



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 09:50 AM EST

PDB ID : 3J0A  
EMDB ID : EMD-5287  
Title : Homology model of human Toll-like receptor 5 fitted into an electron microscopy single particle reconstruction  
Authors : Modis, Y.; Zhou, K.; Kanai, R.; Lee, P.; Wang, H.W.  
Deposited on : 2011-06-02  
Resolution : 26.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

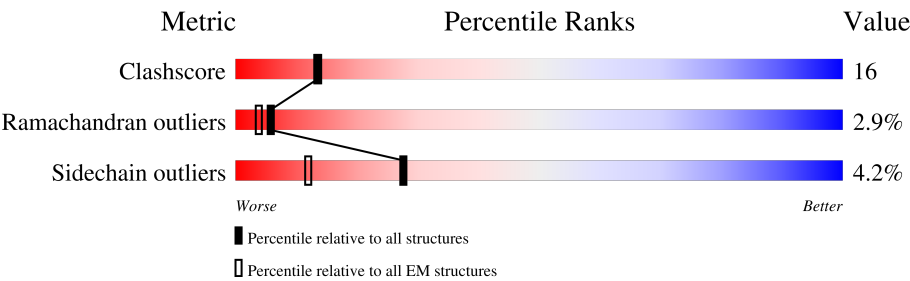
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 26.00 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	844	<div><div>30%</div><div>60%</div><div>31%</div><div>6%</div></div>
1	B	844	<div><div>30%</div><div>46%</div><div>26%</div><div>25%</div></div>
2	C	2	<div><div>100%</div></div>
2	D	2	<div><div>100%</div></div>
2	E	2	<div><div>100%</div></div>
2	F	2	<div><div>50%</div><div>50%</div></div>
2	G	2	<div><div>100%</div></div>
2	H	2	<div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>50%</div><div>50%</div></div>
2	J	2	<div><div></div><div>100%</div><div></div></div>
2	K	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>100%</div><div></div></div>
2	L	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>100%</div><div></div></div>
2	M	2	<div><div></div><div>50%</div><div>50%</div></div>
2	N	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>100%</div><div></div></div>
2	O	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>100%</div><div></div></div>
2	P	2	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11828 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 Toll-like receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6437	4155	1081	1176	25		
1	B	632	Total	C	N	O	S	0	0
			5055	3272	839	927	17		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	859	GLY	-	expression tag	UNP O60602
A	860	SER	-	expression tag	UNP O60602
A	861	HIS	-	expression tag	UNP O60602
A	862	HIS	-	expression tag	UNP O60602
A	863	HIS	-	expression tag	UNP O60602
A	864	HIS	-	expression tag	UNP O60602
A	865	HIS	-	expression tag	UNP O60602
A	866	HIS	-	expression tag	UNP O60602
B	859	GLY	-	expression tag	UNP O60602
B	860	SER	-	expression tag	UNP O60602
B	861	HIS	-	expression tag	UNP O60602
B	862	HIS	-	expression tag	UNP O60602
B	863	HIS	-	expression tag	UNP O60602
B	864	HIS	-	expression tag	UNP O60602
B	865	HIS	-	expression tag	UNP O60602
B	866	HIS	-	expression tag	UNP O60602

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

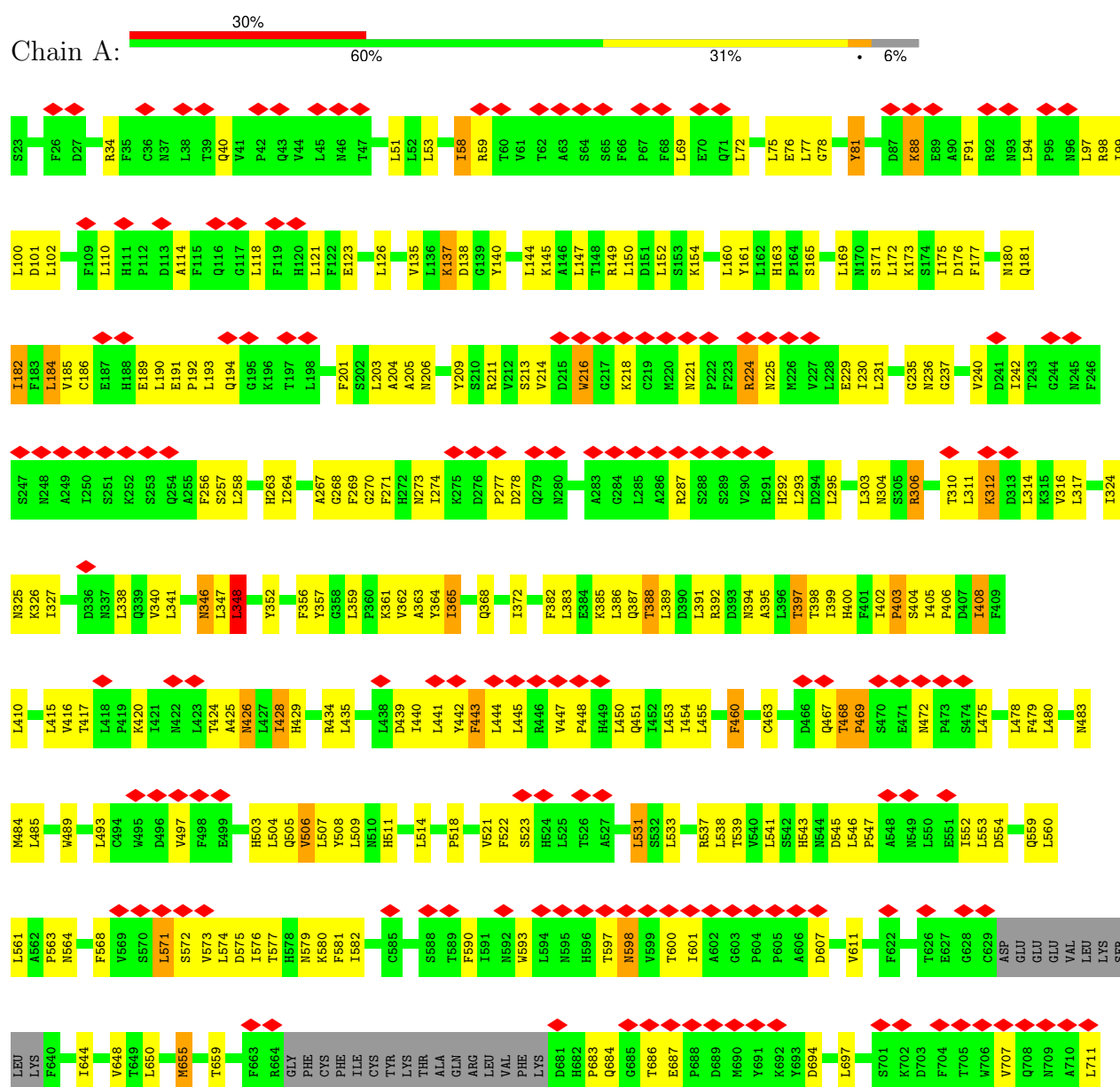


Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total 24	C 14	N 1	O 9	0	0
2	D	2	Total 24	C 14	N 1	O 9	0	0
2	E	2	Total 24	C 14	N 1	O 9	0	0
2	F	2	Total 24	C 14	N 1	O 9	0	0
2	G	2	Total 24	C 14	N 1	O 9	0	0
2	H	2	Total 24	C 14	N 1	O 9	0	0
2	I	2	Total 24	C 14	N 1	O 9	0	0
2	J	2	Total 24	C 14	N 1	O 9	0	0
2	K	2	Total 24	C 14	N 1	O 9	0	0
2	L	2	Total 24	C 14	N 1	O 9	0	0
2	M	2	Total 24	C 14	N 1	O 9	0	0
2	N	2	Total 24	C 14	N 1	O 9	0	0
2	O	2	Total 24	C 14	N 1	O 9	0	0
2	P	2	Total 24	C 14	N 1	O 9	0	0

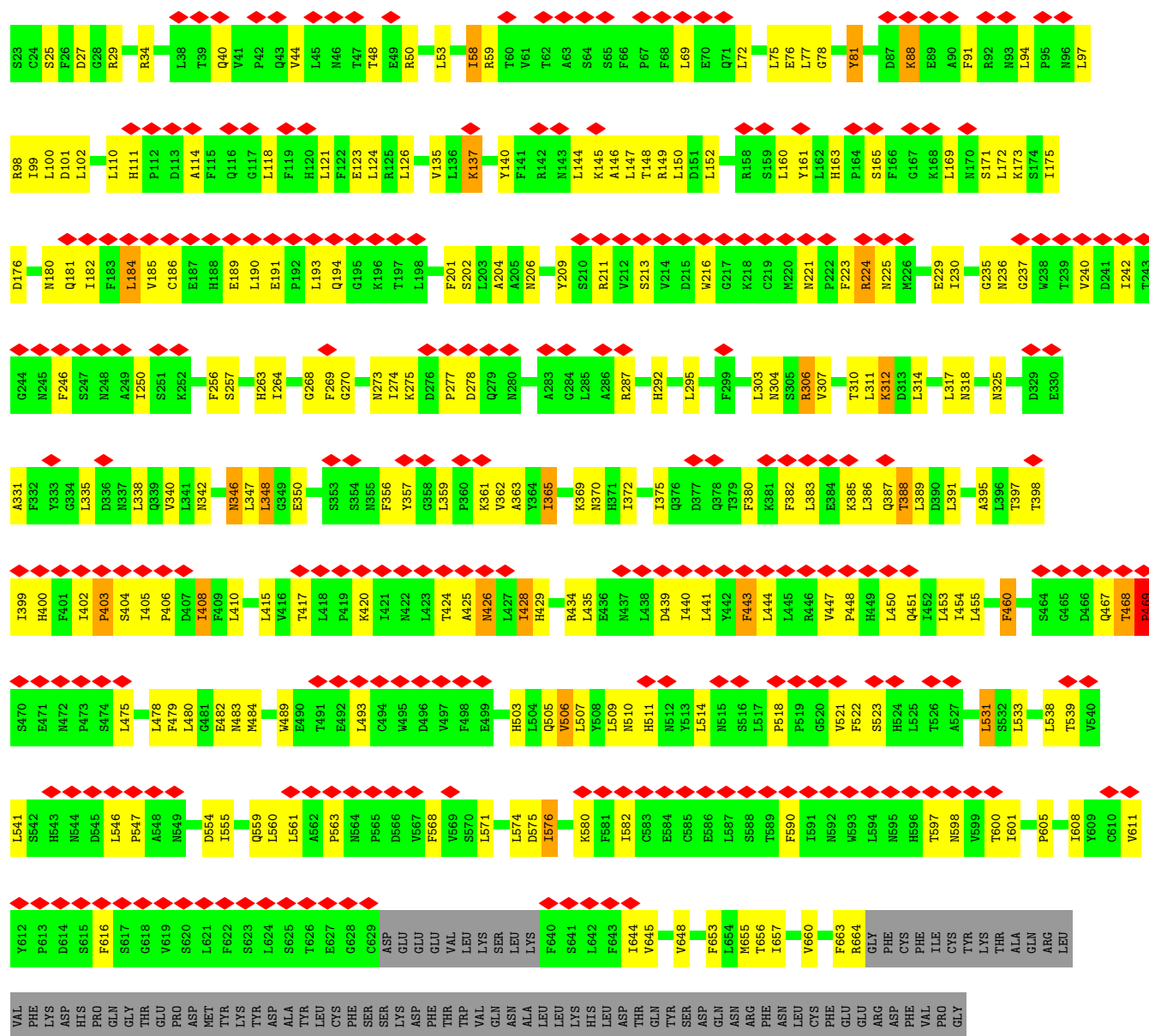
### 3 Residue-property plots

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: Toll-like receptor 5



- Molecule 1: Toll-like receptor 5



GLU ASN ARG ILE ALA ASN ILE ASP ALA TRP ASN SER ARG LYS ILE VAL CYS LEU TRP VAL SER GLU ARG HIS PHE LEU ASP ASP GLY TRP TRP CYS LEU GLU ALA PHE LEU SER TYR ALA GLY ARG CYS LEU SER ASP LEU ASN SER ALA LEU ILE MET VAL VAL GLY SER LEU THR ALA THR ILE

TYR GLN LEU MET HIS HIS HIS HIS HIS HIS SER ILE ARG ALA GLY PHE VAL GLN LYS ARG LYS LYS ILE TYR LEU ARG TRP PRO GLU ARG ASP PHE GLN ASP VAL GLY TRP PHE LEU HIS LEU PHE LEU SER GLN GLN ILE LEU LYS LYS GLU LYS SER ASP ASN ASN ILE PRO VAL LEU THR VAL THR LEU THR ILE

SER  
GLY  
SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%  
100%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%  
100%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%  
100%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%  
100%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%  
100%





- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-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	4241	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	52000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	14.528	Depositor
Minimum map value	-4.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.69	Depositor
Map size ( $\text{\AA}$ )	214.00002, 214.00002, 214.00002	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.14, 2.14, 2.14	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.87	7/6589 (0.1%)	0.61	1/8938 (0.0%)
1	B	0.75	2/5172 (0.0%)	0.59	3/7029 (0.0%)
All	All	0.82	9/11761 (0.1%)	0.61	4/15967 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	GLU	CD-OE1	-28.34	0.94	1.25
1	A	738	GLU	CD-OE2	9.38	1.35	1.25
1	A	582	ILE	C-O	7.25	1.37	1.23
1	A	738	GLU	CA-C	7.20	1.71	1.52
1	B	616	PHE	CE2-CZ	6.46	1.49	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	GLU	OE1-CD-OE2	-11.45	109.56	123.30
1	B	664	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	B	664	ARG	NH1-CZ-NH2	5.22	125.15	119.40
1	B	660	VAL	CG1-CB-CG2	-5.15	102.66	110.90

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	6437	0	6385	214	0
1	B	5055	0	5041	160	0
2	C	24	0	22	0	0
2	D	24	0	22	0	0
2	E	24	0	22	0	0
2	F	24	0	22	1	0
2	G	24	0	22	0	0
2	H	24	0	22	0	0
2	I	24	0	22	1	0
2	J	24	0	22	0	0
2	K	24	0	22	0	0
2	L	24	0	22	0	0
2	M	24	0	22	1	0
2	N	24	0	22	0	0
2	O	24	0	22	0	0
2	P	24	0	22	1	0
All	All	11828	0	11734	372	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 16.

The worst 5 of 372 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:B:514:LEU:HD13	1:B:538:LEU:HG	1.55	0.87
1:A:748:ILE:HG23	1:A:754:ILE:HD11	1.58	0.86
1:A:123:GLU:HG2	1:A:149:ARG:HB3	1.58	0.85
1:B:123:GLU:HG2	1:B:149:ARG:HB3	1.58	0.85
1:A:707:VAL:HG13	1:A:711:LEU:HD23	1.64	0.78

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	791/844 (94%)	621 (78%)	151 (19%)	19 (2%)	5	27
1	B	628/844 (74%)	471 (75%)	135 (22%)	22 (4%)	3	20
All	All	1419/1688 (84%)	1092 (77%)	286 (20%)	41 (3%)	6	23

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	397	THR
1	B	182	ILE
1	B	506	VAL
1	A	181	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	727/770 (94%)	697 (96%)	30 (4%)	26	47
1	B	576/770 (75%)	551 (96%)	25 (4%)	25	46
All	All	1303/1540 (85%)	1248 (96%)	55 (4%)	27	46

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	739	ASN
1	B	145	LYS
1	B	655	MET
1	B	443	PHE
1	A	802	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	GLN
1	B	221	ASN
1	B	510	ASN
1	B	80	GLN
1	B	155	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

28 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	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	1.62	4 (28%)	17,19,21	1.34	2 (11%)
2	FUC	C	2	2	10,10,11	1.71	3 (30%)	14,14,16	1.78	4 (28%)
2	NAG	D	1	1,2	14,14,15	1.88	4 (28%)	17,19,21	1.26	1 (5%)
2	FUC	D	2	2	10,10,11	1.65	4 (40%)	14,14,16	1.43	3 (21%)
2	NAG	E	1	1,2	14,14,15	1.70	3 (21%)	17,19,21	1.70	4 (23%)
2	FUC	E	2	2	10,10,11	1.53	2 (20%)	14,14,16	1.29	1 (7%)
2	NAG	F	1	1,2	14,14,15	1.47	4 (28%)	17,19,21	1.11	0
2	FUC	F	2	2	10,10,11	1.63	4 (40%)	14,14,16	1.72	4 (28%)
2	NAG	G	1	1,2	14,14,15	1.94	2 (14%)	17,19,21	1.40	2 (11%)
2	FUC	G	2	2	10,10,11	1.84	3 (30%)	14,14,16	1.34	2 (14%)
2	NAG	H	1	1,2	14,14,15	1.42	2 (14%)	17,19,21	1.35	3 (17%)
2	FUC	H	2	2	10,10,11	1.88	4 (40%)	14,14,16	2.07	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	1,2	14,14,15	1.53	2 (14%)	17,19,21	1.05	2 (11%)
2	FUC	I	2	2	10,10,11	1.93	4 (40%)	14,14,16	2.06	4 (28%)
2	NAG	J	1	1,2	14,14,15	1.68	2 (14%)	17,19,21	1.32	3 (17%)
2	FUC	J	2	2	10,10,11	1.72	3 (30%)	14,14,16	1.30	3 (21%)
2	NAG	K	1	1,2	14,14,15	1.32	1 (7%)	17,19,21	1.27	4 (23%)
2	FUC	K	2	2	10,10,11	1.56	2 (20%)	14,14,16	1.14	0
2	NAG	L	1	1,2	14,14,15	2.00	4 (28%)	17,19,21	1.16	1 (5%)
2	FUC	L	2	2	10,10,11	1.80	5 (50%)	14,14,16	1.57	3 (21%)
2	NAG	M	1	1,2	14,14,15	1.65	3 (21%)	17,19,21	1.33	1 (5%)
2	FUC	M	2	2	10,10,11	1.66	3 (30%)	14,14,16	1.52	3 (21%)
2	NAG	N	1	1,2	14,14,15	1.96	2 (14%)	17,19,21	1.39	2 (11%)
2	FUC	N	2	2	10,10,11	1.83	3 (30%)	14,14,16	1.34	2 (14%)
2	NAG	O	1	1,2	14,14,15	1.84	5 (35%)	17,19,21	1.06	1 (5%)
2	FUC	O	2	2	10,10,11	1.96	4 (40%)	14,14,16	2.55	5 (35%)
2	NAG	P	1	1,2	14,14,15	1.79	3 (21%)	17,19,21	1.41	3 (17%)
2	FUC	P	2	2	10,10,11	1.81	4 (40%)	14,14,16	1.97	4 (28%)

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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	4/6/23/26	0/1/1/1
2	FUC	J	2	2	-	-	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	NAG	L	1	1,2	-	4/6/23/26	0/1/1/1
2	FUC	L	2	2	-	-	0/1/1/1
2	NAG	M	1	1,2	-	4/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	N	2	2	-	-	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
2	NAG	P	1	1,2	-	4/6/23/26	0/1/1/1
2	FUC	P	2	2	-	-	0/1/1/1

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O5-C1	5.38	1.52	1.43
2	G	1	NAG	O5-C1	5.32	1.52	1.43
2	L	1	NAG	C1-C2	5.13	1.59	1.52
2	E	1	NAG	C4-C5	4.40	1.62	1.53
2	P	1	NAG	C1-C2	4.35	1.58	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	FUC	C6-C5-C4	5.86	123.80	113.08
2	O	2	FUC	C3-C4-C5	5.29	117.86	109.81
2	O	2	FUC	C6-C5-C4	4.74	121.74	113.08
2	C	2	FUC	C1-C2-C3	4.65	116.41	109.64
2	P	2	FUC	C6-C5-C4	4.55	121.41	113.08

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

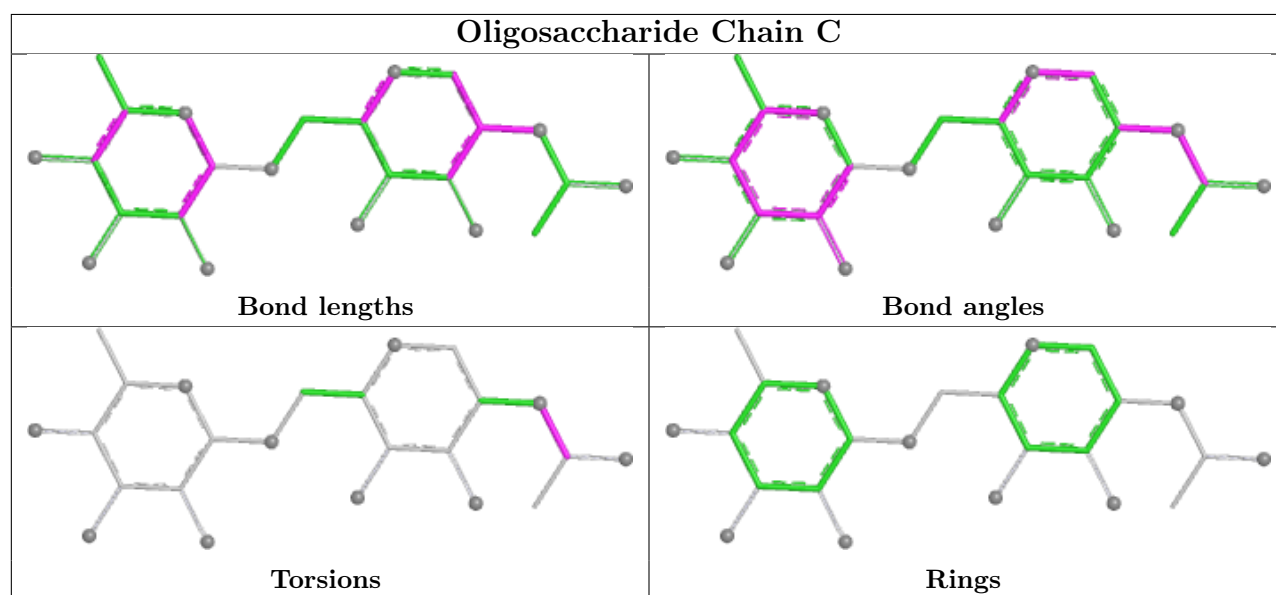
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2

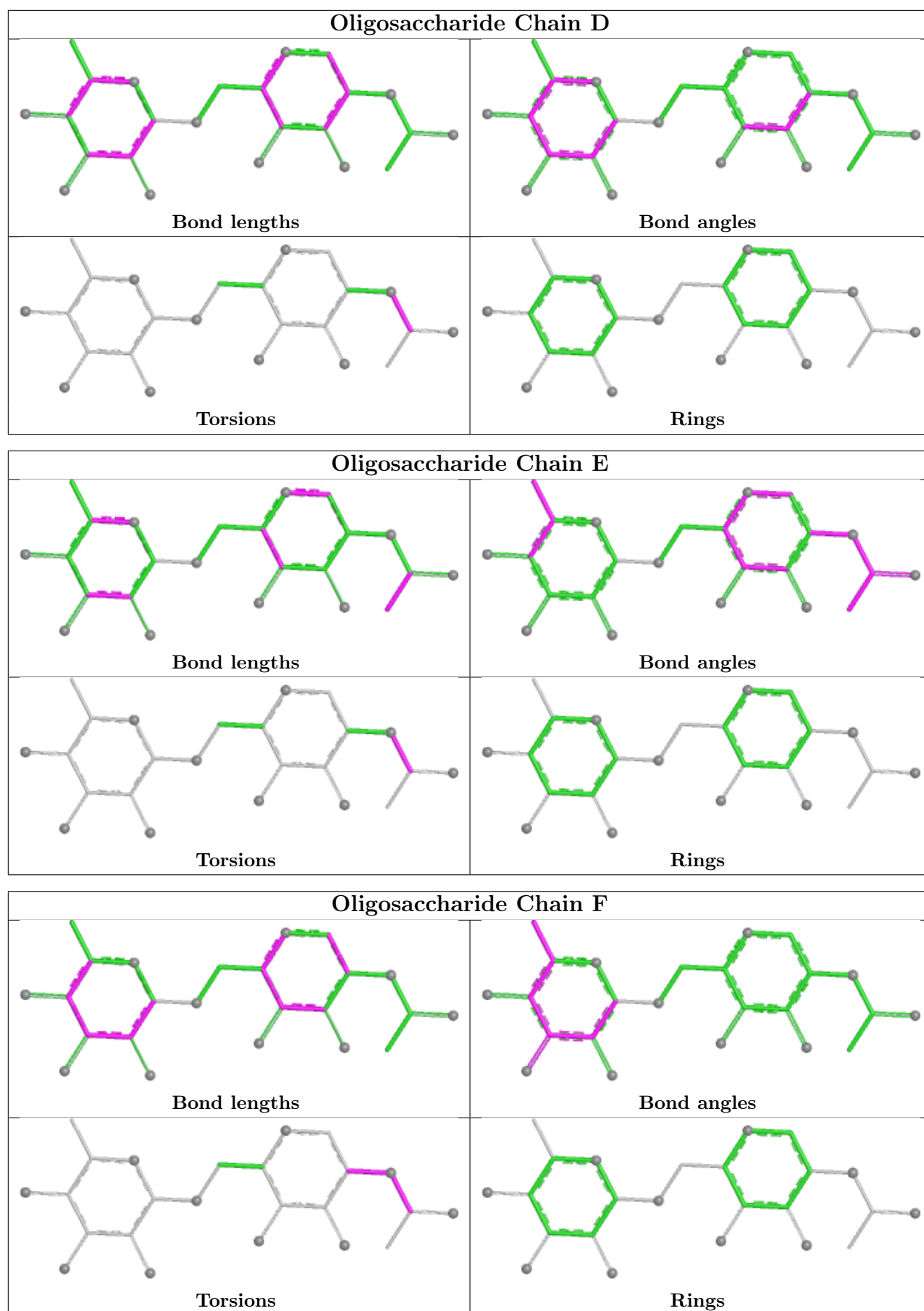
There are no ring outliers.

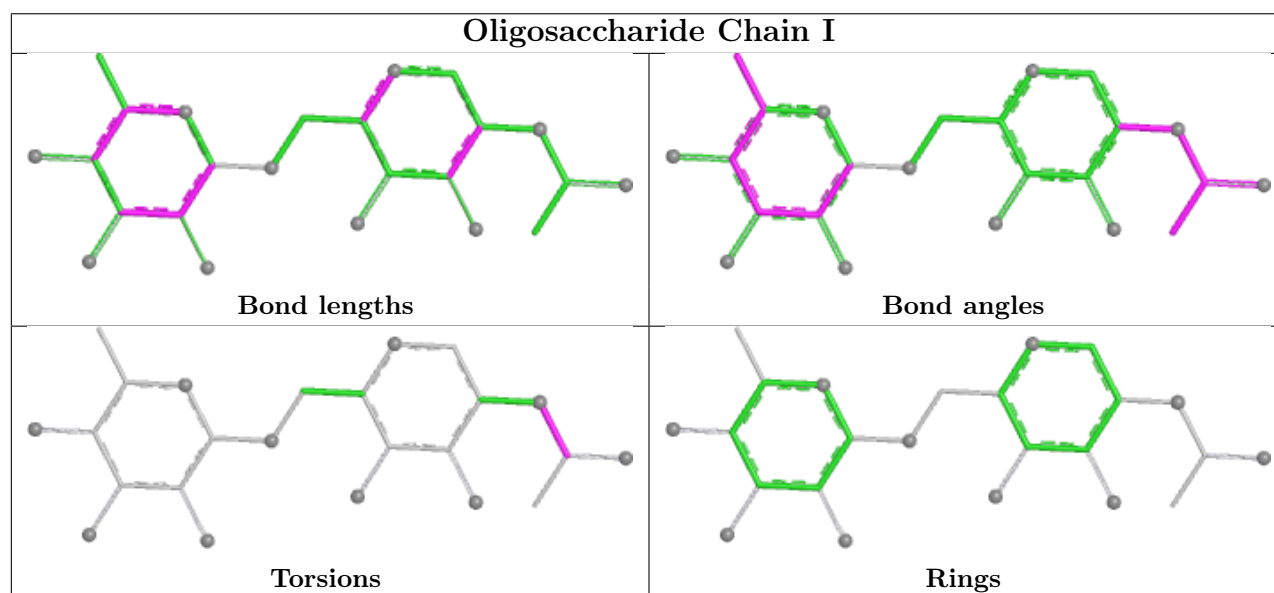
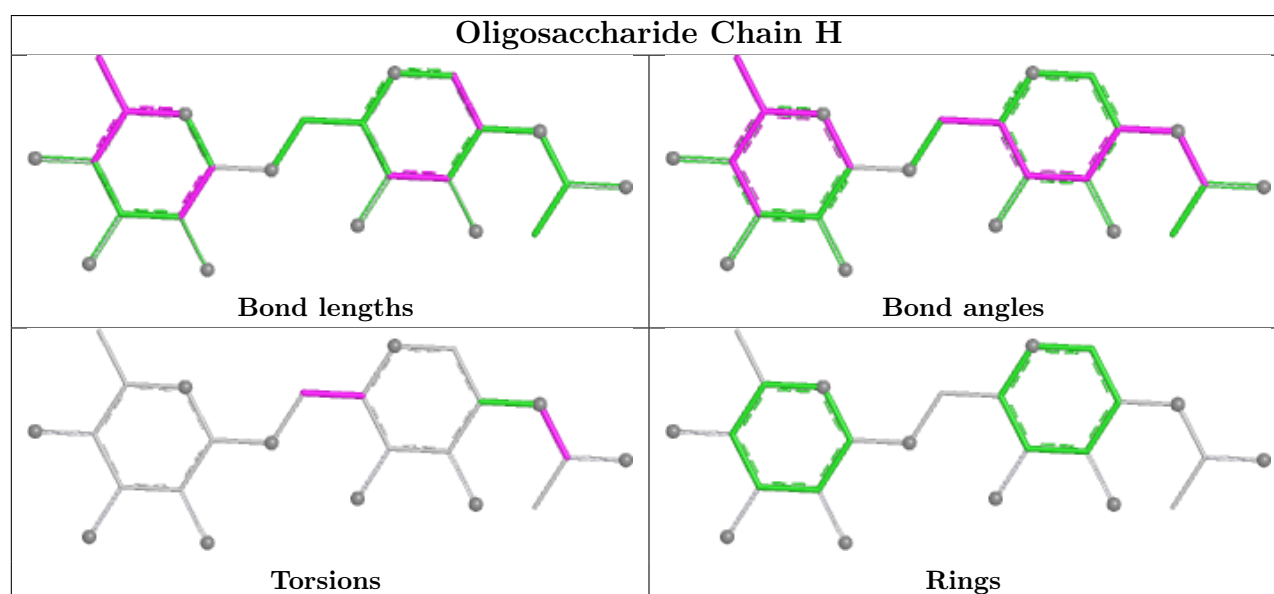
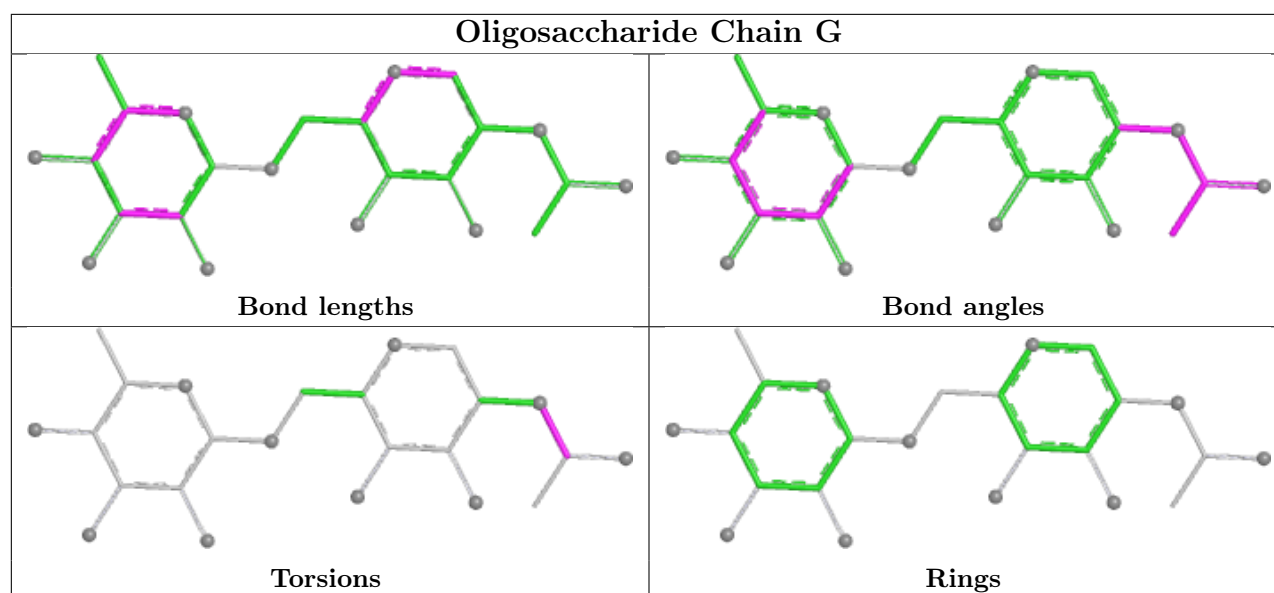
4 monomers are involved in 4 short contacts:

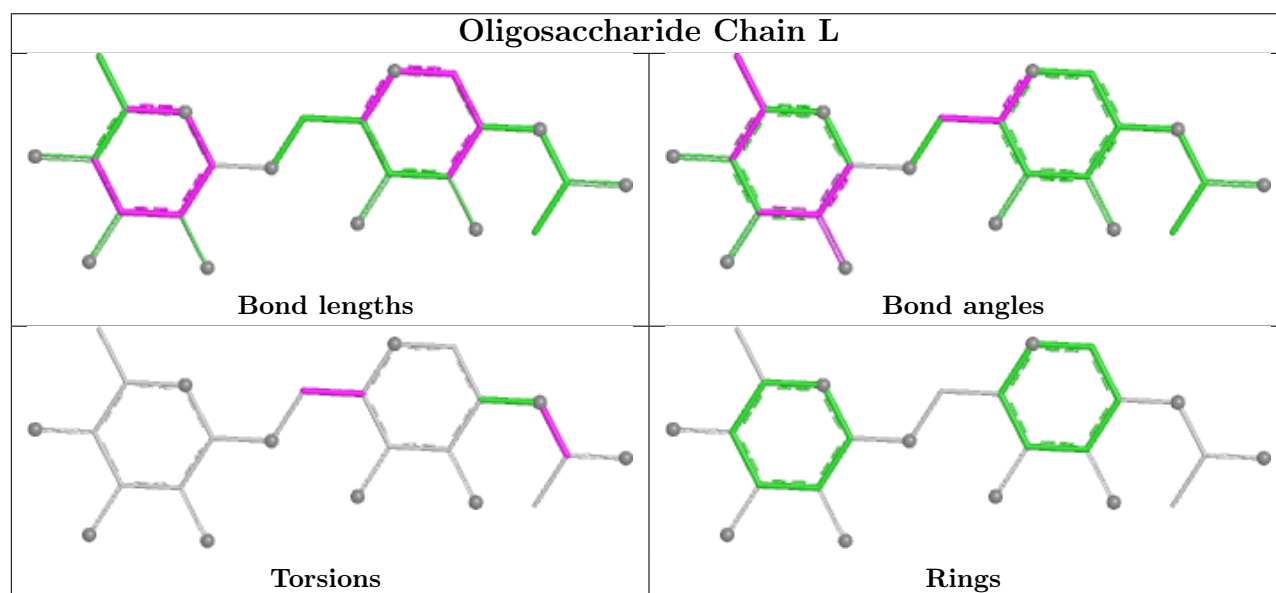
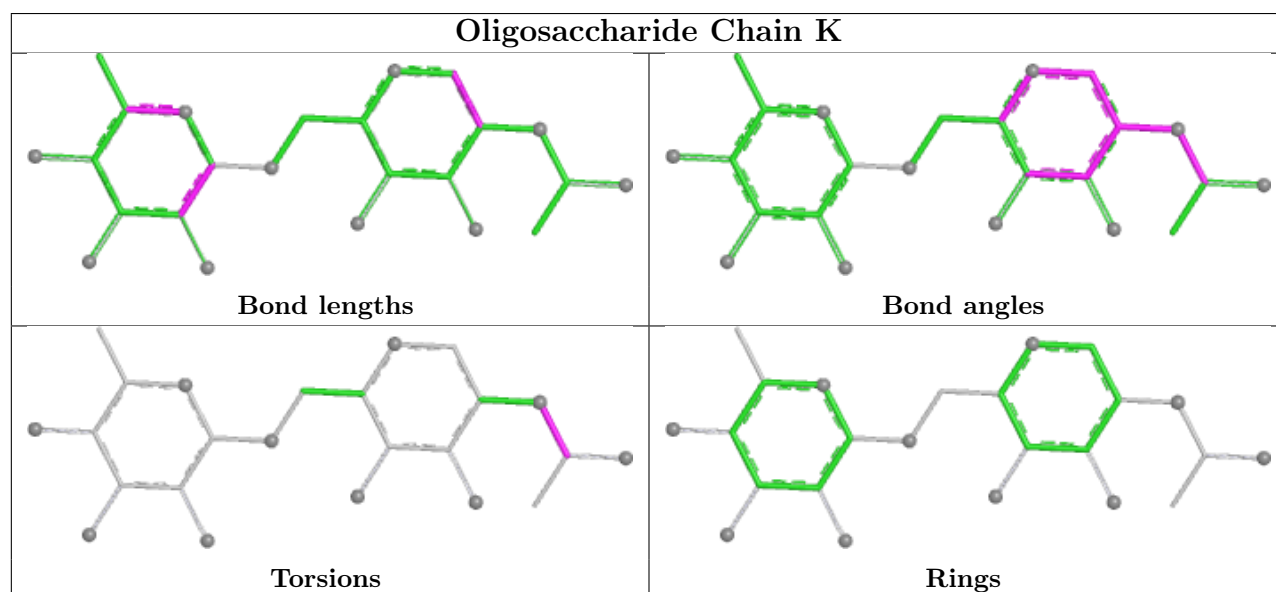
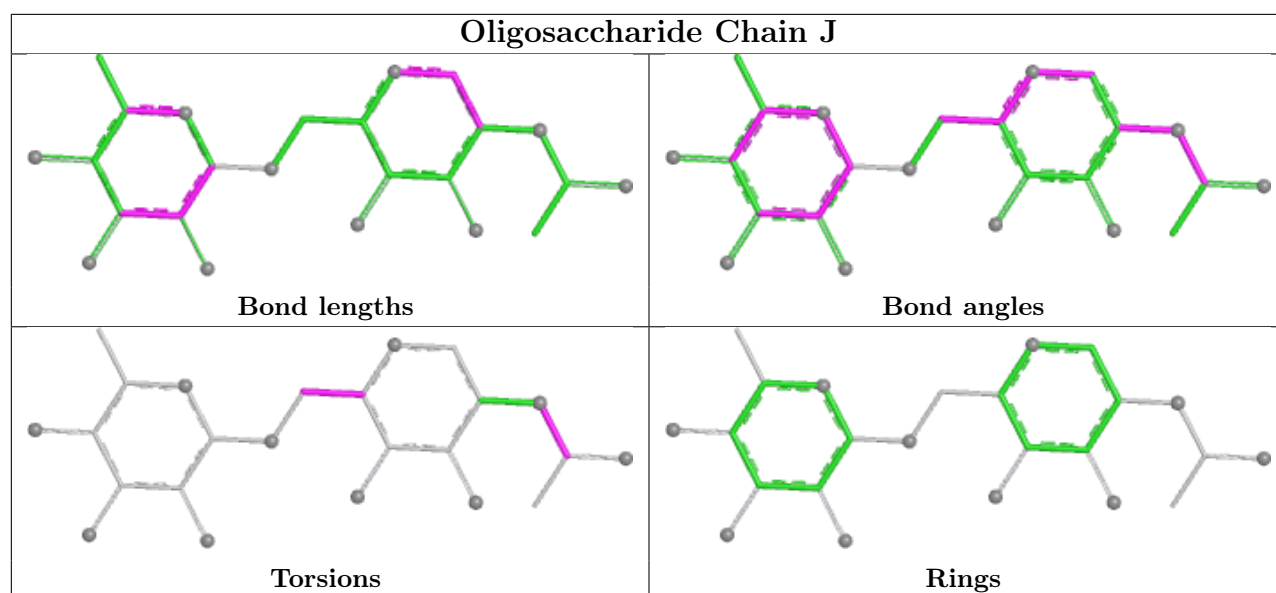
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	M	1	NAG	1	0
2	I	1	NAG	1	0
2	P	1	NAG	1	0

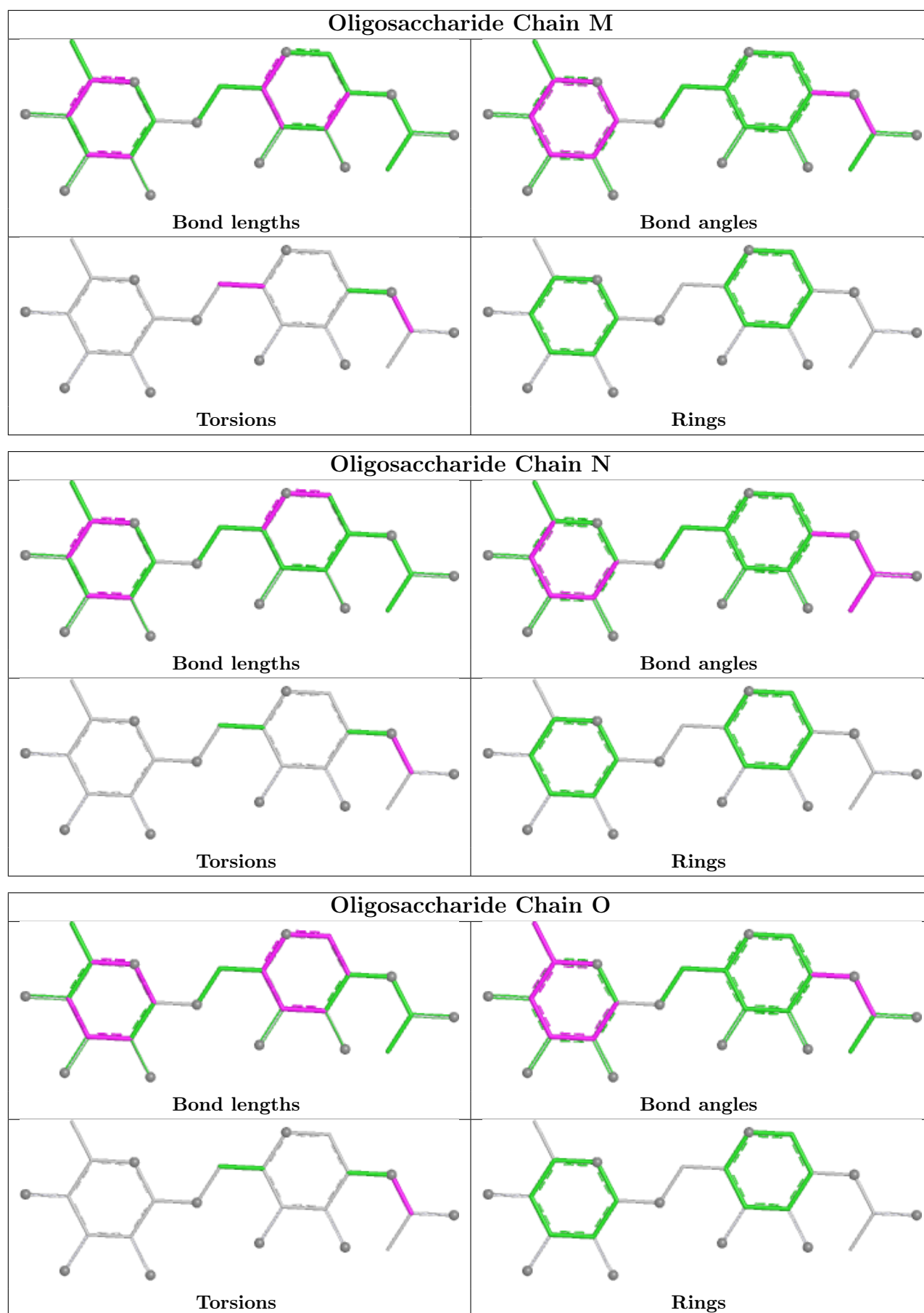
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

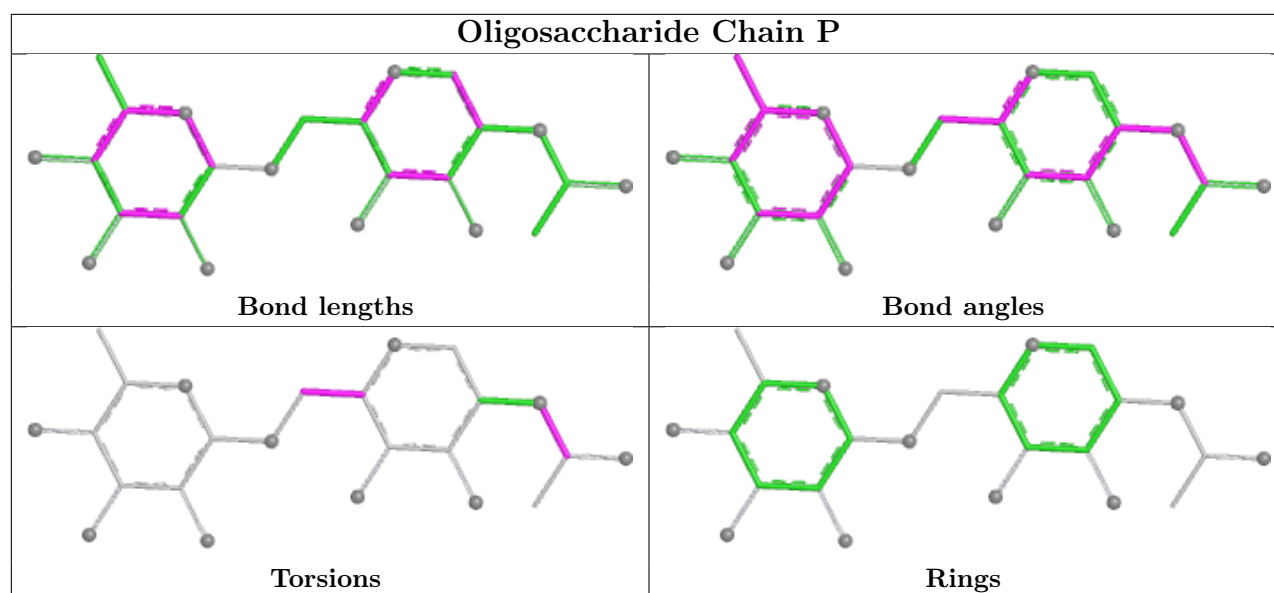












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

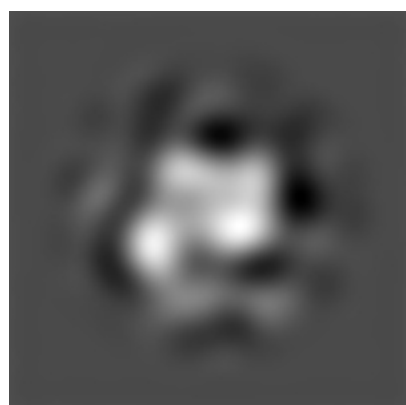
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5287. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y

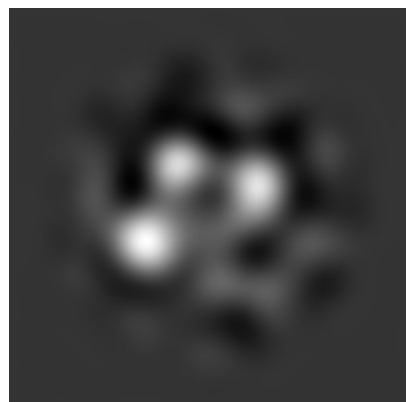


Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 50



Y Index: 50



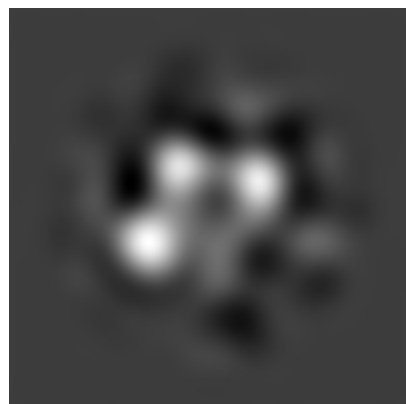
Z Index: 50



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: 53



Y Index: 60

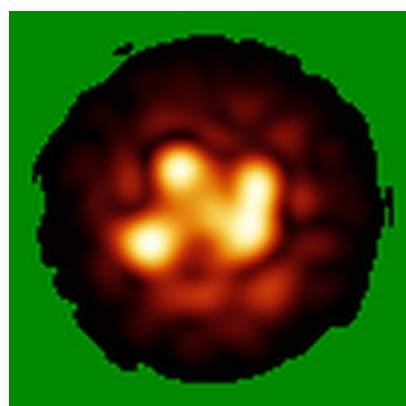


Z Index: 44

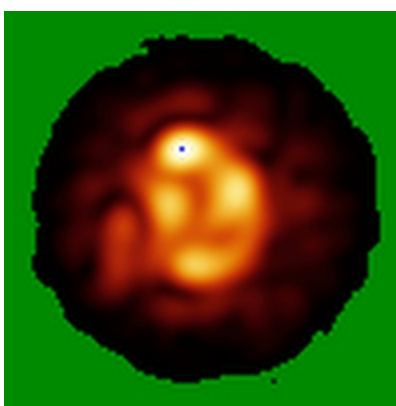
The images above show the largest variance slices of the map in three orthogonal directions.

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

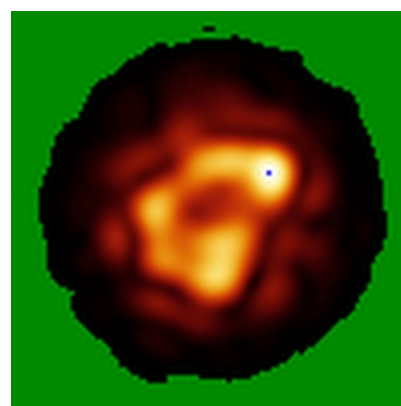
### 6.4.1 Primary map



X



Y

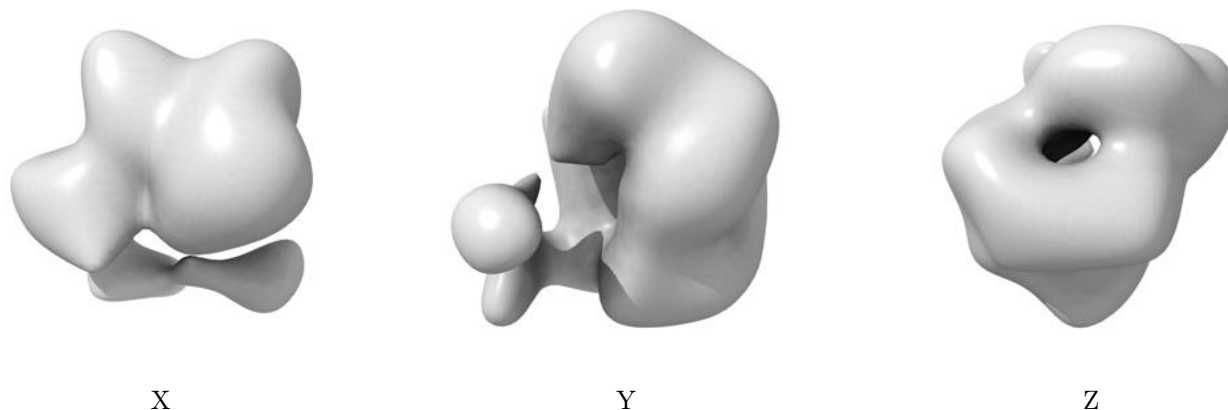


Z

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 2.69. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

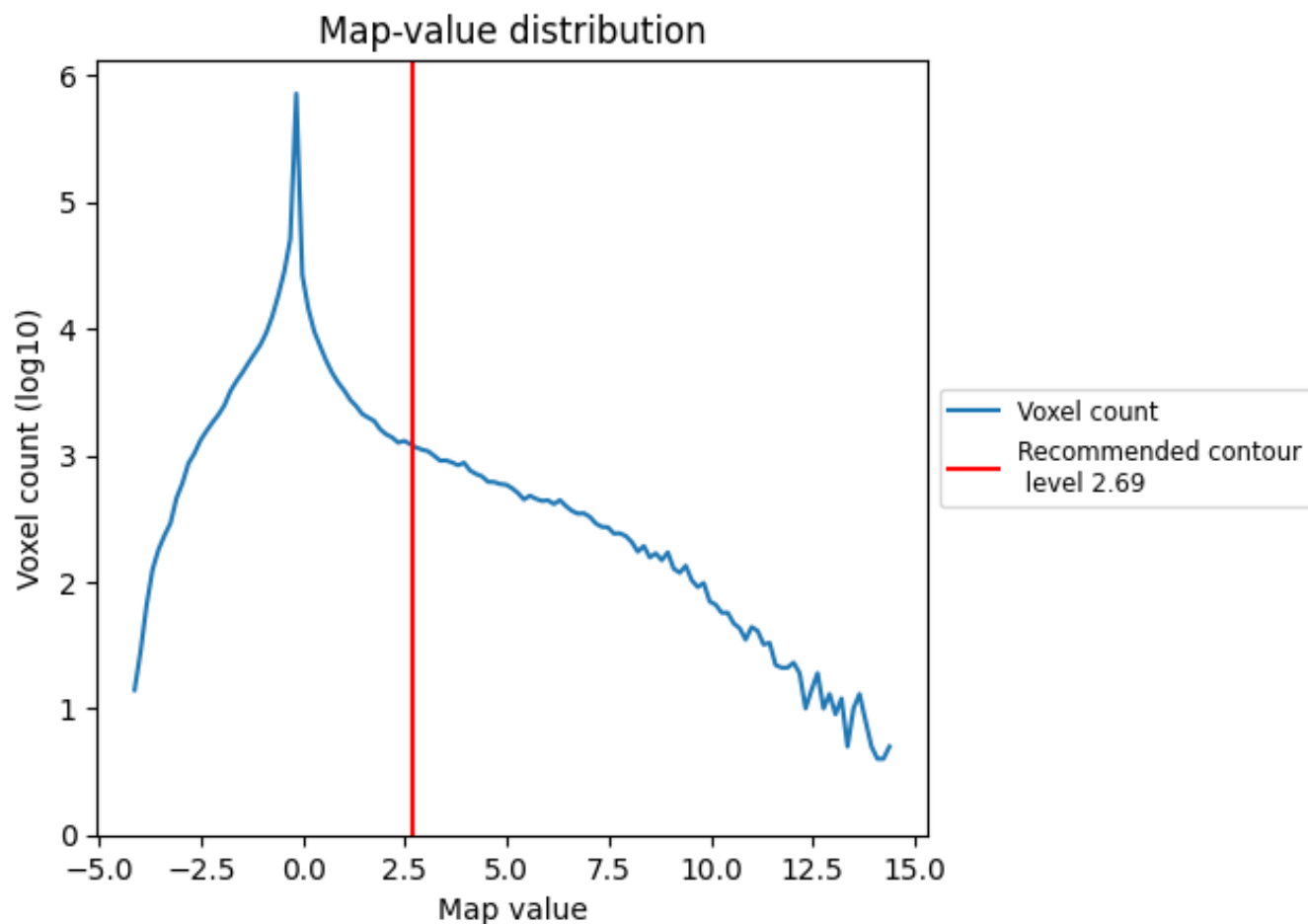
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

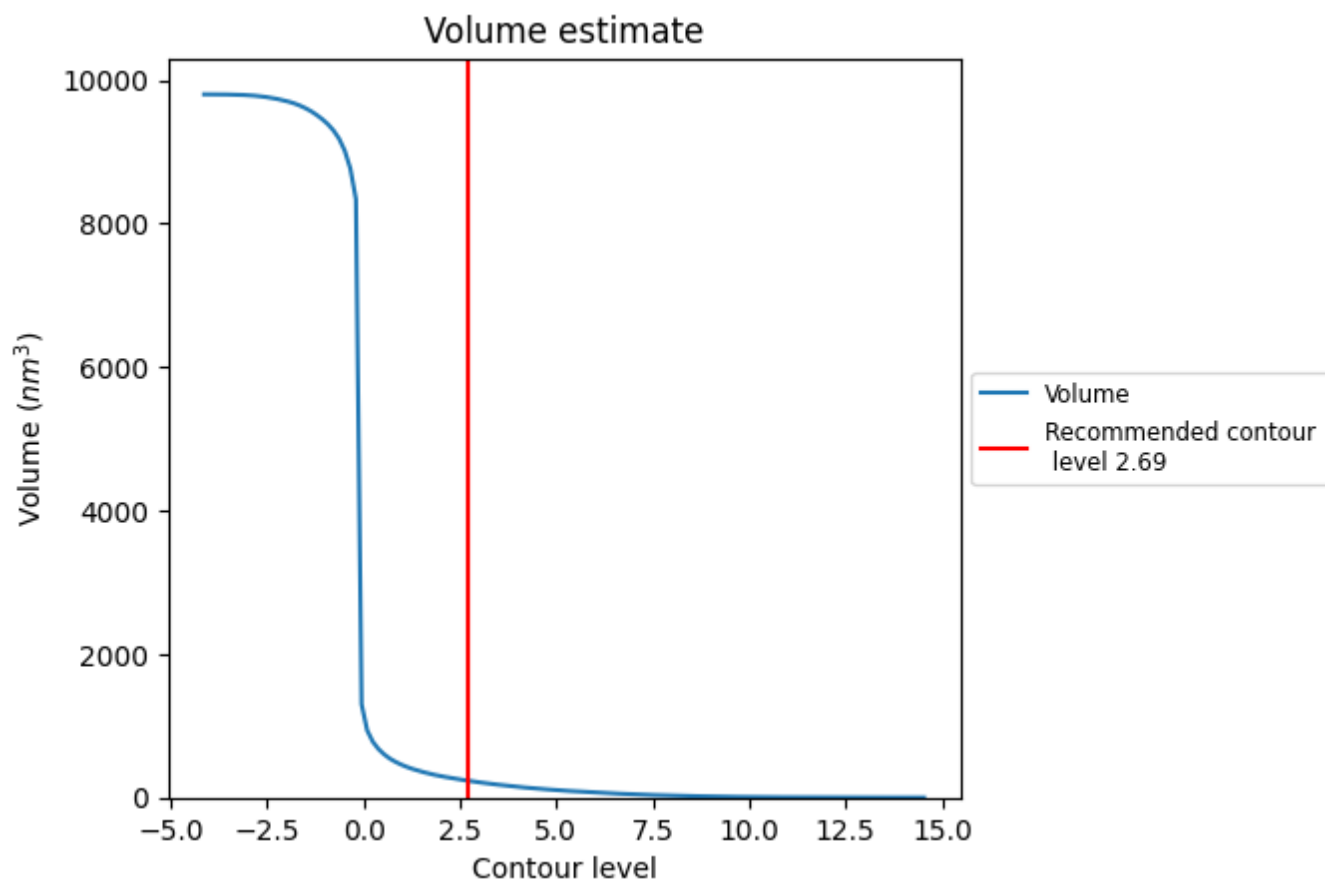
This section contains the results of statistical analysis of the map.

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



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

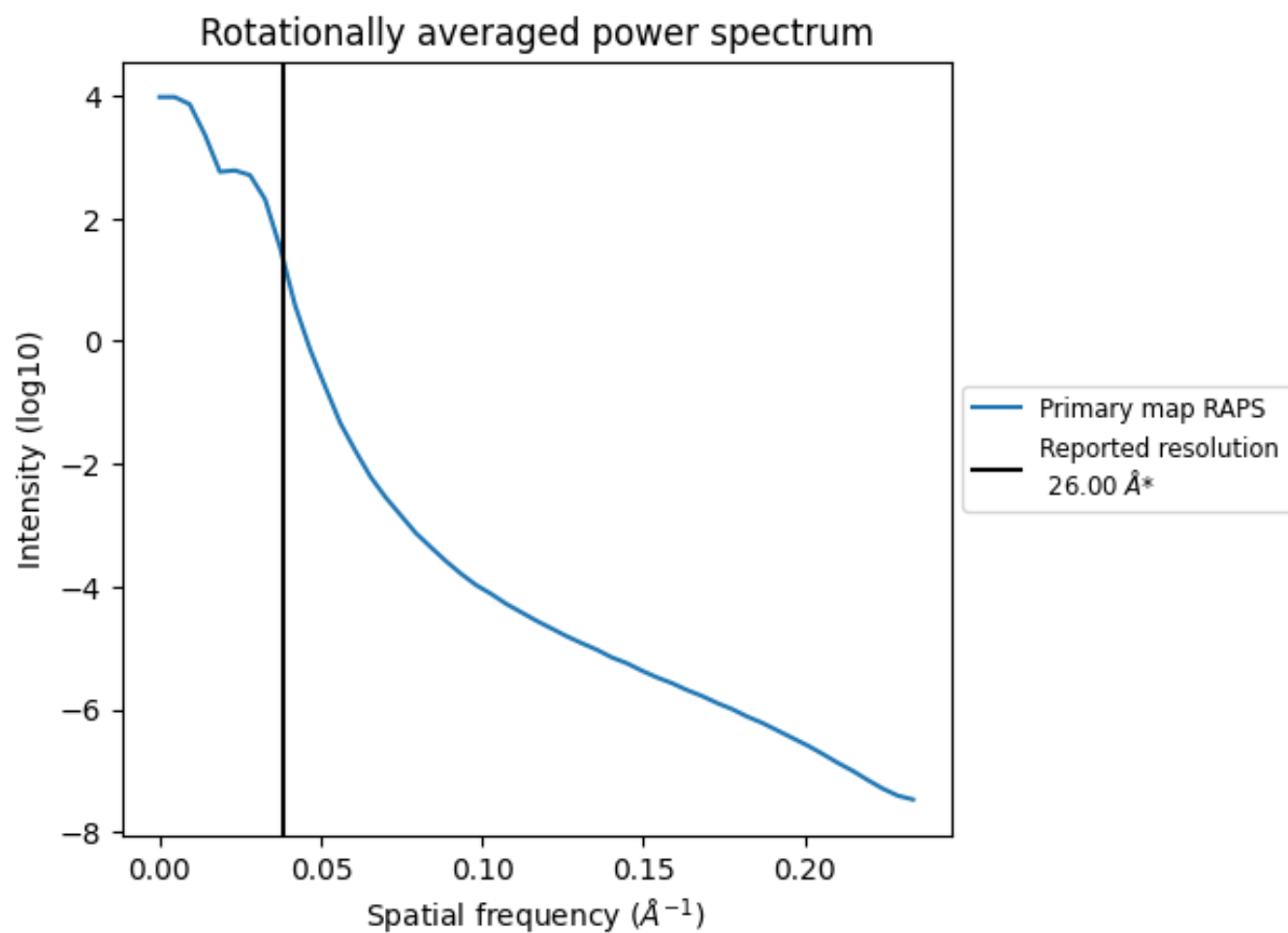
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm<sup>3</sup>; this corresponds to an approximate mass of 214 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 0.038 Å<sup>-1</sup>

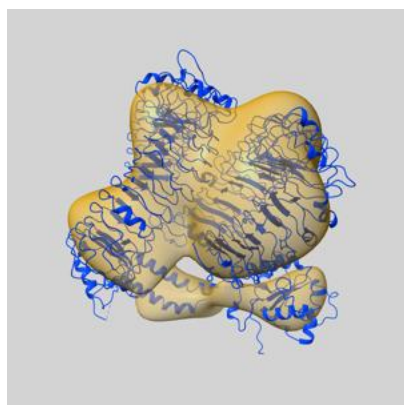
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

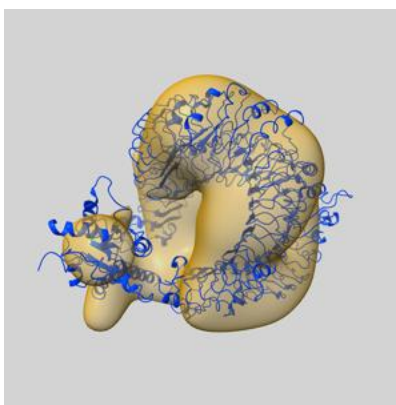
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5287 and PDB model 3J0A. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

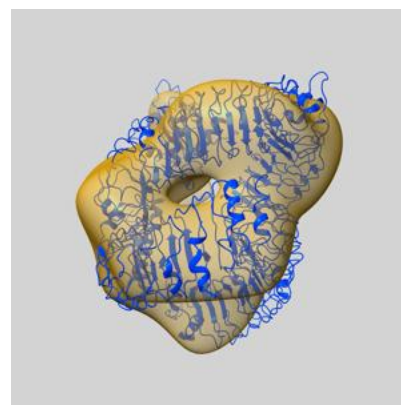
### 9.1 Map-model overlay [i](#)



X



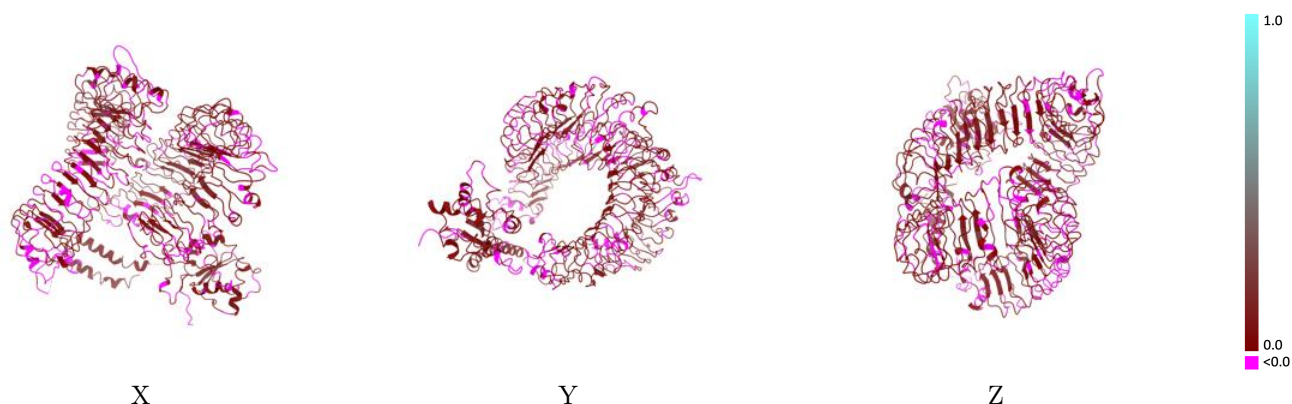
Y



Z

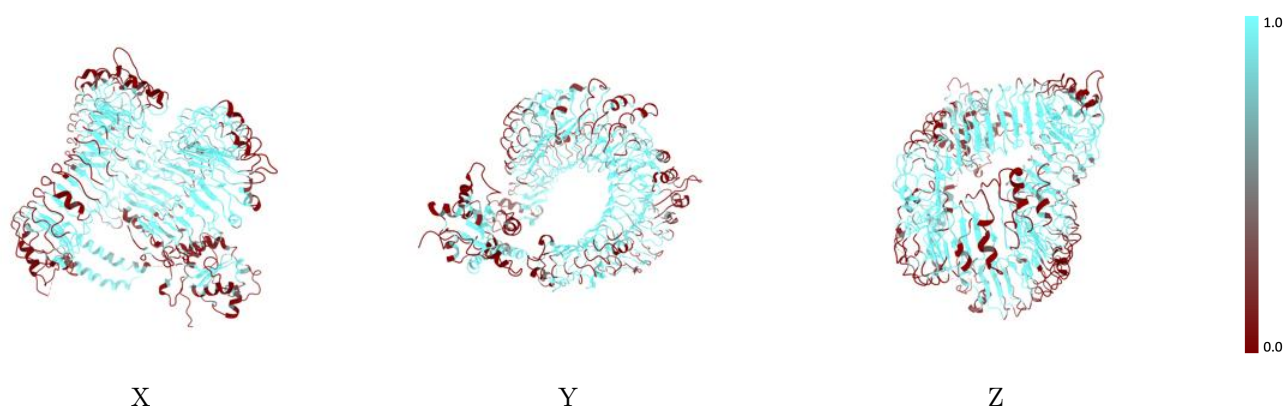
The images above show the 3D surface view of the map at the recommended contour level 2.69 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

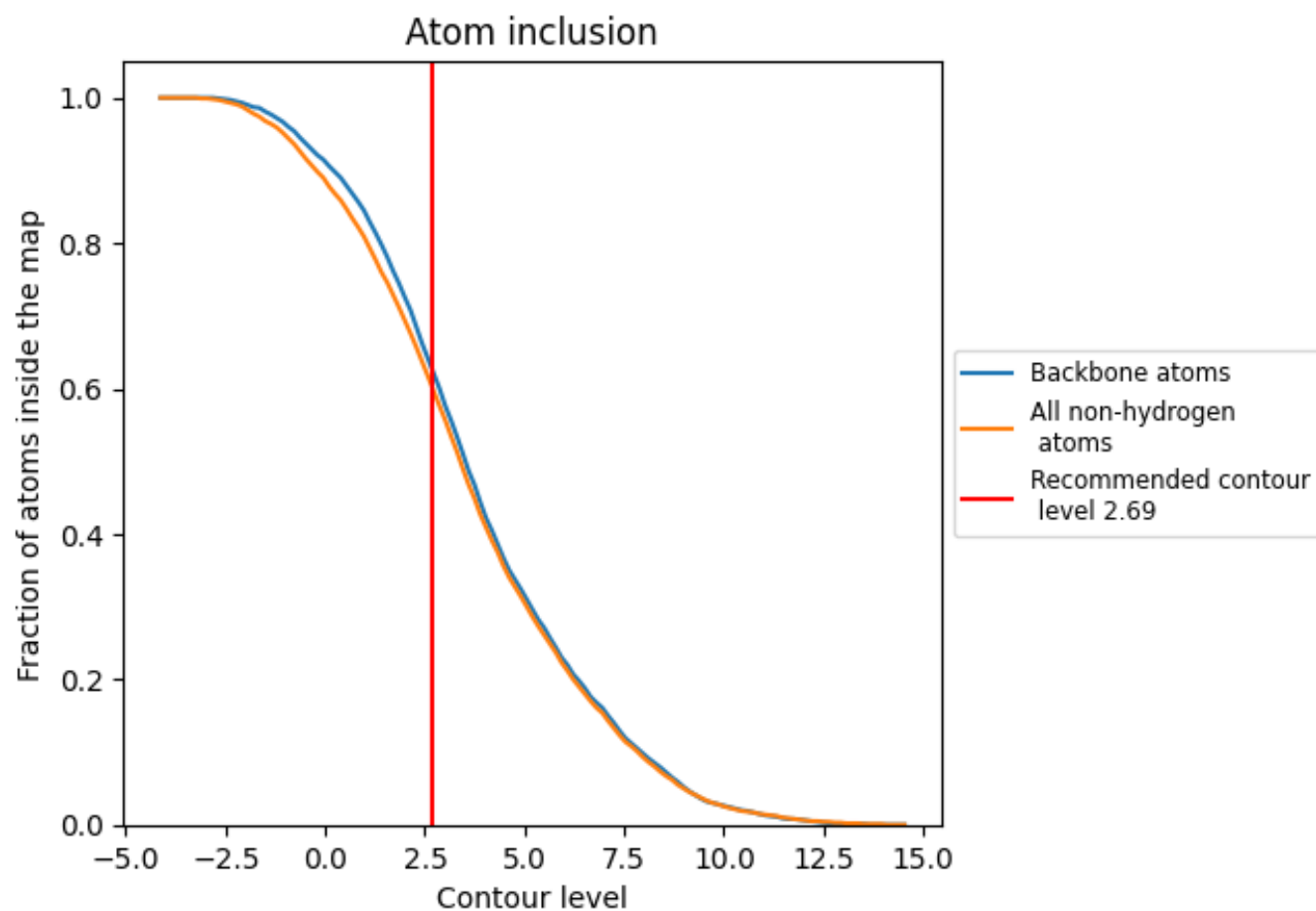
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (2.69).





































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 62% of all backbone atoms, 60% 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 (2.69) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6010	 0.0350
A	 0.6430	 0.0430
B	 0.5750	 0.0280
C	 0.0000	 -0.0090
D	 0.0000	 -0.0270
E	 0.0000	 -0.0710
F	 1.0000	 -0.0210
G	 0.0000	 -0.0420
H	 0.0000	 -0.1140
I	 0.0000	 -0.0730
J	 0.7920	 0.0320
K	 0.0000	 0.1120
L	 0.0000	 -0.1250
M	 1.0000	 0.0360
N	 0.0000	 -0.0070
O	 0.0000	 -0.1860
P	 0.0000	 -0.0140

