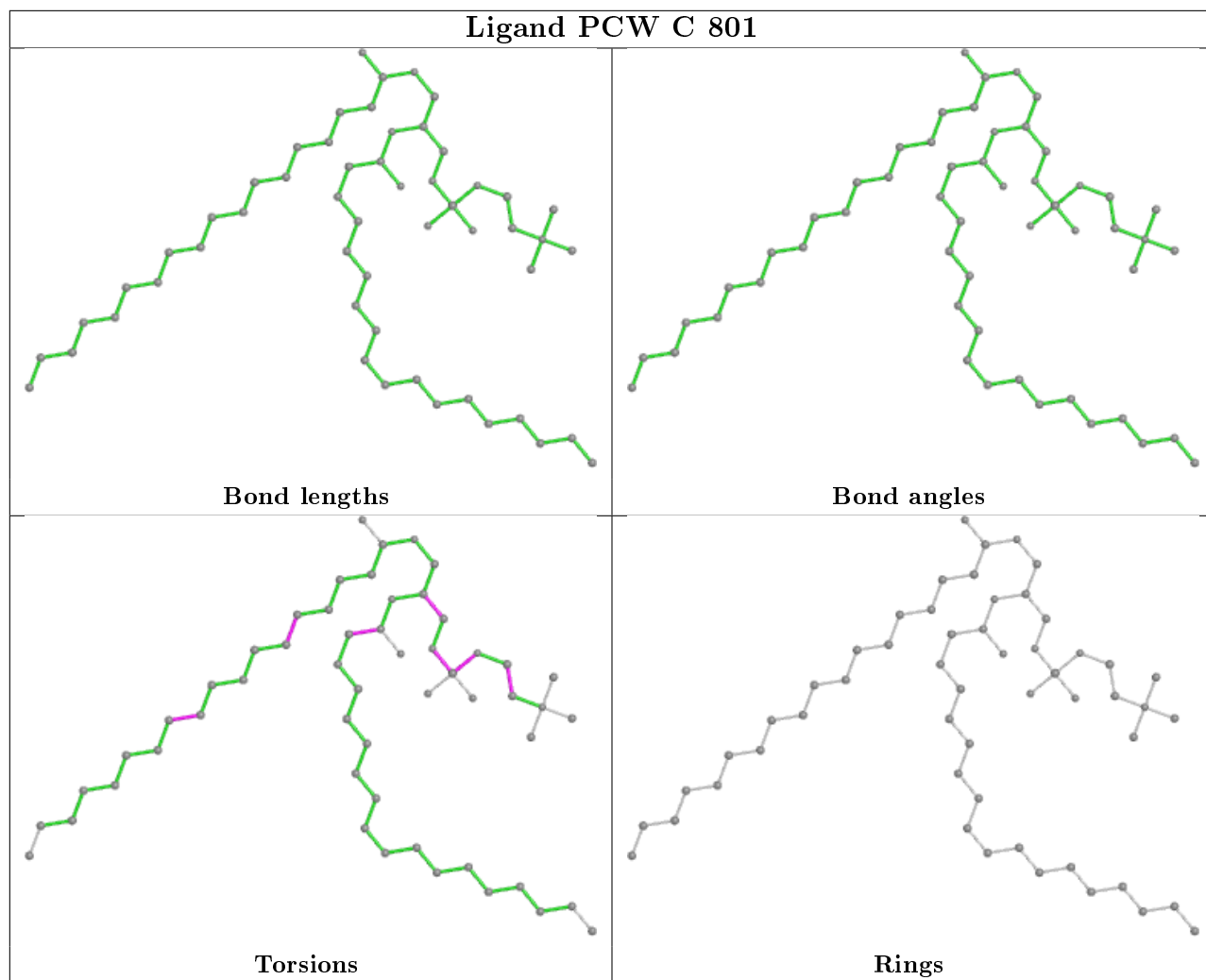
14 monomers are involved in 62 short contacts:

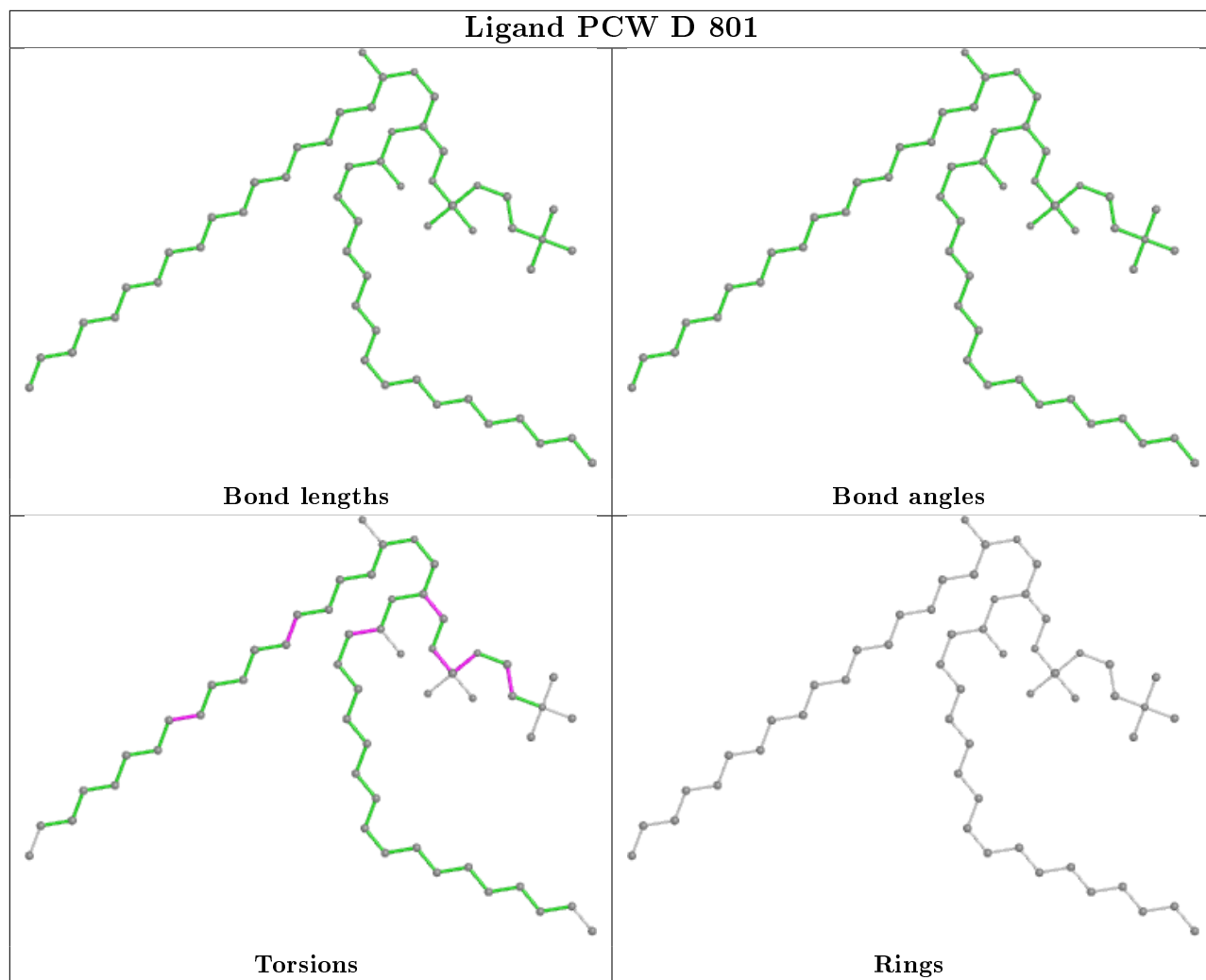
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	LMT	4	0
3	C	802	LMT	3	0
2	C	801	PCW	6	0
2	D	801	PCW	6	0
2	B	801	PCW	6	0
3	B	802	LMT	4	0
3	G	802	LMT	4	0
3	F	802	LMT	3	0
2	G	801	PCW	7	0
3	E	802	LMT	5	0
3	A	802	LMT	3	0
2	A	801	PCW	6	0
2	F	801	PCW	6	0
2	E	801	PCW	7	0

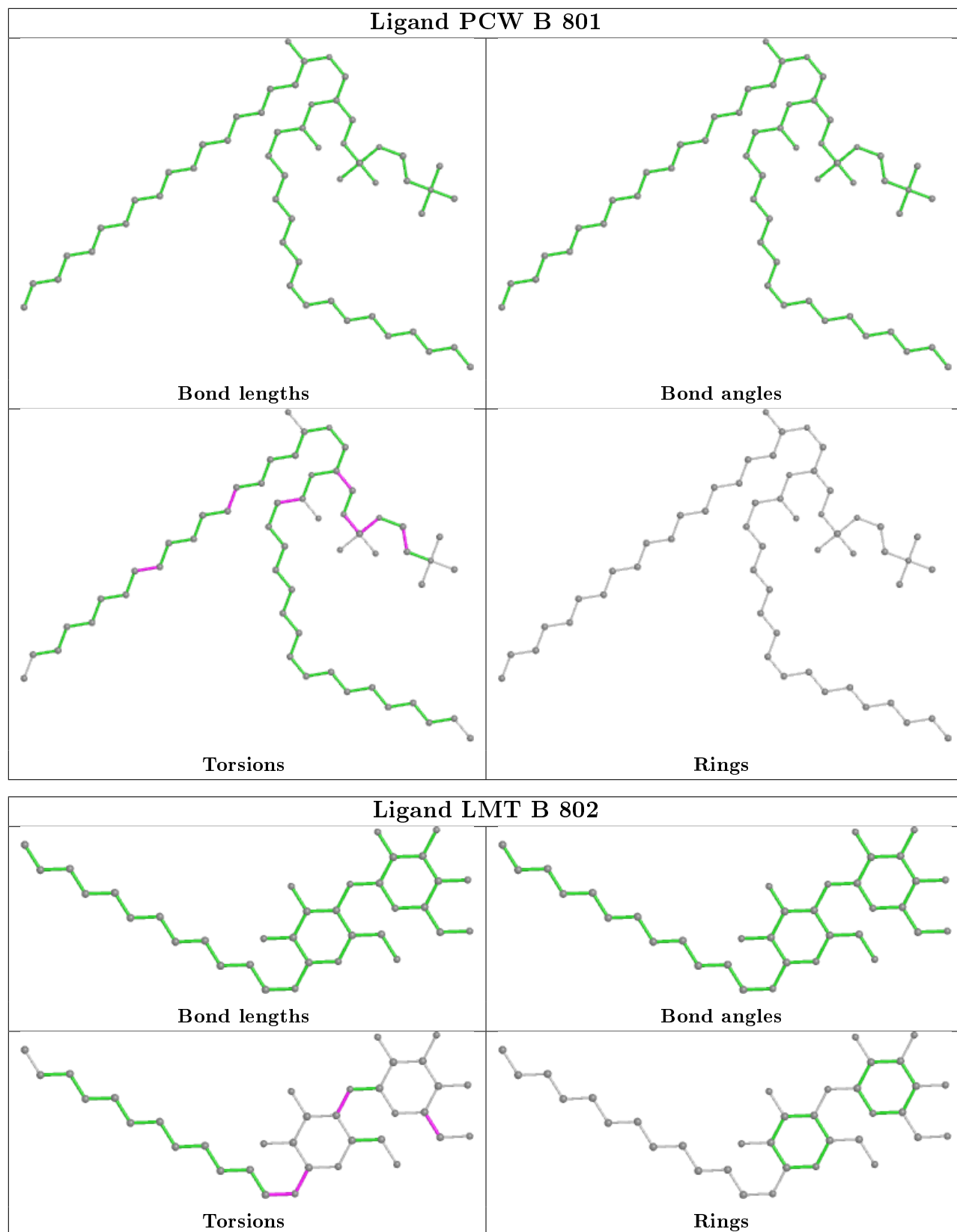
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

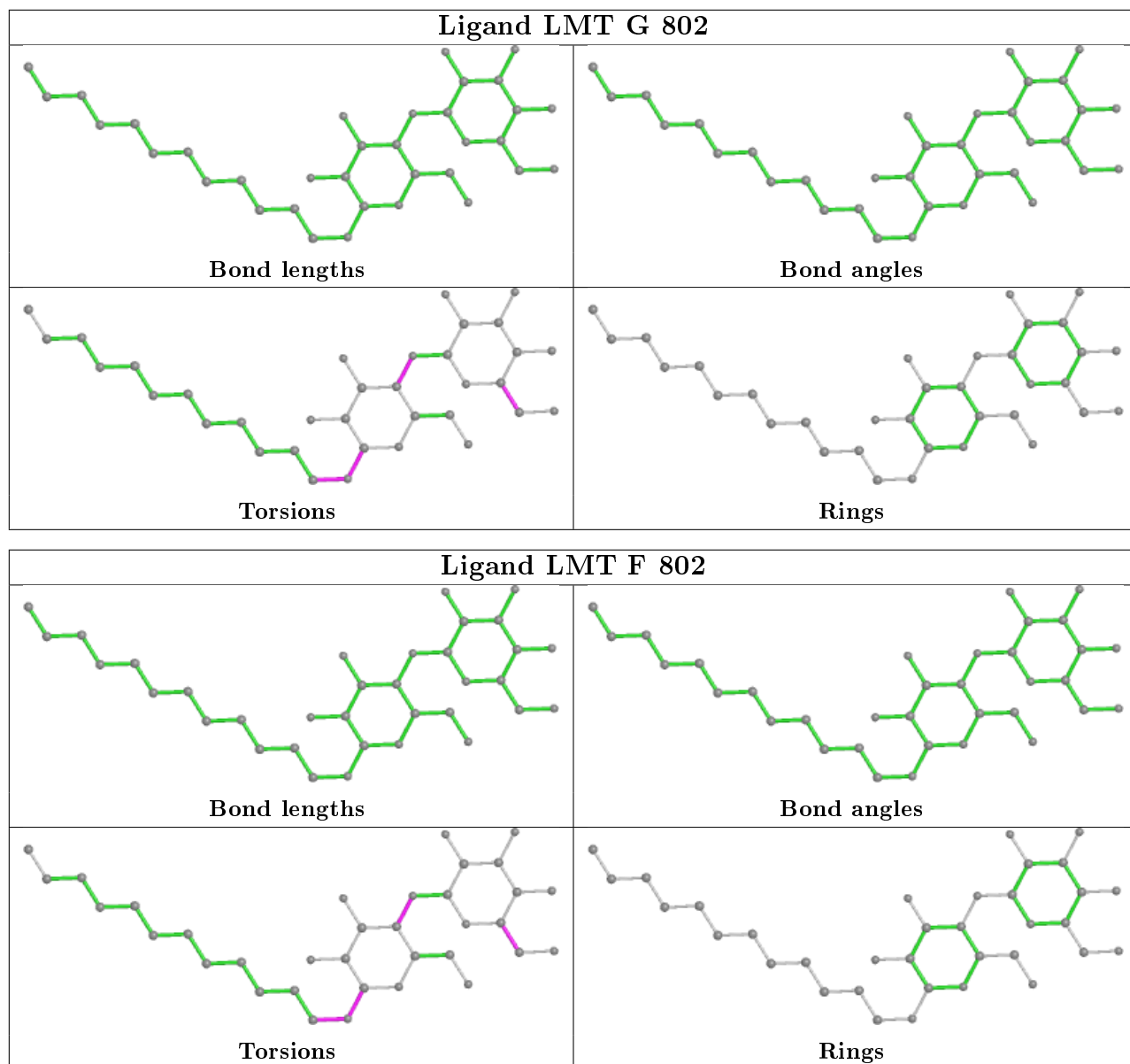
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

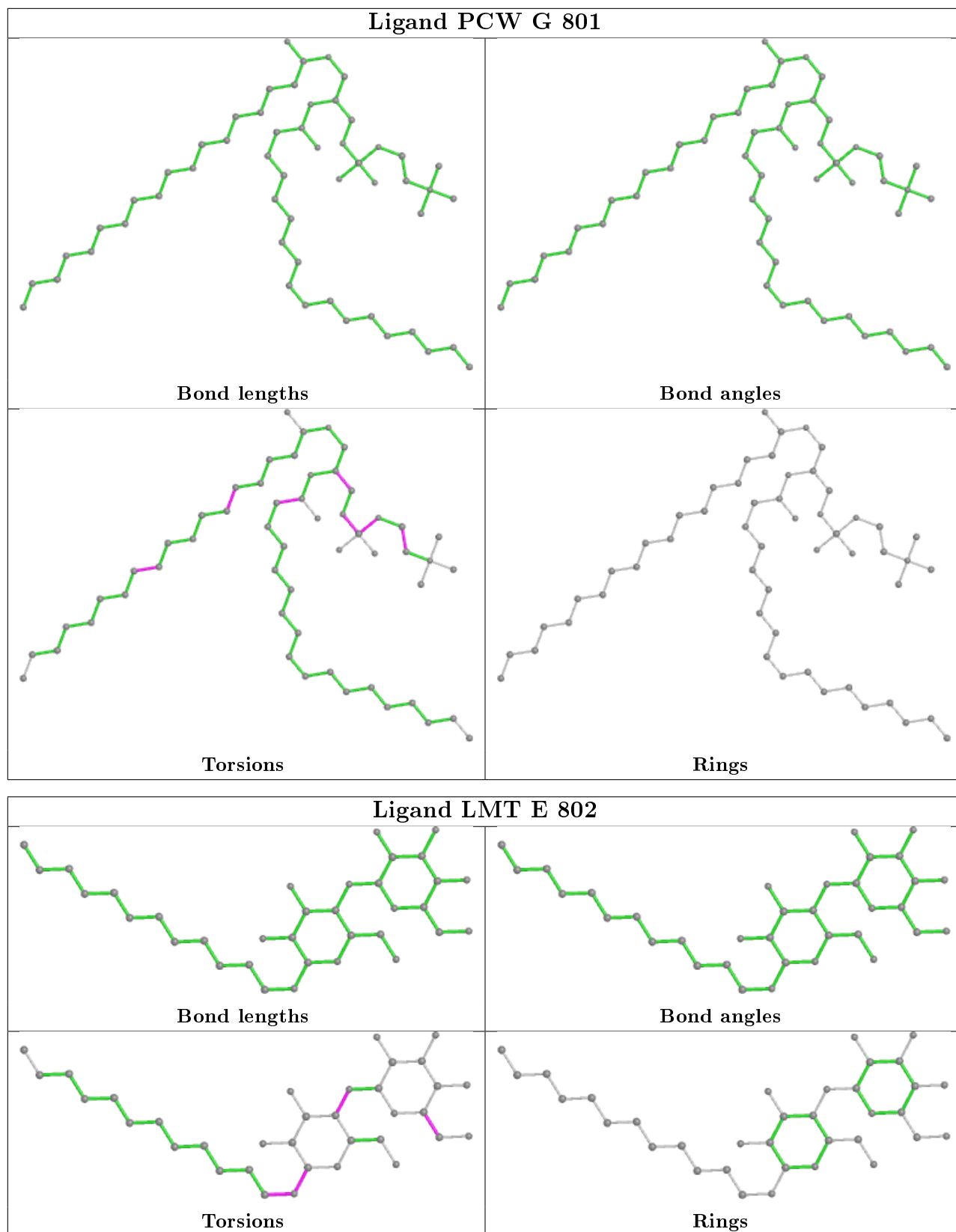


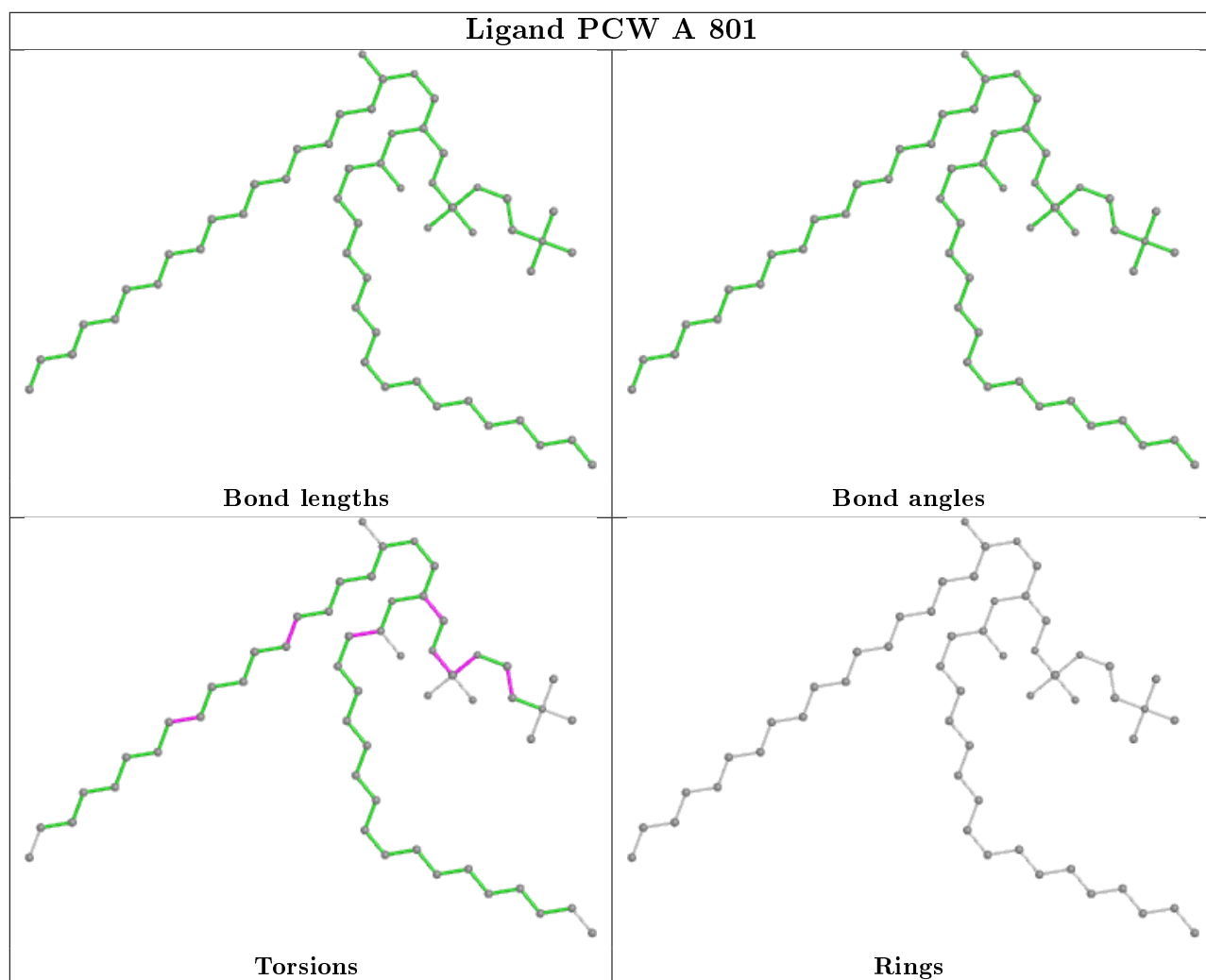
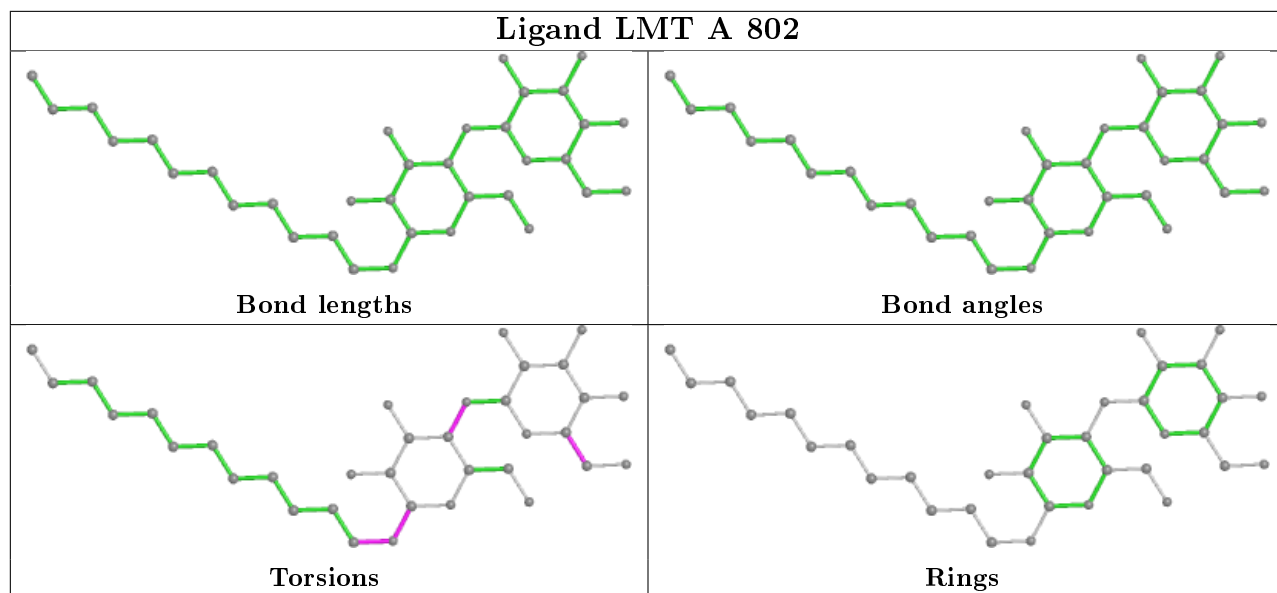


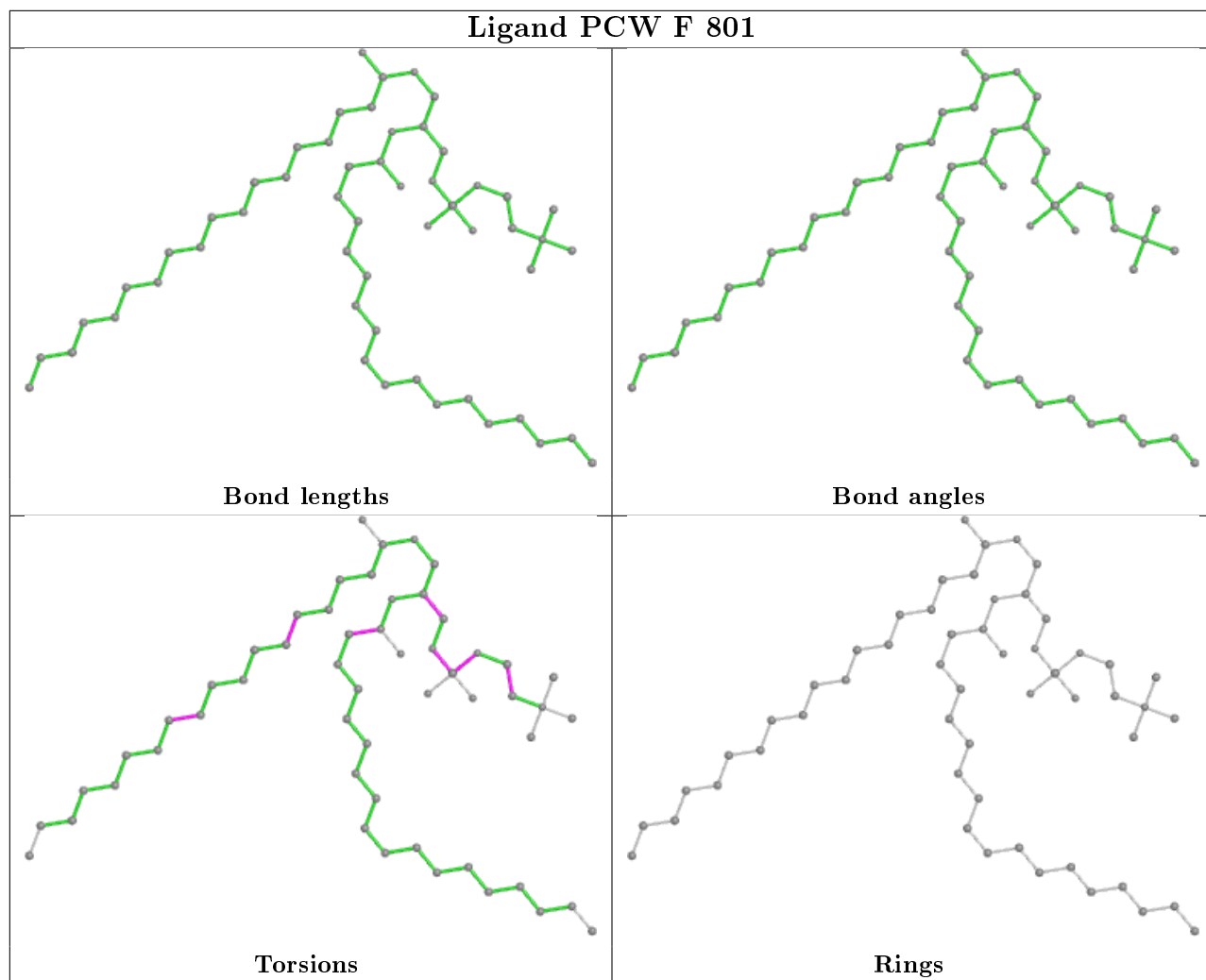


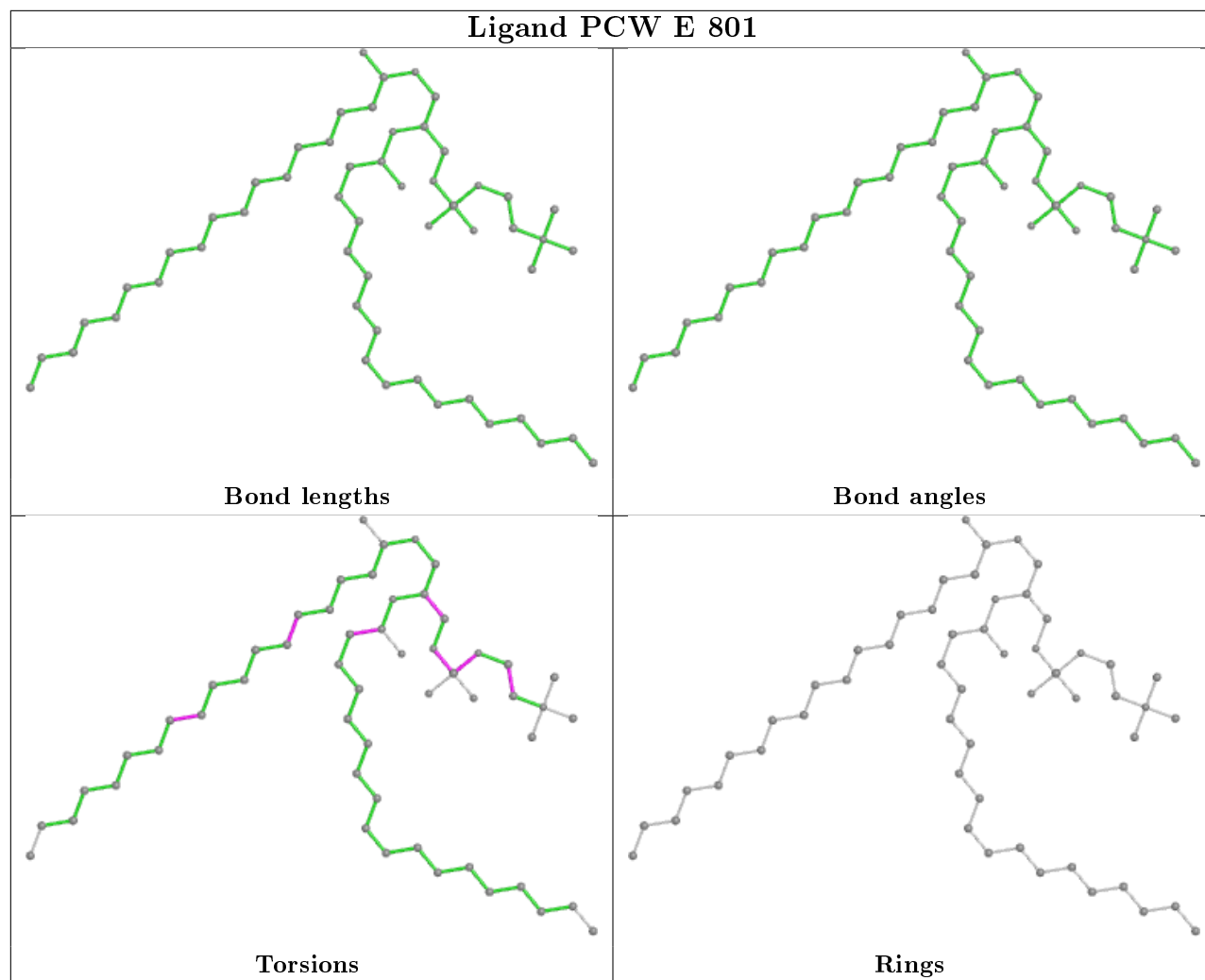












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

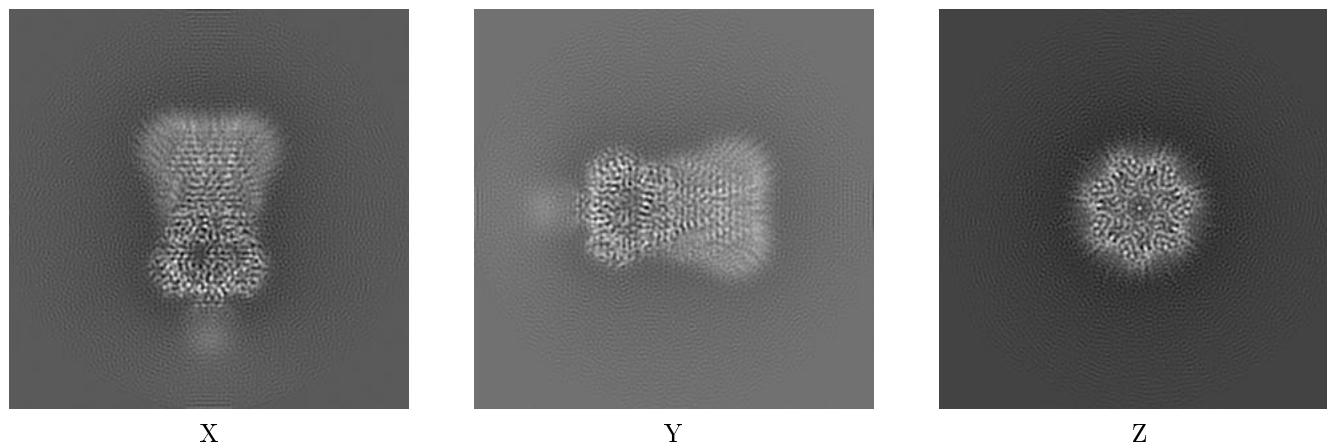
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13006. These allow visual inspection of the internal detail of the map and identification of artifacts.

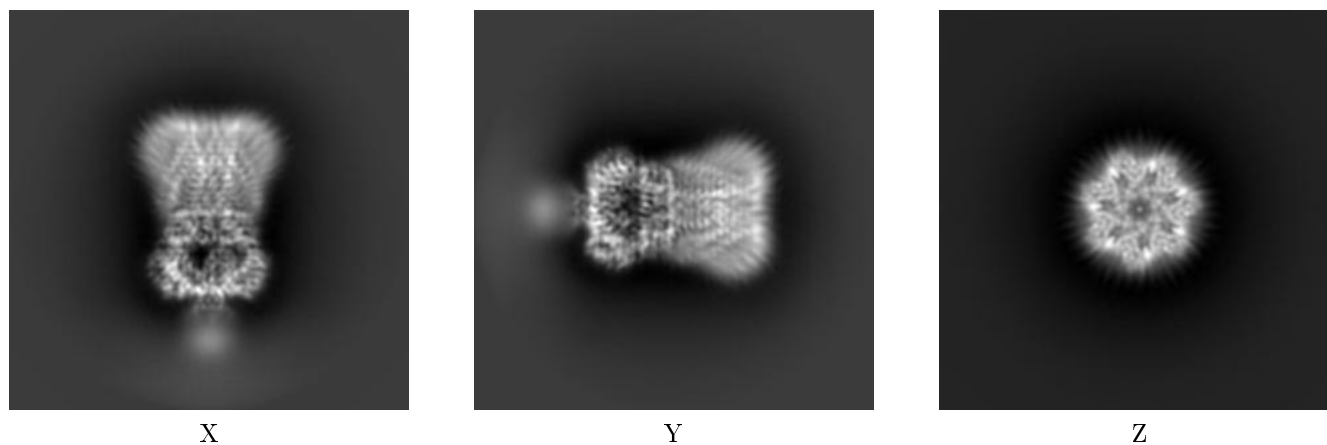
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



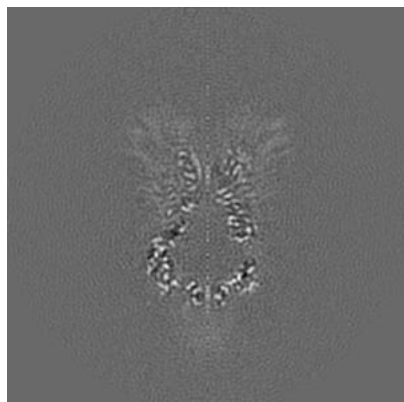
6.1.2 Raw map



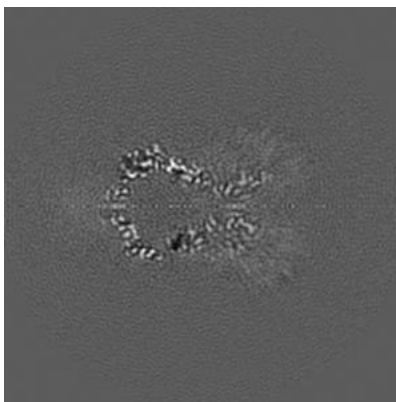
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

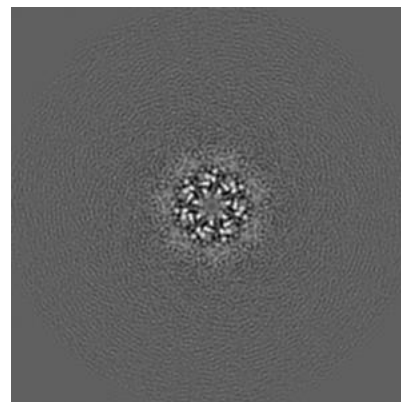
6.2.1 Primary map



X Index: 128

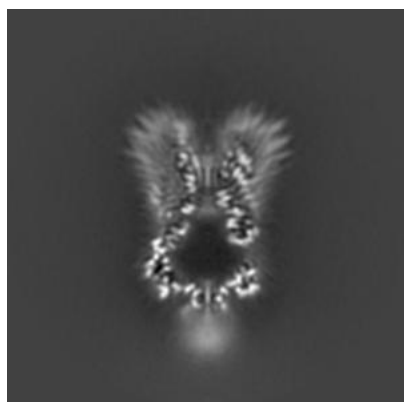


Y Index: 128

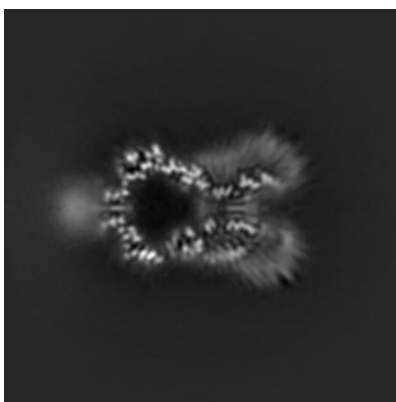


Z Index: 128

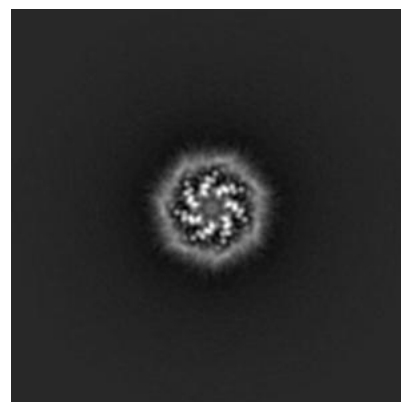
6.2.2 Raw map



X Index: 128



Y Index: 128

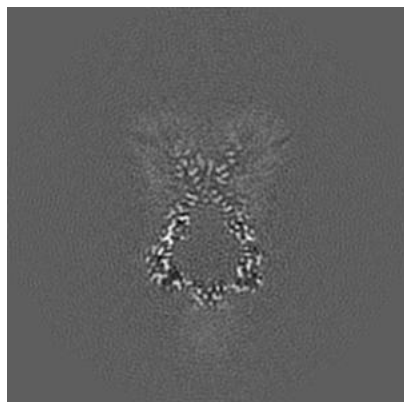


Z Index: 128

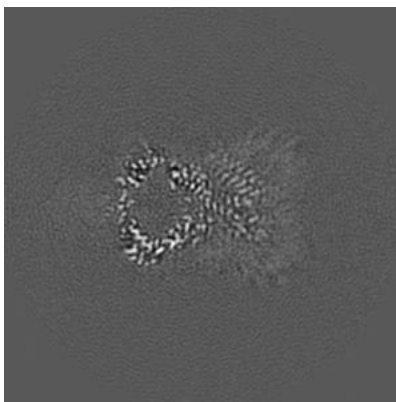
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

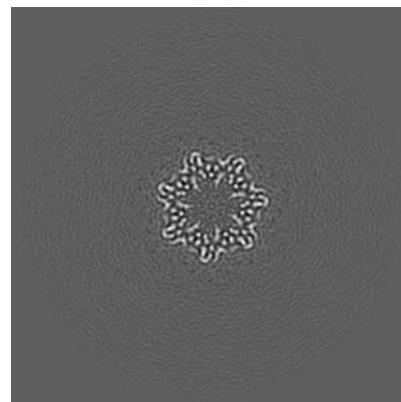
6.3.1 Primary map



X Index: 122

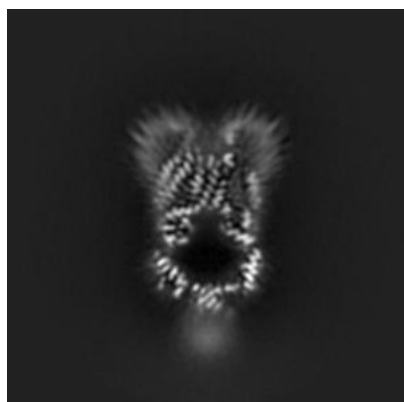


Y Index: 140

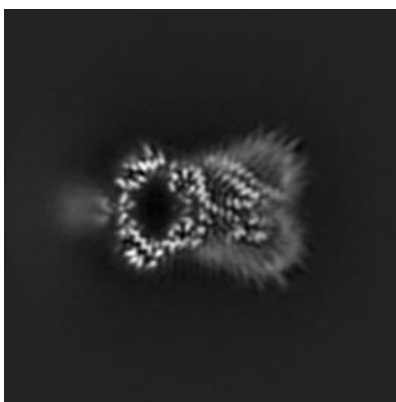


Z Index: 83

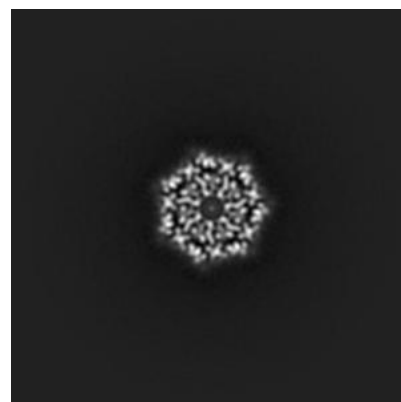
6.3.2 Raw map



X Index: 136



Y Index: 140

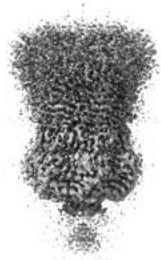


Z Index: 78

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

6.4 Orthogonal surface views [i](#)

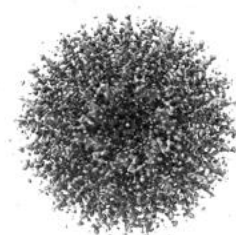
6.4.1 Primary map



X



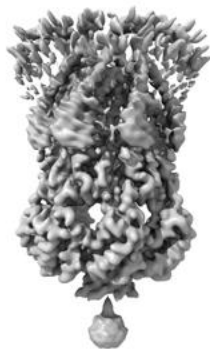
Y



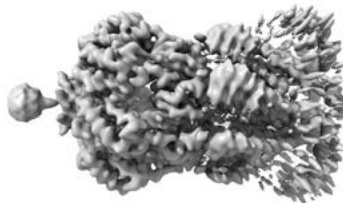
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

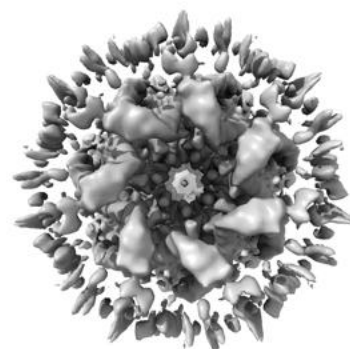
6.4.2 Raw map



X



Y



Z

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

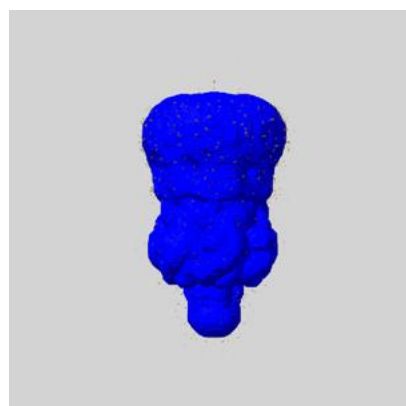
6.5 Mask visualisation [i](#)

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

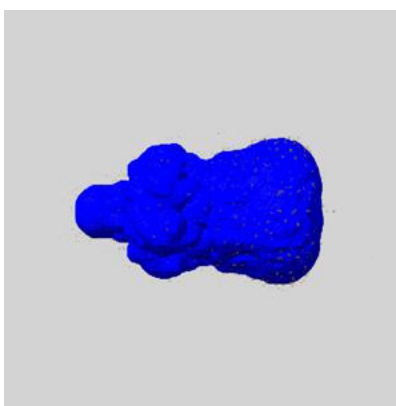
A mask typically either:

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

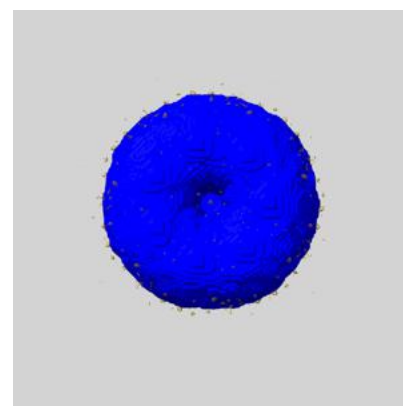
6.5.1 emd_13006_msk_1.map [i](#)



X



Y

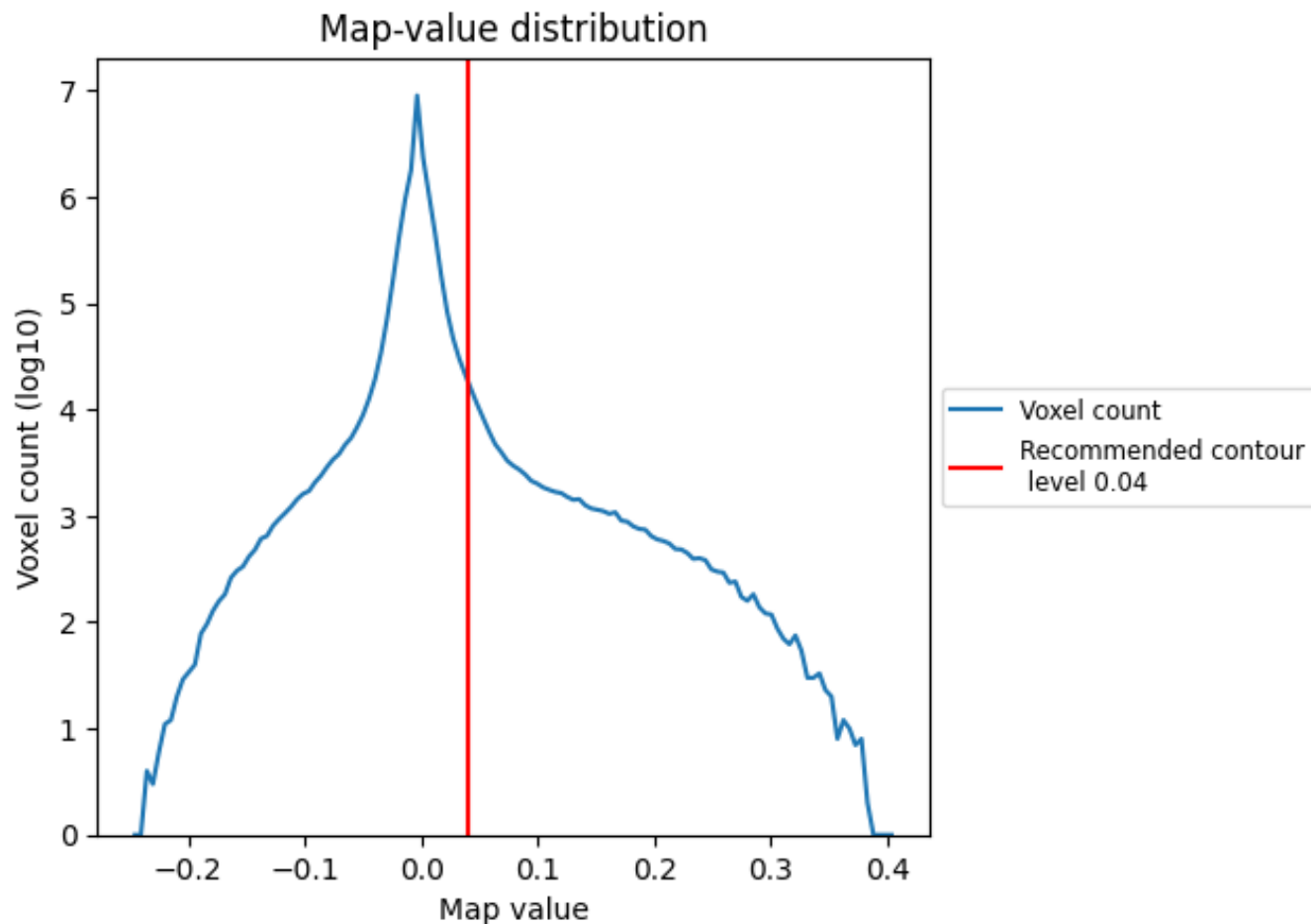


Z

7 Map analysis [i](#)

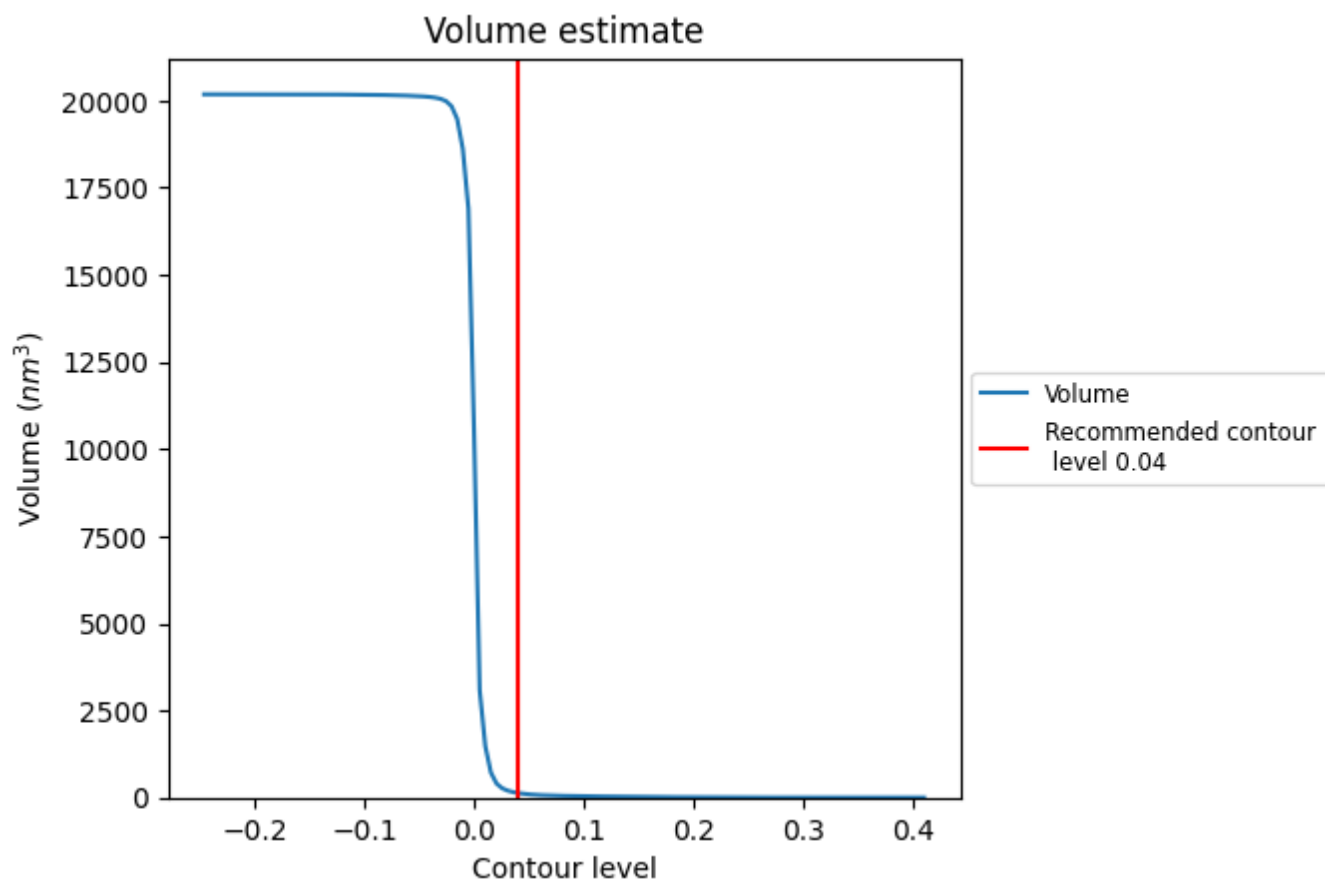
This section contains the results of statistical analysis of the map.

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.

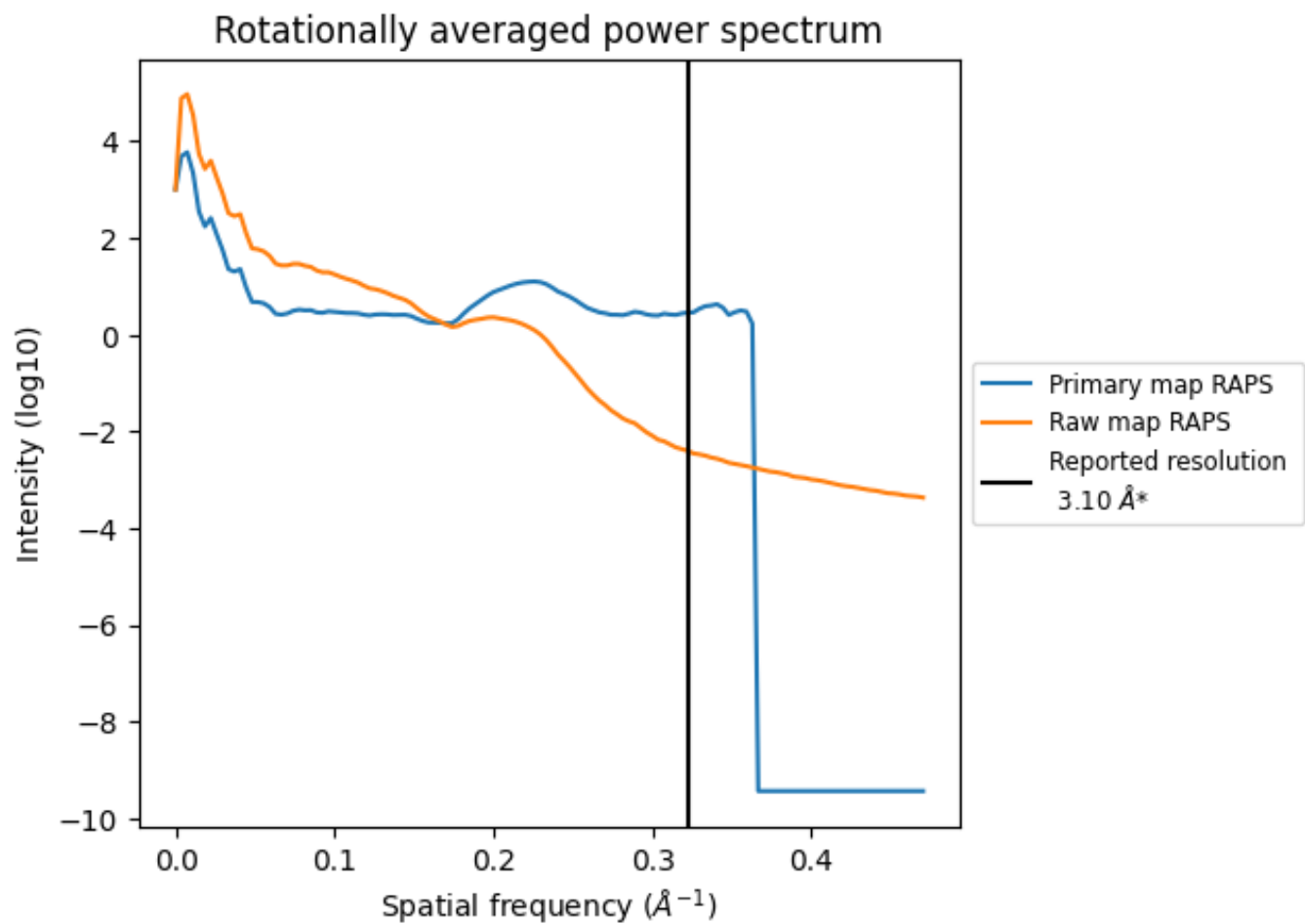
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm^3 ; this corresponds to an approximate mass of 117 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](#)

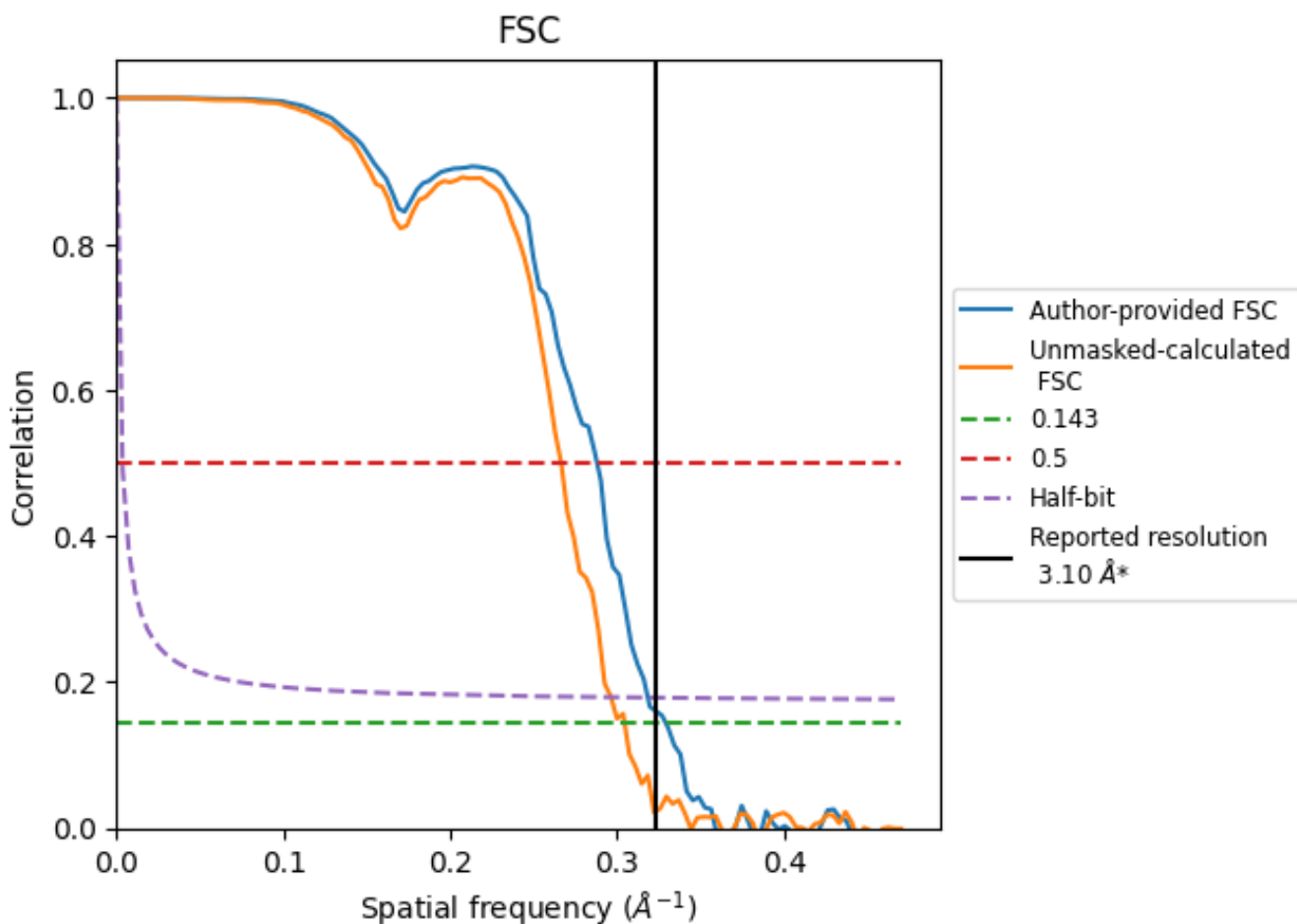


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

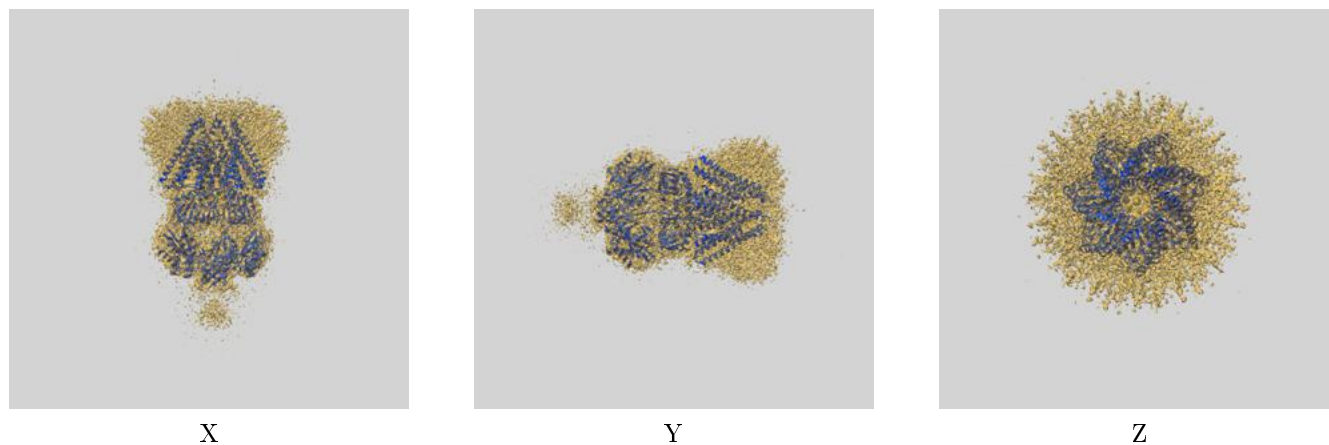
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.47	3.14
Unmasked-calculated*	3.29	3.75	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

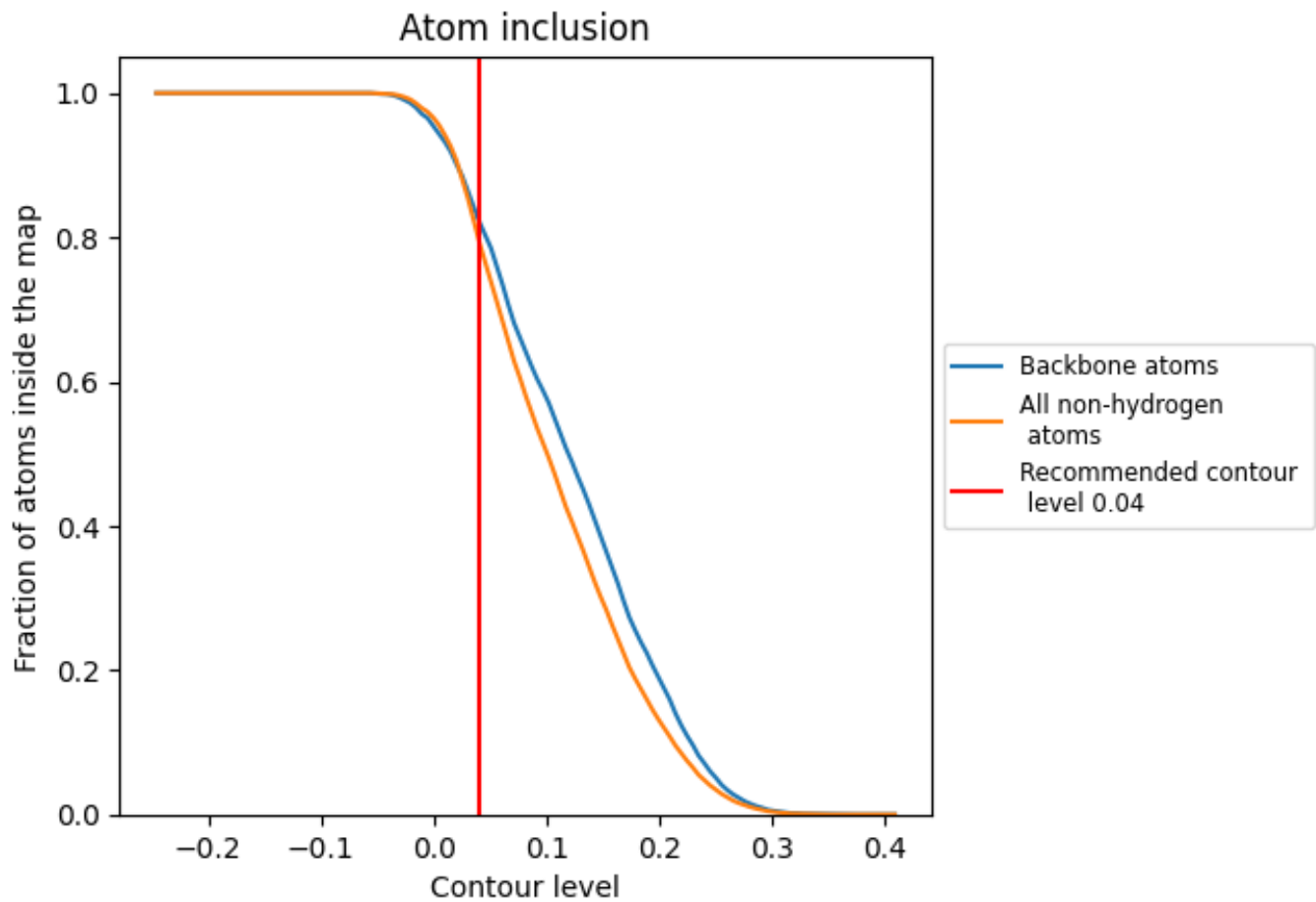
This section contains information regarding the fit between EMDB map EMD-13006 and PDB model 7OO6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.