



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:48 AM UTC

PDB ID : 8C9X / pdb_00008c9x
EMDB ID : EMD-16513
Title : human alpha7 nicotinic receptor in complex with the C4 nanobody
Authors : Prevost, M.S.; Barilone, N.; Dejean de la Batie, G.; Pons, S.; Ayme, G.; England, P.; Gielen, M.; Bontems, F.; Pehau-Arnaudet, G.; Maskos, U.; Lafaye, P.; Corringer, P.-J.
Deposited on : 2023-01-23
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

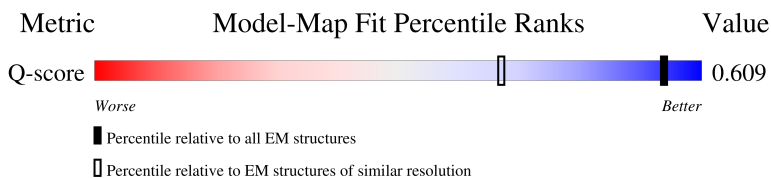
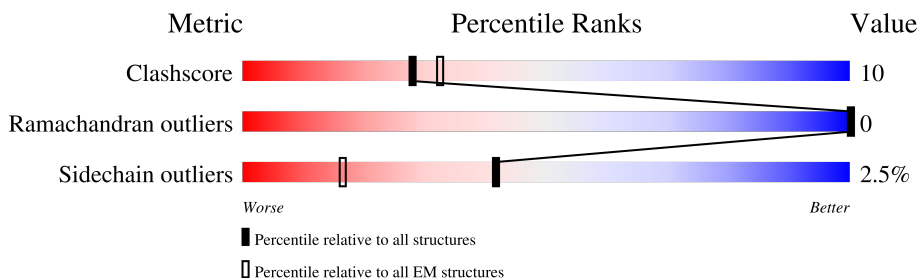
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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.



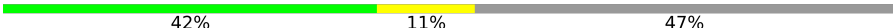
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	388	
1	B	388	
1	C	388	
1	D	388	

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Mol	Chain	Length	Quality of chain
1	E	388	
2	F	147	
2	G	147	
2	H	147	
2	I	147	
2	J	147	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13485 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 Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	207	Total	C	N	O	S	1	0
			1726	1115	287	315	9		
1	B	207	Total	C	N	O	S	1	0
			1726	1115	287	315	9		
1	C	207	Total	C	N	O	S	1	0
			1726	1115	287	315	9		
1	D	207	Total	C	N	O	S	1	0
			1726	1115	287	315	9		
1	E	207	Total	C	N	O	S	1	0
			1726	1115	287	315	9		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASP	-	linker	UNP P36544
A	326	GLY	-	linker	UNP P36544
A	327	VAL	-	linker	UNP P36544
A	376	SER	-	expression tag	UNP P36544
A	377	ALA	-	expression tag	UNP P36544
A	378	GLY	-	expression tag	UNP P36544
A	379	LEU	-	expression tag	UNP P36544
A	380	THR	-	expression tag	UNP P36544
A	381	GLU	-	expression tag	UNP P36544
A	382	THR	-	expression tag	UNP P36544
A	383	SER	-	expression tag	UNP P36544
A	384	GLN	-	expression tag	UNP P36544
A	385	VAL	-	expression tag	UNP P36544
A	386	ALA	-	expression tag	UNP P36544
A	387	PRO	-	expression tag	UNP P36544
A	388	ALA	-	expression tag	UNP P36544
B	325	ASP	-	linker	UNP P36544
B	326	GLY	-	linker	UNP P36544
B	327	VAL	-	linker	UNP P36544
B	376	SER	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	377	ALA	-	expression tag	UNP P36544
B	378	GLY	-	expression tag	UNP P36544
B	379	LEU	-	expression tag	UNP P36544
B	380	THR	-	expression tag	UNP P36544
B	381	GLU	-	expression tag	UNP P36544
B	382	THR	-	expression tag	UNP P36544
B	383	SER	-	expression tag	UNP P36544
B	384	GLN	-	expression tag	UNP P36544
B	385	VAL	-	expression tag	UNP P36544
B	386	ALA	-	expression tag	UNP P36544
B	387	PRO	-	expression tag	UNP P36544
B	388	ALA	-	expression tag	UNP P36544
C	325	ASP	-	linker	UNP P36544
C	326	GLY	-	linker	UNP P36544
C	327	VAL	-	linker	UNP P36544
C	376	SER	-	expression tag	UNP P36544
C	377	ALA	-	expression tag	UNP P36544
C	378	GLY	-	expression tag	UNP P36544
C	379	LEU	-	expression tag	UNP P36544
C	380	THR	-	expression tag	UNP P36544
C	381	GLU	-	expression tag	UNP P36544
C	382	THR	-	expression tag	UNP P36544
C	383	SER	-	expression tag	UNP P36544
C	384	GLN	-	expression tag	UNP P36544
C	385	VAL	-	expression tag	UNP P36544
C	386	ALA	-	expression tag	UNP P36544
C	387	PRO	-	expression tag	UNP P36544
C	388	ALA	-	expression tag	UNP P36544
D	325	ASP	-	linker	UNP P36544
D	326	GLY	-	linker	UNP P36544
D	327	VAL	-	linker	UNP P36544
D	376	SER	-	expression tag	UNP P36544
D	377	ALA	-	expression tag	UNP P36544
D	378	GLY	-	expression tag	UNP P36544
D	379	LEU	-	expression tag	UNP P36544
D	380	THR	-	expression tag	UNP P36544
D	381	GLU	-	expression tag	UNP P36544
D	382	THR	-	expression tag	UNP P36544
D	383	SER	-	expression tag	UNP P36544
D	384	GLN	-	expression tag	UNP P36544
D	385	VAL	-	expression tag	UNP P36544
D	386	ALA	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	387	PRO	-	expression tag	UNP P36544
D	388	ALA	-	expression tag	UNP P36544
E	325	ASP	-	linker	UNP P36544
E	326	GLY	-	linker	UNP P36544
E	327	VAL	-	linker	UNP P36544
E	376	SER	-	expression tag	UNP P36544
E	377	ALA	-	expression tag	UNP P36544
E	378	GLY	-	expression tag	UNP P36544
E	379	LEU	-	expression tag	UNP P36544
E	380	THR	-	expression tag	UNP P36544
E	381	GLU	-	expression tag	UNP P36544
E	382	THR	-	expression tag	UNP P36544
E	383	SER	-	expression tag	UNP P36544
E	384	GLN	-	expression tag	UNP P36544
E	385	VAL	-	expression tag	UNP P36544
E	386	ALA	-	expression tag	UNP P36544
E	387	PRO	-	expression tag	UNP P36544
E	388	ALA	-	expression tag	UNP P36544

- Molecule 2 is a protein called Nanobody C4.

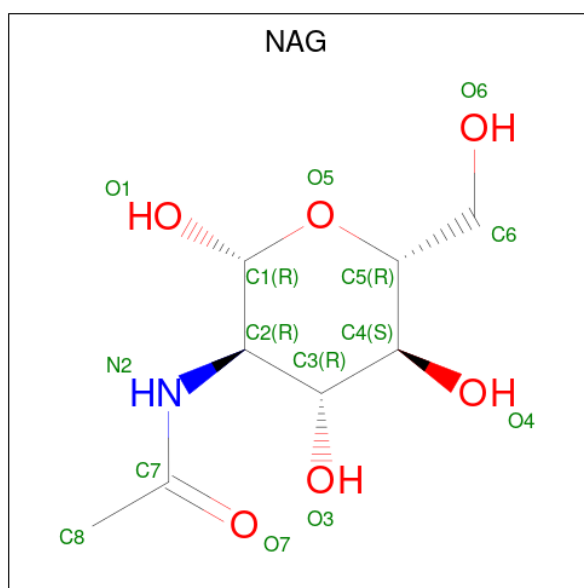
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	120	Total	C	N	O	S	0	0
			915	582	155	175	3		
2	G	120	Total	C	N	O	S	0	0
			915	582	155	175	3		
2	H	120	Total	C	N	O	S	0	0
			915	582	155	175	3		
2	I	120	Total	C	N	O	S	0	0
			915	582	155	175	3		
2	J	120	Total	C	N	O	S	0	0
			915	582	155	175	3		

- Molecule 3 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
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



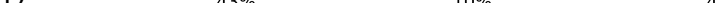
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

VAL	TRP	LEU	E1
GLU	THR	SER	F32
ALA	ARG	LEU	S33
GLY	VAL	THR	L34
VAL	ILE	VAL	L37
LYS	LEU	PHE	N40
ASP	LEU	MET	K45
PHE	ASN	LEU	N46
ALA	TRP	LEU	Q47
SER	CYS	VAL	N52
ALA	ALA	ALA	N54
GLY	TRP	GLU	L55
LEU	PHE	ILE	Q56
THR	LEU	MET	N57
GLU	ARG	PRO	I53
THR	MET	ALA	T200
SER	LYS	THR	V201
GLN	ARG	SER	R205
VAL	GLY	ASP	Q206
ALA	GLY	SER	R207
PRO	VAL	VAL	LEU
ALA	ALA	PRO	T76
	VAL	LEU	V77
	CYS	ILE	R78
	SER	ALA	
	GLU	GLN	P87
	TRP	TYR	D88
	LYS	PHE	I89
	PHE	ALA	I90
	ALA	SER	L91
	ALA	THR	Y92
	CYS	MET	N93
	CYS	ILE	S94
	VAL	VAL	A95
	VAL	LEU	D96
	ASP	VAL	E97
	ARG	GLY	
	LEU	LEU	D100
	CYS	SER	A101
	LEU	VAL	T102
	MET	VAL	
	ALA	VAL	S112
	PHE	THR	G113
	SER	VAL	H114
	VAL	ILE	
	PHE	VAL	P119
	THR	LEU	
	ILE	GLN	T122
	ILE	ALA	
	CYS	HIS	C127
	CYS	SER	
	THR	HIS	G127
	ILE	GLY	
	ILE	GLY	L132
	GLY	ASP	
	ILE	PRO	
	ILE	THR	D137
	LEU	ASP	
	MET	GLY	K144
	SER	GLY	
	ALA	LYS	I145
	PRO	MET	G152
	ASN	THR	W153
	PHE	LYS	

- Chain D:  43% 10% 47%

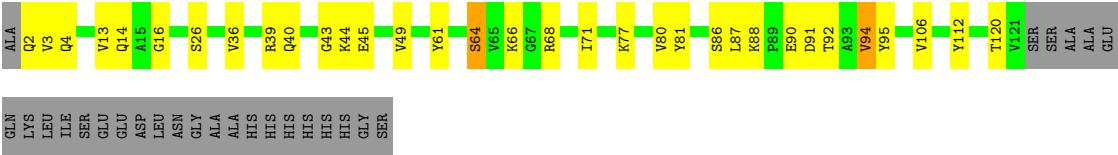
Lys	Leu	Phe	Met	Phe	D174	E1
Asp	Leu	Met	Leu	Leu	I178	F32
Ala	Asn	Leu	Leu	Leu	P179	S33
Ser	Trp	Val	Val	Val	R185	L34
Ala	Ala	Ala	Ala	Ala	F186	M40
Gly	Trp	Glu	Glu	Glu	I187	K45
Leu	Phe	Ile	Ile	Ile	E188	M46
Thr	Leu	Met	Met	Met	T200	Q47
Glu	Arg	Pro	Pro	Pro	V201	
Thr	Met	Ala	Ala	Ala	R205	I53
Ser	Lys	Thr	Thr	Thr	S206	M54
GlN	Arg	Ser	Ser	Ser	T207	L55
Val	Val	Asp	Asp	Asp	Leu	O56
Ala	Gly	Ser	Ser	Val	Tyr	M57
Ala	Val	Val	Val	Pro	Tyr	T76
Val	Val	Leu	Leu	Leu	Gly	V77
Val	Cys	Ile	Ile	Ile	Ala	R78
Asp	Ser	Ala	Ala	Gln	Leu	
Arg	Glu	Trp	Tyr	Tyr	Asn	P87
Leu	Trp	Phe	Phe	Phe	Leu	S88
Leu	Phe	Ala	Ala	Ala	Leu	I89
Leu	Ala	Ser	Ser	Ile	Ile	
Cys	Ala	Thr	Thr	Pro	Pro	Y92
Cys	Ala	Met	Met	Cys	Cys	
Val	Val	Ile	Ile	Val	Val	
Val	Val	Ile	Ile	Val	Leu	A95
Asp	Val	Val	Val	Ile	Ile	D96
Arg	Asp	Gly	Gly	Val	Ser	E97
Leu	Arg	Leu	Leu	Ala	Ala	
Cys	Leu	Ser	Ser	Ala	D100	A100
Leu	Leu	Val	Val	Ala	Ala	T102
Met	Met	Val	Val	Leu	Leu	
Ala	Ala	Val	Val	Leu	Val	H114
Phe	Phe	Thr	Thr	Val	Val	
Val	Val	Val	Val	Phe	Phe	
Val	Val	Ile	Ile	Ile	Leu	Y117
Phe	Val	Val	Val	Val	Leu	L118
Thr	Thr	Leu	Leu	Pro	Pro	P119
Ile	Ile	Gln	Gln	Ala	Ala	
Ile	Ile	Tyr	Tyr	Asp	Asp	I122
Cys	Cys	His	His	Ser	Ser	C127
Ile	Ile	His	His	Gly	Gly	
Gly	Gly	Asp	Asp	Lys	Lys	R132
Ile	Ile	Pro	Pro	Ile	Ile	
Leu	Leu	Asp	Asp	Ser	Ser	D137
Met	Met	Gly	Gly	Leu	Leu	
Ser	Ala	Lys	Lys	Ile	Ile	K144
Pro	Pro	Met	Met	Thr	Thr	
Asn	Asn	Pro	Pro	Val	Val	G152
Phe	Phe	Lys	Lys	Leu	Leu	W153
Val	Val	Trp	Trp	Leu	Leu	S154
Glu	Glu	Thr	Thr	Ser	Ser	
Ala	Ala	Arg	Arg	Leu	Leu	Q160
Ser	Ser	Ile	Ile	Val	Val	
Val	Val	Thr	Thr	Val	Val	N170

- Chain E: 42% 11% 47%

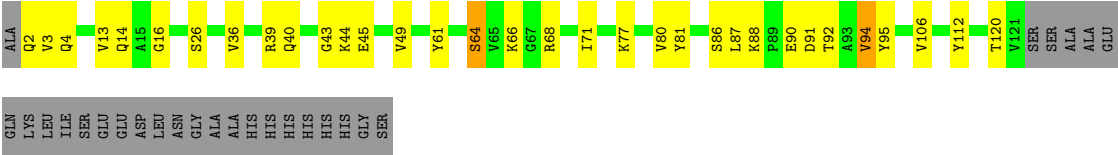
[illegible]

ALA
VAL
SER
LYS
ASP
PHE
ALA
SER
GLY
LEU
THR
GLU
THR
GLN
SER
VAL
ALA
PRO
ALA

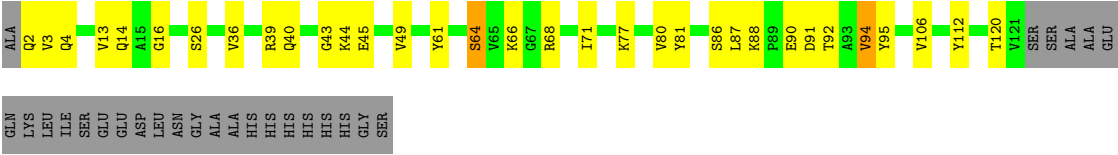
● Molecule 2: Nanobody C4



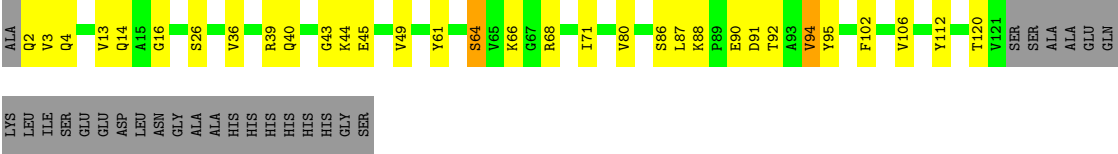
● Molecule 2: Nanobody C4



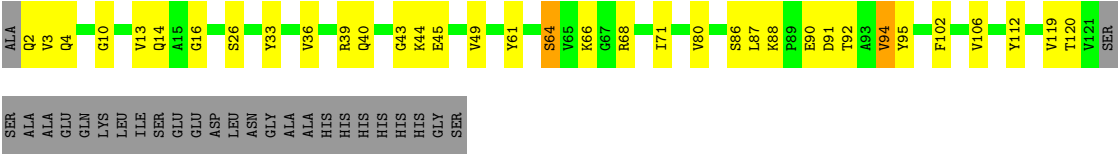
● Molecule 2: Nanobody C4



● Molecule 2: Nanobody C4



● Molecule 2: Nanobody C4



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

Chain P:  50% 50%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	104409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0049	Depositor
Map size (Å)	292.4, 292.4, 292.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/1785	0.33	0/2430
1	B	0.12	0/1785	0.33	0/2430
1	C	0.12	0/1785	0.33	0/2430
1	D	0.12	0/1785	0.33	0/2430
1	E	0.12	0/1785	0.33	0/2430
2	F	0.15	0/937	0.41	0/1270
2	G	0.15	0/937	0.41	0/1270
2	H	0.15	0/937	0.41	0/1270
2	I	0.15	0/937	0.41	0/1270
2	J	0.15	0/937	0.41	0/1270
All	All	0.13	0/13610	0.36	0/18500

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	1646	26	0
1	B	1726	0	1646	29	0
1	C	1726	0	1646	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1726	0	1646	24	0
1	E	1726	0	1646	26	0
2	F	915	0	873	25	0
2	G	915	0	873	26	0
2	H	915	0	873	25	0
2	I	915	0	873	25	0
2	J	915	0	873	27	0
3	P	28	0	25	3	0
3	Q	28	0	25	3	0
3	R	28	0	25	4	0
3	S	28	0	25	2	0
3	T	28	0	25	4	0
4	A	28	0	26	1	0
4	B	28	0	26	1	0
4	C	28	0	26	1	0
4	D	28	0	26	1	0
4	E	28	0	26	1	0
All	All	13485	0	12850	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 254 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:E:34:LEU:HD13	1:E:53:ILE:HG12	1.71	0.73
1:D:34:LEU:HD13	1:D:53:ILE:HG12	1.71	0.73
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.24	0.71
2:I:68:ARG:NH2	2:I:91:ASP:OD2	2.24	0.71
1:B:34:LEU:HD13	1:B:53:ILE:HG12	1.71	0.71

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	206/388 (53%)	198 (96%)	8 (4%)	0	100	100
1	B	206/388 (53%)	198 (96%)	8 (4%)	0	100	100
1	C	206/388 (53%)	198 (96%)	8 (4%)	0	100	100
1	D	206/388 (53%)	198 (96%)	8 (4%)	0	100	100
1	E	206/388 (53%)	198 (96%)	8 (4%)	0	100	100
2	F	118/147 (80%)	116 (98%)	2 (2%)	0	100	100
2	G	118/147 (80%)	116 (98%)	2 (2%)	0	100	100
2	H	118/147 (80%)	116 (98%)	2 (2%)	0	100	100
2	I	118/147 (80%)	116 (98%)	2 (2%)	0	100	100
2	J	118/147 (80%)	116 (98%)	2 (2%)	0	100	100
All	All	1620/2675 (61%)	1570 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/346 (56%)	190 (99%)	2 (1%)	68	82
1	B	192/346 (56%)	190 (99%)	2 (1%)	68	82
1	C	192/346 (56%)	190 (99%)	2 (1%)	68	82
1	D	192/346 (56%)	190 (99%)	2 (1%)	68	82
1	E	192/346 (56%)	190 (99%)	2 (1%)	68	82
2	F	92/112 (82%)	87 (95%)	5 (5%)	20	29
2	G	92/112 (82%)	87 (95%)	5 (5%)	20	29
2	H	92/112 (82%)	87 (95%)	5 (5%)	20	29
2	I	92/112 (82%)	87 (95%)	5 (5%)	20	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	92/112 (82%)	87 (95%)	5 (5%)	20	29
All	All	1420/2290 (62%)	1385 (98%)	35 (2%)	42	60

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	94	VAL
2	I	106	VAL
2	J	80	VAL
2	F	80	VAL
2	F	64	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	15	ASN
2	F	2	GLN
2	I	85	ASN
1	E	65	GLN
2	F	85	ASN

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](#)

10 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
3	NAG	P	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.85	0
3	NAG	P	2	3	14,14,15	0.53	0	17,19,21	0.56	0
3	NAG	Q	1	3,1	14,14,15	0.61	1 (7%)	17,19,21	0.86	0
3	NAG	Q	2	3	14,14,15	0.53	0	17,19,21	0.57	0
3	NAG	R	1	3,1	14,14,15	0.62	1 (7%)	17,19,21	0.86	0
3	NAG	R	2	3	14,14,15	0.52	0	17,19,21	0.56	0
3	NAG	S	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.86	0
3	NAG	S	2	3	14,14,15	0.53	0	17,19,21	0.56	0
3	NAG	T	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.86	0
3	NAG	T	2	3	14,14,15	0.53	0	17,19,21	0.57	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	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	4/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	4/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-2.17	1.40	1.43
3	P	1	NAG	O5-C1	-2.16	1.40	1.43
3	S	1	NAG	O5-C1	-2.15	1.40	1.43
3	R	1	NAG	O5-C1	-2.09	1.40	1.43
3	Q	1	NAG	O5-C1	-2.07	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

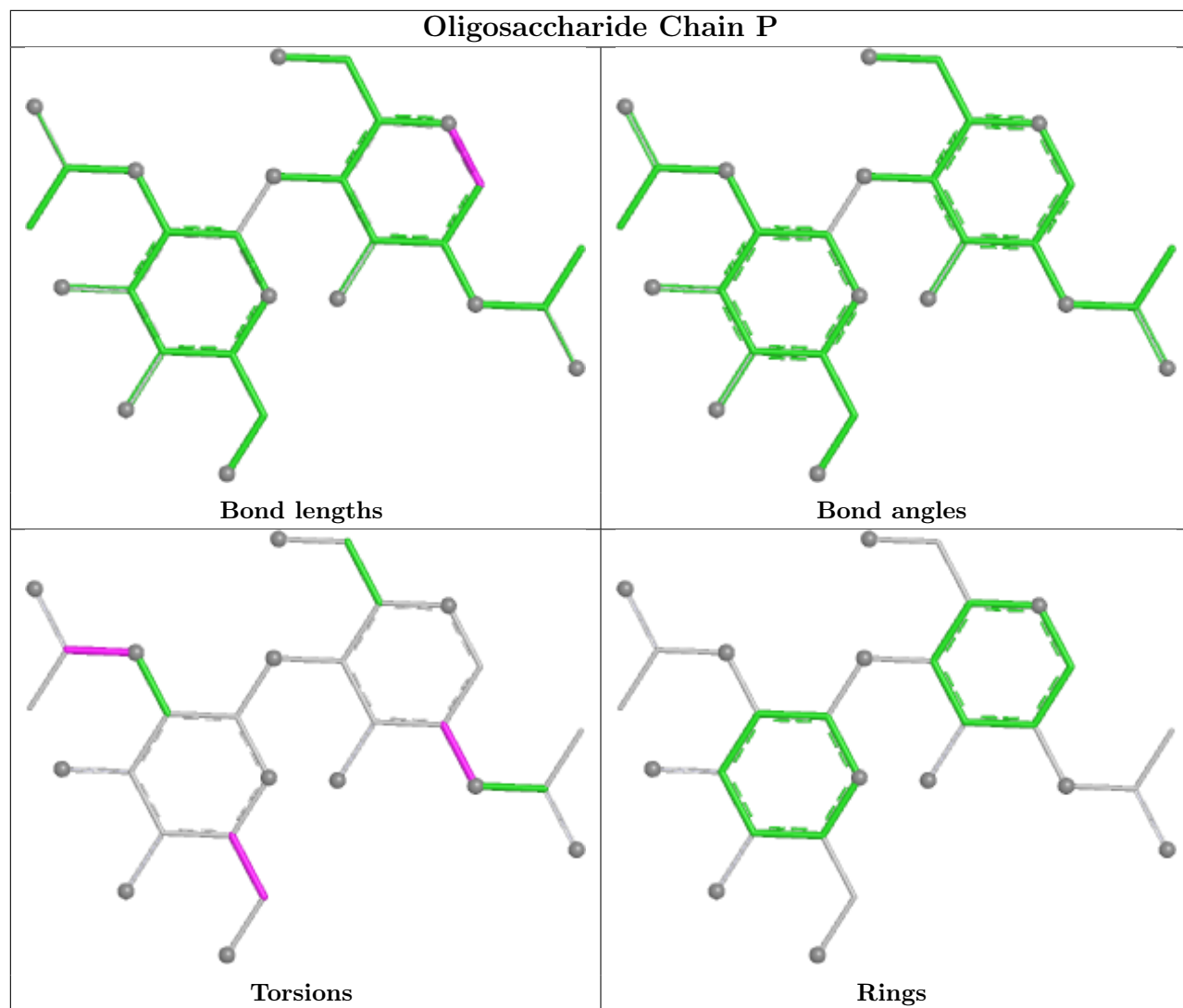
Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2

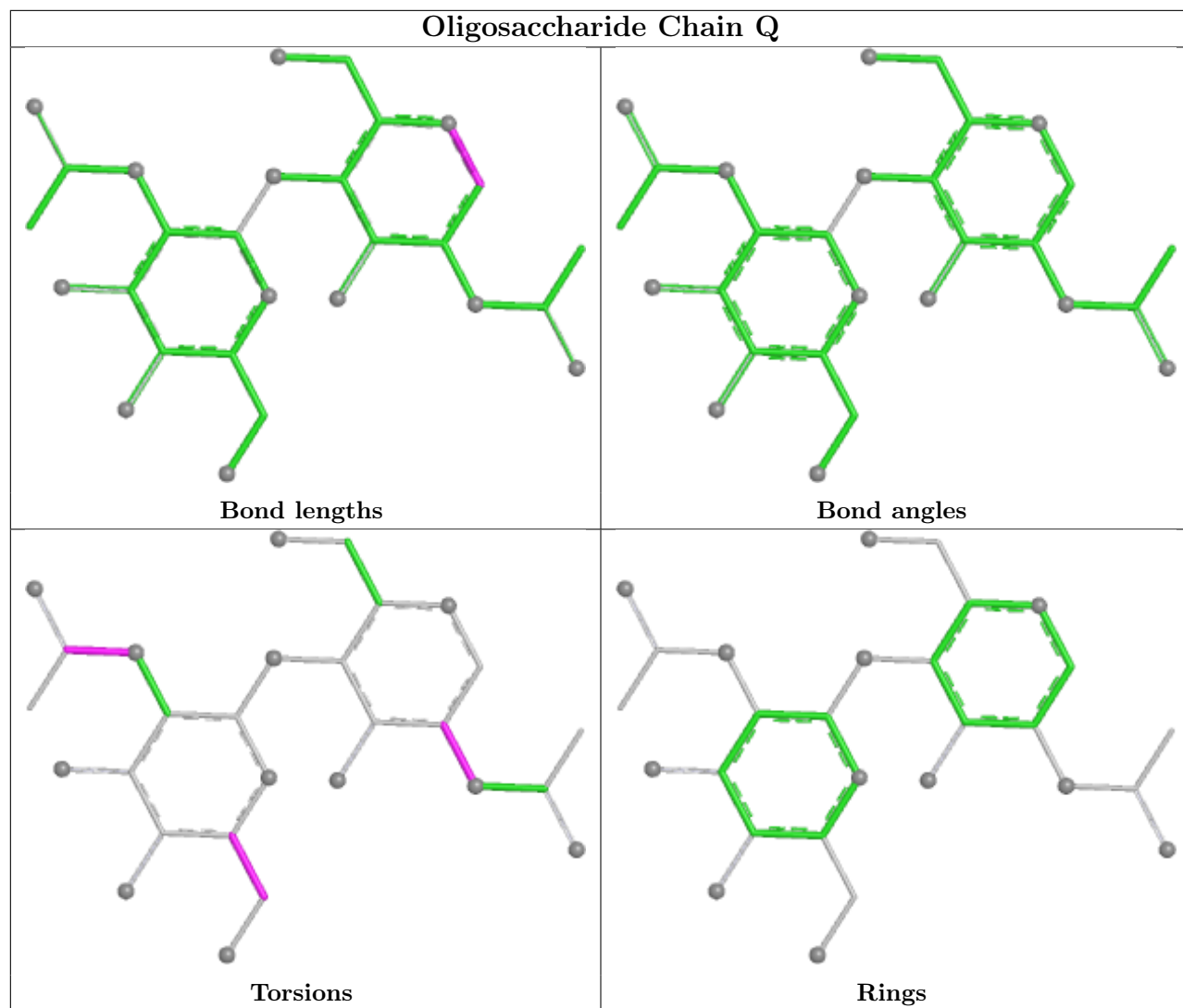
There are no ring outliers.

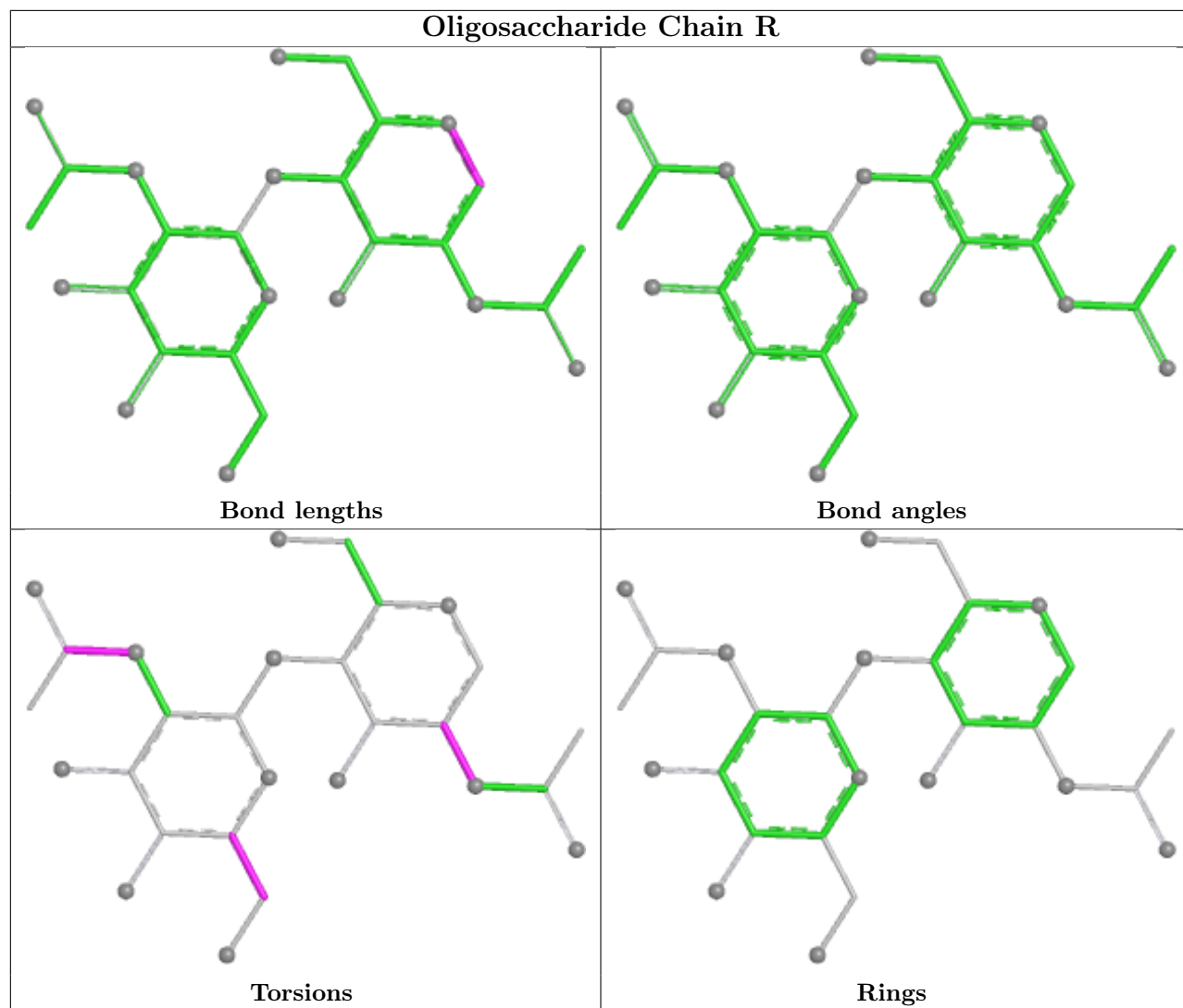
10 monomers are involved in 16 short contacts:

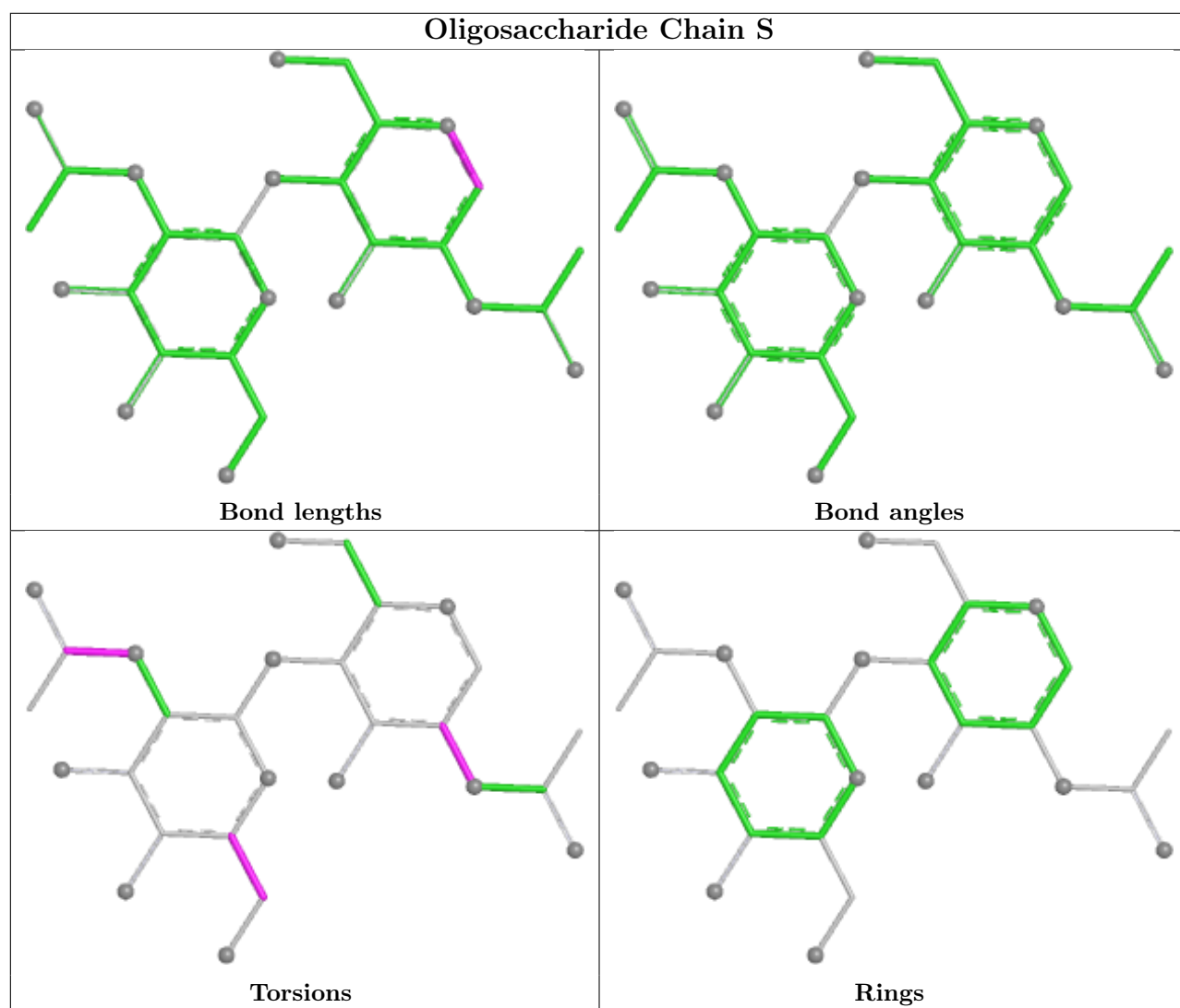
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	4	0
3	P	2	NAG	1	0
3	Q	2	NAG	1	0
3	P	1	NAG	3	0
3	T	1	NAG	4	0
3	T	2	NAG	2	0
3	S	1	NAG	2	0
3	R	2	NAG	2	0
3	Q	1	NAG	3	0
3	S	2	NAG	1	0

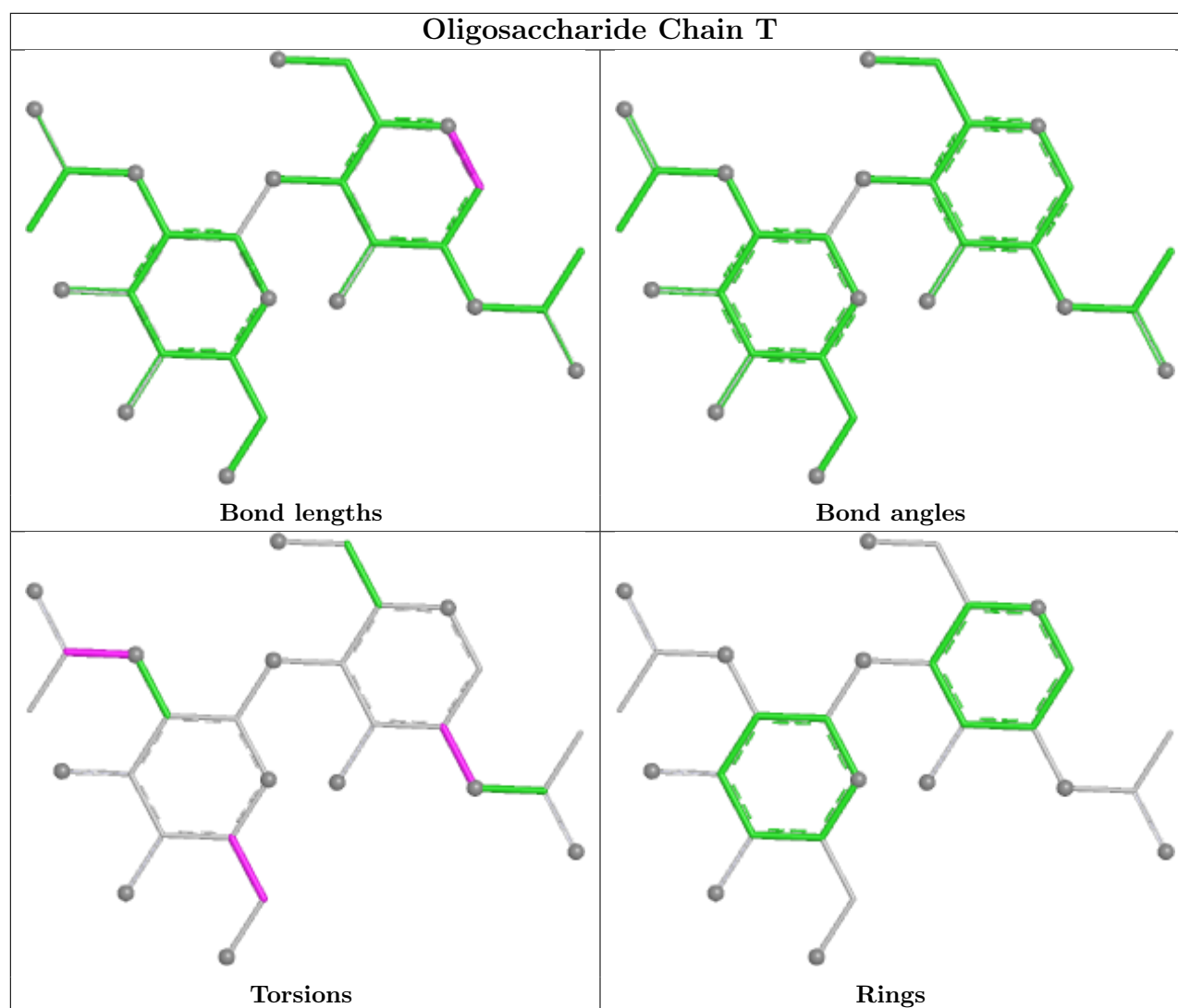
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	NAG	D	401	1	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
4	NAG	B	401	1	14,14,15	0.45	0	17,19,21	1.36	2 (11%)
4	NAG	A	401	1	14,14,15	0.40	0	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	402	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	D	402	1	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	C	402	1	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	B	402	1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	A	402	1	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	E	401	1	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
4	NAG	C	401	1	14,14,15	0.46	0	17,19,21	1.36	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	401	1	-	6/6/23/26	0/1/1/1
4	NAG	B	401	1	-	6/6/23/26	0/1/1/1
4	NAG	A	401	1	-	6/6/23/26	0/1/1/1
4	NAG	E	402	1	-	2/6/23/26	0/1/1/1
4	NAG	D	402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	402	1	-	2/6/23/26	0/1/1/1
4	NAG	E	401	1	-	6/6/23/26	0/1/1/1
4	NAG	C	401	1	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	NAG	C2-N2-C7	4.66	129.14	122.90
4	B	401	NAG	C2-N2-C7	4.65	129.13	122.90
4	A	401	NAG	C2-N2-C7	4.64	129.12	122.90
4	E	401	NAG	C2-N2-C7	4.61	129.08	122.90
4	D	401	NAG	C2-N2-C7	4.60	129.06	122.90

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

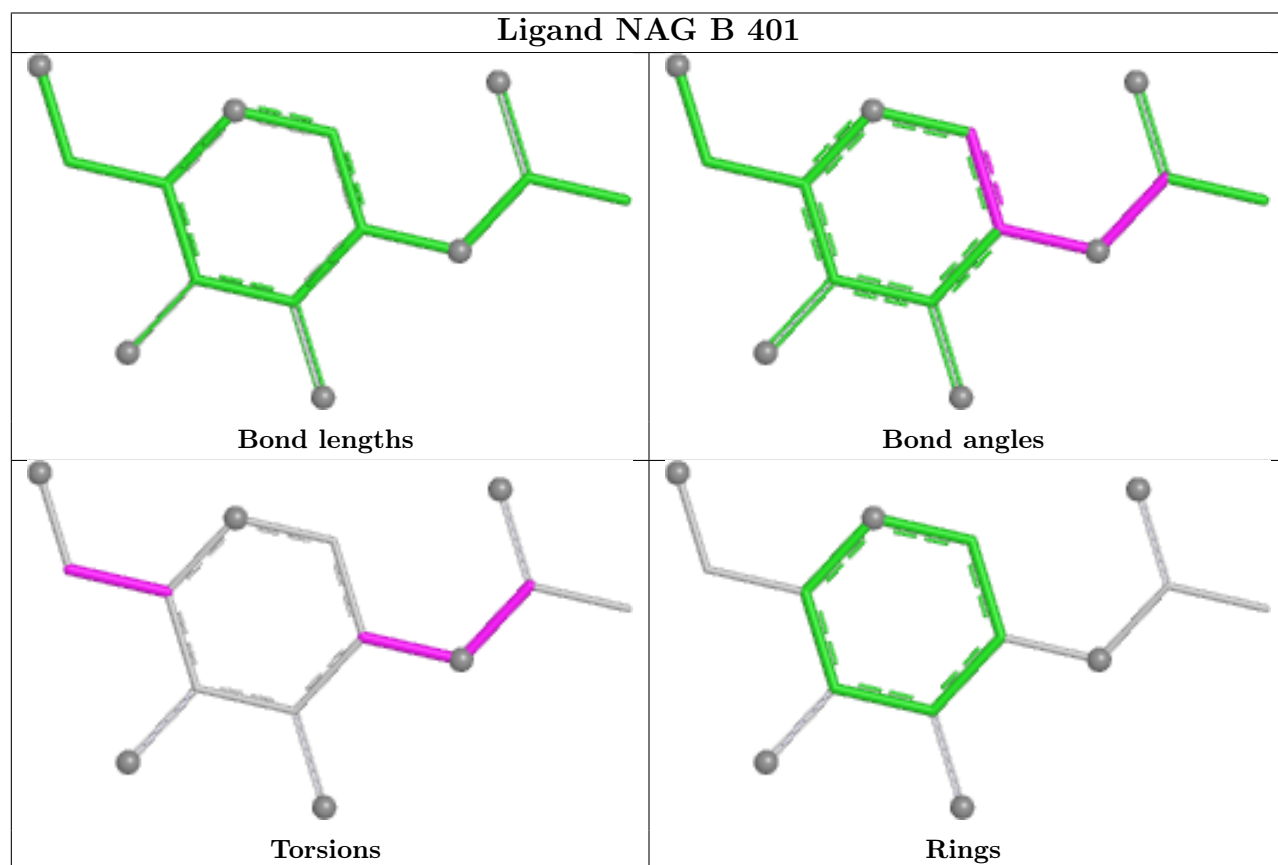
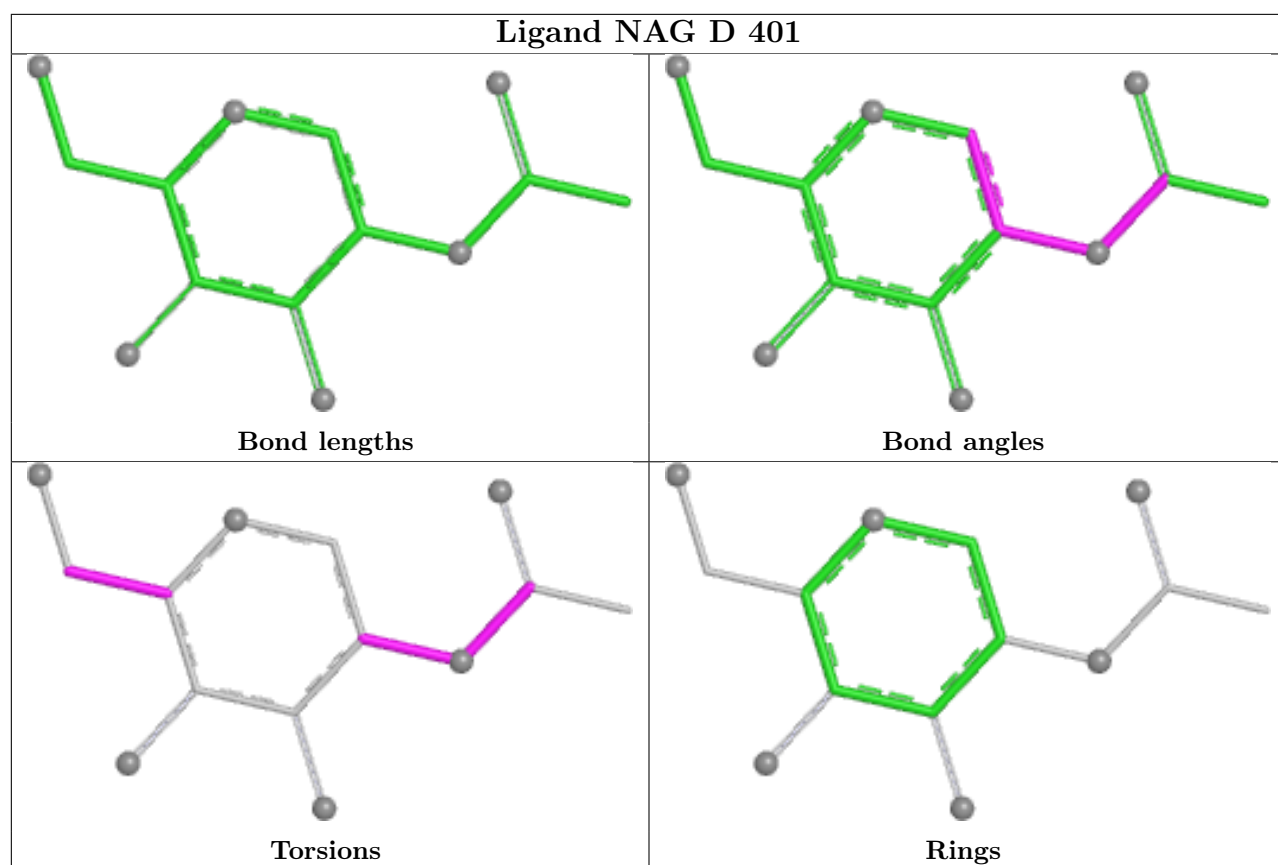
Mol	Chain	Res	Type	Atoms
4	A	402	NAG	O5-C5-C6-O6
4	B	402	NAG	O5-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	D	402	NAG	O5-C5-C6-O6
4	E	402	NAG	O5-C5-C6-O6

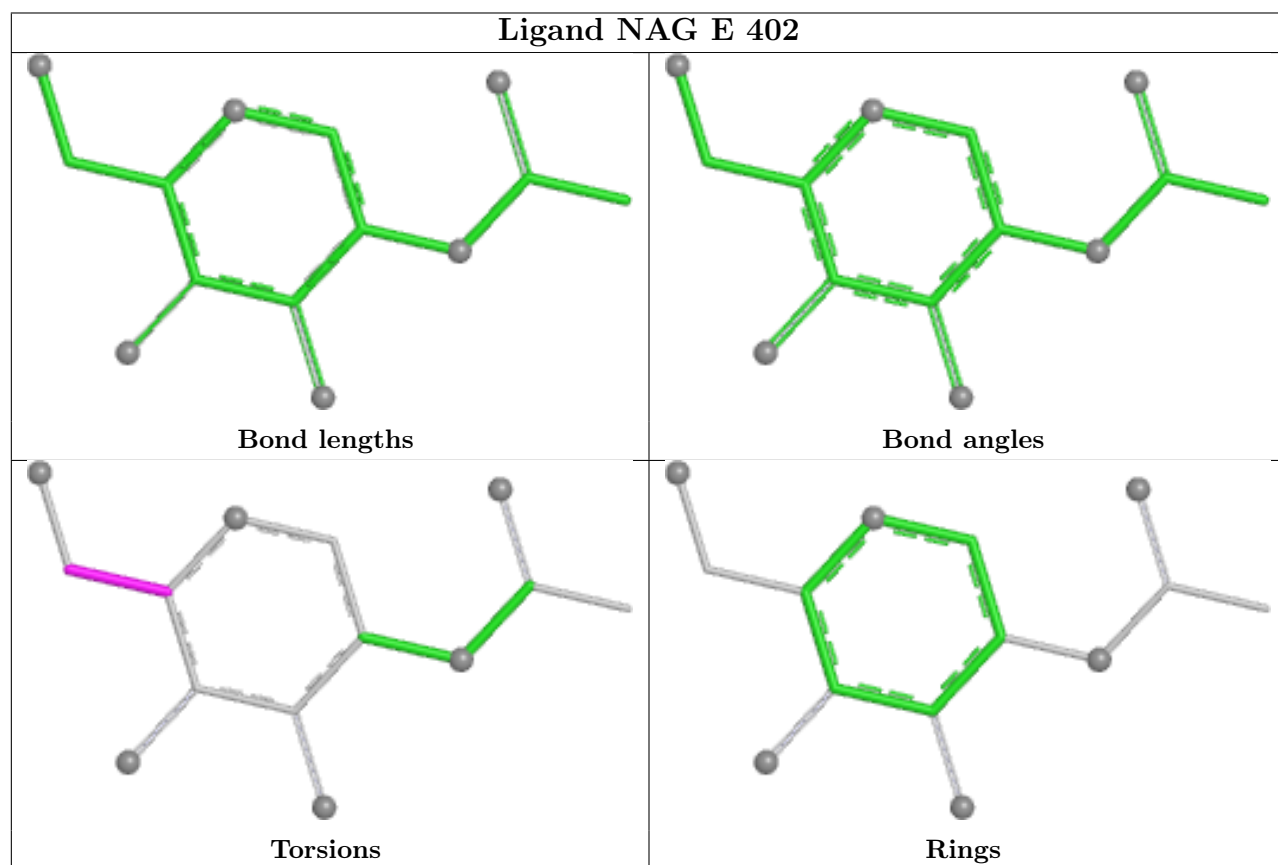
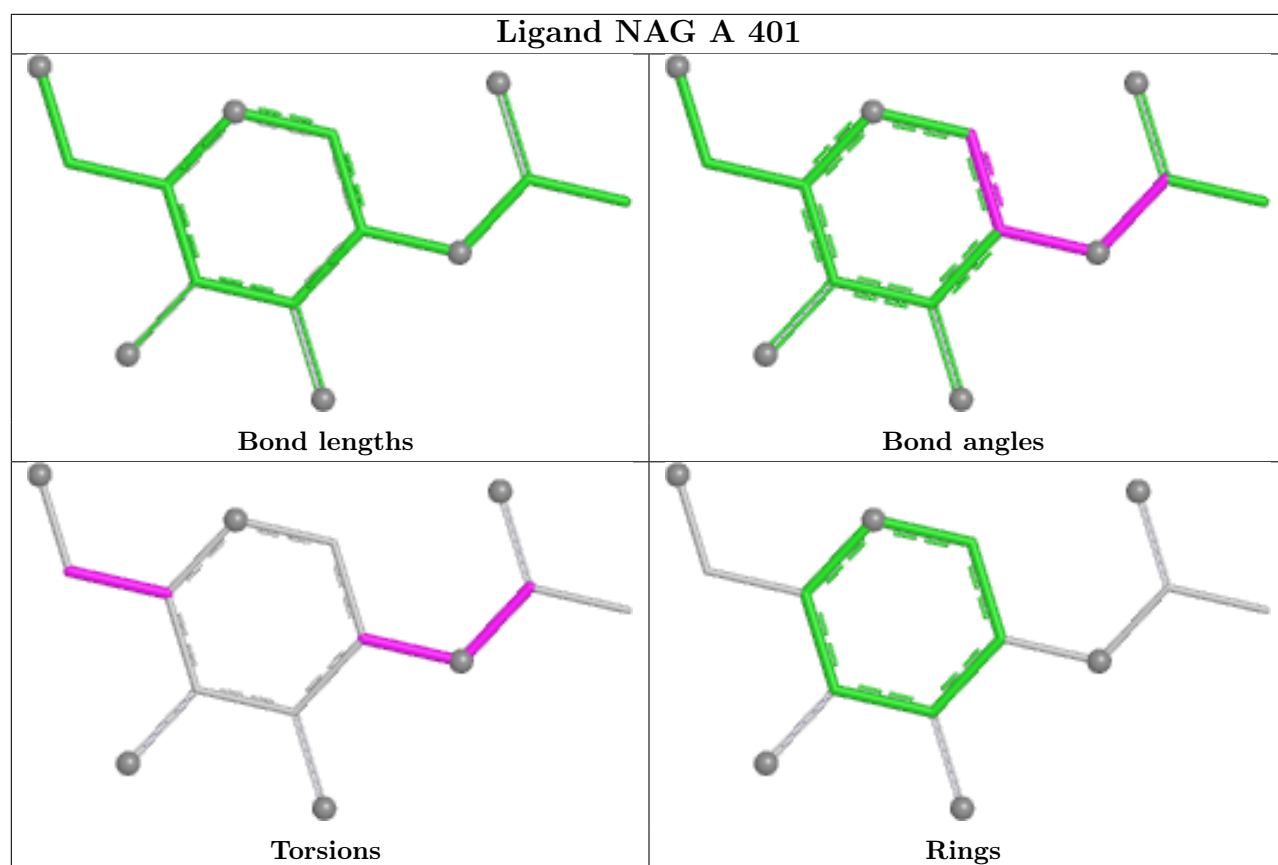
There are no ring outliers.

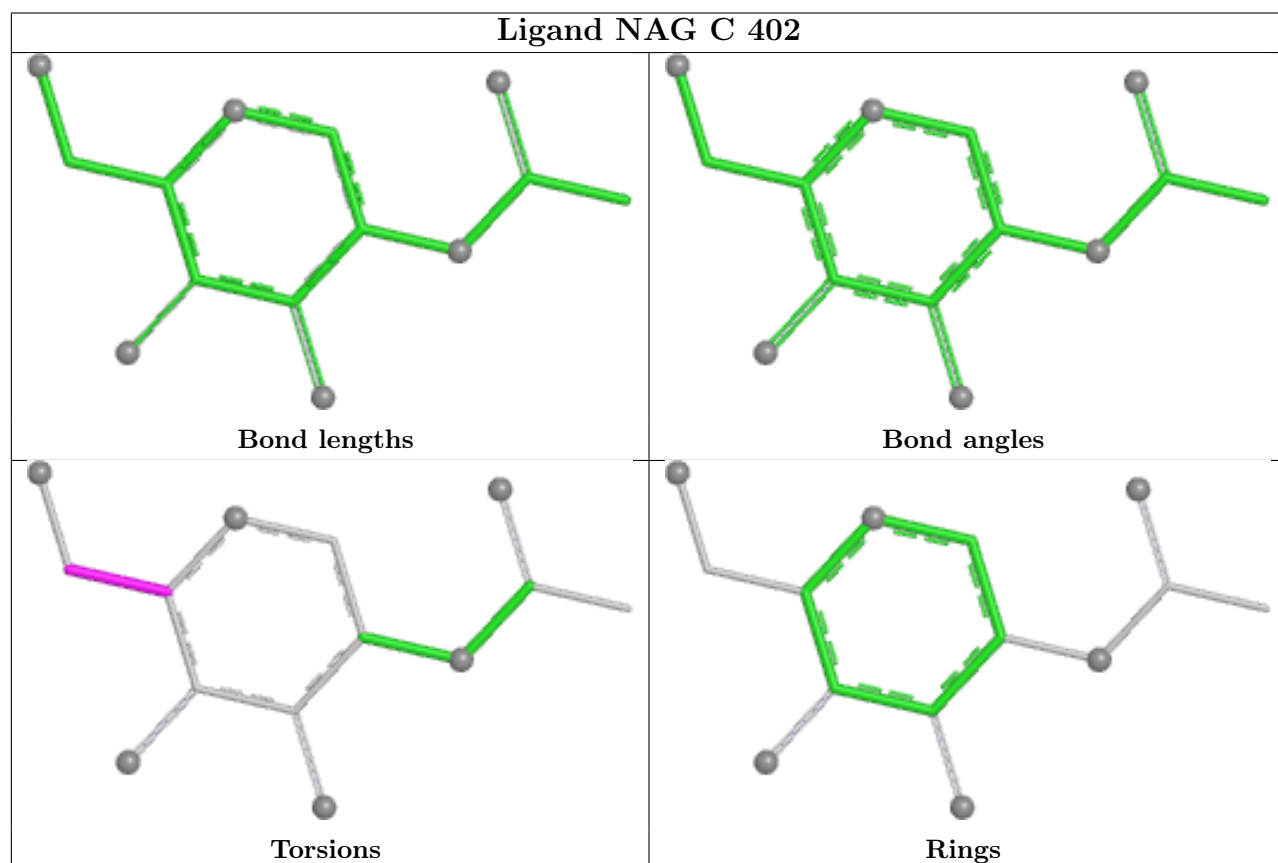
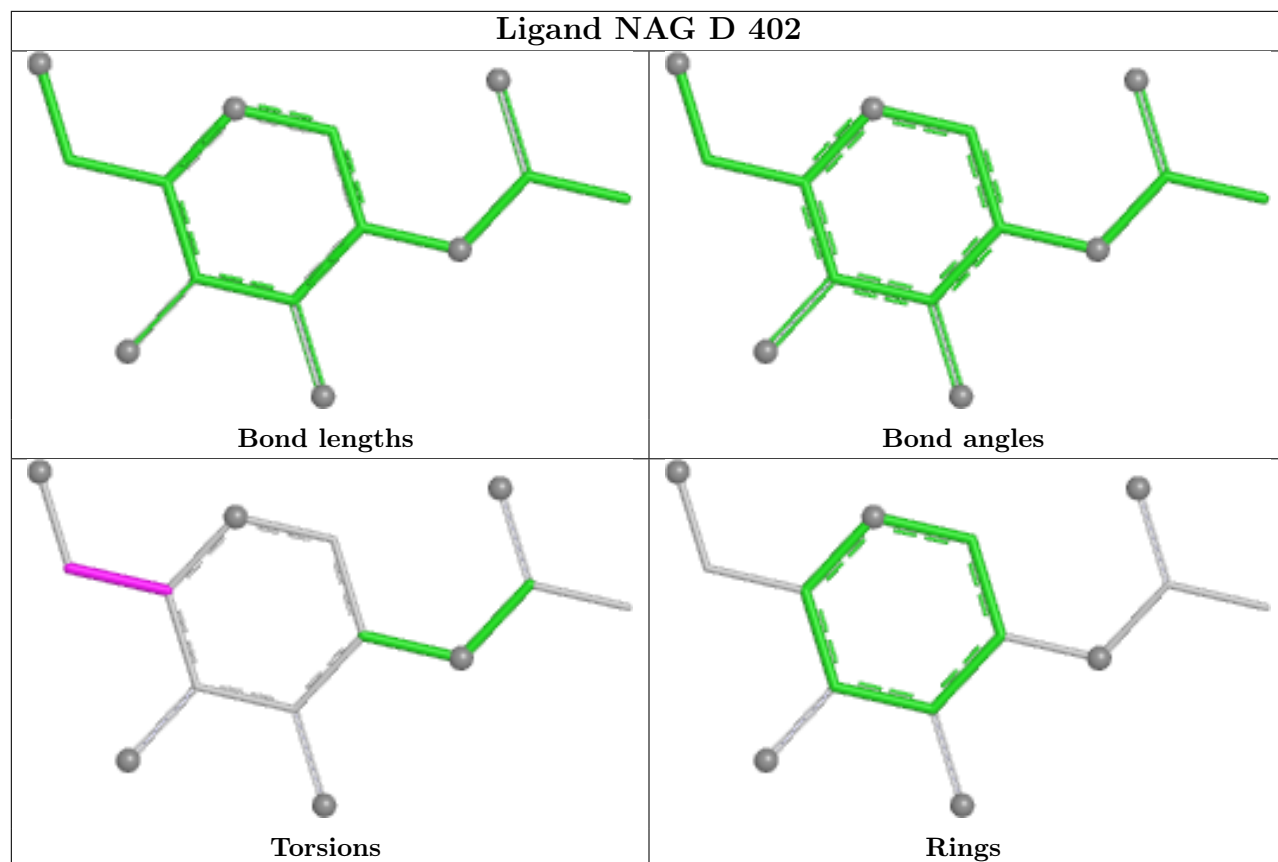
5 monomers are involved in 5 short contacts:

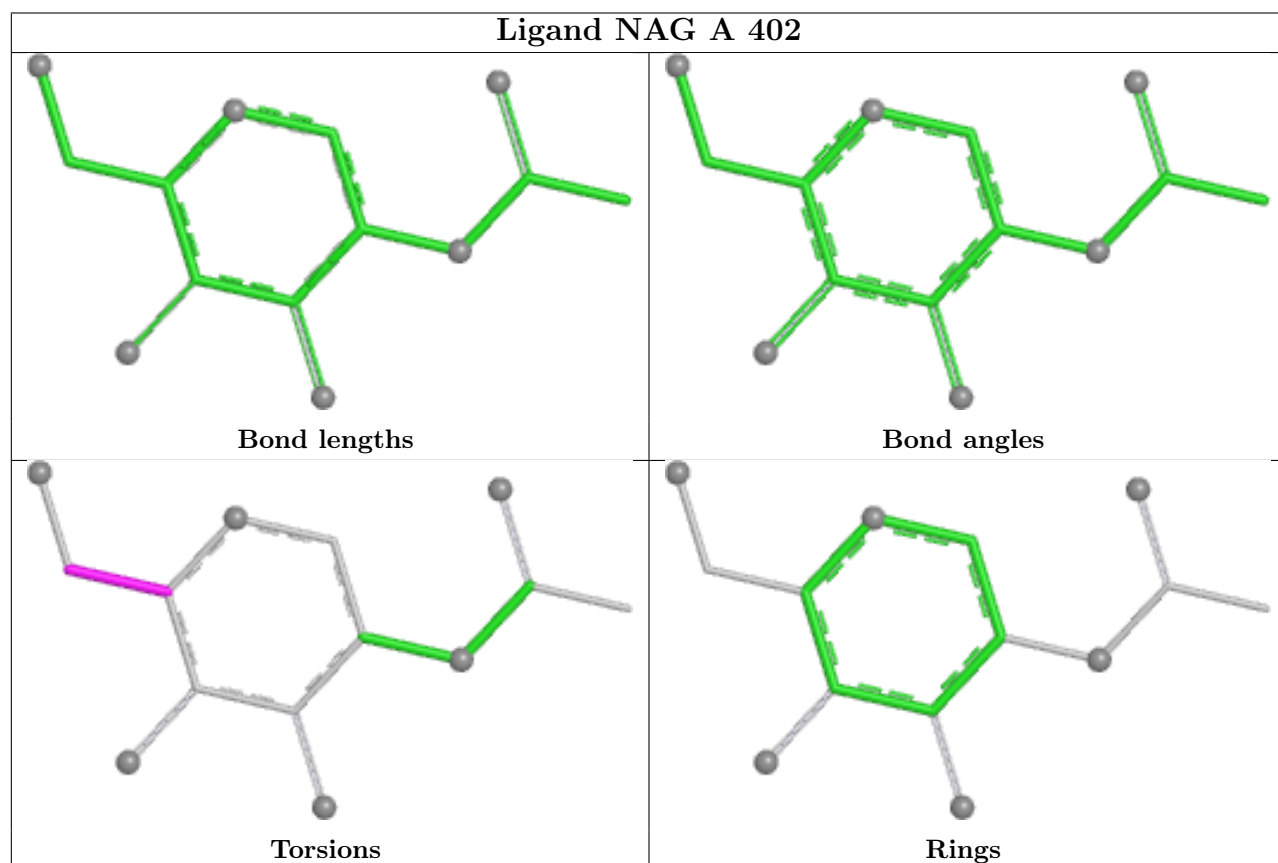
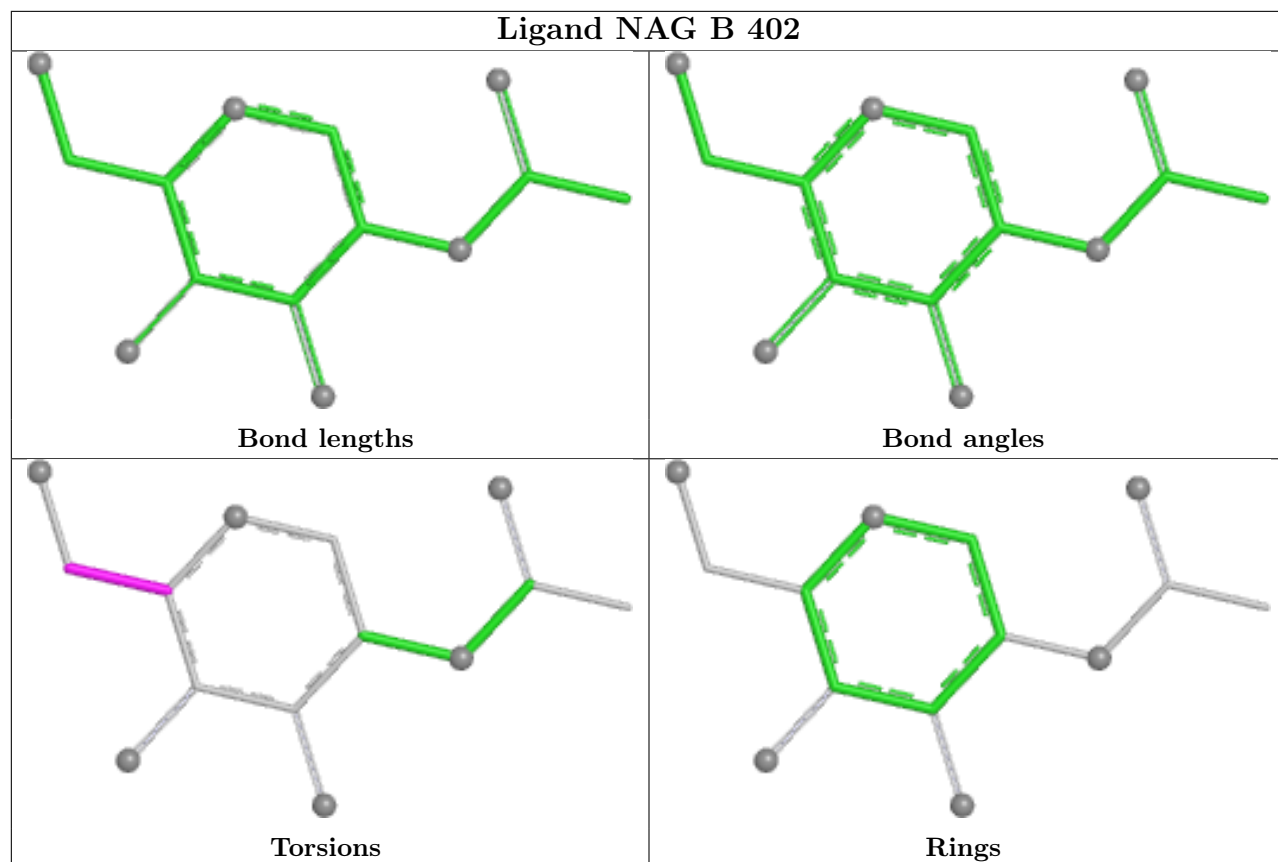
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	NAG	1	0
4	B	401	NAG	1	0
4	A	401	NAG	1	0
4	E	401	NAG	1	0
4	C	401	NAG	1	0

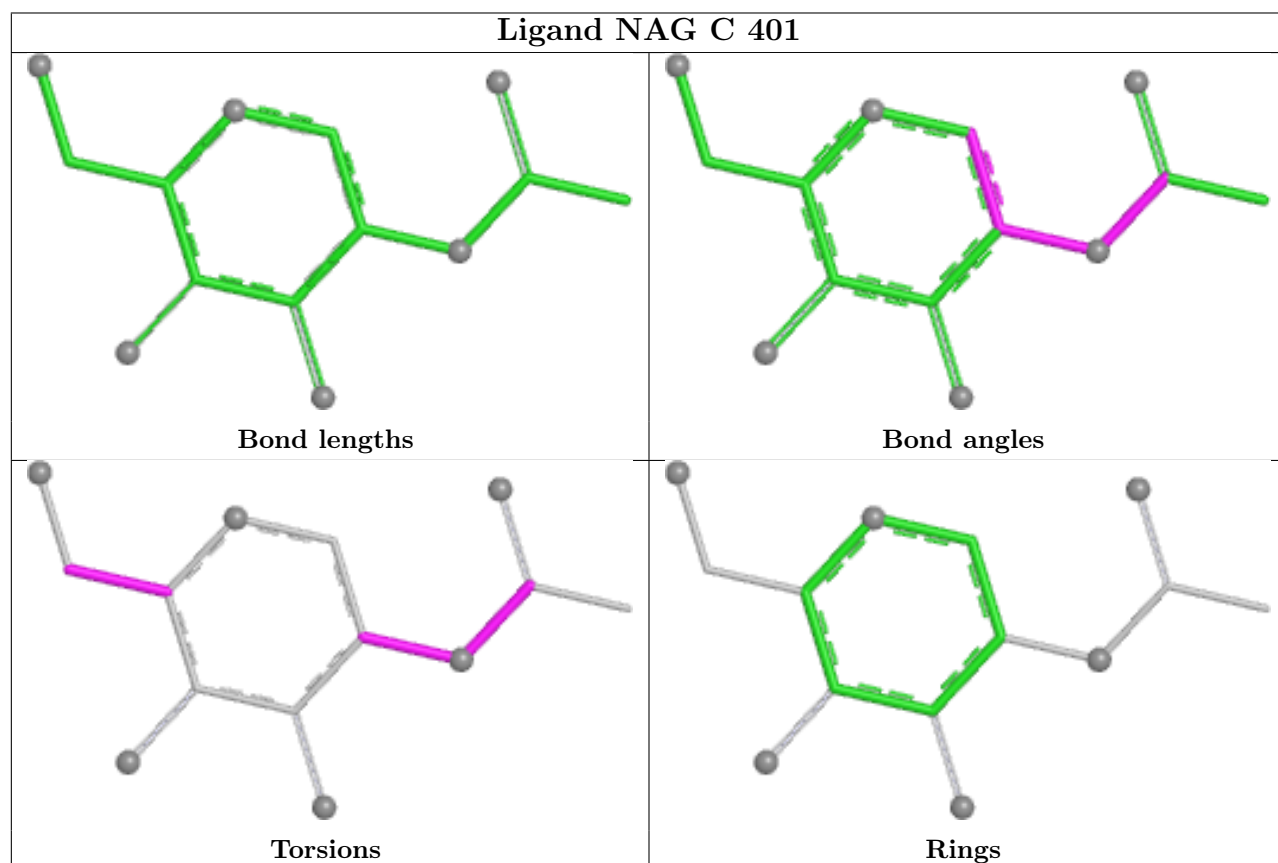
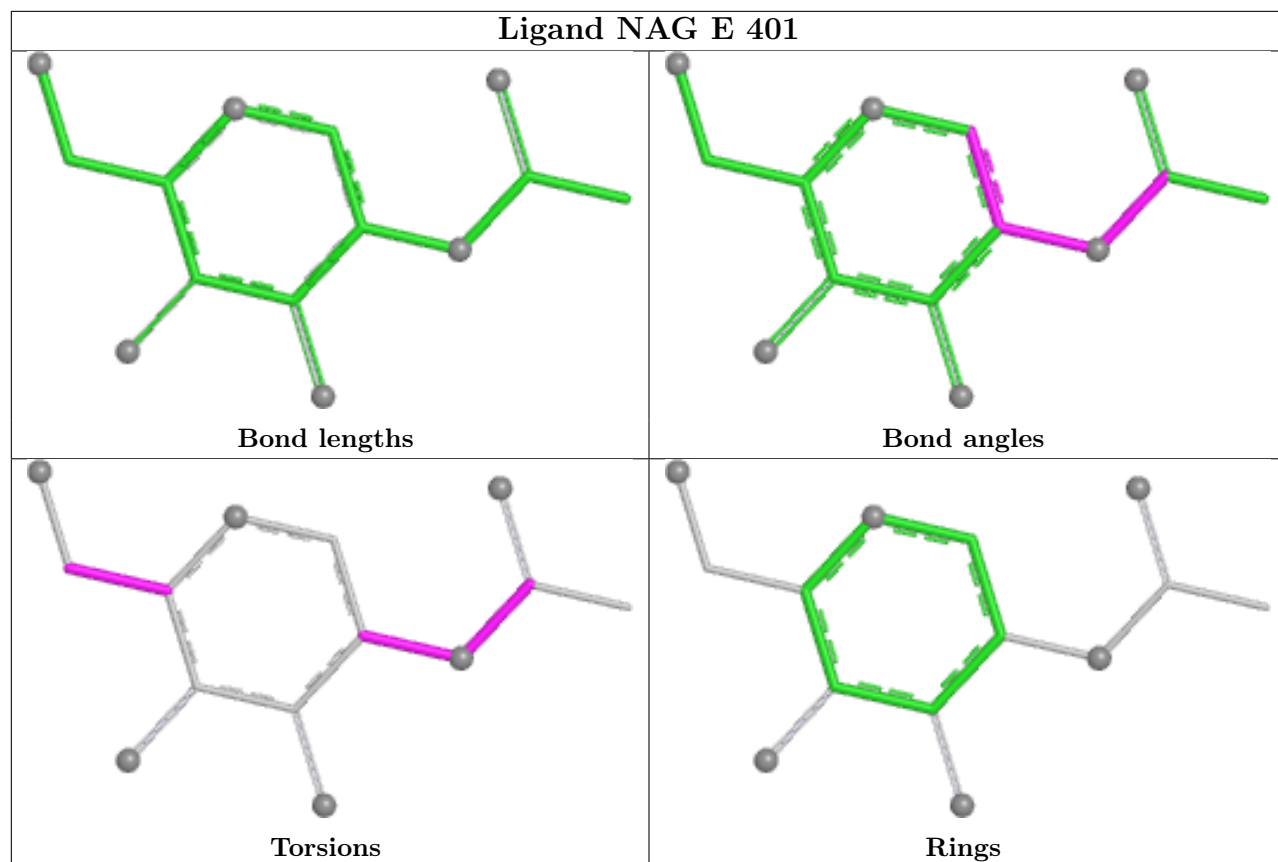
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

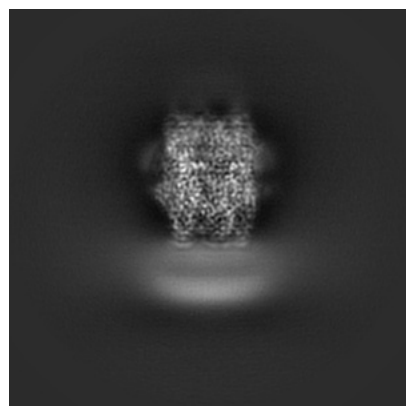
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16513. These allow visual inspection of the internal detail of the map and identification of artifacts.

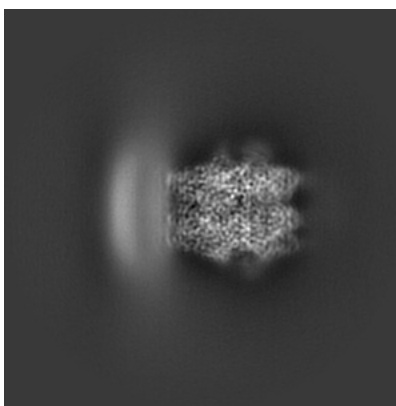
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

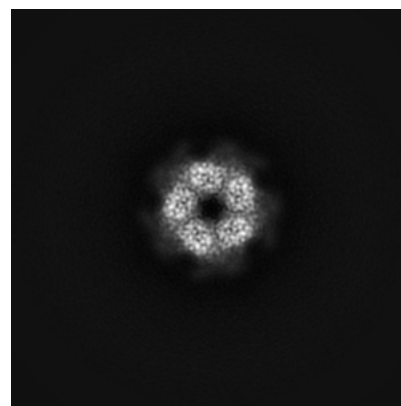
6.1.1 Primary map



X

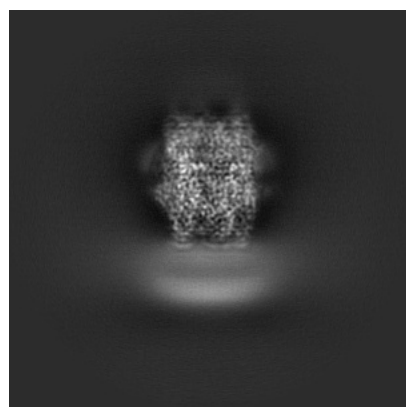


Y

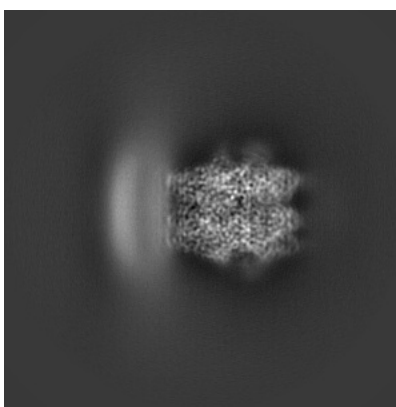


Z

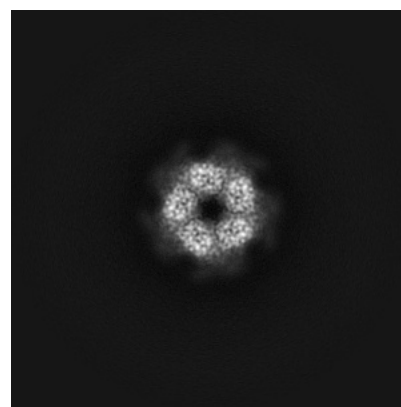
6.1.2 Raw map



X



Y

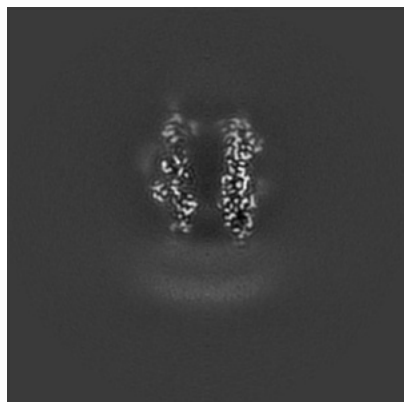


Z

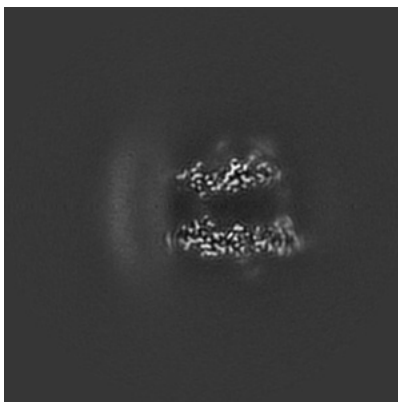
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

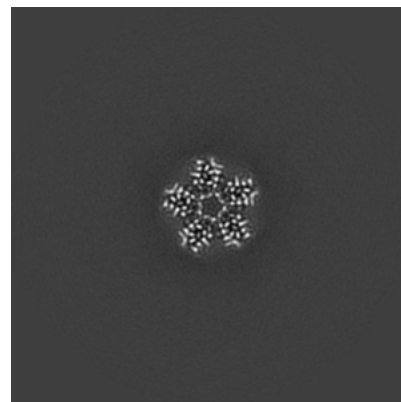
6.2.1 Primary map



X Index: 200

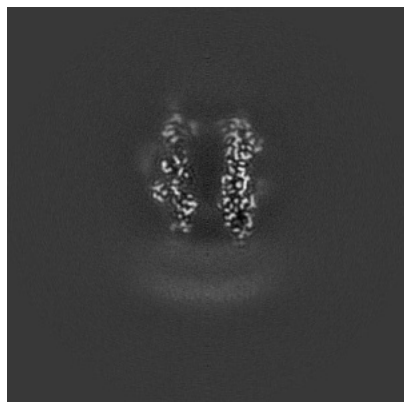


Y Index: 200

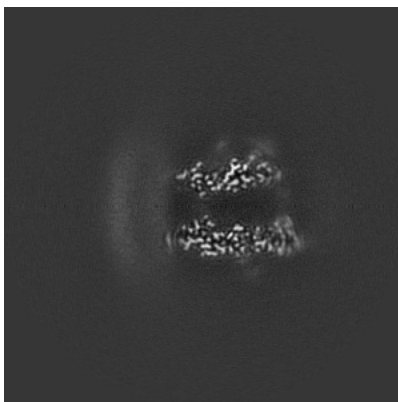


Z Index: 200

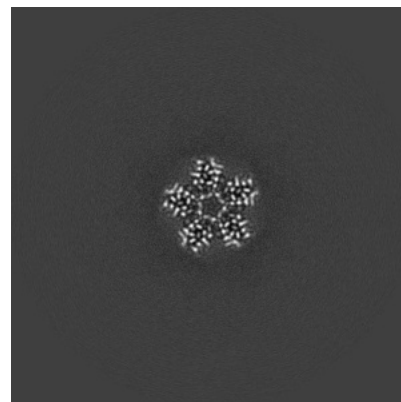
6.2.2 Raw map



X Index: 200



Y Index: 200

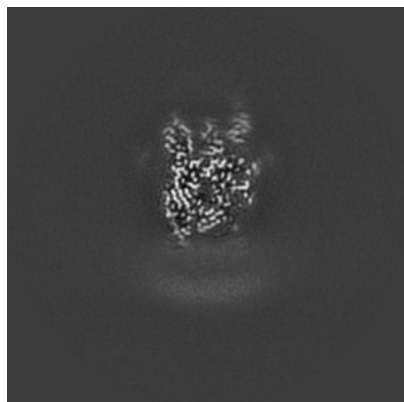


Z Index: 200

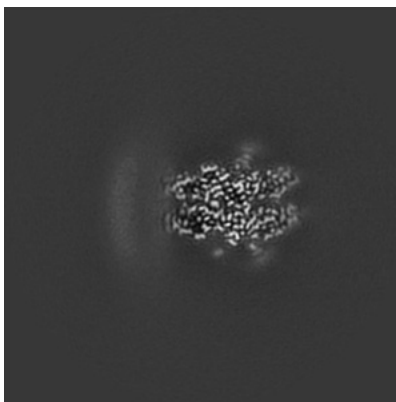
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

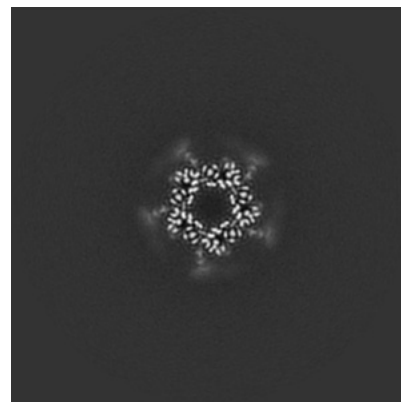
6.3.1 Primary map



X Index: 179

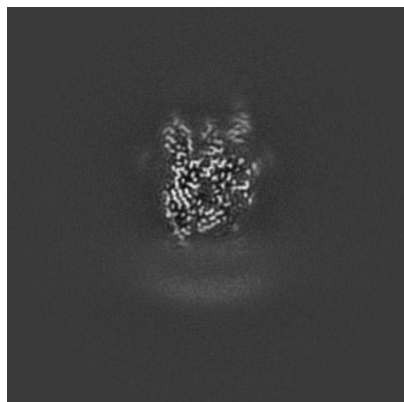


Y Index: 172

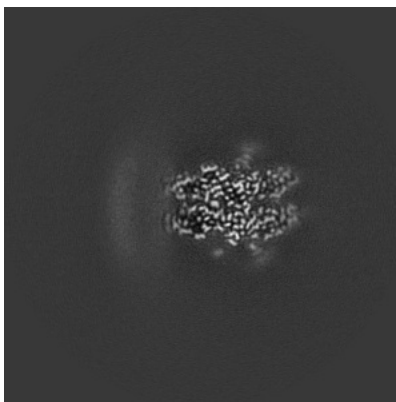


Z Index: 244

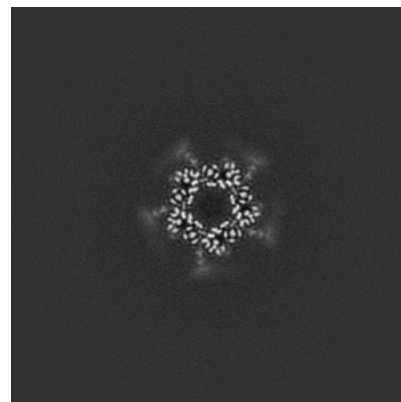
6.3.2 Raw map



X Index: 179



Y Index: 172

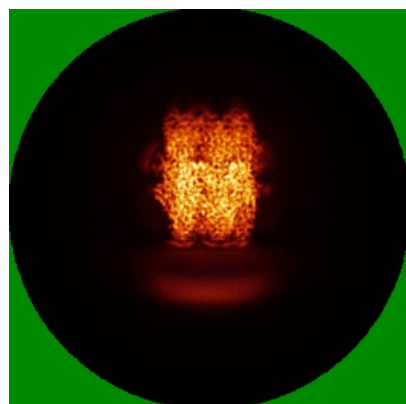


Z Index: 244

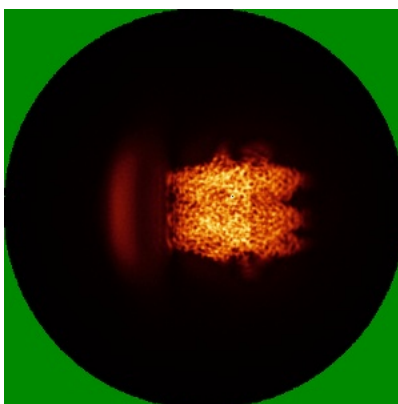
The images above show the largest variance slices of the map in three orthogonal directions.

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

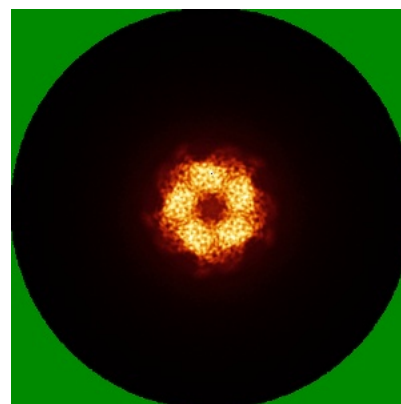
6.4.1 Primary map



X

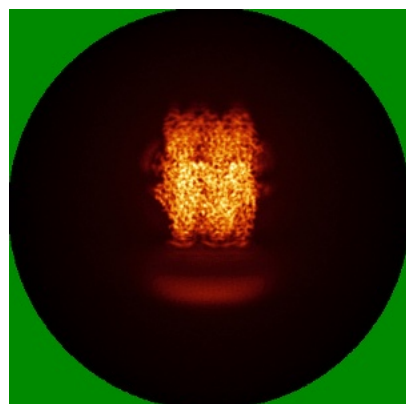


Y

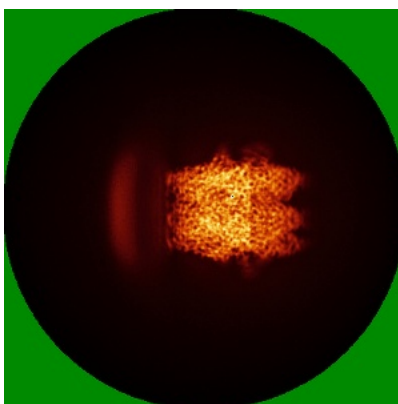


Z

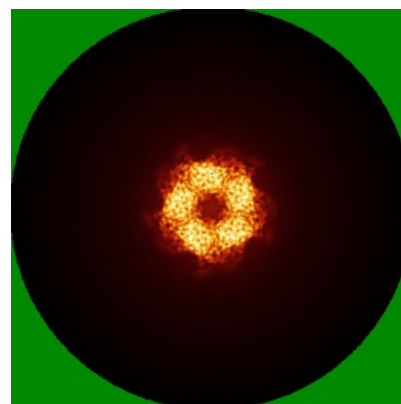
6.4.2 Raw map



X



Y

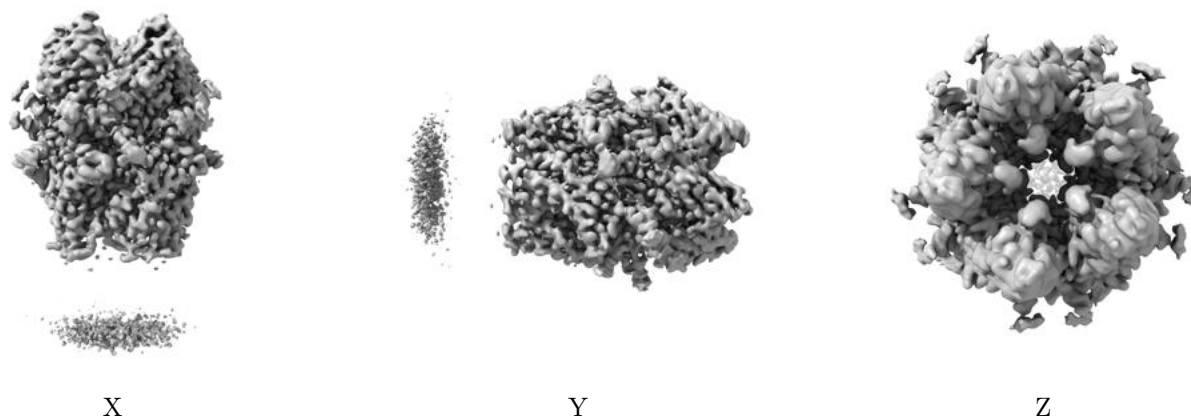


Z

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.

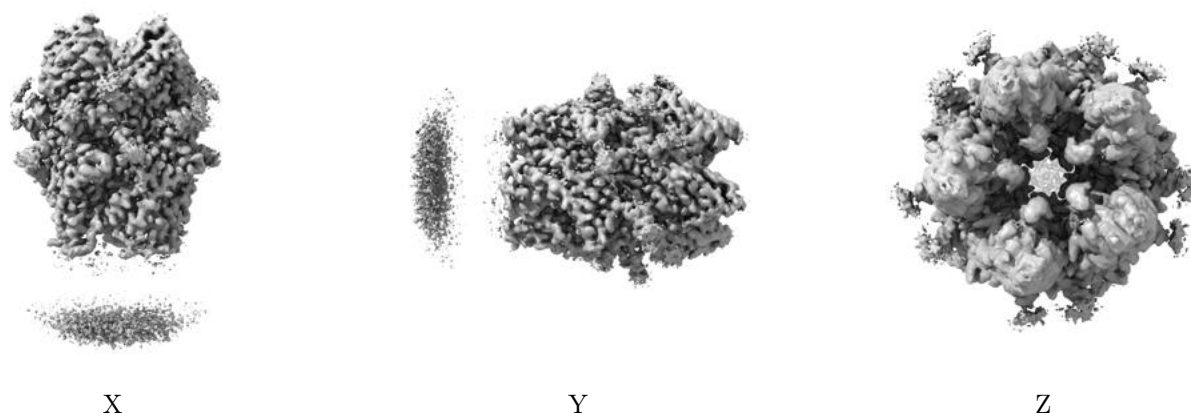
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0049. 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.

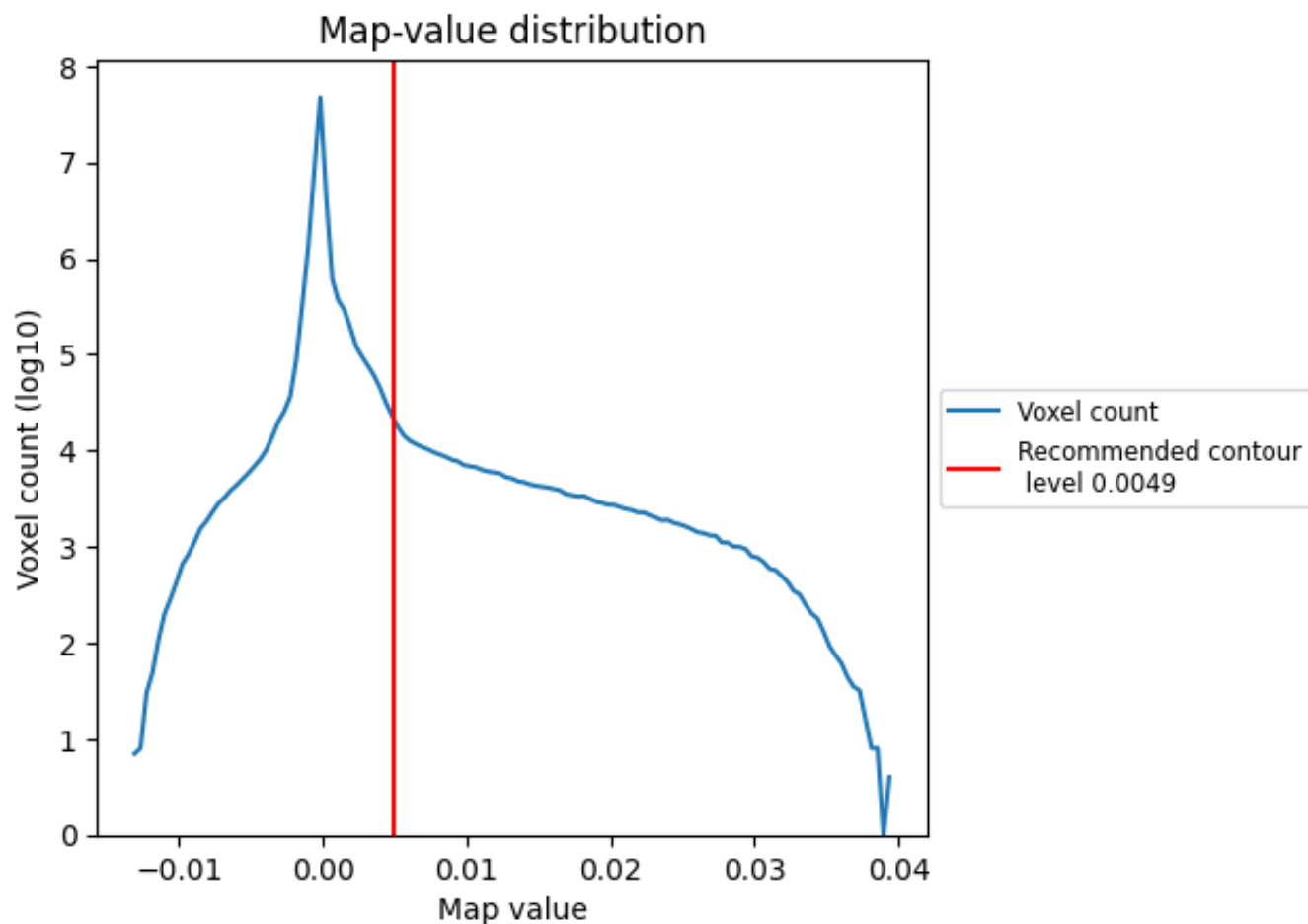
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

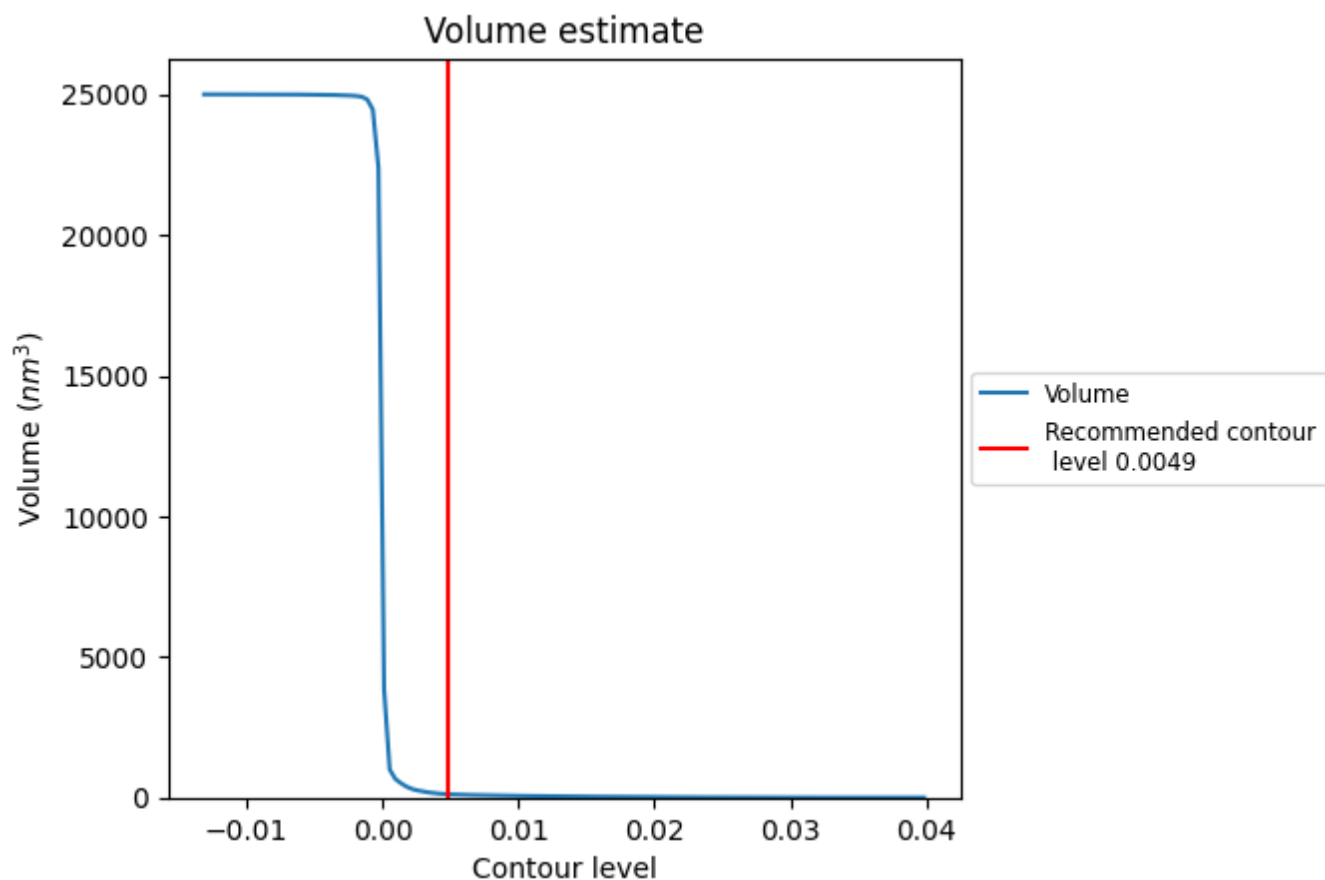
This section contains the results of statistical analysis of the map.

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.

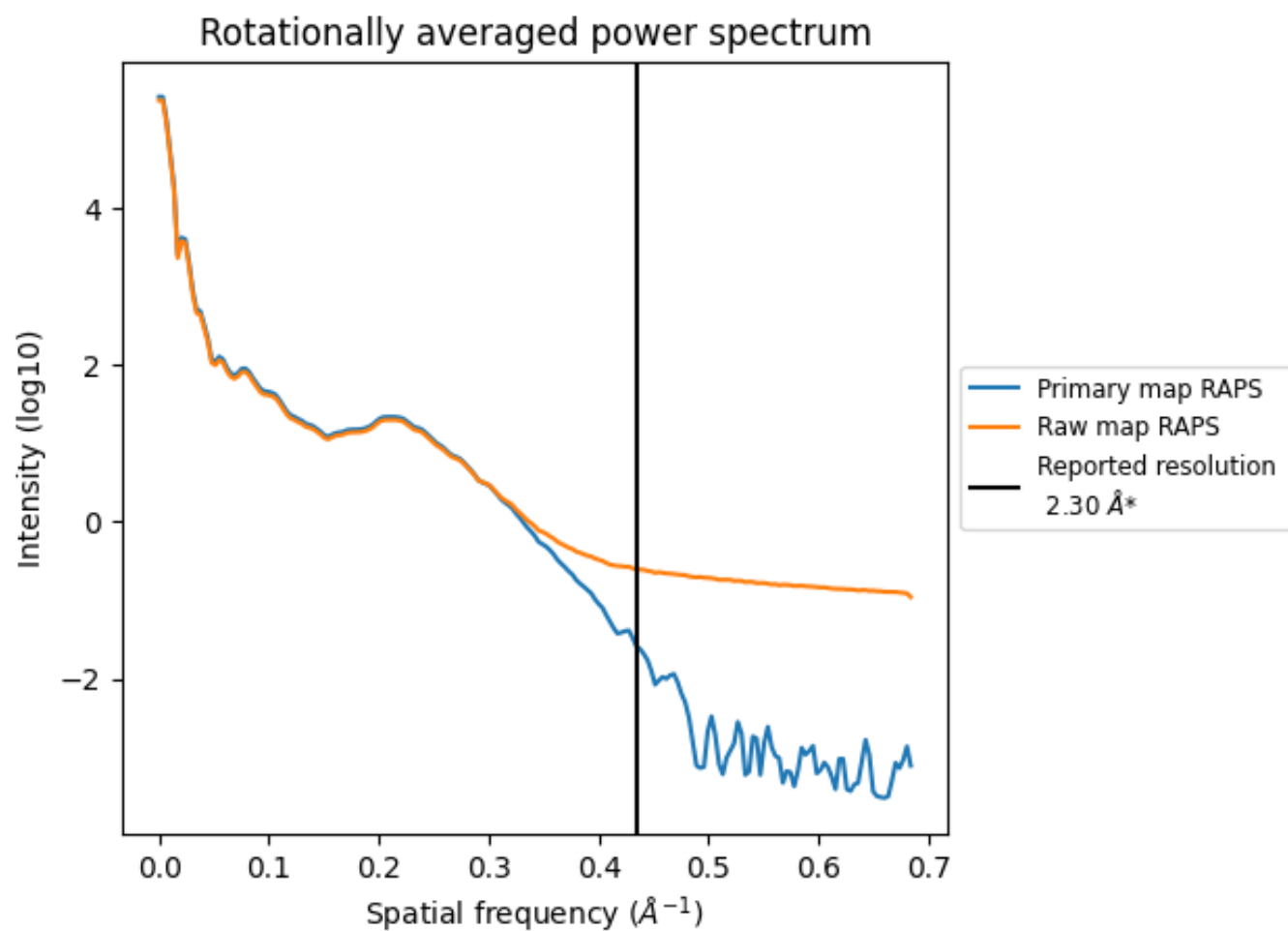
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm^3 ; this corresponds to an approximate mass of 106 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

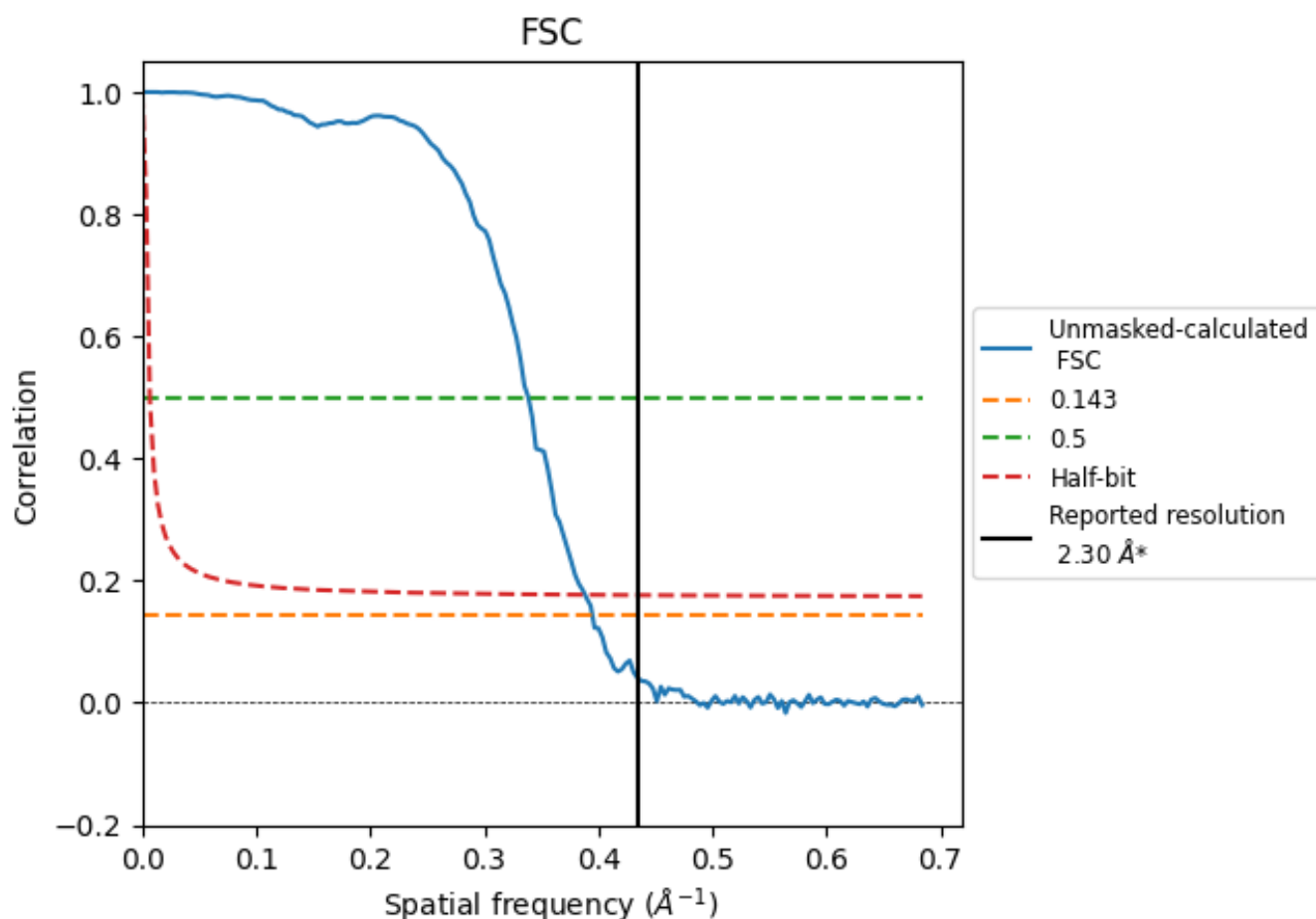


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

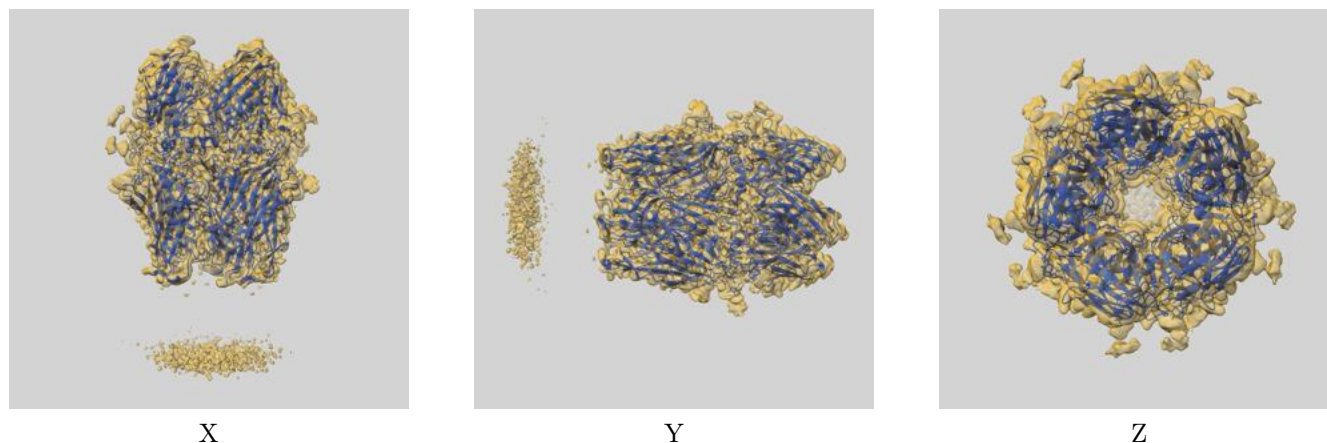
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.53	2.95	2.58

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

9 Map-model fit [i](#)

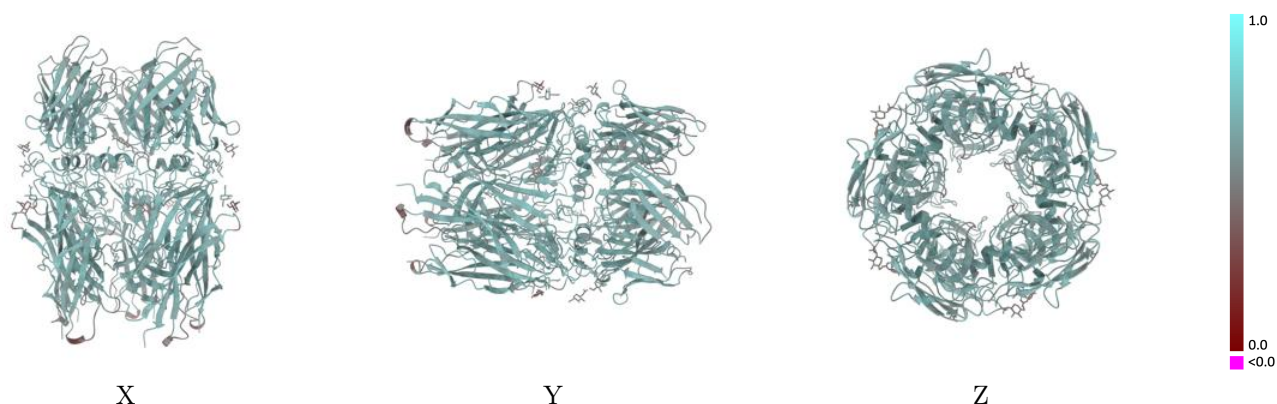
This section contains information regarding the fit between EMDB map EMD-16513 and PDB model 8C9X. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



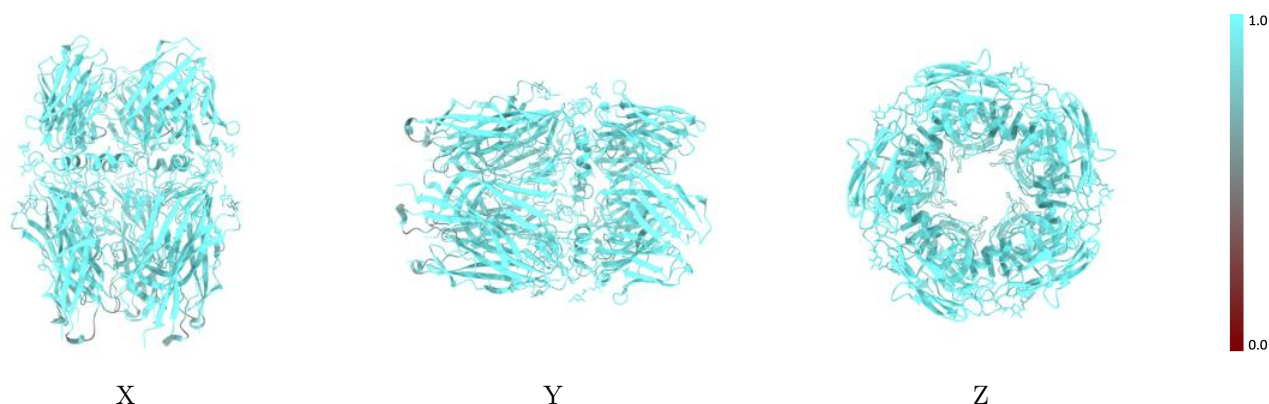
The images above show the 3D surface view of the map at the recommended contour level 0.0049 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



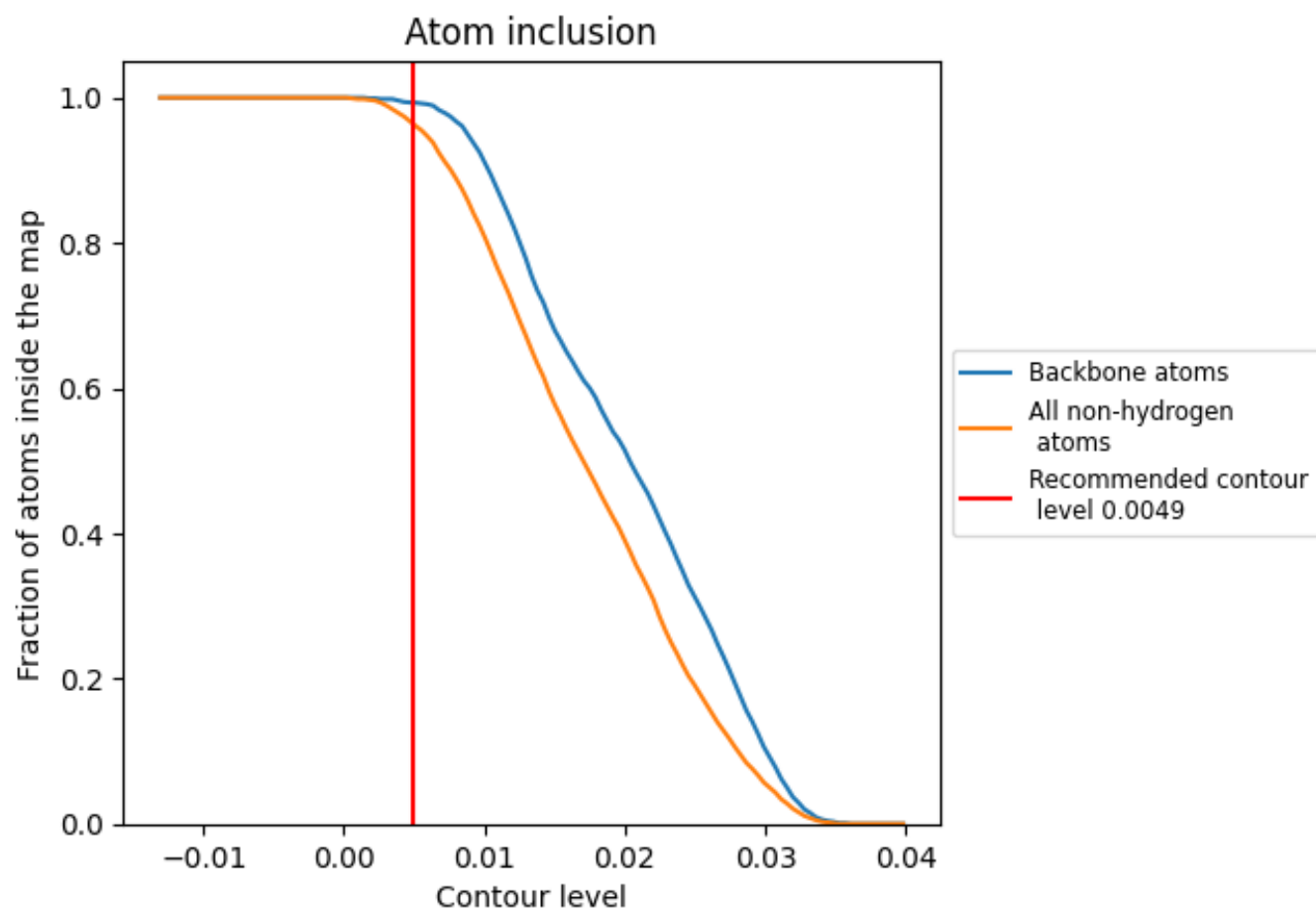
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0049).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.0049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9640	0.6090
A	0.9580	0.6170
B	0.9590	0.6170
C	0.9580	0.6160
D	0.9600	0.6160
E	0.9580	0.6140
F	0.9750	0.6000
G	0.9790	0.6020
H	0.9790	0.5990
I	0.9750	0.5970
J	0.9780	0.6000
P	0.8930	0.4810
Q	0.8930	0.4790
R	0.8930	0.4740
S	0.8930	0.4740
T	0.8930	0.4720

1.0

0.0

<0.0