



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 04:43 PM EDT

PDB ID : 9Z67 / pdb\_00009z67  
EMDB ID : EMD-73838  
Title : Cryo-EM structure of human Wntless-Wnt5a 2:2 complex - Composite map  
Authors : Ge, Y.; de Almeida Magalhaes, T.; Wu, H.; Yadav, G.P.; Wang, Z.; Salic, A.;  
Jiang, J.; Huang, P.  
Deposited on : 2025-11-13  
Resolution : 3.32 Å(reported)

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:

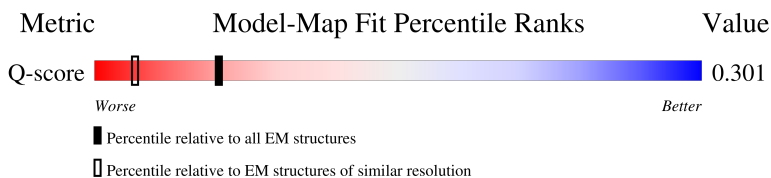
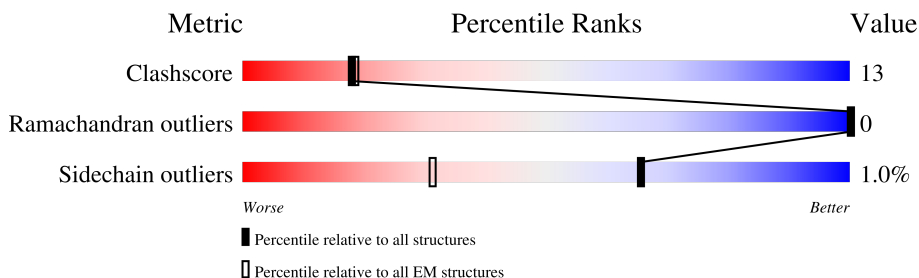
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.32 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.



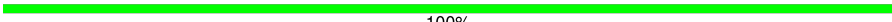
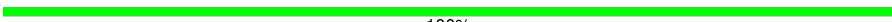
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14518 ( 2.82 - 3.82 )

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	345	<p>33% (Poor fit), 69% (0 outliers), 23% (1 outlier), 7% (2 outliers), 7% (3+ outliers)</p>
1	C	345	<p>35% (Poor fit), 71% (0 outliers), 22% (1 outlier), 7% (2 outliers), 7% (3+ outliers)</p>
2	B	575	<p>20% (Poor fit), 68% (0 outliers), 18% (1 outlier), 14% (2 outliers), 14% (3+ outliers)</p>
2	D	575	<p>22% (Poor fit), 70% (0 outliers), 16% (1 outlier), 14% (2 outliers), 14% (3+ outliers)</p>

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 100%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13366 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 Protein Wnt-5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	321	2521	1551	468	470	32	0	0
1	C	321	2521	1551	468	470	32	0	0

- Molecule 2 is a protein called Protein wntless homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	494	4020	2665	654	664	37	0	0
2	D	494	4020	2665	654	664	37	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	ALA	-	expression tag	UNP Q5T9L3
B	543	ALA	-	expression tag	UNP Q5T9L3
B	544	ALA	-	expression tag	UNP Q5T9L3
B	545	LEU	-	expression tag	UNP Q5T9L3
B	546	GLU	-	expression tag	UNP Q5T9L3
B	547	VAL	-	expression tag	UNP Q5T9L3
B	548	LEU	-	expression tag	UNP Q5T9L3
B	549	PHE	-	expression tag	UNP Q5T9L3
B	550	GLN	-	expression tag	UNP Q5T9L3
B	551	GLY	-	expression tag	UNP Q5T9L3
B	552	PRO	-	expression tag	UNP Q5T9L3
B	553	GLY	-	expression tag	UNP Q5T9L3
B	554	ALA	-	expression tag	UNP Q5T9L3
B	555	ALA	-	expression tag	UNP Q5T9L3
B	556	GLU	-	expression tag	UNP Q5T9L3
B	557	ASP	-	expression tag	UNP Q5T9L3
B	558	GLN	-	expression tag	UNP Q5T9L3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	559	VAL	-	expression tag	UNP Q5T9L3
B	560	ASP	-	expression tag	UNP Q5T9L3
B	561	PRO	-	expression tag	UNP Q5T9L3
B	562	ARG	-	expression tag	UNP Q5T9L3
B	563	LEU	-	expression tag	UNP Q5T9L3
B	564	ILE	-	expression tag	UNP Q5T9L3
B	565	ASP	-	expression tag	UNP Q5T9L3
B	566	GLY	-	expression tag	UNP Q5T9L3
B	567	LYS	-	expression tag	UNP Q5T9L3
B	568	HIS	-	expression tag	UNP Q5T9L3
B	569	HIS	-	expression tag	UNP Q5T9L3
B	570	HIS	-	expression tag	UNP Q5T9L3
B	571	HIS	-	expression tag	UNP Q5T9L3
B	572	HIS	-	expression tag	UNP Q5T9L3
B	573	HIS	-	expression tag	UNP Q5T9L3
B	574	HIS	-	expression tag	UNP Q5T9L3
B	575	HIS	-	expression tag	UNP Q5T9L3
D	542	ALA	-	expression tag	UNP Q5T9L3
D	543	ALA	-	expression tag	UNP Q5T9L3
D	544	ALA	-	expression tag	UNP Q5T9L3
D	545	LEU	-	expression tag	UNP Q5T9L3
D	546	GLU	-	expression tag	UNP Q5T9L3
D	547	VAL	-	expression tag	UNP Q5T9L3
D	548	LEU	-	expression tag	UNP Q5T9L3
D	549	PHE	-	expression tag	UNP Q5T9L3
D	550	GLN	-	expression tag	UNP Q5T9L3
D	551	GLY	-	expression tag	UNP Q5T9L3
D	552	PRO	-	expression tag	UNP Q5T9L3
D	553	GLY	-	expression tag	UNP Q5T9L3
D	554	ALA	-	expression tag	UNP Q5T9L3
D	555	ALA	-	expression tag	UNP Q5T9L3
D	556	GLU	-	expression tag	UNP Q5T9L3
D	557	ASP	-	expression tag	UNP Q5T9L3
D	558	GLN	-	expression tag	UNP Q5T9L3
D	559	VAL	-	expression tag	UNP Q5T9L3
D	560	ASP	-	expression tag	UNP Q5T9L3
D	561	PRO	-	expression tag	UNP Q5T9L3
D	562	ARG	-	expression tag	UNP Q5T9L3
D	563	LEU	-	expression tag	UNP Q5T9L3
D	564	ILE	-	expression tag	UNP Q5T9L3
D	565	ASP	-	expression tag	UNP Q5T9L3
D	566	GLY	-	expression tag	UNP Q5T9L3

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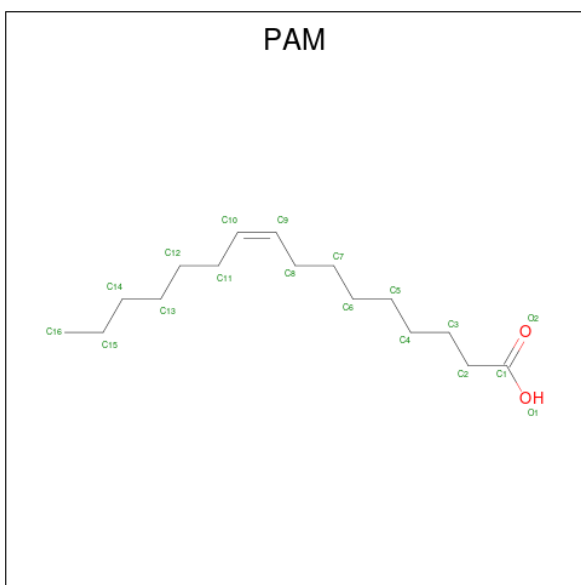
Chain	Residue	Modelled	Actual	Comment	Reference
D	567	LYS	-	expression tag	UNP Q5T9L3
D	568	HIS	-	expression tag	UNP Q5T9L3
D	569	HIS	-	expression tag	UNP Q5T9L3
D	570	HIS	-	expression tag	UNP Q5T9L3
D	571	HIS	-	expression tag	UNP Q5T9L3
D	572	HIS	-	expression tag	UNP Q5T9L3
D	573	HIS	-	expression tag	UNP Q5T9L3
D	574	HIS	-	expression tag	UNP Q5T9L3
D	575	HIS	-	expression tag	UNP Q5T9L3

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



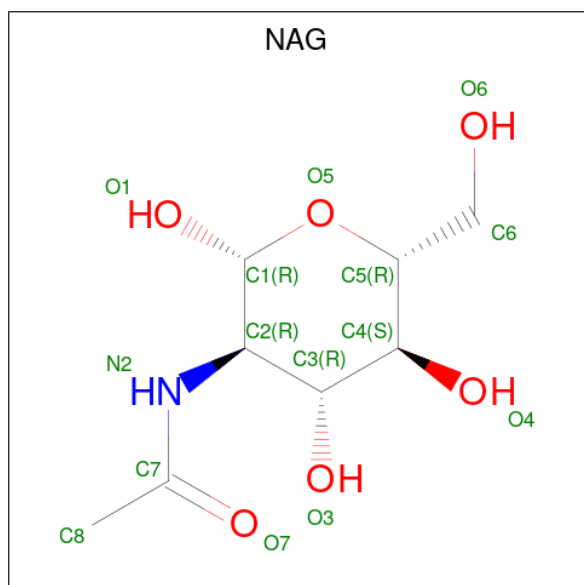
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is PALMITOLEIC ACID (CCD ID: PAM) (formula: C<sub>16</sub>H<sub>30</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



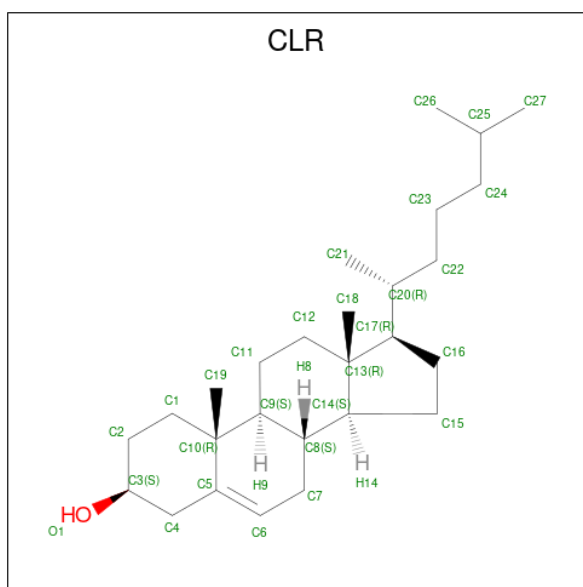
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



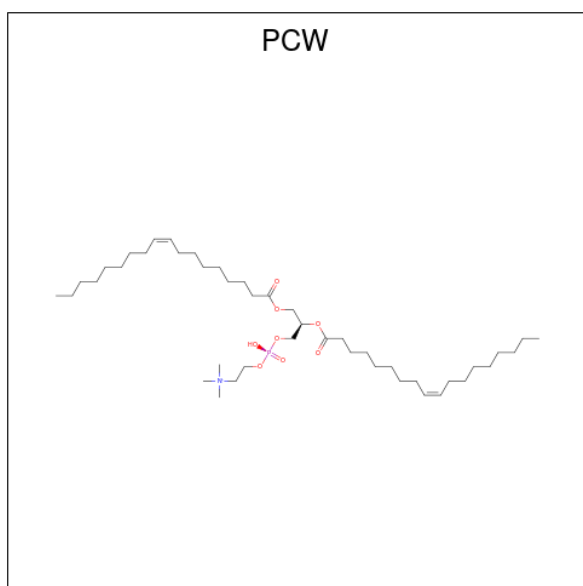
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms				AltConf	
7	B	1	Total	C	N	O	P	0
			41	31	1	8	1	

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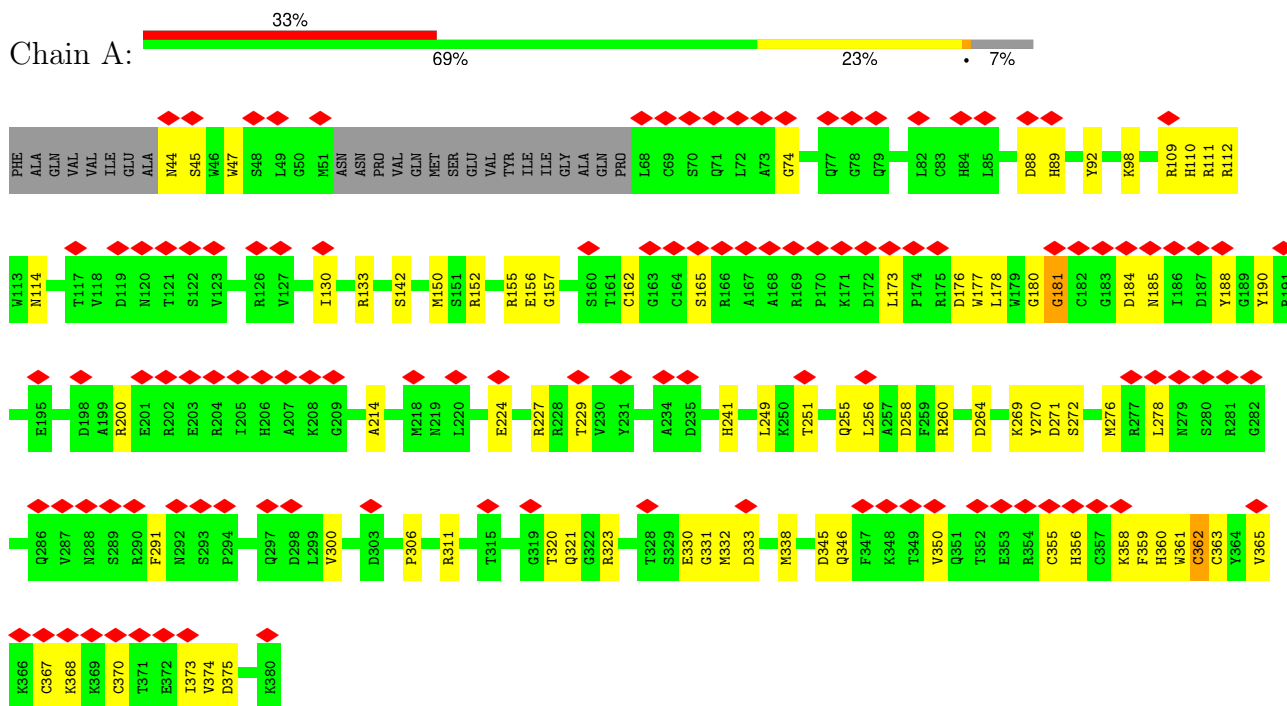
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	D	1	41	31	1	8	1	0

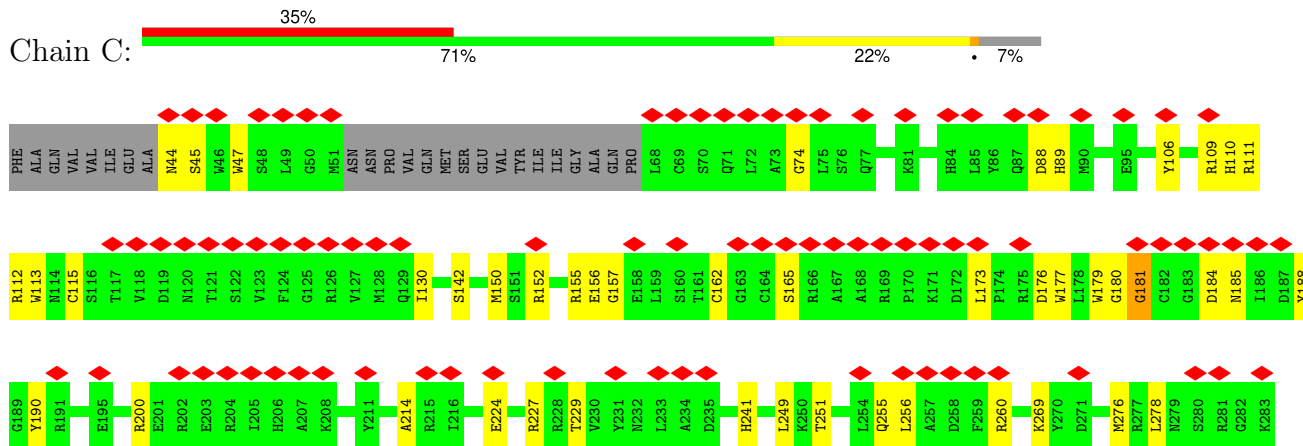
### 3 Residue-property plots

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.

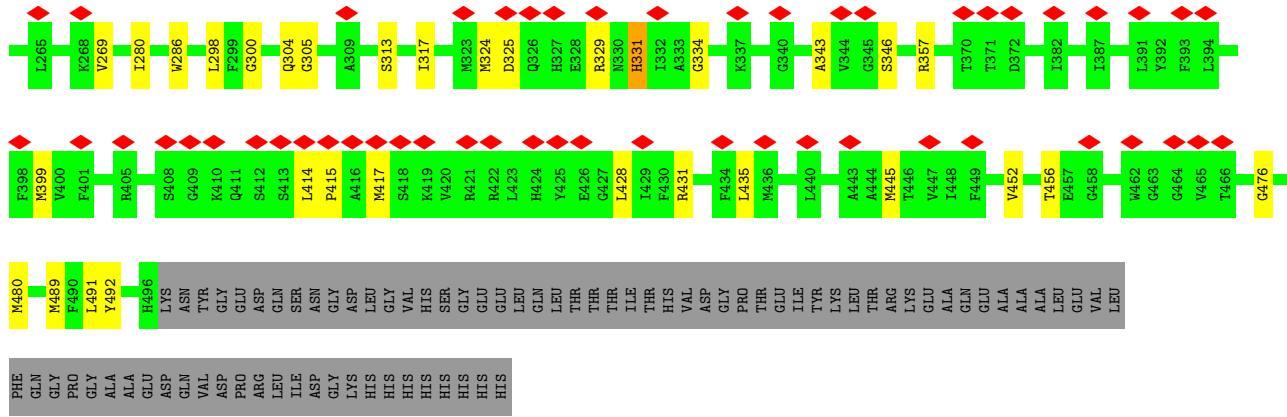
- Molecule 1: Protein Wnt-5a



- Molecule 1: Protein Wnt-5a







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

Chain E:  100%



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

Chain F:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174062	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.83	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00828	Depositor
Map size ( $\text{\AA}$ )	262.4, 262.4, 262.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	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: PCW, CLR, NAG, PAM

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	0.13	0/2569	0.34	0/3450
1	C	0.13	0/2569	0.34	0/3450
2	B	0.14	0/4144	0.33	0/5618
2	D	0.14	0/4144	0.34	0/5618
All	All	0.14	0/13426	0.34	0/18136

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
2	B	0	1
2	D	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLY	Peptide
1	A	181	GLY	Peptide
1	A	362	CYS	Peptide
2	B	59	LYS	Peptide
1	C	180	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	181	GLY	Peptide
1	C	362	CYS	Peptide
2	D	59	LYS	Peptide

## 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	2521	0	2409	157	0
1	C	2521	0	2410	100	0
2	B	4020	0	4035	159	0
2	D	4020	0	4035	107	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	17	0	29	2	0
4	C	17	0	29	4	0
5	A	28	0	26	0	0
5	C	28	0	26	0	0
6	B	28	0	46	1	0
6	D	28	0	46	1	0
7	B	41	0	52	3	0
7	D	41	0	52	3	0
All	All	13366	0	13245	354	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 13.

All (354) 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:360:HIS:NE2	2:B:205:GLU:CD	1.77	1.41
1:A:152:ARG:NH2	2:B:218:ASP:OD1	1.62	1.32
1:A:260:ARG:HG2	2:B:175:ARG:CG	1.63	1.28
1:A:109:ARG:NH2	2:B:171:GLU:HG3	1.54	1.23
1:A:155:ARG:HH21	2:B:46:MET:CE	1.55	1.18
1:C:106:TYR:OH	2:D:171:GLU:O	1.59	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:C	1:C:337:LEU:HD21	1.71	1.15
1:C:152:ARG:NH2	2:D:218:ASP:OD1	1.80	1.12
1:A:152:ARG:NH1	2:B:218:ASP:OD2	1.81	1.12
1:A:260:ARG:HG2	2:B:175:ARG:HG3	1.23	1.10
1:C:155:ARG:HH21	2:D:46:MET:HE2	1.15	1.06
1:A:255:GLN:CG	2:B:220:ARG:NH1	2.20	1.05
1:A:255:GLN:HG2	2:B:220:ARG:HH12	1.19	1.05
1:A:152:ARG:HH22	2:B:218:ASP:CG	1.66	1.03
1:A:255:GLN:HG2	2:B:220:ARG:NH1	1.73	1.02
1:A:155:ARG:HH21	2:B:46:MET:HE2	1.27	0.99
1:C:155:ARG:HH21	2:D:46:MET:CE	1.74	0.99
1:A:173:LEU:HD23	2:B:100:HIS:HB2	1.44	0.99
1:A:271:ASP:O	1:C:344:TYR:O	1.81	0.98
1:A:330:GLU:O	1:C:337:LEU:CD2	2.12	0.97
1:A:185:ASN:ND2	2:B:44:SER:HB2	1.81	0.95
1:A:360:HIS:NE2	2:B:205:GLU:CG	2.29	0.95
1:C:241:HIS:O	1:C:249:LEU:HB3	1.68	0.94
1:A:241:HIS:O	1:A:249:LEU:HB3	1.68	0.93
1:A:155:ARG:HH21	2:B:46:MET:HE1	1.32	0.93
1:A:361:TRP:HD1	2:B:210:ASN:O	1.51	0.93
1:A:330:GLU:O	1:C:337:LEU:HD21	1.68	0.92
1:A:177:TRP:CE2	2:B:101:MET:HE3	2.05	0.91
1:A:260:ARG:CG	2:B:175:ARG:CG	2.49	0.91
1:A:155:ARG:NH2	2:B:46:MET:CE	2.33	0.90
1:A:155:ARG:NH2	2:B:46:MET:HE2	1.87	0.90
1:C:260:ARG:HG2	2:D:175:ARG:CG	2.01	0.90
1:C:360:HIS:CG	2:D:203:VAL:HG11	2.06	0.90
1:A:255:GLN:CD	2:B:220:ARG:HH11	1.80	0.89
1:A:360:HIS:CD2	2:B:205:GLU:OE1	2.24	0.88
1:C:255:GLN:HG2	2:D:220:ARG:NH1	1.88	0.88
1:A:173:LEU:CD2	2:B:100:HIS:HB2	2.03	0.88
1:A:177:TRP:CG	2:B:101:MET:HG2	2.08	0.87
1:A:260:ARG:HG2	2:B:175:ARG:HG2	1.57	0.86
1:C:155:ARG:NH2	2:D:46:MET:HE2	1.90	0.86
1:C:361:TRP:CZ2	2:D:201:LEU:HB2	2.12	0.85
1:C:360:HIS:NE2	2:D:205:GLU:CD	2.36	0.84
1:A:177:TRP:CD2	2:B:101:MET:HE3	2.11	0.84
1:A:109:ARG:HH22	2:B:171:GLU:HG3	1.43	0.84
1:A:361:TRP:CD1	2:B:210:ASN:O	2.31	0.84
1:C:152:ARG:HH22	2:D:218:ASP:CG	1.86	0.83
1:A:360:HIS:NE2	2:B:205:GLU:OE1	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:HG2	2:D:175:ARG:HG3	1.59	0.82
1:C:109:ARG:NH2	2:D:171:GLU:HG3	1.94	0.82
1:A:177:TRP:CD1	2:B:101:MET:HG2	2.16	0.80
1:A:260:ARG:CG	2:B:175:ARG:HG2	2.11	0.80
1:A:255:GLN:CG	2:B:220:ARG:HH11	1.91	0.80
1:C:255:GLN:CG	2:D:220:ARG:NH1	2.46	0.79
1:C:255:GLN:HG2	2:D:220:ARG:HH12	1.48	0.78
1:C:362:CYS:HB3	2:D:87:ALA:HB2	1.63	0.78
1:A:152:ARG:NH2	2:B:218:ASP:CG	2.30	0.77
1:A:360:HIS:CD2	2:B:205:GLU:CD	2.62	0.77
1:A:271:ASP:OD1	1:C:343:GLY:HA2	1.85	0.77
1:A:291:PHE:CE1	1:C:347:PHE:HD1	2.02	0.77
1:A:360:HIS:CG	2:B:203:VAL:HG11	2.22	0.74
1:A:173:LEU:HD23	2:B:100:HIS:CB	2.18	0.74
1:A:156:GLU:HA	2:B:46:MET:O	1.87	0.73
2:D:331:HIS:CE1	2:D:334:GLY:HA3	2.24	0.73
4:A:501:PAM:H62	2:B:305:GLY:HA3	1.71	0.73
1:C:152:ARG:NH1	2:D:218:ASP:OD2	2.19	0.73
1:A:361:TRP:CD1	2:B:203:VAL:HG22	2.23	0.72
2:B:331:HIS:CE1	2:B:334:GLY:HA3	2.24	0.72
1:C:260:ARG:HG2	2:D:175:ARG:HG2	1.72	0.71
1:C:156:GLU:OE1	2:D:75:ARG:NH1	2.23	0.71
1:C:185:ASN:ND2	2:D:44:SER:HB2	2.05	0.71
1:A:367:CYS:SG	1:A:368:LYS:N	2.64	0.70
2:B:25:GLN:HE22	2:B:480:MET:HB2	1.57	0.70
2:D:25:GLN:HE22	2:D:480:MET:HB2	1.57	0.70
1:A:332:MET:SD	1:C:341:GLY:HA3	2.31	0.69
1:C:367:CYS:SG	1:C:368:LYS:N	2.64	0.69
2:D:286:TRP:HB3	6:D:601:CLR:H122	1.75	0.69
1:A:109:ARG:NH2	2:B:171:GLU:CG	2.45	0.69
2:B:286:TRP:HB3	6:B:601:CLR:H122	1.75	0.69
1:A:359:PHE:HA	1:A:365:VAL:HG11	1.76	0.68
1:C:255:GLN:CG	2:D:220:ARG:HH11	2.06	0.68
1:C:359:PHE:HA	1:C:365:VAL:HG11	1.76	0.68
1:C:360:HIS:CD2	2:D:203:VAL:HG11	2.29	0.68
1:A:330:GLU:C	1:C:337:LEU:CD2	2.57	0.68
2:D:117:ASP:OD1	2:D:220:ARG:NE	2.26	0.67
1:C:155:ARG:NH2	2:D:46:MET:CE	2.54	0.67
1:A:156:GLU:O	2:B:48:VAL:HG23	1.95	0.67
1:A:360:HIS:NE2	2:B:205:GLU:OE2	2.24	0.67
2:D:331:HIS:HE1	2:D:334:GLY:HA3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:NE2	2:B:205:GLU:HG2	2.08	0.67
1:A:361:TRP:NE1	2:B:203:VAL:CG2	2.58	0.66
1:C:111:ARG:O	1:C:323:ARG:NH1	2.28	0.66
1:A:177:TRP:CD2	2:B:101:MET:CE	2.79	0.66
2:B:331:HIS:HE1	2:B:334:GLY:HA3	1.60	0.65
2:D:445:MET:HG2	2:D:480:MET:HE1	1.79	0.65
1:A:251:THR:HB	2:B:224:ILE:HD13	1.79	0.65
2:B:115:GLN:HB2	2:B:220:ARG:HB2	1.79	0.65
1:A:264:ASP:OD2	2:B:175:ARG:NH2	2.24	0.65
2:D:115:GLN:HB2	2:D:220:ARG:HB2	1.79	0.64
1:A:152:ARG:CZ	2:B:218:ASP:OD2	2.44	0.64
2:B:445:MET:HG2	2:B:480:MET:HE1	1.79	0.63
1:A:361:TRP:CZ2	2:B:201:LEU:HB2	2.34	0.63
1:A:109:ARG:HH21	2:B:171:GLU:HG3	1.57	0.63
2:D:121:LYS:HA	2:D:173:GLU:HG2	1.80	0.63
1:C:45:SER:OG	1:C:200:ARG:NH1	2.32	0.63
1:A:111:ARG:O	1:A:323:ARG:NH1	2.28	0.63
1:C:89:HIS:HD2	1:C:150:MET:HE1	1.65	0.62
2:B:121:LYS:HA	2:B:173:GLU:HG2	1.80	0.62
4:C:501:PAM:H62	2:D:305:GLY:HA3	1.82	0.62
1:A:45:SER:OG	1:A:200:ARG:NH1	2.32	0.62
1:A:89:HIS:HD2	1:A:150:MET:HE1	1.65	0.62
2:B:117:ASP:OD1	2:B:220:ARG:NE	2.26	0.62
1:A:177:TRP:CE3	2:B:101:MET:CE	2.83	0.61
1:A:156:GLU:O	2:B:48:VAL:CG2	2.49	0.61
2:B:64:VAL:HG23	2:B:70:HIS:HA	1.83	0.61
1:C:361:TRP:CD1	2:D:203:VAL:HG22	2.34	0.61
1:A:177:TRP:CG	2:B:101:MET:CG	2.84	0.61
1:A:155:ARG:O	2:B:46:MET:N	2.28	0.60
2:B:298:LEU:HD13	2:B:357:ARG:HB2	1.84	0.60
1:A:361:TRP:HE1	2:B:203:VAL:CG2	2.15	0.60
1:A:260:ARG:CB	2:B:175:ARG:HG2	2.32	0.60
1:A:177:TRP:CZ2	2:B:101:MET:HE3	2.36	0.59
1:C:360:HIS:NE2	2:D:205:GLU:CG	2.65	0.59
2:D:64:VAL:HG23	2:D:70:HIS:HA	1.83	0.59
1:A:255:GLN:CD	2:B:220:ARG:NH1	2.50	0.59
1:A:255:GLN:NE2	2:B:115:GLN:OE1	2.33	0.58
1:A:185:ASN:ND2	2:B:44:SER:CB	2.63	0.58
1:A:190:TYR:OH	1:A:224:GLU:OE2	2.22	0.58
2:D:298:LEU:HD13	2:D:357:ARG:HB2	1.84	0.58
2:D:300:GLY:O	2:D:304:GLN:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:O	1:C:337:LEU:HD23	2.02	0.58
2:D:428:LEU:HA	2:D:431:ARG:HD3	1.86	0.58
1:A:156:GLU:OE1	2:B:75:ARG:NH1	2.37	0.58
1:C:44:ASN:HB3	1:C:74:GLY:HA2	1.86	0.57
1:C:111:ARG:HD2	1:C:332:MET:HE2	1.86	0.57
2:B:428:LEU:HA	2:B:431:ARG:HD3	1.86	0.57
1:A:177:TRP:CD2	2:B:101:MET:SD	2.98	0.57
2:D:52:ASP:OD2	2:D:200:ARG:NH2	2.37	0.57
2:B:300:GLY:O	2:B:304:GLN:HG2	2.04	0.57
1:A:260:ARG:HG2	2:B:175:ARG:CD	2.32	0.57
2:D:186:GLU:OE2	2:D:357:ARG:NH1	2.38	0.57
1:A:111:ARG:HD2	1:A:332:MET:HE2	1.86	0.57
1:A:258:ASP:HB2	2:B:176:TYR:HB2	1.85	0.57
2:B:186:GLU:OE2	2:B:357:ARG:NH1	2.37	0.57
2:B:414:LEU:HA	2:B:417:MET:HE2	1.86	0.57
1:A:44:ASN:HB3	1:A:74:GLY:HA2	1.86	0.56
1:A:185:ASN:ND2	2:B:44:SER:O	2.39	0.56
2:B:206:LYS:HD3	2:B:206:LYS:N	2.20	0.56
1:A:260:ARG:HG3	2:B:175:ARG:NE	2.21	0.56
2:D:206:LYS:HD3	2:D:206:LYS:N	2.20	0.56
1:A:155:ARG:C	2:B:46:MET:H	2.14	0.56
1:A:260:ARG:HB3	2:B:175:ARG:HG2	1.87	0.56
2:B:59:LYS:O	2:B:61:LYS:N	2.39	0.56
1:A:331:GLY:N	1:C:337:LEU:HD21	2.18	0.56
2:D:112:PHE:HB3	2:D:221:LEU:HD11	1.88	0.56
2:D:414:LEU:HA	2:D:417:MET:HE2	1.86	0.56
2:D:313:SER:O	2:D:317:ILE:HG12	2.06	0.55
2:B:112:PHE:HB3	2:B:221:LEU:HD11	1.88	0.55
1:C:190:TYR:OH	1:C:224:GLU:OE2	2.21	0.55
2:B:313:SER:O	2:B:317:ILE:HG12	2.07	0.55
1:C:255:GLN:CD	2:D:220:ARG:HH11	2.14	0.55
1:C:361:TRP:CD1	2:D:203:VAL:CG2	2.90	0.55
2:D:59:LYS:O	2:D:61:LYS:N	2.39	0.55
1:A:361:TRP:NE1	2:B:203:VAL:HG22	2.20	0.55
1:A:109:ARG:HH22	2:B:171:GLU:CG	2.16	0.55
1:C:157:GLY:HA3	2:D:66:TRP:CD1	2.41	0.55
1:A:130:ILE:HD12	1:A:306:PRO:HG3	1.89	0.55
1:A:176:ASP:O	1:A:181:GLY:HA2	2.07	0.55
4:C:501:PAM:H111	2:D:346:SER:HB3	1.89	0.55
1:C:130:ILE:HD12	1:C:306:PRO:HG3	1.89	0.54
1:C:110:HIS:HB3	1:C:333:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:HB3	1:A:333:ASP:HB3	1.89	0.54
1:C:176:ASP:O	1:C:181:GLY:HA2	2.07	0.54
1:A:255:GLN:HG3	2:B:220:ARG:NH1	2.21	0.54
2:B:269:VAL:HG21	2:B:317:ILE:HG21	1.90	0.54
1:A:152:ARG:CZ	2:B:218:ASP:CG	2.80	0.54
1:A:331:GLY:HA2	1:C:337:LEU:CD2	2.38	0.54
1:C:156:GLU:HA	2:D:46:MET:O	2.08	0.54
1:A:361:TRP:CD1	2:B:203:VAL:CG2	2.89	0.53
1:C:173:LEU:CD2	2:D:100:HIS:HB2	2.38	0.53
1:C:156:GLU:HG3	2:D:46:MET:HB3	1.89	0.53
1:C:355:CYS:SG	1:C:356:HIS:ND1	2.81	0.53
2:D:269:VAL:HG21	2:D:317:ILE:HG21	1.90	0.53
1:A:291:PHE:CE1	1:C:347:PHE:CD1	2.90	0.53
4:C:501:PAM:C6	2:D:305:GLY:HA3	2.38	0.53
1:A:178:LEU:HD11	2:B:102:GLU:O	2.09	0.53
1:C:109:ARG:HH22	2:D:171:GLU:HG3	1.70	0.53
1:A:311:ARG:HH22	1:A:321:GLN:NE2	2.07	0.52
2:B:329:ARG:HH22	2:B:399:MET:HE1	1.74	0.52
1:C:229:THR:OG1	1:C:269:LYS:NZ	2.38	0.52
1:A:355:CYS:SG	1:A:356:HIS:ND1	2.81	0.52
2:B:52:ASP:OD2	2:B:200:ARG:NH2	2.37	0.52
1:A:152:ARG:NH2	2:B:218:ASP:OD2	2.42	0.52
1:A:362:CYS:HB3	2:B:87:ALA:HB2	1.90	0.52
1:C:311:ARG:HH22	1:C:321:GLN:NE2	2.07	0.52
1:A:229:THR:OG1	1:A:269:LYS:NZ	2.38	0.52
1:A:361:TRP:HB3	2:B:213:ILE:HG12	1.92	0.52
2:B:207:LYS:HB2	2:B:209:ILE:HD12	1.92	0.52
2:D:329:ARG:HH22	2:D:399:MET:HE1	1.74	0.52
2:B:96:ILE:HB	2:B:195:TYR:HB2	1.92	0.51
2:B:59:LYS:O	2:B:61:LYS:HB2	2.09	0.51
1:A:331:GLY:HA2	1:C:337:LEU:HD23	1.93	0.51
1:C:177:TRP:CG	2:D:101:MET:HG2	2.45	0.51
2:D:96:ILE:HB	2:D:195:TYR:HB2	1.93	0.51
1:A:255:GLN:NE2	2:B:220:ARG:HH11	2.08	0.50
2:D:59:LYS:O	2:D:61:LYS:HB2	2.09	0.50
1:A:361:TRP:HE1	2:B:203:VAL:HG23	1.76	0.50
4:A:501:PAM:C6	2:B:305:GLY:HA3	2.40	0.50
1:C:345:ASP:OD1	1:C:346:GLN:N	2.44	0.50
2:D:207:LYS:HB2	2:D:209:ILE:HD12	1.92	0.50
1:A:272:SER:HA	1:C:344:TYR:O	2.12	0.50
1:A:345:ASP:OD1	1:A:346:GLN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:ND1	2:B:203:VAL:HG11	2.26	0.50
1:A:177:TRP:CG	2:B:101:MET:SD	3.05	0.49
1:A:177:TRP:CE3	2:B:101:MET:HE3	2.42	0.49
1:A:92:TYR:CE1	2:B:75:ARG:CZ	2.96	0.49
1:A:249:LEU:HD21	2:B:40:THR:HG21	1.95	0.49
1:C:241:HIS:O	1:C:249:LEU:CB	2.52	0.49
1:A:155:ARG:CB	2:B:46:MET:HB2	2.42	0.49
1:C:260:ARG:CG	2:D:175:ARG:HG2	2.39	0.49
1:A:255:GLN:NE2	2:B:220:ARG:NH1	2.61	0.49
1:C:251:THR:HB	2:D:224:ILE:HD13	1.95	0.49
1:A:214:ALA:HB2	1:A:278:LEU:HG	1.95	0.48
1:C:173:LEU:HD23	2:D:100:HIS:HB2	1.95	0.48
1:A:173:LEU:HD11	2:B:101:MET:SD	2.53	0.48
2:B:254:ARG:O	2:B:258:MET:HG3	2.14	0.48
1:C:214:ALA:HB2	1:C:278:LEU:HG	1.95	0.48
2:D:254:ARG:O	2:D:258:MET:HG3	2.14	0.48
1:A:155:ARG:HB2	2:B:46:MET:HB2	1.95	0.48
1:A:249:LEU:HD21	2:B:40:THR:CG2	2.44	0.48
2:D:25:GLN:NE2	2:D:480:MET:HB2	2.26	0.48
1:A:271:ASP:O	1:C:344:TYR:N	2.42	0.48
1:A:276:MET:HG3	1:A:300:VAL:HB	1.96	0.48
2:B:255:ARG:HD3	2:B:258:MET:HE3	1.96	0.47
2:B:435:LEU:HB2	2:B:492:TYR:OH	2.14	0.47
2:D:255:ARG:HD3	2:D:258:MET:HE3	1.96	0.47
1:C:173:LEU:HD11	2:D:101:MET:SD	2.55	0.47
1:C:276:MET:HG3	1:C:300:VAL:HB	1.96	0.47
1:A:355:CYS:HB2	1:A:370:CYS:HB2	1.87	0.47
1:A:362:CYS:C	1:A:363:CYS:SG	2.98	0.47
2:B:75:ARG:HD2	2:B:75:ARG:HA	1.73	0.46
1:C:362:CYS:C	1:C:363:CYS:SG	2.98	0.46
1:A:88:ASP:OD1	1:A:88:ASP:N	2.46	0.46
4:C:501:PAM:H151	2:D:343:ALA:HA	1.97	0.46
1:A:155:ARG:CZ	2:B:46:MET:HE2	2.45	0.46
1:C:88:ASP:OD1	1:C:88:ASP:N	2.45	0.46
2:D:435:LEU:HB2	2:D:492:TYR:OH	2.14	0.46
2:D:280:ILE:HD11	2:D:304:GLN:HA	1.98	0.46
1:A:251:THR:HG21	2:B:224:ILE:HG12	1.97	0.46
1:C:177:TRP:CE2	2:D:101:MET:HE3	2.50	0.46
2:D:81:ILE:HB	2:D:82:PRO:HD3	1.98	0.46
2:B:121:LYS:HG3	2:B:124:ASN:H	1.80	0.46
1:C:152:ARG:NH2	2:D:218:ASP:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:TRP:HD1	2:D:210:ASN:O	1.99	0.46
1:A:47:TRP:HE1	1:A:142:SER:HB3	1.81	0.45
2:B:280:ILE:HD11	2:B:304:GLN:HA	1.98	0.45
2:D:75:ARG:HD2	2:D:75:ARG:HA	1.73	0.45
1:A:133:ARG:HH12	1:C:343:GLY:HA3	1.81	0.45
2:B:62:TRP:CH2	2:B:139:ALA:HB2	2.51	0.45
2:D:62:TRP:CH2	2:D:139:ALA:HB2	2.51	0.45
2:B:6:ILE:HB	2:B:491:LEU:HB3	1.99	0.45
2:B:29:PHE:CE1	2:B:476:GLY:HA3	2.52	0.45
1:C:47:TRP:HE1	1:C:142:SER:HB3	1.81	0.45
1:C:360:HIS:NE2	2:D:205:GLU:HG2	2.30	0.45
2:D:6:ILE:HB	2:D:491:LEU:HB3	1.99	0.45
1:A:177:TRP:CH2	2:B:43:VAL:HG21	2.52	0.45
2:B:78:GLU:OE2	2:B:217:LYS:HE3	2.16	0.45
1:C:350:VAL:HG22	1:C:373:ILE:HG12	1.99	0.45
2:D:78:GLU:OE2	2:D:217:LYS:HE3	2.16	0.45
2:D:121:LYS:HG3	2:D:124:ASN:H	1.81	0.45
1:A:178:LEU:HA	2:B:107:PHE:HZ	1.82	0.45
2:D:80:ALA:HB1	2:D:85:ILE:HB	1.99	0.45
1:A:350:VAL:HG22	1:A:373:ILE:HG12	1.99	0.45
2:B:81:ILE:HB	2:B:82:PRO:HD3	1.98	0.44
2:B:428:LEU:O	2:B:431:ARG:HG2	2.17	0.44
1:C:112:ARG:HG2	1:C:320:THR:HG21	1.99	0.44
7:D:602:PCW:H41	7:D:602:PCW:H63	1.68	0.44
2:D:29:PHE:CE1	2:D:476:GLY:HA3	2.52	0.44
2:D:249:MET:HG2	2:D:489:MET:HE1	2.00	0.44
2:D:428:LEU:O	2:D:431:ARG:HG2	2.17	0.44
1:C:358:LYS:HB3	2:D:205:GLU:OE1	2.18	0.44
1:A:157:GLY:HA3	2:B:66:TRP:CD1	2.53	0.44
2:B:80:ALA:HB1	2:B:85:ILE:HB	1.99	0.44
1:C:179:TRP:NE1	2:D:37:PRO:HB3	2.32	0.44
2:B:414:LEU:HB2	2:B:415:PRO:HD3	2.00	0.44
1:A:177:TRP:CB	2:B:101:MET:HG2	2.46	0.44
1:C:185:ASN:ND2	2:D:44:SER:O	2.50	0.44
2:D:230:PHE:HE1	7:D:602:PCW:H61	1.83	0.44
1:C:89:HIS:CD2	1:C:150:MET:HE1	2.50	0.44
1:C:152:ARG:HH12	2:D:218:ASP:CG	2.19	0.44
2:B:25:GLN:NE2	2:B:480:MET:HB2	2.26	0.44
2:D:414:LEU:HB2	2:D:415:PRO:HD3	2.00	0.43
1:A:251:THR:CG2	2:B:42:ALA:HB2	2.48	0.43
1:A:375:ASP:OD1	1:A:375:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ARG:HH21	2:D:46:MET:HE1	1.72	0.43
2:B:249:MET:HG2	2:B:489:MET:HE1	2.00	0.43
7:B:602:PCW:H63	7:B:602:PCW:H41	1.68	0.43
1:A:112:ARG:HG2	1:A:320:THR:HG21	1.99	0.43
1:C:177:TRP:CD1	2:D:101:MET:HG2	2.53	0.43
1:A:152:ARG:NH1	2:B:218:ASP:CG	2.67	0.43
1:A:260:ARG:CG	2:B:175:ARG:NE	2.81	0.43
1:C:109:ARG:HH21	2:D:171:GLU:HG3	1.80	0.43
2:D:245:ILE:HA	2:D:248:ILE:HG22	2.01	0.43
1:C:162:CYS:HB2	1:C:188:TYR:CD1	2.54	0.43
1:A:162:CYS:HB2	1:A:188:TYR:CD1	2.54	0.42
2:B:62:TRP:HZ2	2:B:150:GLU:HB2	1.84	0.42
2:B:431:ARG:O	2:B:492:TYR:OH	2.37	0.42
2:B:230:PHE:HE1	7:B:602:PCW:H61	1.83	0.42
2:D:452:VAL:O	2:D:456:THR:HG23	2.19	0.42
2:B:96:ILE:HD13	2:B:96:ILE:HA	1.78	0.42
2:B:245:ILE:HA	2:B:248:ILE:HG22	2.01	0.42
2:B:242:THR:HB	2:B:243:PRO:HD3	2.01	0.42
2:D:431:ARG:O	2:D:492:TYR:OH	2.37	0.42
2:B:452:VAL:O	2:B:456:THR:HG23	2.19	0.42
2:D:121:LYS:HB2	2:D:121:LYS:HE2	1.61	0.42
1:A:155:ARG:NH2	2:B:46:MET:HE1	2.13	0.42
2:D:62:TRP:HZ2	2:D:150:GLU:HB2	1.84	0.42
1:A:165:SER:HB2	1:A:184:ASP:HB2	2.01	0.41
1:C:360:HIS:CD2	2:D:205:GLU:CD	2.98	0.41
2:D:325:ASP:OD1	2:D:325:ASP:N	2.53	0.41
1:A:177:TRP:CE3	2:B:101:MET:SD	3.13	0.41
1:C:361:TRP:HD1	2:D:203:VAL:HG22	1.81	0.41
1:C:165:SER:HB2	1:C:184:ASP:HB2	2.01	0.41
1:A:155:ARG:HB3	2:B:46:MET:N	2.35	0.41
2:B:96:ILE:HD12	2:B:112:PHE:CE1	2.56	0.41
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.89	0.41
2:D:96:ILE:HD12	2:D:112:PHE:CE1	2.56	0.41
1:A:360:HIS:HD2	2:B:205:GLU:OE1	1.96	0.41
1:A:114:ASN:OD1	1:A:114:ASN:N	2.53	0.41
1:A:173:LEU:HD21	2:B:100:HIS:HB2	1.93	0.41
1:C:361:TRP:CE3	1:C:362:CYS:HB2	2.56	0.41
1:A:98:LYS:HB3	1:A:98:LYS:HE3	1.84	0.41
2:B:116:LEU:HD12	2:B:160:LEU:HD21	2.03	0.41
2:D:234:TRP:HZ2	7:D:602:PCW:H31	1.86	0.41
1:A:190:TYR:CE2	1:A:227:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:TYR:CE2	1:C:227:ARG:HB3	2.56	0.41
1:A:338:MET:HE2	1:A:338:MET:HB2	1.99	0.41
1:A:358:LYS:HD2	1:A:358:LYS:HA	1.96	0.41
2:B:187:ILE:HG22	2:B:189:SER:H	1.86	0.41
2:B:324:MET:HE3	2:B:324:MET:HB3	1.95	0.41
2:D:242:THR:HB	2:D:243:PRO:HD3	2.02	0.41
1:C:113:TRP:CZ2	1:C:115:CYS:HA	2.56	0.41
1:C:355:CYS:HB2	1:C:370:CYS:HB2	1.87	0.41
1:C:358:LYS:HD2	1:C:358:LYS:HA	1.97	0.41
1:A:133:ARG:NH1	1:C:380:LYS:HD3	2.36	0.40
1:A:271:ASP:HB3	1:C:344:TYR:CD2	2.56	0.40
1:A:361:TRP:CE3	1:A:362:CYS:HB2	2.56	0.40
2:D:187:ILE:HG22	2:D:189:SER:H	1.86	0.40
1:A:89:HIS:CD2	1:A:150:MET:HE1	2.50	0.40
1:A:241:HIS:O	1:A:249:LEU:CB	2.52	0.40
2:D:435:LEU:HD12	2:D:435:LEU:HA	1.84	0.40
1:A:133:ARG:HB3	1:A:270:TYR:CE2	2.56	0.40
2:B:234:TRP:HZ2	7:B:602:PCW:H31	1.86	0.40
2:B:422:ARG:O	2:B:426:GLU:HG3	2.22	0.40
2:D:324:MET:HE3	2:D:324:MET:HB3	1.95	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	317/345 (92%)	301 (95%)	16 (5%)	0	100	100
1	C	317/345 (92%)	301 (95%)	16 (5%)	0	100	100
2	B	492/575 (86%)	479 (97%)	13 (3%)	0	100	100
2	D	492/575 (86%)	479 (97%)	13 (3%)	0	100	100
All	All	1618/1840 (88%)	1560 (96%)	58 (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	A	271/291 (93%)	269 (99%)	2 (1%)	76	79
1	C	271/291 (93%)	269 (99%)	2 (1%)	76	79
2	B	433/499 (87%)	427 (99%)	6 (1%)	59	72
2	D	433/499 (87%)	429 (99%)	4 (1%)	70	77
All	All	1408/1580 (89%)	1394 (99%)	14 (1%)	65	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LEU
1	A	374	VAL
2	B	84	GLU
2	B	101	MET
2	B	122	LEU
2	B	132	VAL
2	B	316	ILE
2	B	331	HIS
1	C	256	LEU
1	C	284	LEU
2	D	84	GLU
2	D	101	MET
2	D	132	VAL
2	D	331	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	C	376	GLN
2	D	8	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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	1	1,3	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

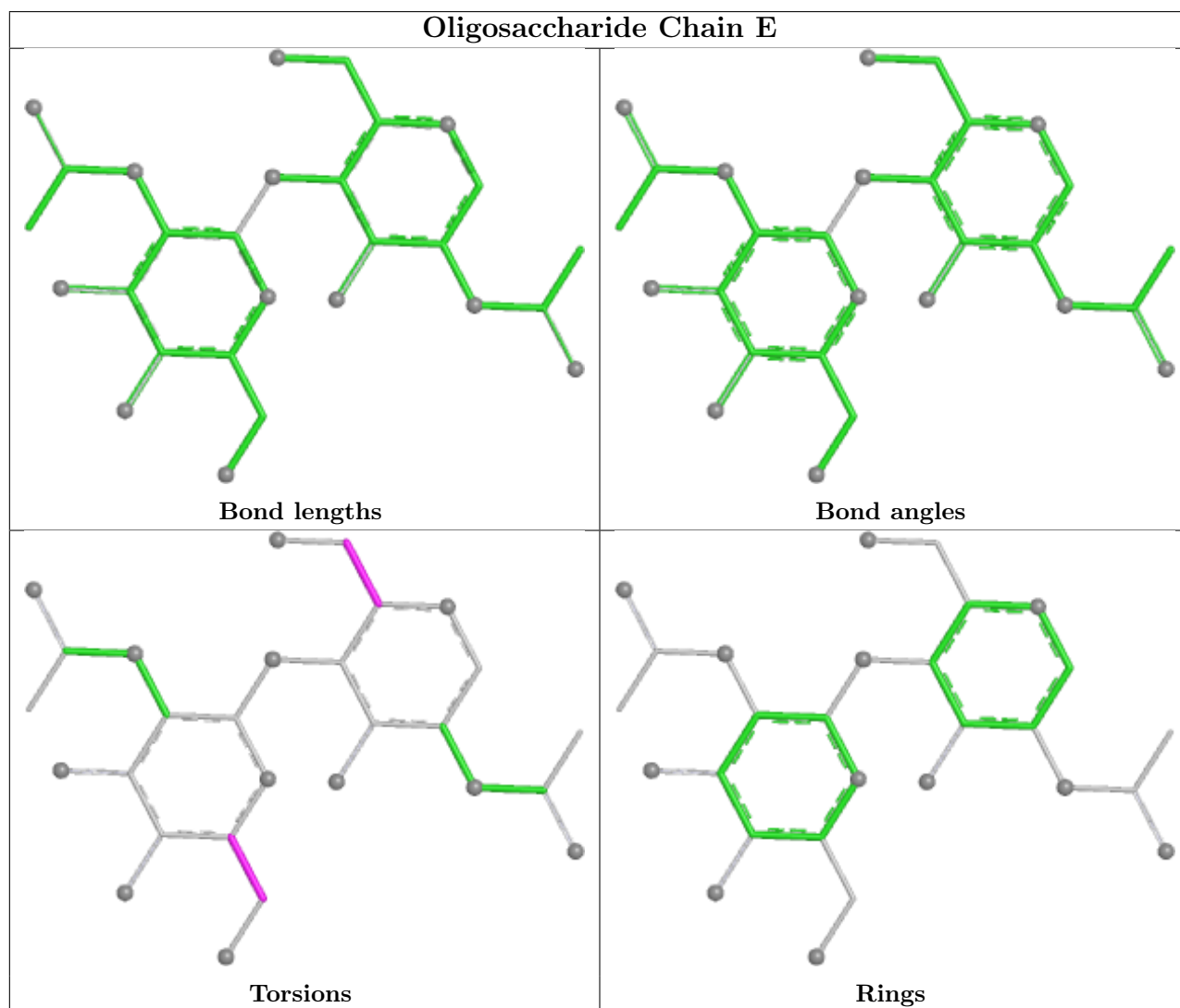
All (8) torsion outliers are listed below:

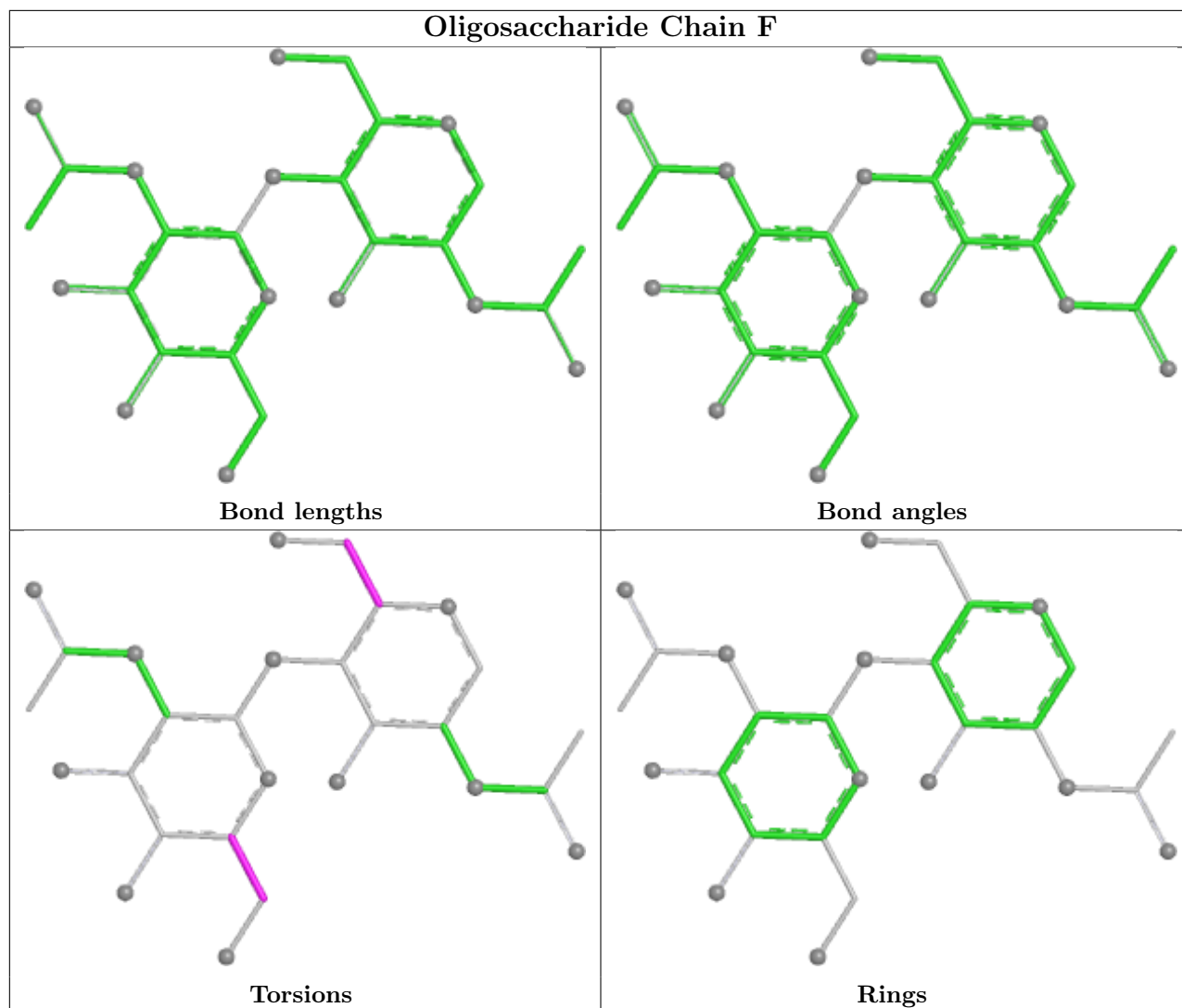
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

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](#)

10 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	$\# Z  > 2$
5	NAG	A	503	1	14,14,15	0.23	0	17,19,21	0.57	0
6	CLR	D	601	-	31,31,31	0.69	0	48,48,48	1.10	2 (4%)
5	NAG	C	502	1	14,14,15	0.20	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PAM	A	501	1	16,16,17	0.86	1 (6%)	15,15,17	0.64	0
5	NAG	A	502	1	14,14,15	0.20	0	17,19,21	0.42	0
7	PCW	B	602	-	40,40,53	1.08	2 (5%)	46,48,61	1.11	3 (6%)
6	CLR	B	601	-	31,31,31	0.69	0	48,48,48	1.09	2 (4%)
4	PAM	C	501	1	16,16,17	0.85	1 (6%)	15,15,17	0.64	0
5	NAG	C	503	1	14,14,15	0.23	0	17,19,21	0.57	0
7	PCW	D	602	-	40,40,53	1.08	2 (5%)	46,48,61	1.11	3 (6%)

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	A	503	1	-	2/6/23/26	0/1/1/1
6	CLR	D	601	-	-	2/10/68/68	0/4/4/4
5	NAG	C	502	1	-	2/6/23/26	0/1/1/1
4	PAM	A	501	1	-	6/14/14/15	-
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
7	PCW	B	602	-	-	4/44/44/57	-
6	CLR	B	601	-	-	2/10/68/68	0/4/4/4
4	PAM	C	501	1	-	6/14/14/15	-
5	NAG	C	503	1	-	2/6/23/26	0/1/1/1
7	PCW	D	602	-	-	4/44/44/57	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	602	PCW	O3-C11	4.28	1.45	1.33
7	D	602	PCW	O3-C11	4.26	1.45	1.33
7	D	602	PCW	O2-C31	4.07	1.45	1.34
7	B	602	PCW	O2-C31	4.05	1.45	1.34
4	A	501	PAM	O1-C1	-3.37	1.24	1.42
4	C	501	PAM	O1-C1	-3.34	1.25	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	602	PCW	O2-C31-C32	4.13	120.42	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	602	PCW	O2-C31-C32	4.12	120.40	111.48
6	B	601	CLR	C8-C7-C6	-2.90	108.75	112.76
6	D	601	CLR	C8-C7-C6	-2.89	108.76	112.76
7	B	602	PCW	O3-C11-C12	2.70	120.07	111.83
7	D	602	PCW	O3-C11-C12	2.70	120.06	111.83
7	D	602	PCW	C2-O2-C31	-2.56	111.68	117.80
7	B	602	PCW	C2-O2-C31	-2.54	111.71	117.80
6	D	601	CLR	C4-C5-C10	2.54	119.68	116.42
6	B	601	CLR	C4-C5-C10	2.47	119.58	116.42

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	O5-C5-C6-O6
5	C	502	NAG	O5-C5-C6-O6
6	B	601	CLR	C17-C20-C22-C23
6	D	601	CLR	C17-C20-C22-C23
5	C	502	NAG	C4-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
6	B	601	CLR	C21-C20-C22-C23
6	D	601	CLR	C21-C20-C22-C23
4	A	501	PAM	C12-C13-C14-C15
4	C	501	PAM	C12-C13-C14-C15
4	A	501	PAM	C6-C7-C8-C9
4	C	501	PAM	C6-C7-C8-C9
4	A	501	PAM	C1-C2-C3-C4
4	C	501	PAM	C1-C2-C3-C4
5	A	503	NAG	C1-C2-N2-C7
5	C	503	NAG	C1-C2-N2-C7
7	B	602	PCW	C39-C40-C41-C42
7	D	602	PCW	C39-C40-C41-C42
7	B	602	PCW	C11-C12-C13-C14
7	D	602	PCW	C11-C12-C13-C14
4	A	501	PAM	C5-C6-C7-C8
4	C	501	PAM	C5-C6-C7-C8
5	A	503	NAG	C3-C2-N2-C7
5	C	503	NAG	C3-C2-N2-C7
4	A	501	PAM	C9-C10-C11-C12
4	C	501	PAM	C9-C10-C11-C12
7	B	602	PCW	C17-C18-C19-C20
7	D	602	PCW	C17-C18-C19-C20

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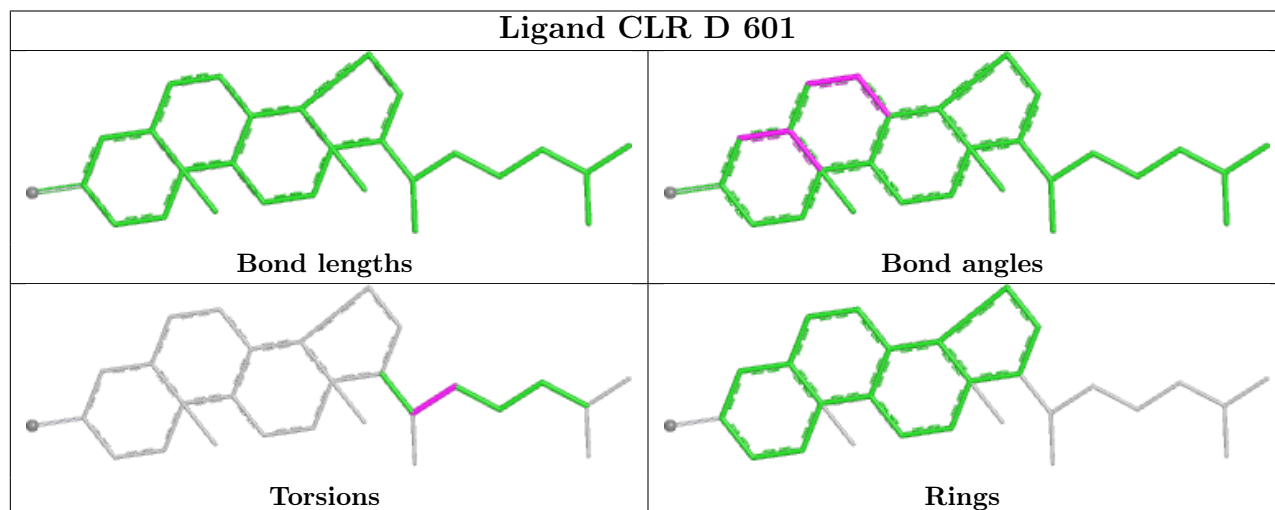
Mol	Chain	Res	Type	Atoms
4	A	501	PAM	C7-C8-C9-C10
4	C	501	PAM	C7-C8-C9-C10
7	B	602	PCW	C37-C38-C39-C40
7	D	602	PCW	C37-C38-C39-C40

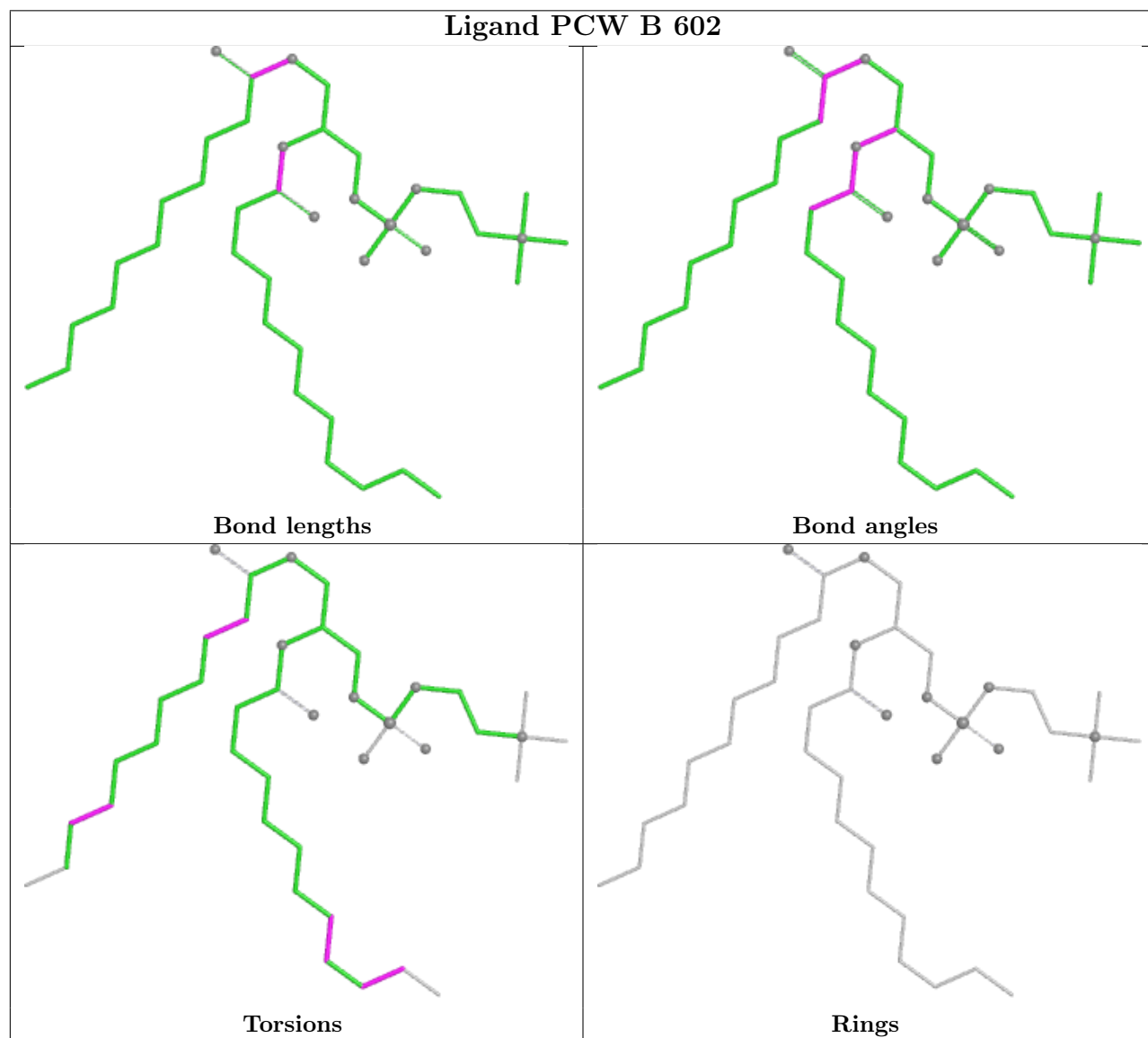
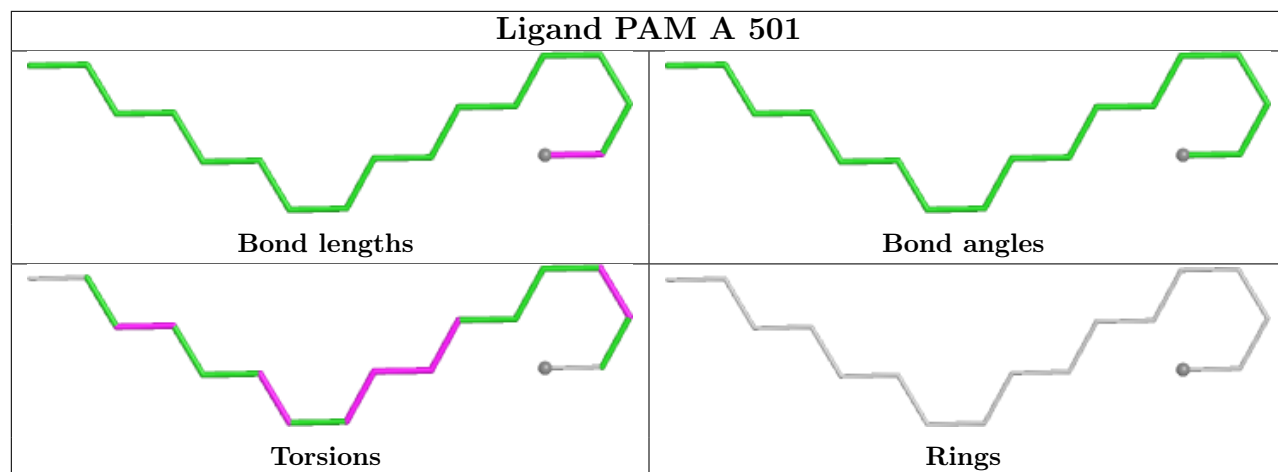
There are no ring outliers.

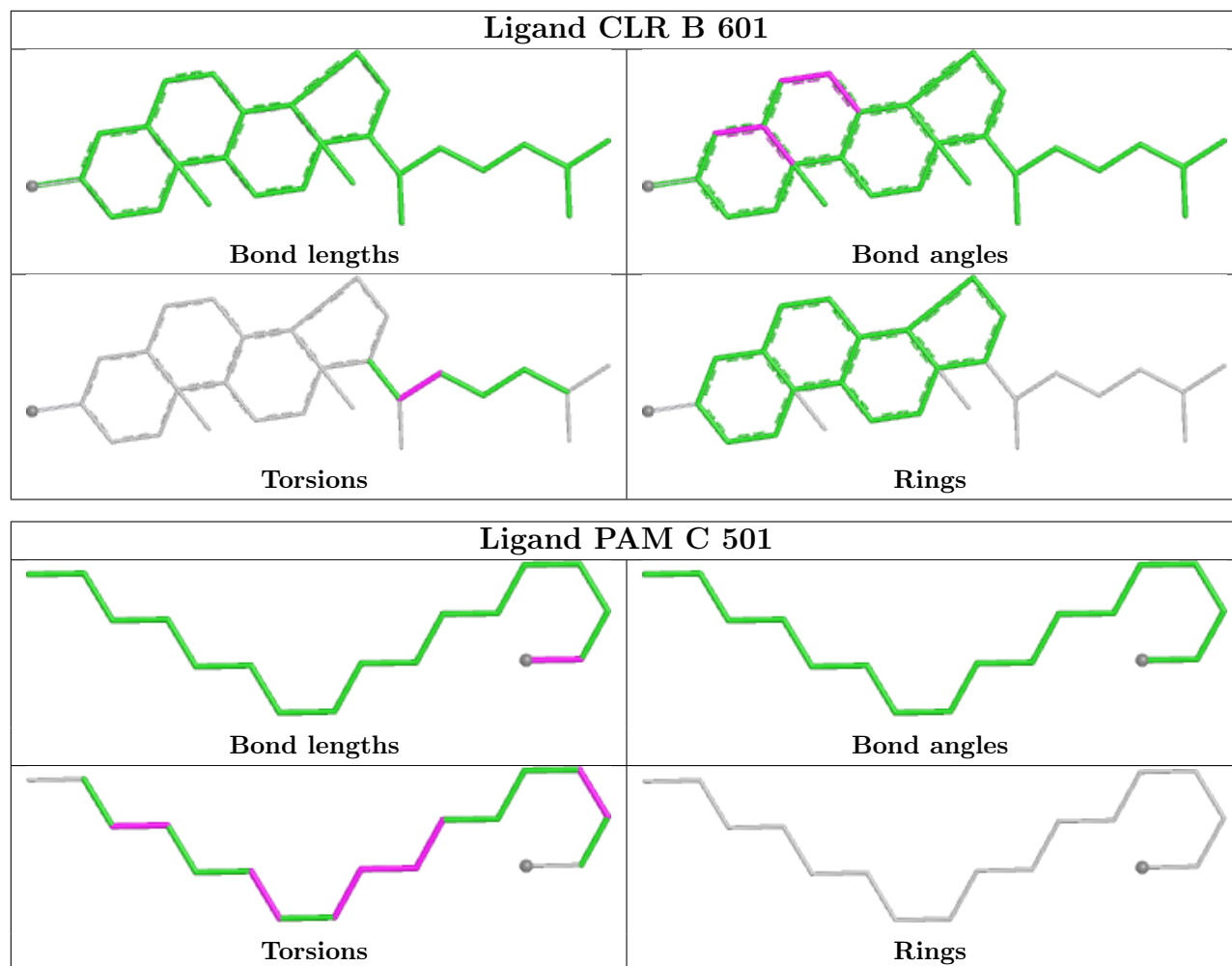
6 monomers are involved in 14 short contacts:

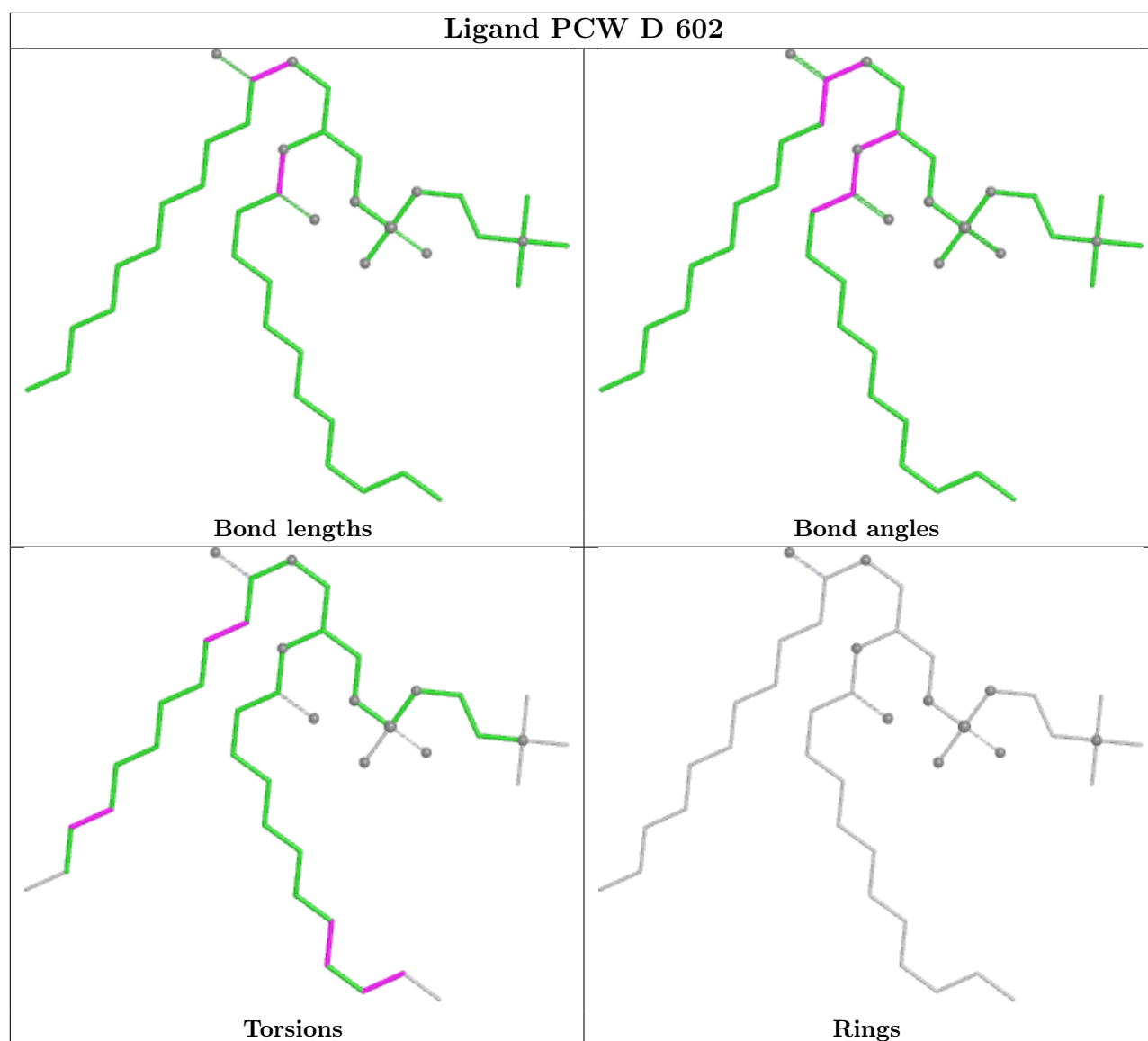
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	CLR	1	0
4	A	501	PAM	2	0
7	B	602	PCW	3	0
6	B	601	CLR	1	0
4	C	501	PAM	4	0
7	D	602	PCW	3	0

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.

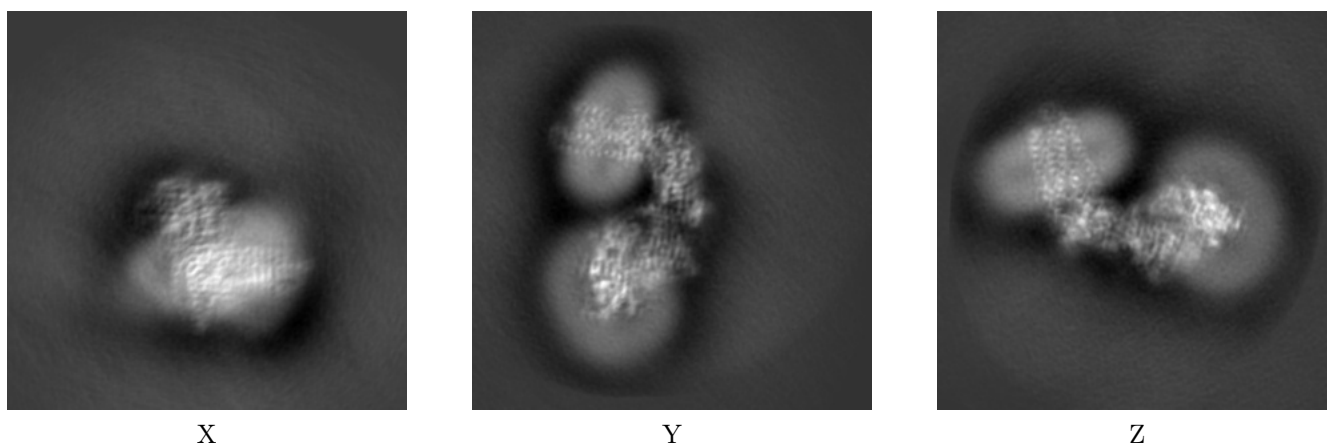
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73838. 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](#)

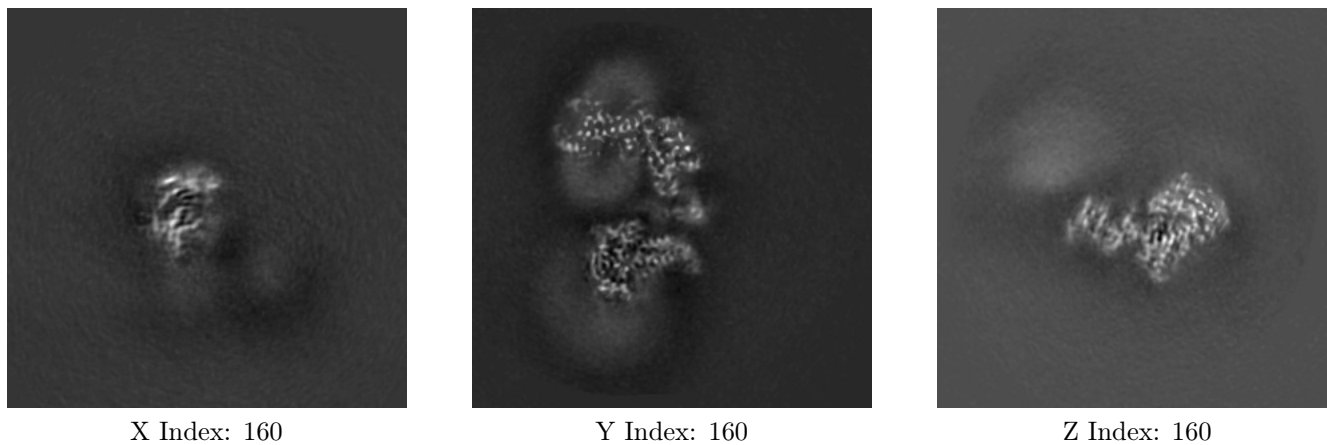
#### 6.1.1 Primary map



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

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

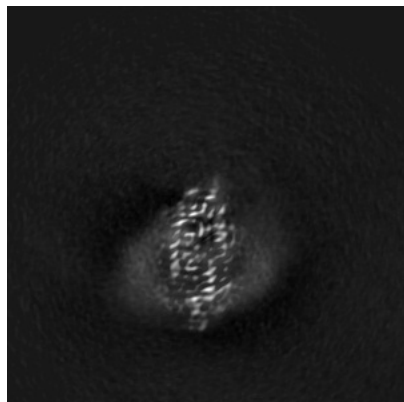
#### 6.2.1 Primary map



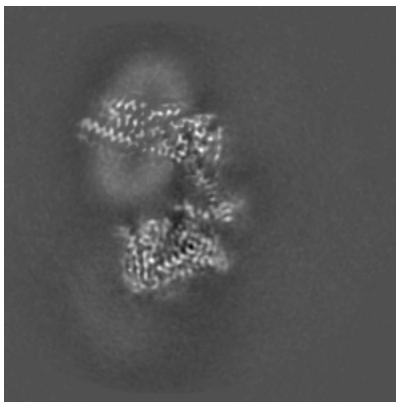
The images above show central slices of the map in three orthogonal directions.

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

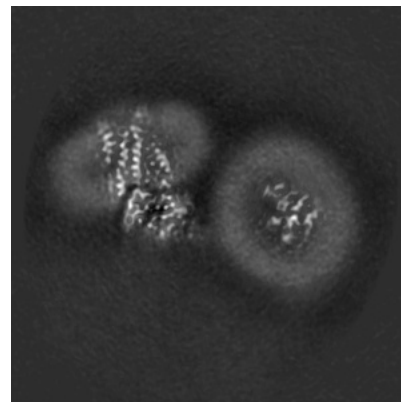
### 6.3.1 Primary map



X Index: 219



Y Index: 151

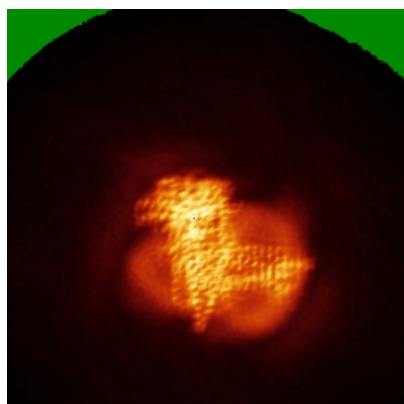


Z Index: 104

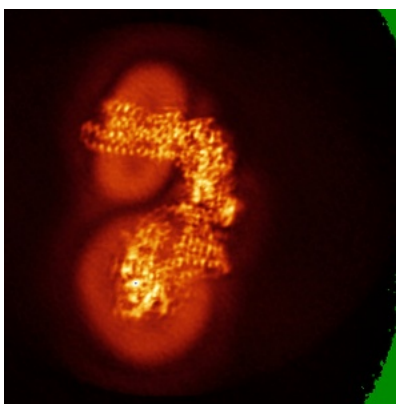
The images above show the largest variance slices of the map in three orthogonal directions.

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

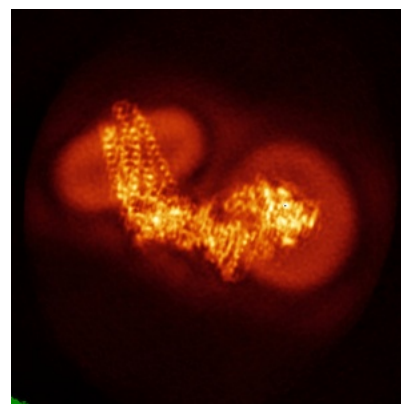
### 6.4.1 Primary map



X



Y

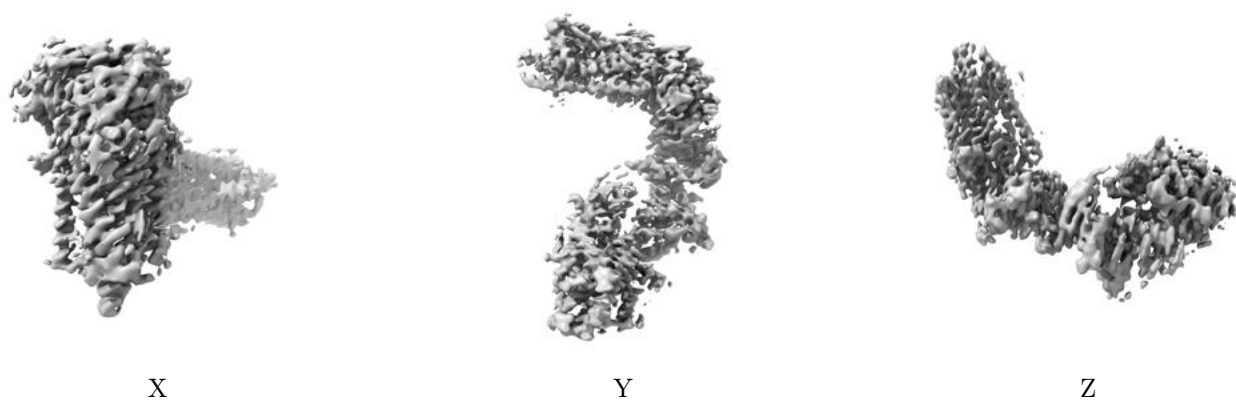


Z

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 0.00828. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

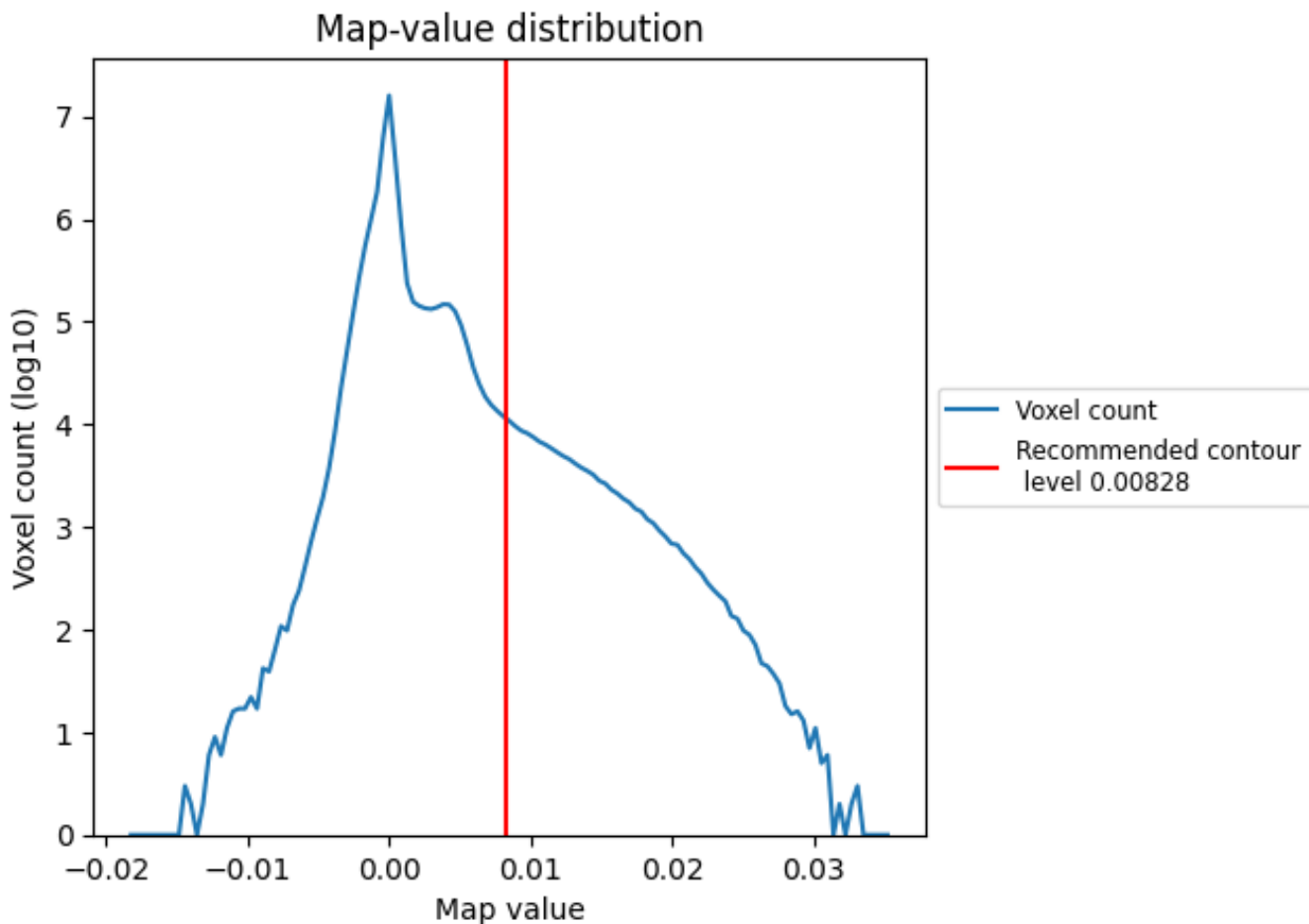
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

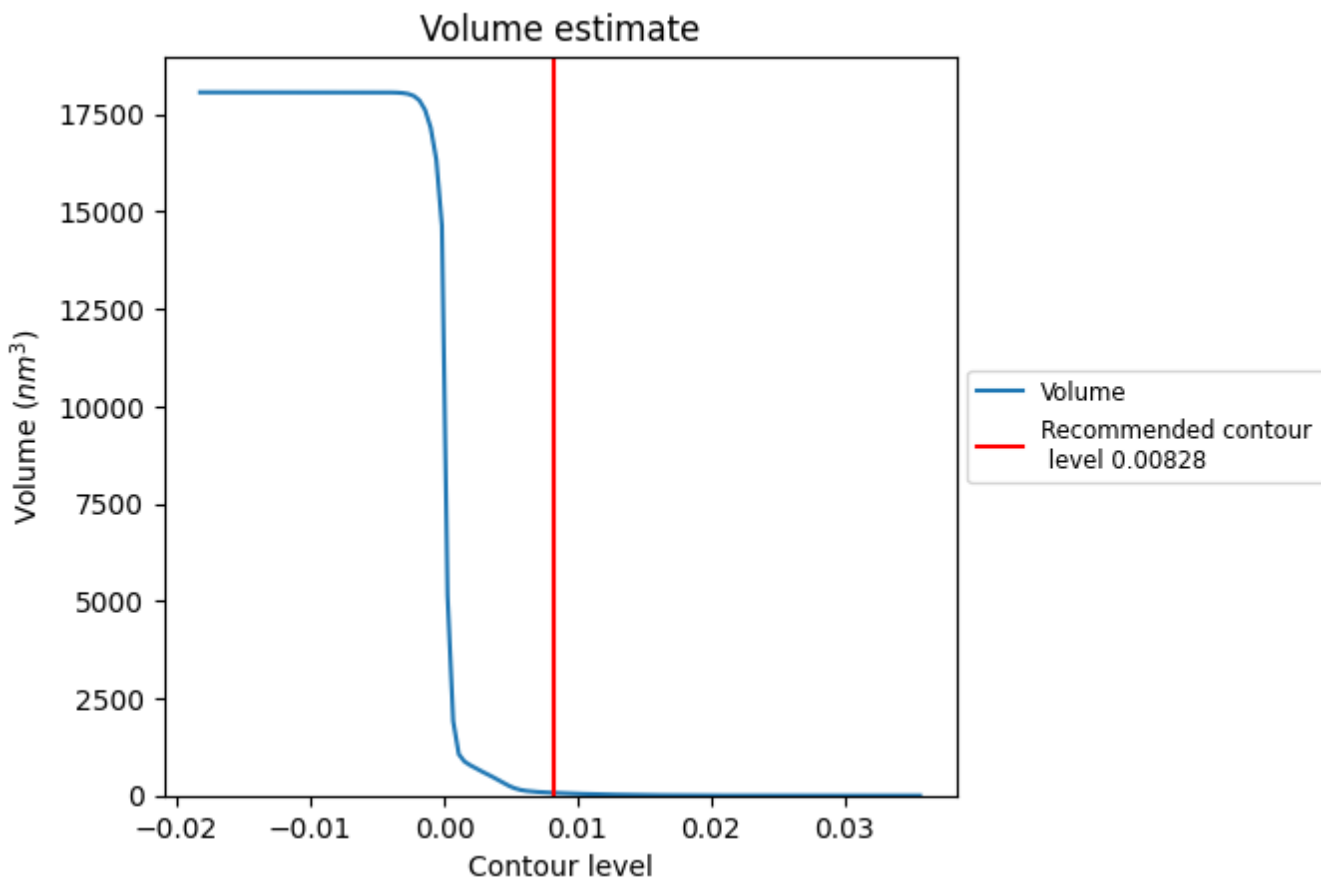
This section contains the results of statistical analysis of the map.

### 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.

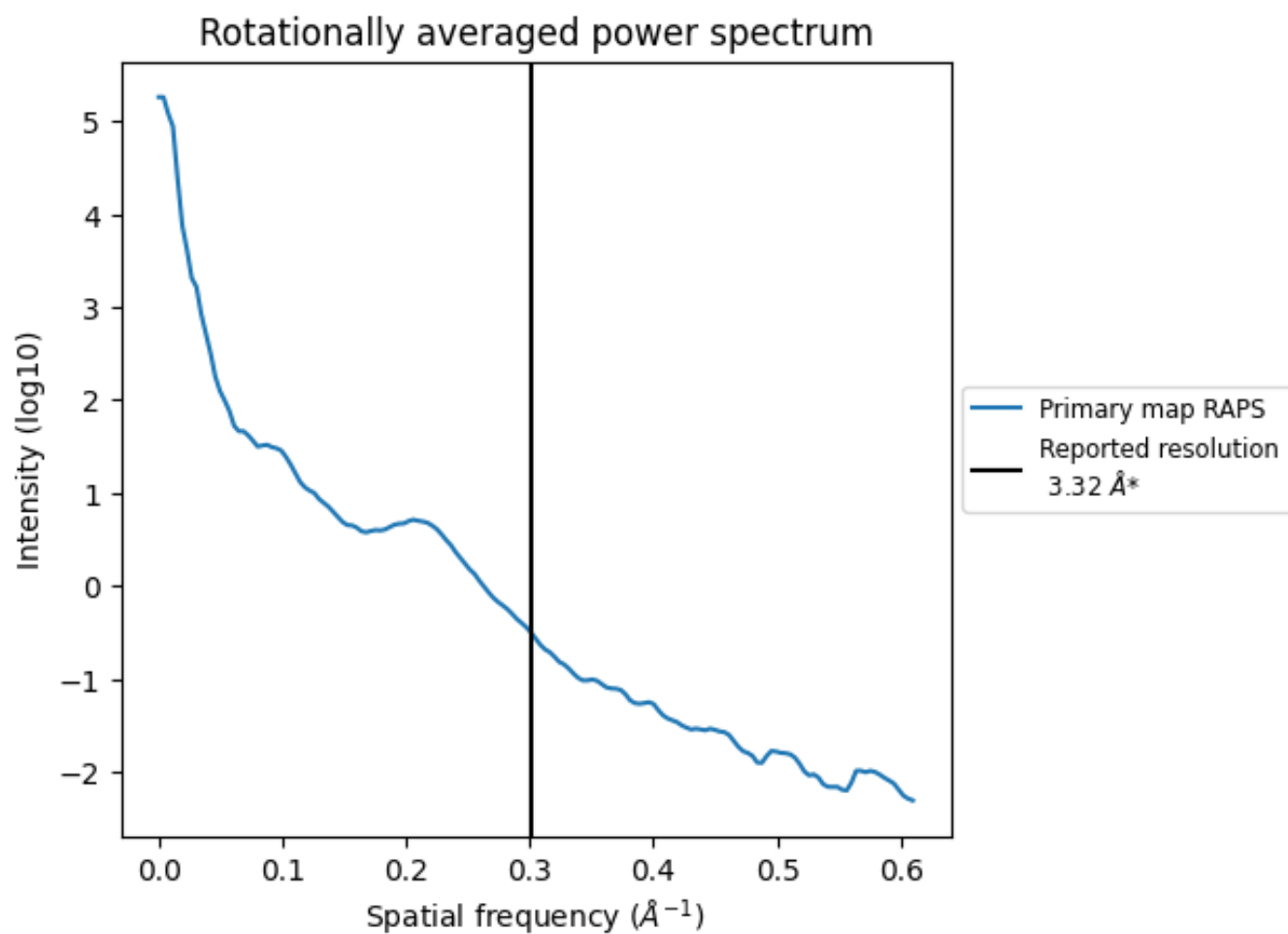
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 68 nm<sup>3</sup>; this corresponds to an approximate mass of 62 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 0.301 Å<sup>-1</sup>

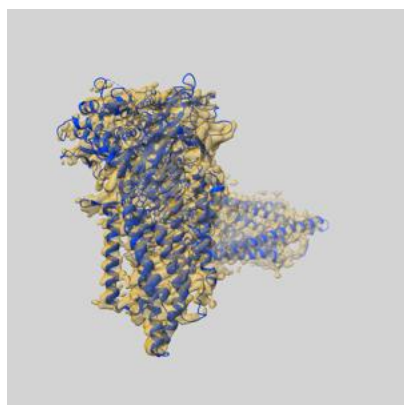
## 8 Fourier-Shell correlation

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

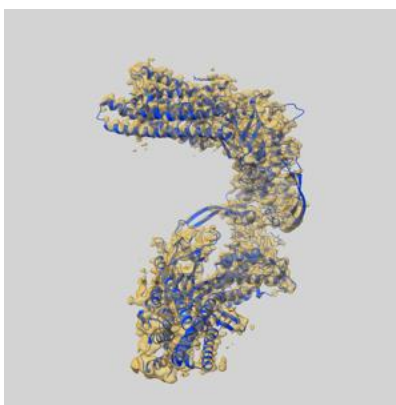
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73838 and PDB model 9Z67. Per-residue inclusion information can be found in section 3 on page 10.

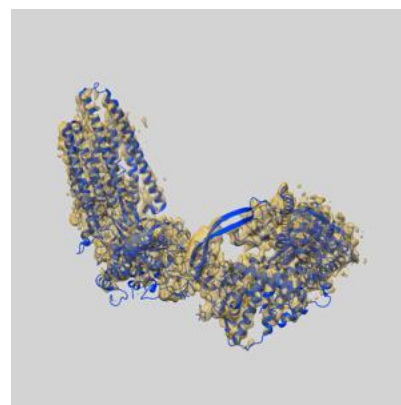
### 9.1 Map-model overlay [i](#)



X



Y



Z

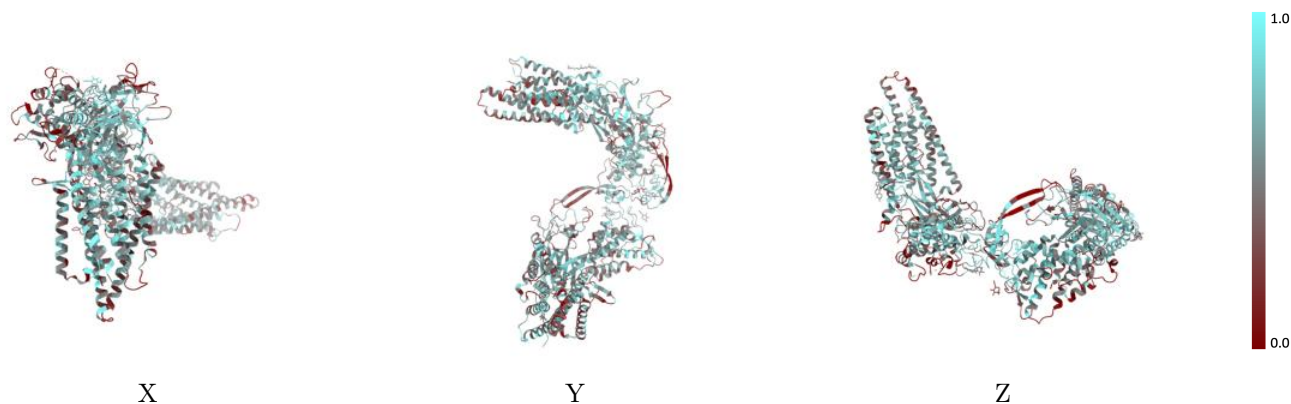
The images above show the 3D surface view of the map at the recommended contour level 0.00828 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



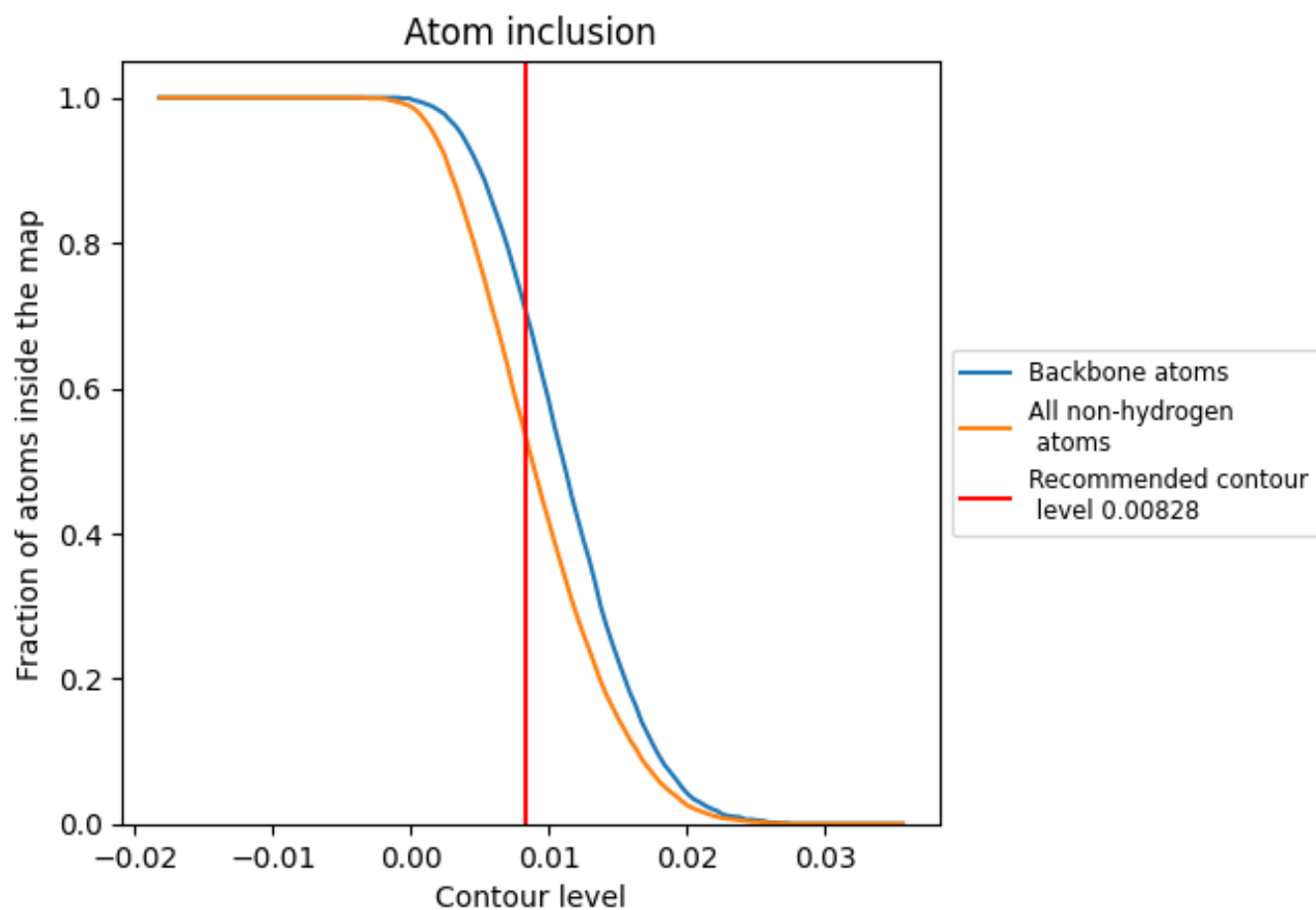
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00828).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.00828) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5340	0.3010
A	0.4970	0.3330
B	0.5720	0.2830
C	0.4800	0.3430
D	0.5490	0.2720
E	0.7860	0.4130
F	0.5710	0.2640

