



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 08:10 am GMT

PDB ID : 6I53
EMDB ID : EMD-4411
Title : Cryo-EM structure of the human synaptic alpha1-beta3-gamma2 GABAA receptor in complex with Megabody38 in a lipid nanodisc
Authors : Lavery, D.; Desai, R.; Uchanski, T.; Masiulis, S.; Wojciech, J.S.; Malinauskas, T.; Zivanov, J.; Pardon, E.; Steyaert, J.; Miller, K.W.; Aricescu, A.R.
Deposited on : 2018-11-12
Resolution : 3.20 Å(reported)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

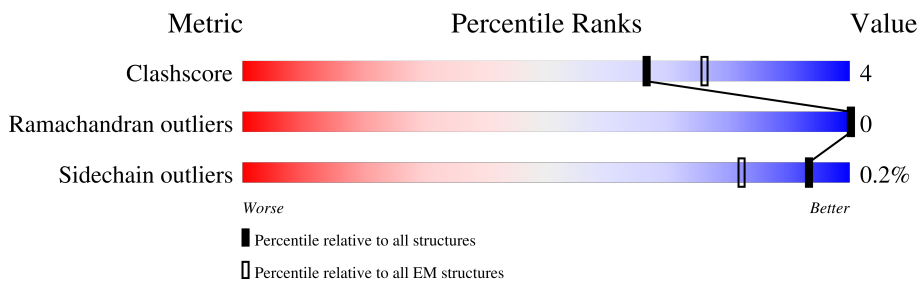
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	473	
1	E	473	
2	A	464	
2	D	464	
3	C	495	
4	G	123	
5	F	5	
5	M	5	

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Mol	Chain	Length	Quality of chain
6	H	2	<p>50% 50%</p>
6	K	2	<p>100%</p>
6	L	2	<p>50% 100%</p>
7	I	7	<p>43% 71% 29%</p>
8	J	6	<p>33% 100%</p>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15362 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 beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	336	Total	C	N	O	S	0	0
			2754	1803	449	487	15		
1	B	338	Total	C	N	O	S	0	0
			2770	1812	452	490	16		

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	349	Total	C	N	O	S	0	0
			2823	1825	475	507	16		
2	D	347	Total	C	N	O	S	0	0
			2805	1814	470	505	16		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	LYS	ARG	conflict	UNP P14867
A	-25	TYR	CYS	conflict	UNP P14867
A	-20	THR	ILE	conflict	UNP P14867
A	-18	PHE	LEU	conflict	UNP P14867
A	-7	ASP	-	insertion	UNP P14867
A	-6	TYR	-	insertion	UNP P14867
A	-5	LYS	-	insertion	UNP P14867
A	-4	ASP	-	insertion	UNP P14867
A	-3	ASP	-	insertion	UNP P14867
A	-2	ASP	-	insertion	UNP P14867
A	-1	ASP	-	insertion	UNP P14867
A	0	LYS	-	insertion	UNP P14867
D	-33	LYS	ARG	conflict	UNP P14867
D	-25	TYR	CYS	conflict	UNP P14867
D	-20	THR	ILE	conflict	UNP P14867
D	-18	PHE	LEU	conflict	UNP P14867
D	-7	ASP	-	insertion	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	TYR	-	insertion	UNP P14867
D	-5	LYS	-	insertion	UNP P14867
D	-4	ASP	-	insertion	UNP P14867
D	-3	ASP	-	insertion	UNP P14867
D	-2	ASP	-	insertion	UNP P14867
D	-1	ASP	-	insertion	UNP P14867
D	0	LYS	-	insertion	UNP P14867

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	328	2701	1766	443	477	15	0	0

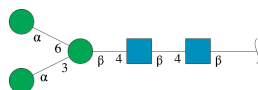
There are 20 discrepancies between the modelled and reference sequences:

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 a protein called Megabody38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	123	949	593	171	181	4	0	0

- Molecule 5 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.



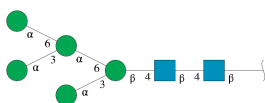
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	5	61	34	2	25	0	0
5	M	5	61	34	2	25	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



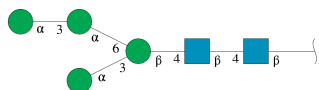
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	2	28	16	2	10	0	0
6	K	2	28	16	2	10	0	0
6	L	2	28	16	2	10	0	0

- Molecule 7 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.



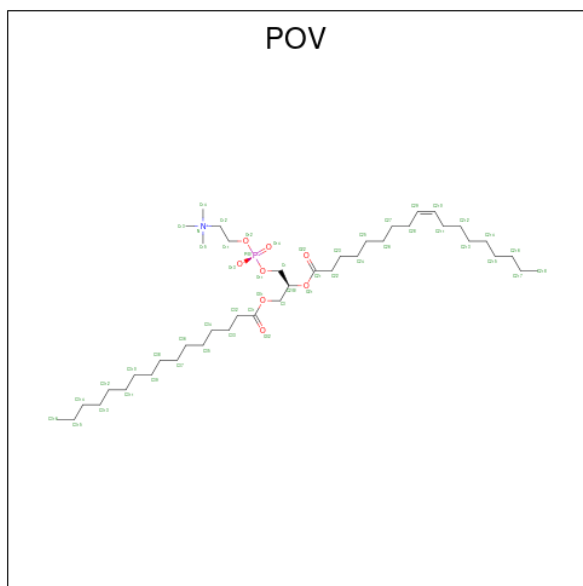
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	I	7	83	46	2	35	0	0

- Molecule 8 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
			Total	C	N	O		
8	J	6	72	40	2	30	0	0

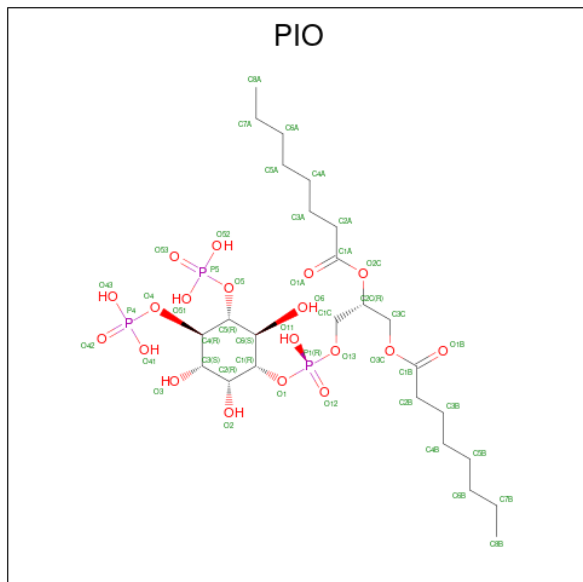
- Molecule 9 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



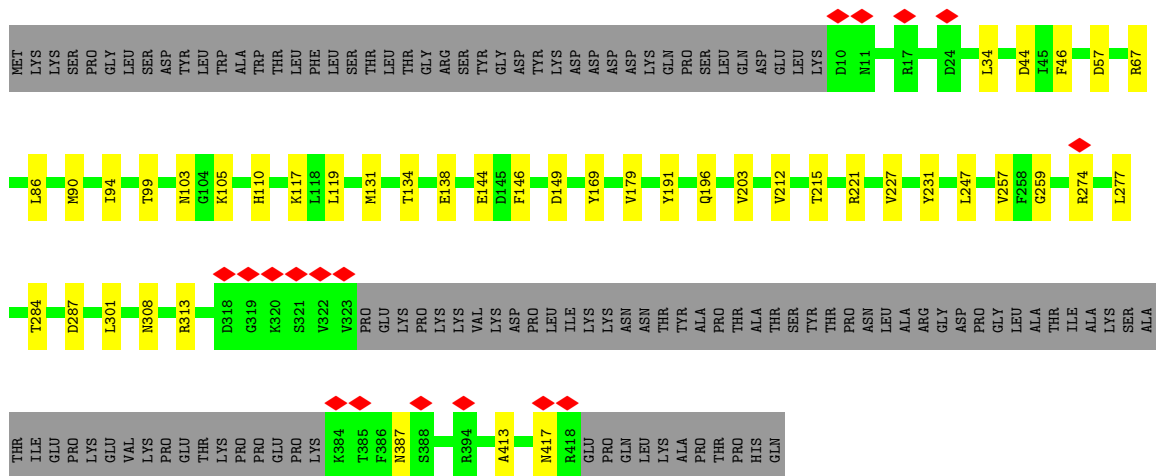
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	E	1	35	26	8	1	0
9	A	1	35	26	8	1	0
9	D	1	35	26	8	1	0

- Molecule 10 is [(2R)-2-octanoyloxy-3-[oxidanyl]-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl

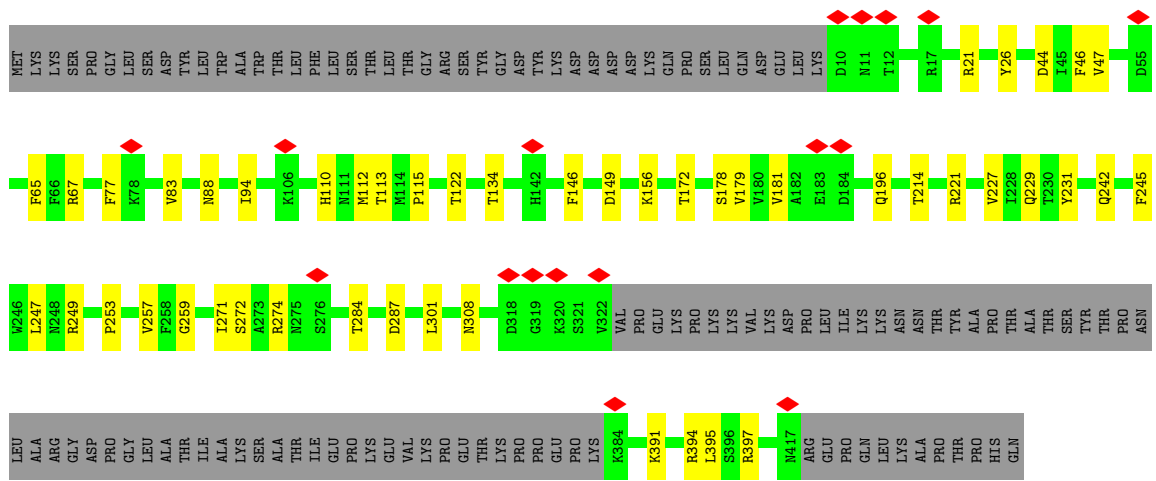
)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C₂₅H₄₉O₁₉P₃).



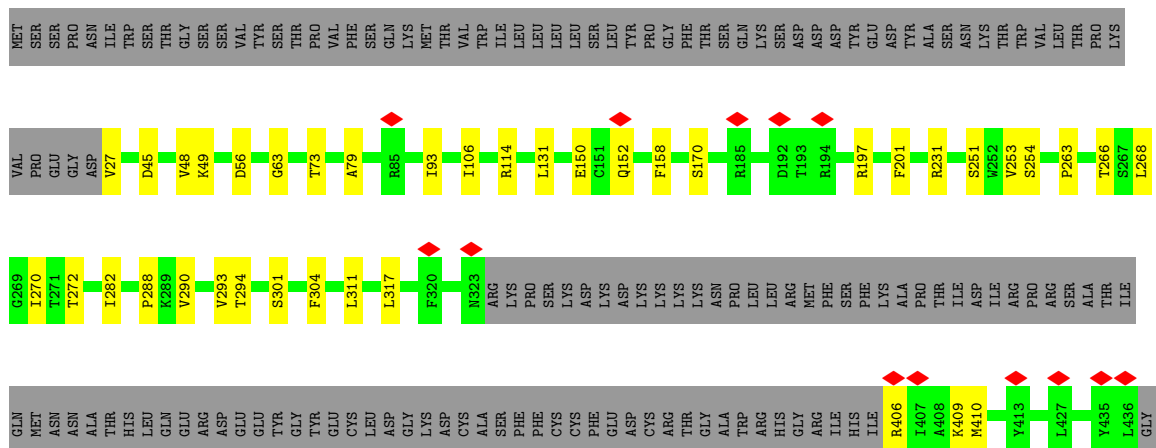
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
10	A	1	47	25	19	3	0
10	D	1	47	25	19	3	0



• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

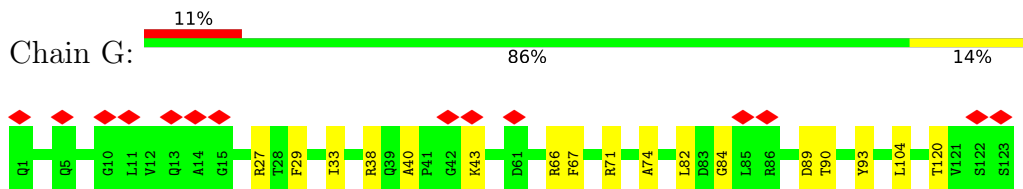


• Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2

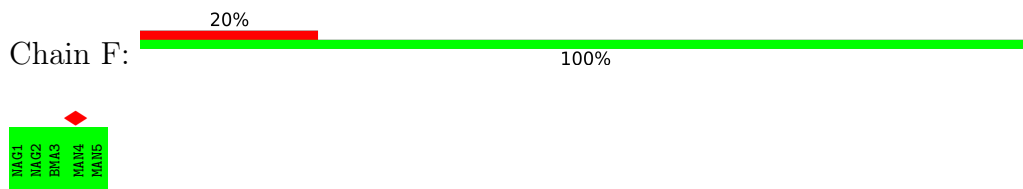


GLY
SER
GLY
GLY
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LYS
THR
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ALA
PRO
ALA

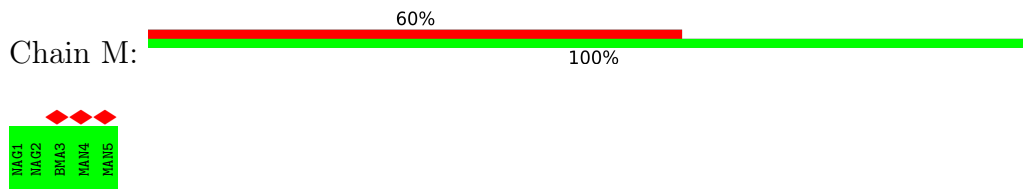
- Molecule 4: Megabody38



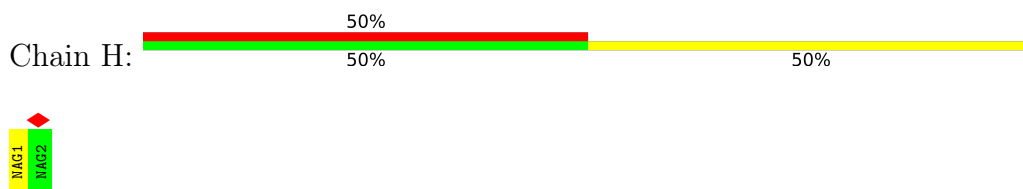
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



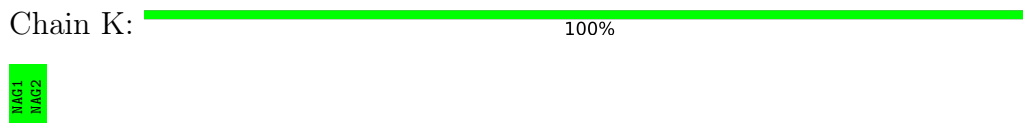
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

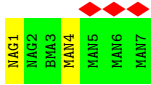
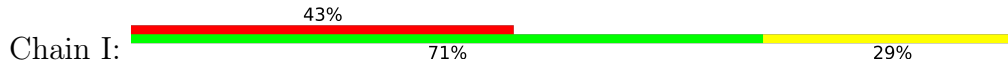


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

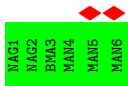




- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF parameters were estimated using GCTF and CTF correction performed in RELION (full phase and amplitude correction).	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.84	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.221	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: PIO, POV, BMA, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.29	0/2844	0.50	0/3870
1	E	0.29	0/2828	0.50	0/3849
2	A	0.29	0/2894	0.49	0/3931
2	D	0.29	0/2876	0.50	0/3907
3	C	0.29	0/2775	0.51	0/3779
4	G	0.29	0/970	0.50	0/1309
All	All	0.29	0/15187	0.50	0/20645

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	B	2770	0	2759	19	0
1	E	2754	0	2744	24	0
2	A	2823	0	2812	27	0
2	D	2805	0	2790	29	0
3	C	2701	0	2693	23	0
4	G	949	0	901	11	0
5	F	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	61	0	52	0	0
6	H	28	0	25	0	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
7	I	83	0	70	0	0
8	J	72	0	61	0	0
9	A	35	0	41	1	0
9	D	35	0	41	1	0
9	E	35	0	41	0	0
10	A	47	0	44	1	0
10	D	47	0	44	3	0
All	All	15362	0	15220	122	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 122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:LYS:HG2	2:D:394:ARG:HH21	1.61	0.66
3:C:48:VAL:HG12	3:C:49:LYS:HG3	1.80	0.64
1:E:235:LEU:HD22	2:A:301:LEU:HD23	1.79	0.63
1:E:98:PHE:HB2	1:E:101:ASP:HB2	1.83	0.61
3:C:251:SER:HB3	3:C:272:THR:HG21	1.82	0.60

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	B	334/473 (71%)	323 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	332/473 (70%)	323 (97%)	9 (3%)	0	100	100
2	A	345/464 (74%)	336 (97%)	9 (3%)	0	100	100
2	D	343/464 (74%)	326 (95%)	17 (5%)	0	100	100
3	C	324/495 (66%)	309 (95%)	15 (5%)	0	100	100
4	G	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
All	All	1799/2492 (72%)	1732 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	B	304/422 (72%)	303 (100%)	1 (0%)	92	96
1	E	302/422 (72%)	302 (100%)	0	100	100
2	A	311/413 (75%)	310 (100%)	1 (0%)	92	96
2	D	309/413 (75%)	308 (100%)	1 (0%)	92	96
3	C	303/448 (68%)	303 (100%)	0	100	100
4	G	93/93 (100%)	93 (100%)	0	100	100
All	All	1622/2211 (73%)	1619 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	308	ASN
1	B	41	ASN
2	D	308	ASN

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

Mol	Chain	Res	Type
1	B	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

29 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	$\# Z > 2$
5	NAG	F	1	1,5	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	F	2	5	14,14,15	0.24	0	17,19,21	0.60	0
5	BMA	F	3	5	11,11,12	0.22	0	15,15,17	0.41	0
5	MAN	F	4	5	11,11,12	0.26	0	15,15,17	0.32	0
5	MAN	F	5	5	11,11,12	0.23	0	15,15,17	0.32	0
6	NAG	H	1	1,6	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
6	NAG	H	2	6	14,14,15	0.24	0	17,19,21	0.47	0
7	NAG	I	1	7,2	14,14,15	0.24	0	17,19,21	0.75	1 (5%)
7	NAG	I	2	7	14,14,15	0.25	0	17,19,21	0.47	0
7	BMA	I	3	7	11,11,12	0.25	0	15,15,17	0.62	0
7	MAN	I	4	7	11,11,12	0.29	0	15,15,17	0.62	1 (6%)
7	MAN	I	5	7	11,11,12	0.32	0	15,15,17	0.43	0
7	MAN	I	6	7	11,11,12	0.24	0	15,15,17	0.35	0
7	MAN	I	7	7	11,11,12	0.28	0	15,15,17	0.47	0
8	NAG	J	1	1,8	14,14,15	0.27	0	17,19,21	0.49	0
8	NAG	J	2	8	14,14,15	0.24	0	17,19,21	0.56	0
8	BMA	J	3	8	11,11,12	0.22	0	15,15,17	0.60	0
8	MAN	J	4	8	11,11,12	0.27	0	15,15,17	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	J	5	8	11,11,12	0.27	0	15,15,17	0.40	0
8	MAN	J	6	8	11,11,12	0.23	0	15,15,17	0.34	0
6	NAG	K	1	1,6	14,14,15	0.25	0	17,19,21	0.51	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	L	1	3,6	14,14,15	0.27	0	17,19,21	0.48	0
6	NAG	L	2	6	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	M	1	2,5	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	M	2	5	14,14,15	0.24	0	17,19,21	0.58	0
5	BMA	M	3	5	11,11,12	0.23	0	15,15,17	0.46	0
5	MAN	M	4	5	11,11,12	0.25	0	15,15,17	0.29	0
5	MAN	M	5	5	11,11,12	0.25	0	15,15,17	0.39	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
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
7	NAG	I	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	1/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	0/2/19/22	0/1/1/1
7	MAN	I	7	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	0/2/19/22	0/1/1/1
8	MAN	J	6	8	-	0/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	NAG	L	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1	NAG	C2-N2-C7	3.06	127.26	122.90
7	I	1	NAG	C1-O5-C5	2.24	115.22	112.19
7	I	4	MAN	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

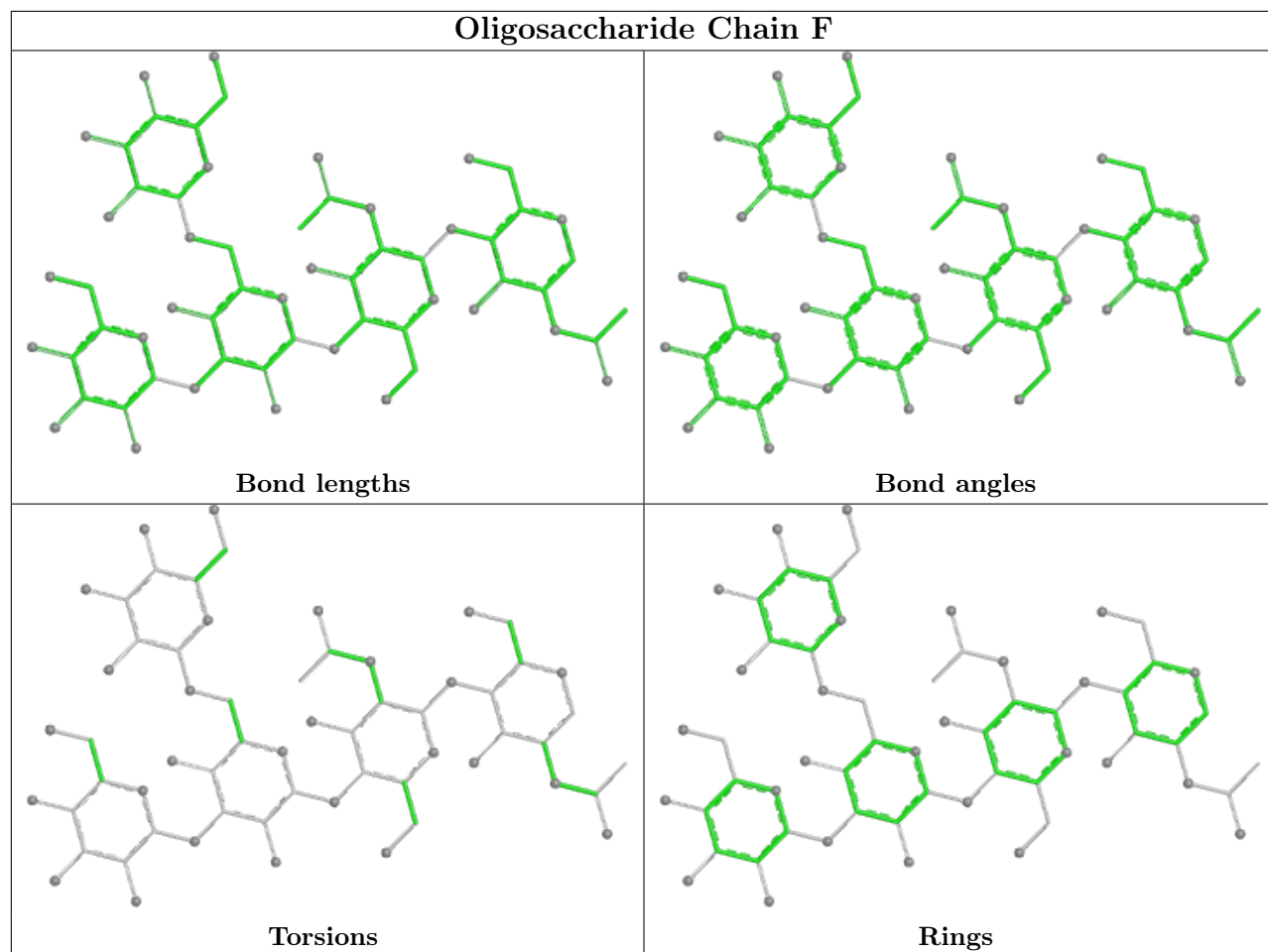
All (4) torsion outliers are listed below:

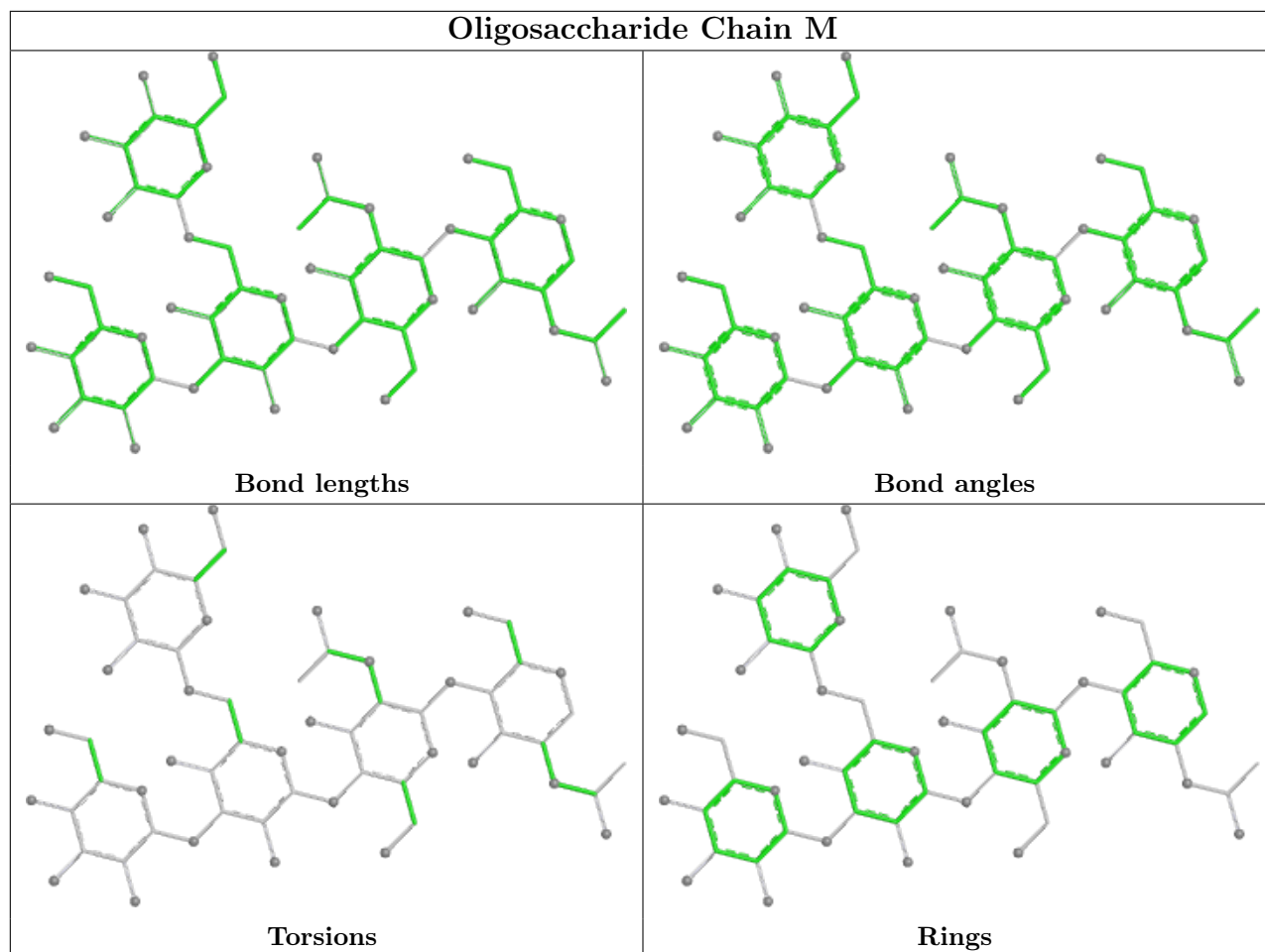
Mol	Chain	Res	Type	Atoms
7	I	4	MAN	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
6	H	1	NAG	C3-C2-N2-C7

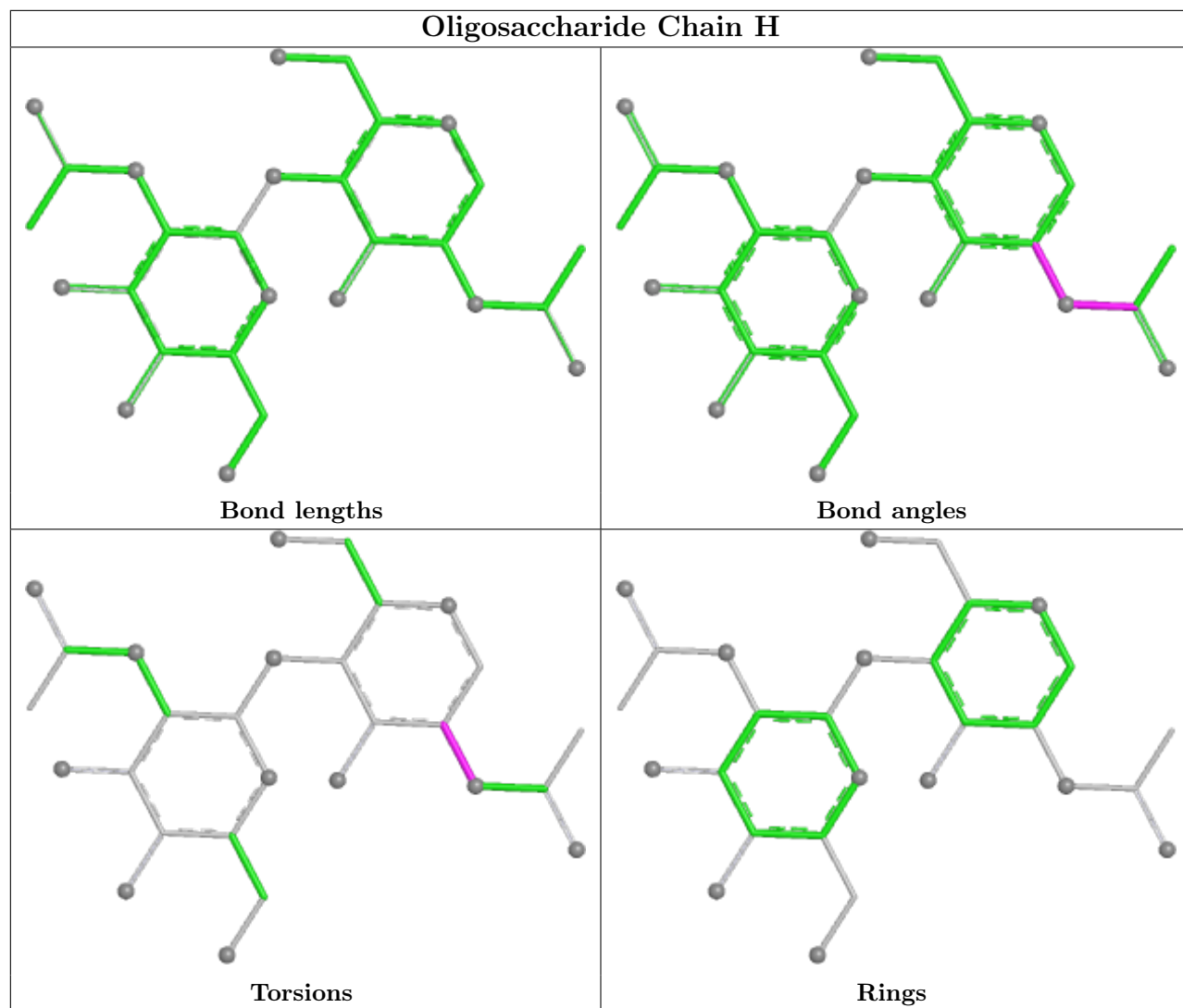
There are no ring outliers.

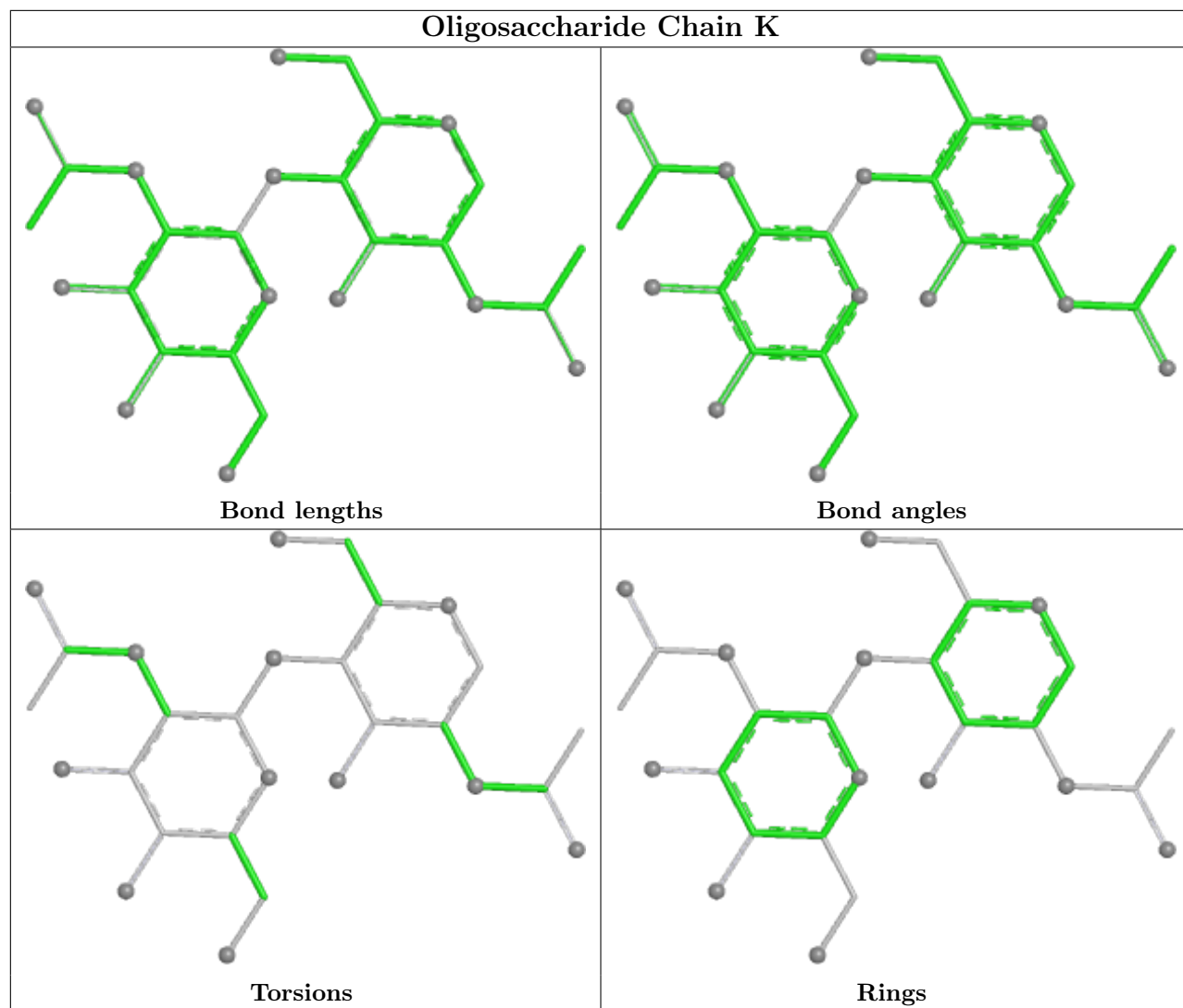
No monomer is involved in short contacts.

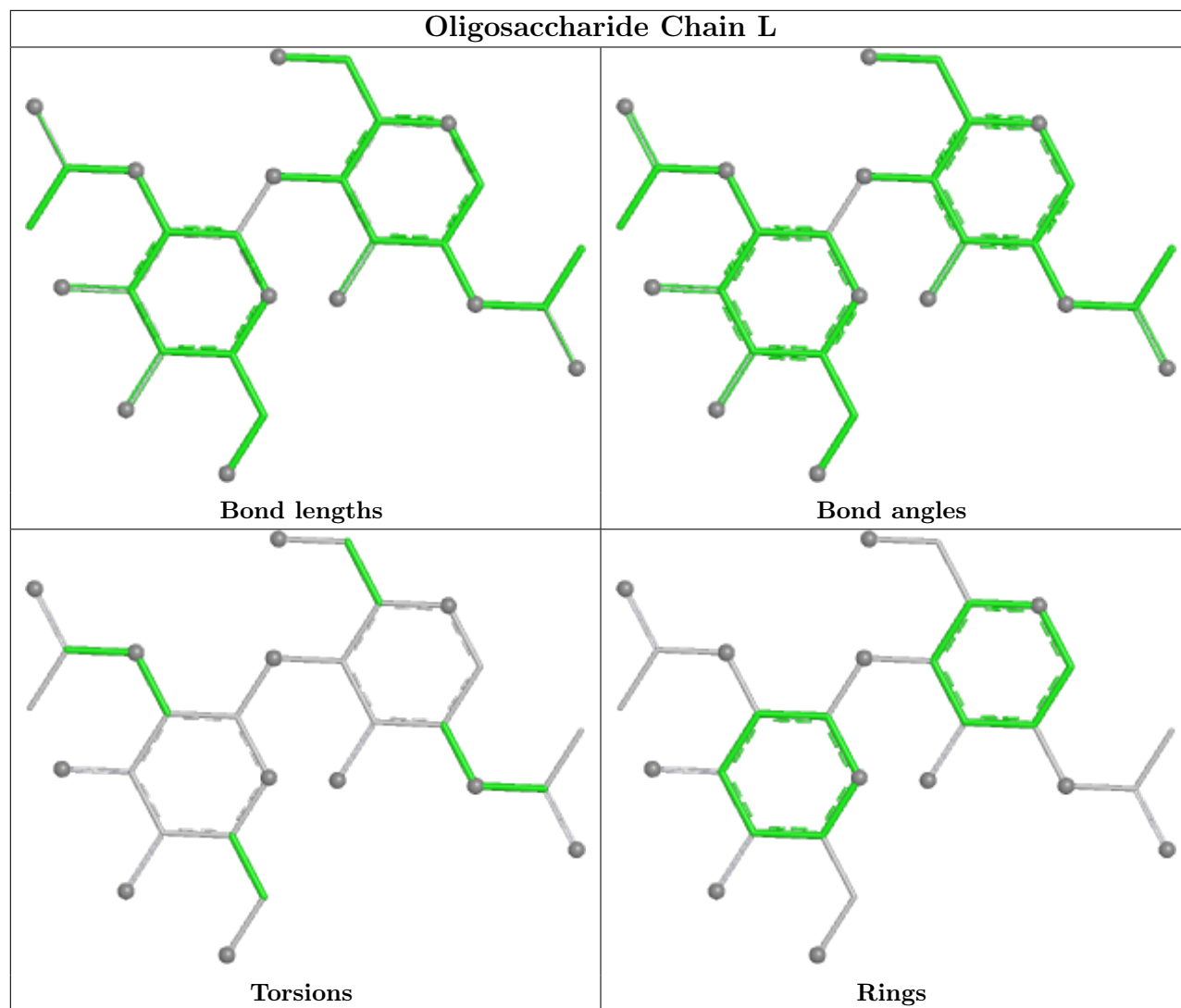
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

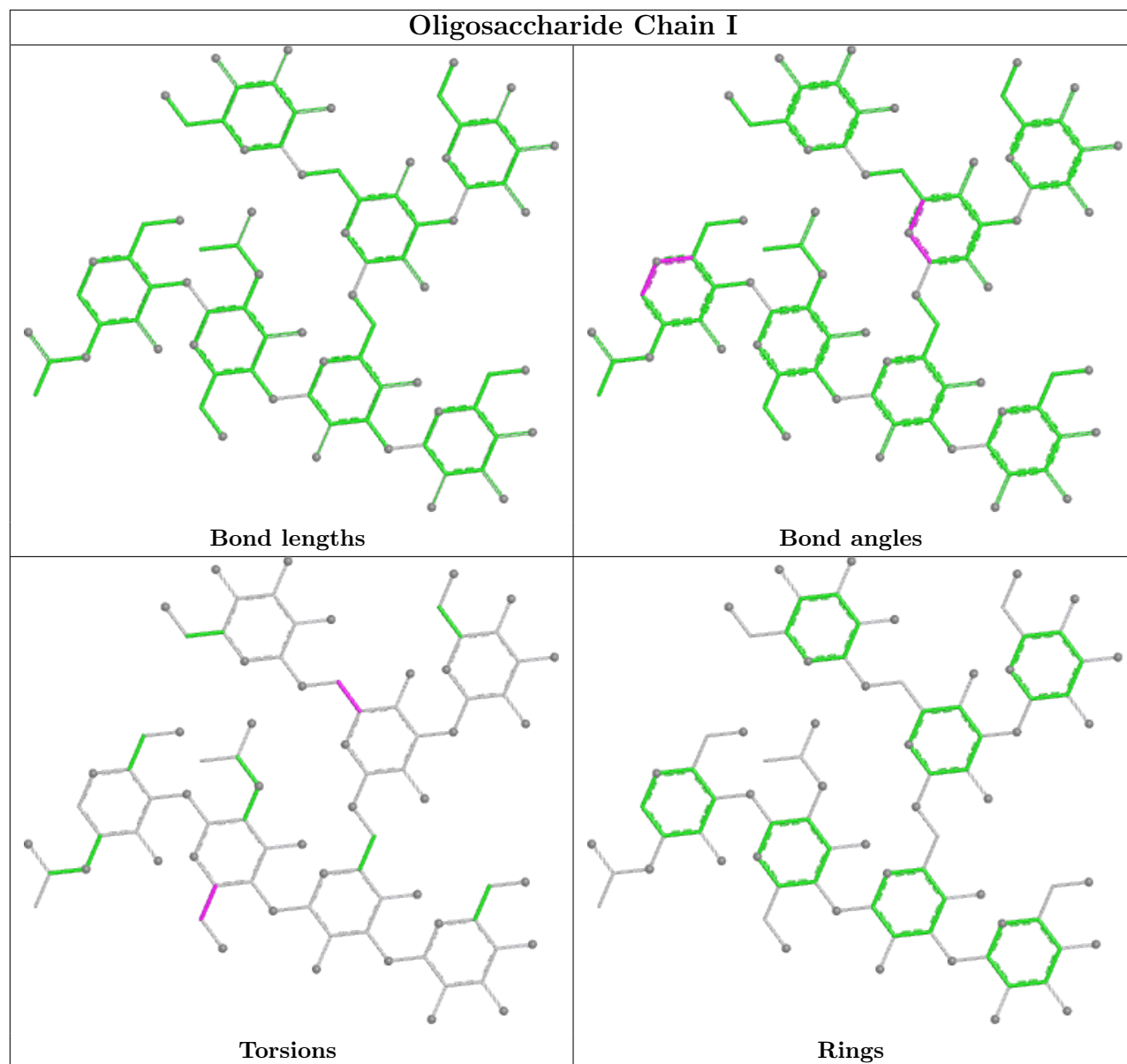


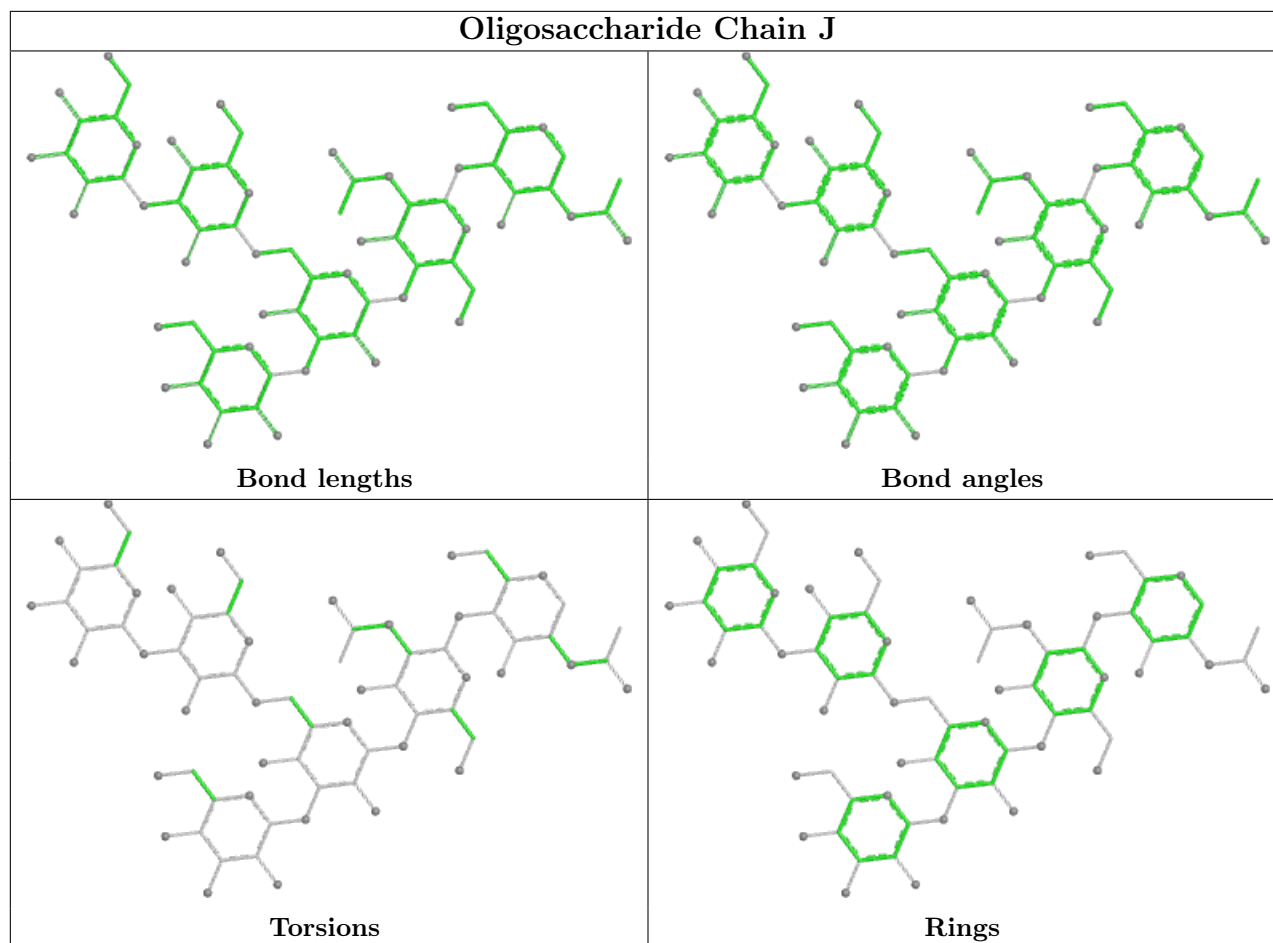












5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	POV	A	609	-	34,34,51	1.66	5 (14%)	38,39,59	1.15	2 (5%)
10	PIO	A	601	-	47,47,47	0.31	0	61,65,65	0.25	0
9	POV	E	508	-	34,34,51	1.65	5 (14%)	38,39,59	1.12	2 (5%)
9	POV	D	507	-	34,34,51	1.64	5 (14%)	38,39,59	1.14	2 (5%)
10	PIO	D	501	-	47,47,47	0.34	0	61,65,65	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	POV	A	609	-	-	16/36/36/55	-
10	PIO	A	601	-	-	5/44/68/68	0/1/1/1
9	POV	E	508	-	-	18/36/36/55	-
9	POV	D	507	-	-	14/36/36/55	-
10	PIO	D	501	-	-	3/44/68/68	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	609	POV	O21-C21	4.79	1.47	1.34
9	E	508	POV	O21-C21	4.77	1.47	1.34
9	D	507	POV	O21-C21	4.74	1.47	1.34
9	A	609	POV	P-O12	4.43	1.71	1.54
9	E	508	POV	P-O12	4.42	1.71	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	507	POV	O21-C21-C22	4.07	120.28	111.50
9	A	609	POV	O21-C21-C22	4.02	120.16	111.50
9	E	508	POV	O21-C21-C22	3.87	119.84	111.50
9	A	609	POV	O31-C31-C32	2.54	119.87	111.91
9	E	508	POV	O31-C31-C32	2.51	119.79	111.91

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

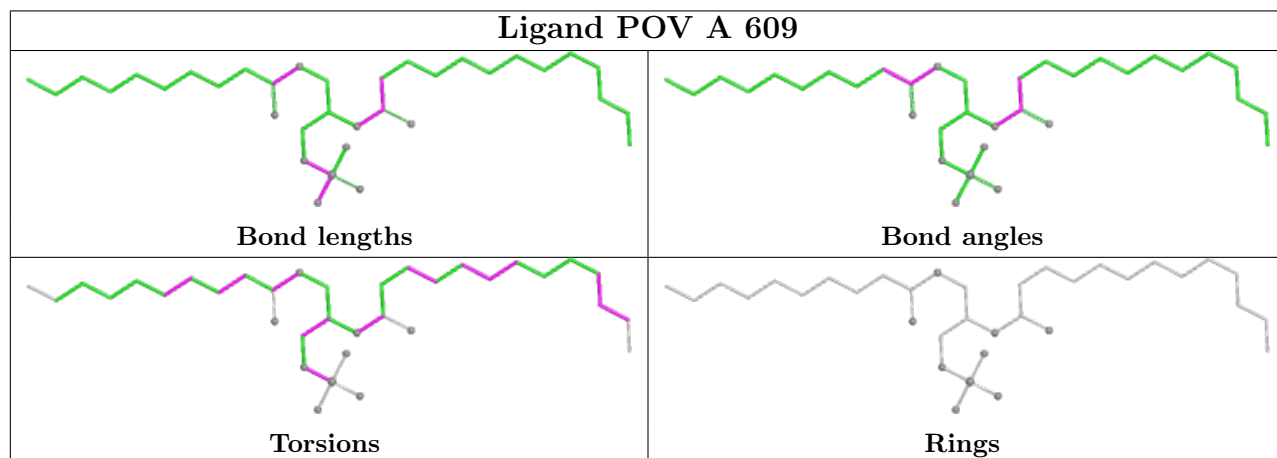
Mol	Chain	Res	Type	Atoms
9	E	508	POV	C210-C211-C212-C213
9	E	508	POV	C22-C21-O21-C2
9	A	609	POV	C1-O11-P-O13
9	A	609	POV	O11-C1-C2-O21
9	A	609	POV	C210-C211-C212-C213

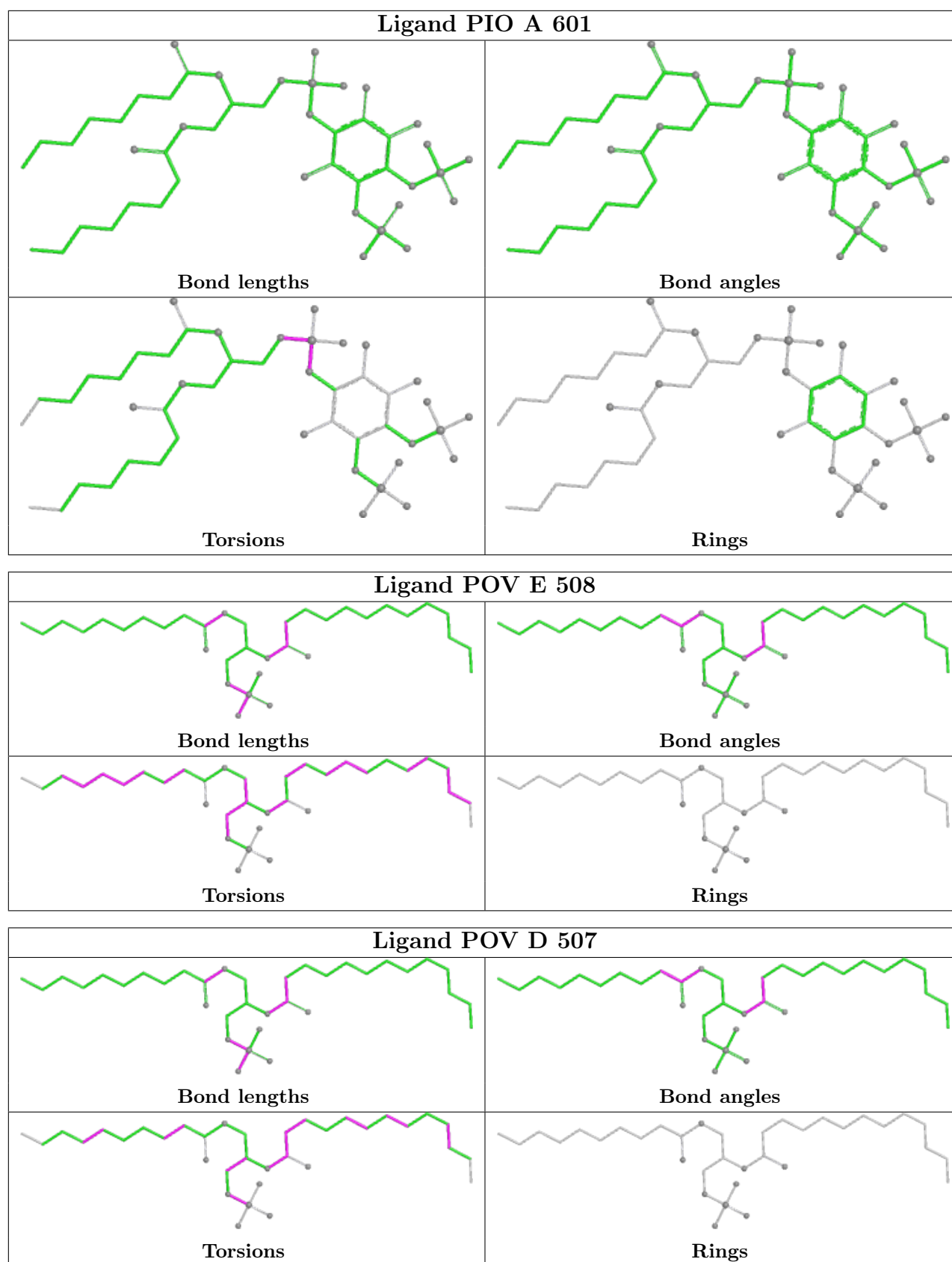
There are no ring outliers.

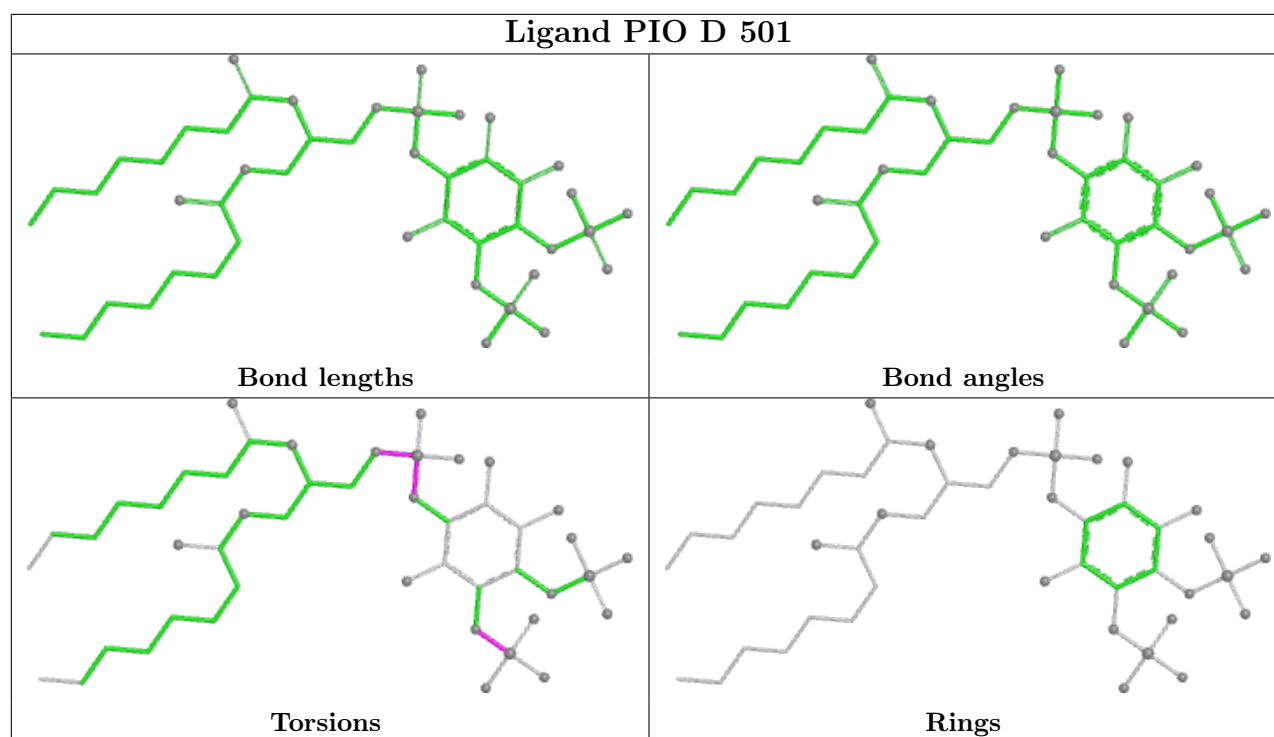
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	609	POV	1	0
10	A	601	PIO	1	0
9	D	507	POV	1	0
10	D	501	PIO	3	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.

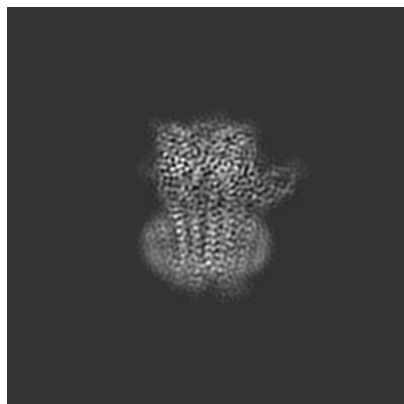
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4411. These allow visual inspection of the internal detail of the map and identification of artifacts.

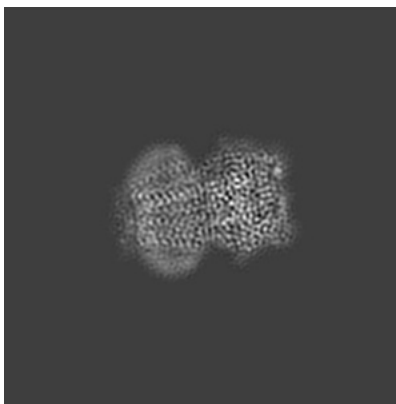
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

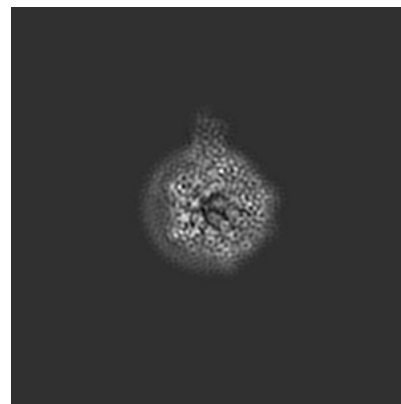
6.1.1 Primary map



X

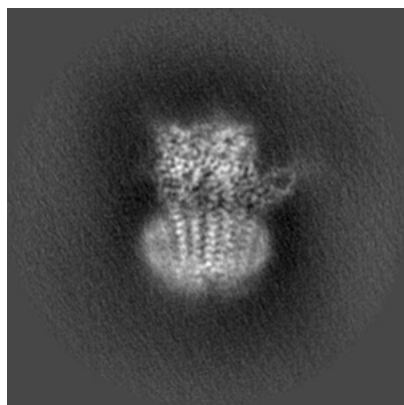


Y

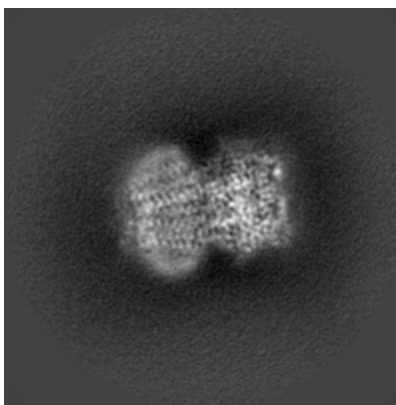


Z

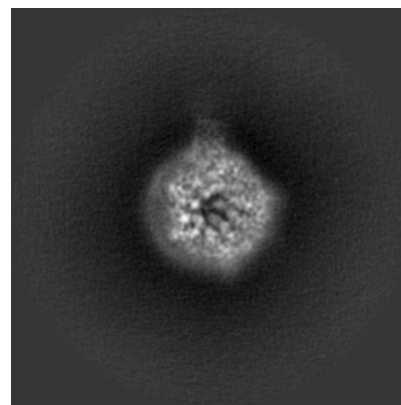
6.1.2 Raw map



X



Y



Z

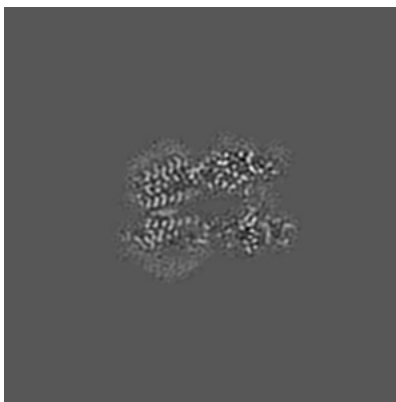
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

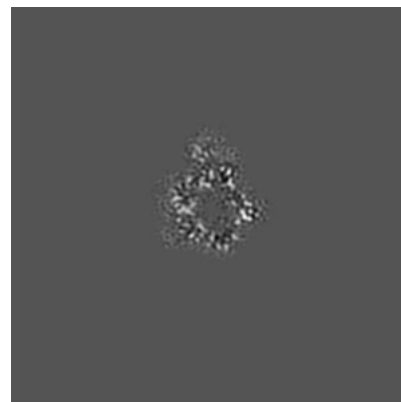
6.2.1 Primary map



X Index: 128

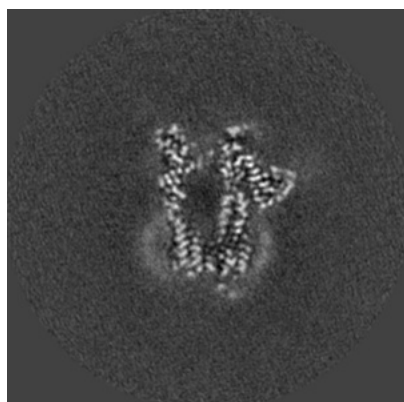


Y Index: 128

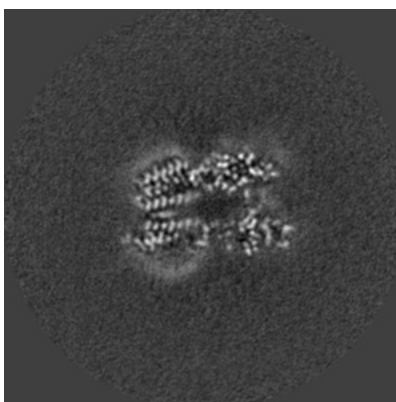


Z Index: 128

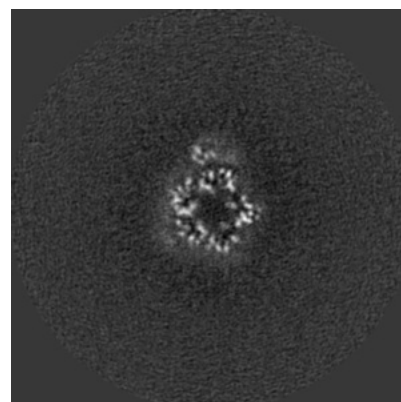
6.2.2 Raw map



X Index: 128



Y Index: 128

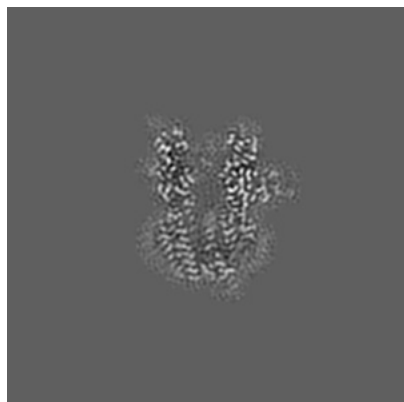


Z Index: 128

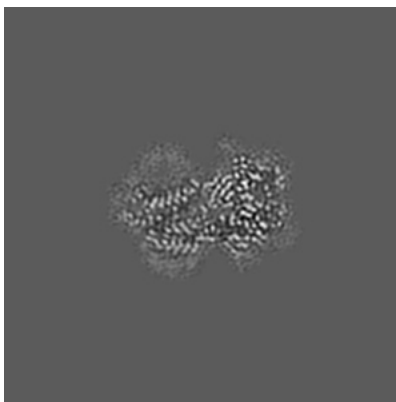
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

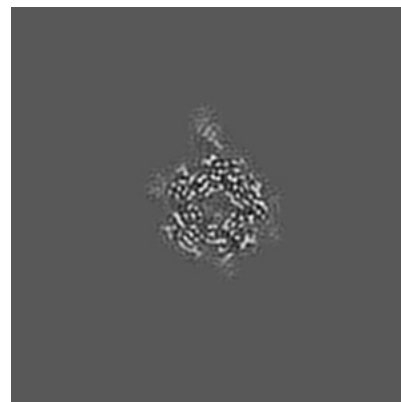
6.3.1 Primary map



X Index: 135

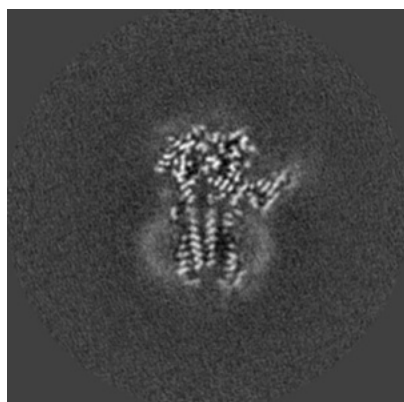


Y Index: 141

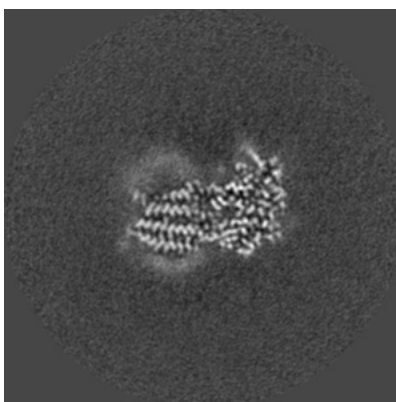


Z Index: 152

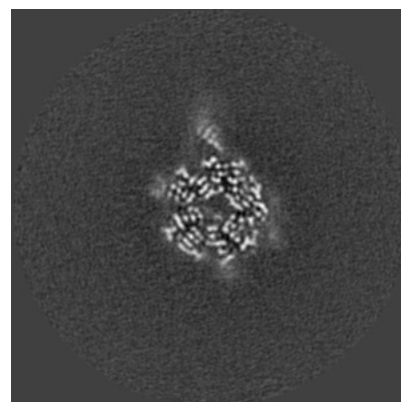
6.3.2 Raw map



X Index: 119



Y Index: 111

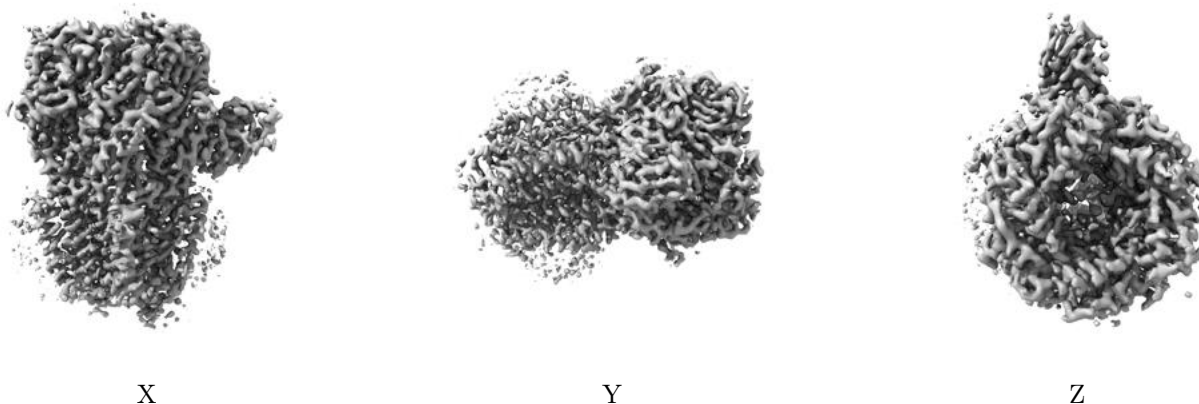


Z Index: 152

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

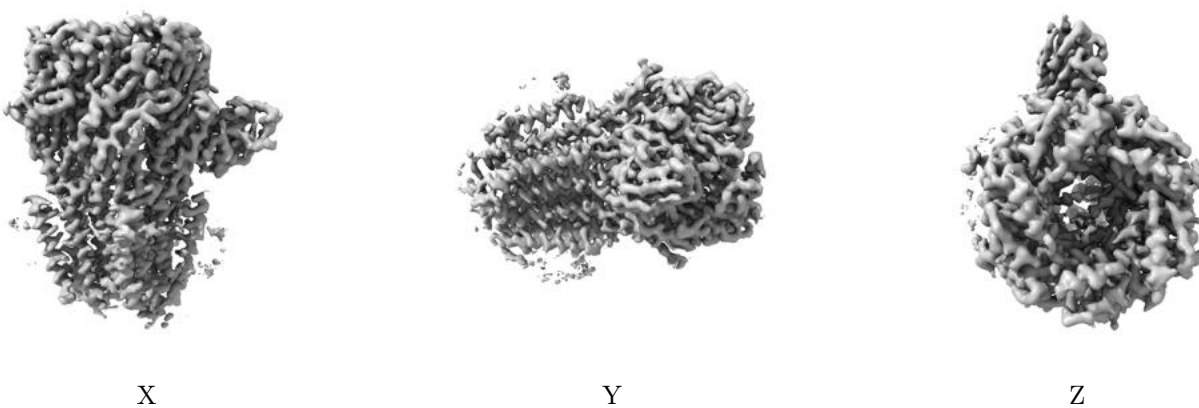
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

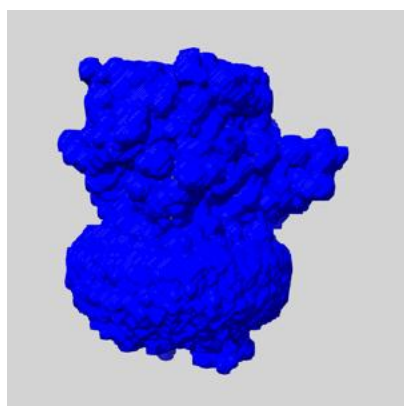
6.5 Mask visualisation [i](#)

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

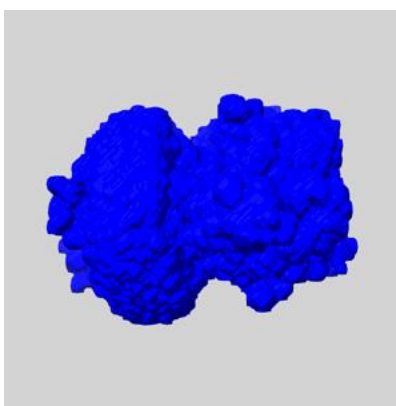
A mask typically either:

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

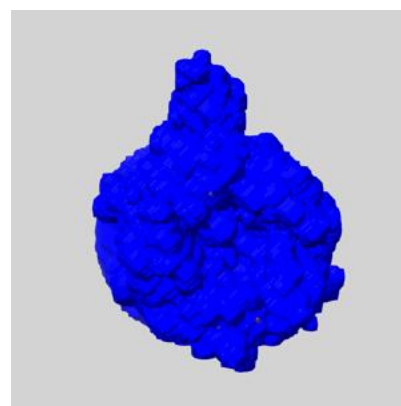
6.5.1 emd_4411_msk_1.map [i](#)



X



Y

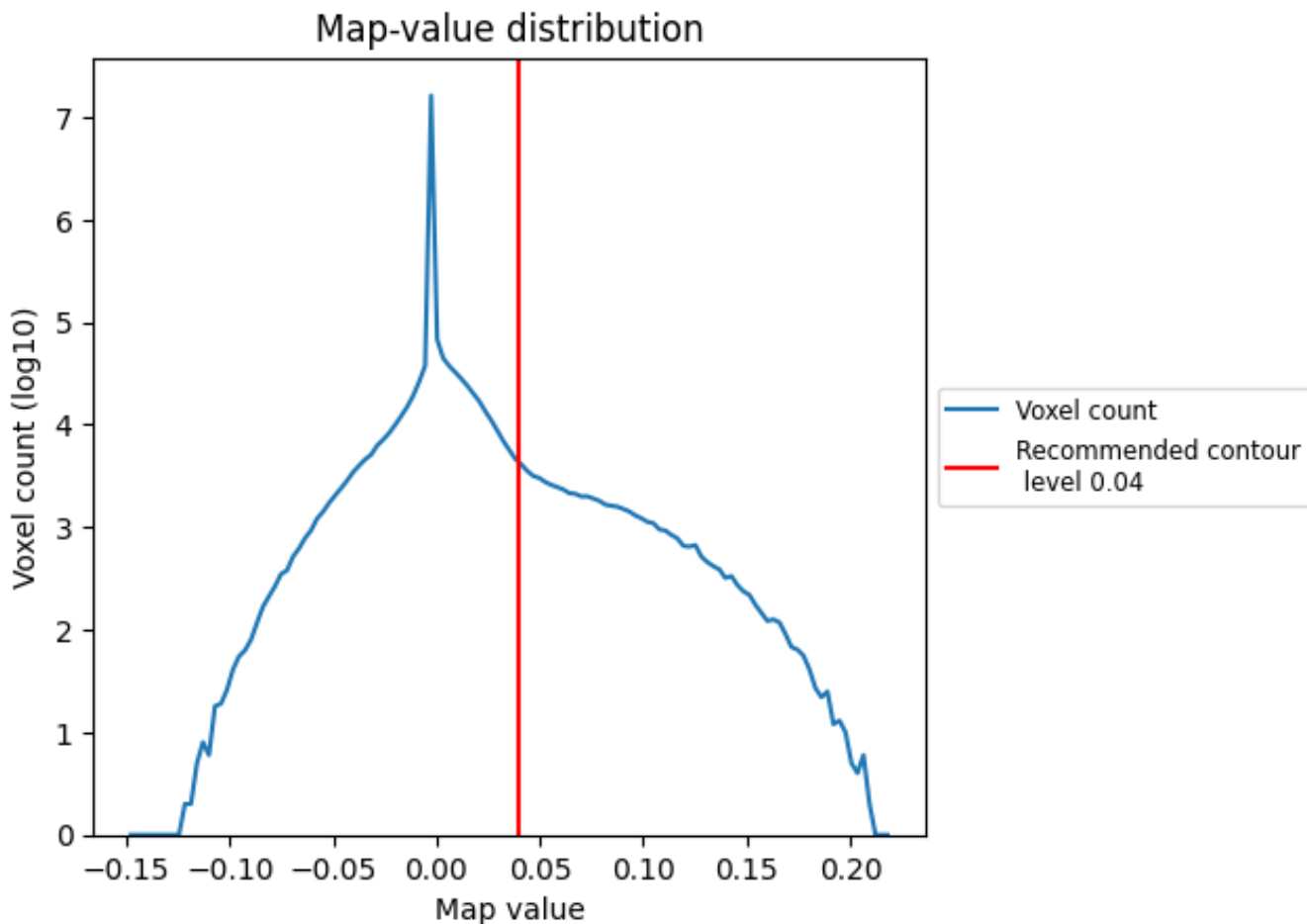


Z

7 Map analysis [i](#)

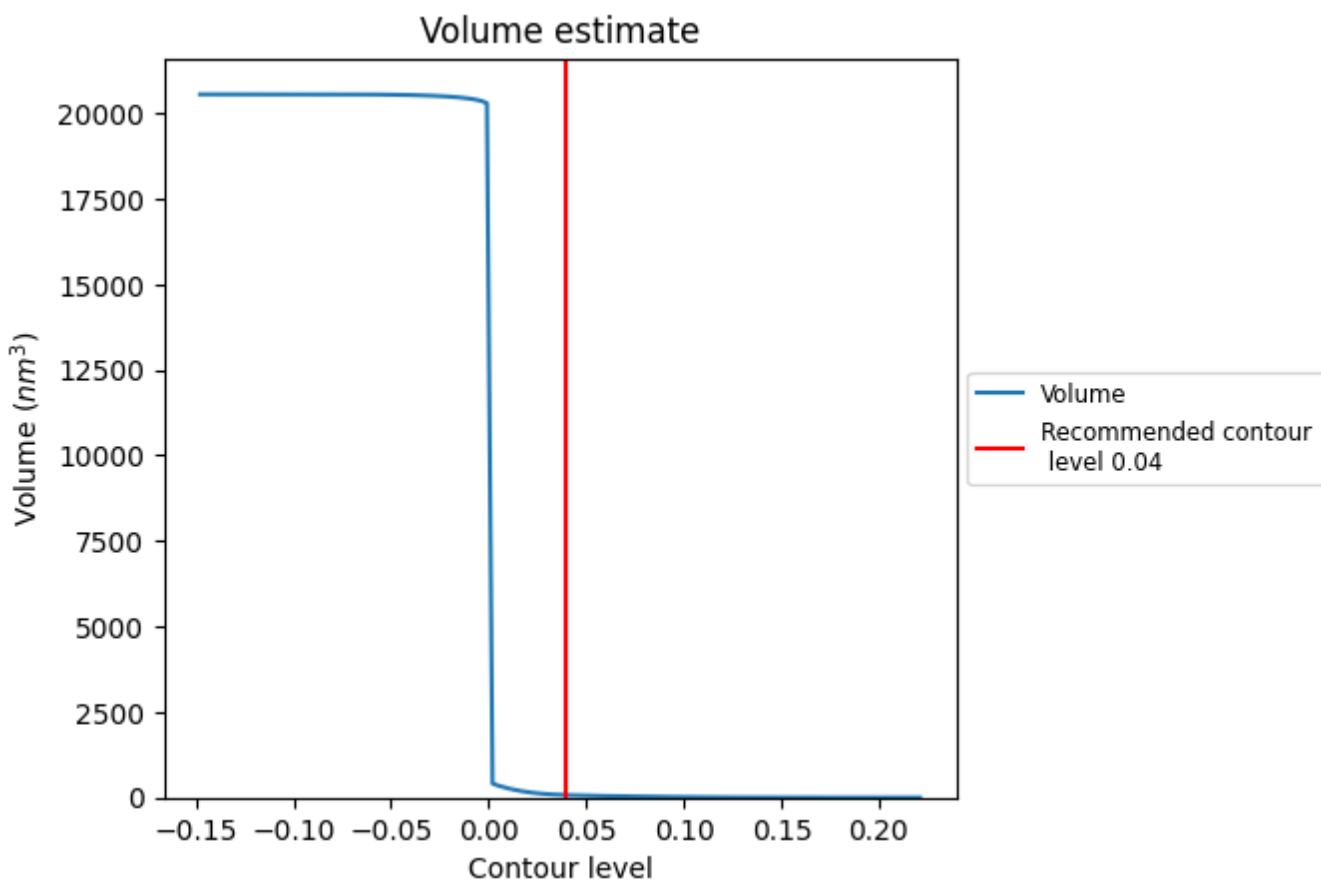
This section contains the results of statistical analysis of the map.

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.

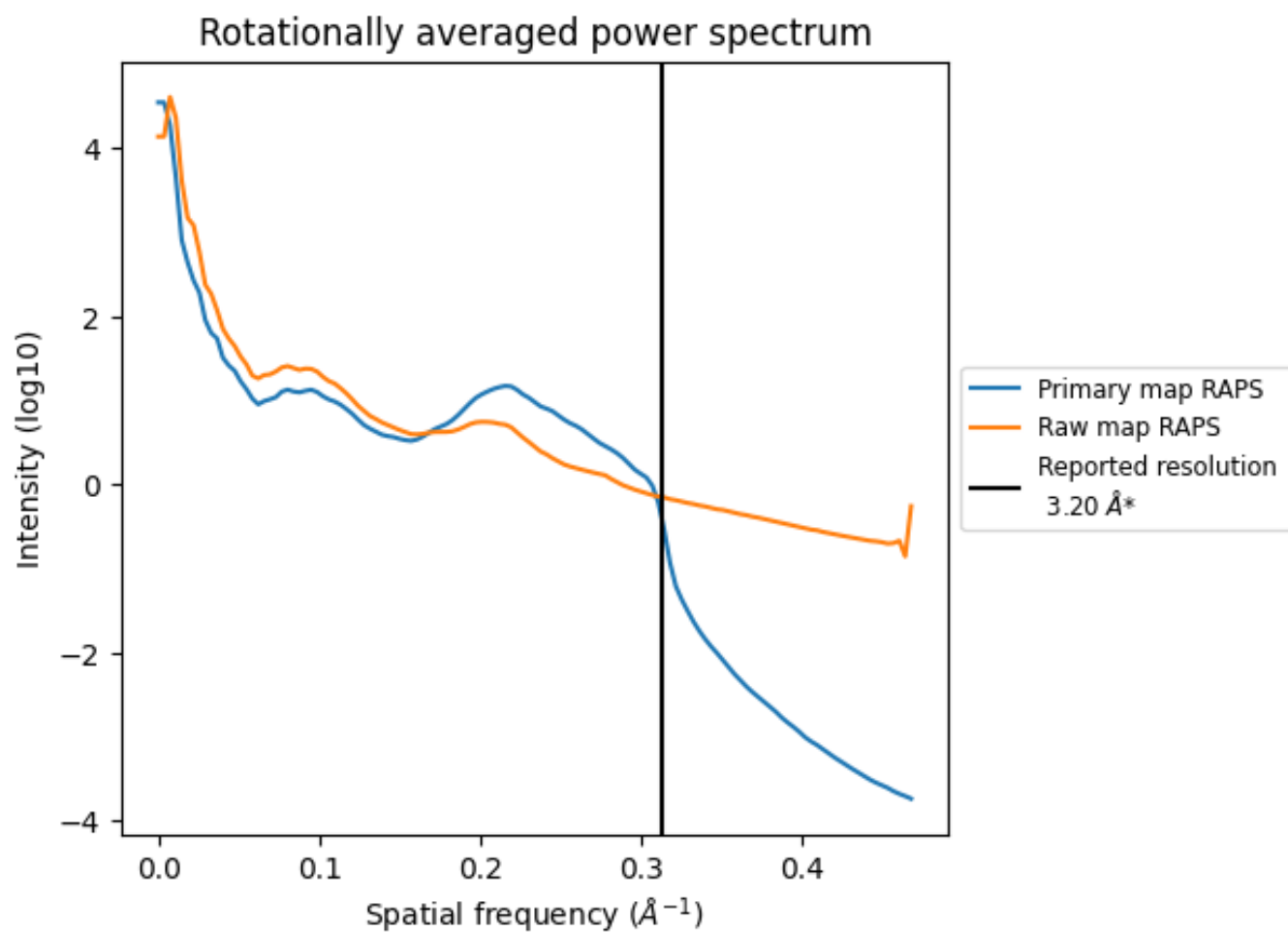
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 kDa.

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

7.3 Rotationally averaged power spectrum i

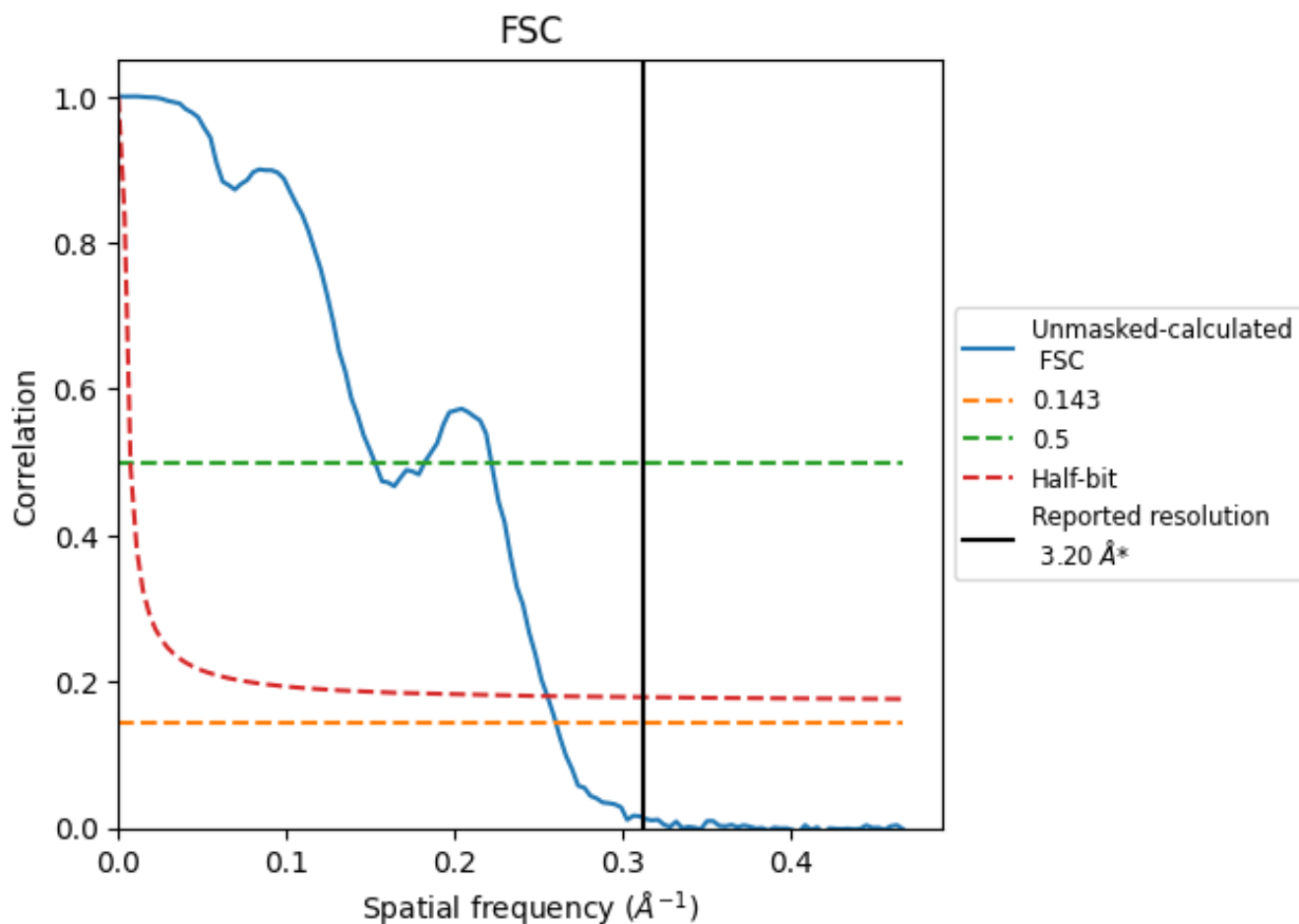


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

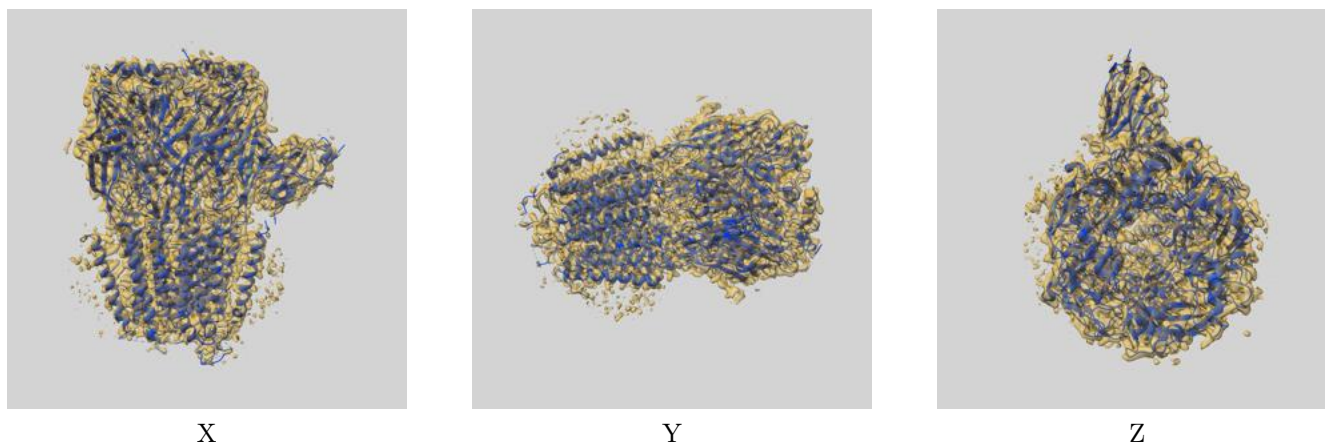
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	6.55	3.91

*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 3.84 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

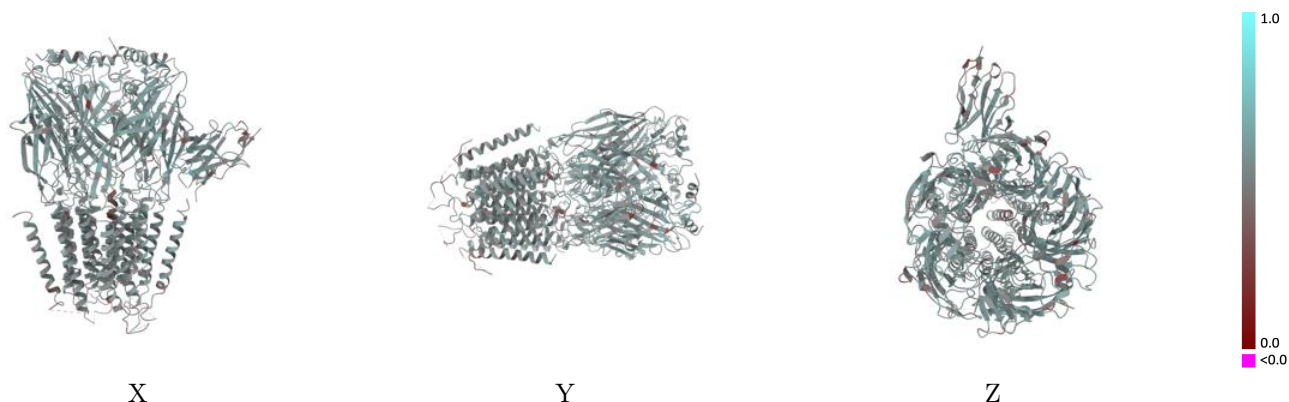
This section contains information regarding the fit between EMDB map EMD-4411 and PDB model 6I53. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



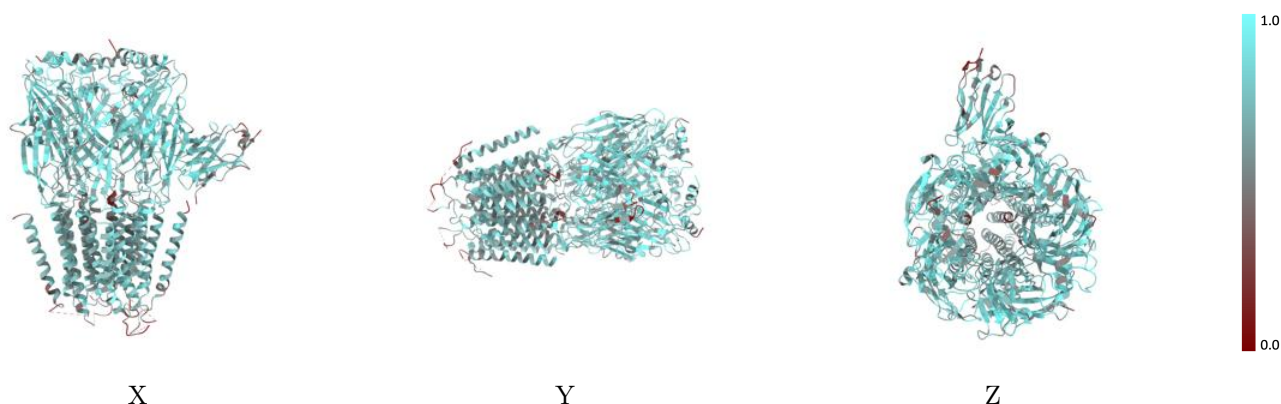
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



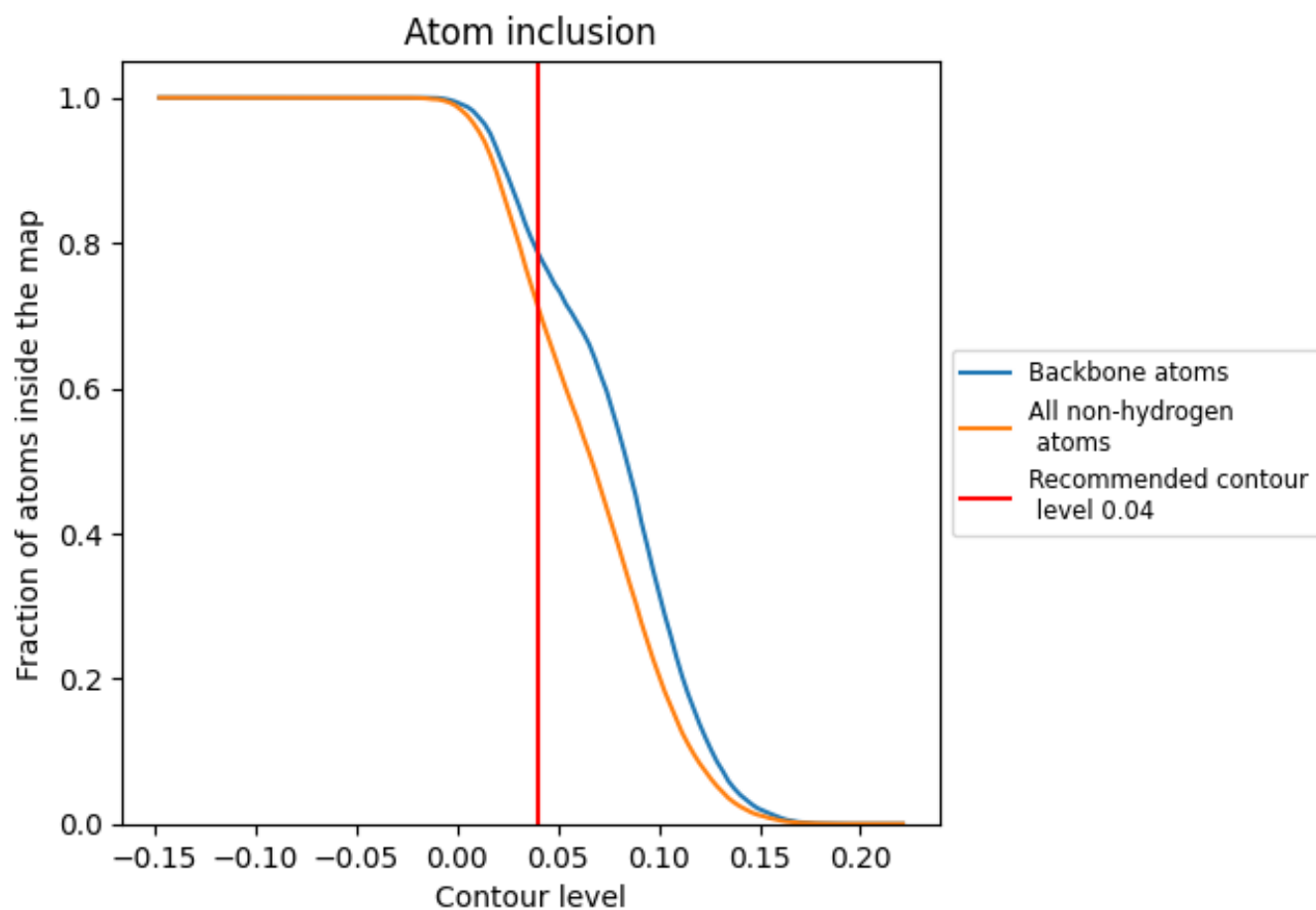
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7127	 0.5290
A	 0.7214	 0.5360
B	 0.7290	 0.5280
C	 0.7211	 0.5290
D	 0.7035	 0.5330
E	 0.7261	 0.5300
F	 0.5574	 0.5060
G	 0.6950	 0.5200
H	 0.4286	 0.4460
I	 0.4458	 0.4580
J	 0.5417	 0.5030
K	 0.6071	 0.4930
L	 0.3929	 0.3540
M	 0.3770	 0.4810

