



## Full wwPDB EM Validation Report ⓘ

May 24, 2025 – 04:16 pm BST

PDB ID : 9FG9 / pdb\_00009fg9  
EMDB ID : EMD-50389  
Title : Cryo-EM structure of the full-length alpha1beta3gamma2 GABA(A) receptor in complex with GABA and Etomidate in the long-lived symmetric desensitised state  
Authors : Mihaylov, D.B.; Malinauskas, T.; Aricescu, A.R.  
Deposited on : 2024-05-23  
Resolution : 2.70 Å (reported)  
Based on initial model : 6HUK

This is a Full wwPDB EM Validation 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.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

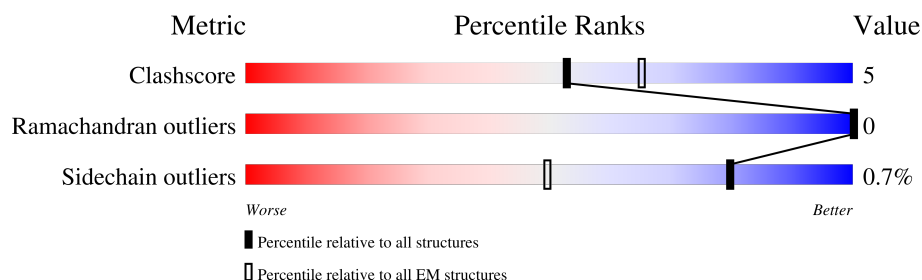
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	464	
1	D	464	
2	B	473	
2	E	473	
3	C	495	
4	a	10	
5	b	2	
5	c	2	

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Mol	Chain	Length	Quality of chain
5	e	2	 100%
6	F	6	 83% 17%
6	G	6	 100%
7	d	5	 100%

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
4	MAN	a	5	X	-	-	-
4	MAN	a	6	X	-	-	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15031 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	349	Total	C	N	O	S	6	0
			2864	1859	479	509	17		
1	D	349	Total	C	N	O	S	6	0
			2864	1860	479	509	16		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P14867
A	-33	LYS	-	expression tag	UNP P14867
A	-32	LYS	-	expression tag	UNP P14867
A	-31	SER	-	expression tag	UNP P14867
A	-30	PRO	-	expression tag	UNP P14867
A	-29	GLY	-	expression tag	UNP P14867
A	-28	LEU	-	expression tag	UNP P14867
A	-27	SER	-	expression tag	UNP P14867
A	-26	ASP	-	expression tag	UNP P14867
A	-25	TYR	-	expression tag	UNP P14867
A	-24	LEU	-	expression tag	UNP P14867
A	-23	TRP	-	expression tag	UNP P14867
A	-22	ALA	-	expression tag	UNP P14867
A	-21	TRP	-	expression tag	UNP P14867
A	-20	THR	-	expression tag	UNP P14867
A	-19	LEU	-	expression tag	UNP P14867
A	-18	PHE	-	expression tag	UNP P14867
A	-17	LEU	-	expression tag	UNP P14867
A	-16	SER	-	expression tag	UNP P14867
A	-15	THR	-	expression tag	UNP P14867
A	-14	LEU	-	expression tag	UNP P14867
A	-13	THR	-	expression tag	UNP P14867
A	-12	GLY	-	expression tag	UNP P14867
A	-11	ARG	-	expression tag	UNP P14867
A	-10	SER	-	expression tag	UNP P14867
A	-9	TYR	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P14867
A	-7	ASP	-	expression tag	UNP P14867
A	-6	TYR	-	expression tag	UNP P14867
A	-5	LYS	-	expression tag	UNP P14867
A	-4	ASP	-	expression tag	UNP P14867
A	-3	ASP	-	expression tag	UNP P14867
A	-2	ASP	-	expression tag	UNP P14867
A	-1	ASP	-	expression tag	UNP P14867
A	0	LYS	-	expression tag	UNP P14867
D	-34	MET	-	initiating methionine	UNP P14867
D	-33	LYS	-	expression tag	UNP P14867
D	-32	LYS	-	expression tag	UNP P14867
D	-31	SER	-	expression tag	UNP P14867
D	-30	PRO	-	expression tag	UNP P14867
D	-29	GLY	-	expression tag	UNP P14867
D	-28	LEU	-	expression tag	UNP P14867
D	-27	SER	-	expression tag	UNP P14867
D	-26	ASP	-	expression tag	UNP P14867
D	-25	TYR	-	expression tag	UNP P14867
D	-24	LEU	-	expression tag	UNP P14867
D	-23	TRP	-	expression tag	UNP P14867
D	-22	ALA	-	expression tag	UNP P14867
D	-21	TRP	-	expression tag	UNP P14867
D	-20	THR	-	expression tag	UNP P14867
D	-19	LEU	-	expression tag	UNP P14867
D	-18	PHE	-	expression tag	UNP P14867
D	-17	LEU	-	expression tag	UNP P14867
D	-16	SER	-	expression tag	UNP P14867
D	-15	THR	-	expression tag	UNP P14867
D	-14	LEU	-	expression tag	UNP P14867
D	-13	THR	-	expression tag	UNP P14867
D	-12	GLY	-	expression tag	UNP P14867
D	-11	ARG	-	expression tag	UNP P14867
D	-10	SER	-	expression tag	UNP P14867
D	-9	TYR	-	expression tag	UNP P14867
D	-8	GLY	-	expression tag	UNP P14867
D	-7	ASP	-	expression tag	UNP P14867
D	-6	TYR	-	expression tag	UNP P14867
D	-5	LYS	-	expression tag	UNP P14867
D	-4	ASP	-	expression tag	UNP P14867
D	-3	ASP	-	expression tag	UNP P14867
D	-2	ASP	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP P14867
D	0	LYS	-	expression tag	UNP P14867

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	340	Total	C	N	O	S	9	0
			2846	1867	466	496	17		
2	E	340	Total	C	N	O	S	3	0
			2811	1842	460	493	16		

- Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	332	Total	C	N	O	S	1	0
			2736	1785	453	483	15		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLY	-	expression tag	UNP P18507
C	438	GLY	-	expression tag	UNP P18507
C	439	SER	-	expression tag	UNP P18507
C	440	GLY	-	expression tag	UNP P18507
C	441	GLY	-	expression tag	UNP P18507
C	442	SER	-	expression tag	UNP P18507
C	443	GLY	-	expression tag	UNP P18507
C	444	GLY	-	expression tag	UNP P18507
C	445	SER	-	expression tag	UNP P18507
C	446	GLY	-	expression tag	UNP P18507
C	447	LYS	-	expression tag	UNP P18507
C	448	THR	-	expression tag	UNP P18507
C	449	GLU	-	expression tag	UNP P18507
C	450	THR	-	expression tag	UNP P18507
C	451	SER	-	expression tag	UNP P18507
C	452	GLN	-	expression tag	UNP P18507
C	453	VAL	-	expression tag	UNP P18507
C	454	ALA	-	expression tag	UNP P18507
C	455	PRO	-	expression tag	UNP P18507
C	456	ALA	-	expression tag	UNP P18507

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	10	Total	C	N	O	0	0
			116	64	2	50		

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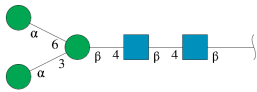
Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	2	Total 28	C 16	N 2	O 10	0	0
5	c	2	Total 28	C 16	N 2	O 10	0	0
5	e	2	Total 28	C 16	N 2	O 10	0	0

- 
- Diagram of a network flow problem with 7 nodes and 10 edges. Nodes 1, 2, and 3 are green circles; nodes 4, 5, and 6 are blue squares. Edges are labeled with capacity (top) and flow (bottom). The network structure is as follows:
- Node 1 (green circle) is connected to Node 2 (green circle) by an edge with capacity 3 and flow  $\alpha$ .
  - Node 2 (green circle) is connected to Node 3 (green circle) by an edge with capacity 3 and flow  $\alpha$ .
  - Node 3 (green circle) is connected to Node 4 (blue square) by an edge with capacity 6 and flow 3.
  - Node 4 (blue square) is connected to Node 5 (blue square) by an edge with capacity 4 and flow  $\beta$ .
  - Node 5 (blue square) is connected to Node 6 (blue square) by an edge with capacity 4 and flow  $\beta$ .
  - Node 6 (blue square) is connected to Node 7 (green circle) by an edge with capacity 4 and flow  $\beta$ .

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	6	Total 72	C 40	N 2	O 30	0	0
6	G	6	Total 72	C 40	N 2	O 30	0	0

- 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-a

cetamido-2-deoxy-beta-D-glucopyranose.

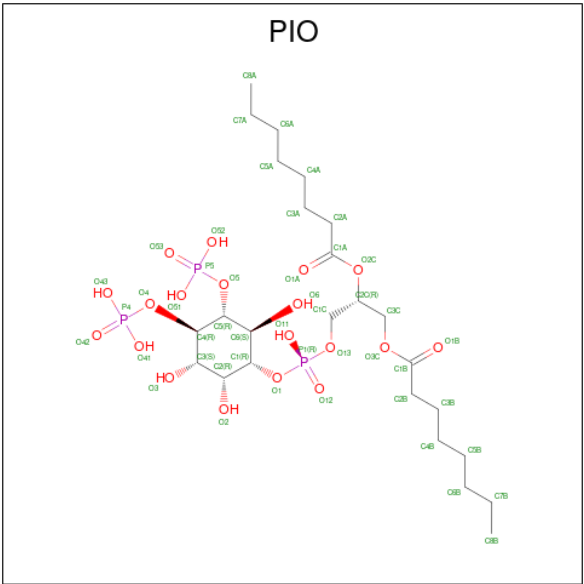


Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Cl	0
			1	1	
8	C	1	Total	Cl	0
			1	1	
8	D	1	Total	Cl	0
			1	1	

- Molecule 9 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>).



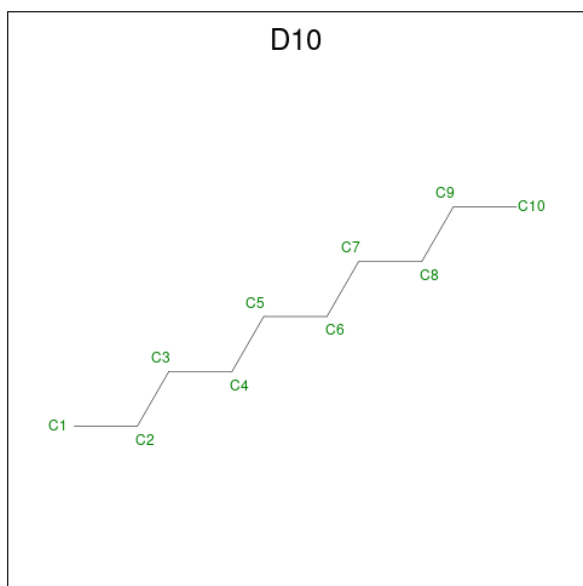
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			47	25	19	3	

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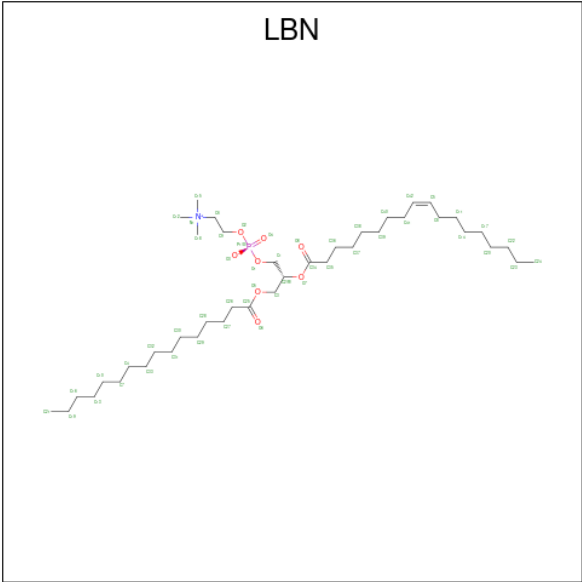
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 10 is DECANE (CCD ID: D10) (formula:  $C_{10}H_{22}$ ).



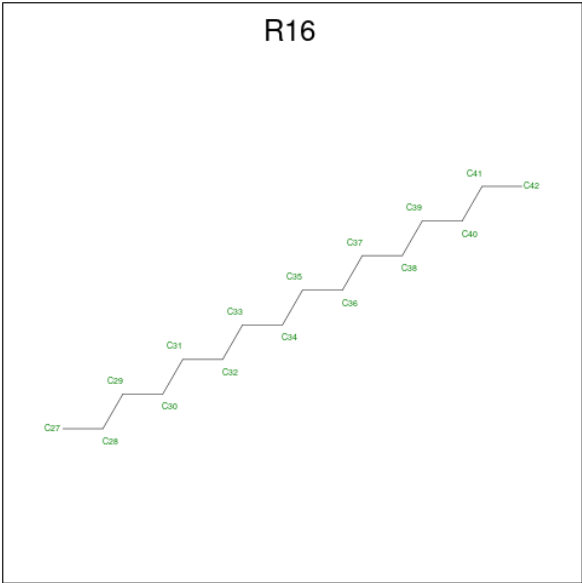
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			10	10	
10	B	1	Total	C	0
			10	10	
10	C	1	Total	C	0
			10	10	
10	D	1	Total	C	0
			10	10	
10	E	1	Total	C	0
			10	10	

- Molecule 11 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula:  $C_{42}H_{82}NO_8P$ ).



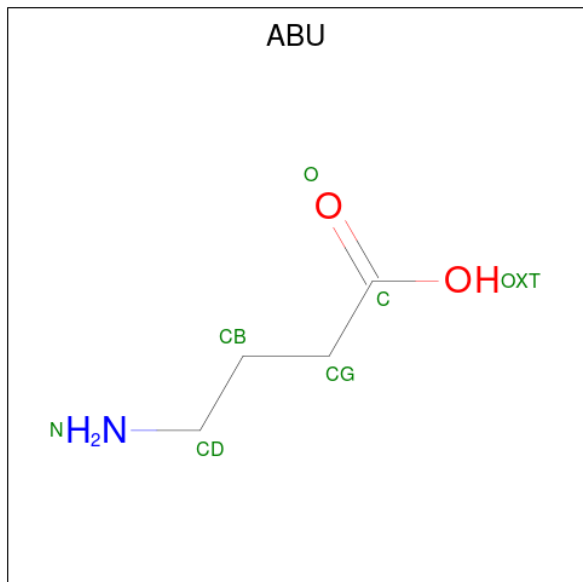
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
11	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 12 is HEXADECANE (CCD ID: R16) (formula: C<sub>16</sub>H<sub>34</sub>).



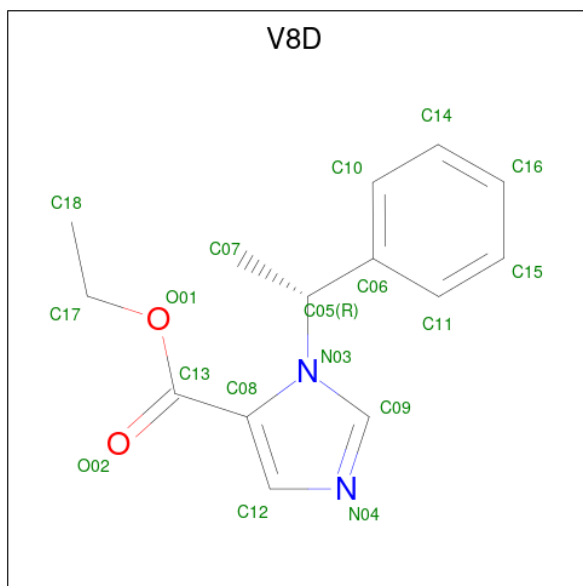
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	C	0
			16	16	
12	E	1	Total	C	0
			16	16	

- Molecule 13 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula:  $C_4H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	N	O	0
			7	4	1	2	
13	E	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 14 is Etomidate (CCD ID: V8D) (formula:  $C_{14}H_{16}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	B	1	Total	C	N	O	0
			18	14	2	2	
14	E	1	Total	C	N	O	0
			18	14	2	2	

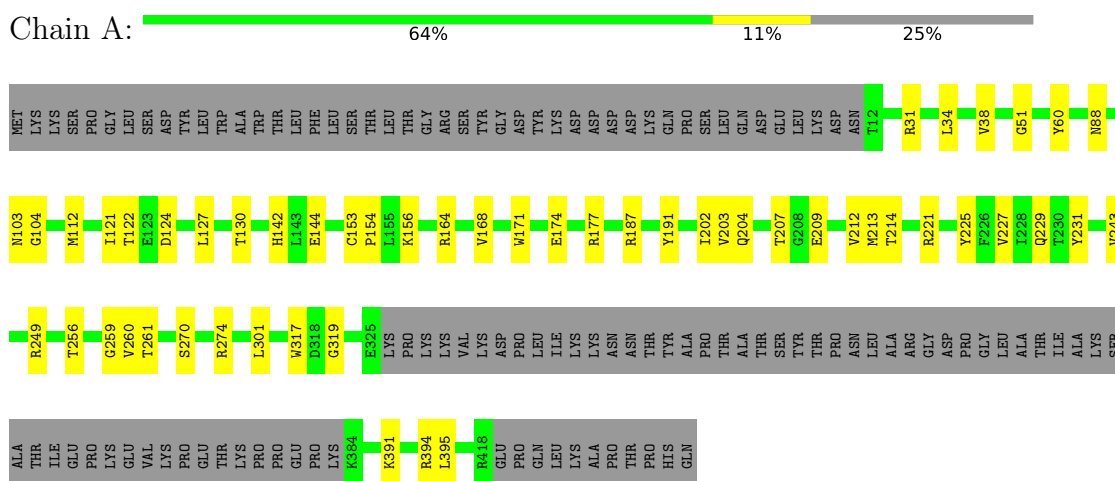
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	30	Total	O	0
			30	30	
15	B	39	Total	O	0
			39	39	
15	C	36	Total	O	0
			36	36	
15	D	33	Total	O	0
			33	33	
15	E	34	Total	O	0
			34	34	

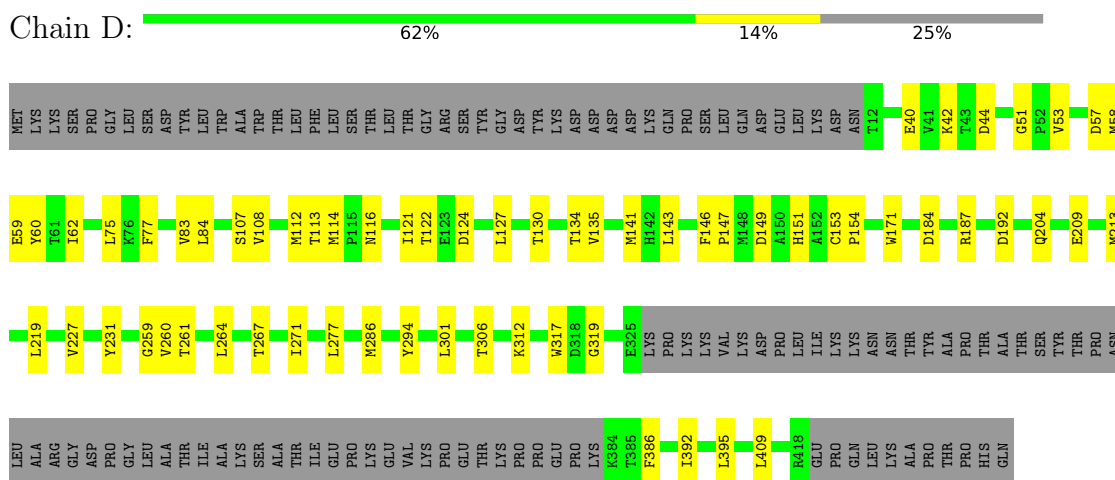
### 3 Residue-property plots

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: Gamma-aminobutyric acid receptor subunit alpha-1



- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1




- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3





- Molecule 4:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -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

Chain a:  90% 10%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 5: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain b:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain c:  100%


MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain e:  100%

MAG1  
MAG2

- Molecule 6:  $\alpha$ -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

Chain F:  83% 17%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 6:  $\alpha$ -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

Chain G:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- 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

Chain d:

100%

MAN1
MAN2
MAN3
MAN4
MAN5

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	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)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.799	Depositor
Minimum map value	-0.612	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	260.28, 260.28, 260.28	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0845, 1.0845, 1.0845	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: LBN, ABU, BMA, R16, D10, CL, V8D, NAG, PIO, MAN

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	0/2956	0.29	0/4015
1	D	0.28	0/2956	0.29	0/4017
2	B	0.28	0/2948	0.32	0/4009
2	E	0.28	0/2895	0.31	0/3939
3	C	0.28	0/2813	0.31	0/3828
All	All	0.28	0/14568	0.31	0/19808

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	2864	0	2872	31	0
1	D	2864	0	2874	40	0
2	B	2846	0	2870	40	0
2	E	2811	0	2815	26	0
3	C	2736	0	2729	28	0
4	a	116	0	97	1	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	28	0	25	0	0
6	F	72	0	61	1	0
6	G	72	0	61	0	0
7	d	61	0	52	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	47	0	44	2	0
9	D	47	0	44	2	0
10	A	10	0	22	1	0
10	B	10	0	22	0	0
10	C	10	0	22	1	0
10	D	10	0	22	1	0
10	E	10	0	22	0	0
11	A	52	0	0	0	0
11	D	52	0	0	0	0
12	B	16	0	34	1	0
12	E	16	0	34	0	0
13	B	7	0	0	0	0
13	E	7	0	0	1	0
14	B	18	0	0	0	0
14	E	18	0	0	0	0
15	A	30	0	0	0	0
15	B	39	0	0	1	0
15	C	36	0	0	1	0
15	D	33	0	0	0	0
15	E	34	0	0	0	0
All	All	15031	0	14772	152	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 5.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD23	2:E:235:LEU:HD11	1.68	0.75
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.20	0.74
1:A:395[A]:LEU:HD23	9:A:502:PIO:H6AA	1.72	0.71
2:B:254:GLY:HA3	2:B:296:LEU:HD13	1.74	0.67
1:A:51:GLY:HA2	1:A:187:ARG:HB2	1.77	0.66
2:B:144:PRO:HD3	2:B:281:ILE:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:PHE:HB2	2:E:101:ASP:HB2	1.78	0.65
2:E:272:LEU:HD13	2:E:279:LYS:HE3	1.80	0.63
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.34	0.62
1:A:270:SER:O	1:A:274:ARG:NH1	2.33	0.62
2:B:306:PHE:HB2	2:B:420:VAL:HG21	1.82	0.61
1:D:143:LEU:HD13	1:D:277:LEU:HD22	1.84	0.60
2:B:272:LEU:HD13	2:B:279:LYS:HE3	1.84	0.59
2:B:41[A]:ASN:ND2	2:B:169:ARG:O	2.36	0.59
1:D:261:THR:HG23	2:E:259[B]:LEU:HD11	1.85	0.58
2:B:192:ARG:NH1	6:F:1:NAG:O7	2.36	0.58
3:C:284:ARG:NH1	3:C:297:ASP:OD2	2.37	0.57
1:A:122:THR:OG1	1:A:124:ASP:OD1	2.22	0.57
3:C:282:ILE:HD13	1:D:271:ILE:HG21	1.88	0.56
3:C:63:GLY:N	3:C:73:THR:O	2.34	0.56
1:D:51:GLY:HA2	1:D:187:ARG:HB2	1.87	0.56
2:B:139:ASP:OD1	2:B:141:ARG:NH1	2.37	0.56
10:C:502:D10:H71	1:D:306:THR:HG22	1.87	0.56
2:E:66[B]:TYR:CZ	2:E:123:THR:HG21	2.41	0.55
2:E:202:THR:OG1	13:E:502:ABU:O	2.24	0.55
3:C:85:ARG:HG2	3:C:88:LYS:HE3	1.89	0.55
2:E:254:GLY:HA3	2:E:296:LEU:HD13	1.90	0.54
2:E:144:PRO:HD3	2:E:281:ILE:HB	1.89	0.54
1:A:261:THR:HG23	2:B:259[B]:LEU:HD11	1.90	0.53
2:B:98:PHE:HB2	2:B:101:ASP:HB2	1.89	0.53
2:B:426:TRP:CE2	2:B:430:VAL:HG21	2.44	0.53
2:B:239:SER:HB3	2:B:253:LEU:HD23	1.91	0.53
1:A:112:MET:HE1	2:B:106:VAL:HG23	1.90	0.53
3:C:69:ASN:O	3:C:117:LYS:NZ	2.41	0.52
10:D:503:D10:H72	2:E:301:PHE:HD1	1.76	0.51
1:D:40[B]:GLU:OE2	1:D:42:LYS:NZ	2.42	0.51
2:B:194:VAL:HB	2:B:209:SER:HB3	1.93	0.51
3:C:110:ASP:OD1	3:C:171:SER:OG	2.26	0.51
1:D:83:VAL:HG22	1:D:122:THR:HG22	1.91	0.51
3:C:101:ASN:O	4:a:5:MAN:O3	2.21	0.50
1:A:164:ARG:HD2	1:A:202:ILE:HD12	1.94	0.50
2:B:66[B]:TYR:CZ	2:B:123:THR:HG21	2.45	0.50
1:D:392:ILE:HG12	9:D:502:PIO:H2AA	1.93	0.50
1:D:114:MET:O	1:D:116:ASN:ND2	2.44	0.49
1:A:174:GLU:OE1	1:A:177:ARG:NH2	2.45	0.49
2:B:66[A]:TYR:CE2	2:B:125:LEU:HD13	2.47	0.49
1:D:149:ASP:OD2	1:D:151:HIS:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:432:SER:HA	3:C:436:LEU:HB2	1.93	0.49
2:B:44:ILE:HG21	2:B:181:ILE:HD11	1.95	0.49
2:E:426:TRP:CE2	2:E:430:VAL:HG21	2.48	0.49
3:C:284:ARG:NH2	3:C:290:VAL:O	2.46	0.48
2:B:302:VAL:HG13	2:B:420:VAL:HG13	1.95	0.48
1:A:227:VAL:HA	1:A:231:TYR:HB2	1.96	0.48
2:B:98:PHE:HA	2:B:153:GLU:O	2.14	0.48
1:D:75:LEU:HD12	1:D:127:LEU:HD11	1.94	0.47
1:A:317:TRP:CZ3	1:A:319:GLY:HA2	2.49	0.47
2:B:48:ASP:OD1	2:B:48:ASP:N	2.47	0.47
3:C:237:THR:HA	3:C:241:TYR:HB2	1.96	0.47
1:D:116:ASN:HD22	1:D:116:ASN:N	2.12	0.47
3:C:56:ASP:HB2	3:C:79:ALA:HB3	1.95	0.47
1:A:207:THR:HG21	2:E:115:MET:HE1	1.96	0.47
1:A:256:THR:O	1:A:260:VAL:HG23	2.14	0.47
2:B:102:LYS:HD2	2:B:135:ALA:HB2	1.96	0.47
1:D:122:THR:OG1	1:D:124:ASP:OD1	2.23	0.47
1:D:317:TRP:CZ3	1:D:319:GLY:HA2	2.49	0.47
1:D:60:TYR:OH	1:D:154:PRO:O	2.27	0.46
1:D:227:VAL:HA	1:D:231:TYR:HB2	1.97	0.46
1:D:121:ILE:HG12	1:D:127:LEU:HD23	1.96	0.46
1:D:171:TRP:CE2	1:D:213:MET:HE3	2.51	0.46
1:D:259:GLY:HA3	1:D:301:LEU:HD13	1.98	0.46
1:A:259:GLY:HA3	1:A:301:LEU:HD13	1.97	0.45
2:B:42:ILE:O	2:B:175:VAL:HA	2.16	0.45
1:D:53:VAL:HG21	1:D:219:LEU:HD13	1.98	0.45
1:A:31:ARG:HG2	1:A:34:LEU:HD12	1.99	0.45
2:B:42:ILE:HB	2:B:175:VAL:HG22	1.98	0.45
1:D:77:PHE:CZ	1:D:84:LEU:HG	2.52	0.45
1:A:156:LYS:HG2	1:A:214:THR:HG23	1.98	0.45
1:D:108:VAL:HB	1:D:134:THR:HB	1.99	0.45
2:E:220:TYR:CZ	2:E:224:GLN:HG3	2.52	0.45
3:C:124:ILE:HA	3:C:125:THR:HA	1.77	0.45
2:B:223:LEU:HD11	3:C:293:VAL:HG22	1.99	0.44
1:D:312:LYS:NZ	9:D:502:PIO:O41	2.35	0.44
2:E:233:THR:O	2:E:236:SER:OG	2.34	0.44
2:B:151:THR:HG22	2:B:211:SER:HB3	2.00	0.44
1:D:261:THR:HG21	2:E:255:ILE:HG23	1.98	0.44
3:C:318:HIS:O	3:C:322:SER:OG	2.29	0.44
3:C:124:ILE:HG13	1:D:107:SER:HB2	1.98	0.44
3:C:183:TRP:CE3	3:C:187:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TRP:CE2	1:A:213:MET:HE3	2.53	0.44
1:A:391:LYS:HG2	1:A:394:ARG:NH2	2.33	0.44
2:B:235:LEU:HD23	2:B:235:LEU:HA	1.85	0.44
2:E:225:THR:HG21	2:E:281:ILE:HD11	2.00	0.44
2:E:262:THR:O	2:E:266:THR:HG23	2.18	0.44
1:A:103:ASN:ND2	1:A:154:PRO:O	2.47	0.44
2:B:57:TYR:OH	2:B:151:THR:O	2.26	0.44
1:D:44:ASP:OD1	1:D:44:ASP:N	2.49	0.44
1:D:267:THR:OG1	1:D:294:TYR:OH	2.26	0.44
3:C:109:PRO:O	15:C:601:HOH:O	2.21	0.44
3:C:155:LEU:HD13	3:C:287:LEU:HD22	1.99	0.44
1:A:60:TYR:CE1	1:A:153:CYS:HB3	2.53	0.43
2:B:224:GLN:NE2	3:C:284:ARG:HD3	2.33	0.43
1:A:112:MET:HE2	1:A:112:MET:HB2	1.89	0.43
3:C:206:LEU:HA	3:C:226:TYR:O	2.18	0.43
2:E:42:ILE:HB	2:E:175:VAL:HG22	1.99	0.43
2:E:44:ILE:HD12	2:E:178:VAL:HG22	2.00	0.43
1:D:146:PHE:CD1	1:D:277:LEU:HD21	2.54	0.43
2:B:44:ILE:HD12	2:B:178:VAL:HG22	2.00	0.43
3:C:34:LEU:HD22	3:C:87:LEU:HA	2.01	0.43
1:A:225:TYR:CE1	1:A:229:GLN:HG3	2.54	0.43
2:B:64[B]:GLN:OE1	15:B:601:HOH:O	2.21	0.43
3:C:72:TYR:CE1	3:C:165:CYS:HB3	2.54	0.42
1:D:146:PHE:CD2	1:D:277:LEU:HD11	2.54	0.42
1:A:191:TYR:OH	1:A:221:ARG:NH2	2.52	0.42
1:D:112:MET:HA	1:D:113:THR:HA	1.81	0.42
1:D:260:VAL:O	1:D:264:LEU:HG	2.18	0.42
1:D:184:ASP:OD1	1:D:184:ASP:N	2.38	0.42
1:A:104:GLY:O	2:E:129:ARG:NH2	2.52	0.42
1:D:57:ASP:HB2	1:D:59:GLU:HG2	2.02	0.42
3:C:102:MET:HE3	3:C:102:MET:HB3	1.93	0.42
1:D:204[A]:GLN:HG2	1:D:209:GLU:HG2	2.02	0.42
2:E:151:THR:HG22	2:E:211:SER:HB3	2.00	0.42
2:E:198:VAL:HG21	2:E:207:ARG:CZ	2.49	0.42
3:C:200:GLN:O	3:C:232:ARG:N	2.45	0.42
2:E:164:ILE:HG23	2:E:206:PRO:HG3	2.02	0.42
3:C:66:ASN:HB3	3:C:71:GLU:HG2	2.01	0.42
3:C:70:MET:HE2	3:C:288:PRO:HG3	2.01	0.42
1:A:121:ILE:HG12	1:A:127:LEU:HD23	2.01	0.41
1:D:62:ILE:HG23	1:D:135:VAL:HB	2.02	0.41
1:A:203:VAL:HB	1:A:212:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:VAL:HA	2:E:181:ILE:HD12	2.02	0.41
2:E:301:PHE:O	2:E:305:ILE:HG12	2.20	0.41
2:B:222:ILE:HA	2:B:226:TYR:HB2	2.03	0.41
1:D:58:MET:HA	1:D:141:MET:HE3	2.01	0.41
2:B:230:ILE:HD13	12:B:501:R16:H371	2.02	0.41
1:D:60:TYR:CE1	1:D:153:CYS:HB3	2.55	0.41
1:A:38:VAL:HG11	1:A:168:VAL:HG13	2.02	0.41
2:B:129:ARG:NH2	3:C:116:SER:O	2.54	0.41
1:D:147:PRO:HD3	1:D:286:MET:HB2	2.02	0.41
1:A:142:HIS:HB3	1:A:144:GLU:OE1	2.21	0.41
2:B:97:TYR:CE1	2:B:155:GLU:HB3	2.56	0.41
2:E:281:ILE:HD12	2:E:281:ILE:HA	1.91	0.41
1:A:204[A]:GLN:OE1	1:A:209:GLU:HG2	2.21	0.41
1:A:243:VAL:HG22	10:A:503:D10:H22	2.03	0.41
1:A:249:ARG:NH2	9:A:502:PIO:O11	2.54	0.41
1:D:192:ASP:O	1:D:219:LEU:HA	2.20	0.41
2:B:145:LEU:HD22	2:B:446:TYR:HB3	2.03	0.40
2:B:251:VAL:HG13	2:B:255:ILE:HD13	2.04	0.40
2:B:424:ASP:O	2:B:428:ARG:HG3	2.22	0.40
2:B:235:LEU:HD22	3:C:311:LEU:HD23	2.04	0.40
1:D:317:TRP:HA	1:D:386:PHE:CD2	2.57	0.40
2:B:99:LEU:HD22	2:B:207:ARG:HH22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/464 (76%)	347 (99%)	4 (1%)	0	100	100
1	D	351/464 (76%)	342 (97%)	9 (3%)	0	100	100
2	B	345/473 (73%)	339 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	339/473 (72%)	335 (99%)	4 (1%)	0	100	100
3	C	329/495 (66%)	314 (95%)	15 (5%)	0	100	100
All	All	1715/2369 (72%)	1677 (98%)	38 (2%)	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	317/413 (77%)	315 (99%)	2 (1%)	84	94
1	D	317/413 (77%)	313 (99%)	4 (1%)	65	85
2	B	315/422 (75%)	312 (99%)	3 (1%)	73	89
2	E	309/422 (73%)	308 (100%)	1 (0%)	91	97
3	C	306/448 (68%)	304 (99%)	2 (1%)	81	93
All	All	1564/2118 (74%)	1552 (99%)	12 (1%)	80	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	130	THR
2	B	255	ILE
2	B	275	ILE
2	B	302	VAL
3	C	208	ASN
3	C	424	LEU
1	D	130	THR
1	D	395[A]	LEU
1	D	395[B]	LEU
1	D	409	LEU
2	E	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	116	ASN
1	A	189	ASN
2	B	54	ASN
2	B	267	HIS
3	C	101	ASN
3	C	128	ASN
3	C	152	GLN
3	C	156	HIS
1	D	242	GLN
2	E	54	ASN
2	E	185	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	$\# Z  > 2$
6	NAG	F	1	2,6	14,14,15	0.26	0	17,19,21	0.53	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.43	0
6	BMA	F	3	6	11,11,12	0.22	0	15,15,17	0.45	0
6	MAN	F	4	6	11,11,12	0.19	0	15,15,17	0.53	0
6	MAN	F	5	6	11,11,12	0.23	0	15,15,17	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	F	6	6	11,11,12	0.18	0	15,15,17	0.35	0
6	NAG	G	1	2,6	14,14,15	0.27	0	17,19,21	0.47	0
6	NAG	G	2	6	14,14,15	0.25	0	17,19,21	0.41	0
6	BMA	G	3	6	11,11,12	0.20	0	15,15,17	0.55	0
6	MAN	G	4	6	11,11,12	0.19	0	15,15,17	0.43	0
6	MAN	G	5	6	11,11,12	0.20	0	15,15,17	0.45	0
6	MAN	G	6	6	11,11,12	0.18	0	15,15,17	0.33	0
4	NAG	a	1	1,4	14,14,15	0.23	0	17,19,21	0.51	0
4	MAN	a	10	4	11,11,12	0.18	0	15,15,17	0.51	0
4	NAG	a	2	4	14,14,15	0.22	0	17,19,21	0.50	0
4	BMA	a	3	4	11,11,12	0.21	0	15,15,17	0.55	0
4	MAN	a	4	4	11,11,12	0.20	0	15,15,17	0.48	0
4	MAN	a	5	4	11,11,12	0.23	0	15,15,17	0.80	0
4	MAN	a	6	4	11,11,12	0.20	0	15,15,17	0.33	0
4	MAN	a	7	4	11,11,12	0.26	0	15,15,17	0.71	0
4	MAN	a	8	4	11,11,12	0.22	0	15,15,17	0.59	0
4	MAN	a	9	4	11,11,12	0.19	0	15,15,17	0.42	0
5	NAG	b	1	2,5	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	b	2	5	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	c	1	3,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	c	2	5	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	d	1	7,1	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	d	2	7	14,14,15	0.22	0	17,19,21	0.63	0
7	BMA	d	3	7	11,11,12	0.17	0	15,15,17	0.36	0
7	MAN	d	4	7	11,11,12	0.24	0	15,15,17	0.30	0
7	MAN	d	5	7	11,11,12	0.22	0	15,15,17	0.48	0
5	NAG	e	1	2,5	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	e	2	5	14,14,15	0.21	0	17,19,21	0.50	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
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	1/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	1/2/19/22	0/1/1/1
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	a	10	4	-	0/2/19/22	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	BMA	a	3	4	-	2/2/19/22	0/1/1/1
4	MAN	a	4	4	-	1/2/19/22	0/1/1/1
4	MAN	a	5	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	a	6	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	a	7	4	-	0/2/19/22	0/1/1/1
4	MAN	a	8	4	-	1/2/19/22	0/1/1/1
4	MAN	a	9	4	-	0/2/19/22	0/1/1/1
5	NAG	b	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	3/6/23/26	0/1/1/1
7	NAG	d	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	BMA	d	3	7	-	0/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
7	MAN	d	5	7	-	0/2/19/22	0/1/1/1
5	NAG	e	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	a	5	MAN	C1
4	a	6	MAN	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	c	2	NAG	C8-C7-N2-C2

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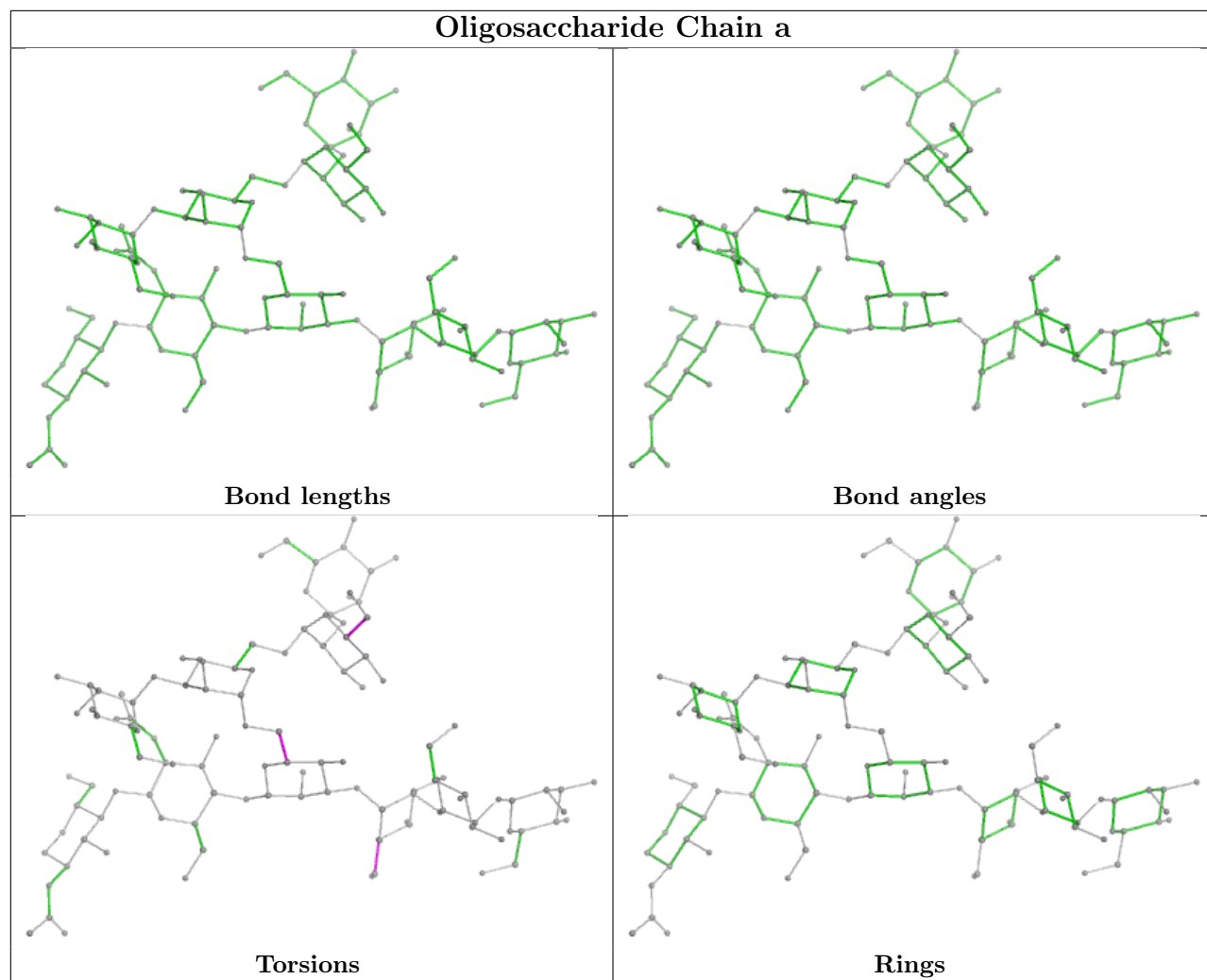
Mol	Chain	Res	Type	Atoms
5	c	2	NAG	O7-C7-N2-C2
4	a	3	BMA	O5-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6
6	F	6	MAN	O5-C5-C6-O6
4	a	4	MAN	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
4	a	8	MAN	O5-C5-C6-O6
4	a	3	BMA	C4-C5-C6-O6

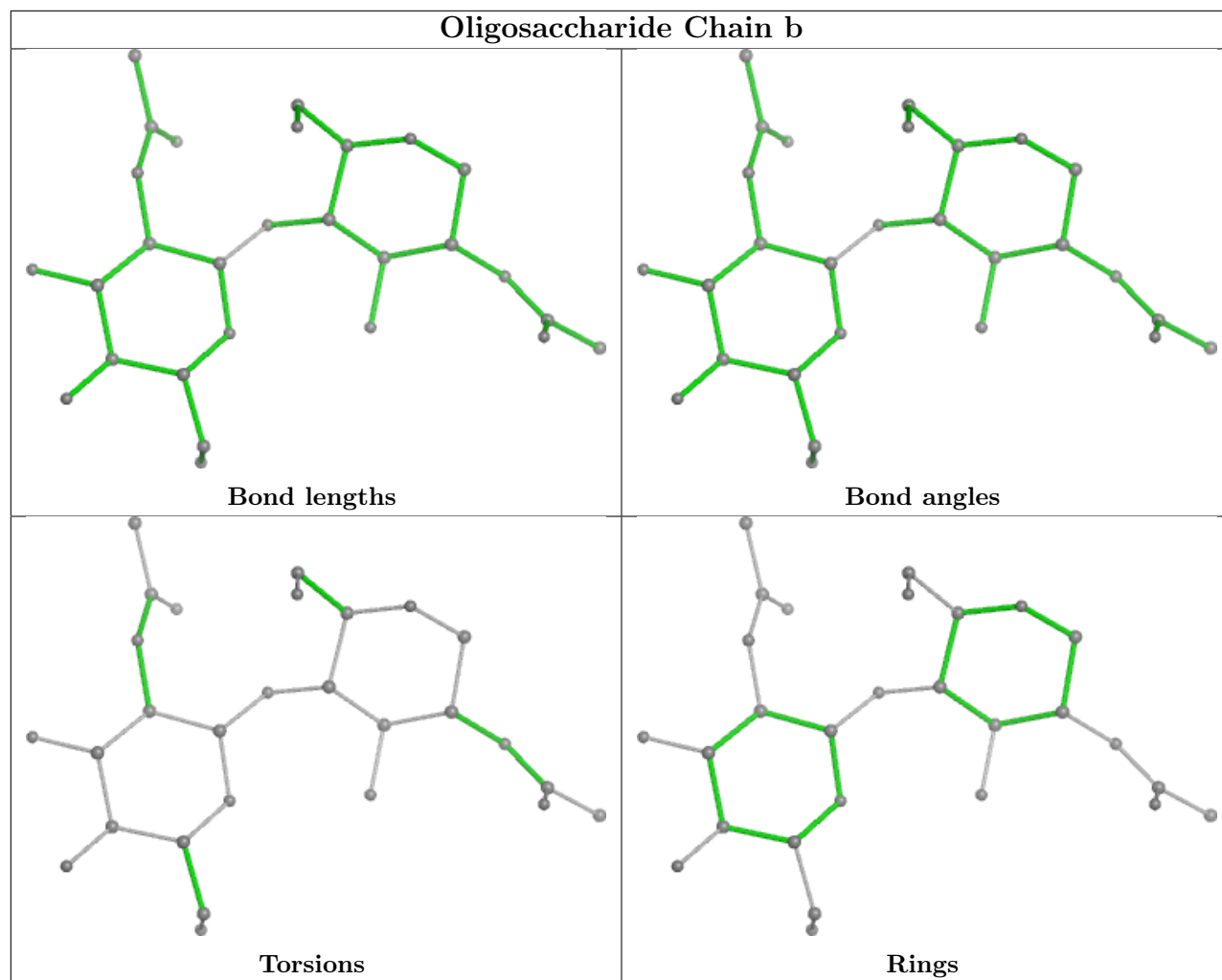
There are no ring outliers.

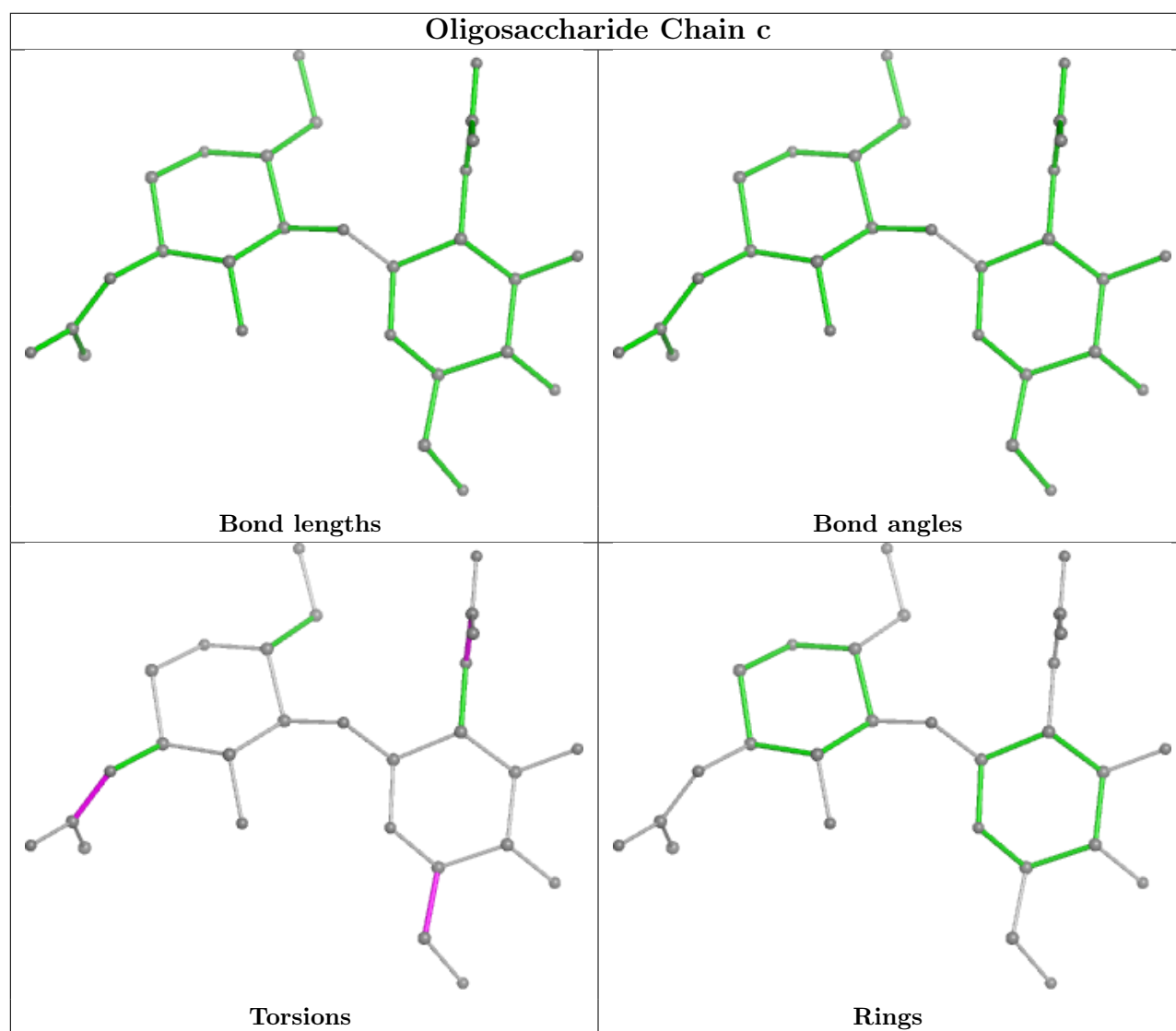
2 monomers are involved in 2 short contacts:

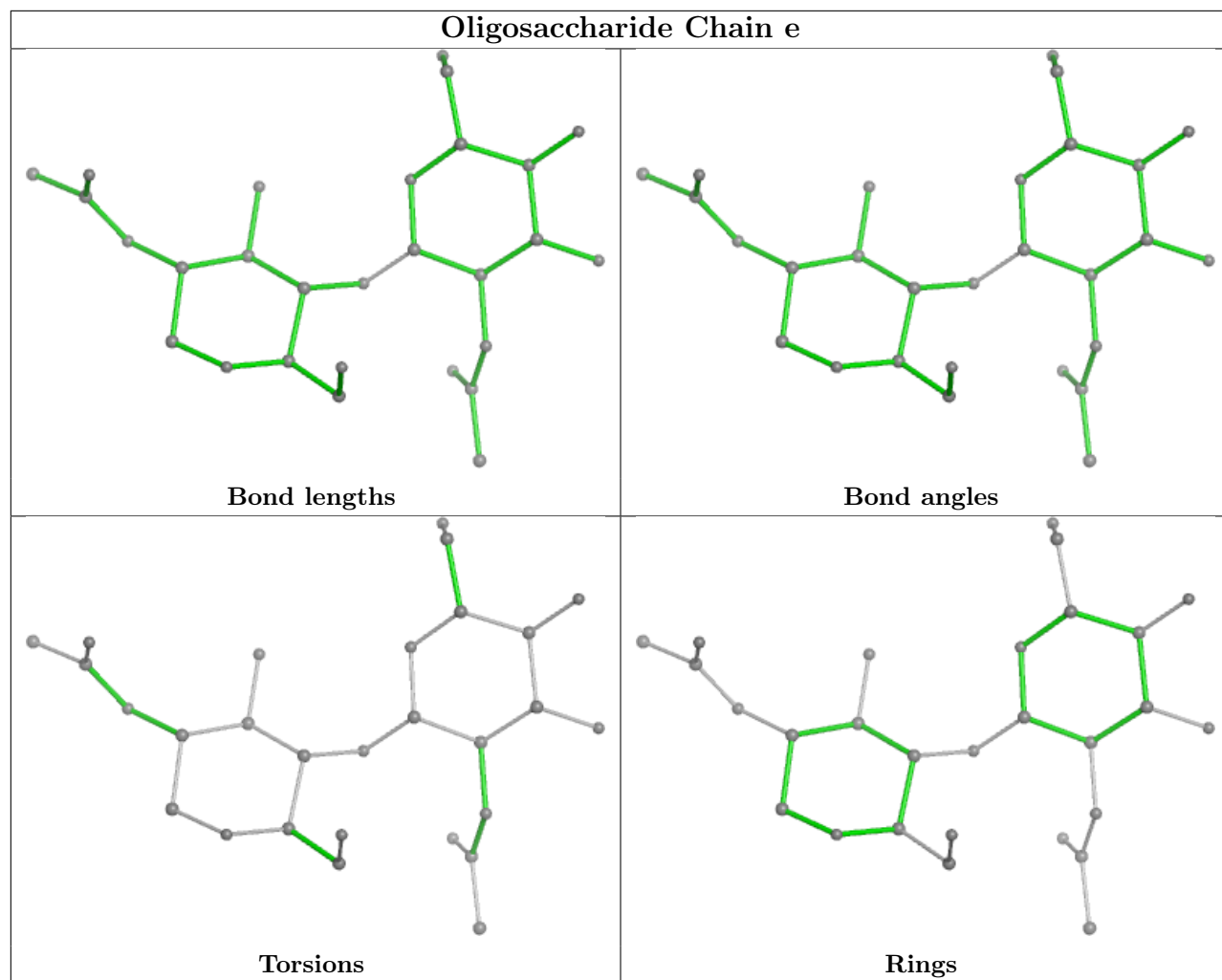
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	5	MAN	1	0
6	F	1	NAG	1	0

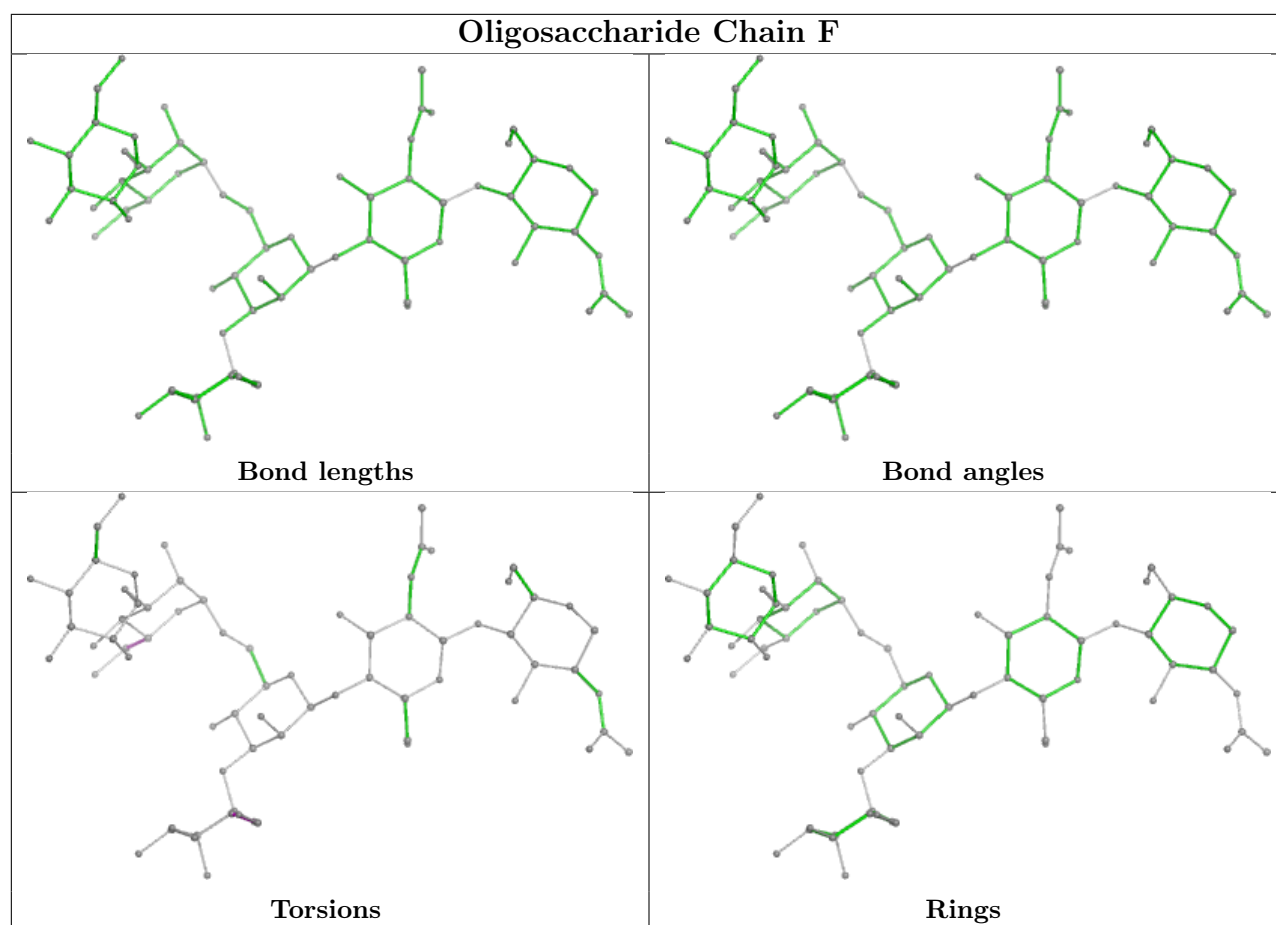
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

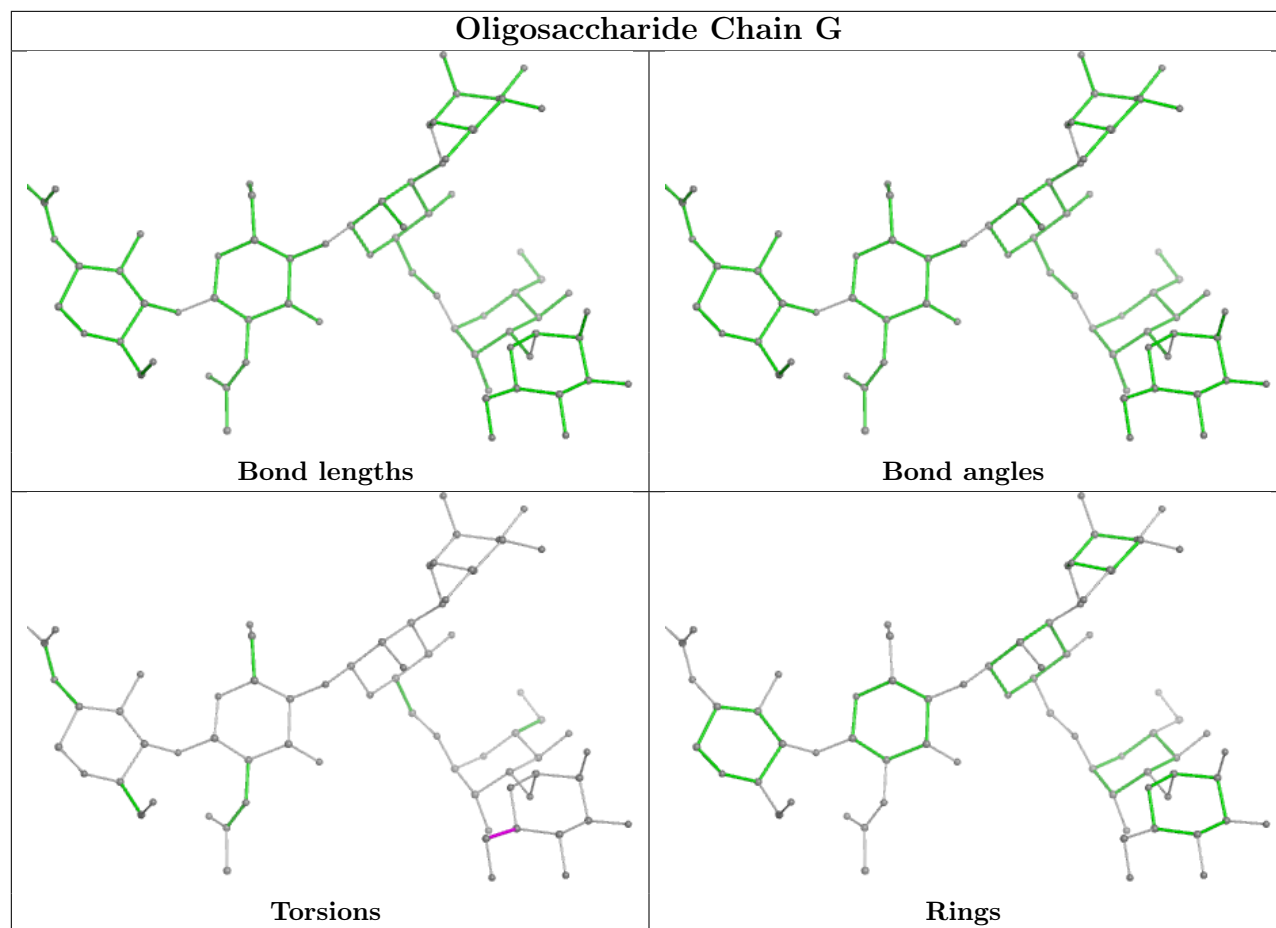


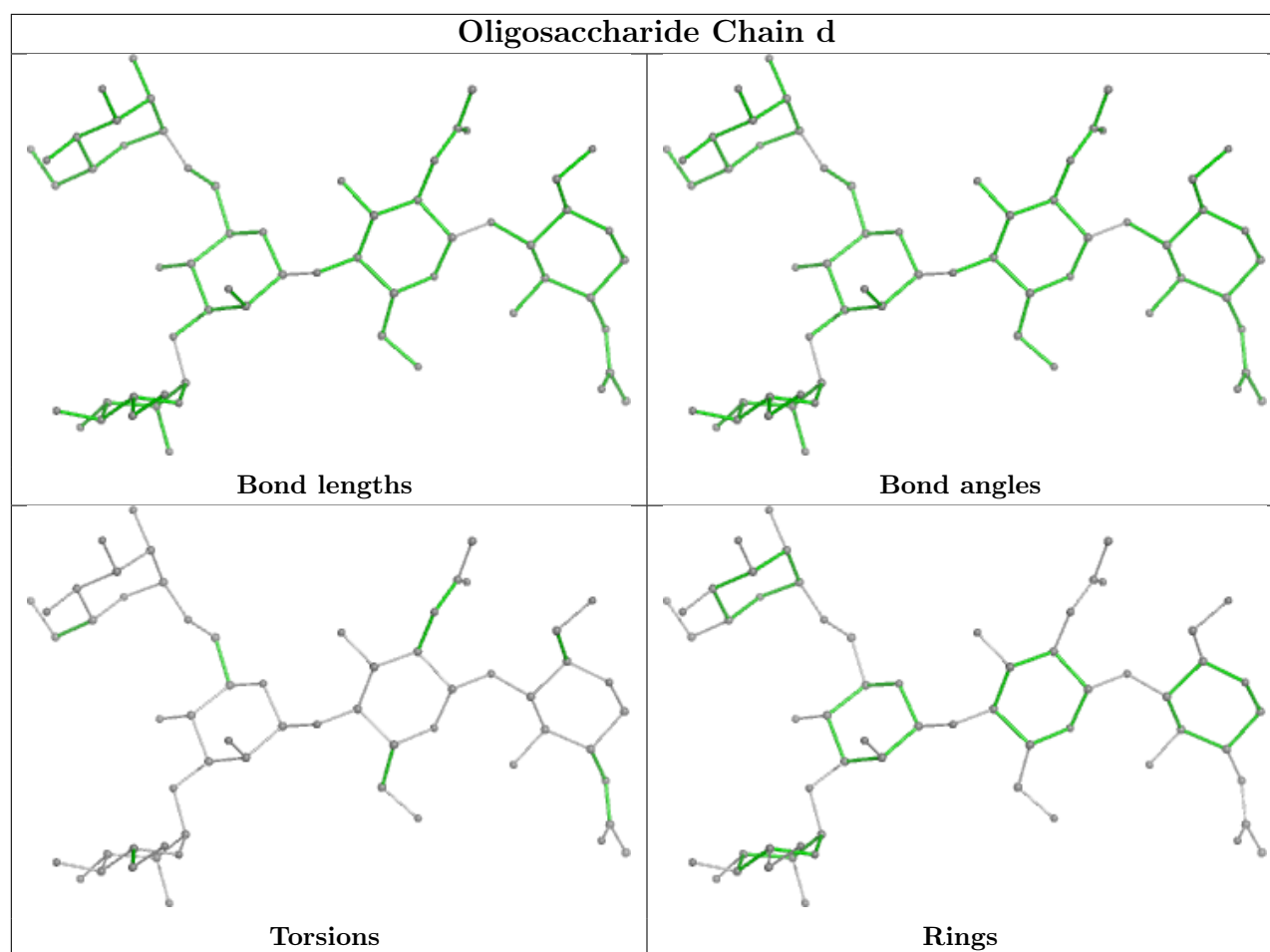












## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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	R16	E	504	-	15,15,15	0.14	0	14,14,14	0.23	0
10	D10	C	502	-	9,9,9	0.14	0	8,8,8	0.12	0
10	D10	B	502	-	9,9,9	0.11	0	8,8,8	0.12	0
11	LBN	D	504	-	51,51,51	0.29	0	57,59,59	0.28	0
10	D10	A	503	-	9,9,9	0.12	0	8,8,8	0.16	0
10	D10	E	501	-	9,9,9	0.12	0	8,8,8	0.11	0
14	V8D	B	504	-	17,19,19	0.47	0	22,25,25	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	ABU	E	502	-	6,6,6	0.89	0	6,6,6	0.91	0
13	ABU	B	503	-	6,6,6	0.77	0	6,6,6	0.77	0
9	PIO	A	502	-	47,47,47	0.56	0	61,65,65	0.45	0
12	R16	B	501	-	15,15,15	0.10	0	14,14,14	0.19	0
9	PIO	D	502	-	47,47,47	0.54	0	61,65,65	0.46	0
10	D10	D	503	-	9,9,9	0.13	0	8,8,8	0.14	0
11	LBN	A	504	-	51,51,51	0.29	0	57,59,59	0.28	0
14	V8D	E	503	-	17,19,19	0.46	0	22,25,25	0.59	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	R16	E	504	-	-	0/13/13/13	-
10	D10	C	502	-	-	0/7/7/7	-
10	D10	B	502	-	-	0/7/7/7	-
11	LBN	D	504	-	-	14/55/55/55	-
10	D10	A	503	-	-	0/7/7/7	-
10	D10	E	501	-	-	0/7/7/7	-
14	V8D	B	504	-	-	0/14/15/15	0/2/2/2
13	ABU	E	502	-	-	0/4/4/4	-
13	ABU	B	503	-	-	0/4/4/4	-
9	PIO	A	502	-	-	8/44/68/68	0/1/1/1
12	R16	B	501	-	-	0/13/13/13	-
9	PIO	D	502	-	-	7/44/68/68	0/1/1/1
10	D10	D	503	-	-	1/7/7/7	-
11	LBN	A	504	-	-	16/55/55/55	-
14	V8D	E	503	-	-	3/14/15/15	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	502	PIO	C4-O4-P4-O42
11	A	504	LBN	C1-O1-P1-O2
11	A	504	LBN	C1-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
11	A	504	LBN	C1-O1-P1-O4
11	A	504	LBN	C9-O2-P1-O1
11	A	504	LBN	C9-O2-P1-O3
11	A	504	LBN	C9-O2-P1-O4
11	D	504	LBN	C9-O2-P1-O3
11	D	504	LBN	C26-C25-O5-C3
11	D	504	LBN	O6-C25-O5-C3
11	D	504	LBN	C9-C6-N1-C12
9	D	502	PIO	C1A-C2A-C3A-C4A
9	A	502	PIO	C1C-O13-P1-O1
11	D	504	LBN	C9-O2-P1-O1
11	D	504	LBN	C9-C6-N1-C18
9	D	502	PIO	O2C-C2C-C3C-O3C
11	D	504	LBN	C9-C6-N1-C15
9	A	502	PIO	C1-O1-P1-O13
11	D	504	LBN	C2-C1-O1-P1
14	E	503	V8D	N03-C05-C06-C10
14	E	503	V8D	N03-C05-C06-C11
9	A	502	PIO	C4-O4-P4-O42
9	D	502	PIO	C1C-C2C-C3C-O3C
11	A	504	LBN	C1-C2-C3-O5
9	D	502	PIO	C5-O5-P5-O52
11	D	504	LBN	C1-O1-P1-O2
9	A	502	PIO	C1C-O13-P1-O11
9	A	502	PIO	C1C-O13-P1-O12
11	A	504	LBN	C6-C9-O2-P1
11	A	504	LBN	N1-C6-C9-O2
11	D	504	LBN	C1-C2-C3-O5
11	D	504	LBN	O7-C2-C3-O5
11	A	504	LBN	O7-C2-C3-O5
11	D	504	LBN	C42-C5-C8-C11
11	D	504	LBN	C40-C41-C42-C5
11	A	504	LBN	O7-C34-C35-C36
9	A	502	PIO	C5-O5-P5-O51
9	A	502	PIO	C5-O5-P5-O52
11	A	504	LBN	C42-C5-C8-C11
14	E	503	V8D	C18-C17-O01-C13
10	D	503	D10	C5-C6-C7-C8
11	A	504	LBN	O8-C34-C35-C36
11	A	504	LBN	C25-C26-C27-C28
9	D	502	PIO	O2C-C1A-C2A-C3A
11	A	504	LBN	O5-C25-C26-C27

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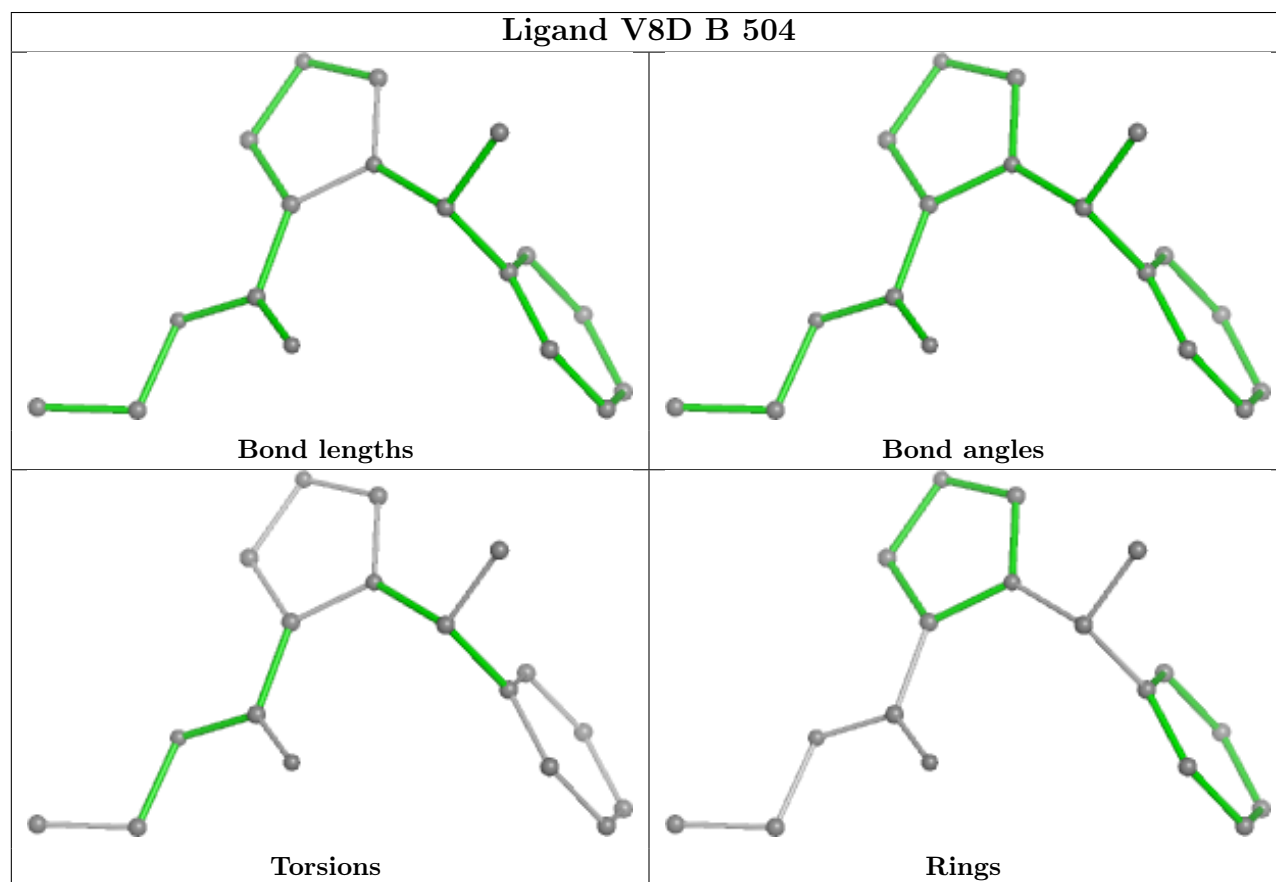
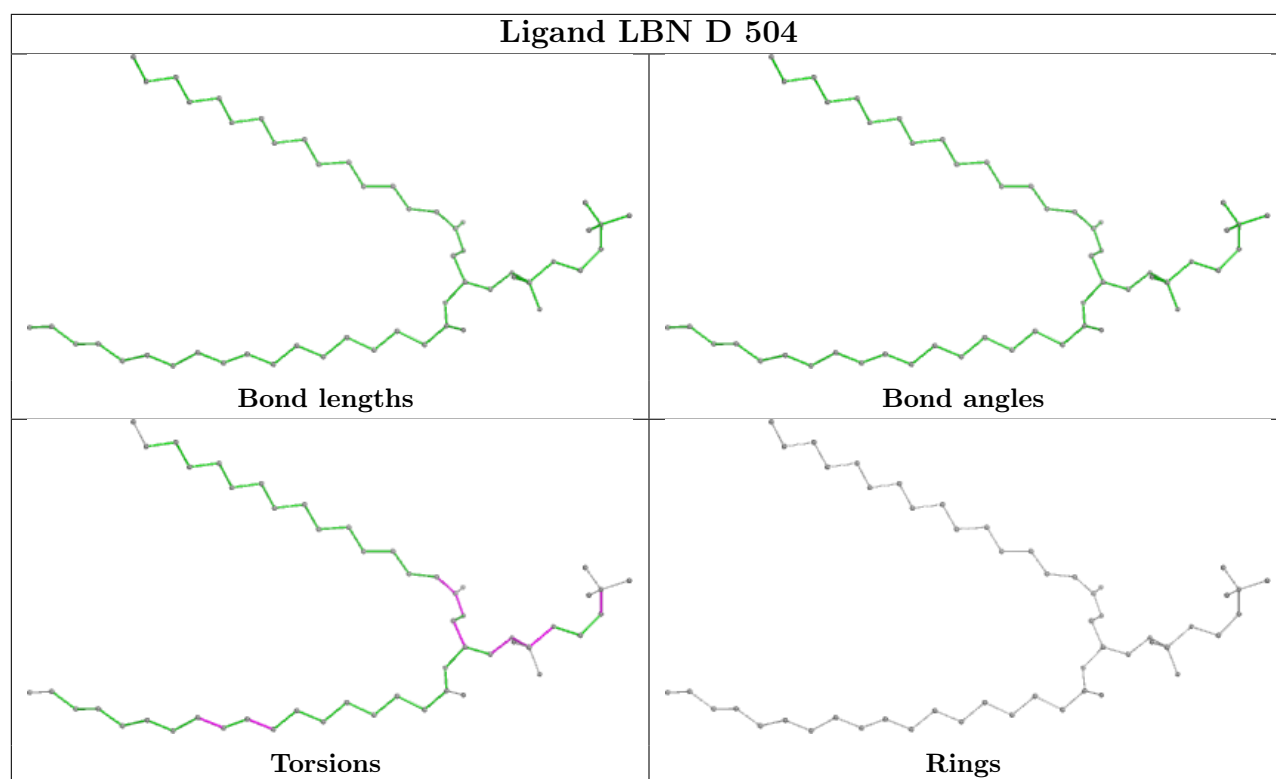
Mol	Chain	Res	Type	Atoms
9	D	502	PIO	O1A-C1A-C2A-C3A
9	A	502	PIO	O2C-C1A-C2A-C3A
11	A	504	LBN	O6-C25-C26-C27
11	D	504	LBN	O5-C25-C26-C27

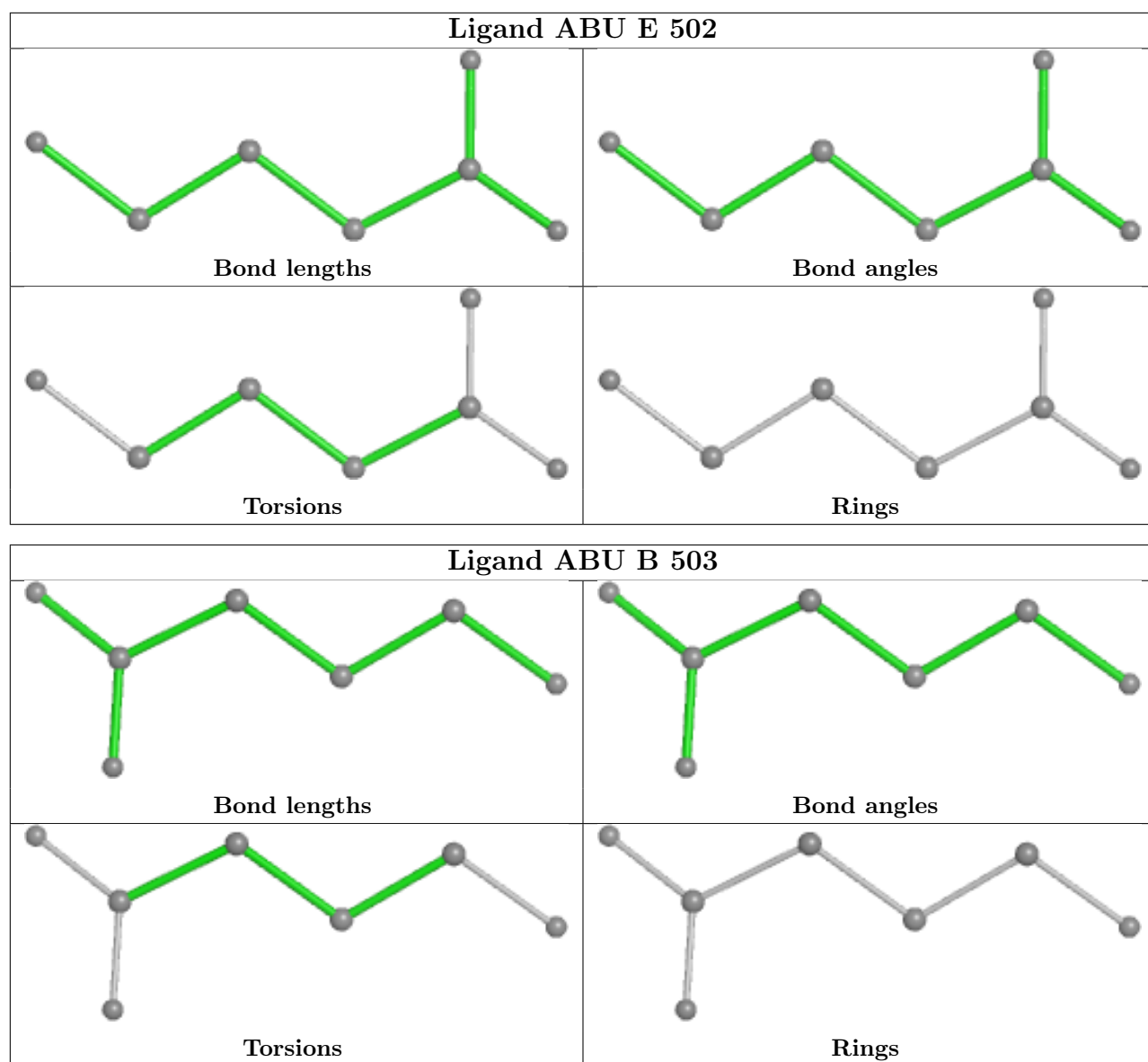
There are no ring outliers.

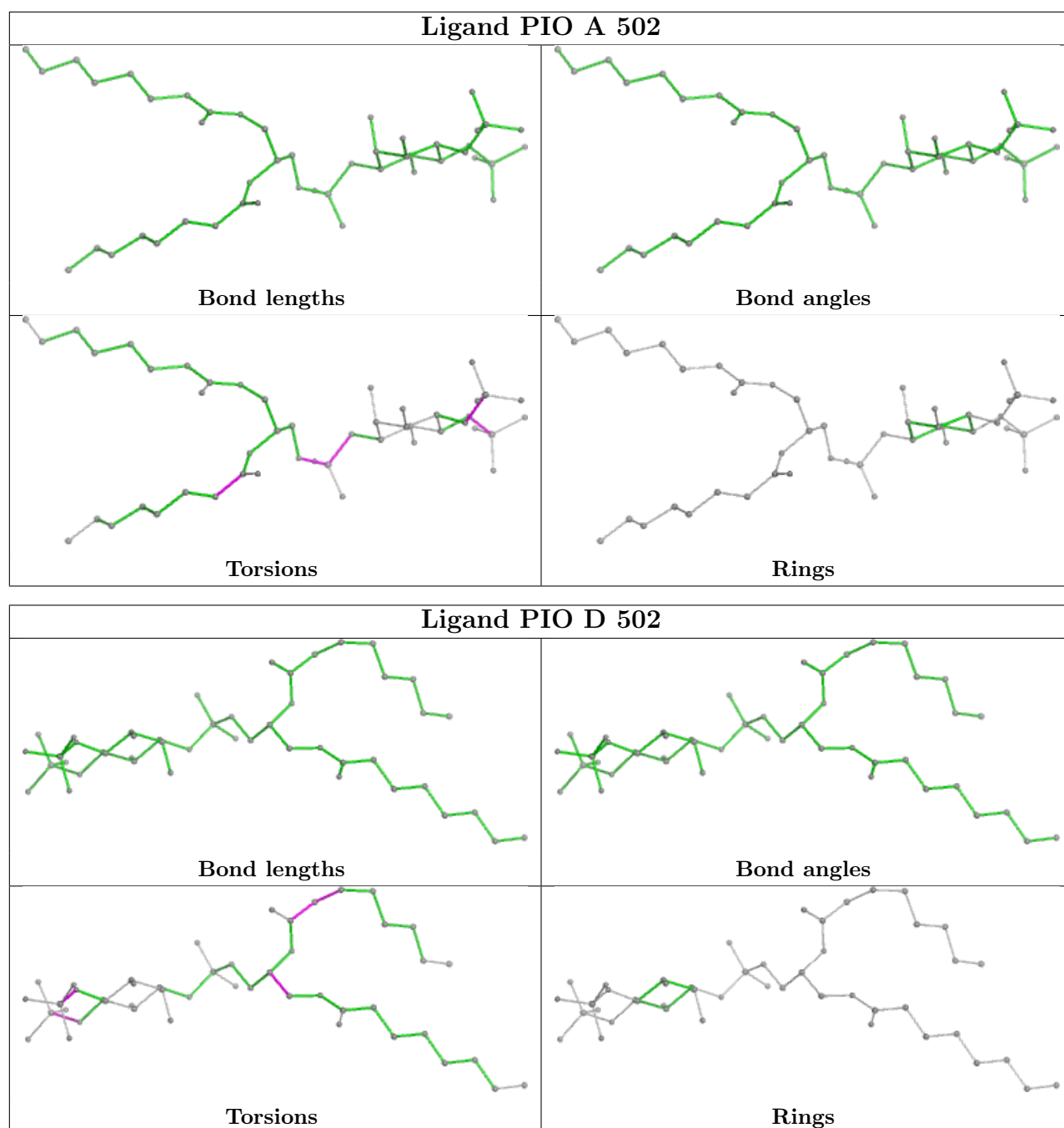
7 monomers are involved in 9 short contacts:

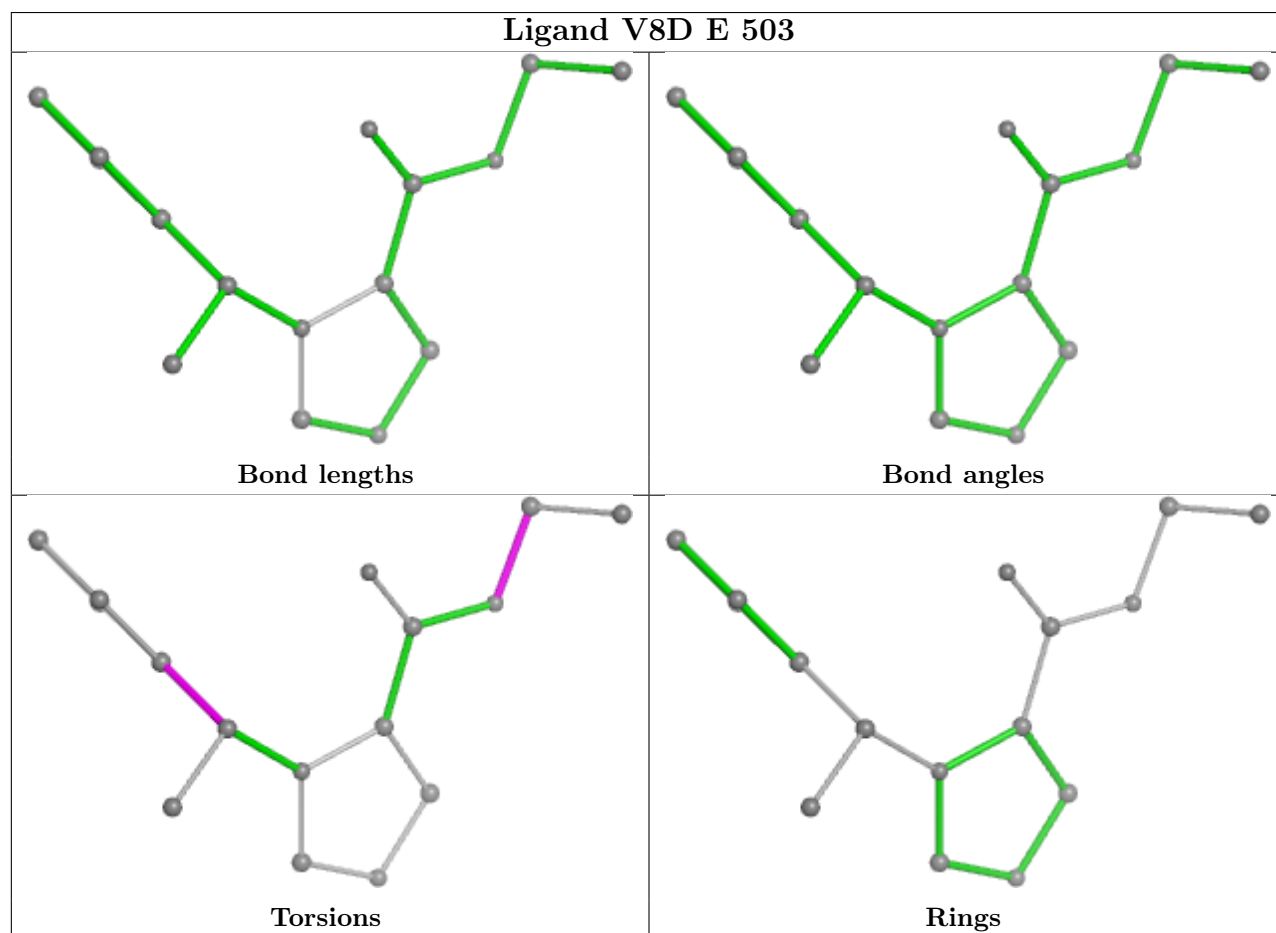
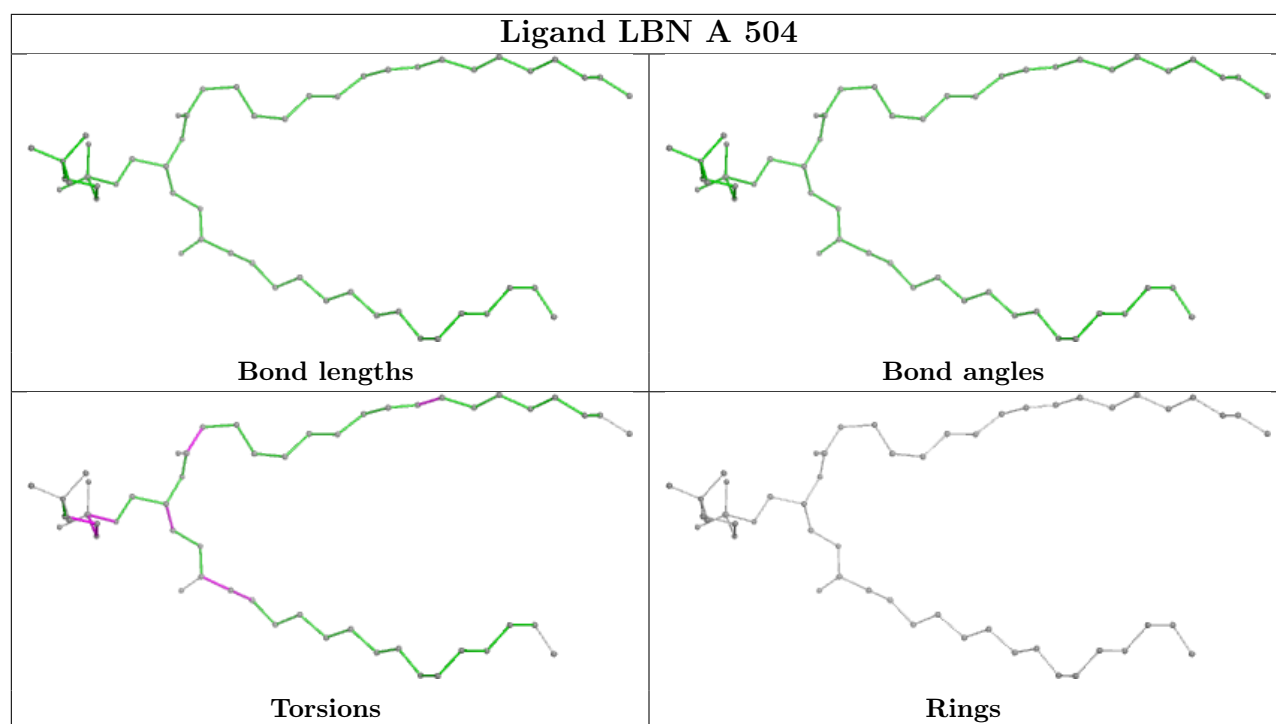
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	502	D10	1	0
10	A	503	D10	1	0
13	E	502	ABU	1	0
9	A	502	PIO	2	0
12	B	501	R16	1	0
9	D	502	PIO	2	0
10	D	503	D10	1	0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

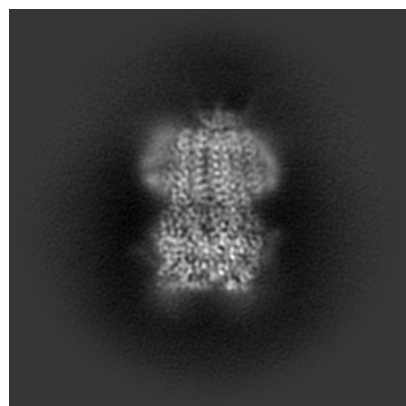
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50389. These allow visual inspection of the internal detail of the map and identification of artifacts.

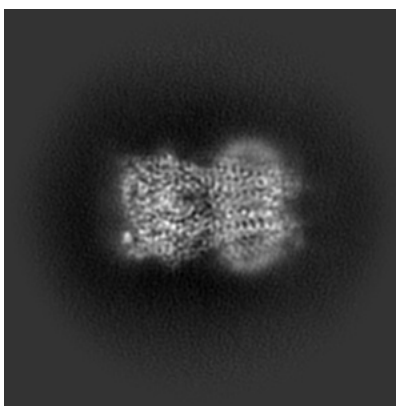
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

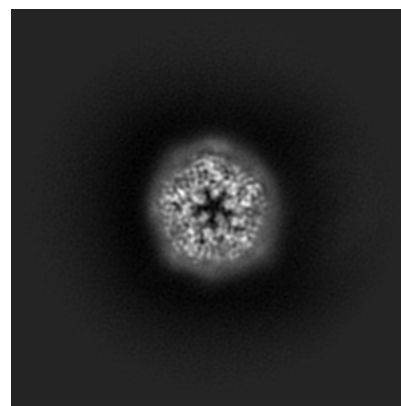
#### 6.1.1 Primary map



X

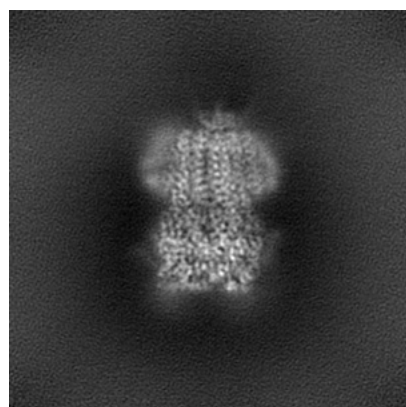


Y

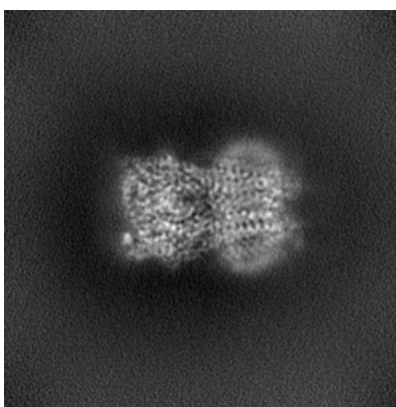


Z

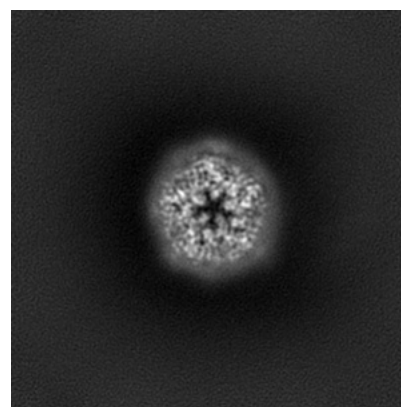
#### 6.1.2 Raw map



X



Y

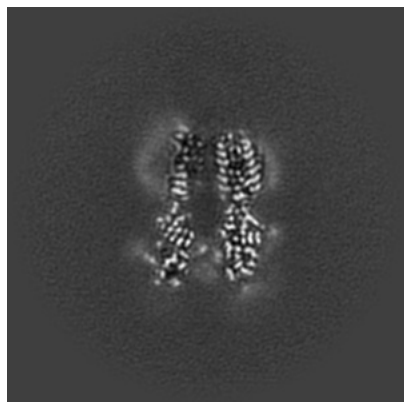


Z

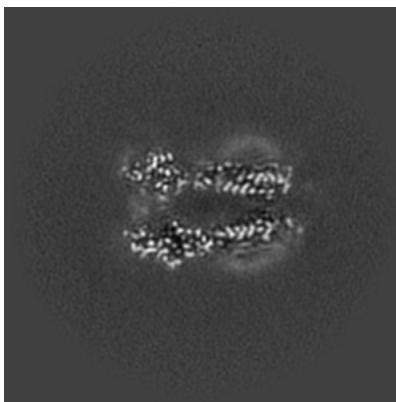
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

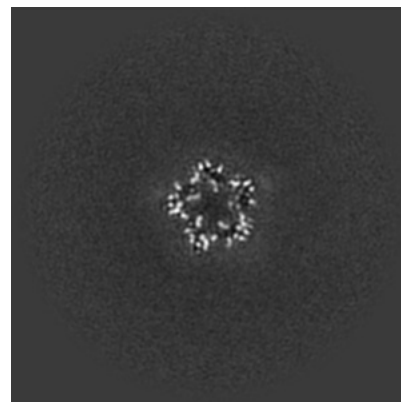
### 6.2.1 Primary map



X Index: 120

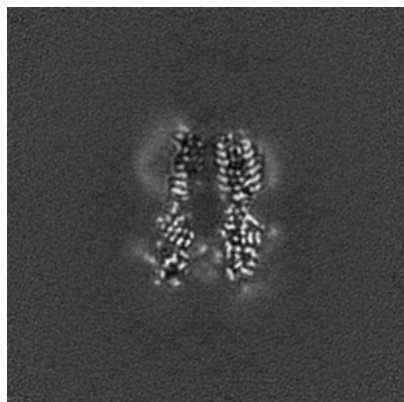


Y Index: 120

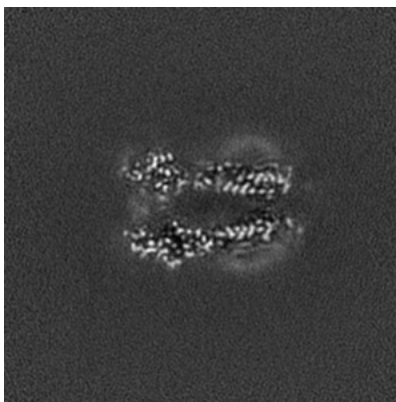


Z Index: 120

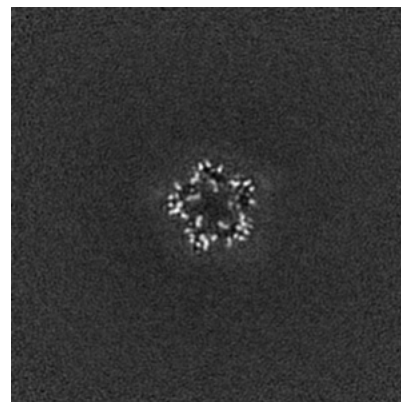
### 6.2.2 Raw map



X Index: 120



Y Index: 120

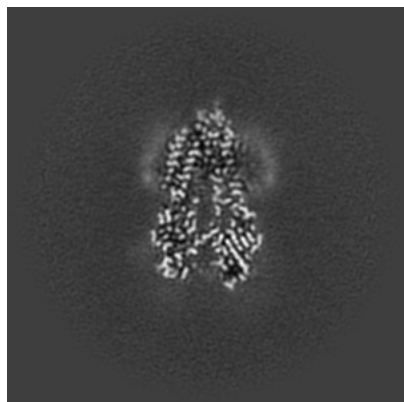


Z Index: 120

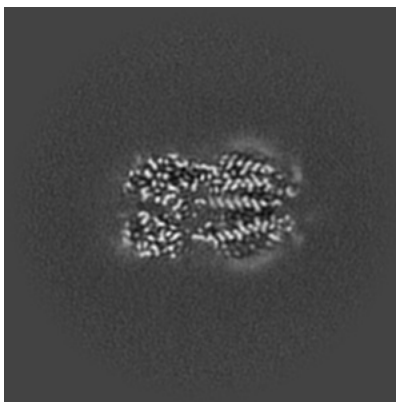
The images above show central slices of the map in three orthogonal directions.

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

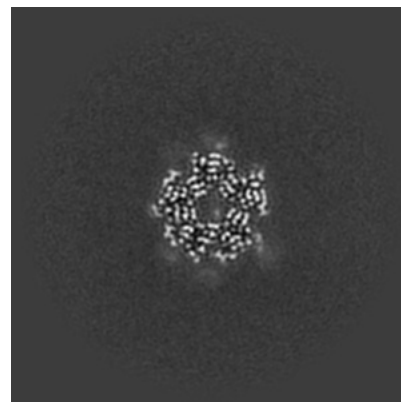
### 6.3.1 Primary map



X Index: 110

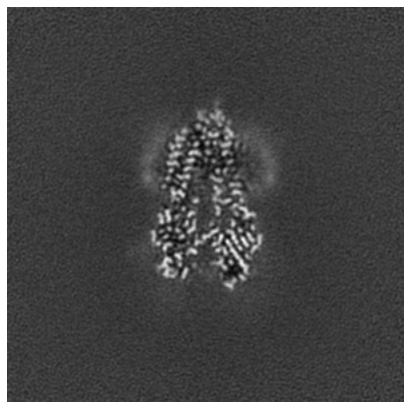


Y Index: 130

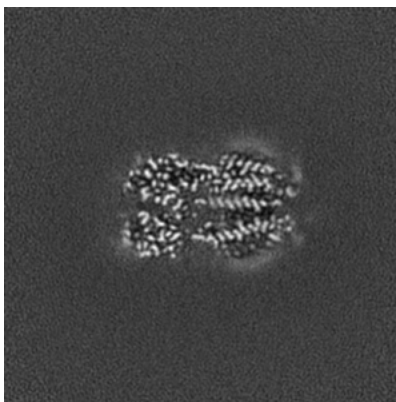


Z Index: 99

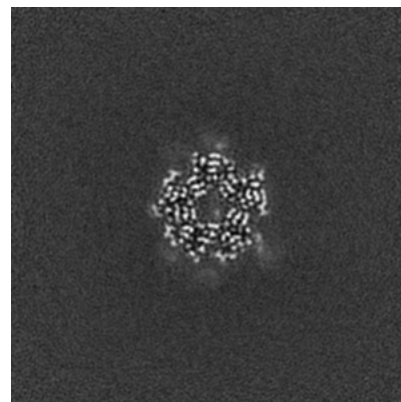
### 6.3.2 Raw map



X Index: 110



Y Index: 130

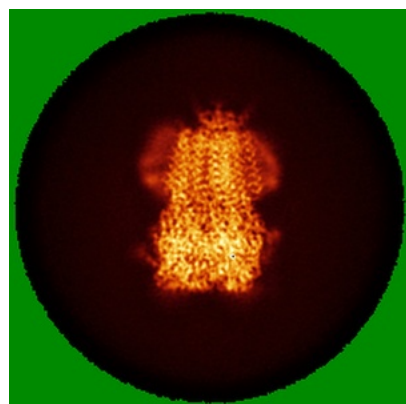


Z Index: 99

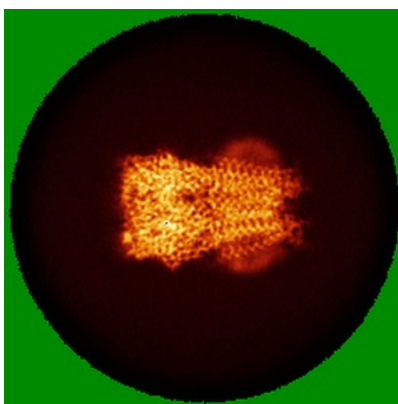
The images above show the largest variance slices of the map in three orthogonal directions.

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

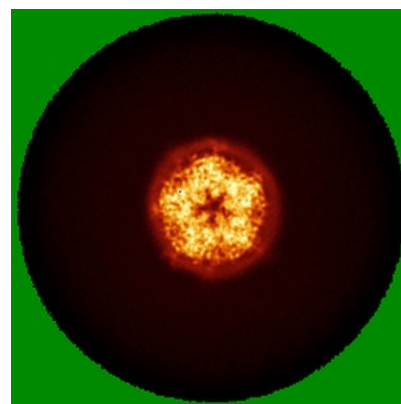
### 6.4.1 Primary map



X

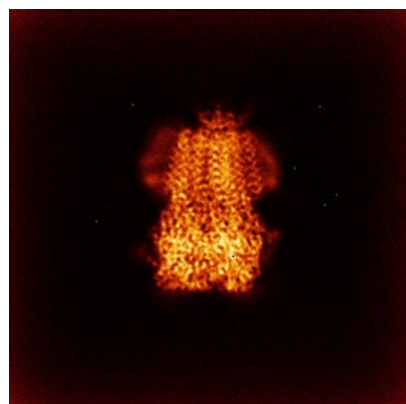


Y

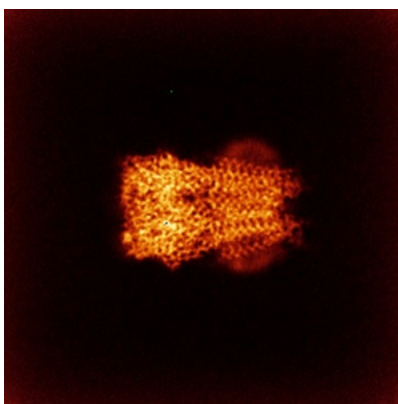


Z

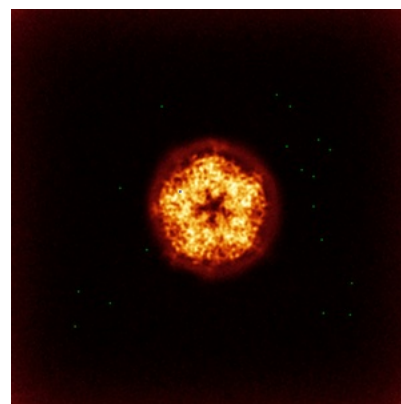
### 6.4.2 Raw map



X



Y

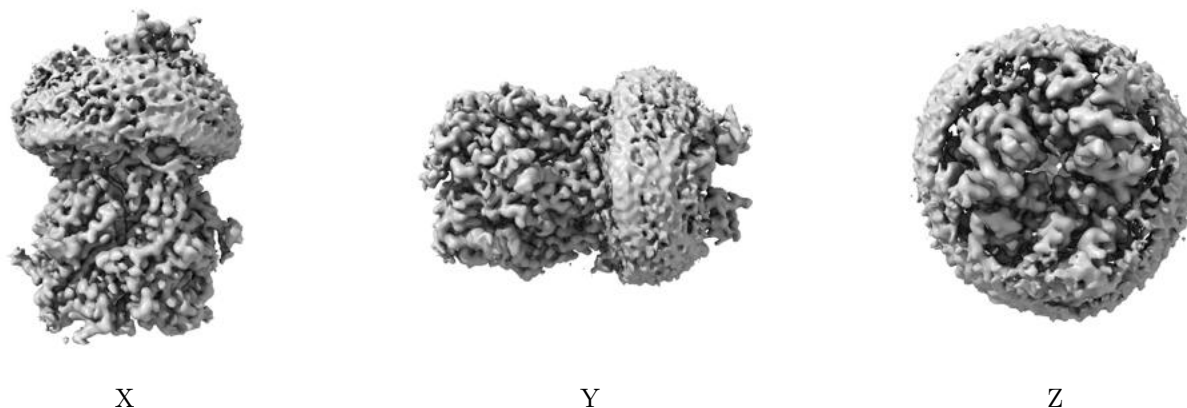


Z

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.

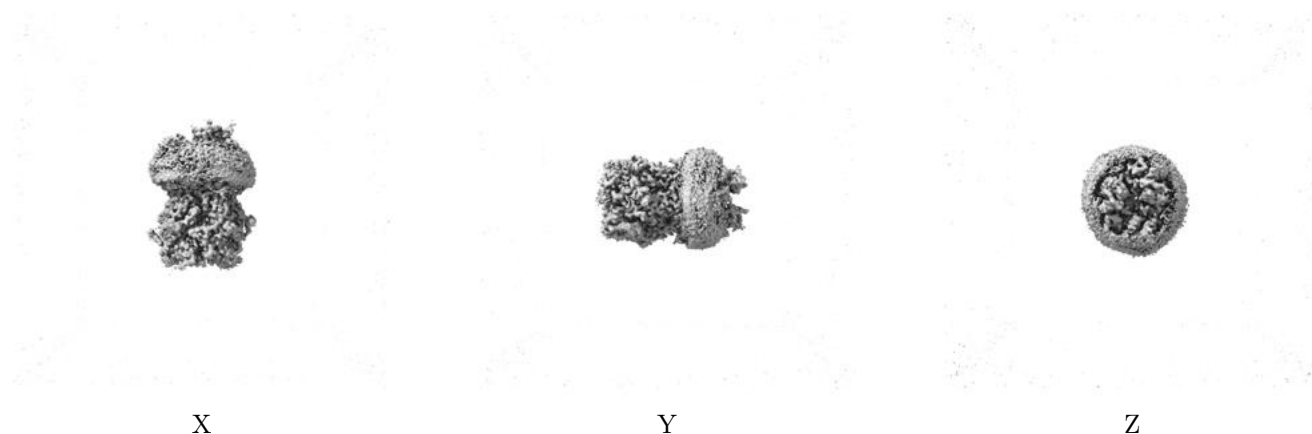
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

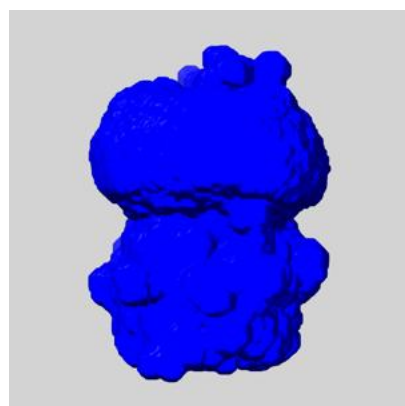
## 6.6 Mask visualisation [i](#)

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

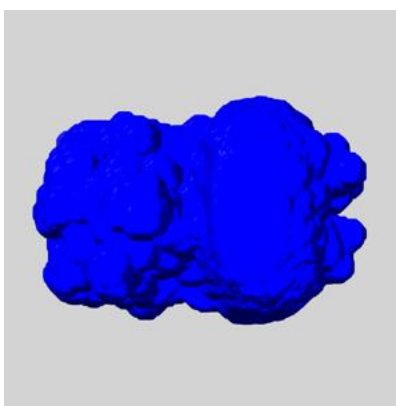
A mask typically either:

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

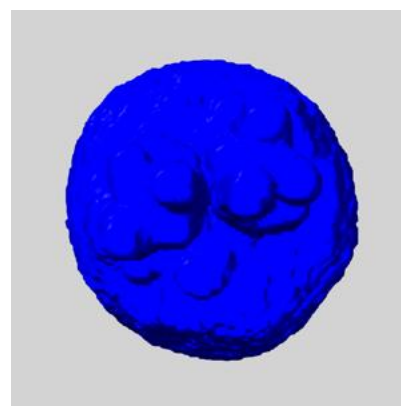
### 6.6.1 emd\_50389\_msk\_1.map [i](#)



X



Y

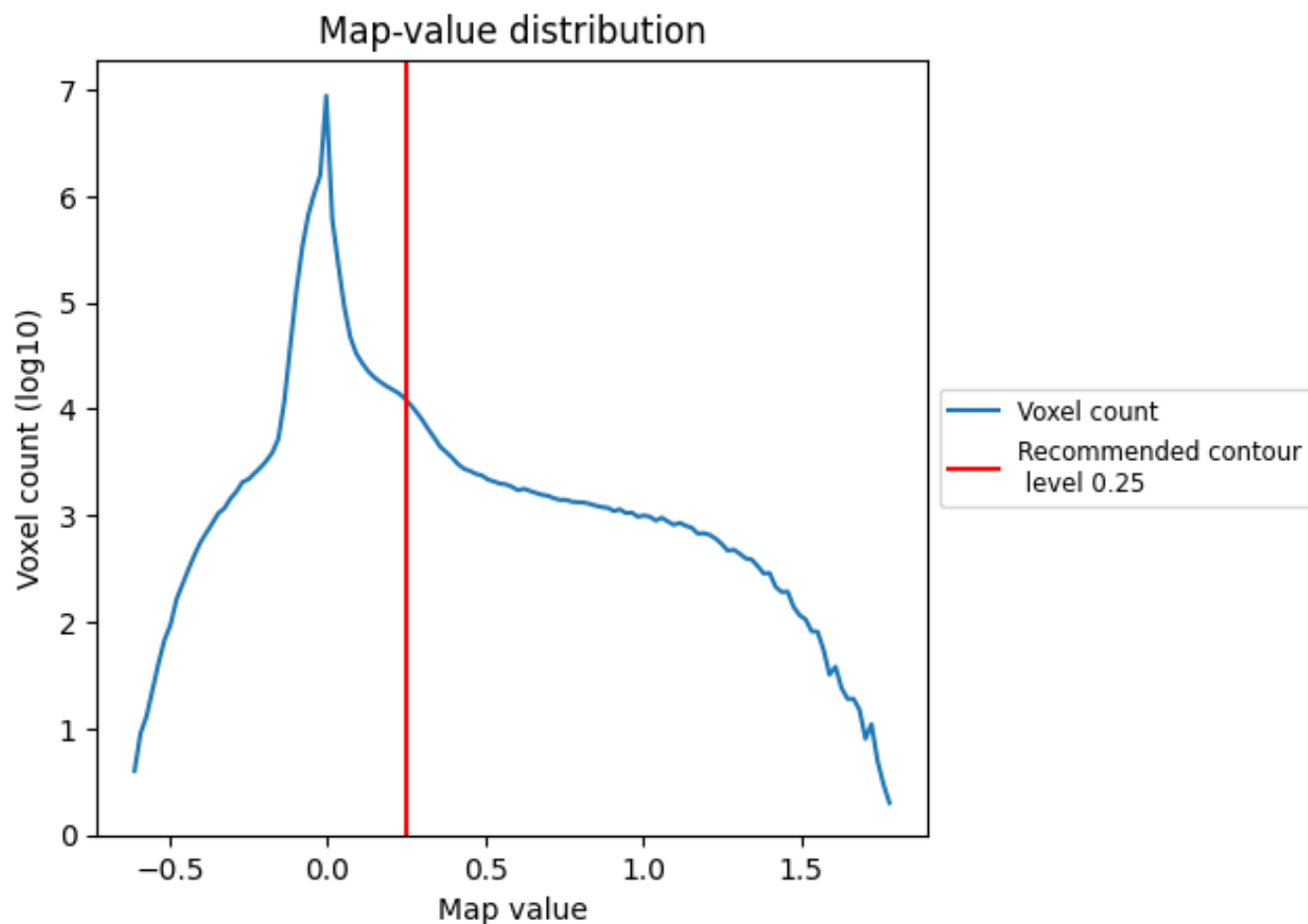


Z

## 7 Map analysis [i](#)

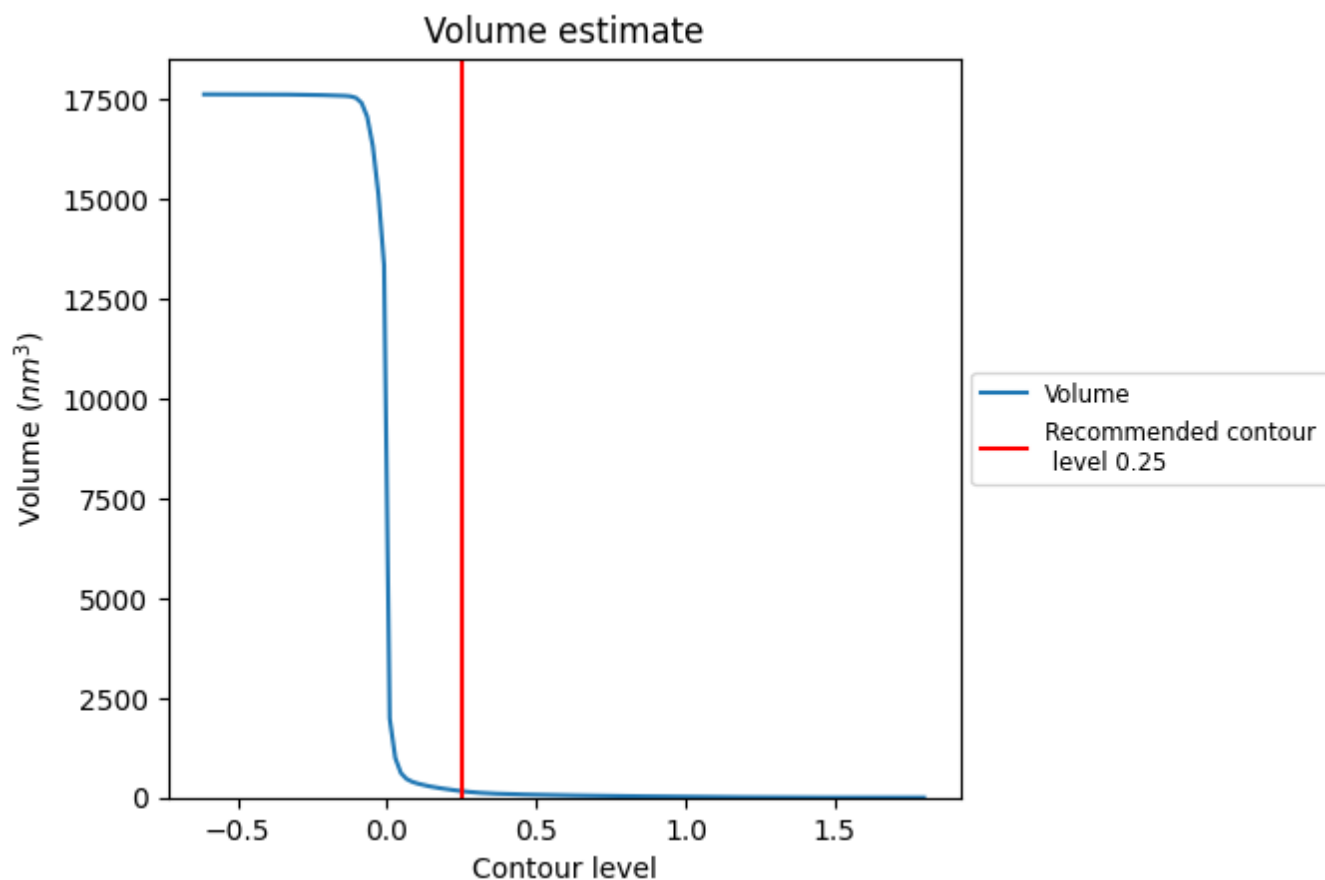
This section contains the results of statistical analysis of the map.

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



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

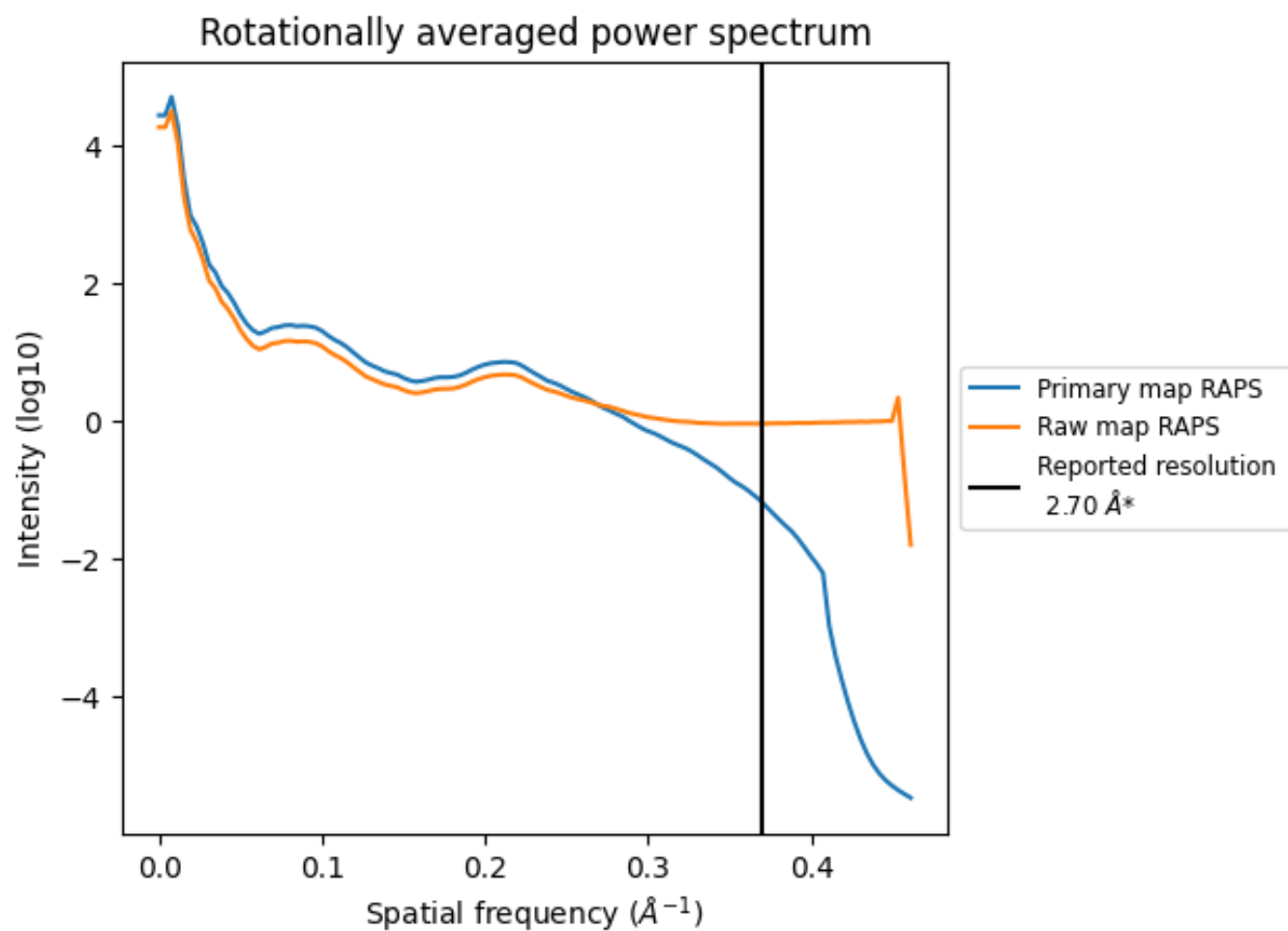
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm<sup>3</sup>; this corresponds to an approximate mass of 146 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 ⓘ

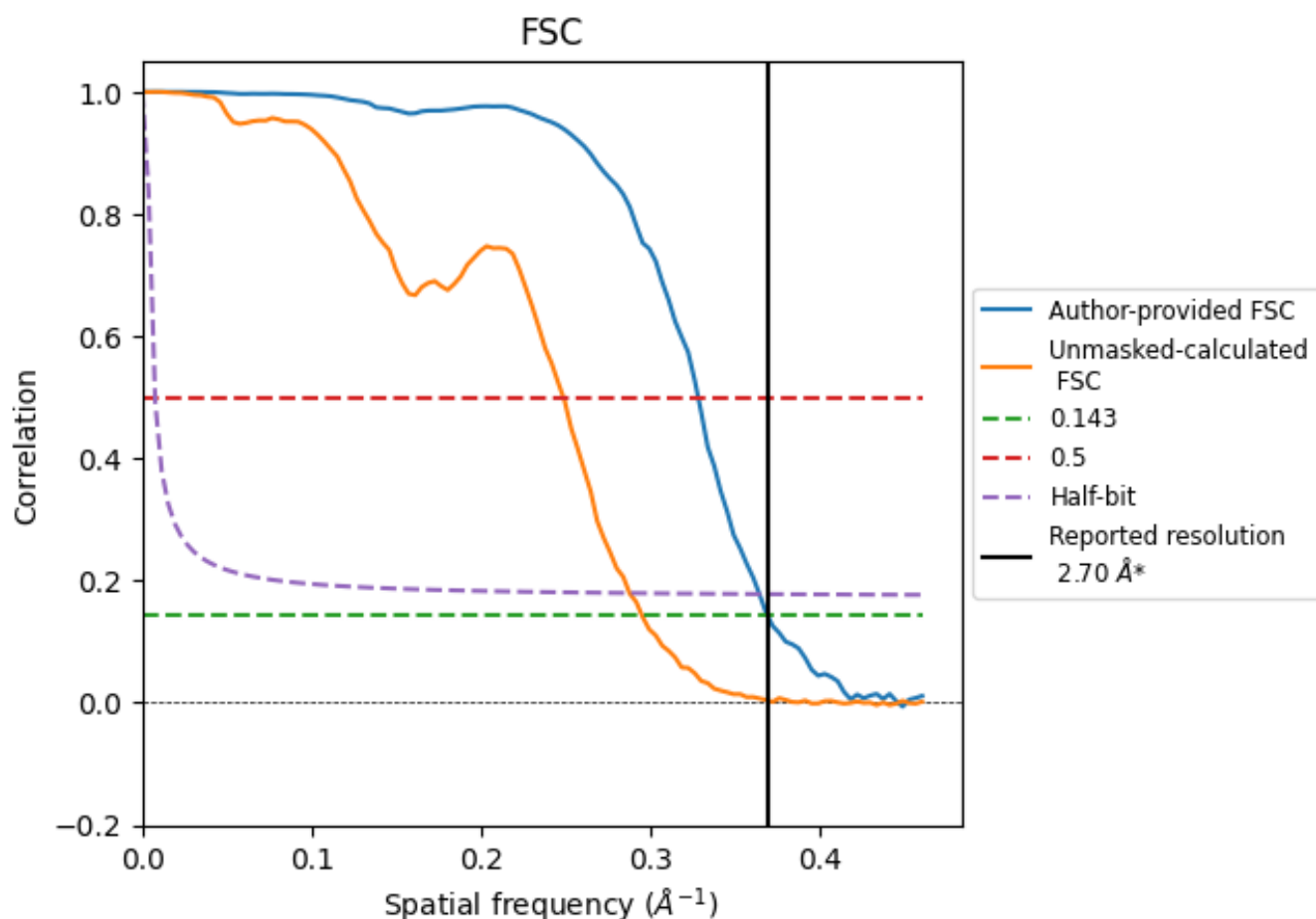


\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

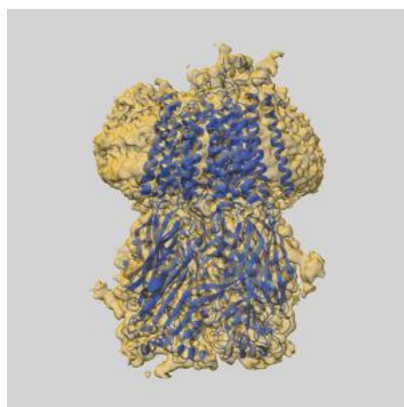
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.04	2.74
Unmasked-calculated*	3.39	4.02	3.47

\*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 3.39 differs from the reported value 2.7 by more than 10 %

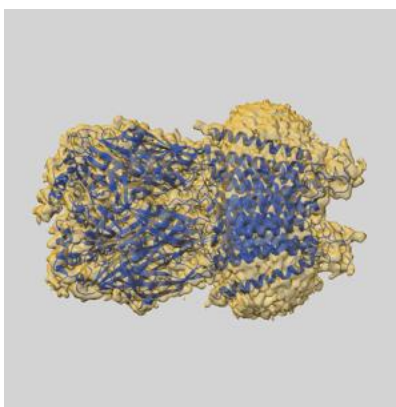
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50389 and PDB model 9FG9. Per-residue inclusion information can be found in section [3](#) on page [13](#).

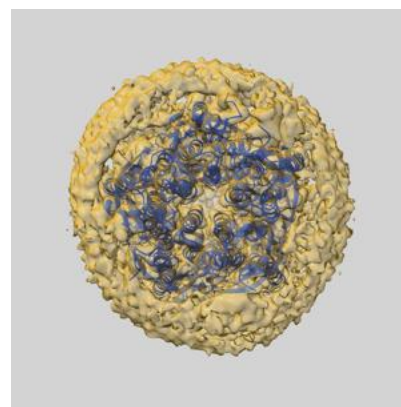
### 9.1 Map-model overlay [i](#)



X



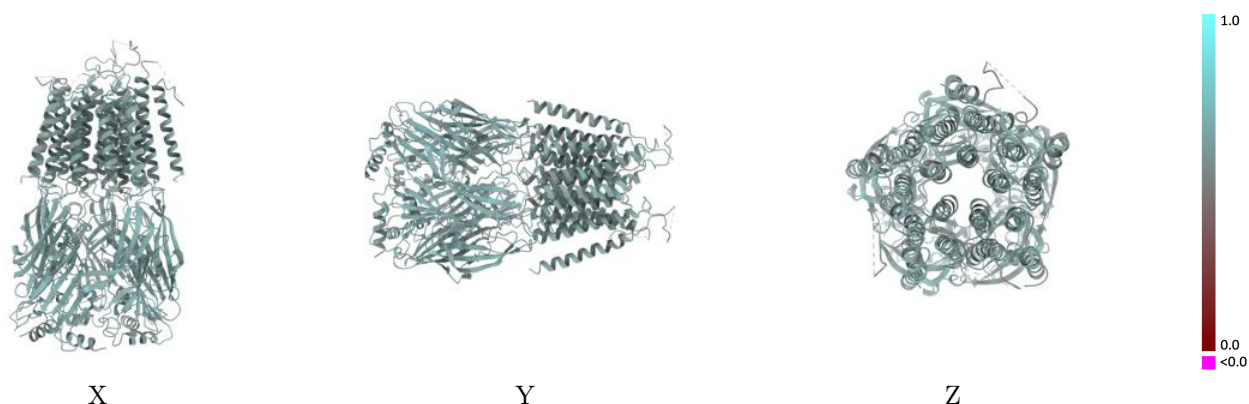
Y



Z

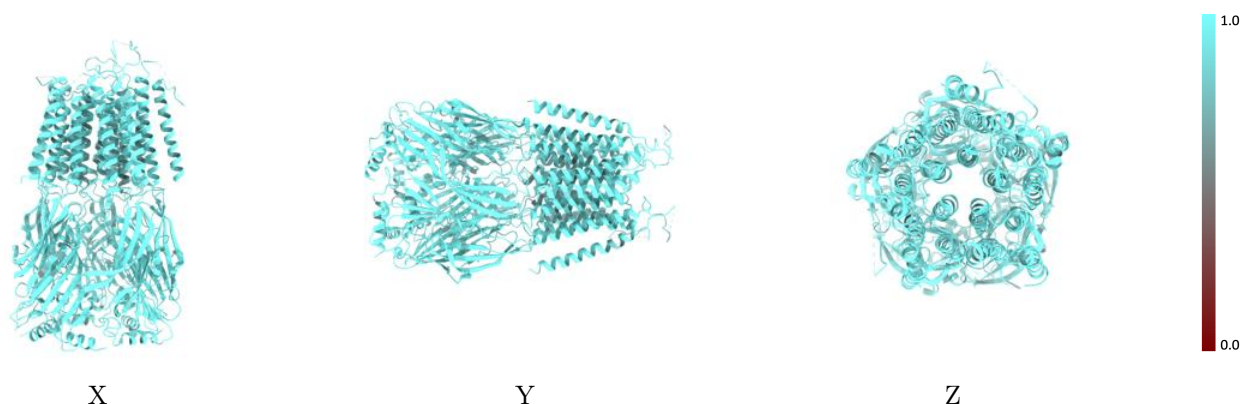
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



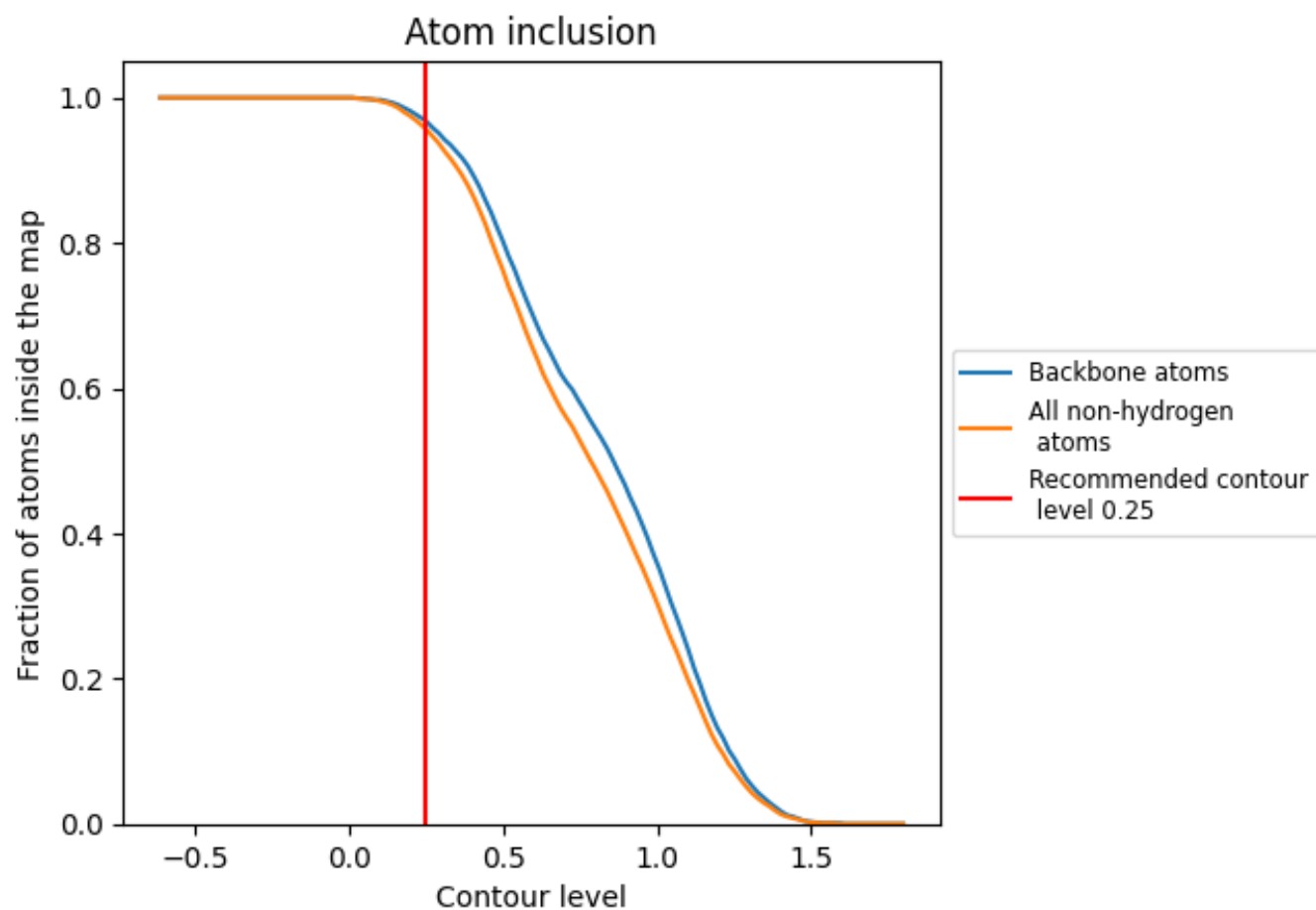
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9570	<div><div></div></div> 0.5840
A	<div><div></div></div> 0.9600	<div><div></div></div> 0.5850
B	<div><div></div></div> 0.9570	<div><div></div></div> 0.5870
C	<div><div></div></div> 0.9650	<div><div></div></div> 0.5850
D	<div><div></div></div> 0.9580	<div><div></div></div> 0.5860
E	<div><div></div></div> 0.9630	<div><div></div></div> 0.5860
F	<div><div></div></div> 0.9310	<div><div></div></div> 0.5360
G	<div><div></div></div> 0.9440	<div><div></div></div> 0.5260
a	<div><div></div></div> 0.8450	<div><div></div></div> 0.4920
b	<div><div></div></div> 0.9640	<div><div></div></div> 0.5140
c	<div><div></div></div> 0.8930	<div><div></div></div> 0.4540
d	<div><div></div></div> 0.8850	<div><div></div></div> 0.5120
e	<div><div></div></div> 0.9290	<div><div></div></div> 0.5180

1.0

0.0

<0.0