



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 02:32 AM EDT

PDB ID : 9BBC
EMDB ID : EMD-44417
Title : TCR GDN detergent micelle
Authors : Notti, R.Q.; Walz, T.
Deposited on : 2024-04-05
Resolution : 3.30 Å(reported)

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.39

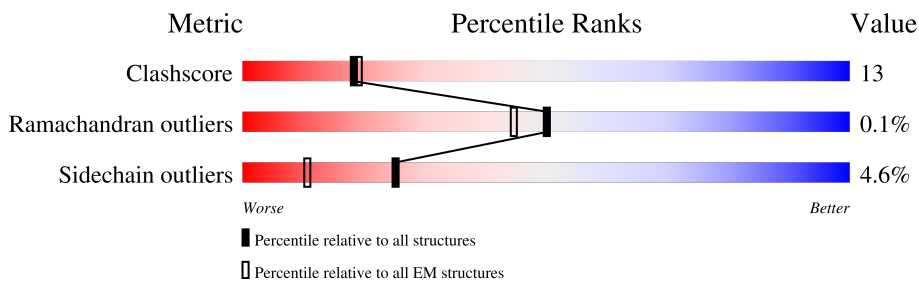
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.




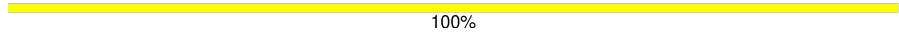

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	273	
2	B	305	
3	D	171	
4	E	207	
4	F	207	
5	G	137	
6	X	164	
6	Y	164	

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Mol	Chain	Length	Quality of chain
7	I	2	 100%
7	R	2	 50% 50%
8	C	3	 100%
8	H	3	 100%
8	O	3	 67% 100%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 8440 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 TCRA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	253	Total	C	N	O	S	0	0
			1932	1215	323	386	8		

- Molecule 2 is a protein called TCRb.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	284	Total	C	N	O	S	0	0
			2206	1399	371	425	11		

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	105	Total	C	N	O	S	0	0
			810	517	134	153	6		

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	119	Total	C	N	O	S	0	0
			930	594	147	181	8		
4	F	119	Total	C	N	O	S	0	0
			936	595	146	187	8		

- Molecule 5 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	114	Total	C	N	O	S	0	0
			888	572	146	163	7		

- Molecule 6 is a protein called T-cell surface glycoprotein CD3 zeta chain.

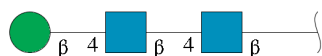
Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	30	Total	C	N	O	S	0	0
			219	148	32	38	1		
6	Y	28	Total	C	N	O	S	0	0
			220	153	33	33	1		

- Molecule 7 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
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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
8	O	3	Total	C	N	O	0	0
			39	22	2	15		
8	C	3	Total	C	N	O	0	0
			39	22	2	15		
8	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

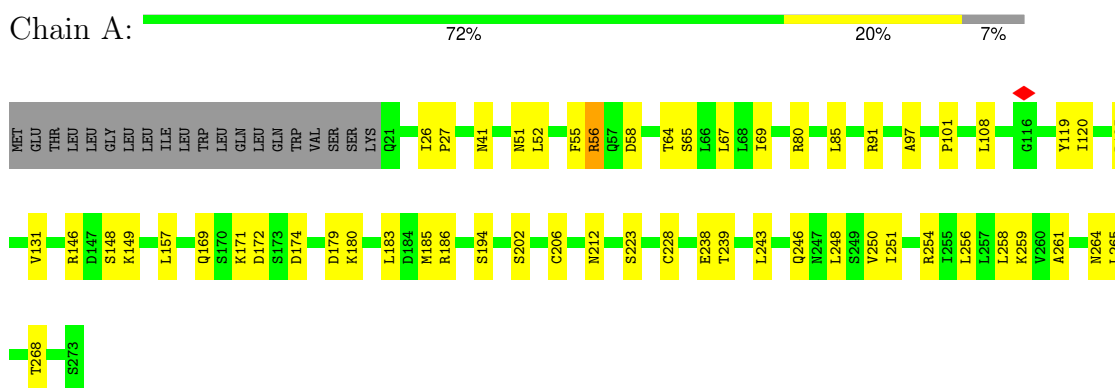


Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			28	27	1	
10	Y	1	Total	C	O	0
			28	27	1	

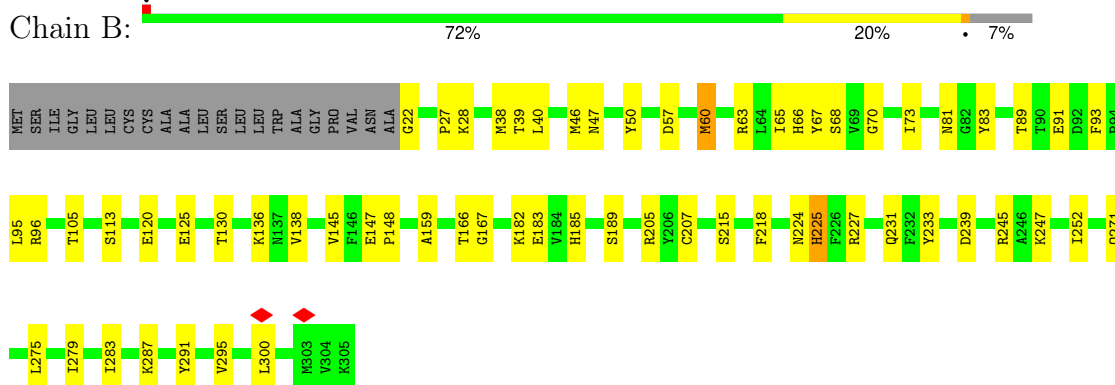
3 Residue-property plots [i](#)

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.

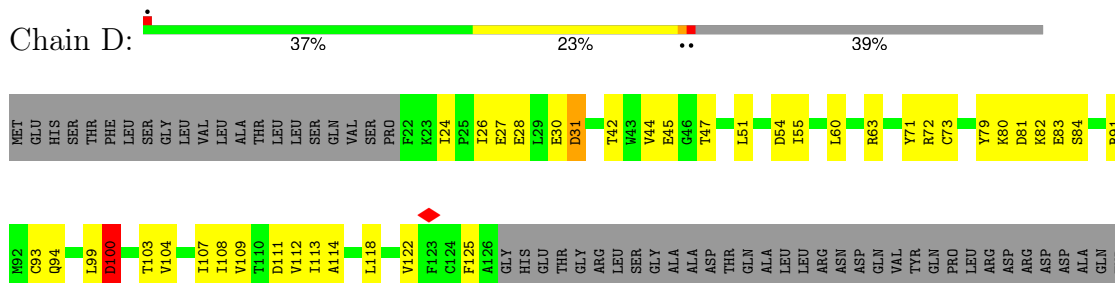
- Molecule 1: TCRA



- Molecule 2: TCRB



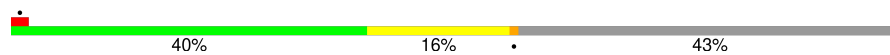
- Molecule 3: T-cell surface glycoprotein CD3 delta chain



SER
HIS
LEU
GLY
GLY
GLY
ASN
TRP
ALA
ARG
ASN
LYS

• Molecule 4: T-cell surface glycoprotein CD3 epsilon chain

Chain E:



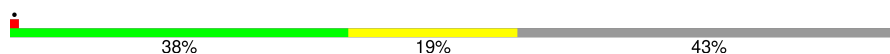
MET
GLN
SER
GLY
THR
HIS
TRP
ARG
VAL
LEU
GLY
LEU
CYS
LEU
SER
SER
VAL
GLY
VAL
TRP
GLY
GLN
ASP
GLY
ASN
GLU
GLU
MET
GLY
ILE
THR
Q33
T34
K37
T43
T48
Q51
S55
E56
I57
Q60
G68
D69
E70
D71
E86
E91
Q92
Y96

V87
C98
Y99
P100
R101
G102
S103
K104
E106
Y113
R117
V118
C119
E120
N121
C122
M123
E124
D126
S129
V130
A131
I133
V136
D137
L144
L147
Y148
Y149
Y150
W151
SER
LYS
ASN
ARG
LYS
ALA
LYS
ALA
PRO
VAL
THR
THR
ARG
GLY
ALA
GLY
ALA
GLY
ARG

GLN
ARG
GLY
GLN
ASN
LYS
GLU
ARG
PRO
PRO
VAL
PRO
ASN
PRO
TYR
GLU
PRO
ILE
ARG
GLN
GLY
ASN
ASP
LEU
TYR
SER
GLY
LEU
ASN
GLN
ARG
ARG
ILE

• Molecule 4: T-cell surface glycoprotein CD3 epsilon chain

Chain F:



MET
GLN
SER
GLY
THR
HIS
TRP
ARG
VAL
LEU
GLY
LEU
CYS
LEU
SER
SER
VAL
GLY
VAL
TRP
GLY
GLN
ASP
GLY
ASN
GLU
GLU
MET
GLY
ILE
THR
Q33
K37
V38
S39
T43
I46
L47
T48
E56
W59
Q60
H61
N62
D63
E70
D71
D78
H81
L82

E86
F87
S88
Q92
S93
Y99
P100
R101
G102
S103
K104
P105
E106
F110
R115
A116
V118
C119
C122
M123
E124
S129
T132
I133
V136
D137
I138
T141
L144
L145
Y149
W151
SER
LYS
ASN
ARG
LYS
ALA
LYS
ALA
PRO
VAL
THR
ARG
GLY
ALA

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

• Molecule 5: T-cell surface glycoprotein CD3 gamma chain

Chain G:



MET
GLU
GLN
GLY
LYS
GLY
LEU
ALA
VAL
LEU
ILE
LEU
ALA
ILE
ILE
LEU
LEU
LEU
GLN
GLY
THR
S24
I25
K26
V31
K32
V33
Y34
D35
V36
Q37
E38
L43
D47
A48
E49
F56
D68
K71
K79
D80
F81
Q86
C87
K88
G89
S90
Q91
N92
K93

P96
L97
Q98
M103
C104
Q106
C107
M111
I115
F118
L119
F120
A121
E122
I123
V124
S125
I126
F127
V128
L129
A130
G131
G132
Y134
F135
I136
A137

• Molecule 6: T-cell surface glycoprotein CD3 zeta chain

Chain X:



MET
LYS
TRP
LYS
ALA
LEU
PHE
THR
ALA
ALA
LEU
LEU
GLN
ALA
GLN
LEU
LEU
LEU
ILE
THR
GLU
ALA
Q22
L26
L27
E28
P29
Y33
L34
L35
D36
G37
I38
L39
F40
I41
L45
L46
L49
F50
L51
ARG
VAL
LEU
GLN
LYS
PHE
SER
SER
ARG
SER
SER
ALA
ASP
ALA
PRO
TYR
SER
GLU
TYR
ILE
GLN
GLY

GLN
ASN
LEU
LEU
TYR
ASN
GLU
LEU
ASN
GLN
GLU
TYR
ASP
ARG
ARG
GLY
ARG
ASP
PRO
GLU
MET
GLY
GLY
LYS
PRO
GLN
ARG
ARG
LYS
ASN
ASN
GLN
GLU
GLY
LEU
TYR
ASN

MET
LYS
GLY
GLU
ARG
ARG
ARG
GLY
LYS
GLY
HIS
ASP
GLY
LEU
TYR
GLN
GLY
SER
THR
ALA
LYS
LEU
MET
GLN
ALA
LEU
PRO
PRO
ARG

- Molecule 6: T-cell surface glycoprotein CD3 zeta chain

Chain Y: 9% 7% 83%

MET
LYS
TRP
LYS
ALA
LEU
PHE
THR
ALA
ASN
ILE
LEU
GLN
ALA
LEU
GLN
PRO
ILE
THR
GLU
ALA
GLN
VAL
SER
PHE
GLY
LEU
LEU
D28
P29
K30
L31
C32
Y33
L34
L35
D36
G37
I38
L39
F40
I41
V44
T47
A48
L49
F50
L51
R52
F55
SER
ARG
SER
MET
ALA
ASP
GLU
ALA
TYR

TYR
GLN
GLY
ASN
GLN
LEU
TYR
ASN
LEU
GLY
HIS
GLY
ASP
GLY
LEU
TYR
GLN
LEU
VAL
SER
THR
ALA
THR
LYS
ASP
THR
TYR
ASP
ALA
LEU
MET
GLY
GLY
LYS
PRO
GLN
ARG
ARG
GLY
ASP
THR
TYR
ASP
ALA
LEU
MET
GLY
GLY
LYS
PRO
GLN
ARG
ARG
LYS
ASN
PRO
GLN
GLY
GLY
LEU
TYR
ASN
GLY
LEU
GLN
LYS
ASP
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MET
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ALA
TYR

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

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 50% 50% 50%

MAG1
MAG2

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

Chain O: 67% 100%

MAG1
MAG2
BMA3

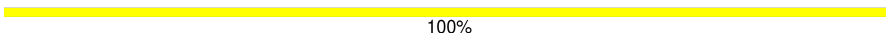
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

MAG1
MAG2
BMA3

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

Chain H:



100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.362	Depositor
Minimum map value	-0.595	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: BMA, NAG, CLR

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	0.27	0/1971	0.53	1/2682 (0.0%)
2	B	0.27	0/2261	0.53	0/3081
3	D	0.28	0/822	0.69	2/1119 (0.2%)
4	E	0.28	0/951	0.64	2/1295 (0.2%)
4	F	0.26	0/957	0.56	0/1303
5	G	0.30	0/906	0.69	1/1222 (0.1%)
6	X	0.25	0/223	0.71	0/302
6	Y	0.31	0/225	0.84	0/304
All	All	0.27	0/8316	0.60	6/11308 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	G	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	31	ASP	CB-CG-OD1	5.62	123.36	118.30
3	D	100	ASP	CB-CG-OD2	5.31	123.08	118.30
4	E	126	ASP	CB-CG-OD1	5.12	122.91	118.30
4	E	137	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	256	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	104	CYS	Peptide

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	1932	0	1851	43	0
2	B	2206	0	2105	41	0
3	D	810	0	813	31	0
4	E	930	0	881	25	0
4	F	936	0	884	26	0
5	G	888	0	861	39	0
6	X	219	0	210	11	0
6	Y	220	0	228	16	0
7	I	28	0	25	0	0
7	R	28	0	25	0	0
8	C	39	0	34	0	0
8	H	39	0	34	0	0
8	O	39	0	34	0	0
9	A	56	0	52	0	0
9	G	14	0	13	0	0
10	A	28	0	46	5	0
10	Y	28	0	46	2	0
All	All	8440	0	8142	213	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 13.

The worst 5 of 213 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:248:LEU:HA	1:A:251:ILE:HD12	1.66	0.78
6:Y:47:THR:HA	6:Y:50:PHE:CE1	2.21	0.76
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.69	0.75
4:F:37:LYS:HB2	4:F:48:THR:HB	1.69	0.74
1:A:41:ASN:HB3	1:A:91:ARG:HH22	1.53	0.73

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	251/273 (92%)	242 (96%)	8 (3%)	1 (0%)	30	61
2	B	282/305 (92%)	279 (99%)	3 (1%)	0	100	100
3	D	103/171 (60%)	95 (92%)	8 (8%)	0	100	100
4	E	117/207 (56%)	111 (95%)	6 (5%)	0	100	100
4	F	117/207 (56%)	111 (95%)	6 (5%)	0	100	100
5	G	112/137 (82%)	107 (96%)	5 (4%)	0	100	100
6	X	28/164 (17%)	27 (96%)	1 (4%)	0	100	100
6	Y	26/164 (16%)	25 (96%)	1 (4%)	0	100	100
All	All	1036/1628 (64%)	997 (96%)	38 (4%)	1 (0%)	50	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	SER

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	218/245 (89%)	211 (97%)	7 (3%)	34	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	238/259 (92%)	230 (97%)	8 (3%)	32	59
3	D	91/147 (62%)	85 (93%)	6 (7%)	14	40
4	E	102/177 (58%)	95 (93%)	7 (7%)	13	38
4	F	105/177 (59%)	101 (96%)	4 (4%)	28	56
5	G	92/114 (81%)	90 (98%)	2 (2%)	47	69
6	X	21/135 (16%)	17 (81%)	4 (19%)	1	5
6	Y	22/135 (16%)	19 (86%)	3 (14%)	3	14
All	All	889/1389 (64%)	848 (95%)	41 (5%)	25	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	63	ASP
6	X	36	ASP
4	F	110	PHE
5	G	68	ASP
6	X	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	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](#)

13 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
8	NAG	C	1	3,8	14,14,15	0.73	0	17,19,21	1.64	3 (17%)
8	NAG	C	2	8	14,14,15	0.73	0	17,19,21	1.27	1 (5%)
8	BMA	C	3	8	11,11,12	0.85	0	15,15,17	2.08	3 (20%)
8	NAG	H	1	3,8	14,14,15	0.77	0	17,19,21	2.04	4 (23%)
8	NAG	H	2	8	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
8	BMA	H	3	8	11,11,12	0.85	0	15,15,17	2.08	3 (20%)
7	NAG	I	1	7,1	14,14,15	0.74	0	17,19,21	0.97	1 (5%)
7	NAG	I	2	7	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
8	NAG	O	1	8,2	14,14,15	0.88	0	17,19,21	2.06	6 (35%)
8	NAG	O	2	8	14,14,15	0.70	0	17,19,21	2.71	5 (29%)
8	BMA	O	3	8	11,11,12	0.89	0	15,15,17	2.68	6 (40%)
7	NAG	R	1	7,5	14,14,15	0.80	0	17,19,21	1.21	2 (11%)
7	NAG	R	2	7	14,14,15	0.72	0	17,19,21	0.81	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
8	NAG	C	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	BMA	C	3	8	-	1/2/19/22	0/1/1/1
8	NAG	H	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	H	2	8	-	0/6/23/26	0/1/1/1
8	BMA	H	3	8	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
8	NAG	O	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	BMA	O	3	8	-	2/2/19/22	0/1/1/1
7	NAG	R	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	O	3	BMA	C1-O5-C5	8.49	123.56	112.19
8	O	2	NAG	C2-N2-C7	7.54	133.01	122.90
8	H	1	NAG	C1-O5-C5	6.44	120.81	112.19
8	C	3	BMA	C1-O5-C5	6.42	120.79	112.19
8	H	3	BMA	C1-O5-C5	6.16	120.44	112.19

There are no chirality outliers.

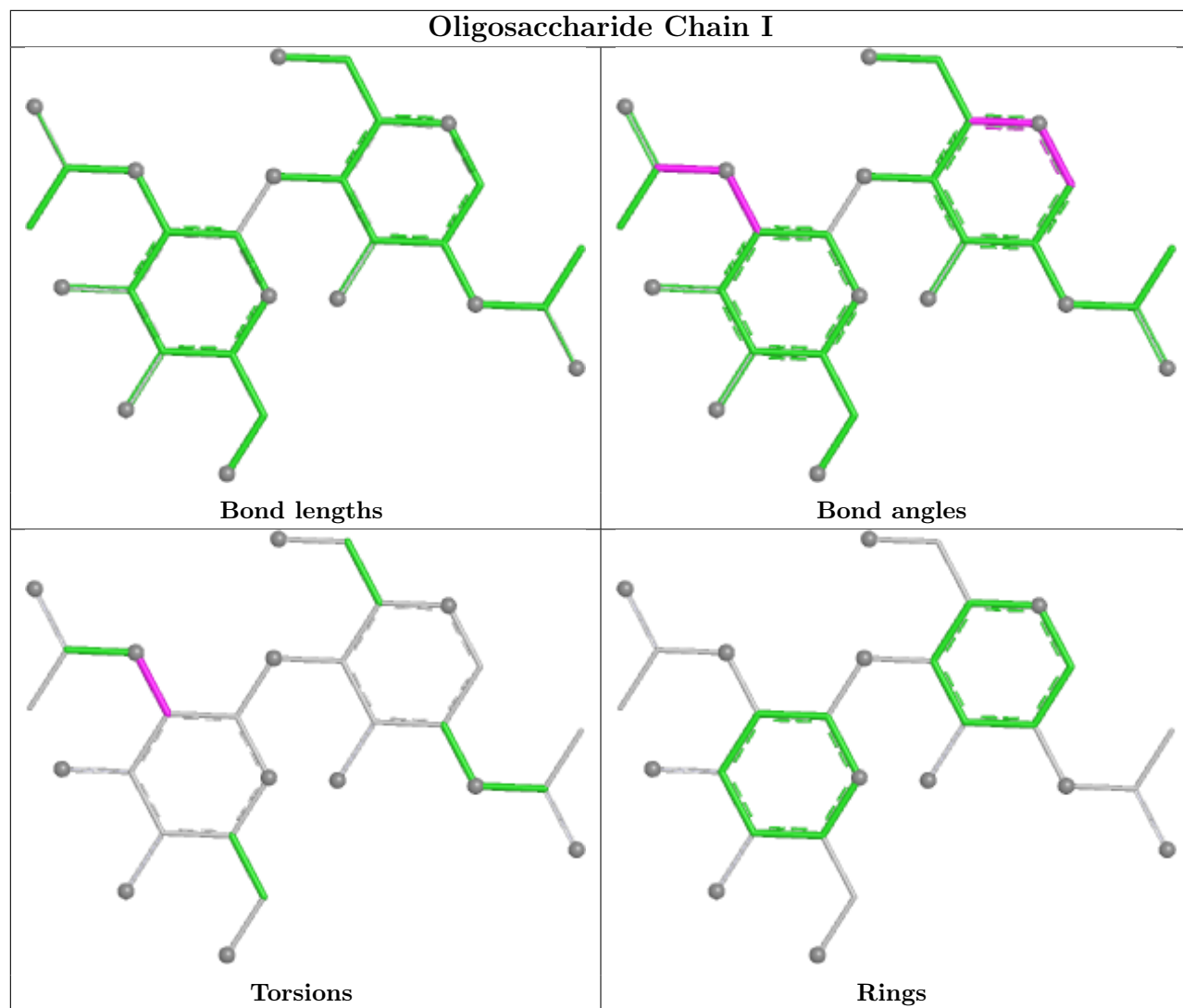
5 of 15 torsion outliers are listed below:

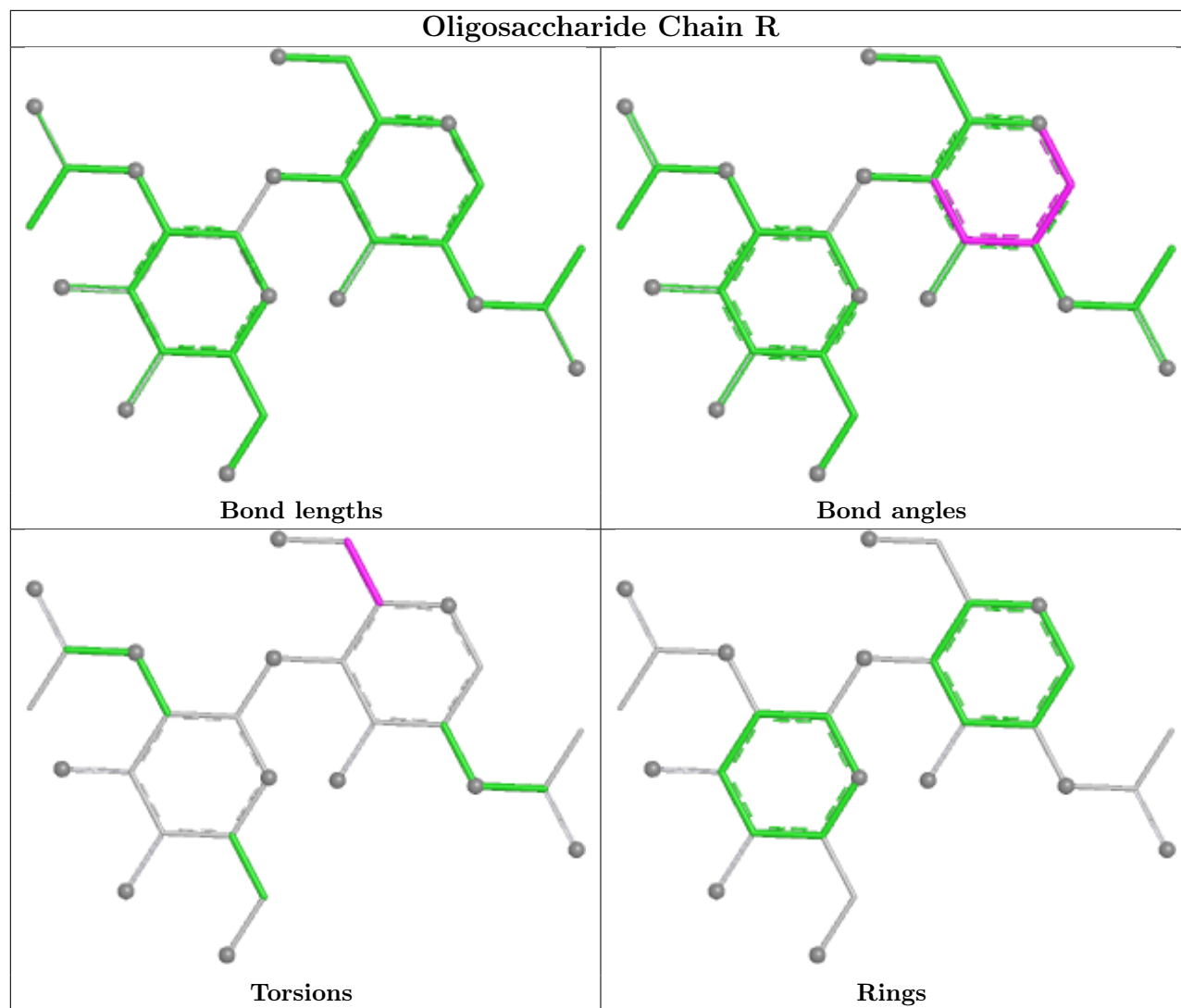
Mol	Chain	Res	Type	Atoms
8	O	2	NAG	C3-C2-N2-C7
8	H	1	NAG	C4-C5-C6-O6
8	H	1	NAG	O5-C5-C6-O6
8	O	1	NAG	C8-C7-N2-C2
8	O	1	NAG	O7-C7-N2-C2

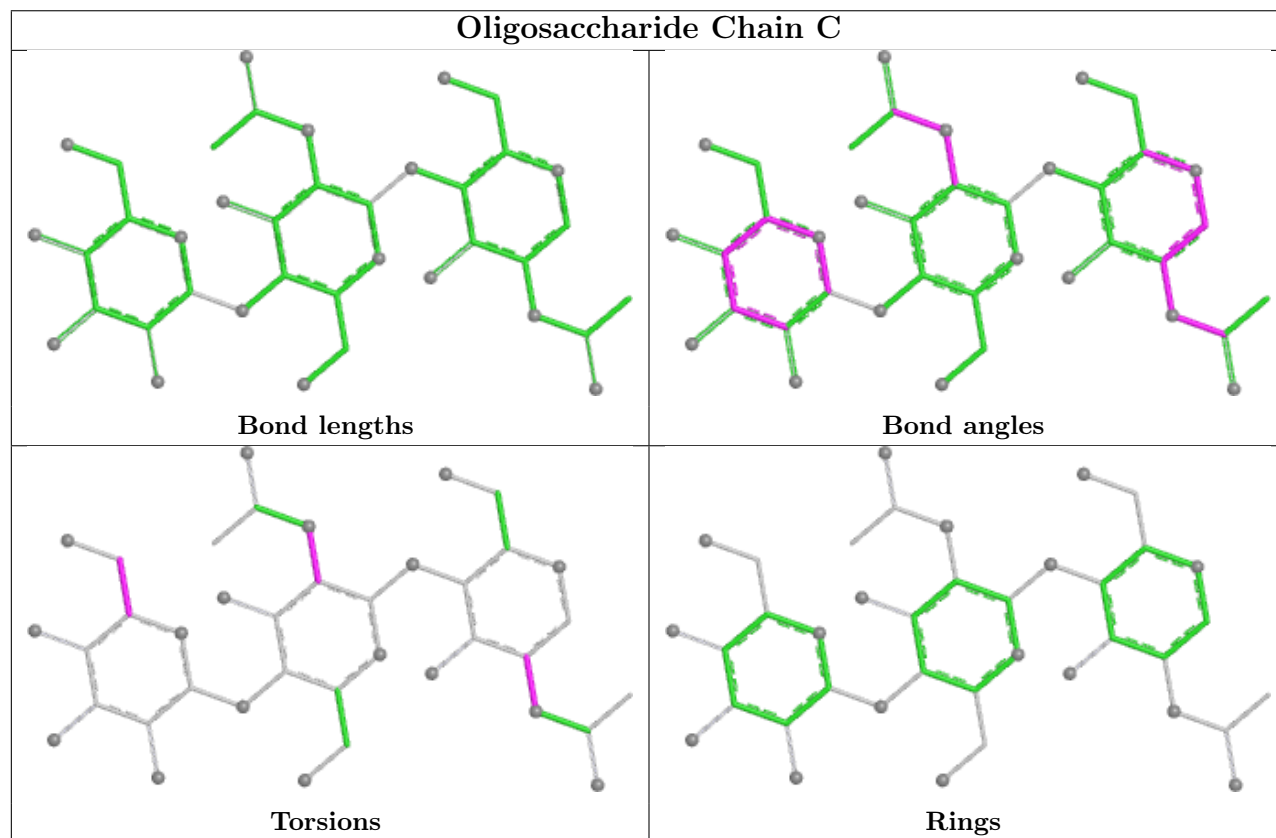
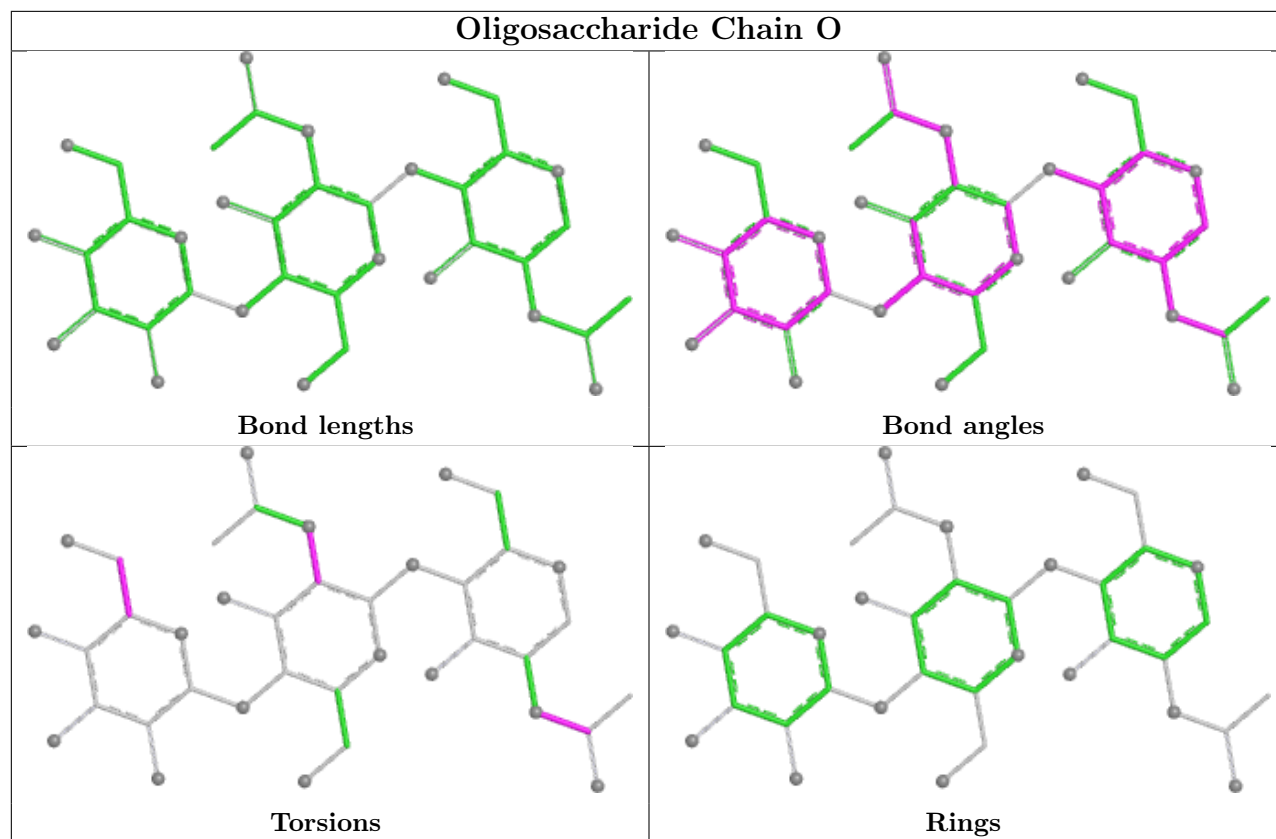
There are no ring outliers.

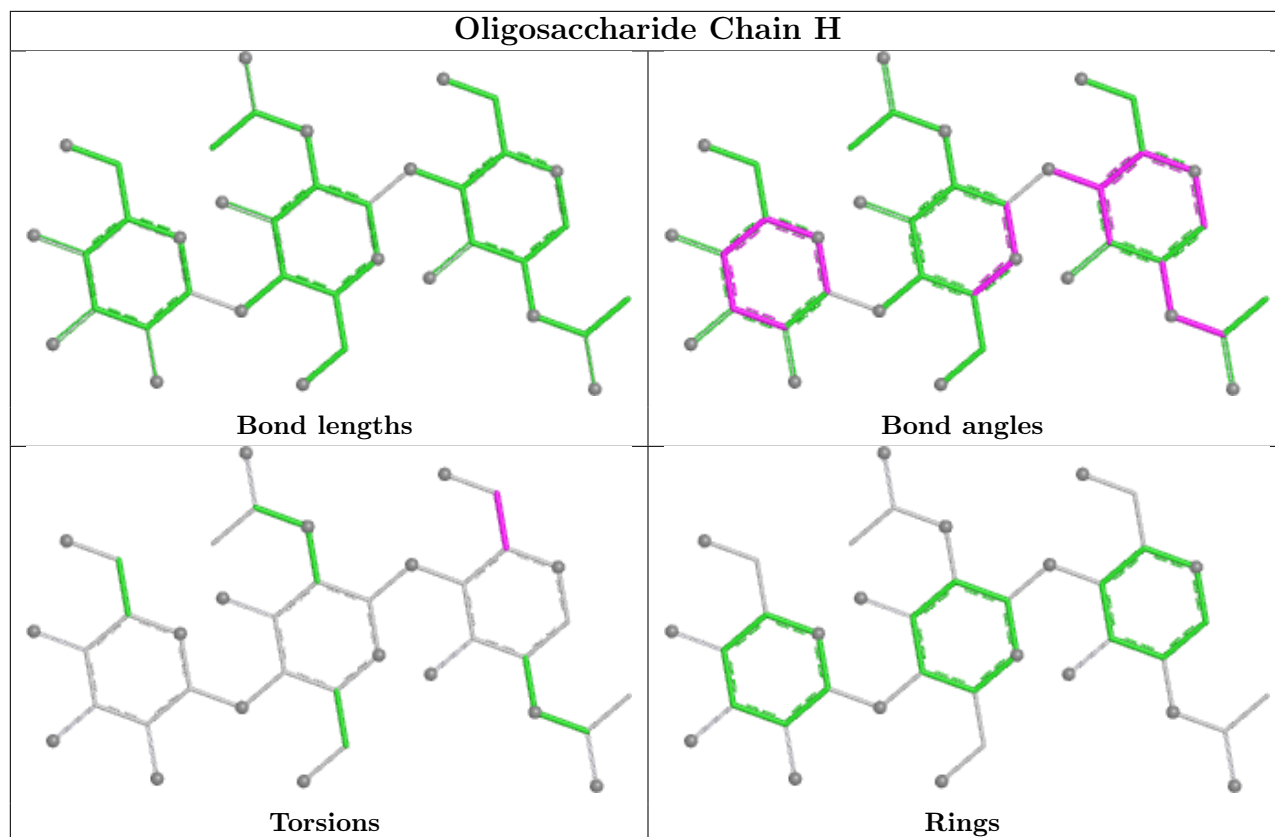
No monomer is involved in short contacts.

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](#)

7 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	$\# Z > 2$
9	NAG	A	304	1	14,14,15	0.72	0	17,19,21	1.19	1 (5%)
9	NAG	A	303	1	14,14,15	0.75	0	17,19,21	0.84	0
10	CLR	Y	201	-	31,31,31	0.38	0	48,48,48	0.61	0
9	NAG	A	301	1	14,14,15	0.69	0	17,19,21	1.18	1 (5%)
9	NAG	G	201	5	14,14,15	0.95	1 (7%)	17,19,21	3.17	6 (35%)
9	NAG	A	302	1	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
10	CLR	A	305	-	31,31,31	0.40	0	48,48,48	0.70	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
9	NAG	A	304	1	-	2/6/23/26	0/1/1/1
9	NAG	A	303	1	-	0/6/23/26	0/1/1/1
10	CLR	Y	201	-	-	4/10/68/68	0/4/4/4
9	NAG	A	301	1	-	3/6/23/26	0/1/1/1
9	NAG	G	201	5	-	5/6/23/26	0/1/1/1
9	NAG	A	302	1	-	2/6/23/26	0/1/1/1
10	CLR	A	305	-	-	3/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	201	NAG	C1-C2	2.56	1.55	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	201	NAG	C2-N2-C7	8.35	134.09	122.90
9	G	201	NAG	C1-O5-C5	7.35	122.03	112.19
9	G	201	NAG	O5-C1-C2	4.53	118.30	111.29
9	A	301	NAG	C2-N2-C7	3.24	127.24	122.90
9	A	304	NAG	C2-N2-C7	3.22	127.22	122.90

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

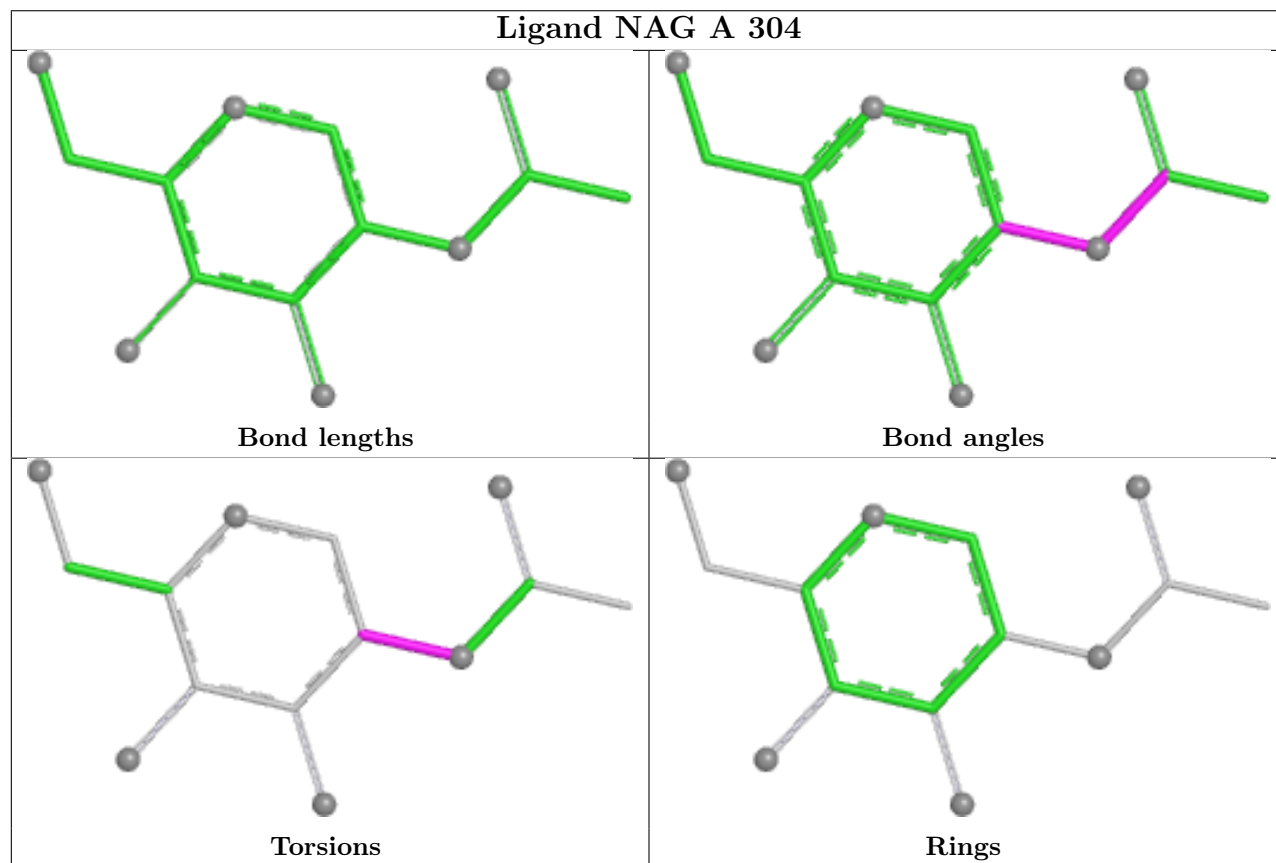
Mol	Chain	Res	Type	Atoms
10	Y	201	CLR	C21-C20-C22-C23
10	Y	201	CLR	C17-C20-C22-C23
9	G	201	NAG	C8-C7-N2-C2
9	G	201	NAG	O7-C7-N2-C2
10	Y	201	CLR	C20-C22-C23-C24

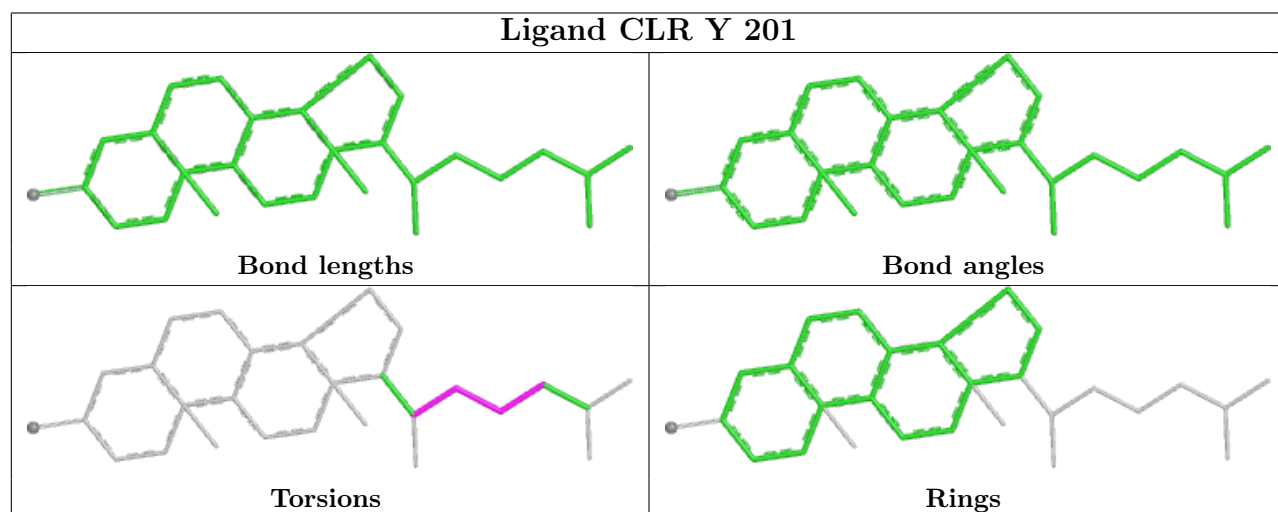
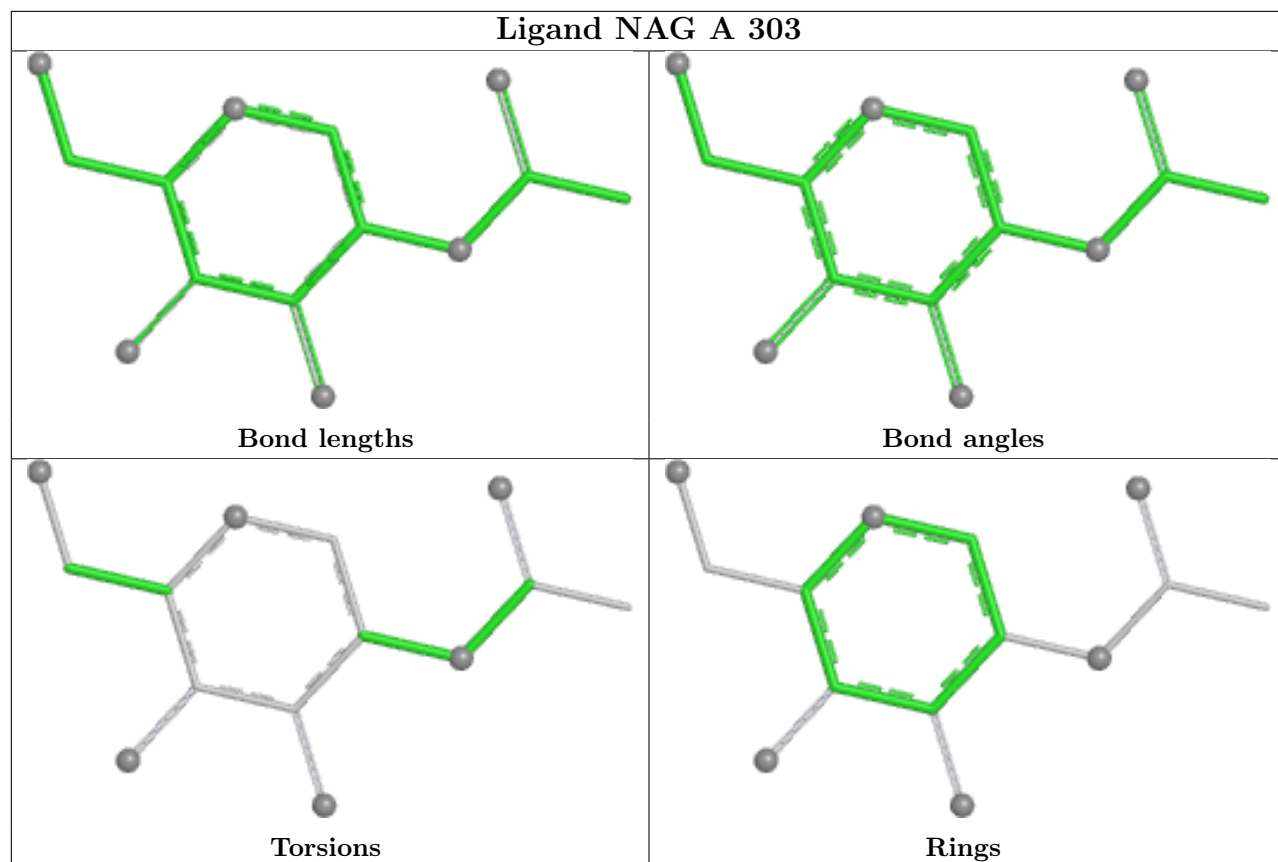
There are no ring outliers.

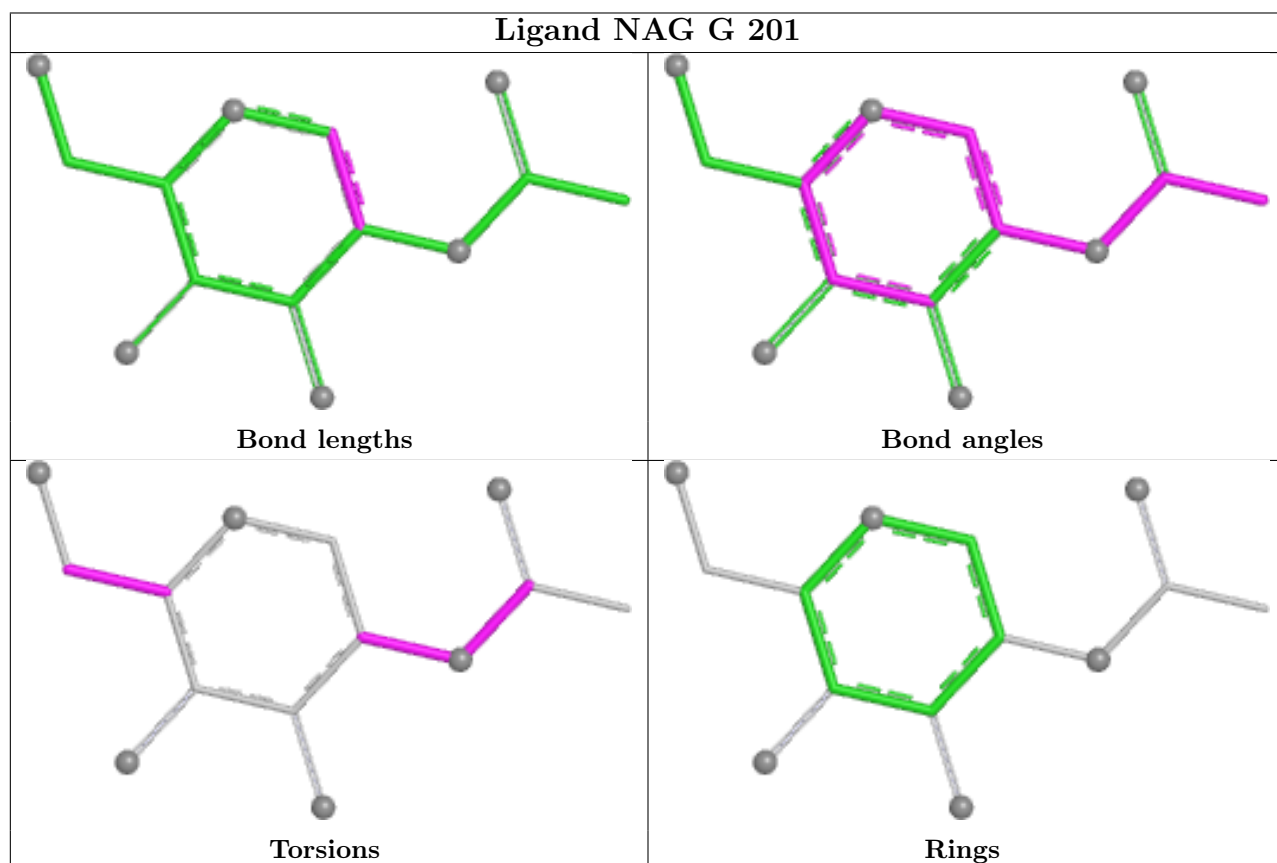
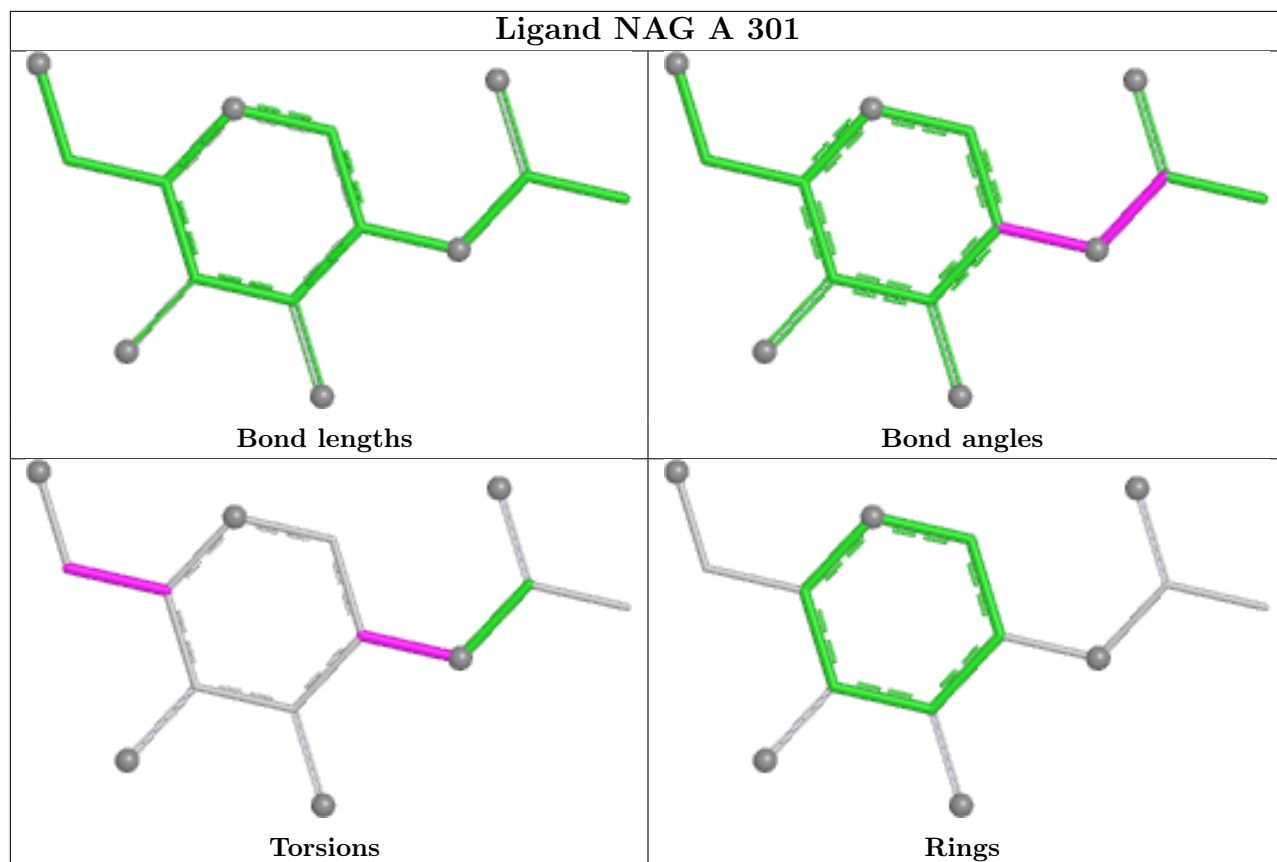
2 monomers are involved in 7 short contacts:

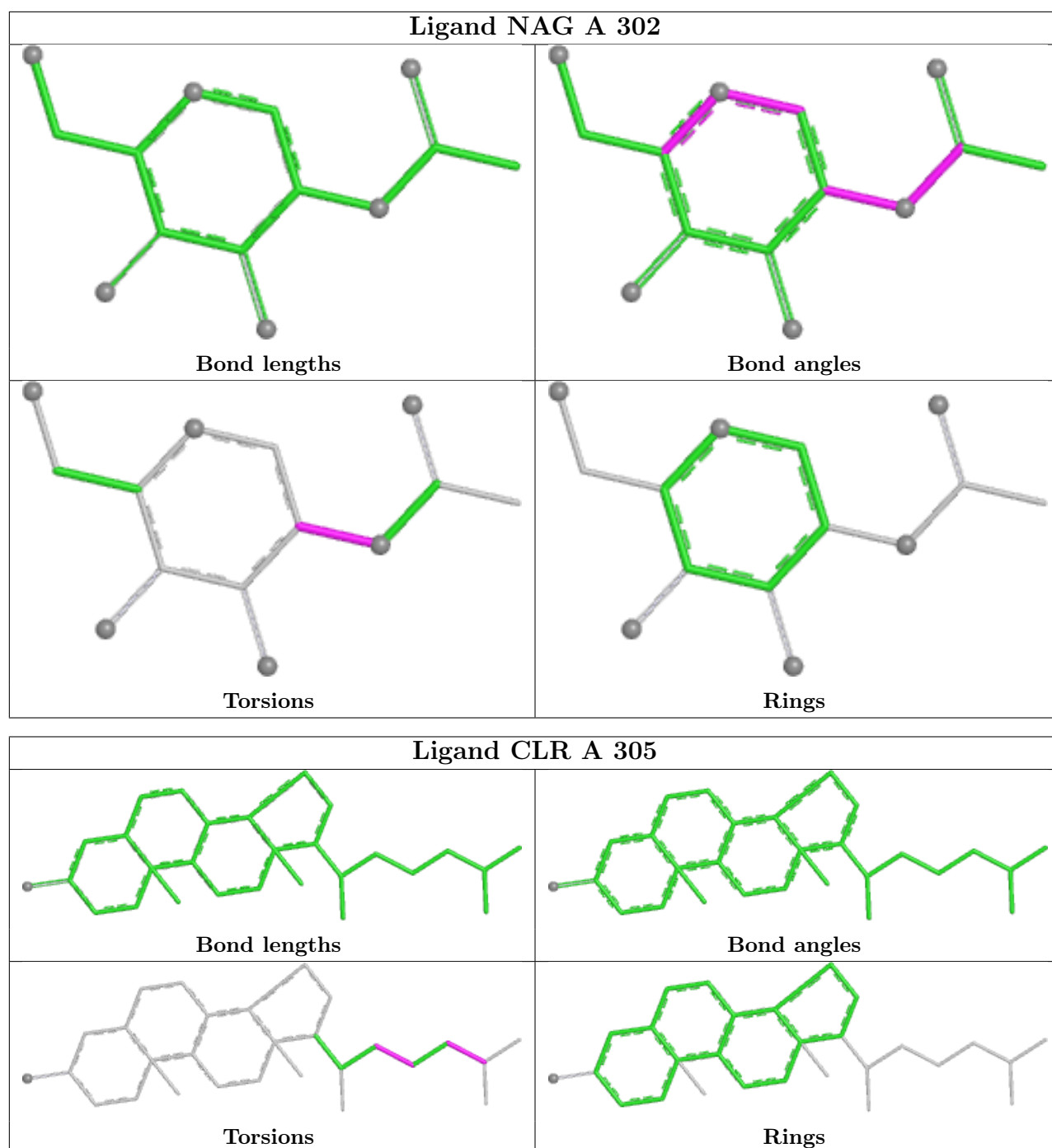
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Y	201	CLR	2	0
10	A	305	CLR	5	0

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.

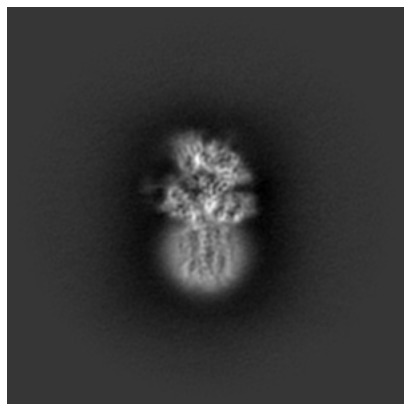
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44417. These allow visual inspection of the internal detail of the map and identification of artifacts.

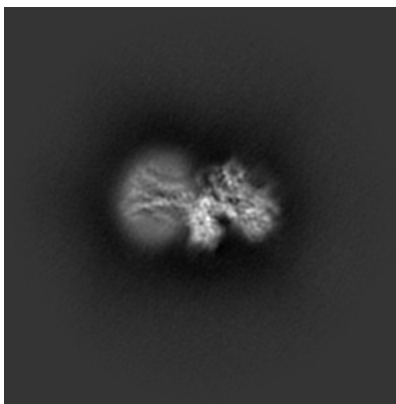
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

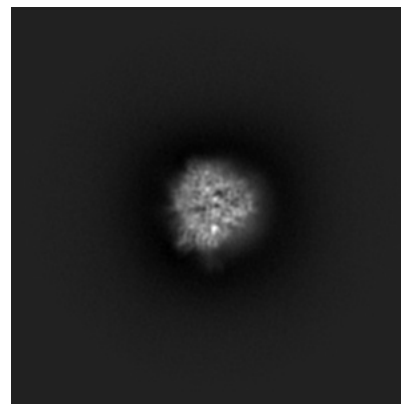
6.1.1 Primary map



X

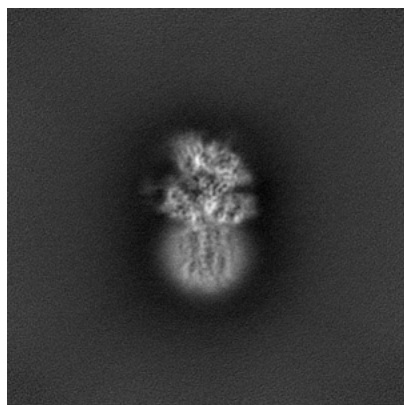


Y

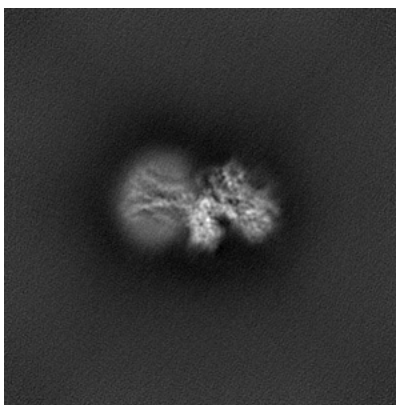


Z

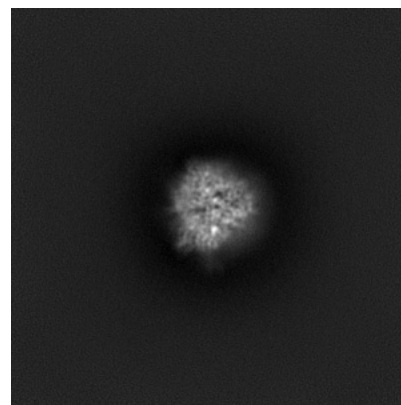
6.1.2 Raw map



X



Y

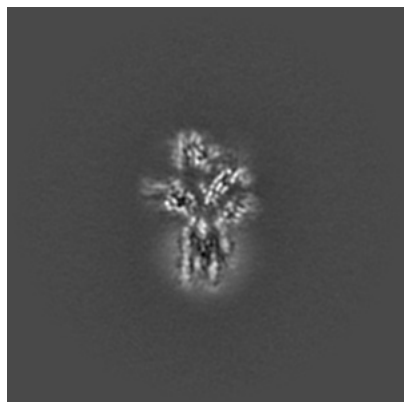


Z

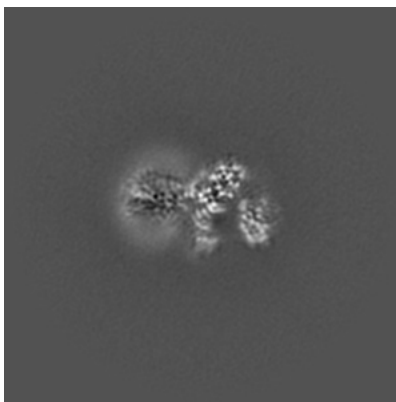
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

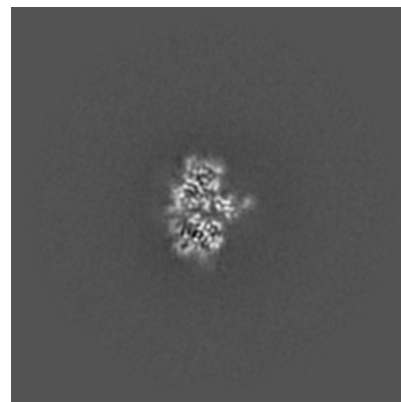
6.2.1 Primary map



X Index: 150

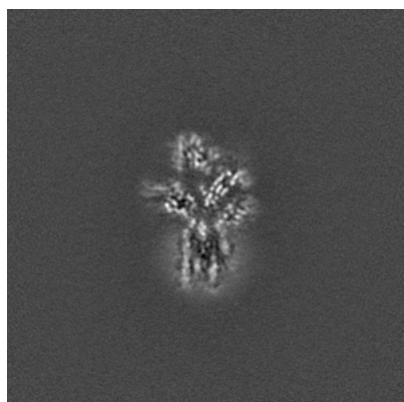


Y Index: 150

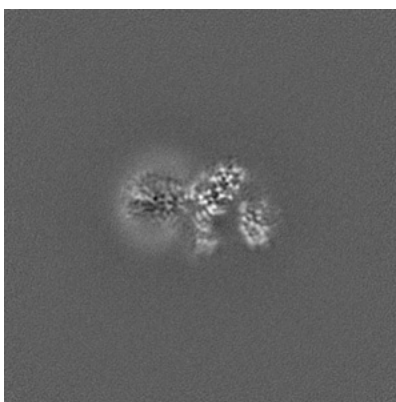


Z Index: 150

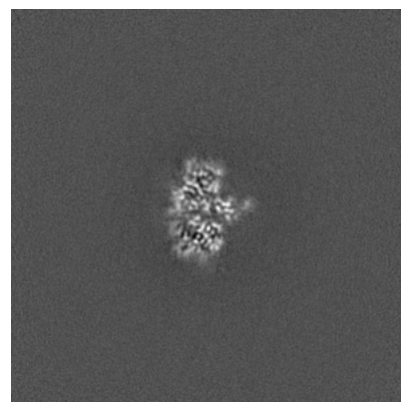
6.2.2 Raw map



X Index: 150



Y Index: 150

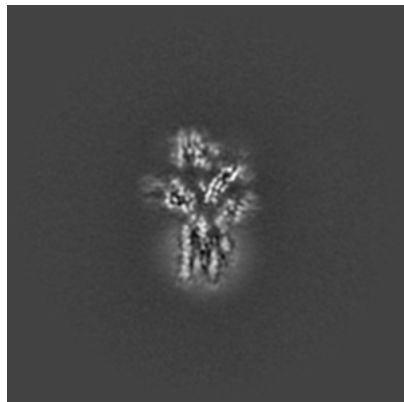


Z Index: 150

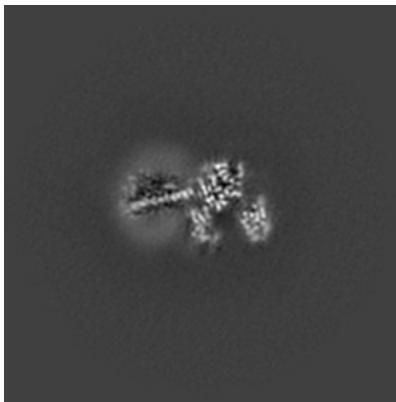
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

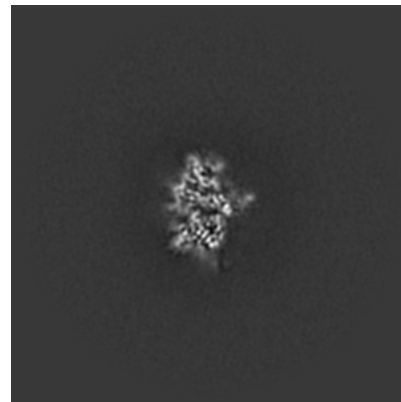
6.3.1 Primary map



X Index: 151

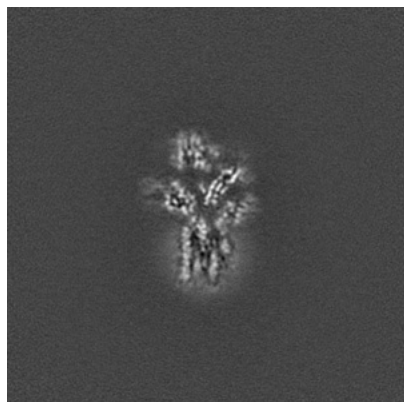


Y Index: 153

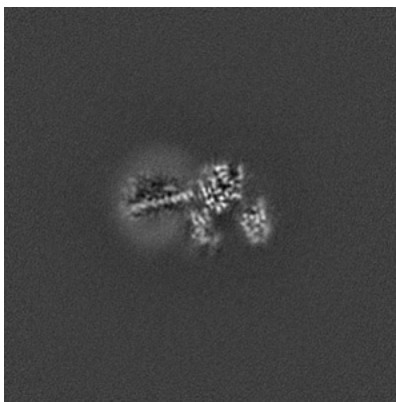


Z Index: 152

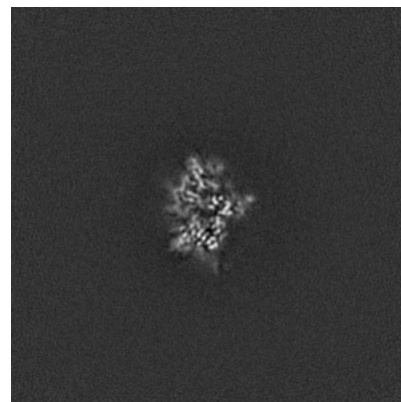
6.3.2 Raw map



X Index: 151



Y Index: 153

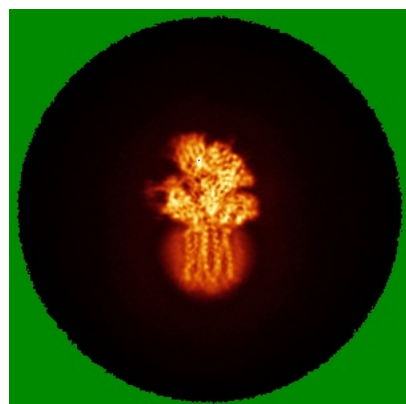


Z Index: 153

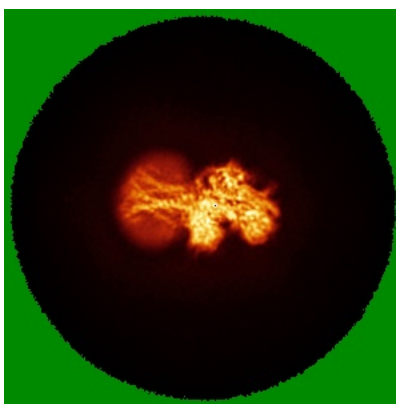
The images above show the largest variance slices of the map in three orthogonal directions.

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

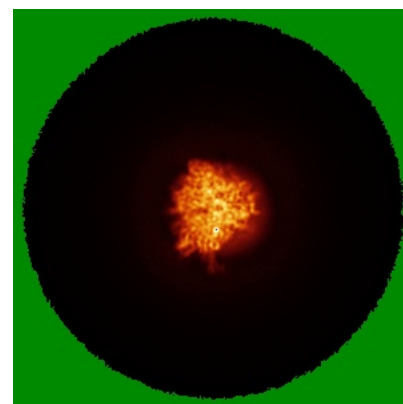
6.4.1 Primary map



X

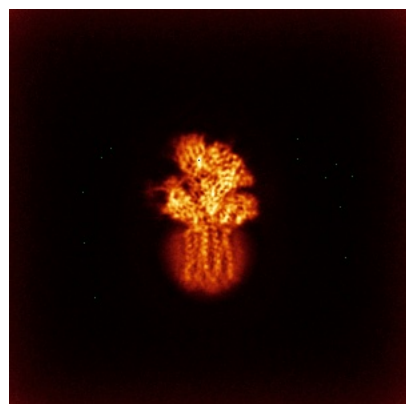


Y

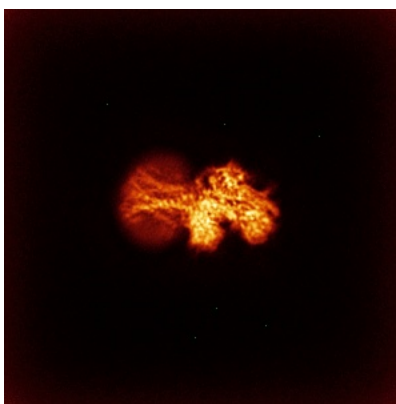


Z

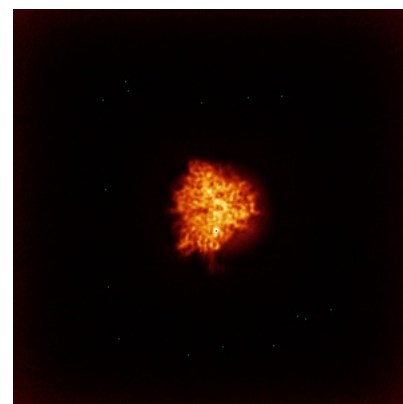
6.4.2 Raw map



X



Y



Z

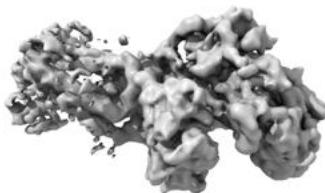
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

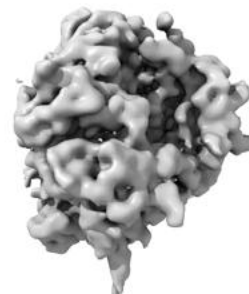
6.5.1 Primary map



X



Y



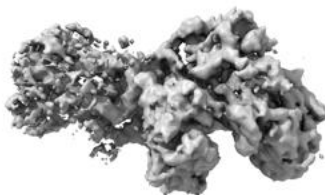
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

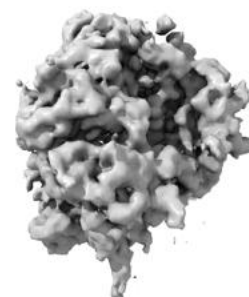
6.5.2 Raw map



X



Y



Z

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

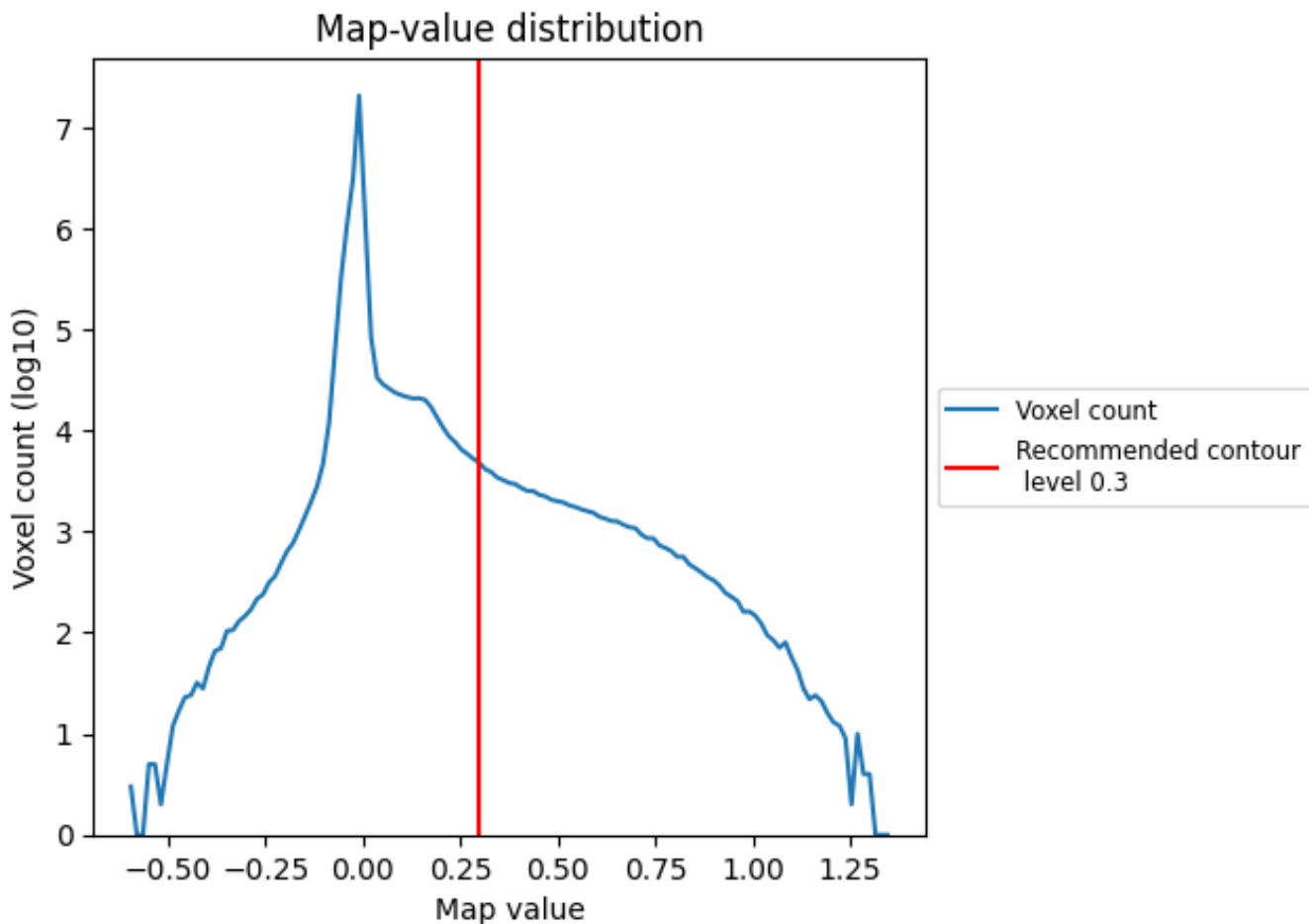
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

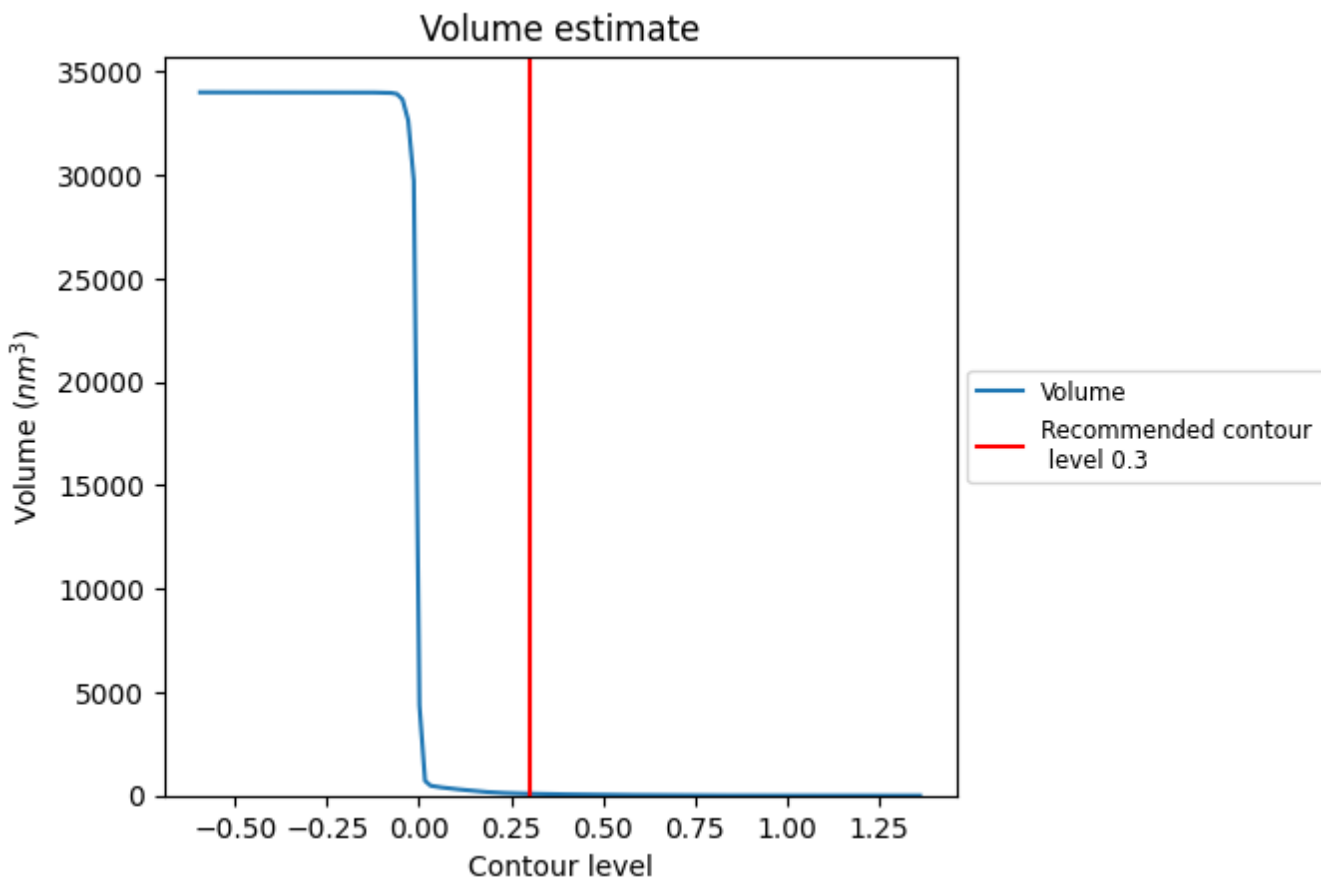
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

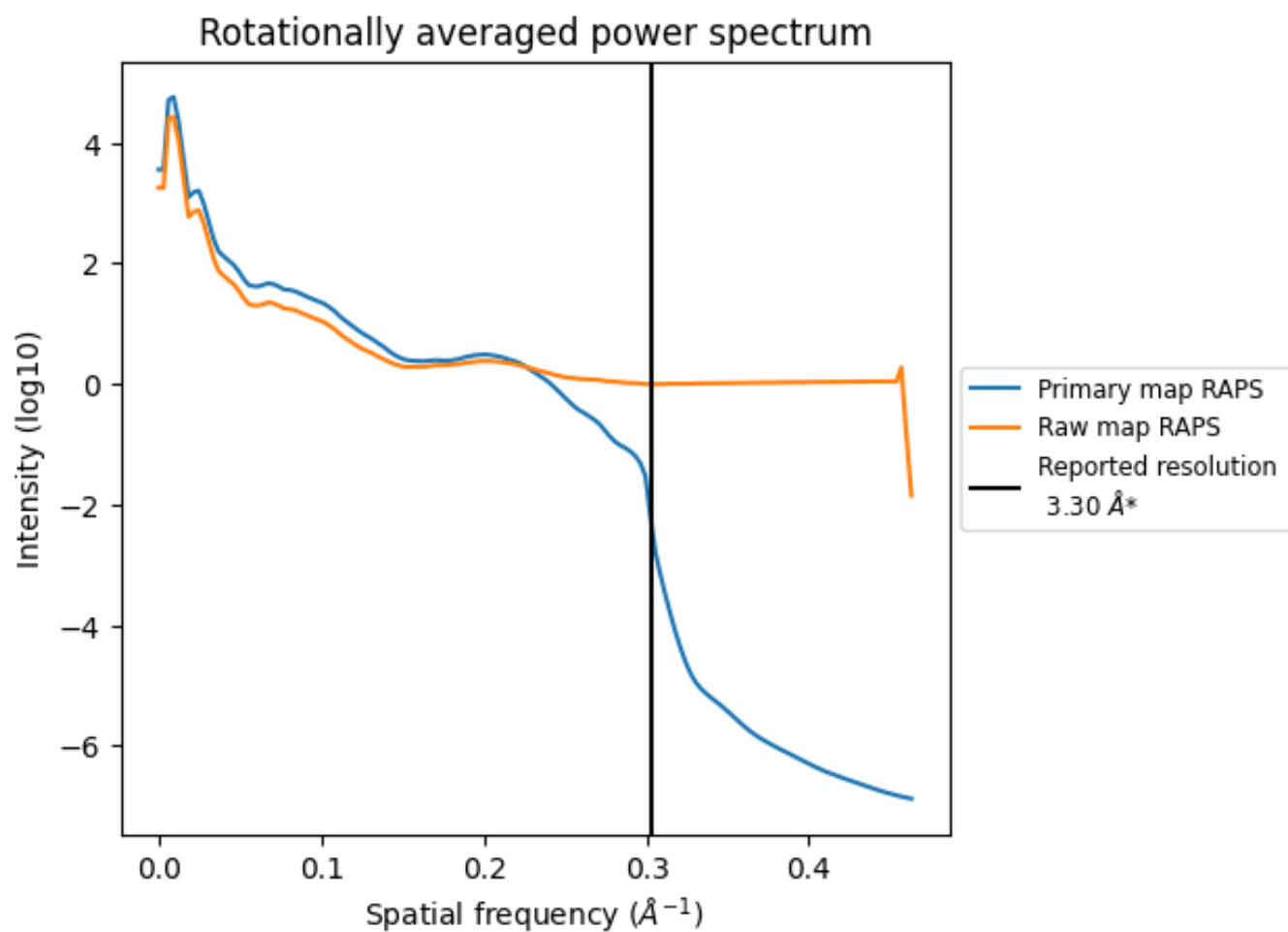
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 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

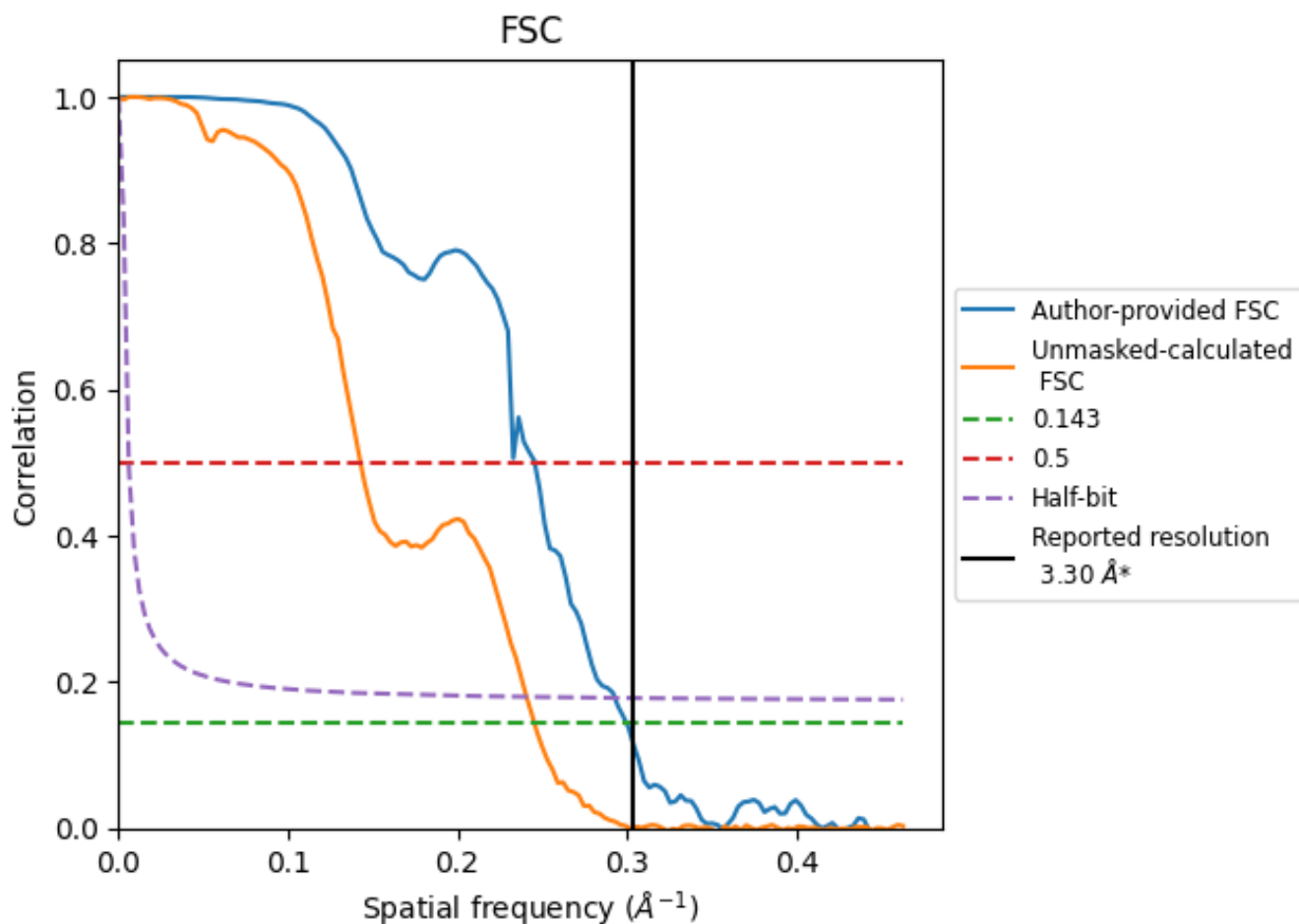


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

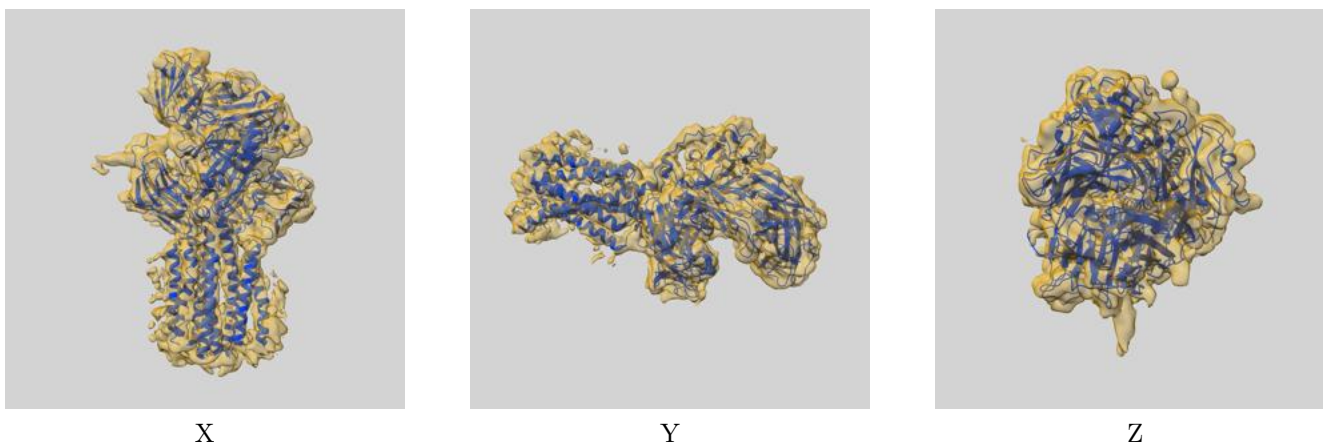
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	4.07	3.41
Unmasked-calculated*	4.07	7.00	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

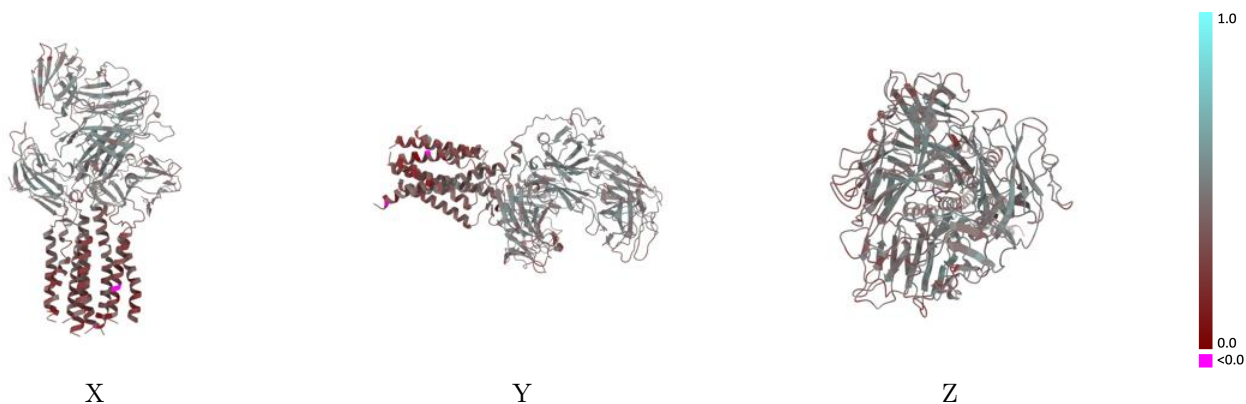
This section contains information regarding the fit between EMDB map EMD-44417 and PDB model 9BBC. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



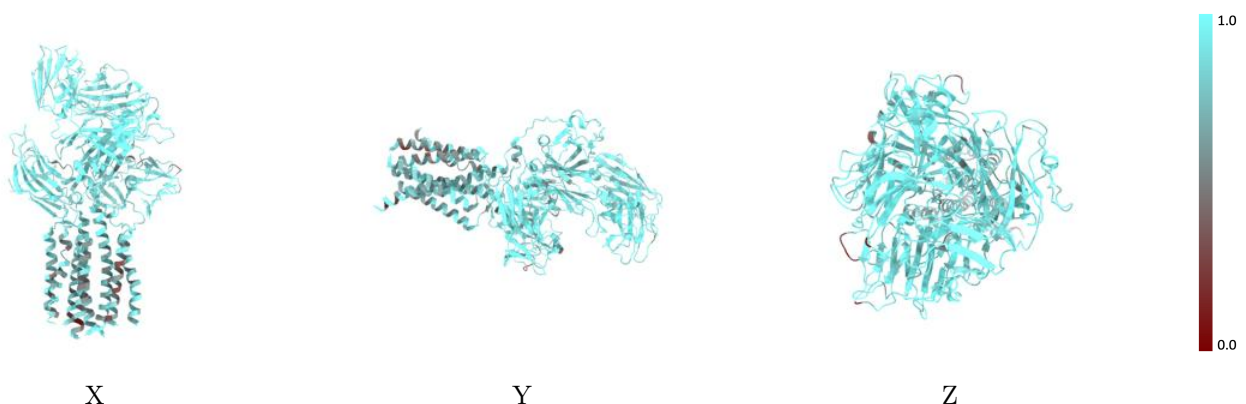
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



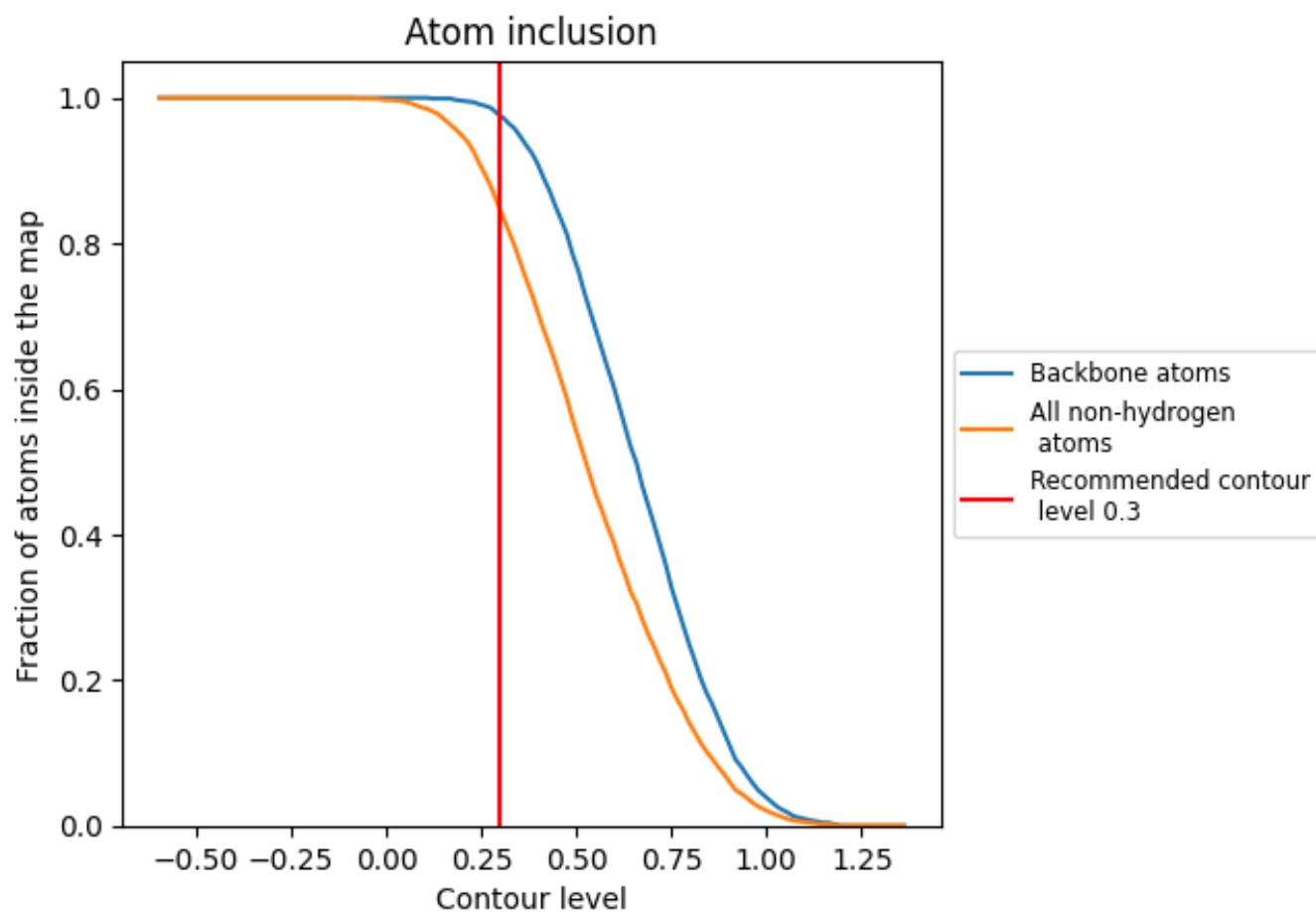
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 85% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.4110
A	 0.8620	 0.4300
B	 0.8990	 0.4470
C	 0.7690	 0.3980
D	 0.8620	 0.4270
E	 0.8570	 0.3970
F	 0.8580	 0.3900
G	 0.8080	 0.3810
H	 0.6150	 0.3190
I	 0.8210	 0.4430
O	 0.3080	 0.2510
R	 0.3570	 0.2780
X	 0.7060	 0.3220
Y	 0.5700	 0.2740

