



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 01:58 am GMT

PDB ID : 8CAU
EMDB ID : EMD-16534
Title : human alpha7 nicotinic receptor in complex with the C4 nanobody and nicotine
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 : 2023-01-24
Resolution : 3.40 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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

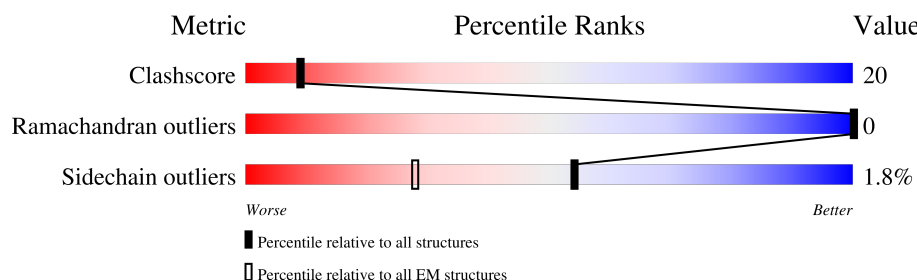
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	492	28% 14% 58%
1	B	492	28% 13% 58%
1	C	492	27% 14% 58%
1	D	492	28% 13% 58%
1	E	492	29% 13% 58%
2	F	147	48% 32% • 18%
2	G	147	52% 27% • 18%
2	H	147	50% 30% • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	147	 47% 35% 18%
2	J	147	 48% 33% 18%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 100%
3	T	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13615 atoms, of which 70 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	206	Total	C	N	O	S	1	0
			1721	1112	286	314	9		
1	B	206	Total	C	N	O	S	1	0
			1721	1112	286	314	9		
1	C	206	Total	C	N	O	S	1	0
			1721	1112	286	314	9		
1	D	206	Total	C	N	O	S	1	0
			1721	1112	286	314	9		
1	E	206	Total	C	N	O	S	1	0
			1721	1112	286	314	9		

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	SER	-	expression tag	UNP P36544
A	481	ALA	-	expression tag	UNP P36544
A	482	GLY	-	expression tag	UNP P36544
A	483	LEU	-	expression tag	UNP P36544
A	484	THR	-	expression tag	UNP P36544
A	485	GLU	-	expression tag	UNP P36544
A	486	THR	-	expression tag	UNP P36544
A	487	SER	-	expression tag	UNP P36544
A	488	GLN	-	expression tag	UNP P36544
A	489	VAL	-	expression tag	UNP P36544
A	490	ALA	-	expression tag	UNP P36544
A	491	PRO	-	expression tag	UNP P36544
A	492	ALA	-	expression tag	UNP P36544
B	480	SER	-	expression tag	UNP P36544
B	481	ALA	-	expression tag	UNP P36544
B	482	GLY	-	expression tag	UNP P36544
B	483	LEU	-	expression tag	UNP P36544
B	484	THR	-	expression tag	UNP P36544
B	485	GLU	-	expression tag	UNP P36544
B	486	THR	-	expression tag	UNP P36544

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	487	SER	-	expression tag	UNP P36544
B	488	GLN	-	expression tag	UNP P36544
B	489	VAL	-	expression tag	UNP P36544
B	490	ALA	-	expression tag	UNP P36544
B	491	PRO	-	expression tag	UNP P36544
B	492	ALA	-	expression tag	UNP P36544
C	480	SER	-	expression tag	UNP P36544
C	481	ALA	-	expression tag	UNP P36544
C	482	GLY	-	expression tag	UNP P36544
C	483	LEU	-	expression tag	UNP P36544
C	484	THR	-	expression tag	UNP P36544
C	485	GLU	-	expression tag	UNP P36544
C	486	THR	-	expression tag	UNP P36544
C	487	SER	-	expression tag	UNP P36544
C	488	GLN	-	expression tag	UNP P36544
C	489	VAL	-	expression tag	UNP P36544
C	490	ALA	-	expression tag	UNP P36544
C	491	PRO	-	expression tag	UNP P36544
C	492	ALA	-	expression tag	UNP P36544
D	480	SER	-	expression tag	UNP P36544
D	481	ALA	-	expression tag	UNP P36544
D	482	GLY	-	expression tag	UNP P36544
D	483	LEU	-	expression tag	UNP P36544
D	484	THR	-	expression tag	UNP P36544
D	485	GLU	-	expression tag	UNP P36544
D	486	THR	-	expression tag	UNP P36544
D	487	SER	-	expression tag	UNP P36544
D	488	GLN	-	expression tag	UNP P36544
D	489	VAL	-	expression tag	UNP P36544
D	490	ALA	-	expression tag	UNP P36544
D	491	PRO	-	expression tag	UNP P36544
D	492	ALA	-	expression tag	UNP P36544
E	480	SER	-	expression tag	UNP P36544
E	481	ALA	-	expression tag	UNP P36544
E	482	GLY	-	expression tag	UNP P36544
E	483	LEU	-	expression tag	UNP P36544
E	484	THR	-	expression tag	UNP P36544
E	485	GLU	-	expression tag	UNP P36544
E	486	THR	-	expression tag	UNP P36544
E	487	SER	-	expression tag	UNP P36544
E	488	GLN	-	expression tag	UNP P36544
E	489	VAL	-	expression tag	UNP P36544

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	490	ALA	-	expression tag	UNP P36544
E	491	PRO	-	expression tag	UNP P36544
E	492	ALA	-	expression tag	UNP P36544

- Molecule 2 is a protein called Nanobody C4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	121	Total	C	N	O	S	0	0
			920	585	156	176	3		
2	G	121	Total	C	N	O	S	0	0
			920	585	156	176	3		
2	H	121	Total	C	N	O	S	0	0
			920	585	156	176	3		
2	I	121	Total	C	N	O	S	0	0
			920	585	156	176	3		
2	J	121	Total	C	N	O	S	0	0
			920	585	156	176	3		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



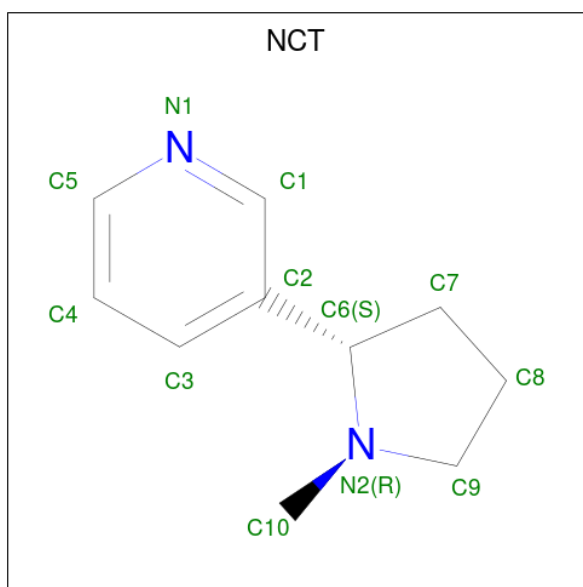
Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (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	
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	

- Molecule 5 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: C₁₀H₁₄N₂) (labeled as "Ligand of Interest" by depositor).

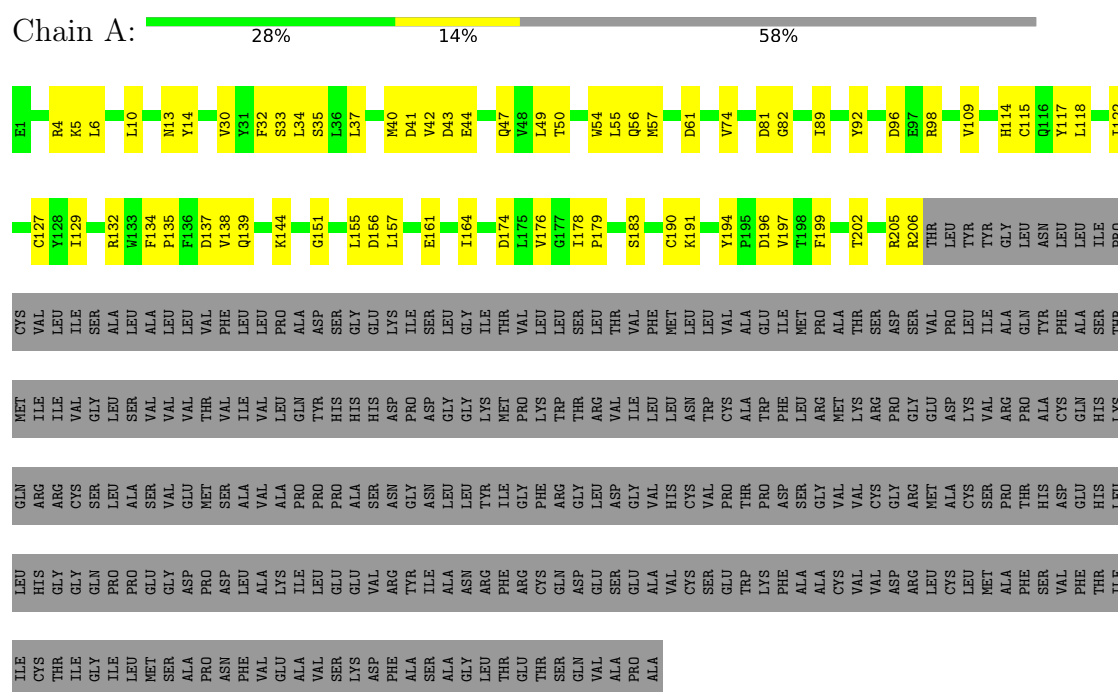


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	N	0
			26	10	14	2	
5	B	1	Total	C	H	N	0
			26	10	14	2	
5	C	1	Total	C	H	N	0
			26	10	14	2	
5	D	1	Total	C	H	N	0
			26	10	14	2	
5	E	1	Total	C	H	N	0
			26	10	14	2	

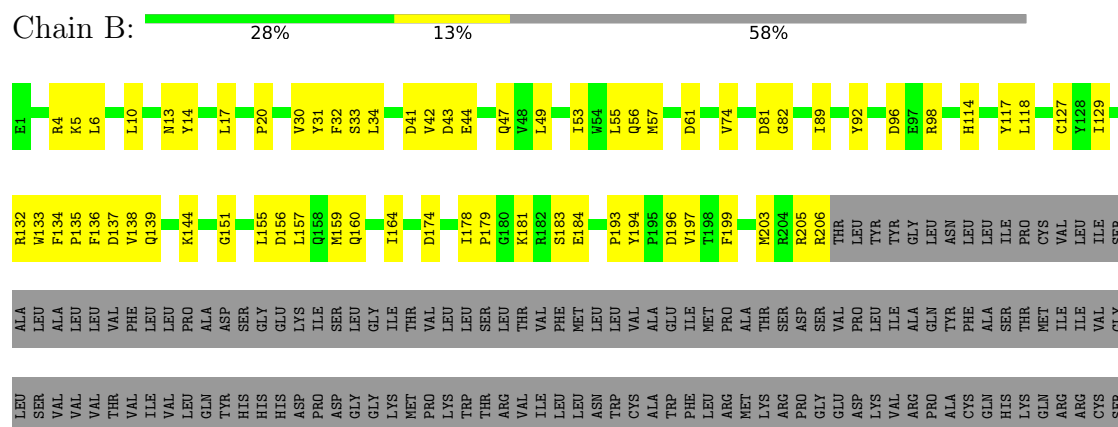
3 Residue-property plots

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: Neuronal acetylcholine receptor subunit alpha-7



• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



[illegible]

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

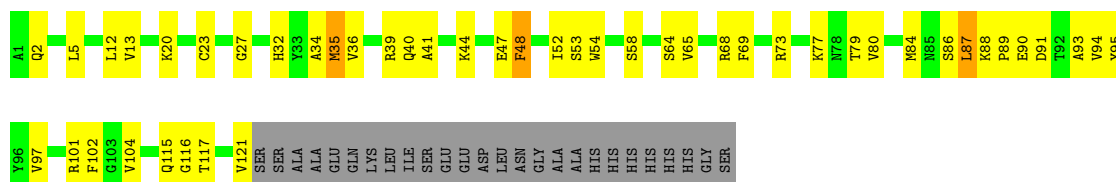
Chain C:  27% 14% 58%

[illegible]

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

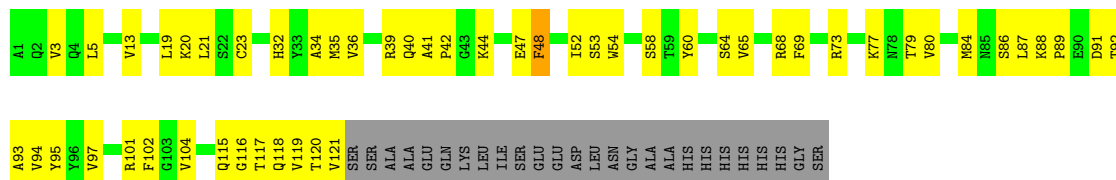
Chain D: 28% 13% 58%

His	Arg	Ile	Val	Y117	E1
	Gly	Ile	Leu	L118	
Gly	Arg	Val	Ile		R4
	GLN	Gly	Ser	I122	K5
Pro	Leu	Leu	Ala		L6
	Pro	Ser	Leu	C127	
Glu	Ser	Val	Ala	I126	L10
	Gly	Val	Leu	I129	
Asp	Glu	Thr	Leu		N13
	Pro	Thr	Val	R132	Y14
Asp	Ser	Val	Phe	W133	
	Leu	Ile	Leu	F134	V30
Ala	Val	Val	Leu	P135	T31
	lys	Leu	Pro	F136	F32
Ile	Pro	GLN	Ala	D137	S33
	Leu	Tyr	Asp	W138	L34
Glu	Pro	His	Ser	Q139	S35
	Glu	His	Gly	L136	L36
Val	Ser	His	Glu	K144	L37
	Arg	Asp	Lys		
Arg	ASN	Asp	Lys		M40
	Tyr	Gly	Ile	L155	D41
Ile	ASN	Asp	Ser	D156	V42
	Ala	Gly	Leu	L157	D43
ASN	Leu	Gly	Gly	O158	E44
	Arg	Lys	Ile	M159	
Phe	Ile	Met	Thr	Q160	
	Arg	Pro	Val		Q47
Cys	Phe	Lys	Leu	I164	V48
	GLN	Trp	Leu	L49	L50
Asp	Gly	Thr	Ser	E172	
	Glu	Arg	Leu		T53
Ser	Ser	Val	Thr	I178	W54
	Glu	Ile	Val	P179	L55
Ala	Val	Leu	Phe		O56
	Val	Leu	Met	S183	M57
Cys	His	Leu	Met	E184	
	Ser	Trp	Leu		T60
Ser	Val	Trp	Val	C189	
	Glu	Cys	Ala	Ala	D61
Trp	Thr	Trp	Glu	P193	
	Lys	Phe	Ile		L64
Phe	Asp	Leu	Met	D196	V74
	Ala	Arg	Pro	V197	
Ala	Gly	Met	Ala	I198	
	Val	Lys	Thr	F199	D81
Val	Val	Arg	Ser		G82
	Asp	Pro	Asp	R205	
Arg	Gly	Gly	Ser	T206	T69
	Arg	Glu	Val	Thr	
Cys	Ala	Asp	Pro	Leu	Y92
	Leu	Lys	Leu	Tyr	
Met	Ser	Val	Ile	Tyr	D96
	Ala	Arg	Ala	Gly	F87
Ala	Pro	Pro	GLN	Leu	R98
	Phe	Thr	Ala	Asn	
Ser	His	Ala	Tyr	Leu	V109
	Val	Cys	Phe	Leu	
Phe	Glu	GLN	Ala	Leu	H114
	Thr	His	Ser	Ile	C115
Ile	Lys	Lys	Thr	Pro	
	Leu	Cln	Met	Cys	G116



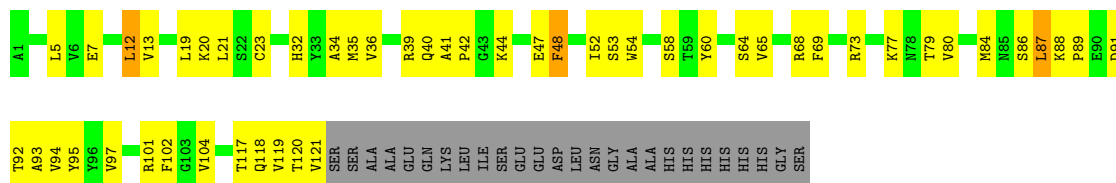
- Molecule 2: Nanobody C4

Chain I: 47% 35% 18%



- Molecule 2: Nanobody C4

Chain J: 48% 33% 18%



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

Chain P: 100%



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

Chain Q: 100%



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

Chain R: 100%




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

Chain S:  100%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	73690	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)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00248	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/1780	0.48	0/2423
1	B	0.26	0/1780	0.47	0/2423
1	C	0.25	0/1780	0.47	0/2423
1	D	0.25	0/1780	0.48	0/2423
1	E	0.26	0/1780	0.47	0/2423
2	F	0.26	0/942	0.49	0/1277
2	G	0.26	0/942	0.48	0/1277
2	H	0.26	0/942	0.48	0/1277
2	I	0.26	0/942	0.49	0/1277
2	J	0.26	0/942	0.49	0/1277
All	All	0.26	0/13610	0.48	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 [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	1721	0	1644	57	0
1	B	1721	0	1644	53	0
1	C	1721	0	1644	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1721	0	1644	56	0
1	E	1721	0	1644	52	0
2	F	920	0	881	51	0
2	G	920	0	881	44	0
2	H	920	0	881	42	0
2	I	920	0	881	52	0
2	J	920	0	881	56	0
3	P	28	0	25	6	0
3	Q	28	0	25	5	0
3	R	28	0	25	4	0
3	S	28	0	25	6	0
3	T	28	0	25	5	0
4	A	28	0	26	4	0
4	B	28	0	26	4	0
4	C	28	0	26	4	0
4	D	28	0	26	4	0
4	E	28	0	26	4	0
5	A	12	14	14	1	0
5	B	12	14	14	0	0
5	C	12	14	14	0	0
5	D	12	14	14	1	0
5	E	12	14	14	1	0
All	All	13545	70	12950	539	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 20.

The worst 5 of 539 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)
2:F:92:THR:HG23	2:F:121:VAL:HG12	1.50	0.91
2:F:90:GLU:N	2:F:90:GLU:OE1	2.03	0.91
4:A:501:NAG:H3	4:A:501:NAG:H83	1.54	0.89
4:C:501:NAG:H83	4:C:501:NAG:H3	1.54	0.89
4:D:501:NAG:H3	4:D:501:NAG:H83	1.54	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/492 (42%)	191 (93%)	14 (7%)	0	100	100
1	B	205/492 (42%)	188 (92%)	17 (8%)	0	100	100
1	C	205/492 (42%)	187 (91%)	18 (9%)	0	100	100
1	D	205/492 (42%)	187 (91%)	18 (9%)	0	100	100
1	E	205/492 (42%)	188 (92%)	17 (8%)	0	100	100
2	F	119/147 (81%)	110 (92%)	9 (8%)	0	100	100
2	G	119/147 (81%)	107 (90%)	12 (10%)	0	100	100
2	H	119/147 (81%)	109 (92%)	10 (8%)	0	100	100
2	I	119/147 (81%)	109 (92%)	10 (8%)	0	100	100
2	J	119/147 (81%)	109 (92%)	10 (8%)	0	100	100
All	All	1620/3195 (51%)	1485 (92%)	135 (8%)	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	192/433 (44%)	190 (99%)	2 (1%)	73	83
1	B	192/433 (44%)	189 (98%)	3 (2%)	58	75
1	C	192/433 (44%)	190 (99%)	2 (1%)	73	83
1	D	192/433 (44%)	189 (98%)	3 (2%)	58	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	192/433 (44%)	191 (100%)	1 (0%)	86	91
2	F	92/112 (82%)	89 (97%)	3 (3%)	33	58
2	G	92/112 (82%)	88 (96%)	4 (4%)	25	50
2	H	92/112 (82%)	88 (96%)	4 (4%)	25	50
2	I	92/112 (82%)	91 (99%)	1 (1%)	70	81
2	J	92/112 (82%)	89 (97%)	3 (3%)	33	58
All	All	1420/2725 (52%)	1394 (98%)	26 (2%)	54	73

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	5	LEU
2	G	87	LEU
2	J	48	PHE
2	G	48	PHE
2	H	12	LEU

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](#)

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	1,3	14,14,15	0.40	0	17,19,21	0.59	0
3	NAG	P	2	3	14,14,15	0.40	0	17,19,21	0.37	0
3	NAG	Q	1	1,3	14,14,15	0.41	0	17,19,21	0.58	0
3	NAG	Q	2	3	14,14,15	0.38	0	17,19,21	0.38	0
3	NAG	R	1	1,3	14,14,15	0.39	0	17,19,21	0.58	0
3	NAG	R	2	3	14,14,15	0.41	0	17,19,21	0.38	0
3	NAG	S	1	1,3	14,14,15	0.38	0	17,19,21	0.58	0
3	NAG	S	2	3	14,14,15	0.36	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	T	2	3	14,14,15	0.39	0	17,19,21	0.38	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	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

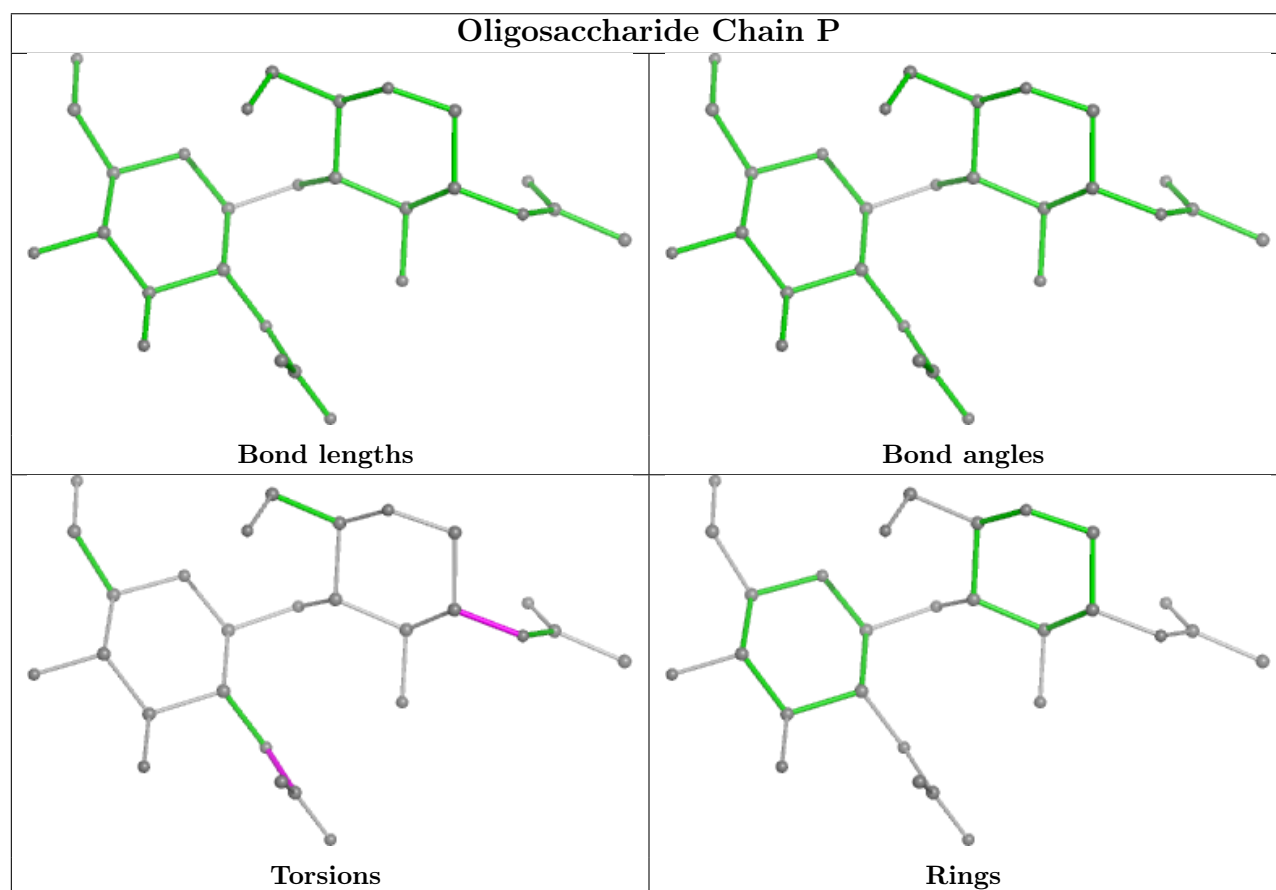
Mol	Chain	Res	Type	Atoms
3	R	1	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2

There are no ring outliers.

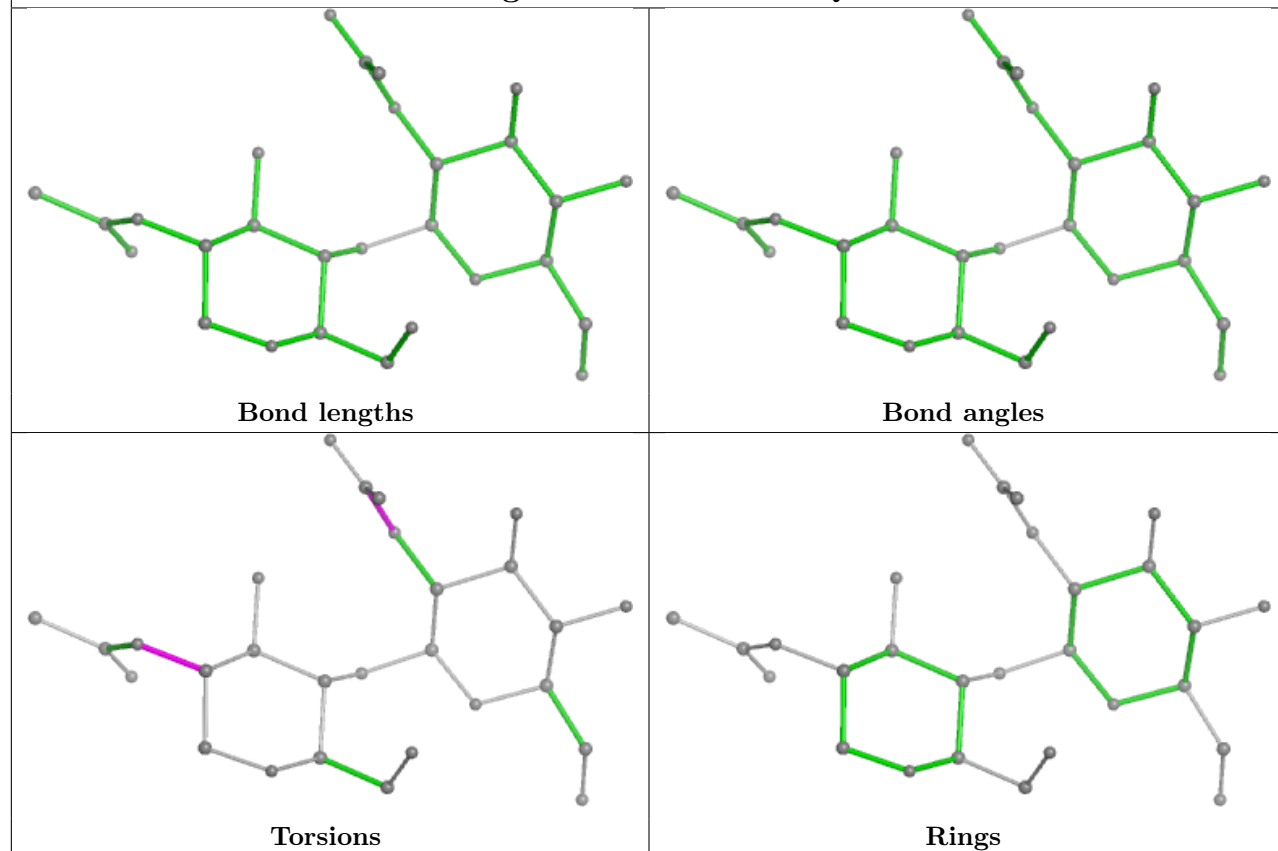
10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	2	NAG	2	0
3	P	1	NAG	5	0
3	R	2	NAG	2	0
3	S	2	NAG	3	0
3	P	2	NAG	3	0
3	R	1	NAG	3	0
3	Q	1	NAG	4	0
3	S	1	NAG	5	0
3	T	2	NAG	3	0
3	T	1	NAG	4	0

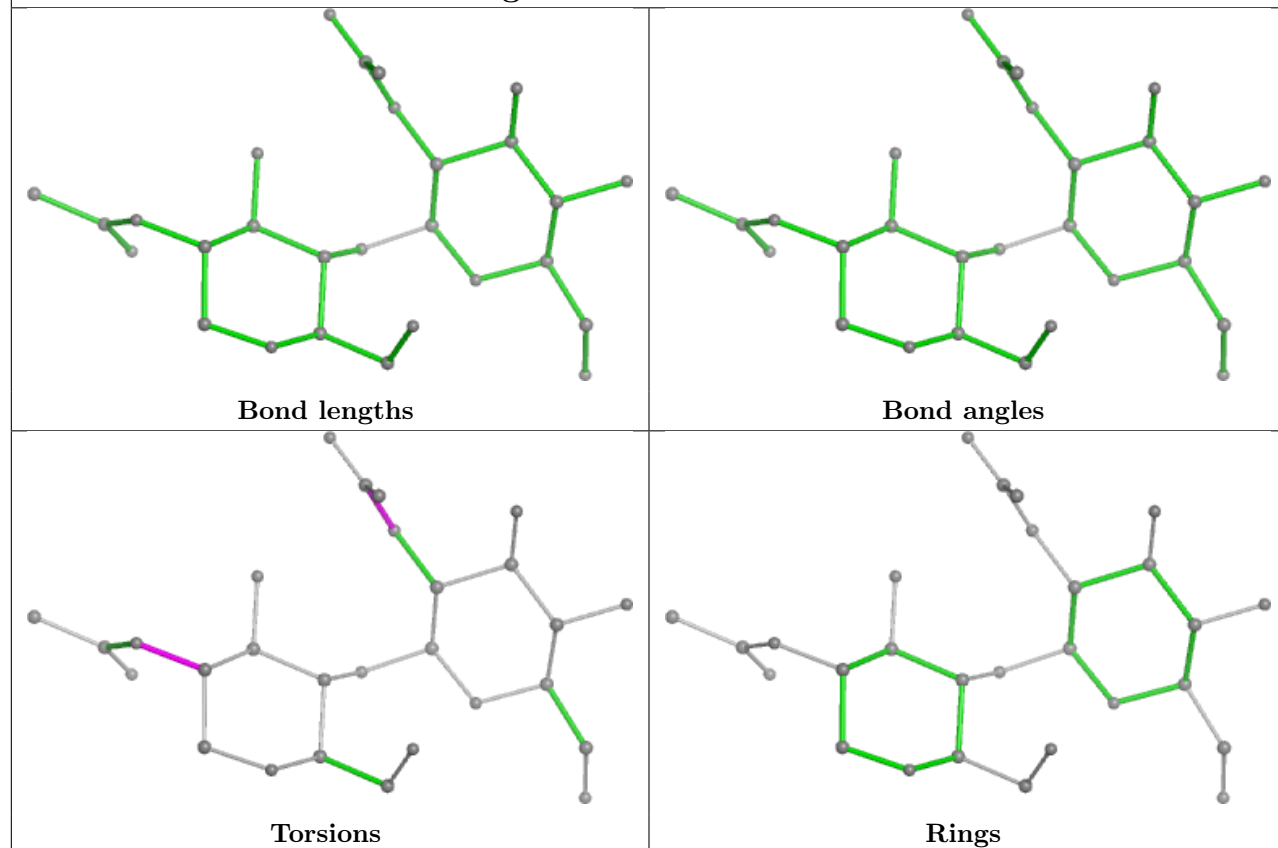
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



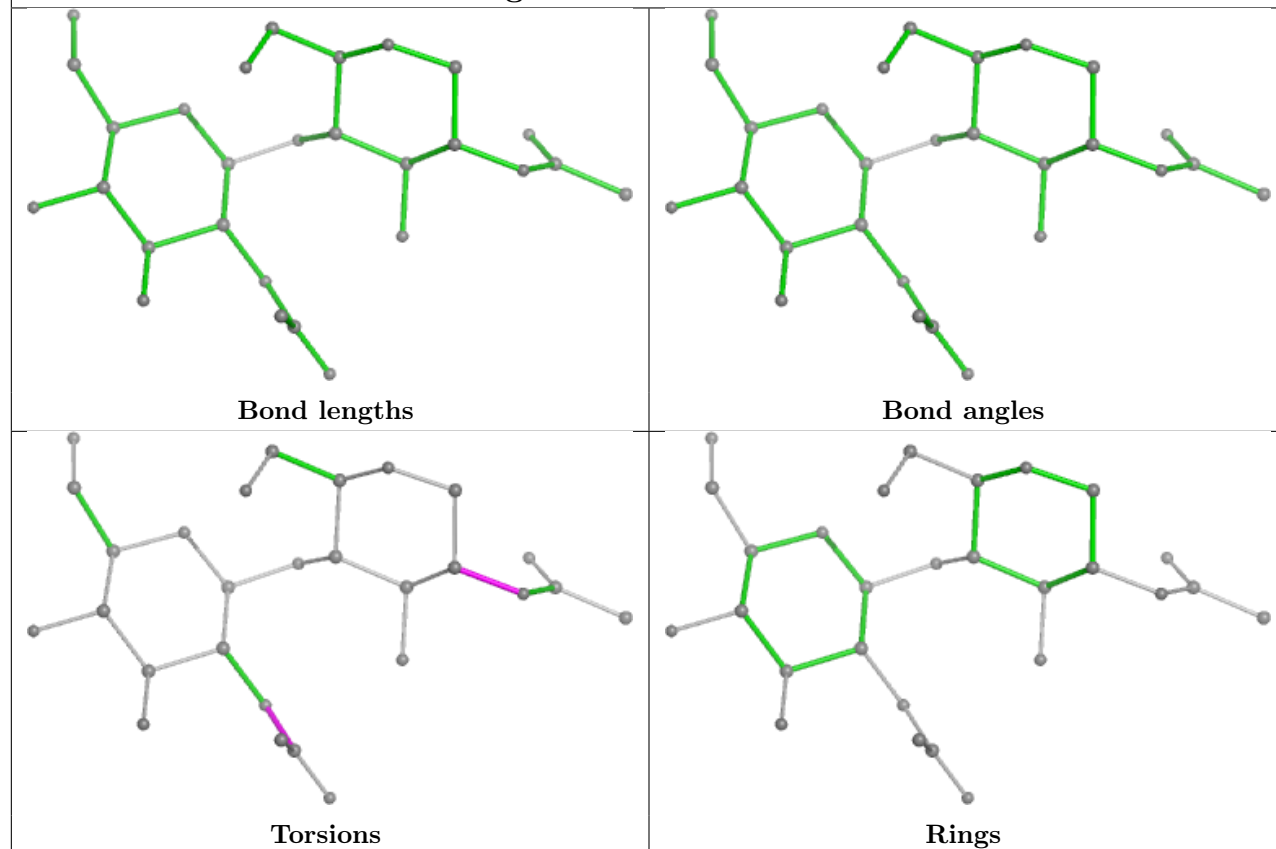
Oligosaccharide Chain Q



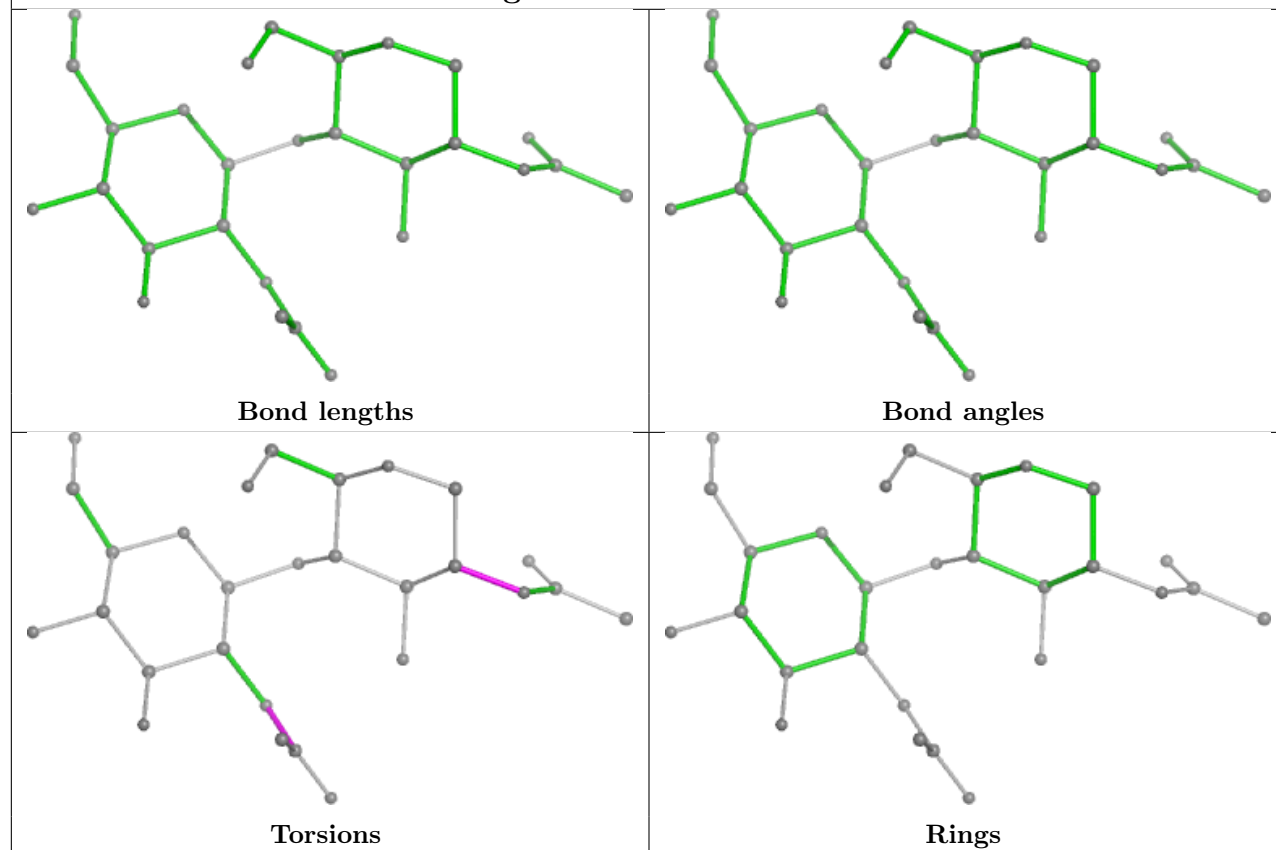
Oligosaccharide Chain R



Oligosaccharide Chain S



Oligosaccharide Chain T



5.6 Ligand geometry

15 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	C	502	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NCT	A	503	-	13,13,13	0.49	0	17,17,17	0.52	0
4	NAG	E	501	1	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	C	501	1	14,14,15	0.23	0	17,19,21	0.56	0
4	NAG	D	502	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	E	502	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NCT	B	503	-	13,13,13	0.49	0	17,17,17	0.48	0
4	NAG	B	501	1	14,14,15	0.22	0	17,19,21	0.55	0
5	NCT	C	503	-	13,13,13	0.46	0	17,17,17	0.59	0
5	NCT	E	503	-	13,13,13	0.44	0	17,17,17	0.63	0
4	NAG	A	502	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	B	502	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.55	0
5	NCT	D	503	-	13,13,13	0.44	0	17,17,17	0.62	0
4	NAG	D	501	1	14,14,15	0.22	0	17,19,21	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	502	1	-	3/6/23/26	0/1/1/1
5	NCT	A	503	-	-	0/4/14/14	0/2/2/2
4	NAG	E	501	1	-	5/6/23/26	0/1/1/1
4	NAG	C	501	1	-	5/6/23/26	0/1/1/1
4	NAG	D	502	1	-	3/6/23/26	0/1/1/1
4	NAG	E	502	1	-	3/6/23/26	0/1/1/1
5	NCT	B	503	-	-	4/4/14/14	0/2/2/2
4	NAG	B	501	1	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NCT	C	503	-	-	0/4/14/14	0/2/2/2
5	NCT	E	503	-	-	2/4/14/14	0/2/2/2
4	NAG	A	502	1	-	3/6/23/26	0/1/1/1
4	NAG	B	502	1	-	3/6/23/26	0/1/1/1
4	NAG	A	501	1	-	5/6/23/26	0/1/1/1
5	NCT	D	503	-	-	2/4/14/14	0/2/2/2
4	NAG	D	501	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	503	NCT	C1-C2-C6-C7
5	E	503	NCT	C1-C2-C6-C7
4	A	501	NAG	O5-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6

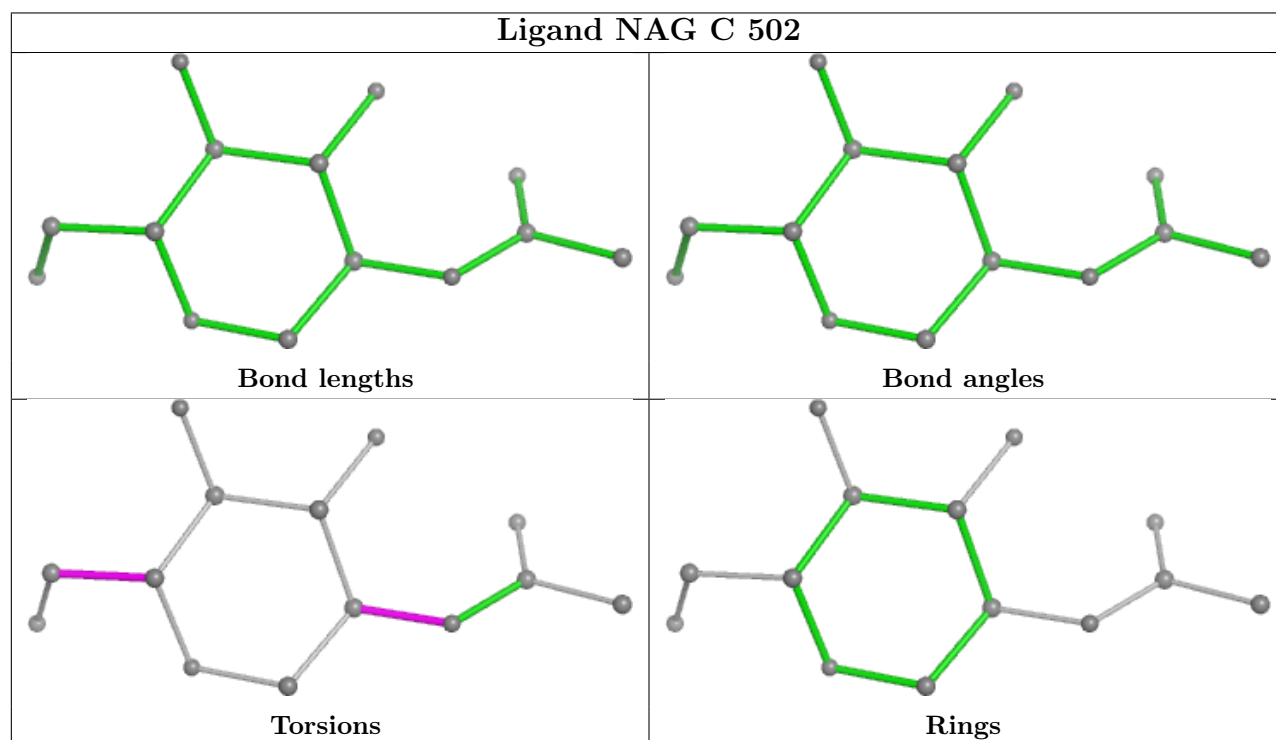
There are no ring outliers.

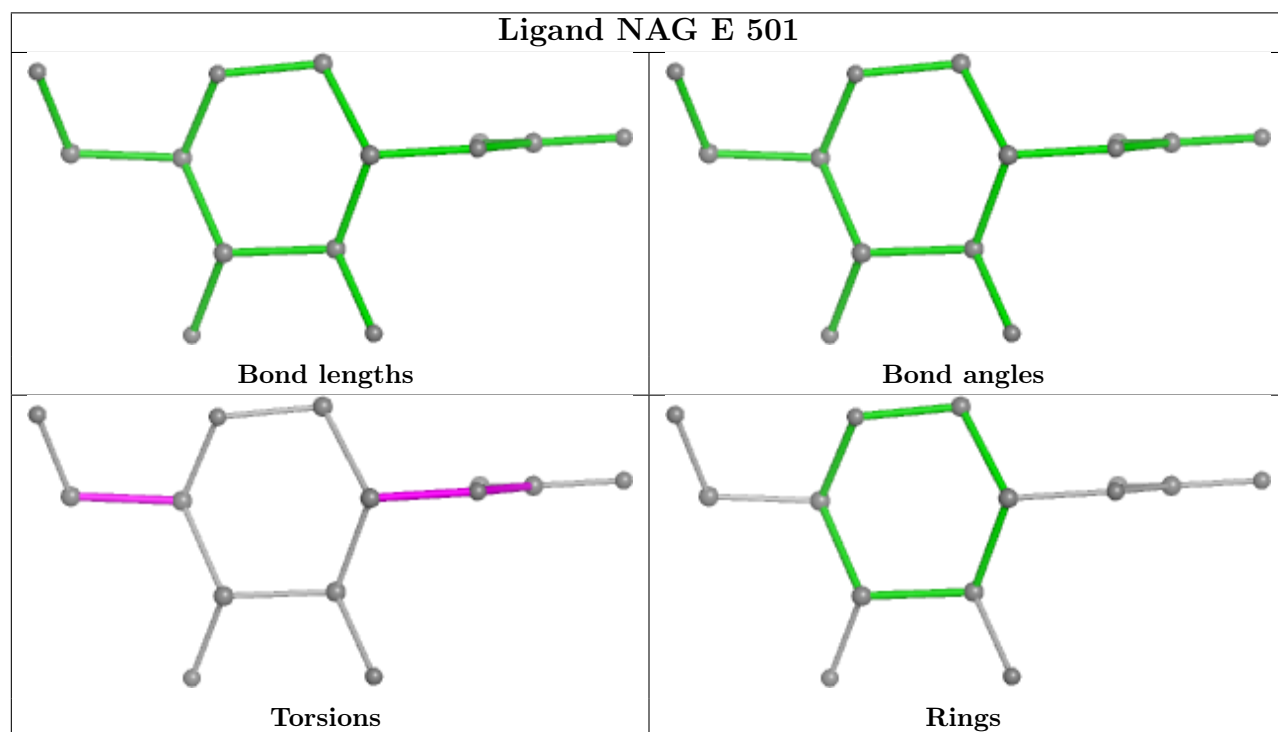
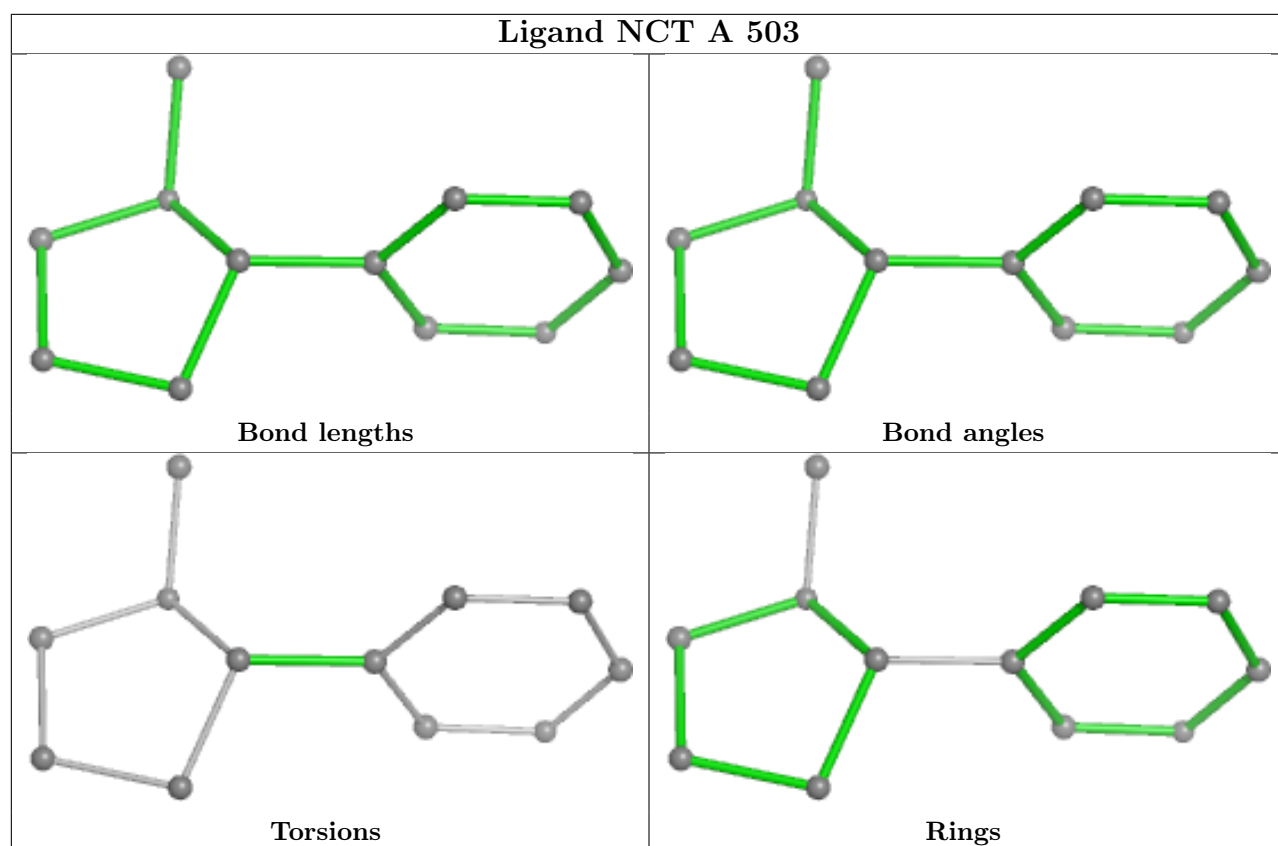
8 monomers are involved in 23 short contacts:

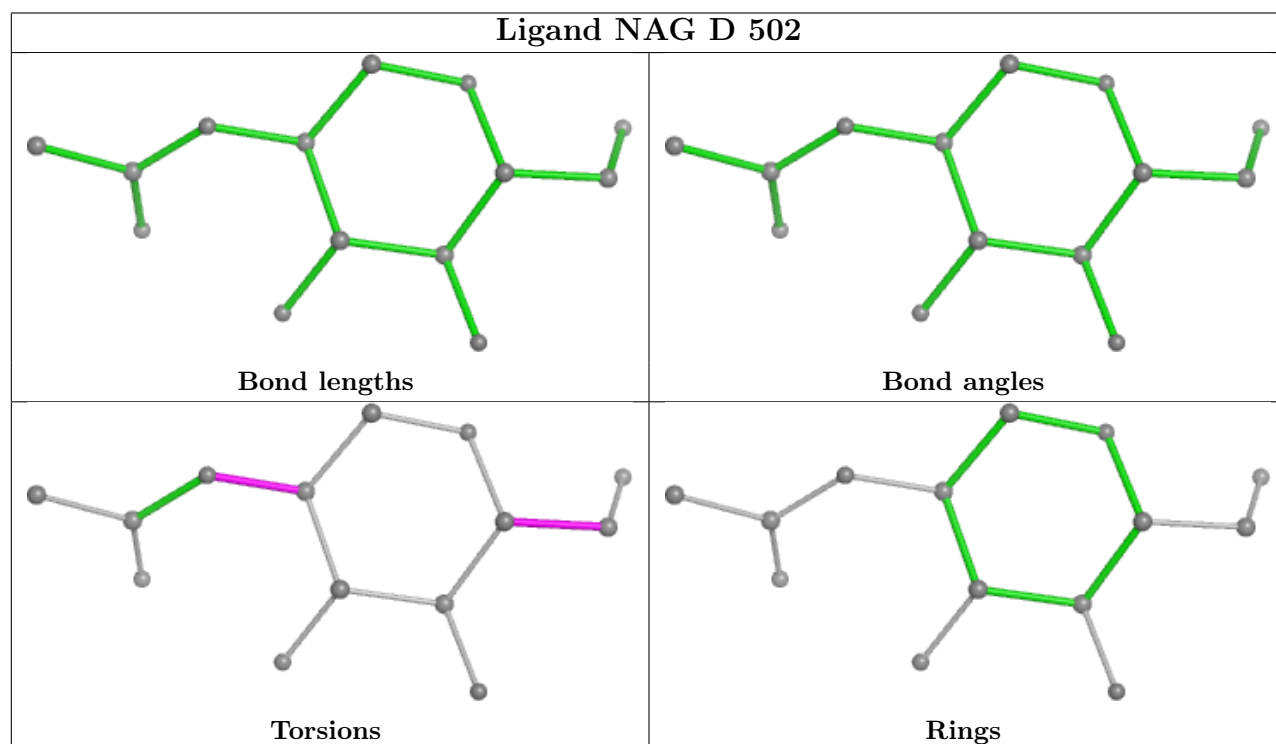
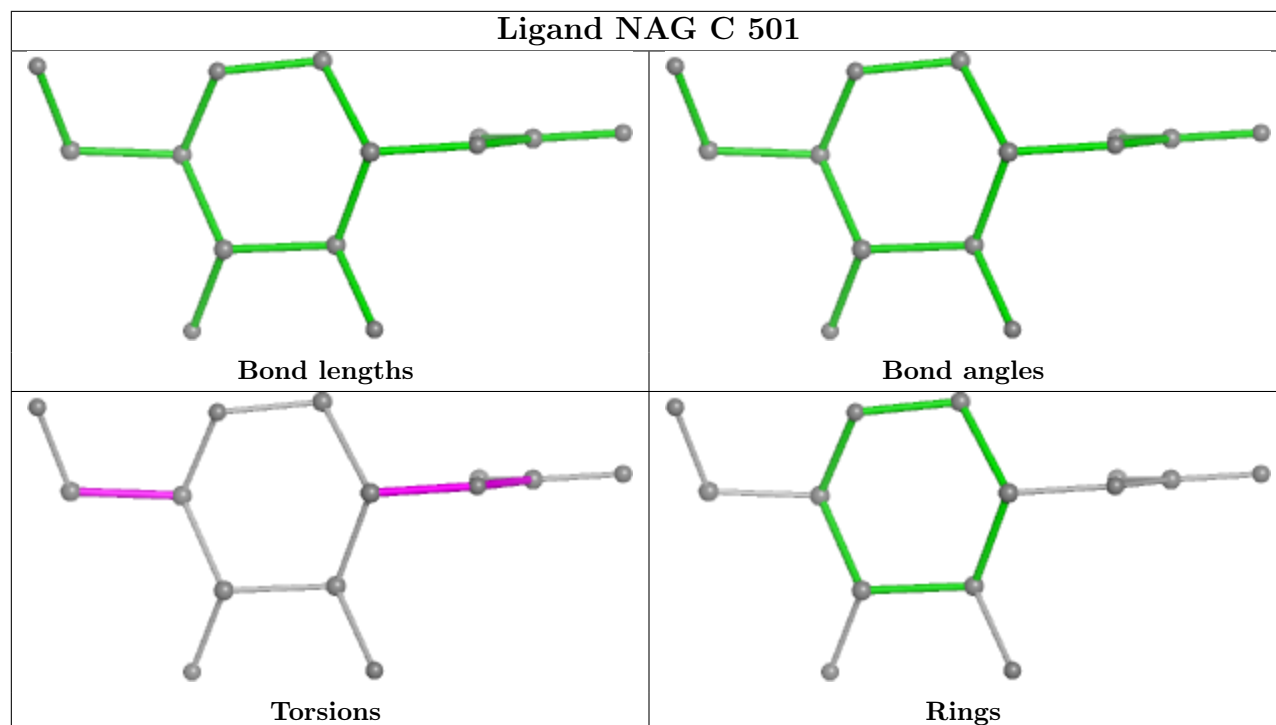
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	NCT	1	0
4	E	501	NAG	4	0
4	C	501	NAG	4	0
4	B	501	NAG	4	0
5	E	503	NCT	1	0
4	A	501	NAG	4	0
5	D	503	NCT	1	0
4	D	501	NAG	4	0

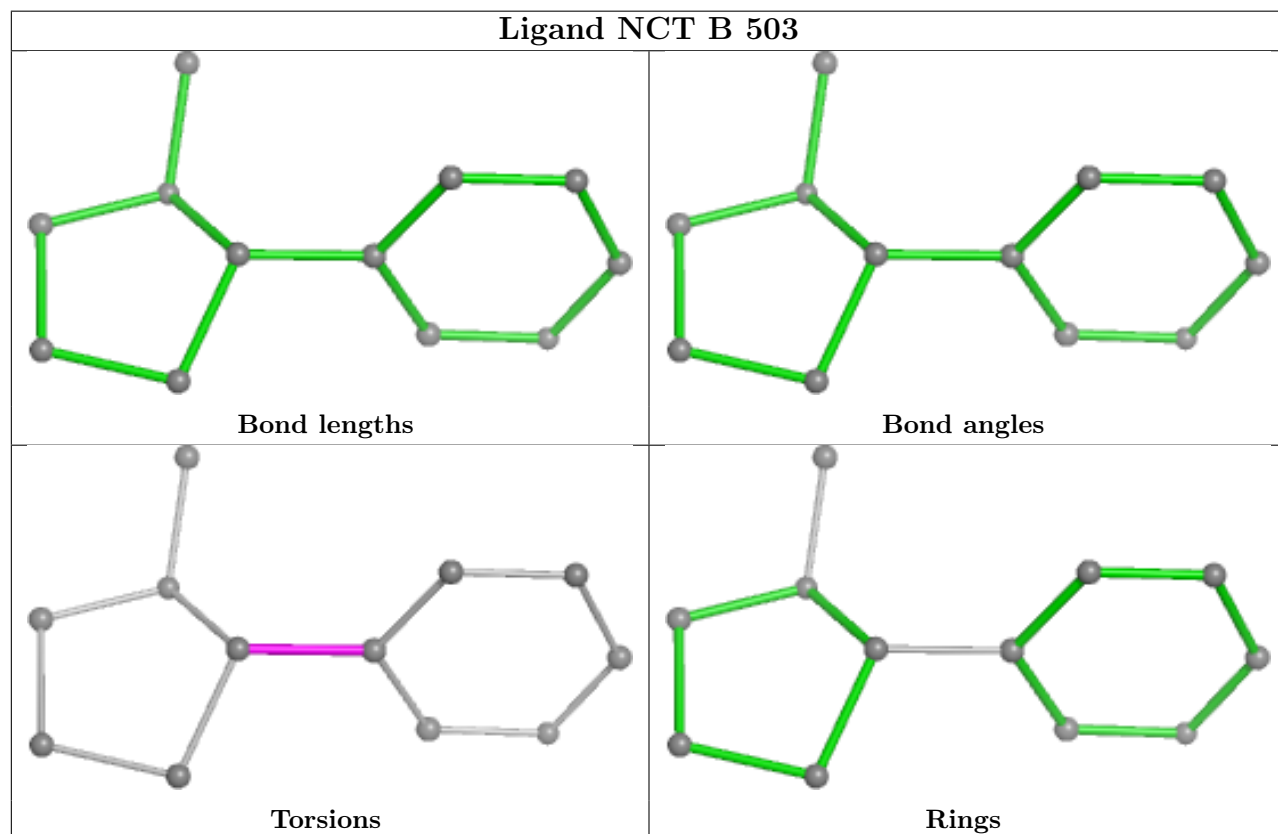
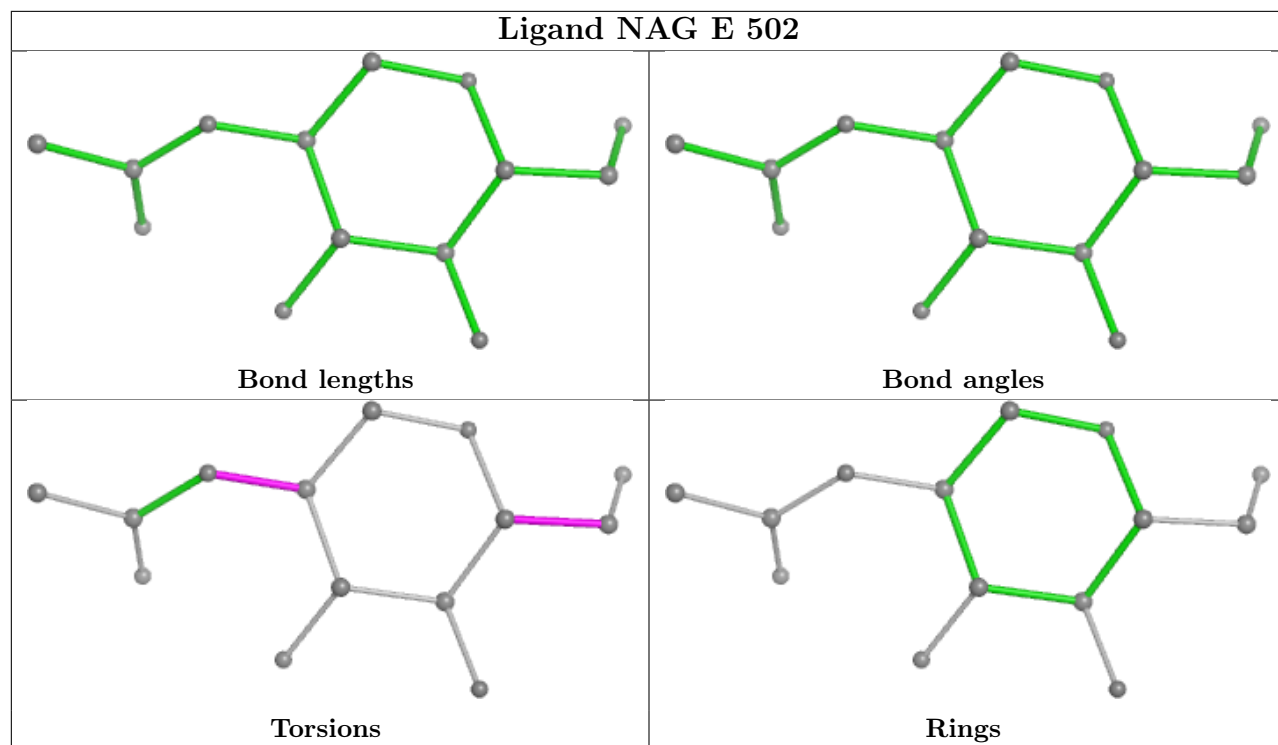
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

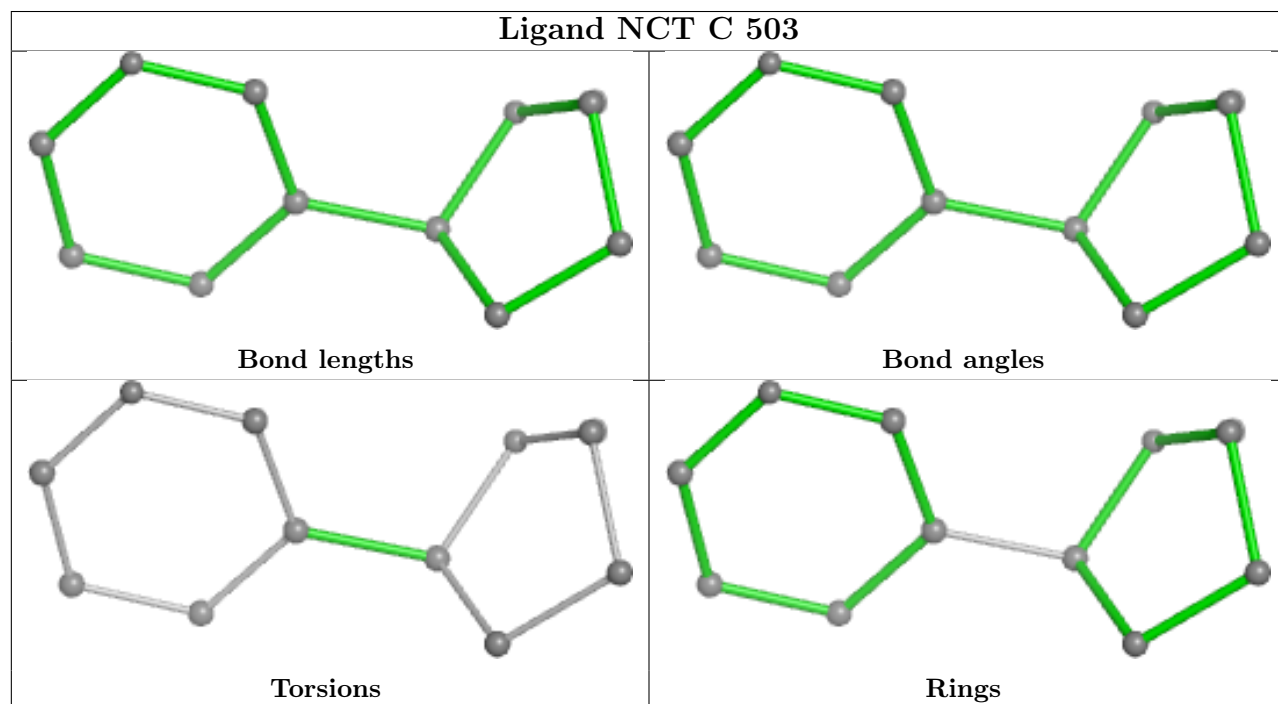
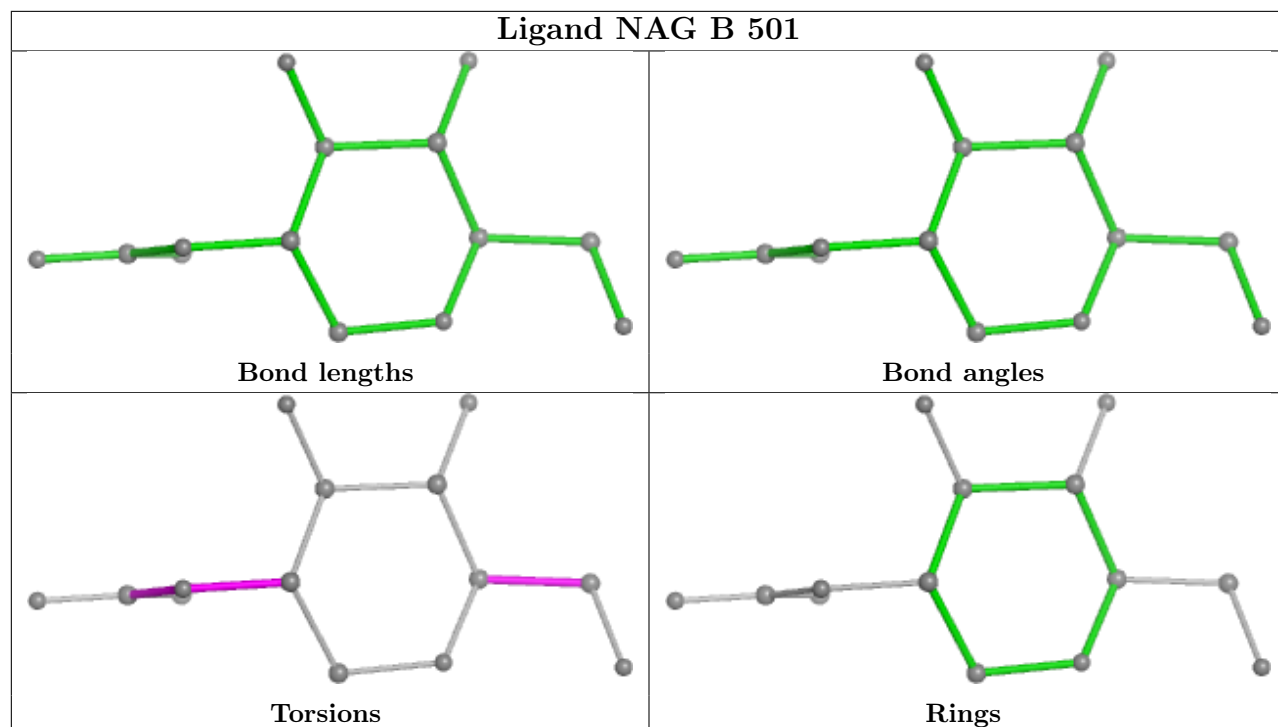
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

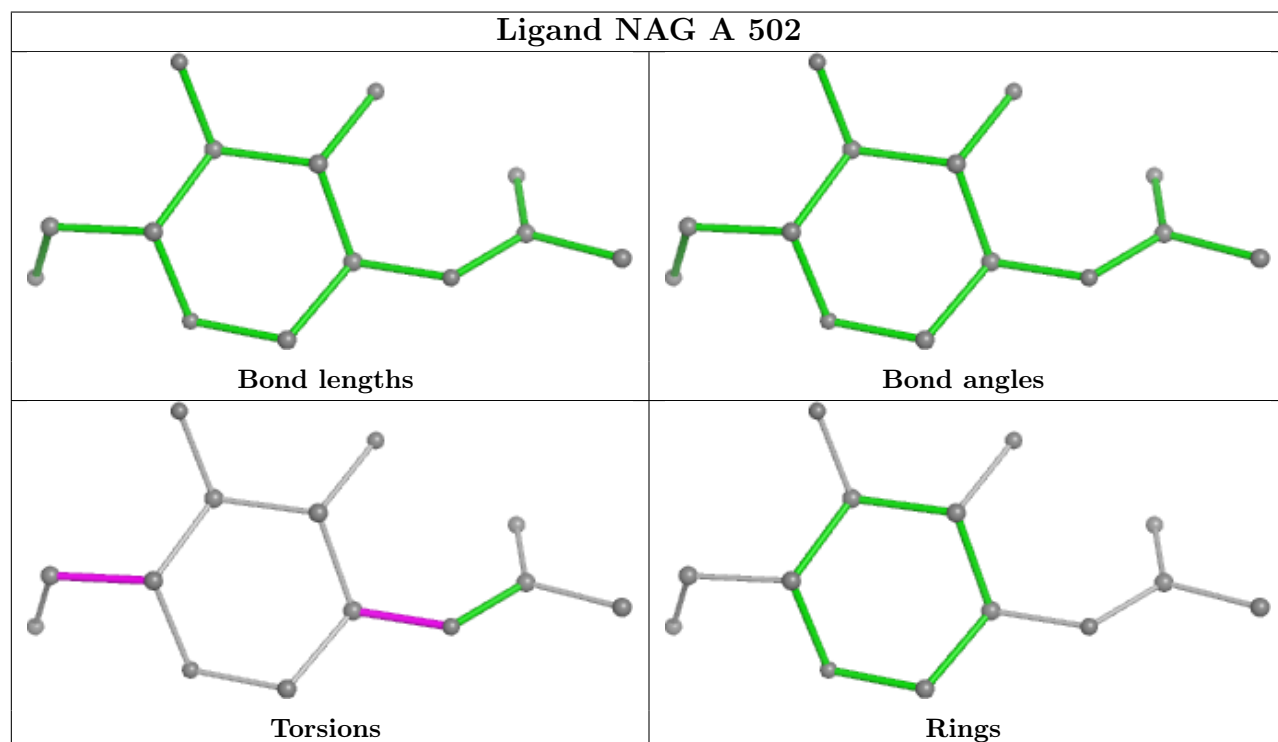
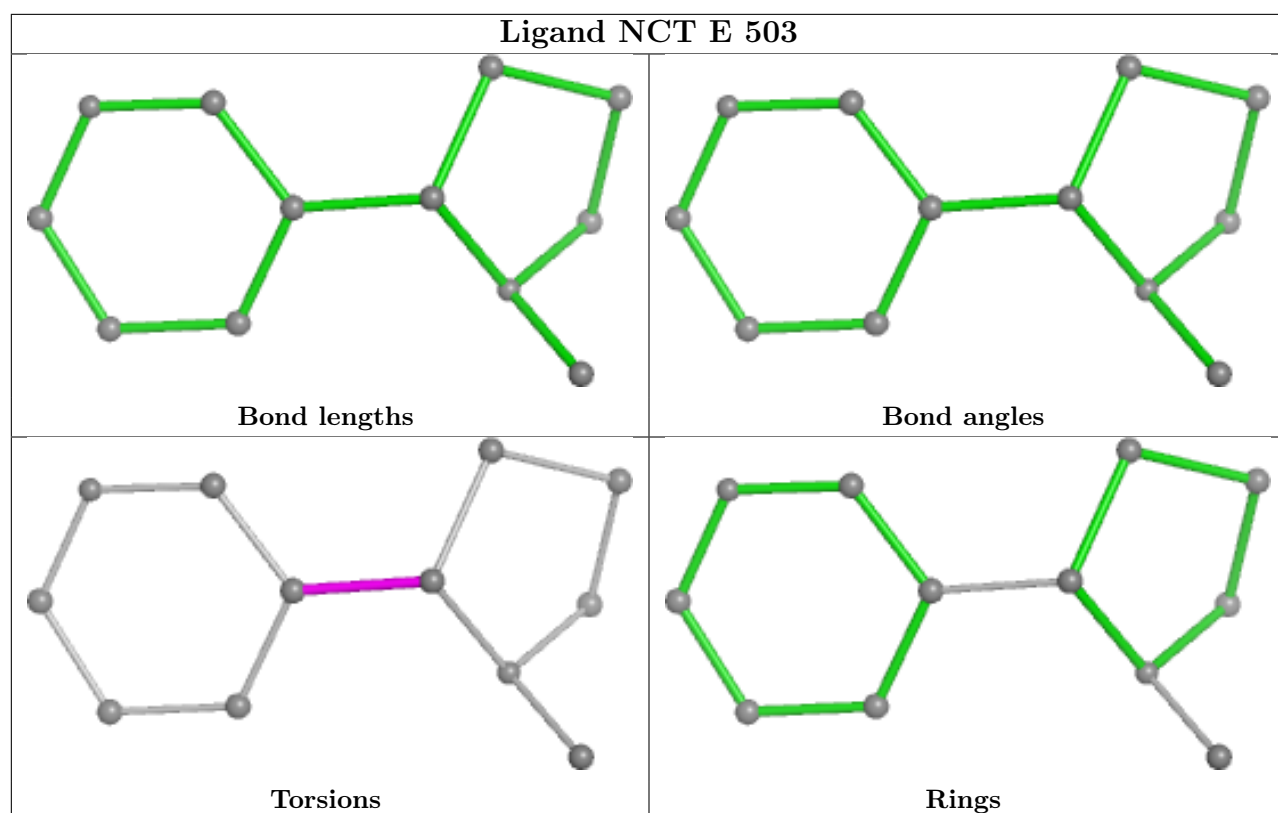


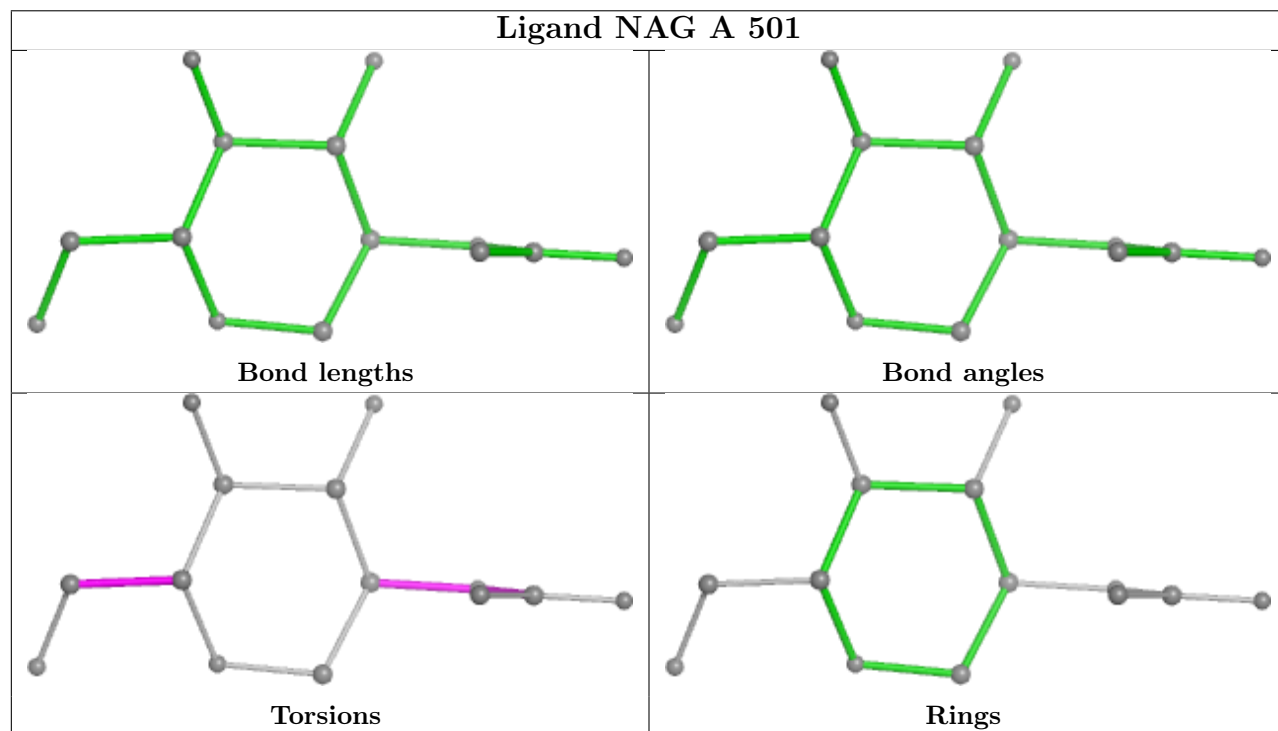
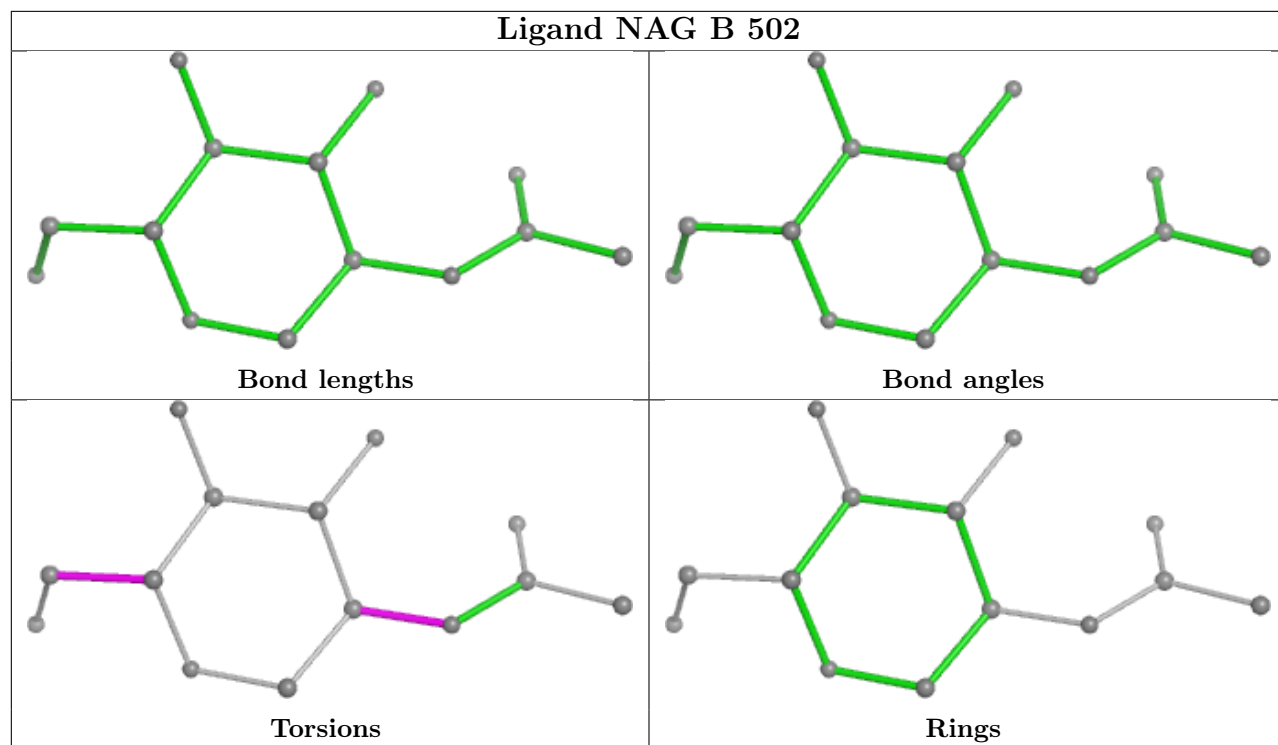


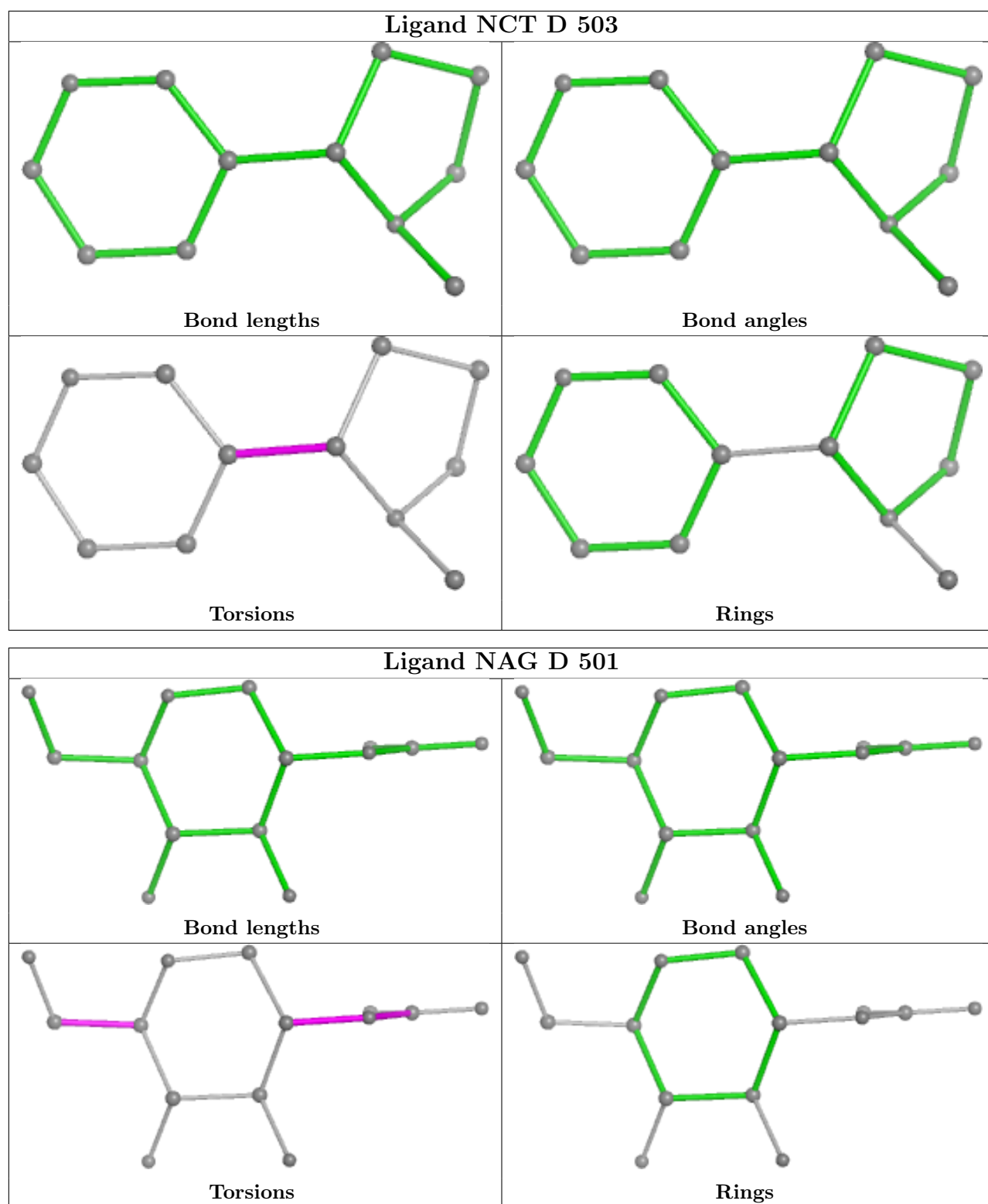












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

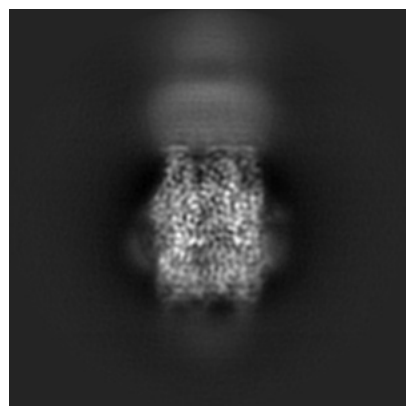
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16534. These allow visual inspection of the internal detail of the map and identification of artifacts.

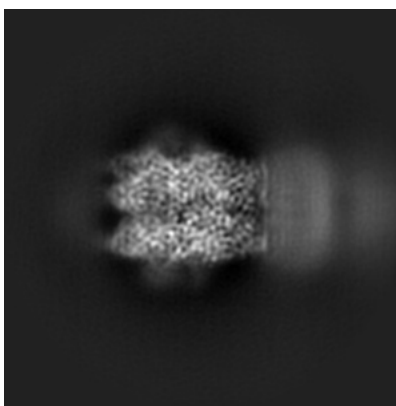
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

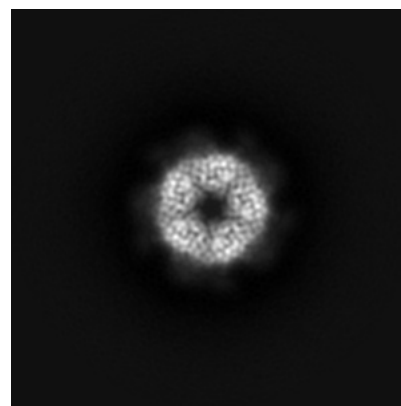
6.1.1 Primary map



X

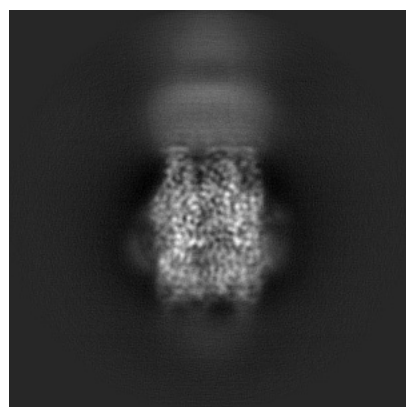


Y

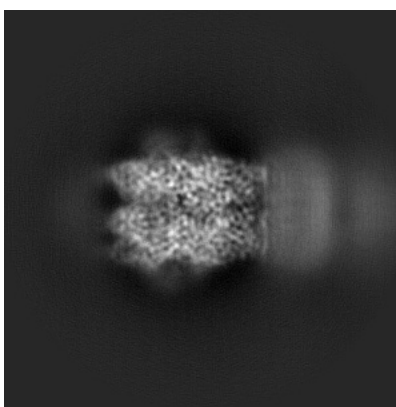


Z

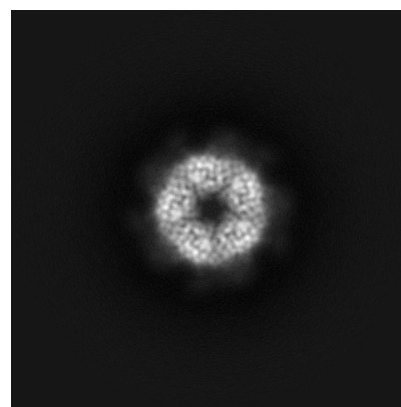
6.1.2 Raw map



X



Y

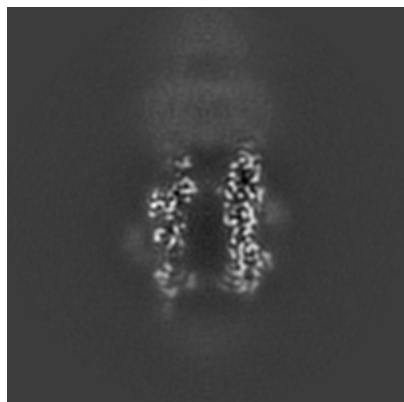


Z

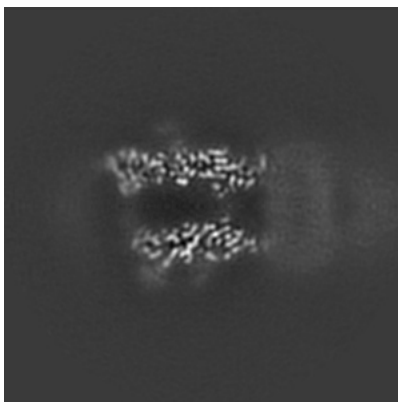
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

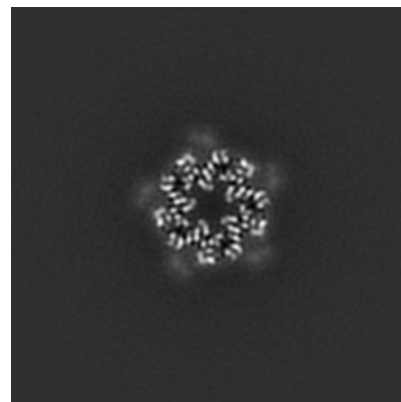
6.2.1 Primary map



X Index: 150

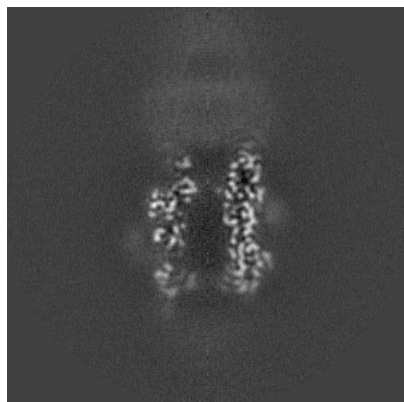


Y Index: 150

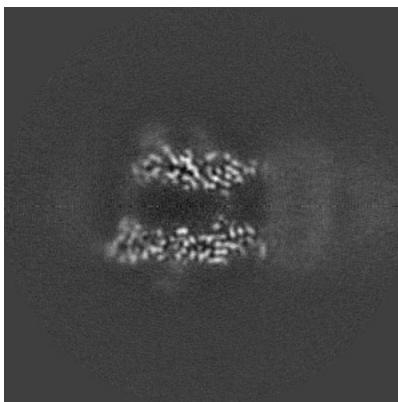


Z Index: 150

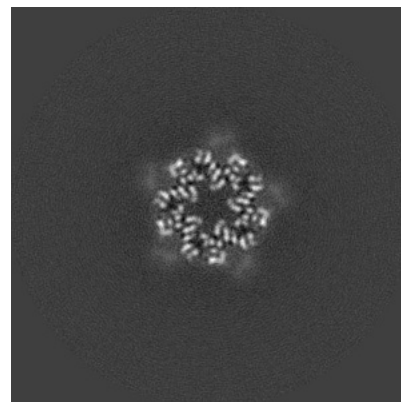
6.2.2 Raw map



X Index: 150



Y Index: 150

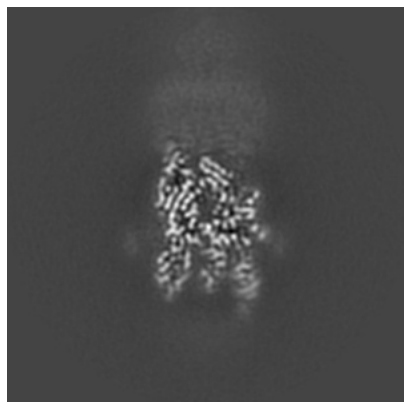


Z Index: 150

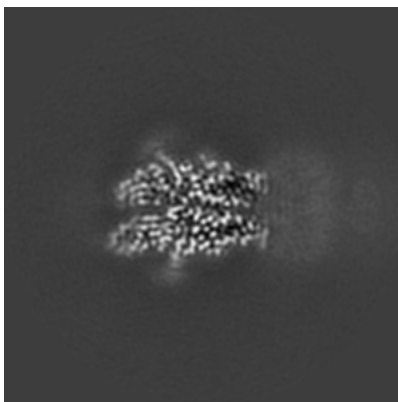
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

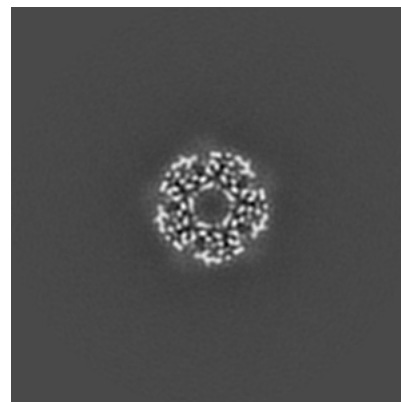
6.3.1 Primary map



X Index: 168

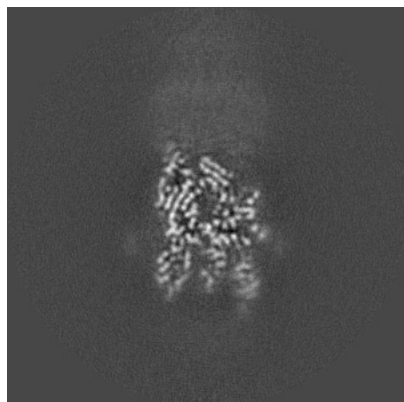


Y Index: 128

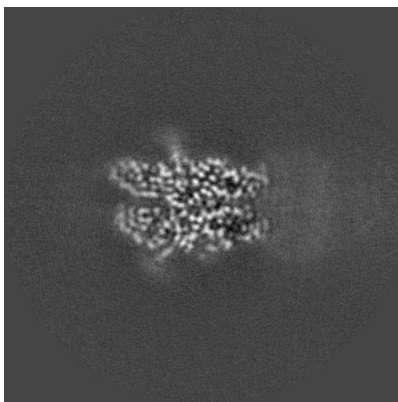


Z Index: 157

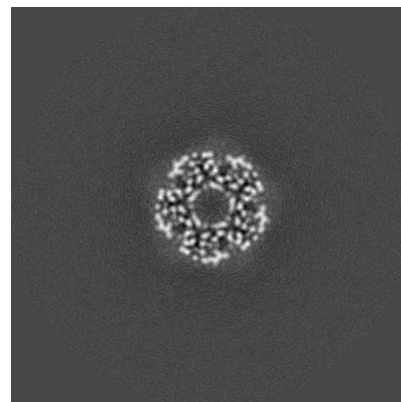
6.3.2 Raw map



X Index: 132



Y Index: 127

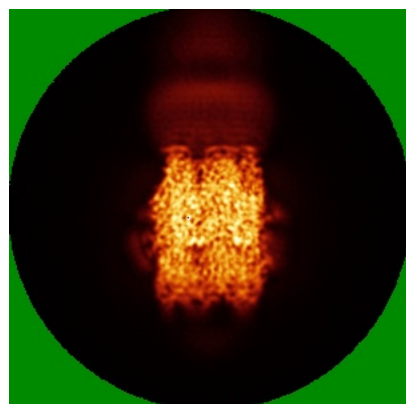


Z Index: 157

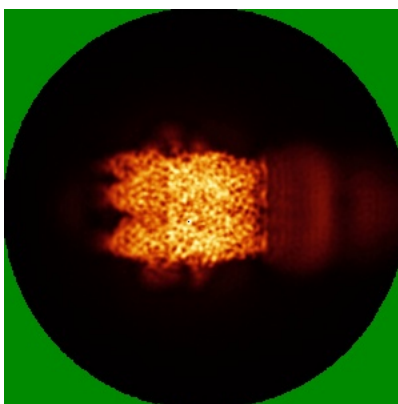
The images above show the largest variance slices of the map in three orthogonal directions.

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

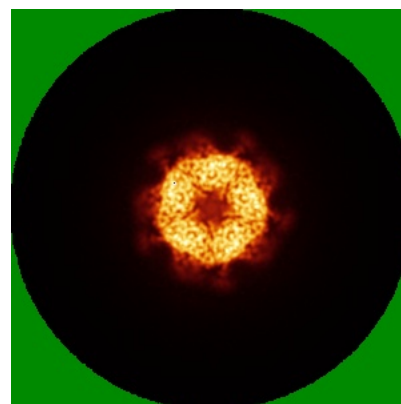
6.4.1 Primary map



X

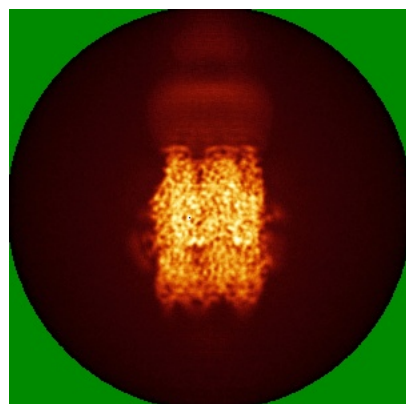


Y

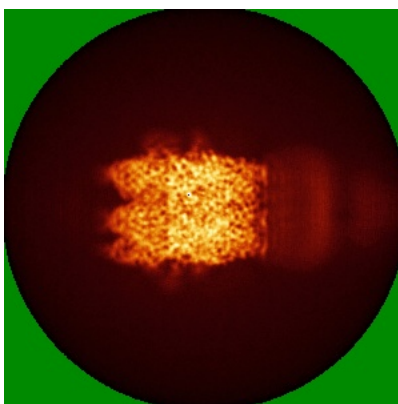


Z

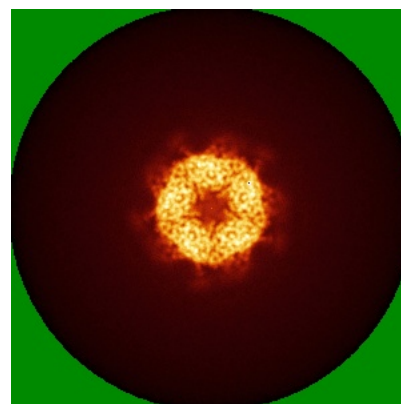
6.4.2 Raw map



X



Y

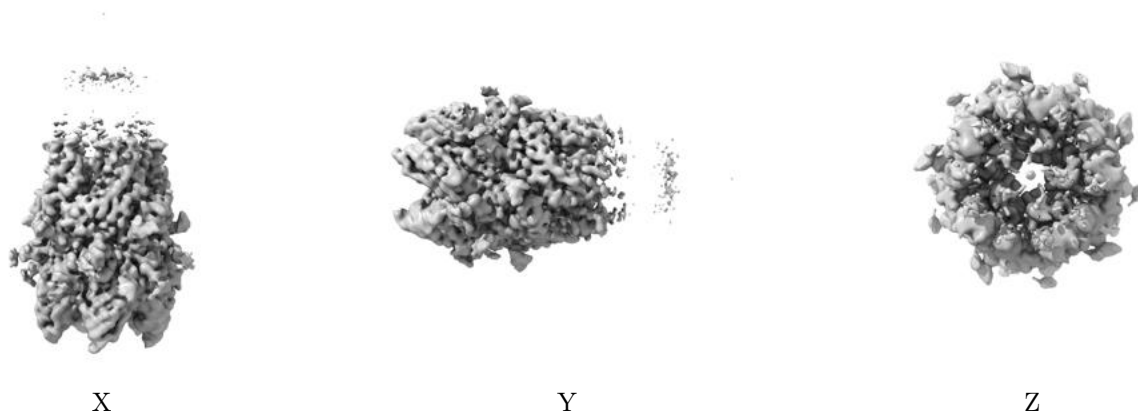


Z

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.

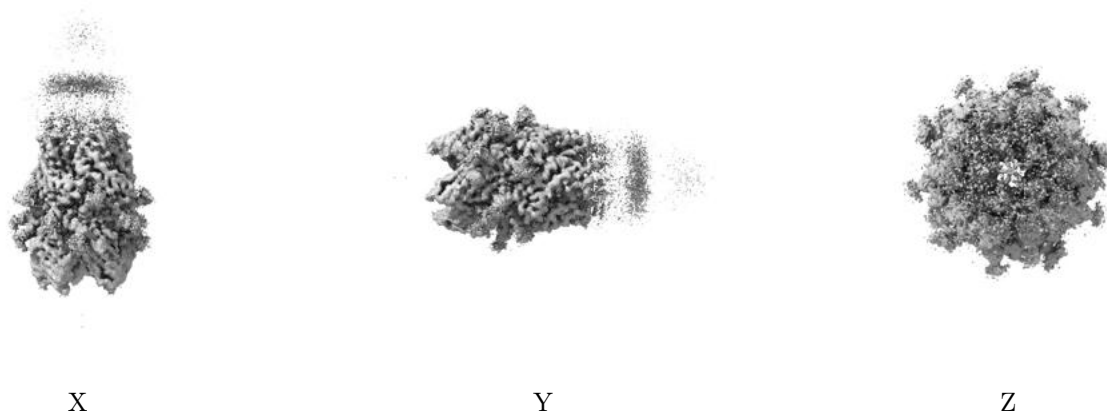
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00248. 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.

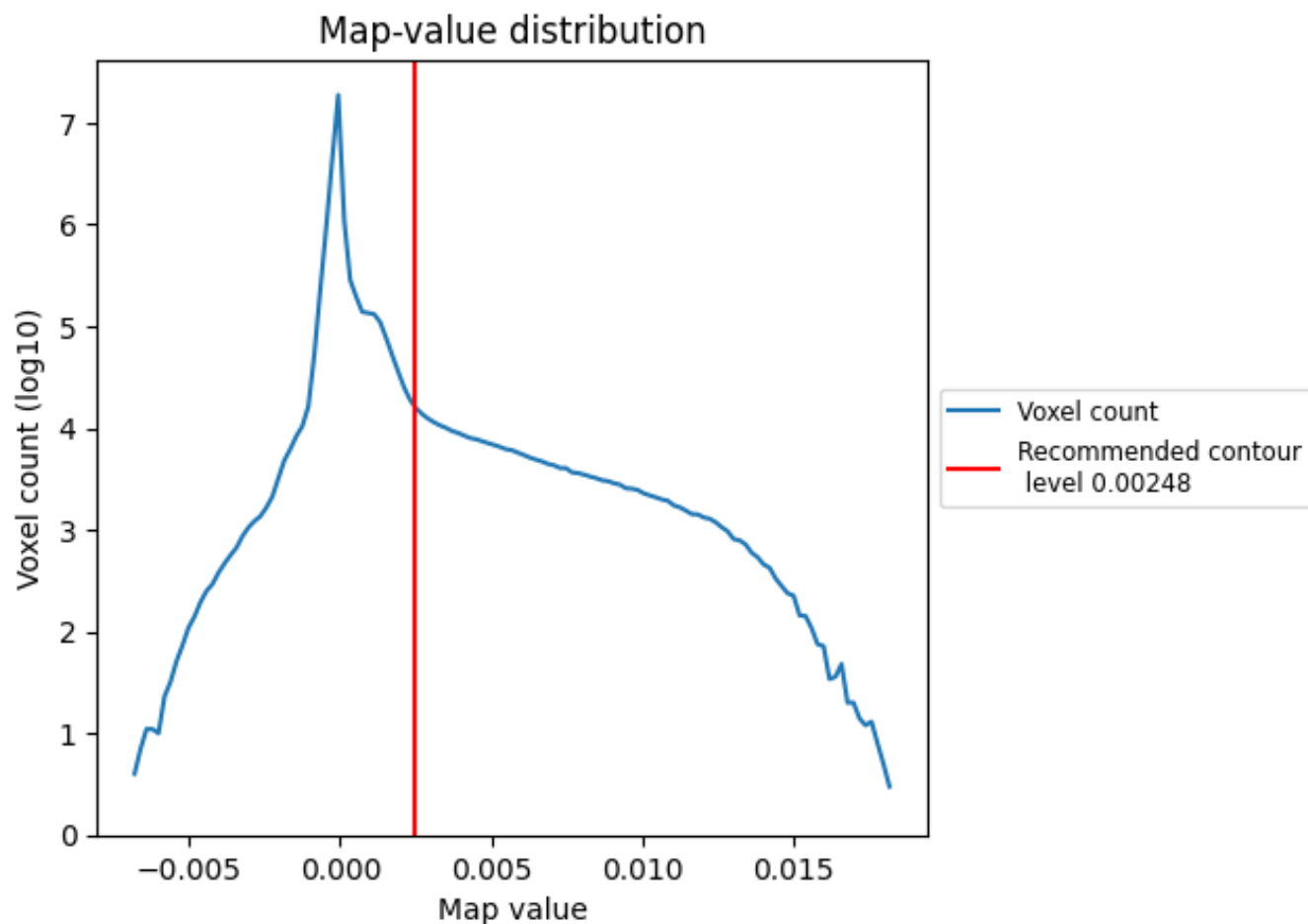
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

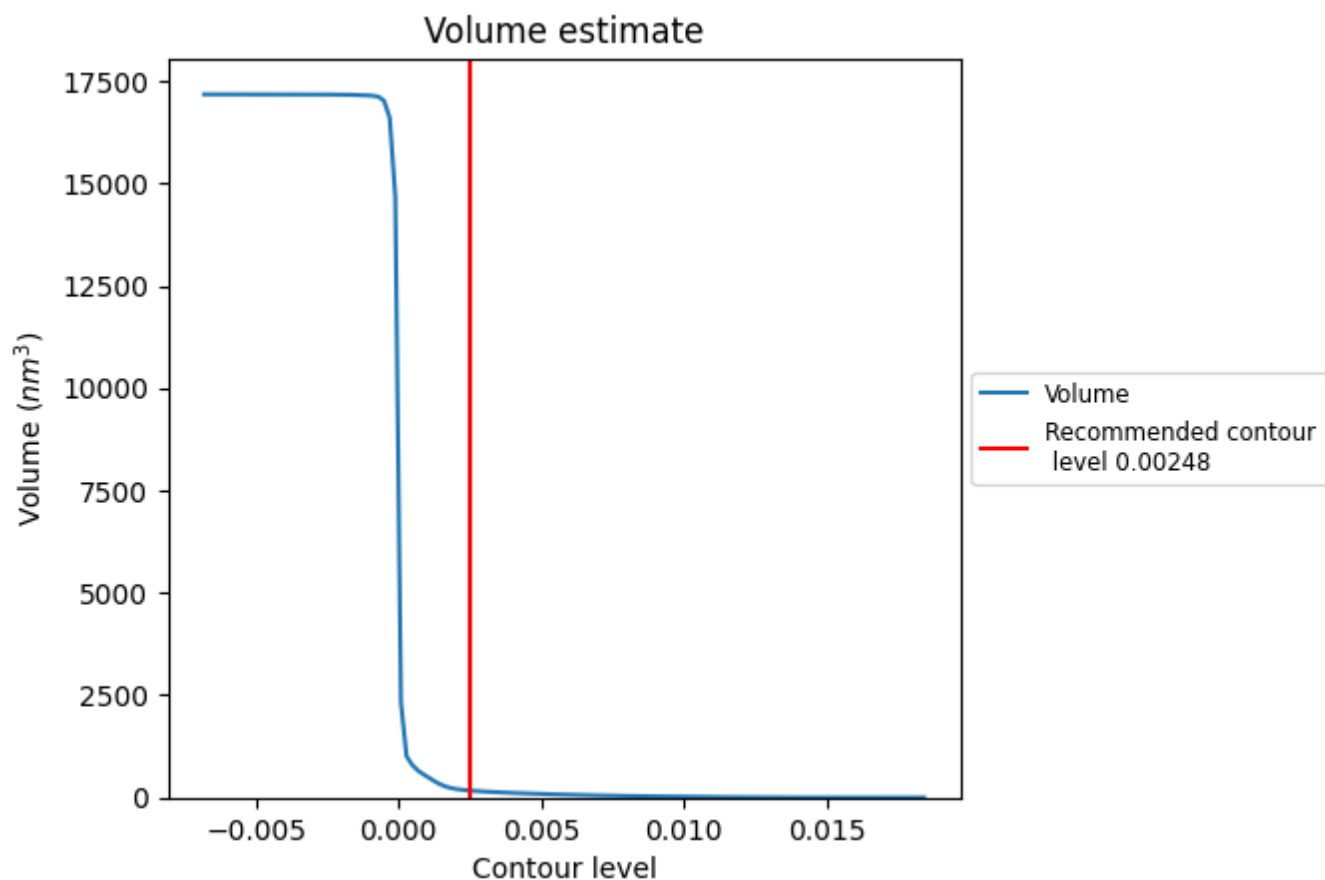
This section contains the results of statistical analysis of the map.

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.

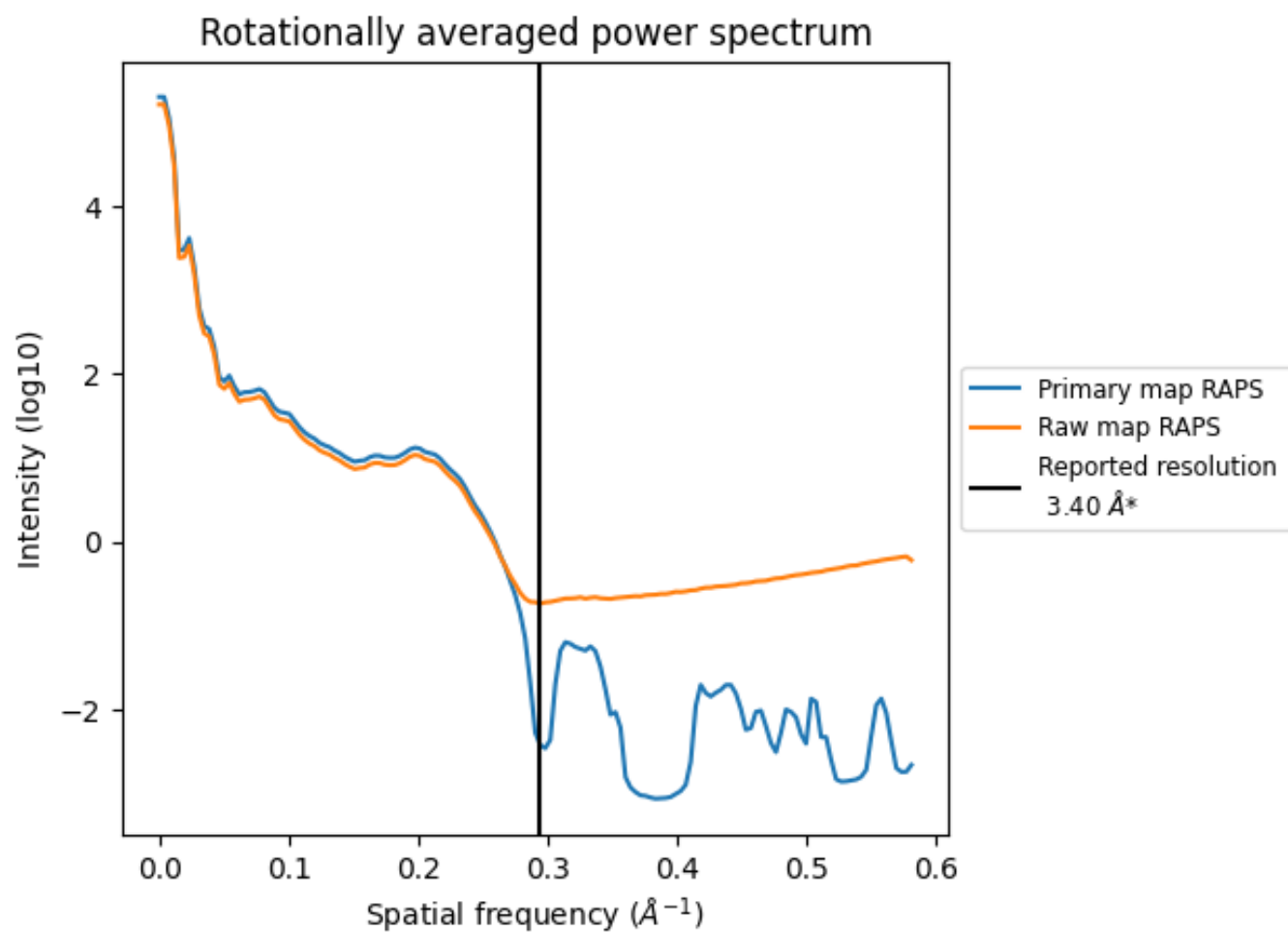
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm³; this corresponds to an approximate mass of 155 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 ⓘ

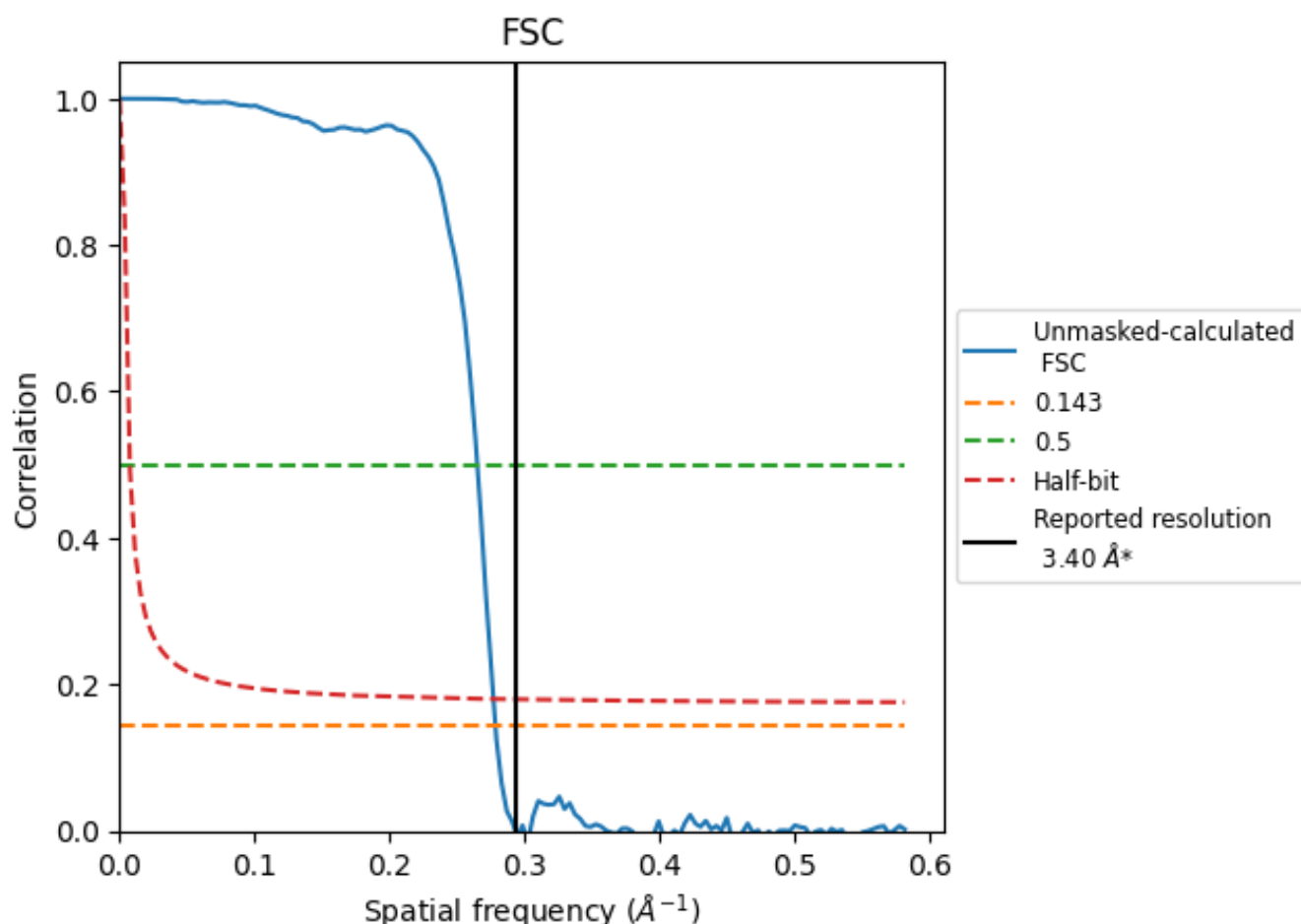


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

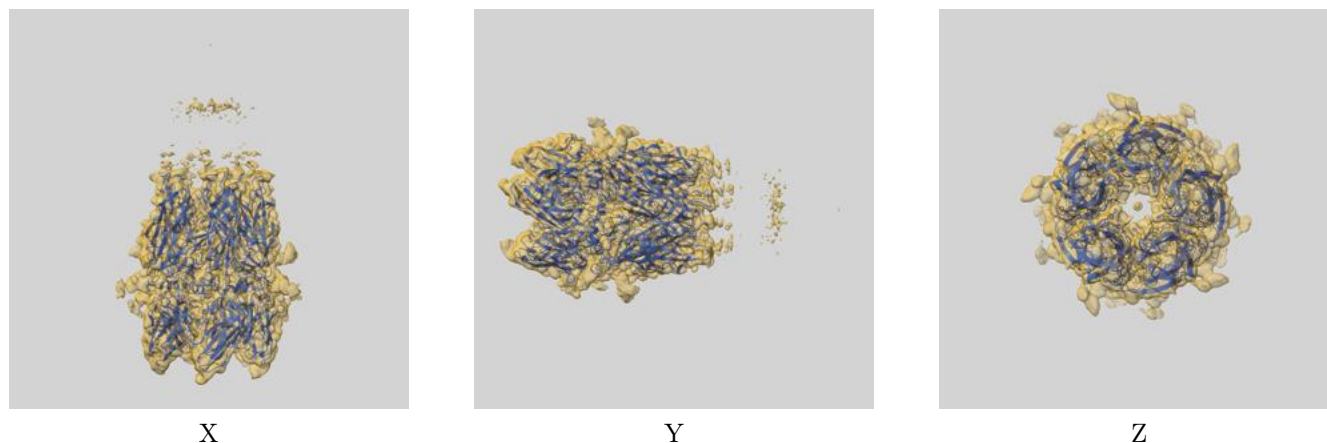
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	3.78	3.61

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

9 Map-model fit [i](#)

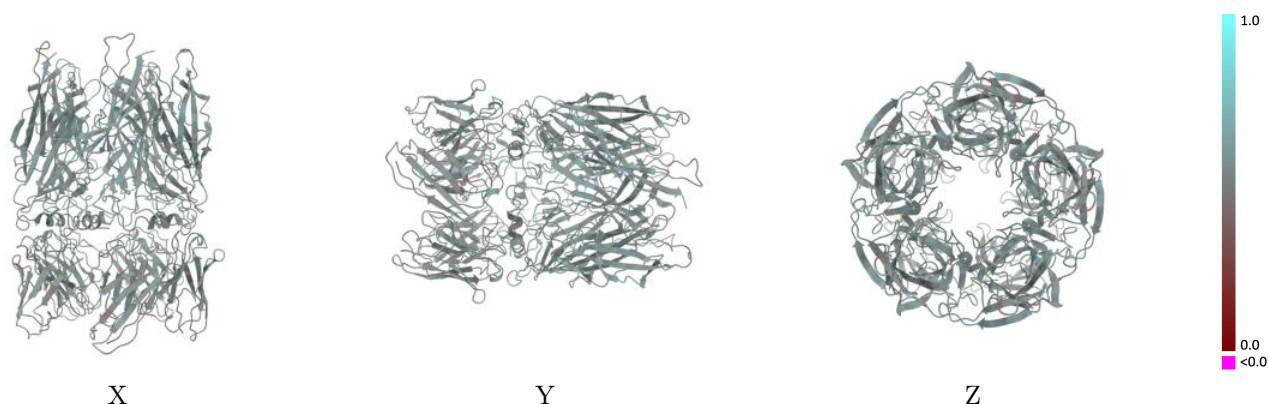
This section contains information regarding the fit between EMDB map EMD-16534 and PDB model 8CAU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



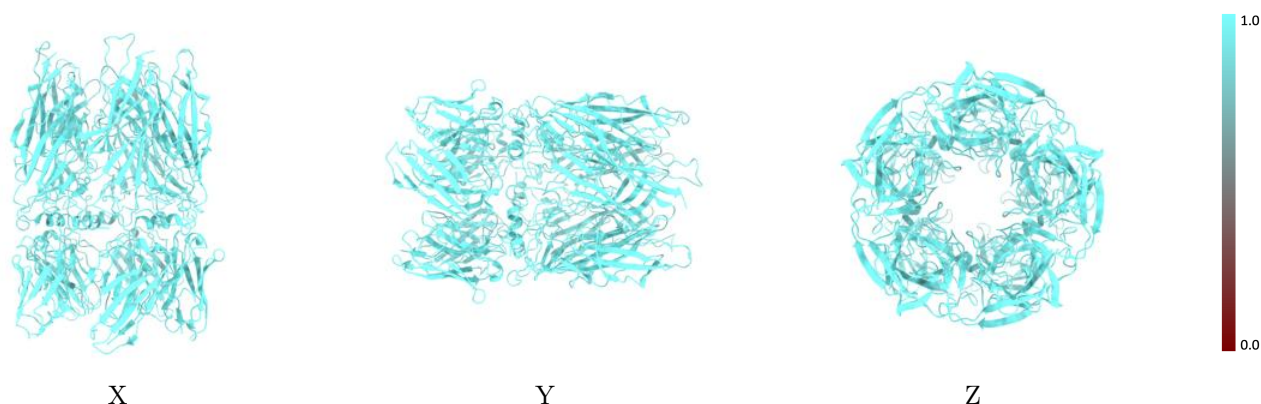
The images above show the 3D surface view of the map at the recommended contour level 0.00248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



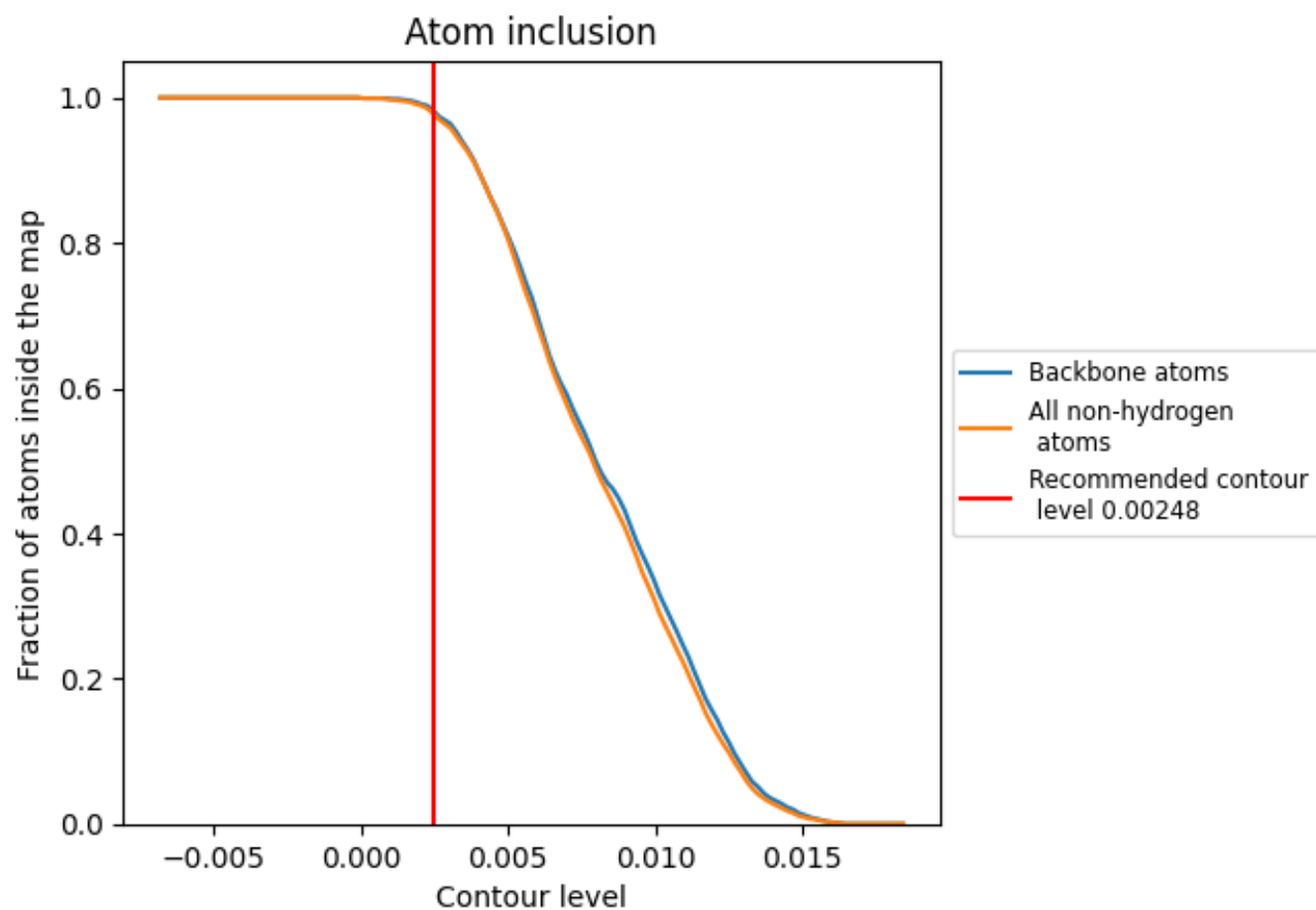
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00248).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.00248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9770	<div></div> 0.5230
A	<div></div> 0.9780	<div></div> 0.5340
B	<div></div> 0.9780	<div></div> 0.5330
C	<div></div> 0.9770	<div></div> 0.5350
D	<div></div> 0.9770	<div></div> 0.5360
E	<div></div> 0.9740	<div></div> 0.5340
F	<div></div> 0.9800	<div></div> 0.5030
G	<div></div> 0.9790	<div></div> 0.5050
H	<div></div> 0.9800	<div></div> 0.5050
I	<div></div> 0.9800	<div></div> 0.5030
J	<div></div> 0.9800	<div></div> 0.5020
P	<div></div> 0.9290	<div></div> 0.4100
Q	<div></div> 0.9290	<div></div> 0.4100
R	<div></div> 0.9290	<div></div> 0.4180
S	<div></div> 0.9290	<div></div> 0.4220
T	<div></div> 0.9290	<div></div> 0.4270

