



## wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 12:20 PM EDT

PDB ID : 9DMQ / pdb\_00009dmq  
EMDB ID : EMD-47013  
Title : Human muscle nAChR with fab3-bound  
Authors : Li, H.; Hibbs, R.E.  
Deposited on : 2024-09-14  
Resolution : 2.06 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
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) : 2.42

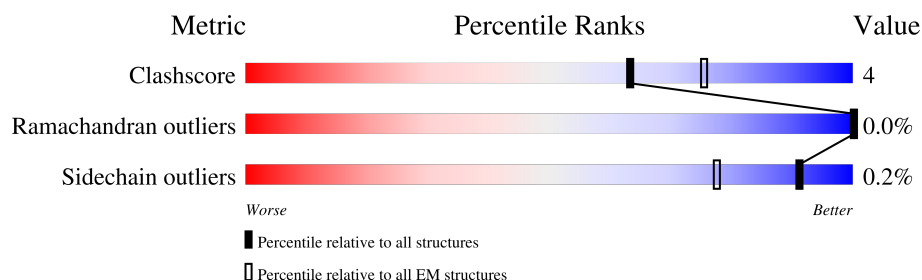
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.06 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  $\geq 3$ , 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	457	
1	C	457	
2	E	503	
3	D	517	
4	B	493	
5	F	275	
6	G	235	
7	H	5	

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Mol	Chain	Length	Quality of chain
7	N	5	
8	I	7	
9	J	6	
9	L	6	
10	K	2	
10	M	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	POV	B	503	-	-	X	-
14	NAG	D	501	X	-	-	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 41371 atoms, of which 20734 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 Acetylcholine receptor subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	399	Total	C	H	N	O	S	0	0
			6436	2093	3234	513	577	19		
1	C	401	Total	C	H	N	O	S	0	0
			6487	2109	3264	516	579	19		

- Molecule 2 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	405	Total	C	H	N	O	S	0	0
			6576	2139	3295	541	591	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	479	SER	-	expression tag	UNP P11230
E	480	ARG	-	expression tag	UNP P11230

- Molecule 3 is a protein called Acetylcholine receptor subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	433	Total	C	H	N	O	S	0	0
			7054	2295	3534	582	629	14		

- Molecule 4 is a protein called Acetylcholine receptor subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	411	Total	C	H	N	O	S	0	0
			6482	2102	3230	533	603	14		

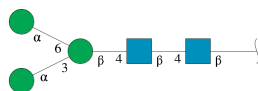
- Molecule 5 is a protein called Fab3 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	227	Total	C	H	N	O	S	0	0
			3426	1104	1689	297	332	4		

- Molecule 6 is a protein called Fab3 light chain.

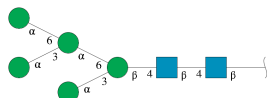
Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	213	Total	C	H	N	O	S	0	0
			3242	1028	1592	285	331	6		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



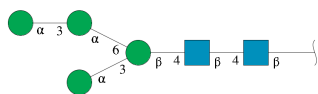
Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	5	Total	C	H	N	O	0	0
			113	34	52	2	25		
7	N	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	I	7	Total	C	H	N	O	0	0
			153	46	70	2	35		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



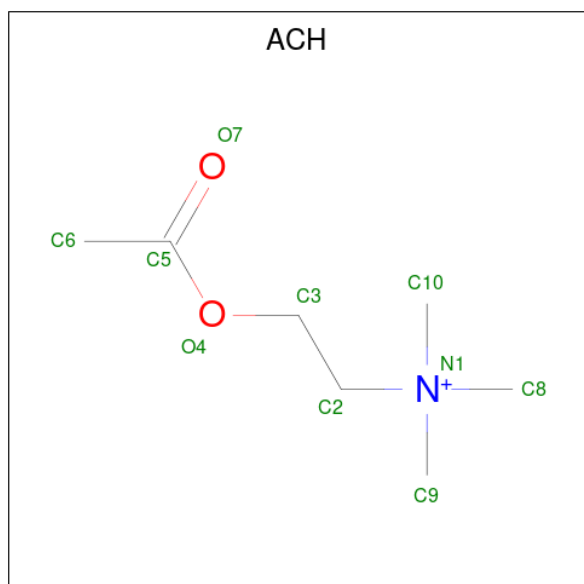
Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	6	Total	C	H	N	O	0	0
			133	40	61	2	30		
9	L	6	Total	C	H	N	O	0	0
			133	40	61	2	30		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



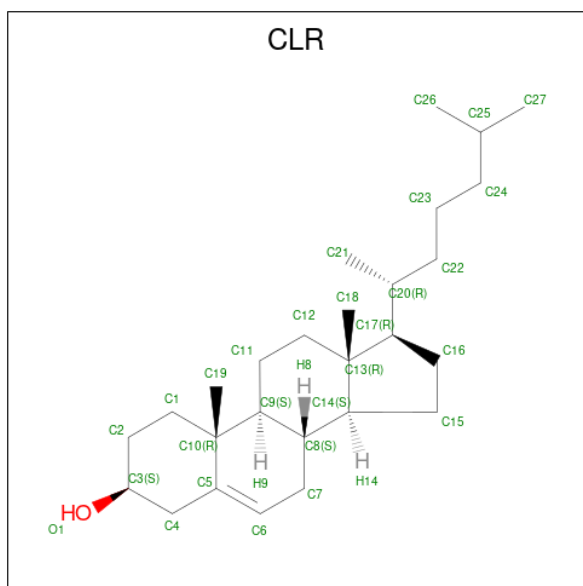
Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
10	M	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 11 is ACETYLCHOLINE (CCD ID: ACH) (formula:  $C_7H_{16}NO_2$ ) (labeled as "Ligand of Interest" by depositor).



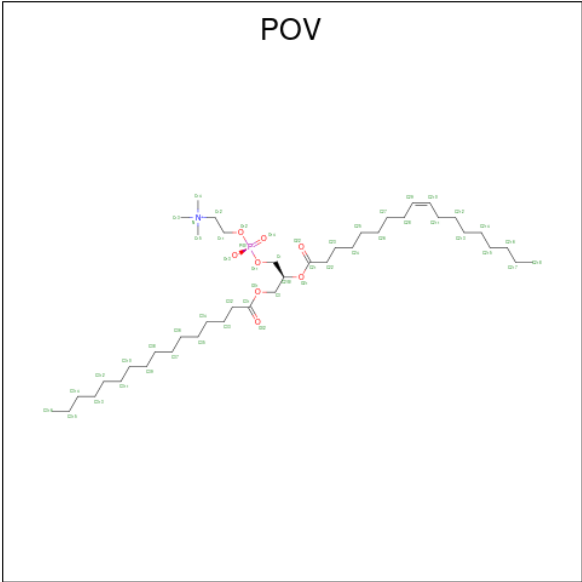
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	H	N	O	0
			26	7	16	1	2	

- Molecule 12 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



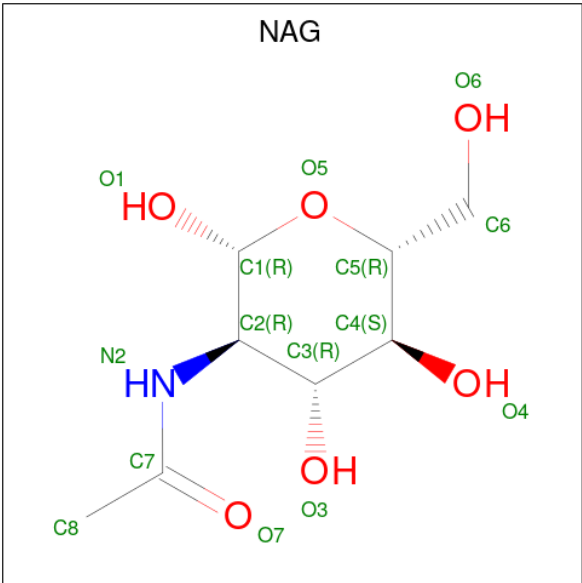
Mol	Chain	Residues	Atoms				AltConf
12	E	1	Total	C	H	O	0
			74	27	46	1	
12	D	1	Total	C	H	O	0
			74	27	46	1	
12	D	1	Total	C	H	O	0
			74	27	46	1	
12	D	1	Total	C	H	O	0
			74	27	46	1	
12	B	1	Total	C	H	O	0
			74	27	46	1	
12	B	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 13 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula:  $C_{42}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms						AltConf
13	E	1	Total	C	H	N	O	P	0
			86	28	48	1	8	1	
13	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
13	D	1	Total	C	H	N	O	P	0
			92	30	52	1	8	1	
13	B	1	Total	C	H	N	O	P	0
			107	34	63	1	8	1	

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms					AltConf
14	D	1	Total	C	H	N	O	0
			27	8	13	1	5	

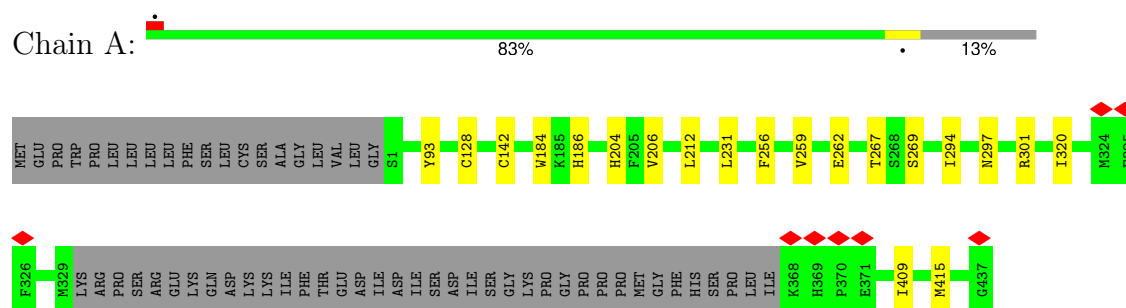
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	O	0
			1	1	

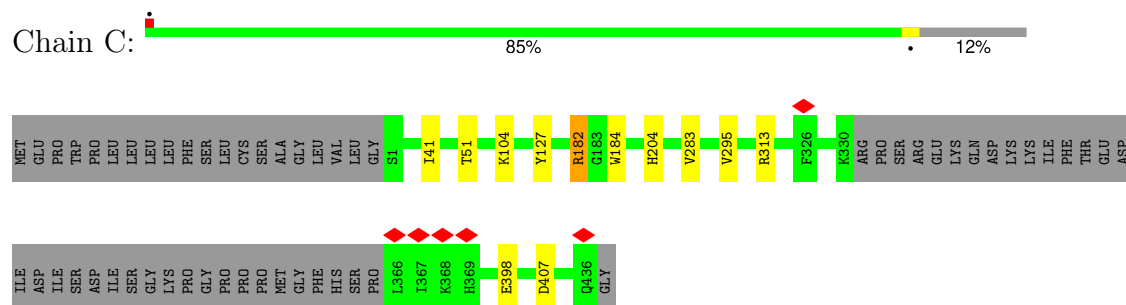
### 3 Residue-property plots

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.

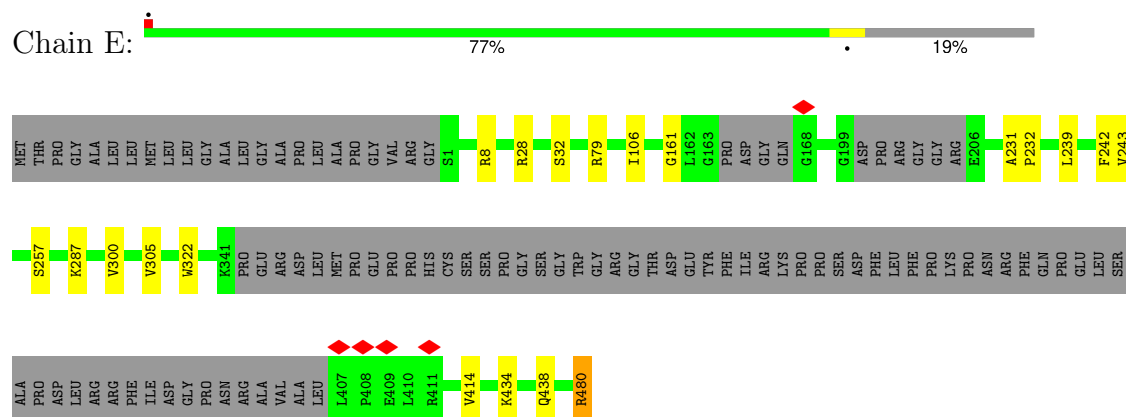
- Molecule 1: Acetylcholine receptor subunit alpha




- Molecule 1: Acetylcholine receptor subunit alpha

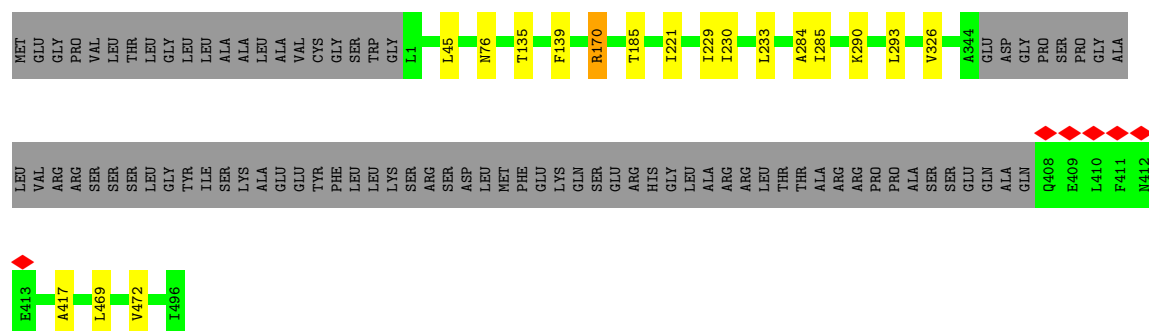


- Molecule 2: Acetylcholine receptor subunit beta




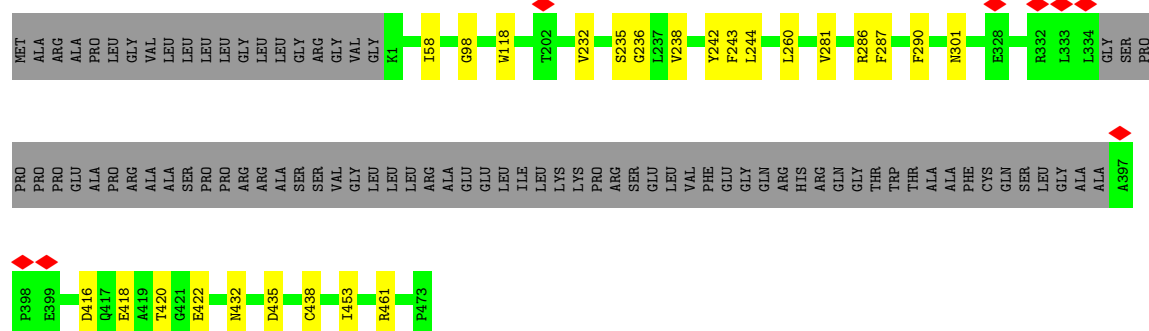
- Molecule 3: Acetylcholine receptor subunit delta

Chain D: 




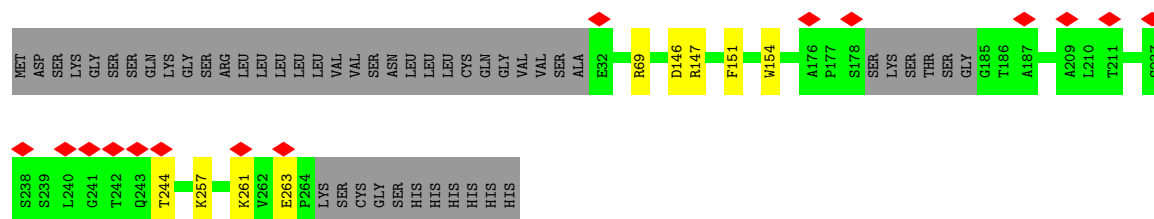
- Molecule 4: Acetylcholine receptor subunit epsilon

Chain B: 




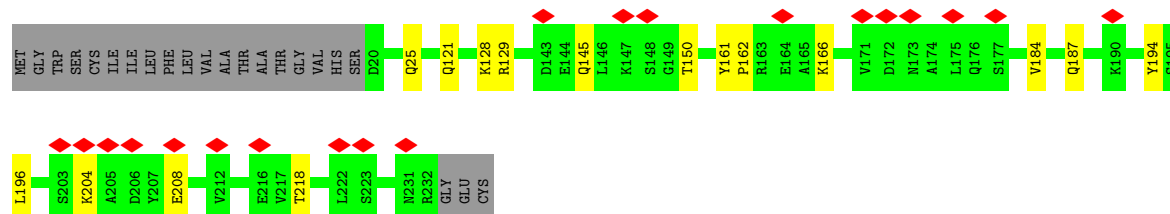
- Molecule 5: Fab3 heavy chain

Chain F: 

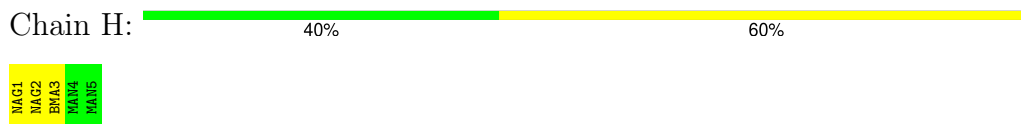


- Molecule 6: Fab3 light chain

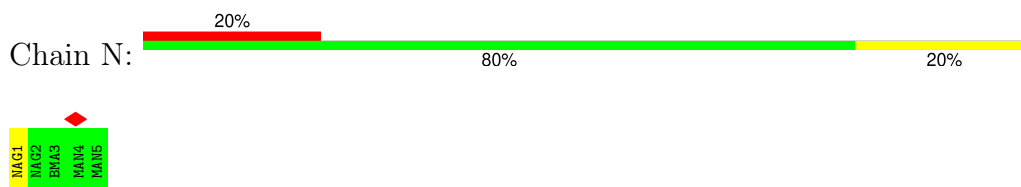
Chain G: 



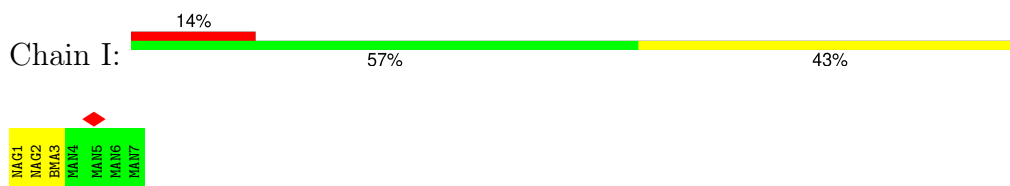
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



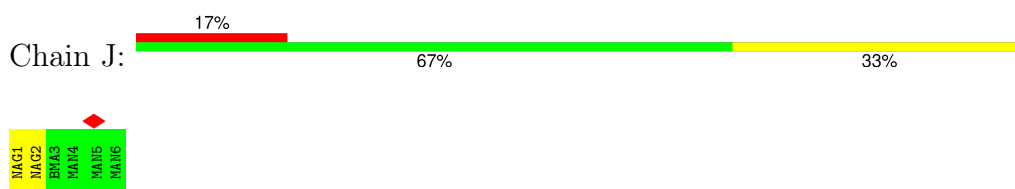
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



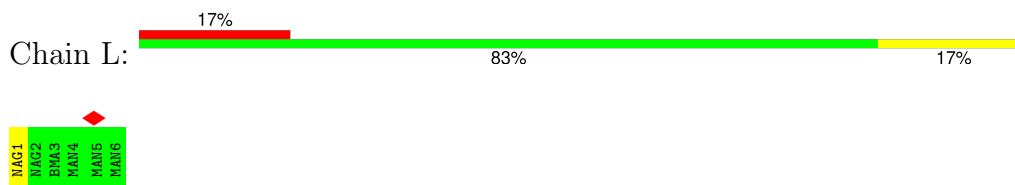
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1  
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	339630	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.543	Depositor
Minimum map value	-0.722	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	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, ACH, BMA, POV, MAN, 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	0.28	0/3285	0.54	0/4479
1	C	0.29	0/3306	0.54	0/4507
2	E	0.28	0/3367	0.57	0/4588
3	D	0.28	0/3616	0.56	0/4934
4	B	0.28	0/3330	0.57	0/4554
5	F	0.36	0/1784	0.60	0/2435
6	G	0.36	0/1688	0.60	0/2296
All	All	0.30	0/20376	0.56	0/27793

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
1	C	0	1
2	E	0	2
3	D	0	1
4	B	0	1
5	F	0	1
6	G	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	461	ARG	Sidechain
1	C	182	ARG	Sidechain
3	D	170	ARG	Sidechain
2	E	28	ARG	Sidechain
2	E	480	ARG	Sidechain

## 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	3202	3234	3235	19	0
1	C	3223	3264	3265	13	0
2	E	3281	3295	3294	22	0
3	D	3520	3534	3535	42	0
4	B	3252	3230	3231	42	0
5	F	1737	1689	1687	5	0
6	G	1650	1592	1591	9	0
7	H	61	52	52	5	0
7	N	61	52	52	0	0
8	I	83	70	70	3	0
9	J	72	61	61	1	0
9	L	72	61	61	0	0
10	K	28	25	25	1	0
10	M	28	25	25	4	0
11	A	10	16	16	1	0
12	B	56	92	92	11	0
12	D	84	138	138	32	0
12	E	28	46	46	5	0
13	B	44	63	63	21	0
13	D	92	134	134	18	0
13	E	38	48	48	7	0
14	D	14	13	13	1	0
15	B	1	0	0	0	0
All	All	20637	20734	20734	164	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 4.

The worst 5 of 164 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)
3:D:472:VAL:HG22	12:D:505:CLR:C7	1.71	1.21
1:A:297:ASN:HD21	13:B:503:POV:H11	1.07	1.10
1:A:297:ASN:ND2	13:B:503:POV:H11	1.66	1.09
2:E:322:TRP:HE1	13:E:502:POV:C13	1.63	1.09
2:E:322:TRP:HE1	13:E:502:POV:H13	1.20	1.06

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	395/457 (86%)	388 (98%)	7 (2%)	0	100	100
1	C	397/457 (87%)	386 (97%)	11 (3%)	0	100	100
2	E	397/503 (79%)	390 (98%)	6 (2%)	1 (0%)	37	31
3	D	429/517 (83%)	422 (98%)	7 (2%)	0	100	100
4	B	407/493 (83%)	400 (98%)	7 (2%)	0	100	100
5	F	223/275 (81%)	219 (98%)	4 (2%)	0	100	100
6	G	211/235 (90%)	202 (96%)	9 (4%)	0	100	100
All	All	2459/2937 (84%)	2407 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	106	ILE

### 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	367/419 (88%)	365 (100%)	2 (0%)	86	88
1	C	370/419 (88%)	370 (100%)	0	100	100
2	E	372/450 (83%)	372 (100%)	0	100	100
3	D	399/466 (86%)	399 (100%)	0	100	100
4	B	363/424 (86%)	361 (99%)	2 (1%)	84	85
5	F	191/233 (82%)	191 (100%)	0	100	100
6	G	187/204 (92%)	187 (100%)	0	100	100
All	All	2249/2615 (86%)	2245 (100%)	4 (0%)	91	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	PHE
1	A	301	ARG
4	B	260	LEU
4	B	435	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
2	E	438	GLN
3	D	70	ASN
4	B	301	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

33 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	$\# Z  > 2$
7	NAG	H	1	7,1	14,14,15	0.37	0	17,19,21	0.59	0
7	NAG	H	2	7	14,14,15	0.37	0	17,19,21	0.65	0
7	BMA	H	3	7	11,11,12	0.29	0	15,15,17	0.55	0
7	MAN	H	4	7	11,11,12	0.29	0	15,15,17	0.51	0
7	MAN	H	5	7	11,11,12	0.26	0	15,15,17	0.50	0
8	NAG	I	1	8,1	14,14,15	0.36	0	17,19,21	0.67	0
8	NAG	I	2	8	14,14,15	0.37	0	17,19,21	0.79	0
8	BMA	I	3	8	11,11,12	0.28	0	15,15,17	0.57	0
8	MAN	I	4	8	11,11,12	0.27	0	15,15,17	0.51	0
8	MAN	I	5	8	11,11,12	0.28	0	15,15,17	0.48	0
8	MAN	I	6	8	11,11,12	0.31	0	15,15,17	0.51	0
8	MAN	I	7	8	11,11,12	0.28	0	15,15,17	0.49	0
9	NAG	J	1	9,2	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
9	NAG	J	2	9	14,14,15	0.37	0	17,19,21	0.52	0
9	BMA	J	3	9	11,11,12	0.35	0	15,15,17	0.45	0
9	MAN	J	4	9	11,11,12	0.31	0	15,15,17	0.47	0
9	MAN	J	5	9	11,11,12	0.27	0	15,15,17	0.50	0
9	MAN	J	6	9	11,11,12	0.30	0	15,15,17	0.47	0
10	NAG	K	1	3,10	14,14,15	0.41	0	17,19,21	0.65	0
10	NAG	K	2	10	14,14,15	0.37	0	17,19,21	0.59	0
9	NAG	L	1	3,9	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
9	NAG	L	2	9	14,14,15	0.39	0	17,19,21	0.55	0
9	BMA	L	3	9	11,11,12	0.23	0	15,15,17	0.56	0
9	MAN	L	4	9	11,11,12	0.30	0	15,15,17	0.52	0
9	MAN	L	5	9	11,11,12	0.28	0	15,15,17	0.50	0
9	MAN	L	6	9	11,11,12	0.30	0	15,15,17	0.47	0
10	NAG	M	1	4,10	14,14,15	0.38	0	17,19,21	0.63	0
10	NAG	M	2	10	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
7	NAG	N	1	4,7	14,14,15	0.40	0	17,19,21	0.93	2 (11%)
7	NAG	N	2	7	14,14,15	0.36	0	17,19,21	0.49	0
7	BMA	N	3	7	11,11,12	0.29	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	N	4	7	11,11,12	0.28	0	15,15,17	0.48	0
7	MAN	N	5	7	11,11,12	0.30	0	15,15,17	0.49	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
7	NAG	H	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
7	MAN	H	5	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
8	MAN	I	6	8	-	0/2/19/22	0/1/1/1
8	MAN	I	7	8	-	2/2/19/22	0/1/1/1
9	NAG	J	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	3/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	1/2/19/22	0/1/1/1
9	MAN	J	5	9	-	1/2/19/22	0/1/1/1
9	MAN	J	6	9	-	2/2/19/22	0/1/1/1
10	NAG	K	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	K	2	10	-	4/6/23/26	0/1/1/1
9	NAG	L	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	L	2	9	-	2/6/23/26	0/1/1/1
9	BMA	L	3	9	-	0/2/19/22	0/1/1/1
9	MAN	L	4	9	-	0/2/19/22	0/1/1/1
9	MAN	L	5	9	-	1/2/19/22	0/1/1/1
9	MAN	L	6	9	-	0/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	M	2	10	-	1/6/23/26	0/1/1/1
7	NAG	N	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	2	NAG	O5-C5-C6	6.53	120.37	107.66
7	N	1	NAG	C1-O5-C5	2.74	115.86	112.19
10	M	2	NAG	C4-C3-C2	2.71	114.99	111.02
9	L	1	NAG	C1-O5-C5	2.48	115.51	112.19
10	M	2	NAG	O3-C3-C4	2.47	116.21	110.38

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

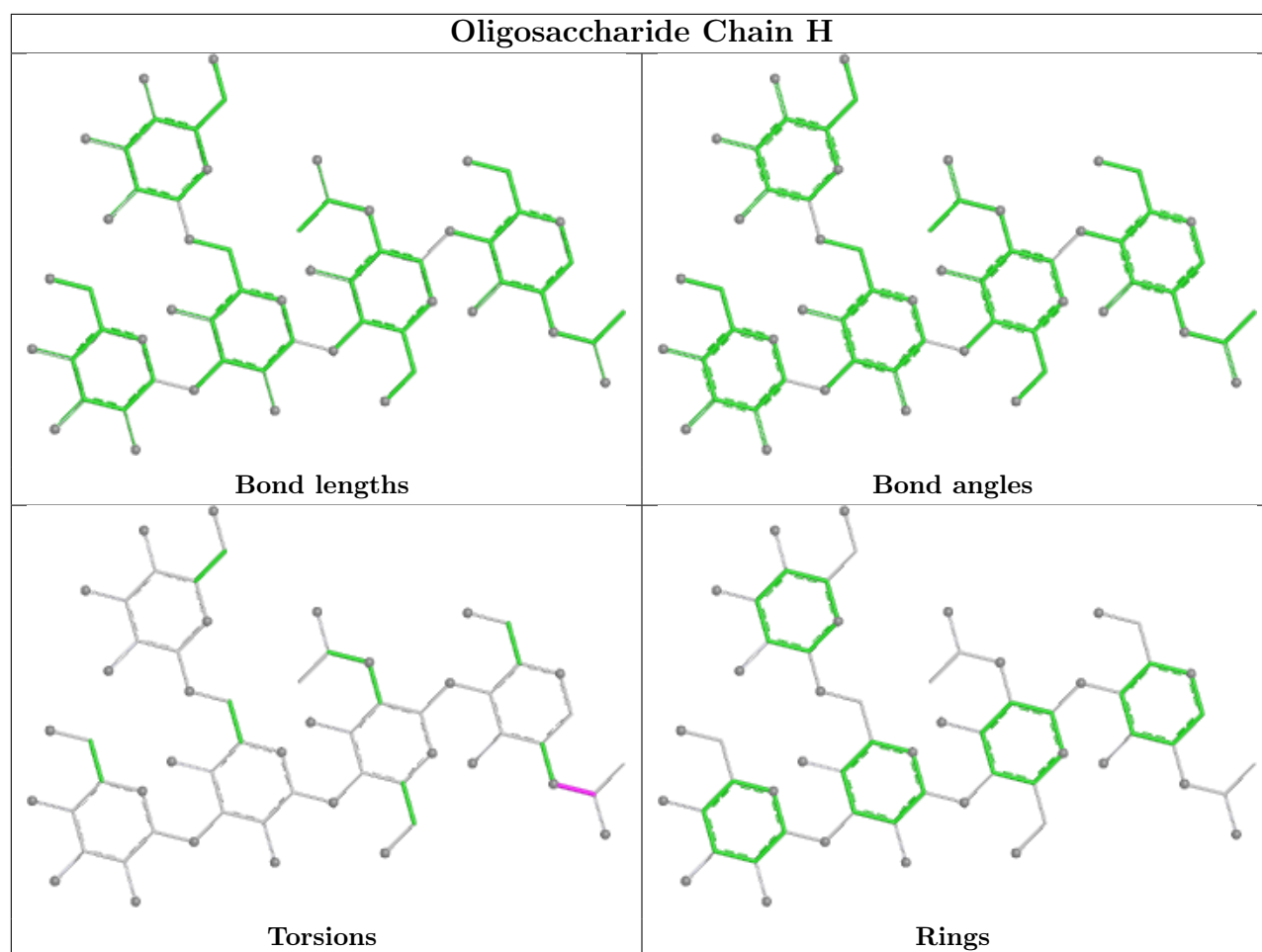
Mol	Chain	Res	Type	Atoms
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
10	M	2	NAG	C3-C2-N2-C7
10	K	2	NAG	O5-C5-C6-O6
8	I	1	NAG	C8-C7-N2-C2

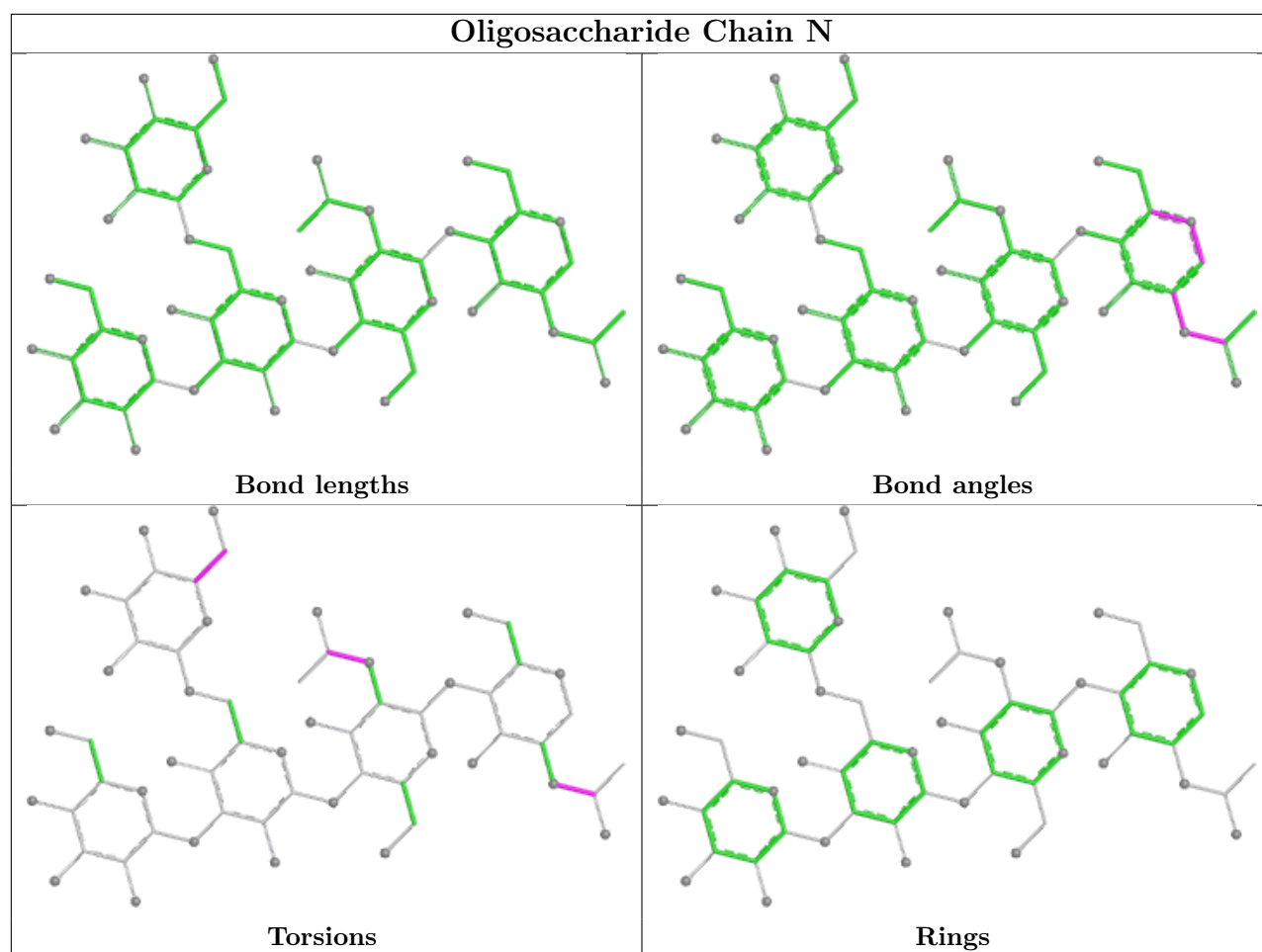
There are no ring outliers.

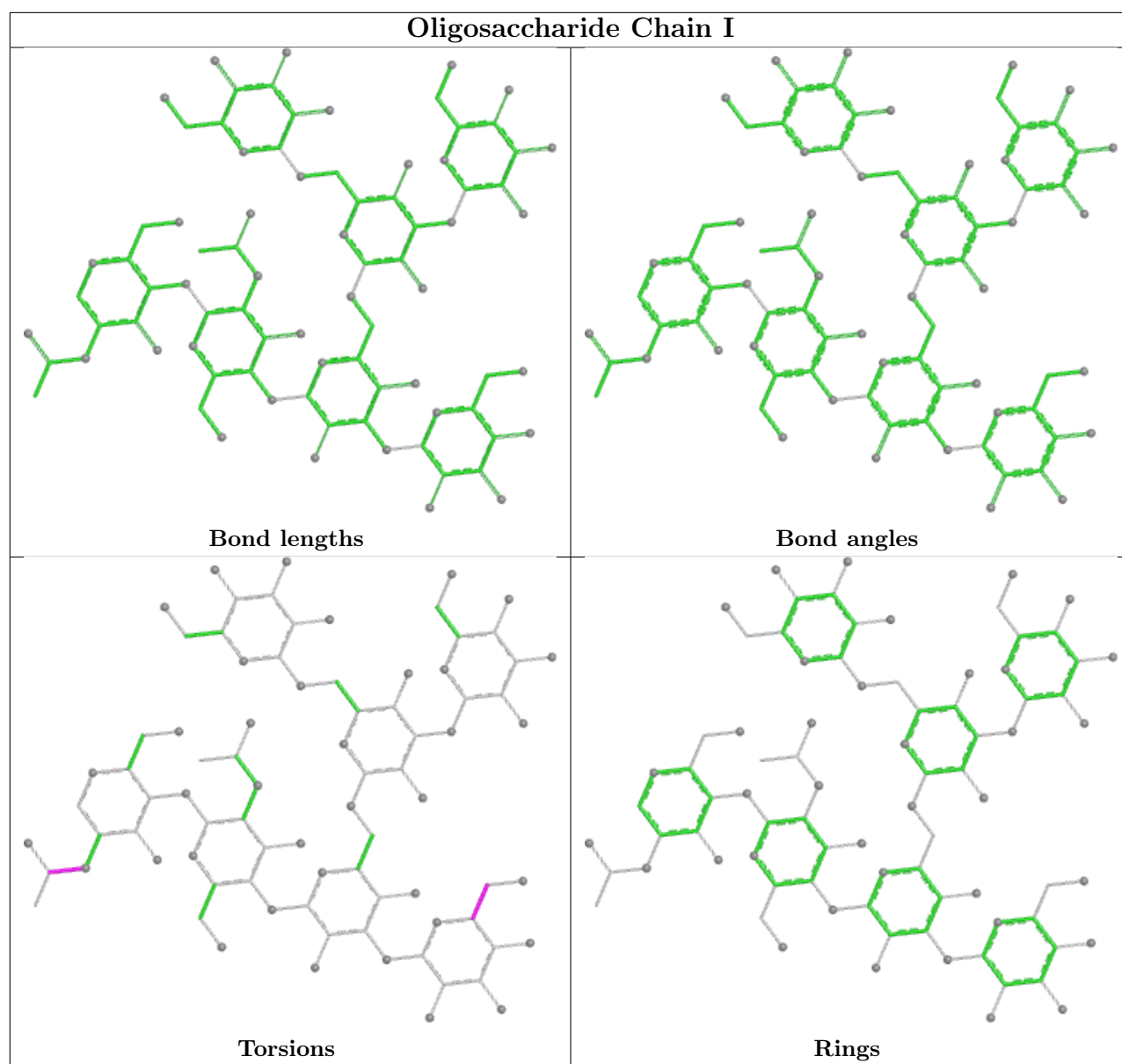
10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	3	BMA	2	0
7	H	2	NAG	2	0
7	H	1	NAG	3	0
10	M	2	NAG	4	0
9	J	2	NAG	1	0
8	I	2	NAG	1	0
10	K	1	NAG	1	0
10	M	1	NAG	2	0
8	I	1	NAG	1	0
7	H	3	BMA	1	0

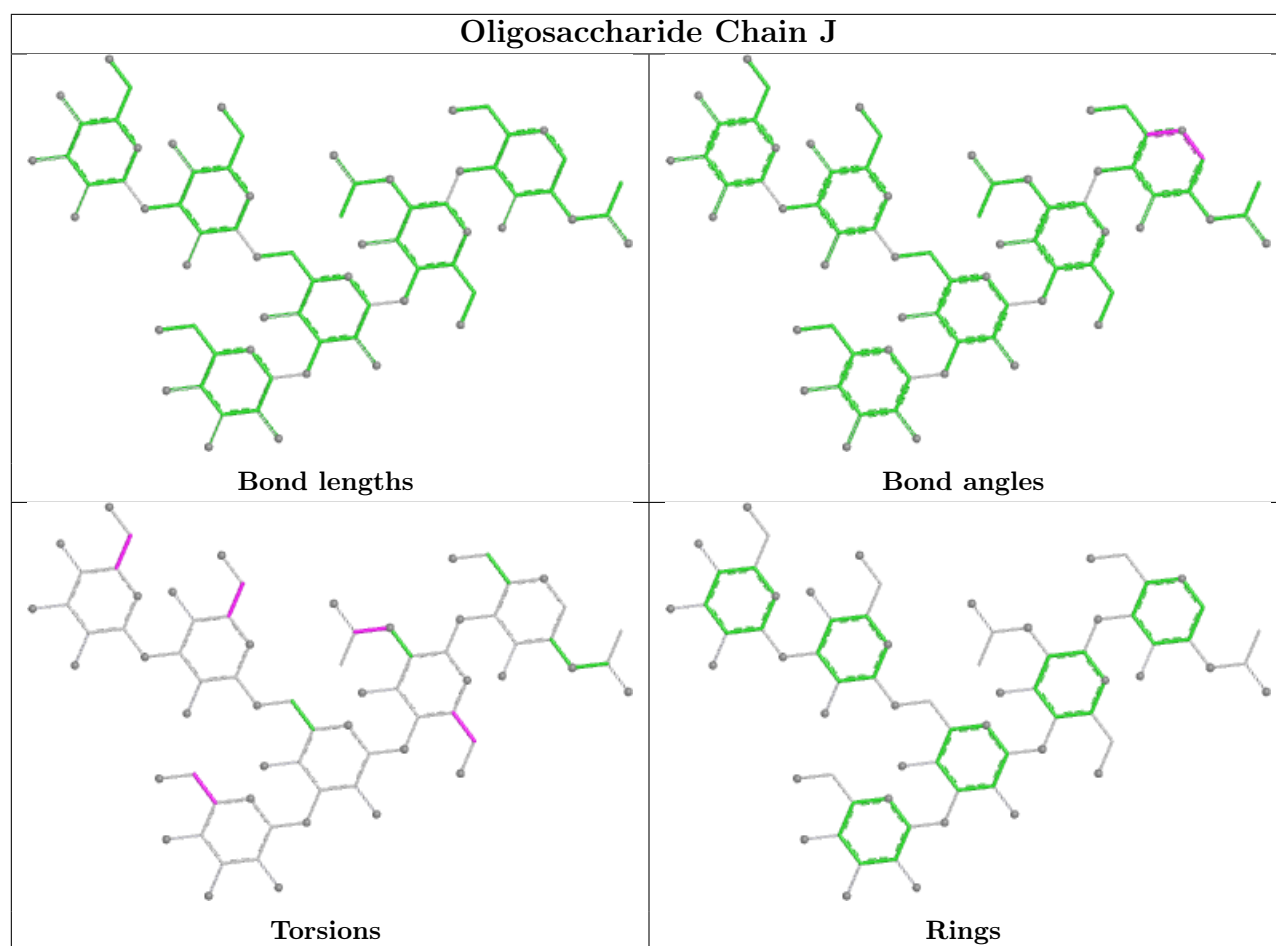
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

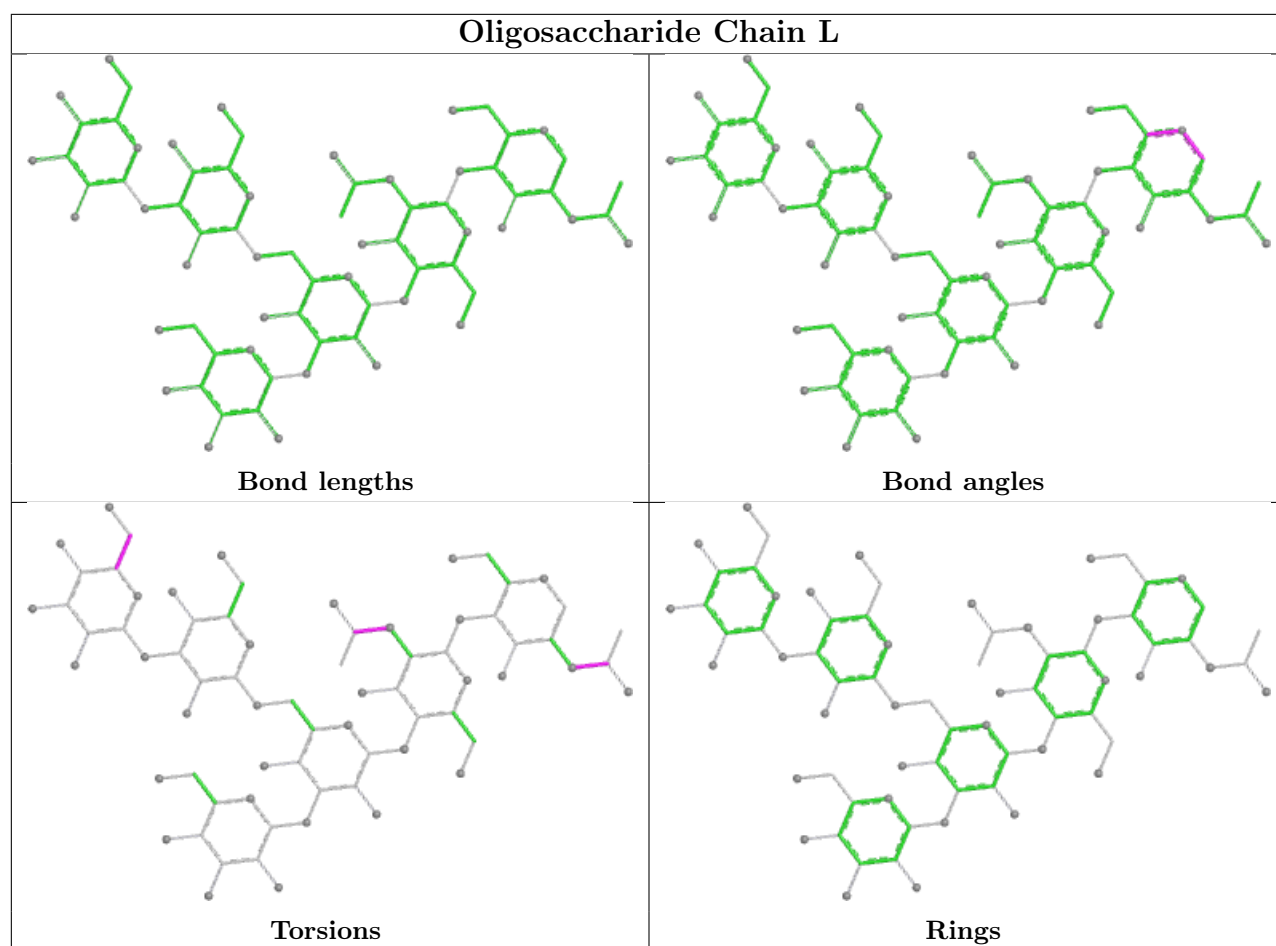


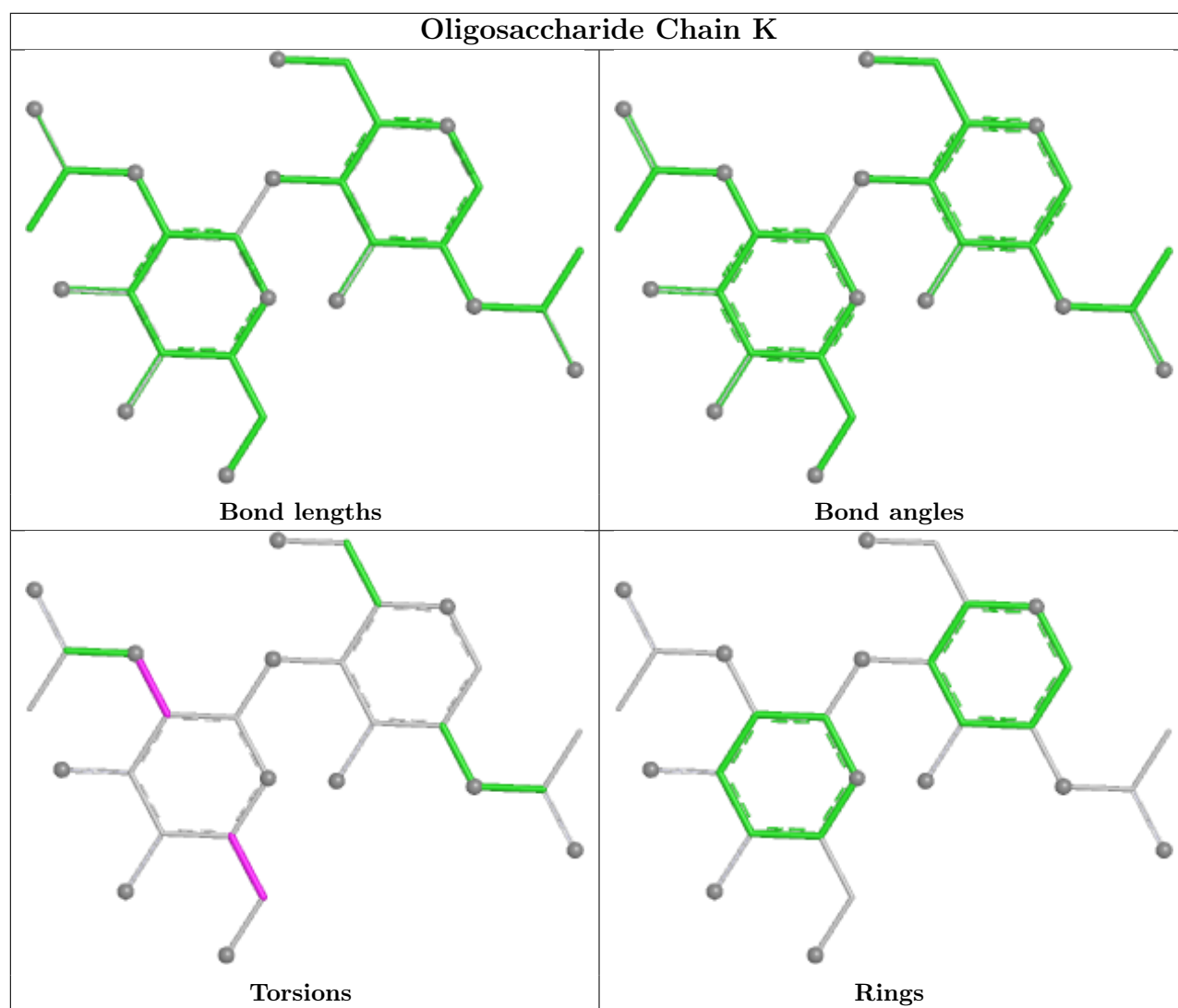


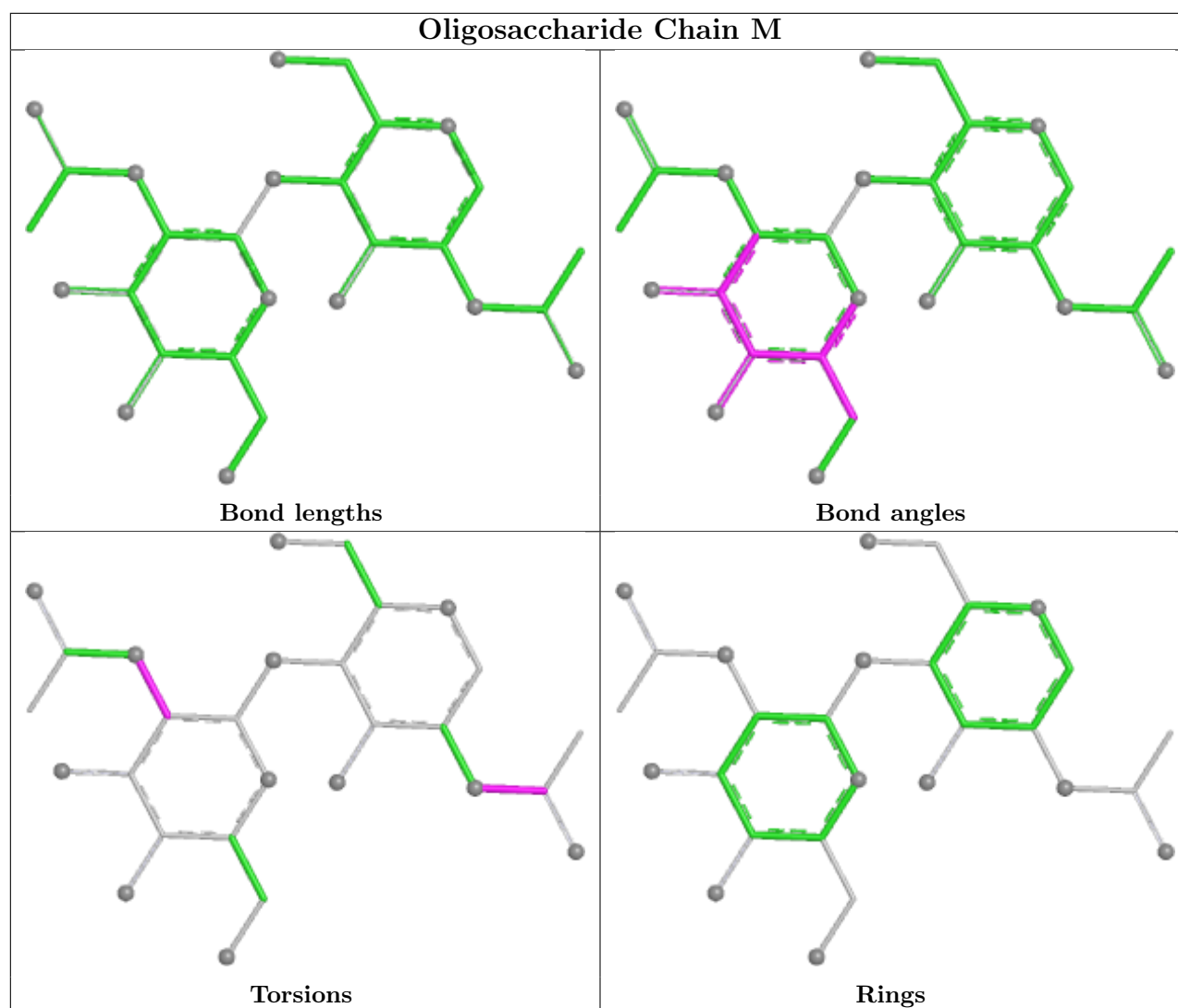












## 5.6 Ligand geometry [i](#)

12 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	$\# Z  > 2$
12	CLR	D	502	-	31,31,31	0.29	0	48,48,48	0.40	0
12	CLR	B	501	-	31,31,31	0.29	0	48,48,48	0.39	0
13	POV	E	502	-	37,37,51	0.34	0	43,45,59	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	NAG	D	501	3	14,14,15	0.42	0	17,19,21	1.28	3 (17%)
12	CLR	B	502	-	31,31,31	0.31	0	48,48,48	0.40	0
12	CLR	E	501	-	31,31,31	0.26	0	48,48,48	0.41	0
12	CLR	D	505	-	31,31,31	0.31	0	48,48,48	0.79	2 (4%)
13	POV	D	506	-	39,39,51	0.32	0	45,47,59	0.34	0
11	ACH	A	501	-	9,9,9	0.32	0	12,12,12	0.29	0
13	POV	D	503	-	51,51,51	0.31	0	57,59,59	0.30	0
12	CLR	D	504	-	31,31,31	0.28	0	48,48,48	0.68	1 (2%)
13	POV	B	503	-	43,43,51	0.34	0	49,51,59	0.31	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
12	CLR	D	502	-	-	0/10/68/68	0/4/4/4
12	CLR	B	501	-	-	2/10/68/68	0/4/4/4
13	POV	E	502	-	-	14/41/41/55	-
14	NAG	D	501	3	1/1/6/7	1/6/23/26	0/1/1/1
12	CLR	B	502	-	-	2/10/68/68	0/4/4/4
12	CLR	E	501	-	-	3/10/68/68	0/4/4/4
12	CLR	D	505	-	-	4/10/68/68	0/4/4/4
13	POV	D	506	-	-	4/43/43/55	-
11	ACH	A	501	-	-	0/7/7/7	-
13	POV	D	503	-	-	22/55/55/55	-
12	CLR	D	504	-	-	6/10/68/68	0/4/4/4
13	POV	B	503	-	-	5/47/47/55	-

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(°)
14	D	501	NAG	C1-C2-N2	3.29	115.62	110.43
14	D	501	NAG	O5-C1-C2	2.82	115.66	111.29
12	D	505	CLR	C9-C10-C5	-2.35	106.22	109.65
14	D	501	NAG	C2-N2-C7	2.32	126.01	122.90
12	D	504	CLR	C16-C17-C20	2.22	115.54	112.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	501	NAG	C1

5 of 63 torsion outliers are listed below:

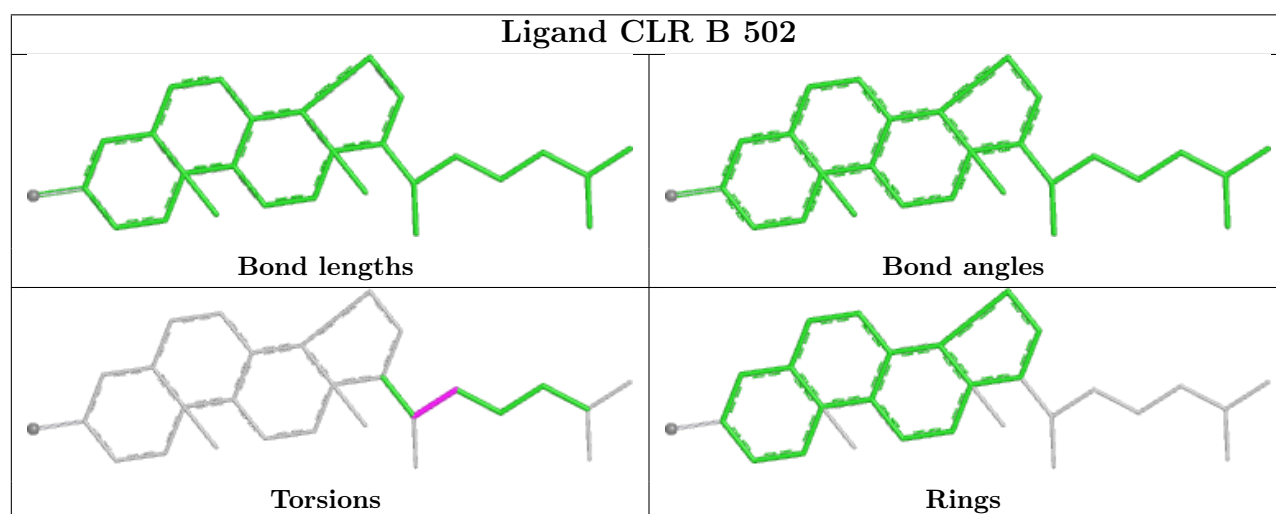
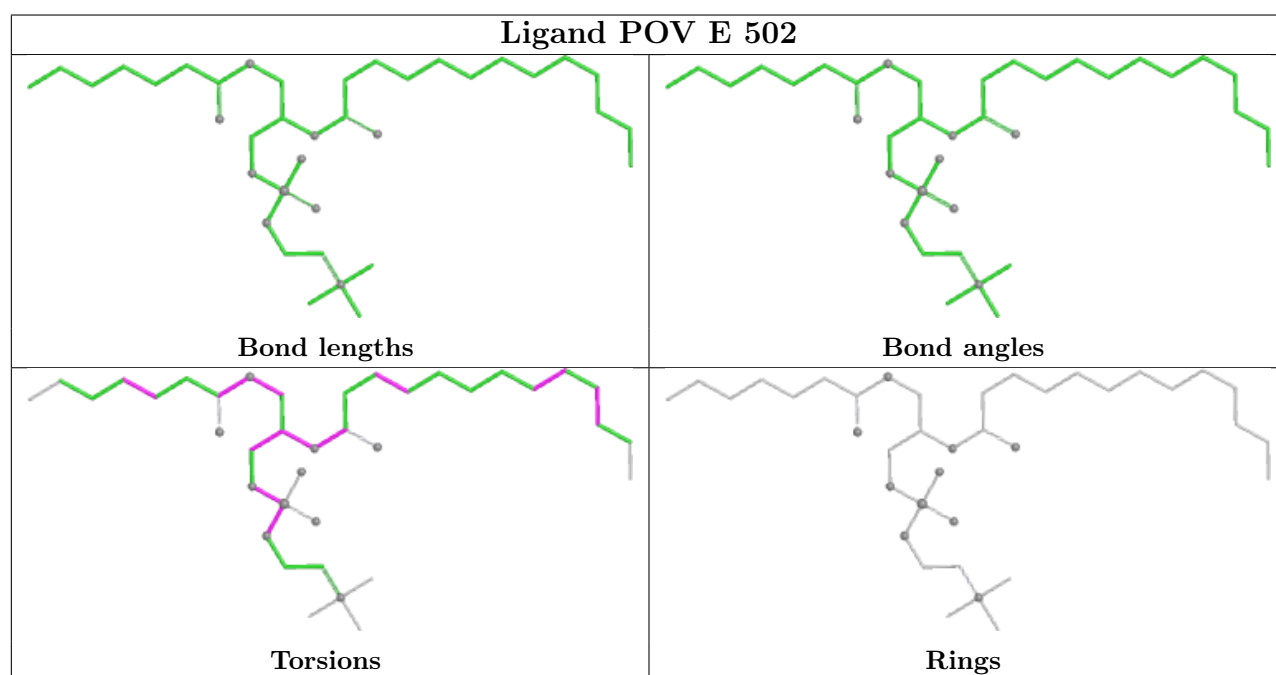
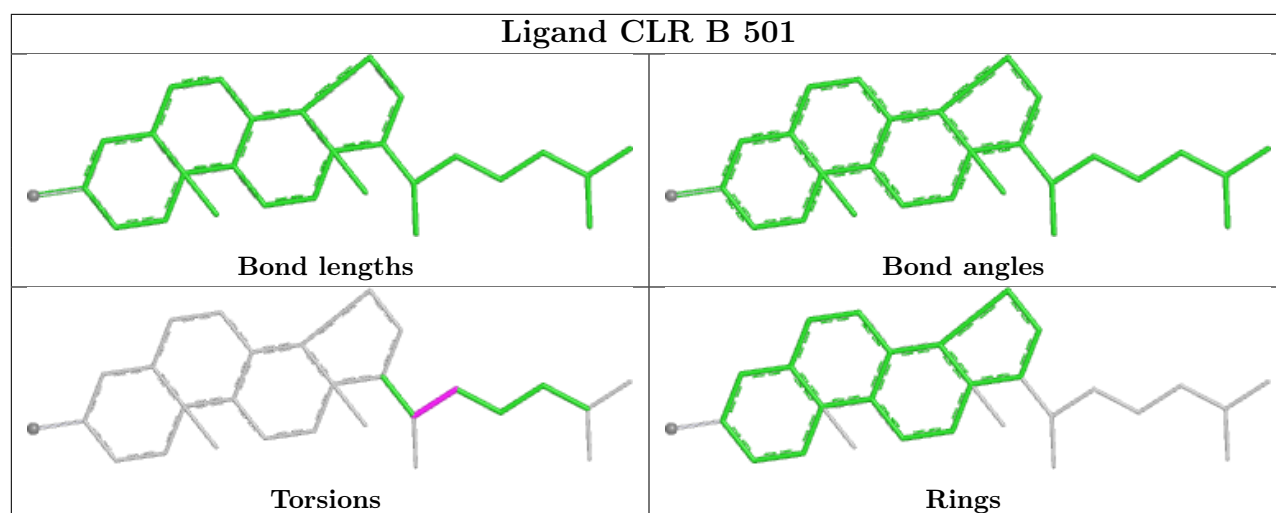
Mol	Chain	Res	Type	Atoms
13	E	502	POV	C1-O11-P-O14
13	D	503	POV	C1-O11-P-O14
13	B	503	POV	O12-C11-C12-N
13	D	506	POV	C32-C31-O31-C3
13	D	506	POV	O32-C31-O31-C3

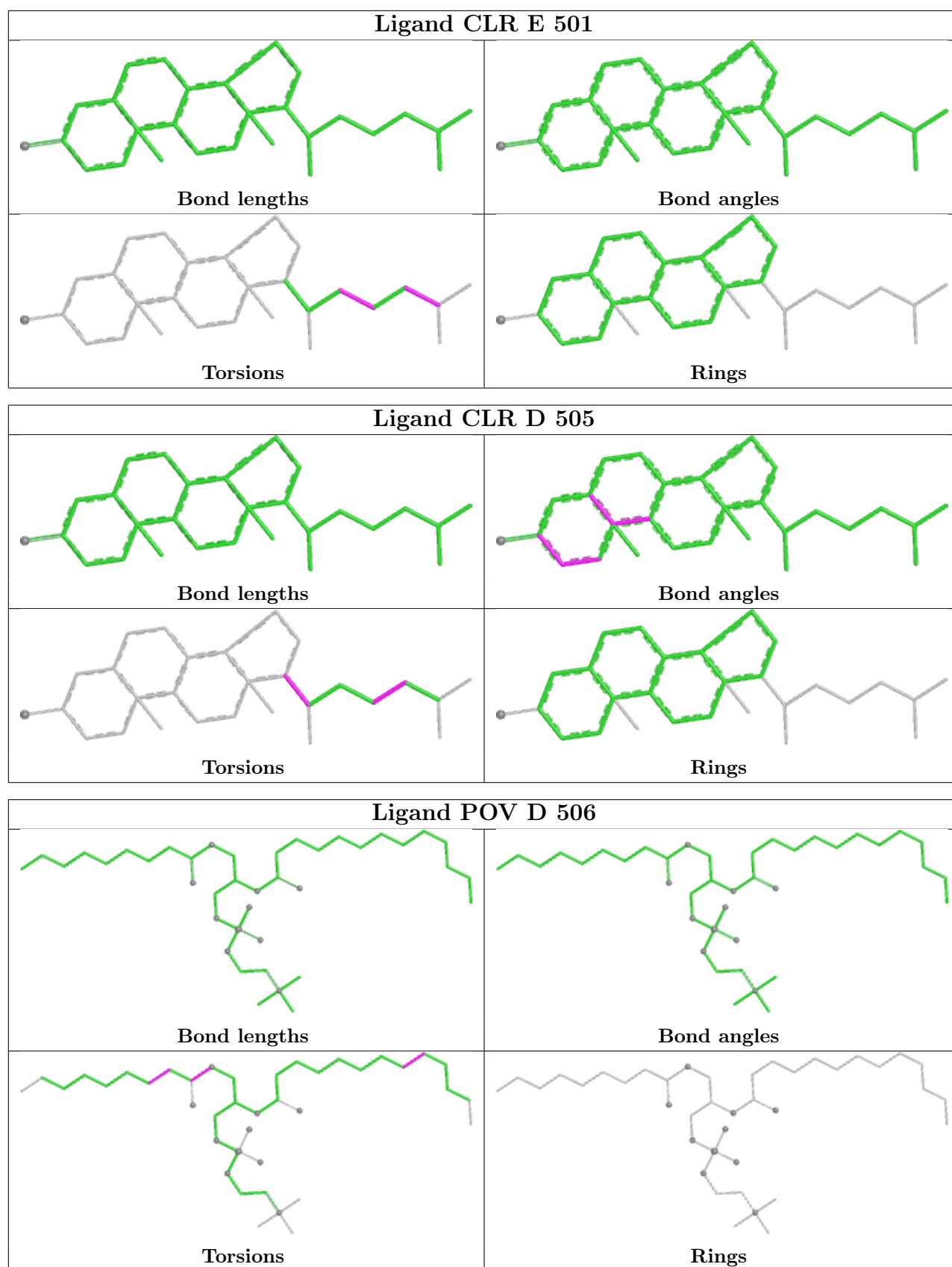
There are no ring outliers.

12 monomers are involved in 96 short contacts:

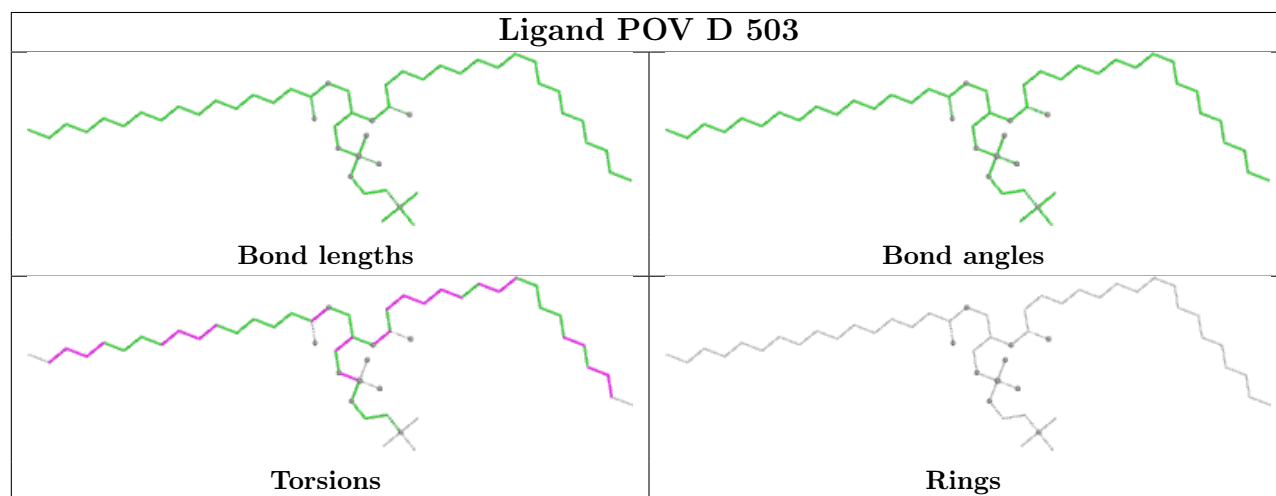
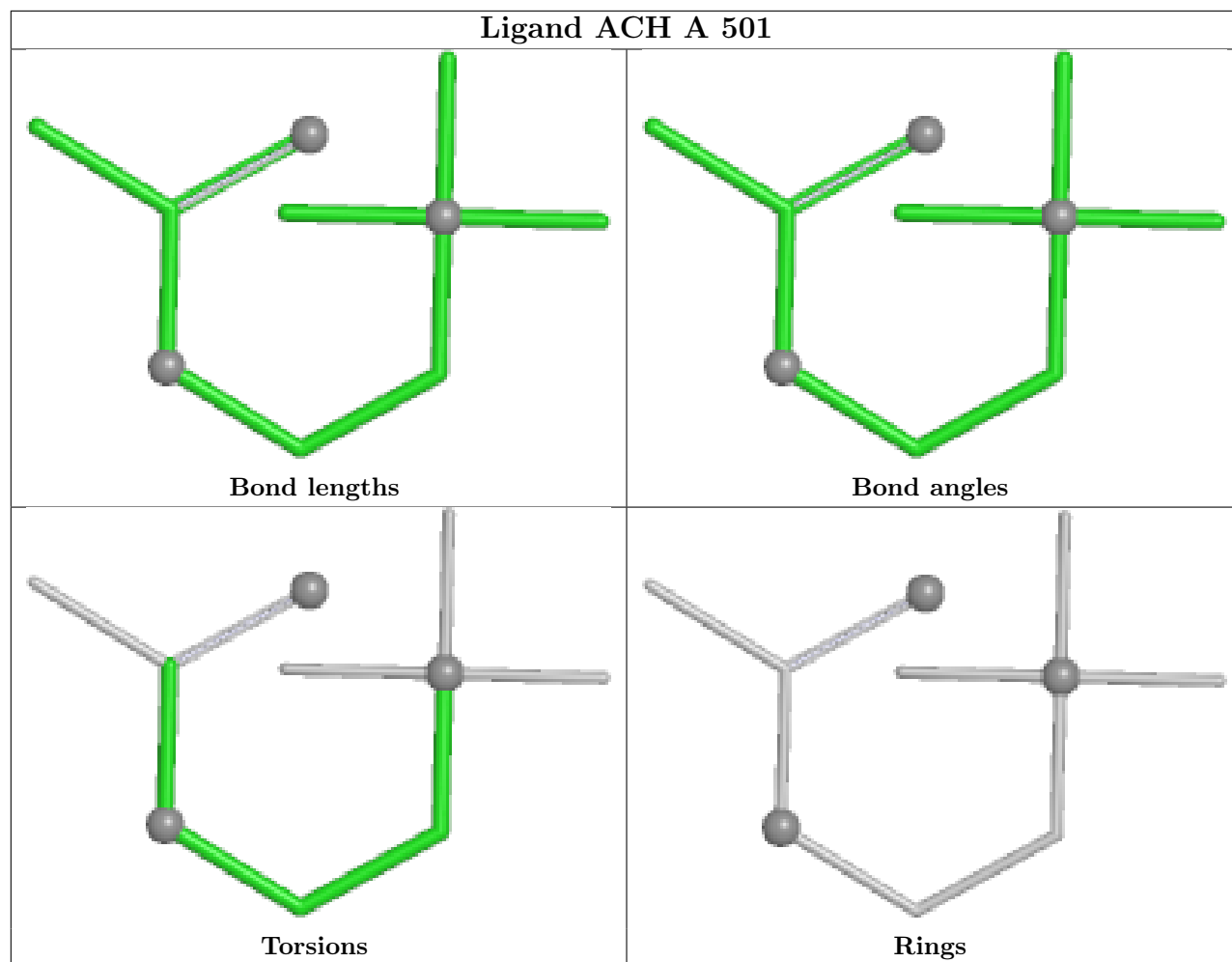
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	502	CLR	9	0
12	B	501	CLR	5	0
13	E	502	POV	7	0
14	D	501	NAG	1	0
12	B	502	CLR	6	0
12	E	501	CLR	5	0
12	D	505	CLR	17	0
13	D	506	POV	14	0
11	A	501	ACH	1	0
13	D	503	POV	4	0
12	D	504	CLR	11	0
13	B	503	POV	21	0

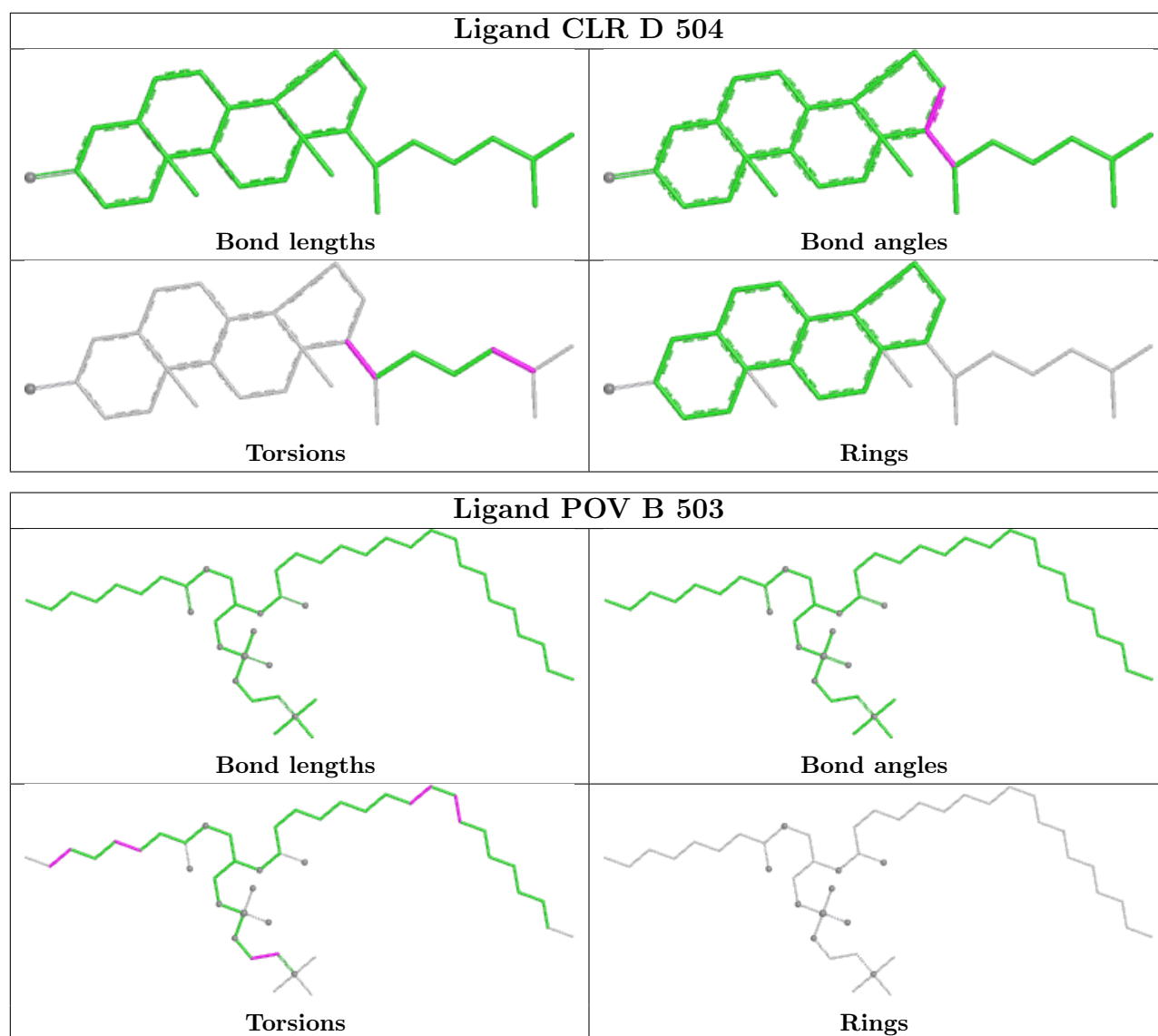
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

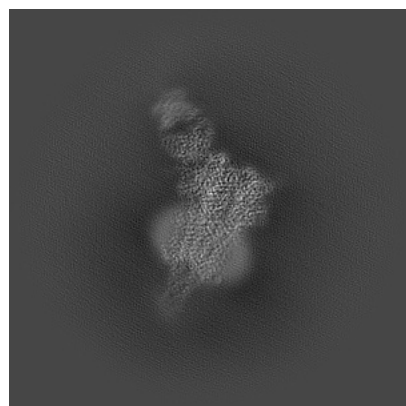
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47013. These allow visual inspection of the internal detail of the map and identification of artifacts.

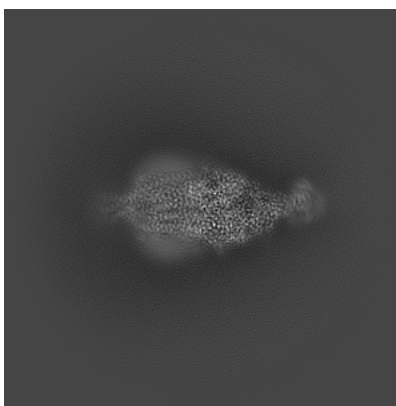
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

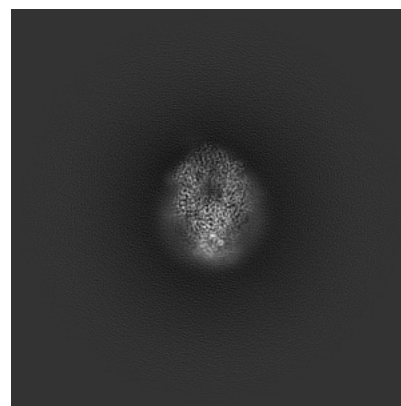
#### 6.1.1 Primary map



X

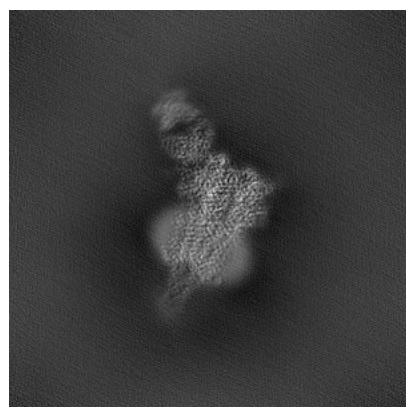


Y

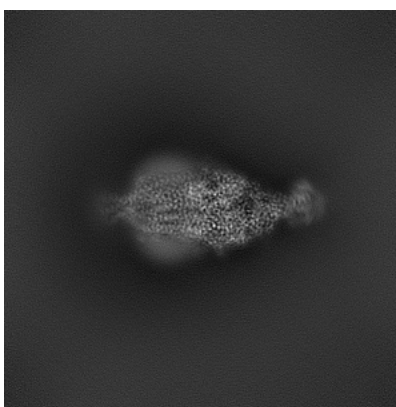


Z

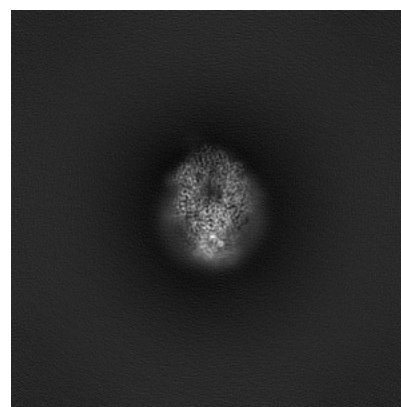
#### 6.1.2 Raw map



X



Y

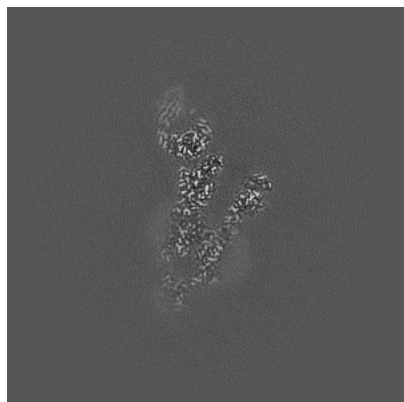


Z

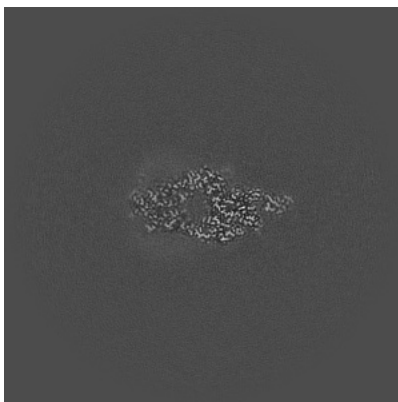
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

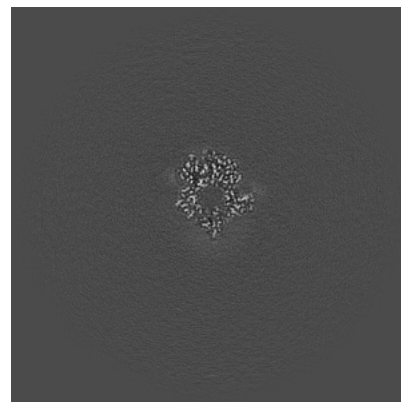
### 6.2.1 Primary map



X Index: 200

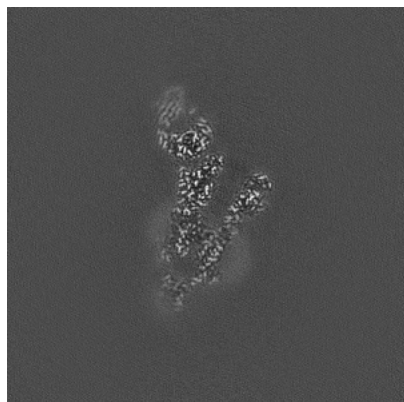


Y Index: 200

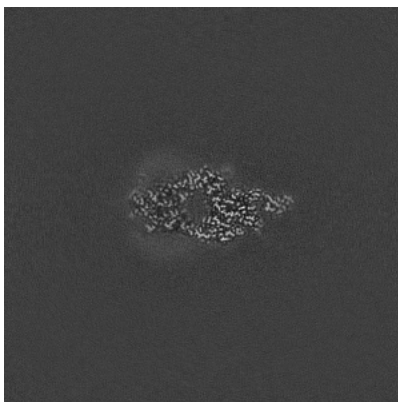


Z Index: 200

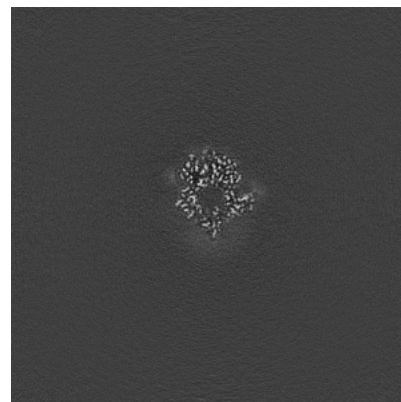
### 6.2.2 Raw map



X Index: 200



Y Index: 200

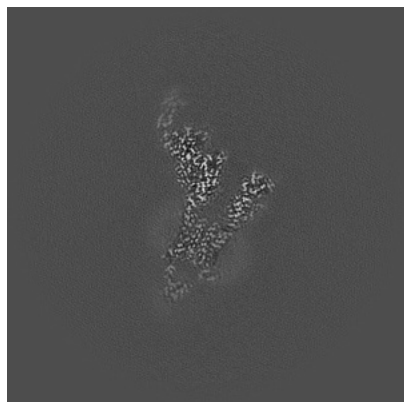


Z Index: 200

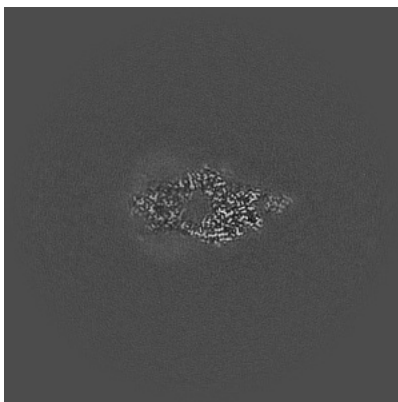
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

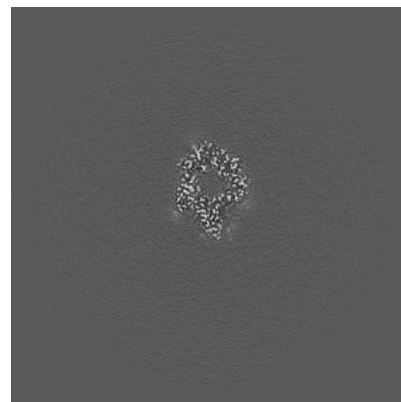
### 6.3.1 Primary map



X Index: 193

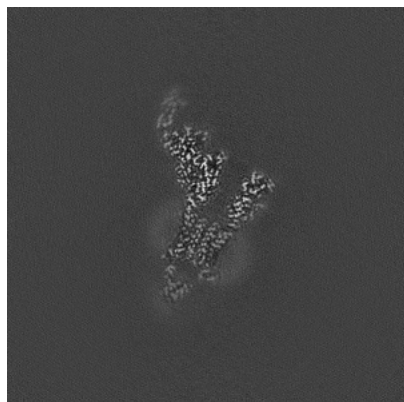


Y Index: 201

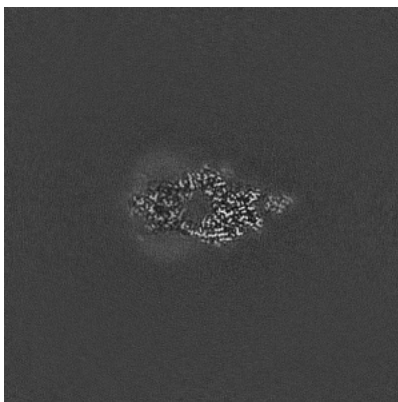


Z Index: 223

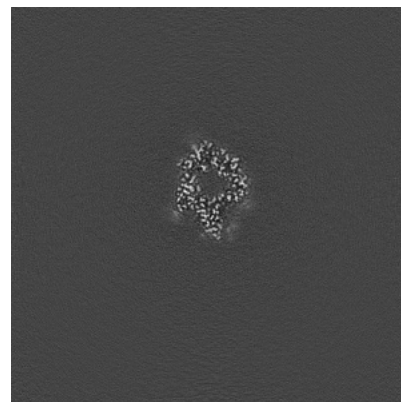
### 6.3.2 Raw map



X Index: 193



Y Index: 201

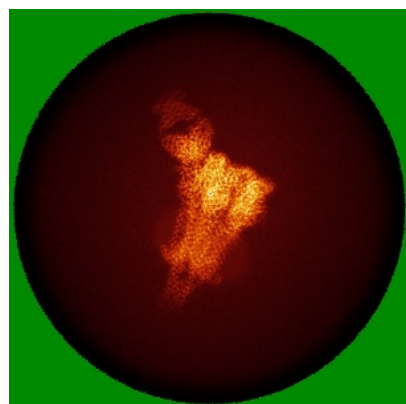


Z Index: 223

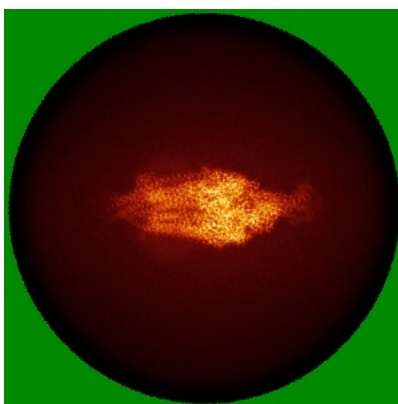
The images above show the largest variance slices of the map in three orthogonal directions.

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

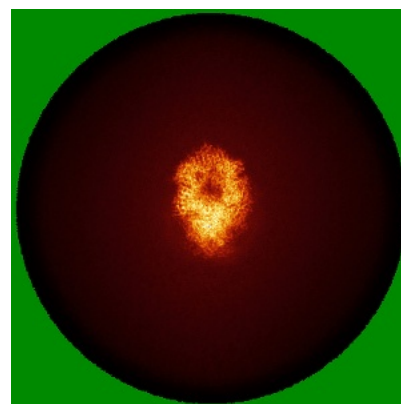
### 6.4.1 Primary map



X



Y

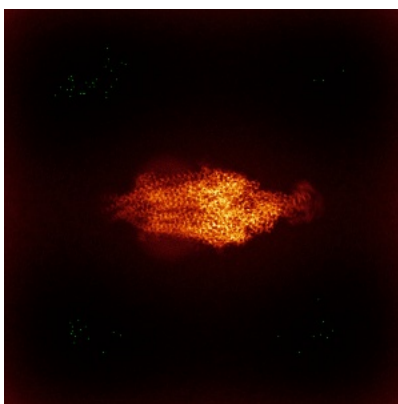


Z

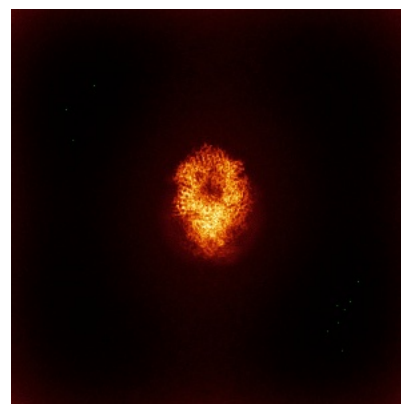
### 6.4.2 Raw map



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 0.095. 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.

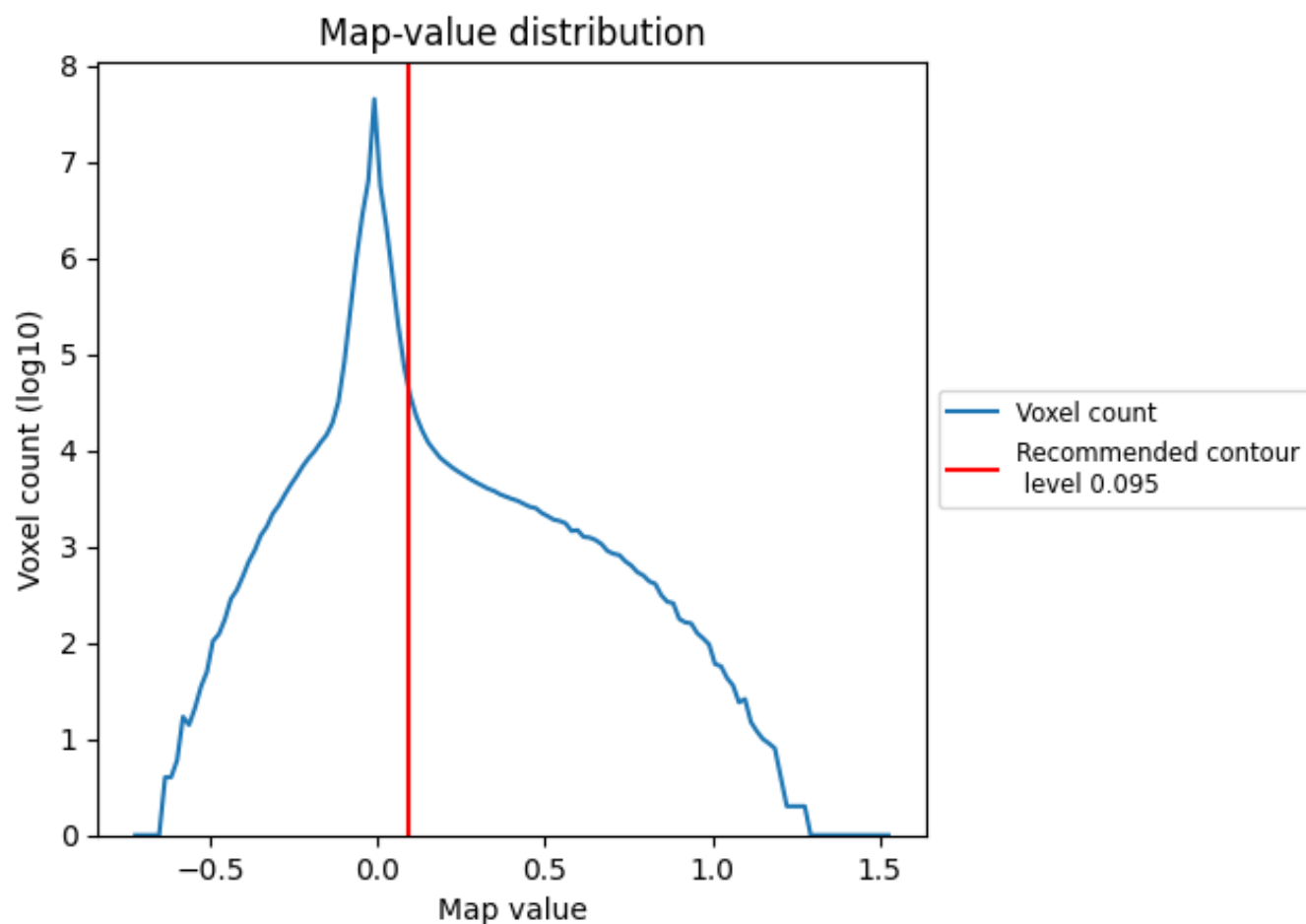
## 6.6 Mask visualisation [i](#)

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.

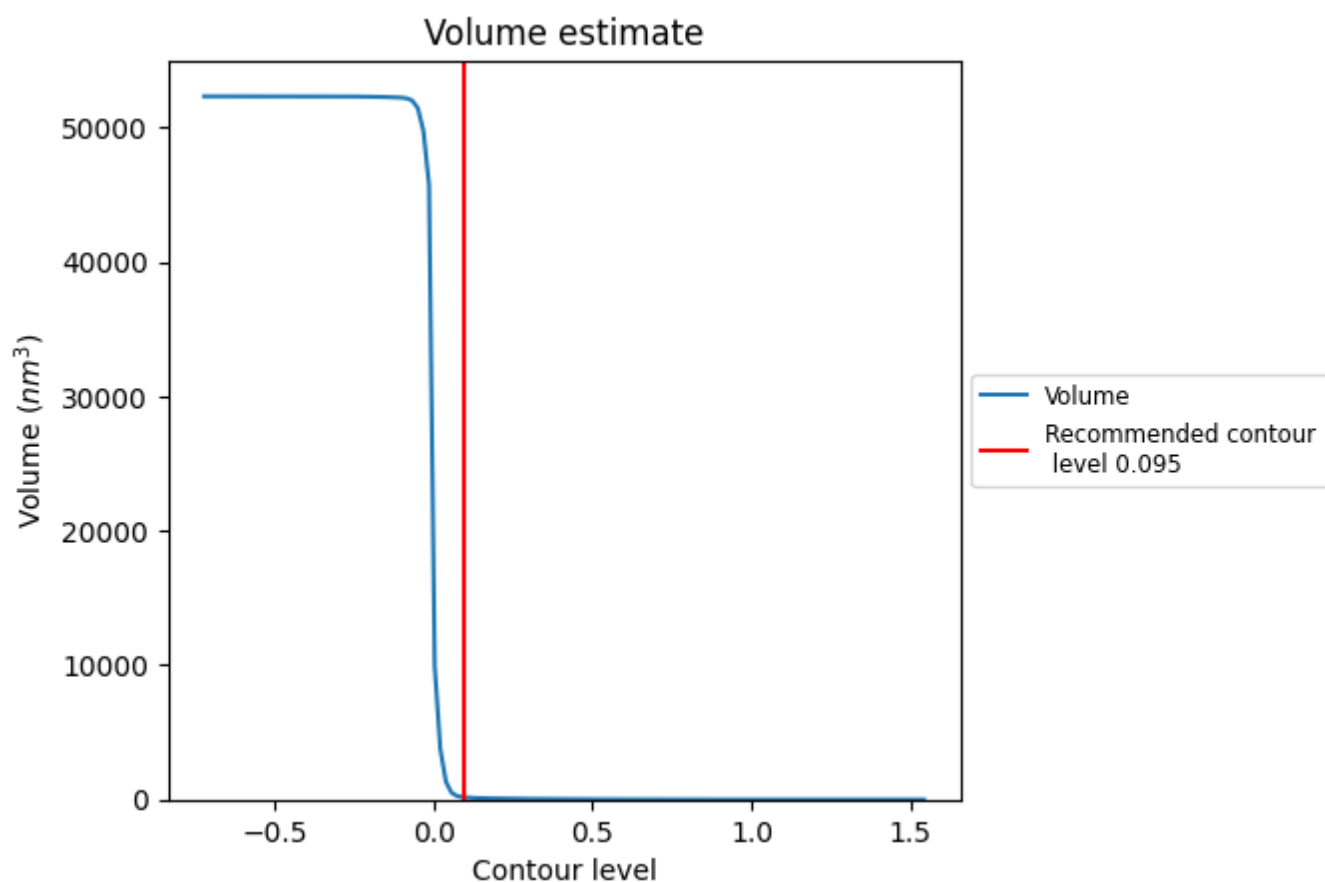
### 7.1 Map-value distribution [i](#)



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.



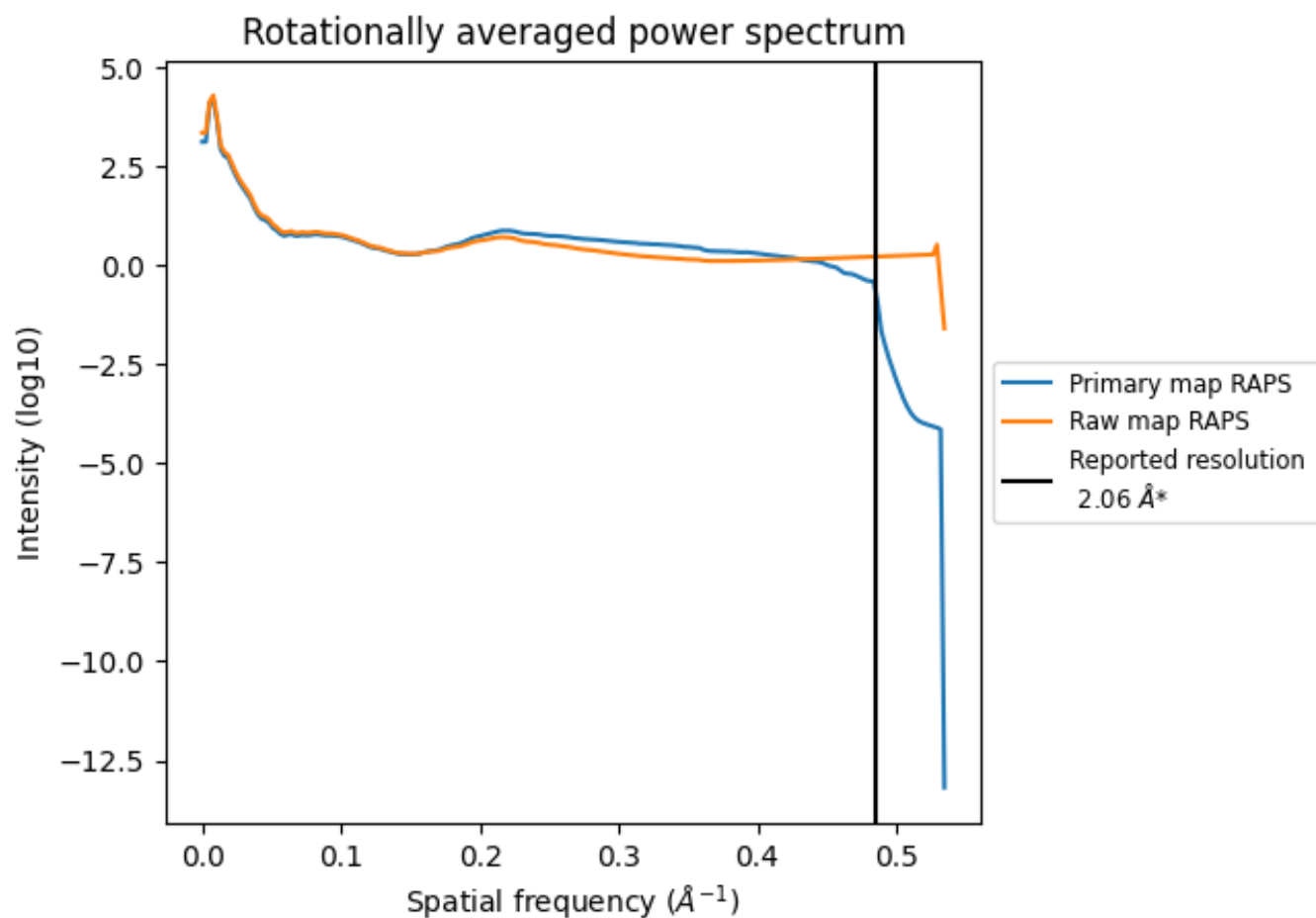
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173  $\text{nm}^3$ ; this corresponds to an approximate mass of 156 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 ⓘ

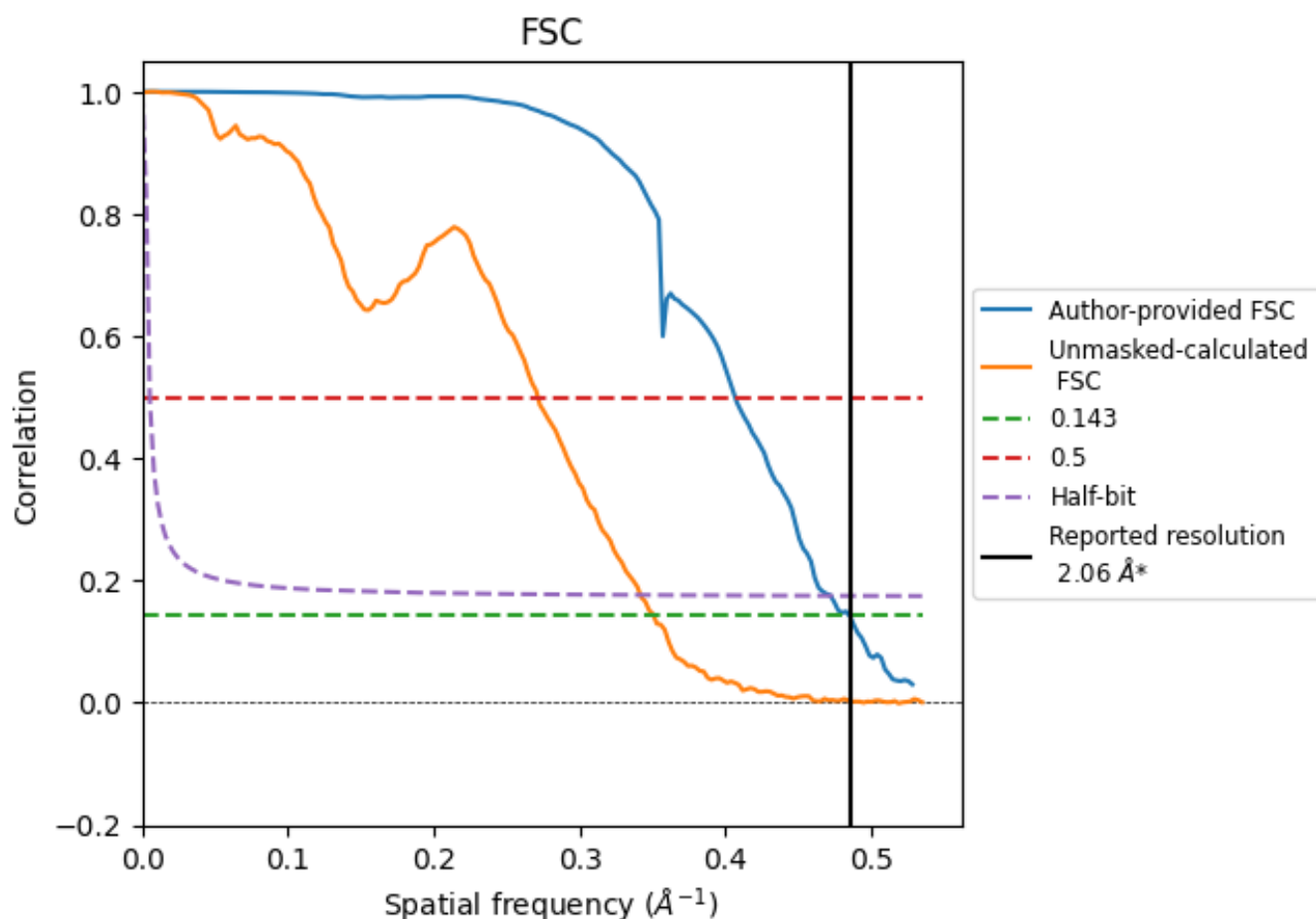


\*Reported resolution corresponds to spatial frequency of 0.485  $\text{\AA}^{-1}$

## 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  $0.485 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.46	2.12
Unmasked-calculated*	2.85	3.69	2.93

\*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 2.85 differs from the reported value 2.06 by more than 10 %

## 9 Map-model fit [i](#)

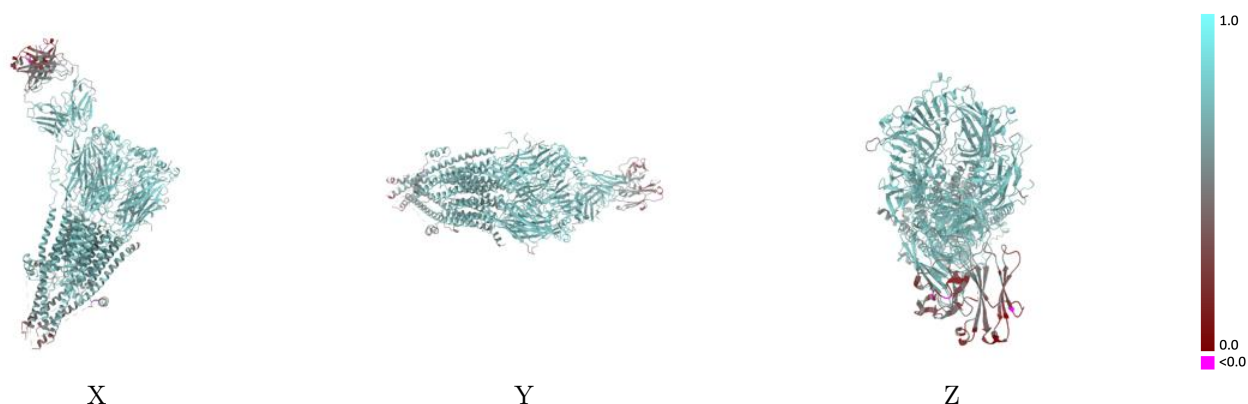
This section contains information regarding the fit between EMDB map EMD-47013 and PDB model 9DMQ. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



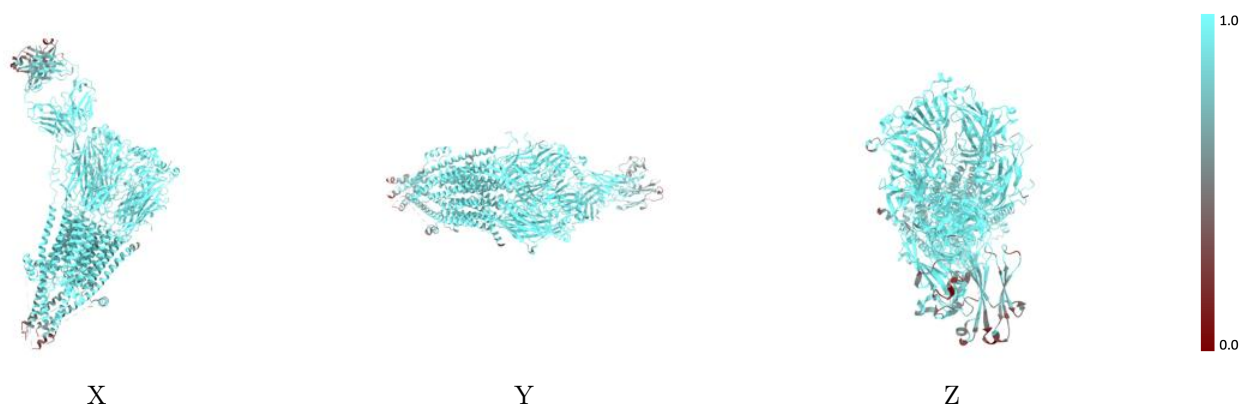
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



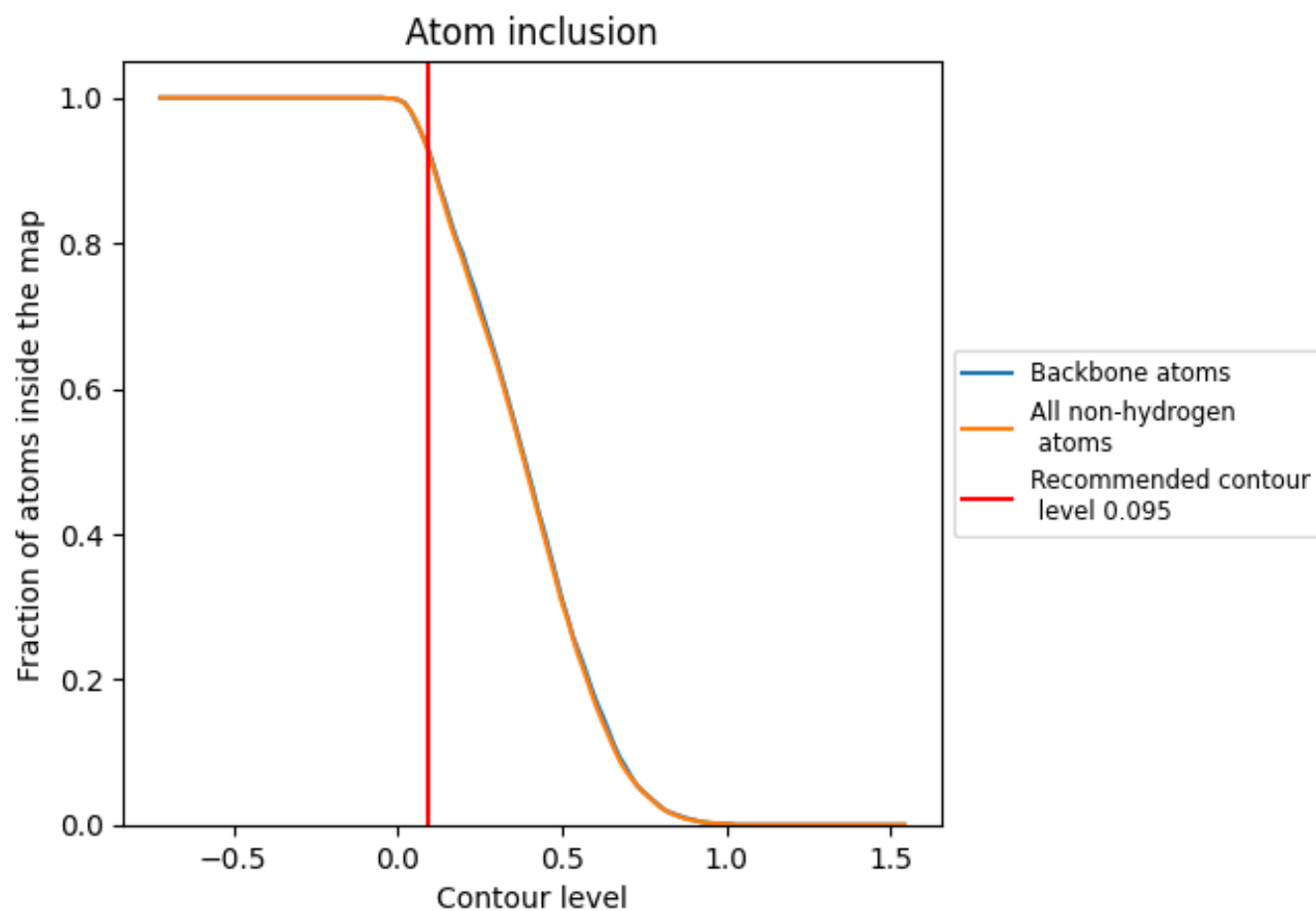
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9250	<div></div> 0.6550
A	<div></div> 0.9410	<div></div> 0.6690
B	<div></div> 0.9320	<div></div> 0.6650
C	<div></div> 0.9430	<div></div> 0.6810
D	<div></div> 0.9440	<div></div> 0.6840
E	<div></div> 0.9520	<div></div> 0.6870
F	<div></div> 0.8660	<div></div> 0.5880
G	<div></div> 0.8200	<div></div> 0.5350
H	<div></div> 0.9670	<div></div> 0.5850
I	<div></div> 0.8070	<div></div> 0.5470
J	<div></div> 0.6940	<div></div> 0.4990
K	<div></div> 0.6430	<div></div> 0.4190
L	<div></div> 0.7920	<div></div> 0.5150
M	<div></div> 0.5000	<div></div> 0.4210
N	<div></div> 0.7050	<div></div> 0.4990

1.0

0.0

<0.0