



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 6M1Y / pdb_00006m1y
EMDB ID : EMD-30049
Title : The overall structure of KCC3
Authors : Chi, X.M.; Li, X.R.; Chen, Y.; Zhang, Y.Y.; Su, Q.; Zhou, Q.
Deposited on : 2020-02-26
Resolution : 3.20 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

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>.

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

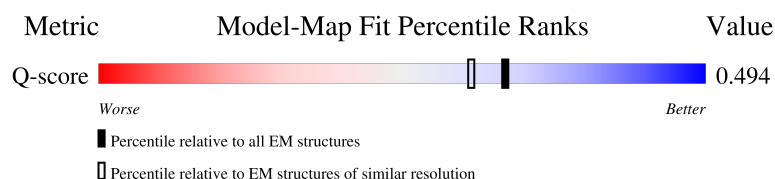
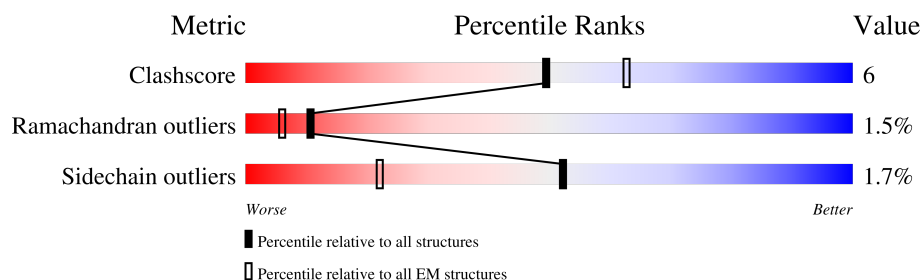
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	A	1112	74% 8% • 16%
1	B	1112	75% 8% • 16%
2	C	2	50% 50%
2	D	2	100%

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Mol	Chain	Length	Quality of chain
2	E	2	 50%50%
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14858 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 Solute carrier family 12 member 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	938	Total	C	N	O	P	S	0	0
			7313	4733	1228	1296	2	54		
1	B	938	Total	C	N	O	P	S	0	0
			7313	4733	1228	1296	2	54		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q9UHW9
A	-11	ALA	-	expression tag	UNP Q9UHW9
A	-10	ASP	-	expression tag	UNP Q9UHW9
A	-9	TYR	-	expression tag	UNP Q9UHW9
A	-8	LYS	-	expression tag	UNP Q9UHW9
A	-7	ASP	-	expression tag	UNP Q9UHW9
A	-6	ASP	-	expression tag	UNP Q9UHW9
A	-5	ASP	-	expression tag	UNP Q9UHW9
A	-4	ASP	-	expression tag	UNP Q9UHW9
A	-3	LYS	-	expression tag	UNP Q9UHW9
A	-2	SER	-	expression tag	UNP Q9UHW9
A	-1	GLY	-	expression tag	UNP Q9UHW9
A	0	ARG	-	expression tag	UNP Q9UHW9
B	-12	MET	-	initiating methionine	UNP Q9UHW9
B	-11	ALA	-	expression tag	UNP Q9UHW9
B	-10	ASP	-	expression tag	UNP Q9UHW9
B	-9	TYR	-	expression tag	UNP Q9UHW9
B	-8	LYS	-	expression tag	UNP Q9UHW9
B	-7	ASP	-	expression tag	UNP Q9UHW9
B	-6	ASP	-	expression tag	UNP Q9UHW9
B	-5	ASP	-	expression tag	UNP Q9UHW9
B	-4	ASP	-	expression tag	UNP Q9UHW9
B	-3	LYS	-	expression tag	UNP Q9UHW9
B	-2	SER	-	expression tag	UNP Q9UHW9
B	-1	GLY	-	expression tag	UNP Q9UHW9
B	0	ARG	-	expression tag	UNP Q9UHW9

- Molecule 2 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
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		

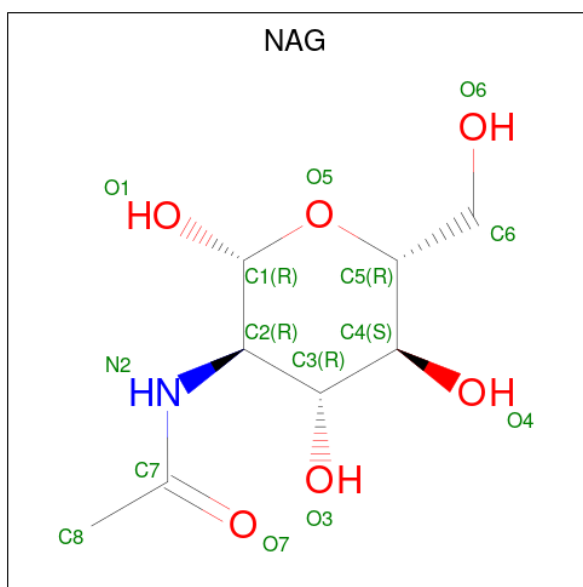
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	K	0
			1	1	
3	B	1	Total	K	0
			1	1	

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Cl	0
			2	2	
4	B	2	Total	Cl	0
			2	2	

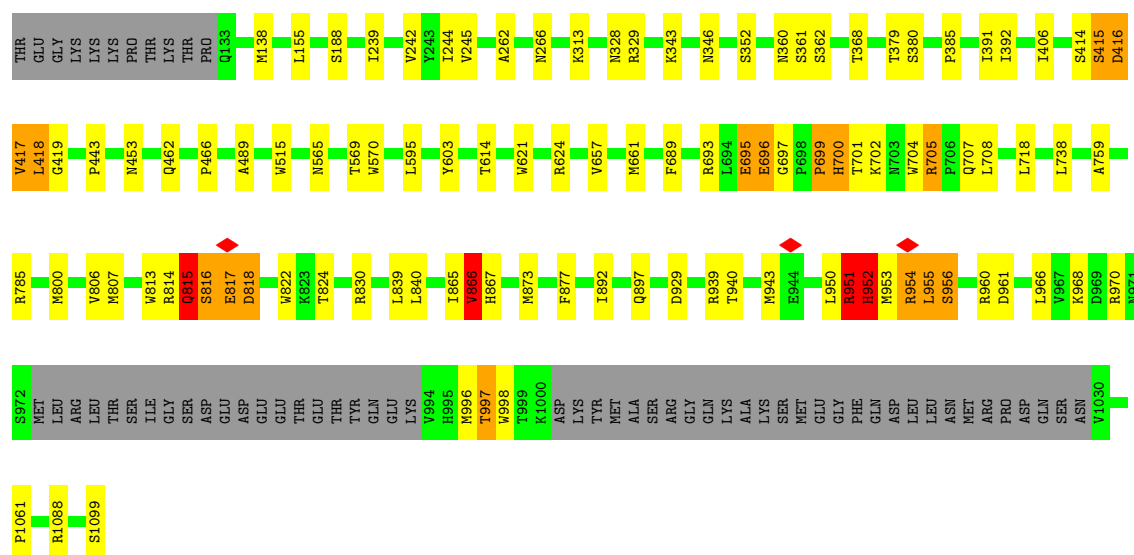
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	O	0
			1	1	
6	B	1	Total	O	0
			1	1	



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

Chain C: 50% 50%



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

Chain D: 100%



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

Chain E: 50% 50%



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

Chain F: 50% 50%



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

Chain G:  100%

HA01
HA02

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

Chain H:  50%  50%

HA01
HA02

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	453155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: CL, K, NAG, TPO

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	0.25	1/7452 (0.0%)	0.54	4/10100 (0.0%)
1	B	0.25	1/7452 (0.0%)	0.54	4/10100 (0.0%)
All	All	0.25	2/14904 (0.0%)	0.54	8/20200 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	GLY	C-N	5.16	1.39	1.33
1	B	697	GLY	C-N	5.16	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	GLY	CA-C-N	-6.20	114.00	120.38
1	A	697	GLY	C-N-CA	-6.20	114.00	120.38
1	B	697	GLY	CA-C-N	-6.20	114.00	120.38
1	B	697	GLY	C-N-CA	-6.20	114.00	120.38
1	A	705	ARG	CA-C-N	-5.53	114.23	119.76
1	A	705	ARG	C-N-CA	-5.53	114.23	119.76
1	B	705	ARG	CA-C-N	-5.53	114.23	119.76
1	B	705	ARG	C-N-CA	-5.53	114.23	119.76

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	7313	0	7424	90	0
1	B	7313	0	7424	81	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
5	A	28	0	26	2	0
5	B	28	0	26	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	14858	0	15050	171	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 6.

All (171) 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:702:LYS:NZ	1:B:953:MET:SD	2.39	0.94
1:A:702:LYS:NZ	1:A:953:MET:SD	2.39	0.93
1:A:952:HIS:HB3	1:A:953:MET:CE	2.04	0.86
1:B:952:HIS:HB3	1:B:953:MET:CE	2.04	0.86
1:B:953:MET:SD	1:B:953:MET:N	2.57	0.75
1:A:953:MET:SD	1:A:953:MET:N	2.57	0.74
1:B:704:TRP:O	1:B:705:ARG:HD3	1.87	0.74
1:A:704:TRP:O	1:A:705:ARG:HD3	1.87	0.73
1:B:954:ARG:O	1:B:954:ARG:HD2	1.88	0.72
1:A:954:ARG:O	1:A:954:ARG:HD2	1.88	0.72
1:B:816:SER:O	1:B:817:GLU:HG3	1.89	0.72
1:A:816:SER:O	1:A:817:GLU:HG3	1.89	0.70
1:A:951:ARG:O	1:A:953:MET:N	2.24	0.70
1:A:865:ILE:O	1:A:866:VAL:HG22	1.91	0.70
1:B:865:ILE:O	1:B:866:VAL:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:951:ARG:O	1:B:953:MET:N	2.24	0.69
1:B:603:TYR:OH	4:B:1102:CL:CL	2.50	0.66
1:B:952:HIS:HB3	1:B:953:MET:HE1	1.78	0.65
1:A:815:GLN:O	1:A:816:SER:HB3	1.97	0.65
1:B:695:GLU:O	1:B:696:GLU:HB3	1.95	0.64
1:B:418:LEU:HG	1:B:419:GLY:N	2.11	0.64
1:A:695:GLU:O	1:A:696:GLU:HB3	1.95	0.64
1:A:952:HIS:HB3	1:A:953:MET:HE1	1.78	0.64
1:A:418:LEU:HG	1:A:419:GLY:N	2.11	0.64
1:B:815:GLN:O	1:B:816:SER:HB3	1.97	0.64
1:A:954:ARG:HD2	1:A:954:ARG:C	2.23	0.63
1:B:954:ARG:HD2	1:B:954:ARG:C	2.23	0.63
1:A:603:TYR:OH	4:A:1102:CL:CL	2.50	0.62
1:A:417:VAL:HG23	1:A:417:VAL:O	2.00	0.62
1:B:417:VAL:O	1:B:417:VAL:HG23	2.00	0.61
1:B:188:SER:HB2	1:B:466:PRO:HB3	1.84	0.59
1:A:188:SER:HB2	1:A:466:PRO:HB3	1.84	0.59
1:A:815:GLN:HA	1:A:815:GLN:OE1	2.01	0.58
1:B:815:GLN:OE1	1:B:815:GLN:HA	2.01	0.58
1:B:866:VAL:HA	1:B:968:LYS:NZ	2.17	0.58
1:A:866:VAL:HA	1:A:968:LYS:NZ	2.17	0.58
1:B:155:LEU:HD11	1:B:239:ILE:HD11	1.85	0.58
1:B:839:LEU:HB3	1:B:1088:ARG:HB3	1.85	0.58
1:A:839:LEU:HB3	1:A:1088:ARG:HB3	1.85	0.57
1:A:155:LEU:HD11	1:A:239:ILE:HD11	1.85	0.56
1:B:707:GLN:O	1:B:708:LEU:HB2	2.05	0.56
1:A:707:GLN:O	1:A:708:LEU:HB2	2.05	0.56
1:A:817:GLU:O	1:A:818:ASP:HB2	2.05	0.56
1:A:866:VAL:HG23	1:A:867:HIS:CG	2.41	0.55
1:A:950:LEU:HD21	1:A:966:LEU:HD21	1.88	0.55
1:A:952:HIS:HB3	1:A:953:MET:HE3	1.88	0.55
1:B:950:LEU:HD21	1:B:966:LEU:HD21	1.88	0.55
1:B:707:GLN:O	1:B:738:LEU:O	2.25	0.54
1:A:956:SER:O	1:A:960:ARG:HG3	2.07	0.54
1:B:866:VAL:HG23	1:B:867:HIS:CG	2.41	0.54
1:B:817:GLU:O	1:B:818:ASP:HB2	2.05	0.54
1:A:954:ARG:O	1:A:955:LEU:HD12	2.08	0.54
1:A:707:GLN:O	1:A:738:LEU:O	2.25	0.54
1:B:956:SER:O	1:B:960:ARG:HG3	2.07	0.53
1:A:699:PRO:C	1:A:700:HIS:CG	2.85	0.53
1:B:954:ARG:O	1:B:955:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:PRO:C	1:B:700:HIS:CG	2.85	0.53
1:A:961:ASP:OD1	1:A:970:ARG:NH1	2.42	0.53
1:B:328:ASN:HB3	1:B:414:SER:HB3	1.91	0.53
1:B:392:ILE:HD12	1:B:489:ALA:HB2	1.92	0.52
1:B:961:ASP:OD1	1:B:970:ARG:NH1	2.42	0.52
1:B:718:LEU:HD23	1:B:759:ALA:HB2	1.91	0.52
1:A:897:GLN:NE2	1:A:929:ASP:OD2	2.43	0.52
1:B:866:VAL:HA	1:B:968:LYS:HZ1	1.74	0.52
1:A:392:ILE:HD12	1:A:489:ALA:HB2	1.92	0.51
1:A:806:VAL:HG22	1:A:840:LEU:HB2	1.91	0.51
1:B:343:LYS:HB2	1:B:352:SER:HB3	1.93	0.51
1:A:329:ARG:HG2	1:A:406:ILE:HG21	1.92	0.51
1:B:785:ARG:HG2	1:B:824:THR:HG23	1.92	0.51
1:A:718:LEU:HD23	1:A:759:ALA:HB2	1.91	0.51
1:B:806:VAL:HG22	1:B:840:LEU:HB2	1.91	0.51
1:B:814:ARG:O	1:B:814:ARG:HG3	2.10	0.51
1:B:897:GLN:NE2	1:B:929:ASP:OD2	2.43	0.51
1:A:814:ARG:O	1:A:814:ARG:HG3	2.10	0.51
1:A:328:ASN:HB3	1:A:414:SER:HB3	1.91	0.51
1:A:785:ARG:HG2	1:A:824:THR:HG23	1.92	0.51
1:A:343:LYS:HB2	1:A:352:SER:HB3	1.93	0.50
1:B:329:ARG:HG2	1:B:406:ILE:HG21	1.92	0.50
1:B:952:HIS:HB3	1:B:953:MET:HE3	1.88	0.50
1:A:866:VAL:HA	1:A:968:LYS:HZ1	1.77	0.50
1:A:700:HIS:ND1	1:A:700:HIS:N	2.60	0.49
1:A:953:MET:HG2	1:A:955:LEU:CD1	2.43	0.49
1:A:385:PRO:HG3	1:A:391:ILE:HD12	1.94	0.49
1:A:702:LYS:HG3	1:A:955:LEU:HD11	1.95	0.49
1:B:738:LEU:HD22	1:B:800:MET:HG2	1.95	0.49
1:B:385:PRO:HG3	1:B:391:ILE:HD12	1.94	0.48
1:B:702:LYS:HG3	1:B:955:LEU:HD11	1.95	0.48
1:B:953:MET:HG2	1:B:955:LEU:CD1	2.43	0.48
1:B:368:THR:OG1	5:B:1111:NAG:O7	2.31	0.48
1:A:368:THR:OG1	5:A:1111:NAG:O7	2.31	0.48
1:A:738:LEU:HD22	1:A:800:MET:HG2	1.95	0.48
1:B:700:HIS:N	1:B:700:HIS:ND1	2.60	0.48
1:A:109:THR:HA	1:A:453:ASN:HB2	1.95	0.48
1:A:360:ASN:OD1	1:A:360:ASN:N	2.47	0.48
1:A:877:PHE:HE2	1:A:1099:SER:HB2	1.79	0.48
1:B:262:ALA:O	1:B:266:ASN:ND2	2.47	0.47
1:B:877:PHE:HE2	1:B:1099:SER:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:THR:OG1	1:B:380:SER:N	2.48	0.47
1:B:109:THR:HA	1:B:453:ASN:HB2	1.95	0.47
1:A:262:ALA:O	1:A:266:ASN:ND2	2.47	0.47
1:A:346:ASN:OD1	1:A:346:ASN:N	2.48	0.46
1:A:379:THR:OG1	1:A:380:SER:N	2.48	0.46
1:A:244:ILE:HG22	1:A:245:VAL:HG22	1.98	0.46
1:B:244:ILE:HG22	1:B:245:VAL:HG22	1.98	0.46
1:B:569:THR:OG1	1:B:570:TRP:N	2.49	0.46
1:A:813:TRP:HB2	1:A:822:TRP:HB3	1.98	0.46
1:A:569:THR:OG1	1:A:570:TRP:N	2.49	0.45
1:A:866:VAL:HG23	1:A:867:HIS:ND1	2.32	0.45
1:A:830:ARG:NH2	1:A:1061:PRO:O	2.49	0.45
1:B:866:VAL:HG23	1:B:867:HIS:ND1	2.32	0.45
1:A:997:TPO:OG1	1:A:998:TRP:N	2.50	0.45
1:B:360:ASN:OD1	1:B:360:ASN:N	2.47	0.45
1:B:830:ARG:NH2	1:B:1061:PRO:O	2.49	0.45
1:A:939:ARG:O	1:A:943:MET:N	2.50	0.45
1:B:702:LYS:HA	1:B:702:LYS:HD3	1.69	0.45
1:B:113:LYS:HE3	1:B:113:LYS:HB3	1.82	0.45
1:B:346:ASN:N	1:B:346:ASN:OD1	2.48	0.45
1:B:689:PHE:HE2	1:B:693:ARG:HH11	1.65	0.45
1:B:997:TPO:OG1	1:B:998:TRP:N	2.50	0.44
1:A:953:MET:HG2	1:A:955:LEU:HD12	1.98	0.44
1:B:813:TRP:HB2	1:B:822:TRP:HB3	1.98	0.44
1:B:953:MET:HG2	1:B:955:LEU:HD12	1.98	0.44
1:B:138:MET:HE3	1:B:138:MET:HB3	1.93	0.44
1:A:138:MET:HE3	1:A:138:MET:HB3	1.93	0.44
1:A:702:LYS:HD3	1:A:702:LYS:HA	1.69	0.44
1:B:313:LYS:HD2	1:B:515:TRP:HD1	1.83	0.44
1:B:807:MET:HE2	1:B:839:LEU:HD11	1.99	0.44
1:A:313:LYS:HD2	1:A:515:TRP:HD1	1.83	0.43
1:A:565:ASN:N	1:A:565:ASN:OD1	2.51	0.43
1:A:689:PHE:HE2	1:A:693:ARG:HH11	1.65	0.43
1:B:816:SER:C	1:B:817:GLU:HG3	2.43	0.43
1:B:956:SER:O	1:B:960:ARG:CG	2.66	0.43
1:A:614:THR:HB	1:A:621:TRP:HE1	1.83	0.43
1:A:807:MET:HE2	1:A:839:LEU:HD11	1.99	0.43
1:A:816:SER:C	1:A:817:GLU:HG3	2.43	0.43
1:A:956:SER:O	1:A:960:ARG:CG	2.66	0.43
1:B:939:ARG:O	1:B:943:MET:N	2.50	0.43
1:A:361:SER:OG	1:A:362:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:THR:HB	1:B:621:TRP:HE1	1.83	0.43
1:A:597:MET:HE2	1:A:597:MET:HB2	1.91	0.42
1:A:702:LYS:CE	1:A:953:MET:SD	3.07	0.42
1:B:702:LYS:CE	1:B:953:MET:SD	3.07	0.42
1:B:361:SER:OG	1:B:362:SER:N	2.51	0.42
1:A:462:GLN:OE1	1:A:624:ARG:NH2	2.53	0.42
1:A:733:LYS:HA	1:A:733:LYS:HD2	1.90	0.42
1:B:873:MET:HE2	1:B:892:ILE:HD13	2.02	0.42
1:A:845:ILE:HD12	1:A:845:ILE:HA	1.94	0.41
1:A:873:MET:HE2	1:A:892:ILE:HD13	2.02	0.41
1:B:657:VAL:O	1:B:661:MET:N	2.47	0.41
1:A:1033:MET:HE3	1:A:1033:MET:HB3	1.89	0.41
1:B:360:ASN:HB3	5:B:1111:NAG:HN2	1.85	0.41
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.95	0.41
1:A:707:GLN:HE21	1:A:738:LEU:HB3	1.86	0.41
1:B:565:ASN:N	1:B:565:ASN:OD1	2.51	0.41
1:B:815:GLN:HB3	1:B:816:SER:H	1.66	0.41
1:B:328:ASN:CB	1:B:414:SER:HB3	2.51	0.41
1:A:360:ASN:HB3	5:A:1111:NAG:HN2	1.85	0.41
1:A:951:ARG:O	1:A:953:MET:SD	2.79	0.41
1:A:443:PRO:HB3	1:A:595:LEU:HD11	2.03	0.41
1:B:952:HIS:HB3	1:B:953:MET:SD	2.61	0.41
1:B:951:ARG:O	1:B:953:MET:SD	2.79	0.41
1:B:443:PRO:HB3	1:B:595:LEU:HD11	2.03	0.40
1:B:462:GLN:OE1	1:B:624:ARG:NH2	2.53	0.40
1:A:328:ASN:CB	1:A:414:SER:HB3	2.51	0.40
1:A:499:LYS:H	1:A:499:LYS:HG2	1.71	0.40
1:A:933:SER:HA	1:A:936:THR:HG22	2.03	0.40
1:A:954:ARG:O	1:A:955:LEU:HG	2.22	0.40
1:A:699:PRO:HB2	1:A:700:HIS:ND1	2.36	0.40
1:A:699:PRO:O	1:A:700:HIS:CG	2.75	0.40
1:A:700:HIS:O	1:A:701:THR:C	2.65	0.40
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	928/1112 (84%)	824 (89%)	90 (10%)	14 (2%)	8	37
1	B	928/1112 (84%)	824 (89%)	90 (10%)	14 (2%)	8	37
All	All	1856/2224 (84%)	1648 (89%)	180 (10%)	28 (2%)	11	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	SER
1	A	416	ASP
1	A	696	GLU
1	A	815	GLN
1	A	818	ASP
1	A	952	HIS
1	B	415	SER
1	B	416	ASP
1	B	696	GLU
1	B	815	GLN
1	B	818	ASP
1	B	952	HIS
1	A	417	VAL
1	A	701	THR
1	A	951	ARG
1	B	417	VAL
1	B	701	THR
1	B	951	ARG
1	A	956	SER
1	A	996	MET
1	B	956	SER
1	B	996	MET
1	A	699	PRO
1	A	816	SER
1	B	699	PRO

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Mol	Chain	Res	Type
1	B	816	SER
1	A	866	VAL
1	B	866	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	786/940 (84%)	773 (98%)	13 (2%)	53	75
1	B	786/940 (84%)	773 (98%)	13 (2%)	53	75
All	All	1572/1880 (84%)	1546 (98%)	26 (2%)	52	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	A	415	SER
1	A	416	ASP
1	A	418	LEU
1	A	695	GLU
1	A	700	HIS
1	A	815	GLN
1	A	817	GLU
1	A	866	VAL
1	A	951	ARG
1	A	952	HIS
1	A	954	ARG
1	A	955	LEU
1	B	242	VAL
1	B	415	SER
1	B	416	ASP
1	B	418	LEU
1	B	695	GLU
1	B	700	HIS
1	B	815	GLN

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Mol	Chain	Res	Type
1	B	817	GLU
1	B	866	VAL
1	B	951	ARG
1	B	952	HIS
1	B	954	ARG
1	B	955	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	115	HIS
1	A	265	ASN
1	A	290	ASN
1	A	399	ASN
1	A	423	HIS
1	A	507	ASN
1	A	607	ASN
1	A	613	GLN
1	A	707	GLN
1	A	761	GLN
1	A	1040	ASN
1	B	107	ASN
1	B	115	HIS
1	B	147	ASN
1	B	290	ASN
1	B	399	ASN
1	B	423	HIS
1	B	507	ASN
1	B	607	ASN
1	B	613	GLN
1	B	707	GLN
1	B	719	HIS
1	B	761	GLN
1	B	1040	ASN
1	B	1045	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPO	A	997	1	8,10,11	1.65	1 (12%)	10,14,16	2.21	2 (20%)
1	TPO	B	940	1	8,10,11	1.14	0	10,14,16	1.87	2 (20%)
1	TPO	B	997	1	8,10,11	1.65	1 (12%)	10,14,16	2.21	2 (20%)
1	TPO	A	940	1	8,10,11	1.14	0	10,14,16	1.87	2 (20%)

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
1	TPO	A	997	1	-	3/9/11/13	-
1	TPO	B	940	1	-	5/9/11/13	-
1	TPO	B	997	1	-	3/9/11/13	-
1	TPO	A	940	1	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	997	TPO	P-O1P	3.50	1.61	1.50
1	B	997	TPO	P-O1P	3.50	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	997	TPO	P-OG1-CB	-6.21	106.45	123.33
1	B	997	TPO	P-OG1-CB	-6.21	106.45	123.33
1	A	940	TPO	P-OG1-CB	-4.41	111.35	123.33
1	B	940	TPO	P-OG1-CB	-4.41	111.35	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	940	TPO	CG2-CB-CA	-3.13	107.17	113.26
1	B	940	TPO	CG2-CB-CA	-3.13	107.17	113.26
1	A	997	TPO	CG2-CB-CA	-2.30	108.77	113.26
1	B	997	TPO	CG2-CB-CA	-2.30	108.77	113.26

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	940	TPO	N-CA-CB-CG2
1	A	940	TPO	N-CA-CB-OG1
1	A	940	TPO	C-CA-CB-CG2
1	A	997	TPO	N-CA-CB-OG1
1	B	940	TPO	N-CA-CB-CG2
1	B	940	TPO	N-CA-CB-OG1
1	B	940	TPO	C-CA-CB-CG2
1	B	997	TPO	N-CA-CB-OG1
1	A	940	TPO	CB-OG1-P-O1P
1	B	940	TPO	CB-OG1-P-O1P
1	A	997	TPO	CB-OG1-P-O3P
1	B	997	TPO	CB-OG1-P-O3P
1	A	940	TPO	O-C-CA-CB
1	A	997	TPO	O-C-CA-CB
1	B	940	TPO	O-C-CA-CB
1	B	997	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	997	TPO	1	0
1	B	997	TPO	1	0

5.5 Carbohydrates

12 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	0.42	0	17,19,21	0.76	1 (5%)
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	D	1	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.35	0	17,19,21	0.57	0
2	NAG	E	1	1,2	14,14,15	0.72	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.58	0
2	NAG	F	1	1,2	14,14,15	0.42	0	17,19,21	0.76	1 (5%)
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	0.57	0
2	NAG	H	1	1,2	14,14,15	0.72	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.58	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.41	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-2.41	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	F	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	E	1	NAG	C3-C4-C5	2.18	114.18	110.23
2	H	1	NAG	C3-C4-C5	2.18	114.18	110.23

There are no chirality outliers.

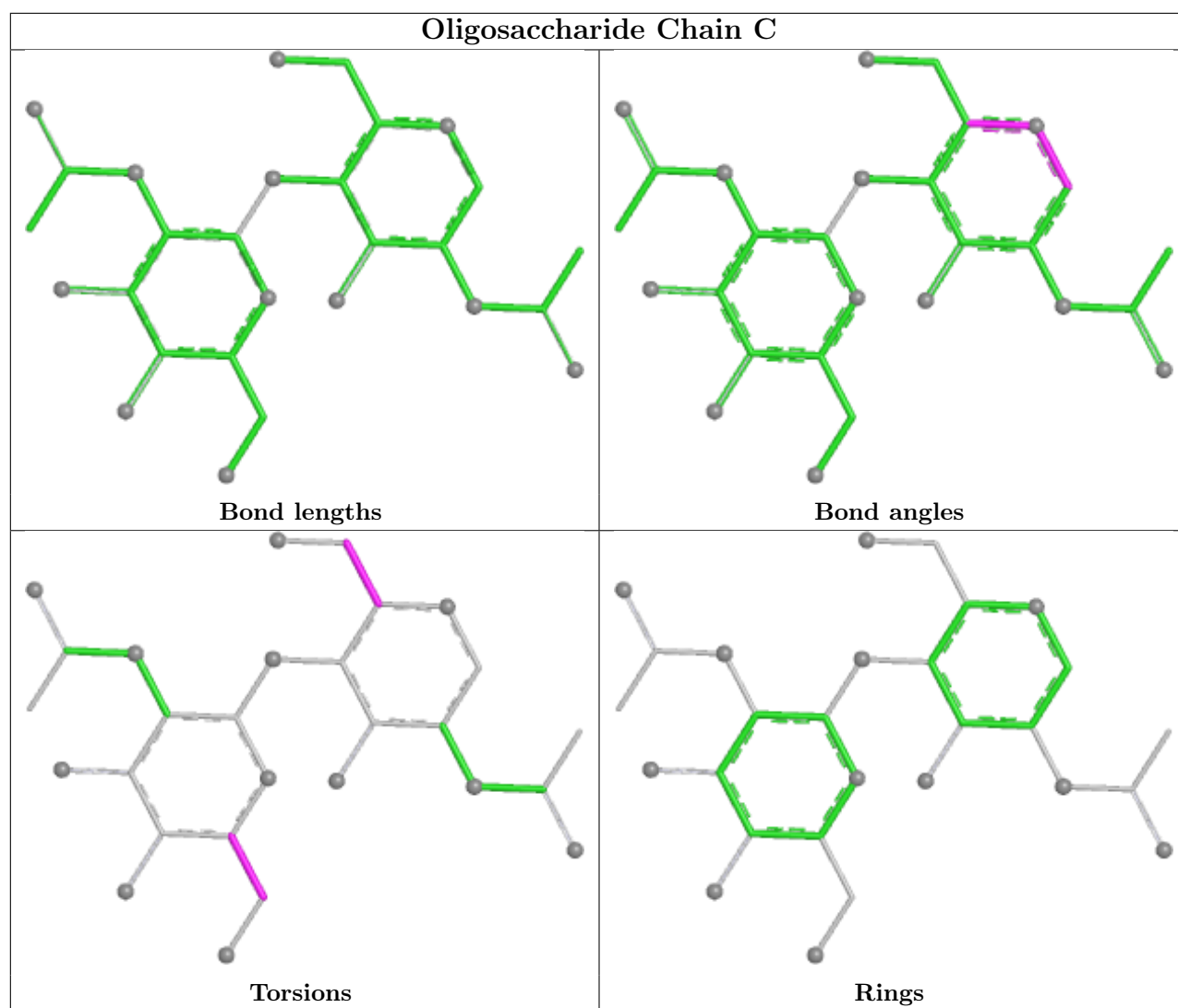
All (20) torsion outliers are listed below:

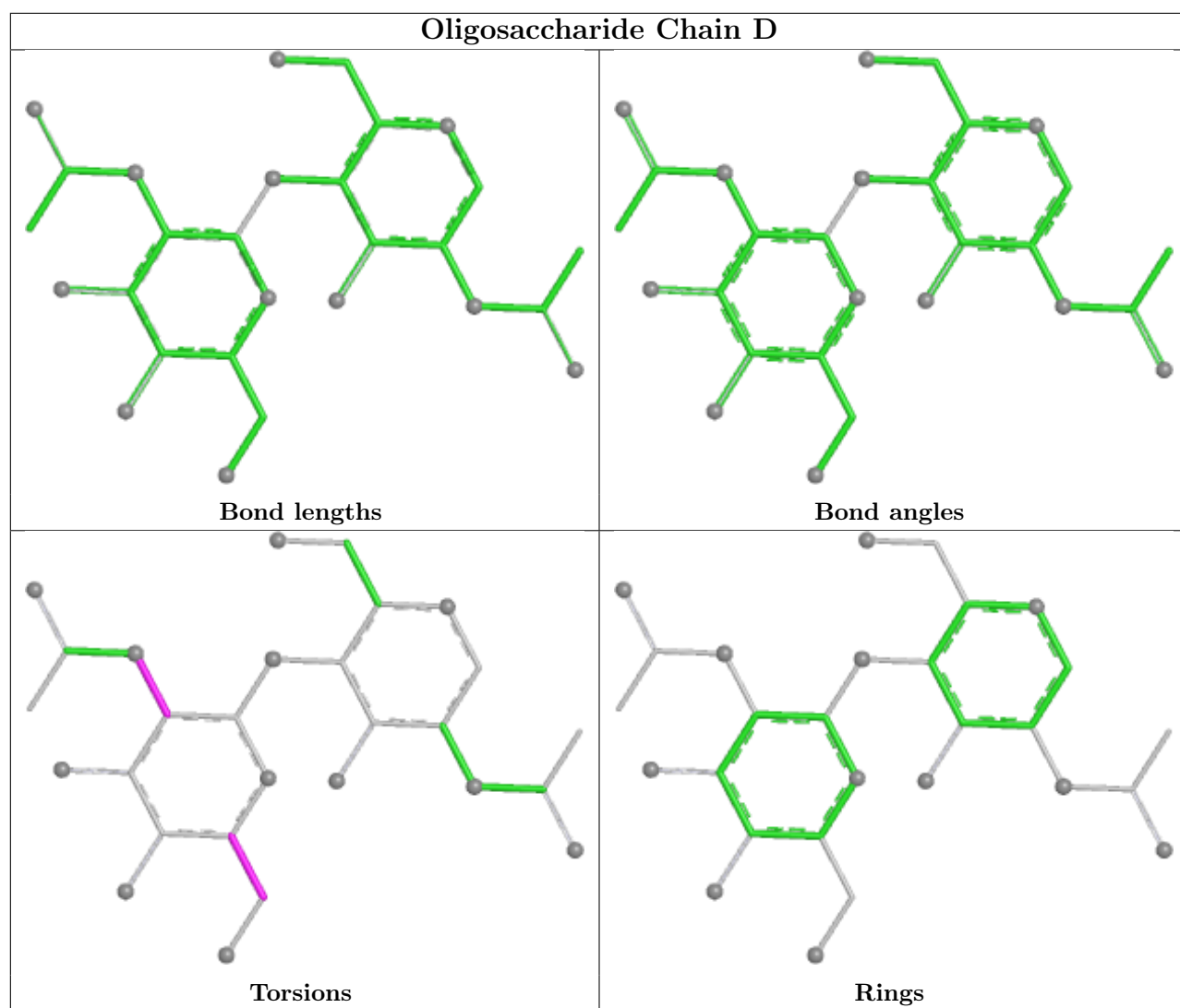
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6

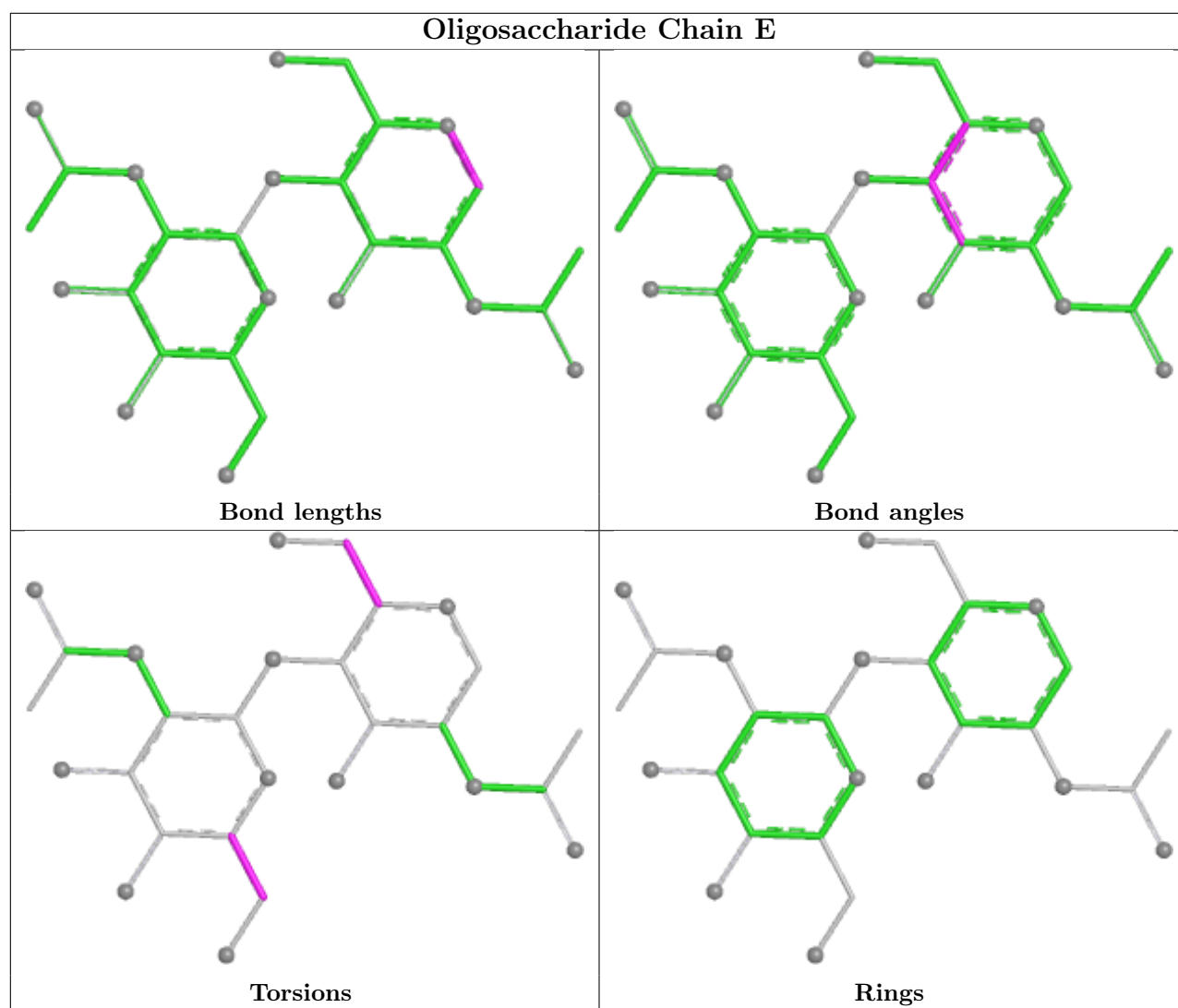
There are no ring outliers.

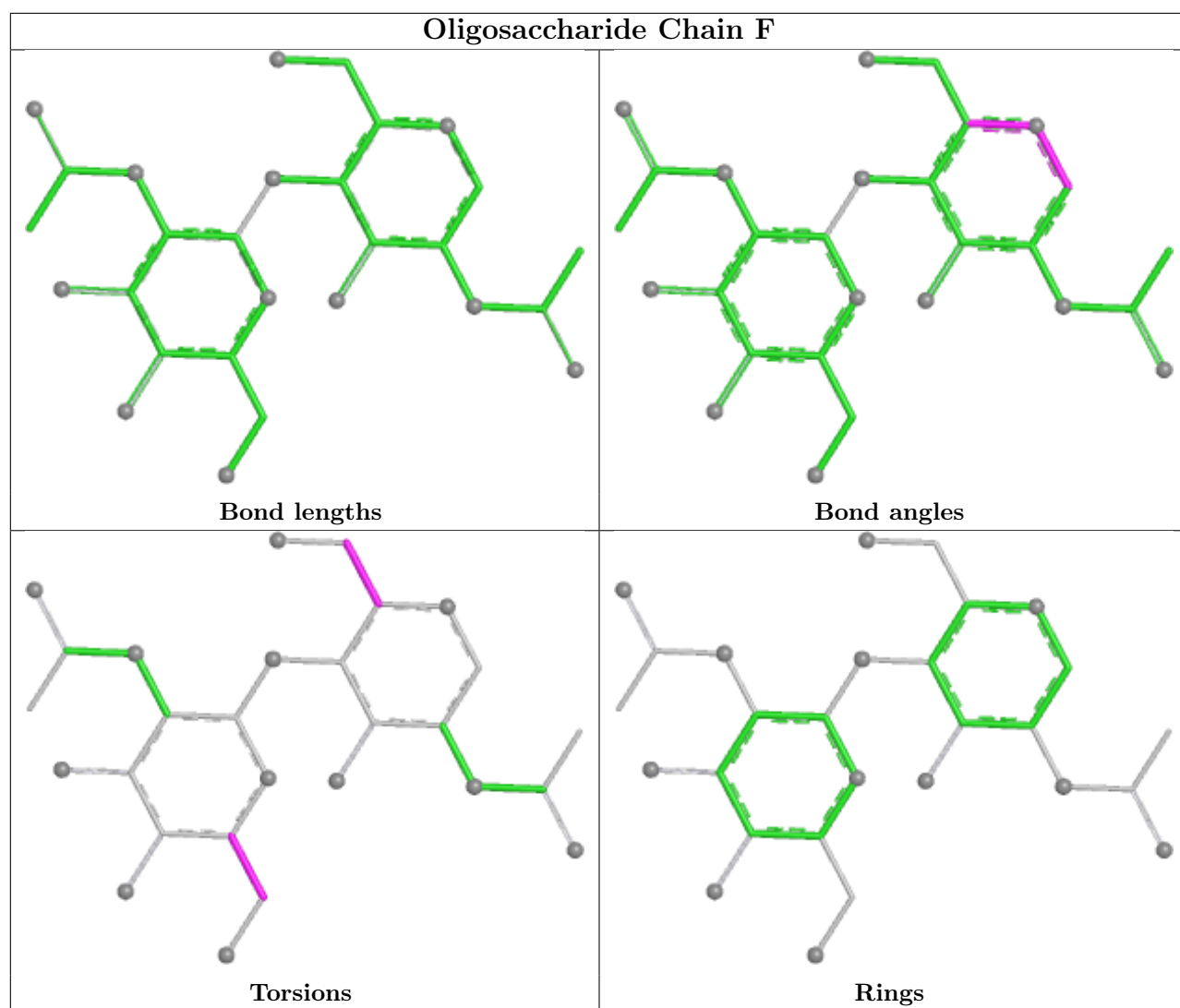
No monomer is involved in short contacts.

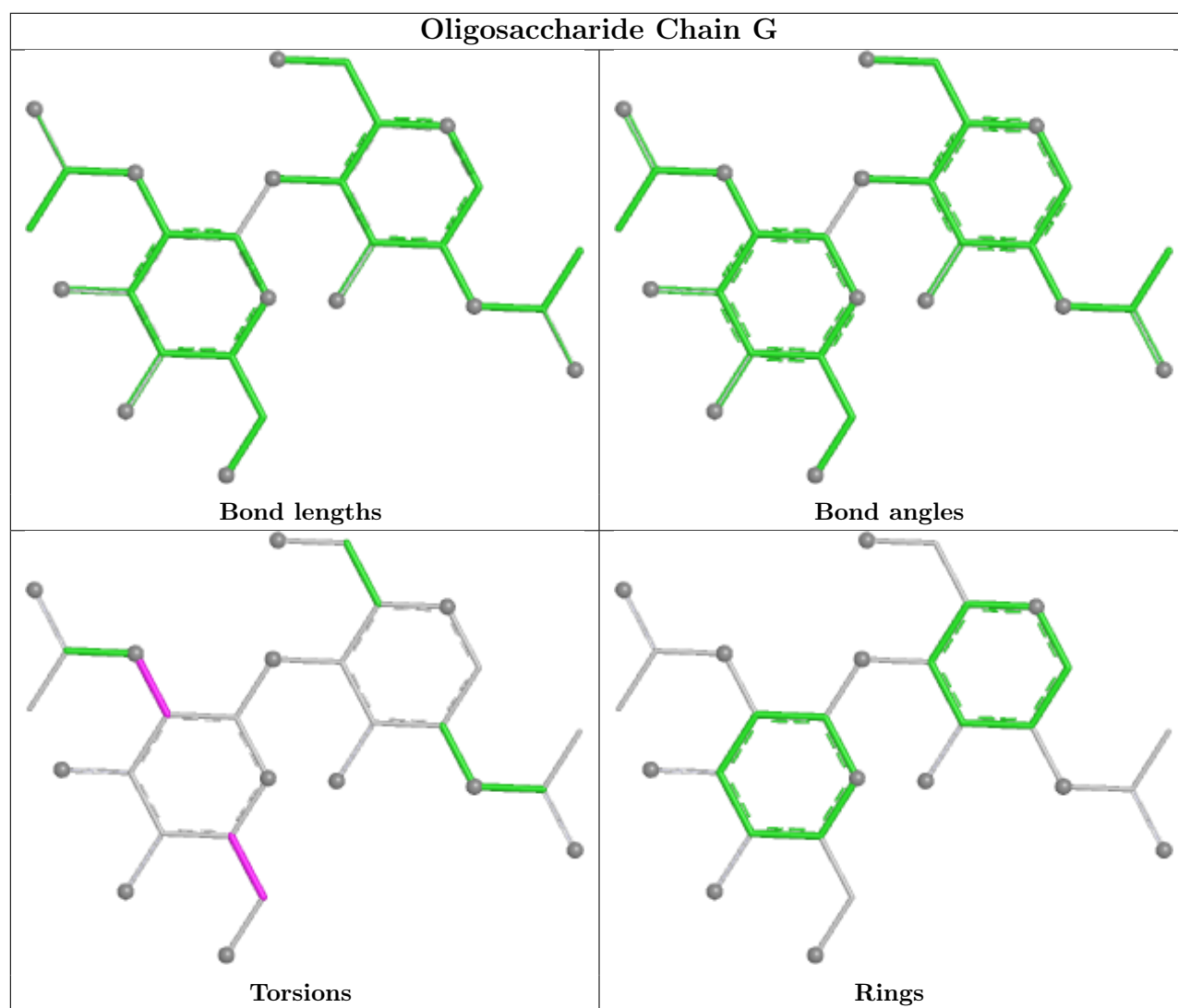
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

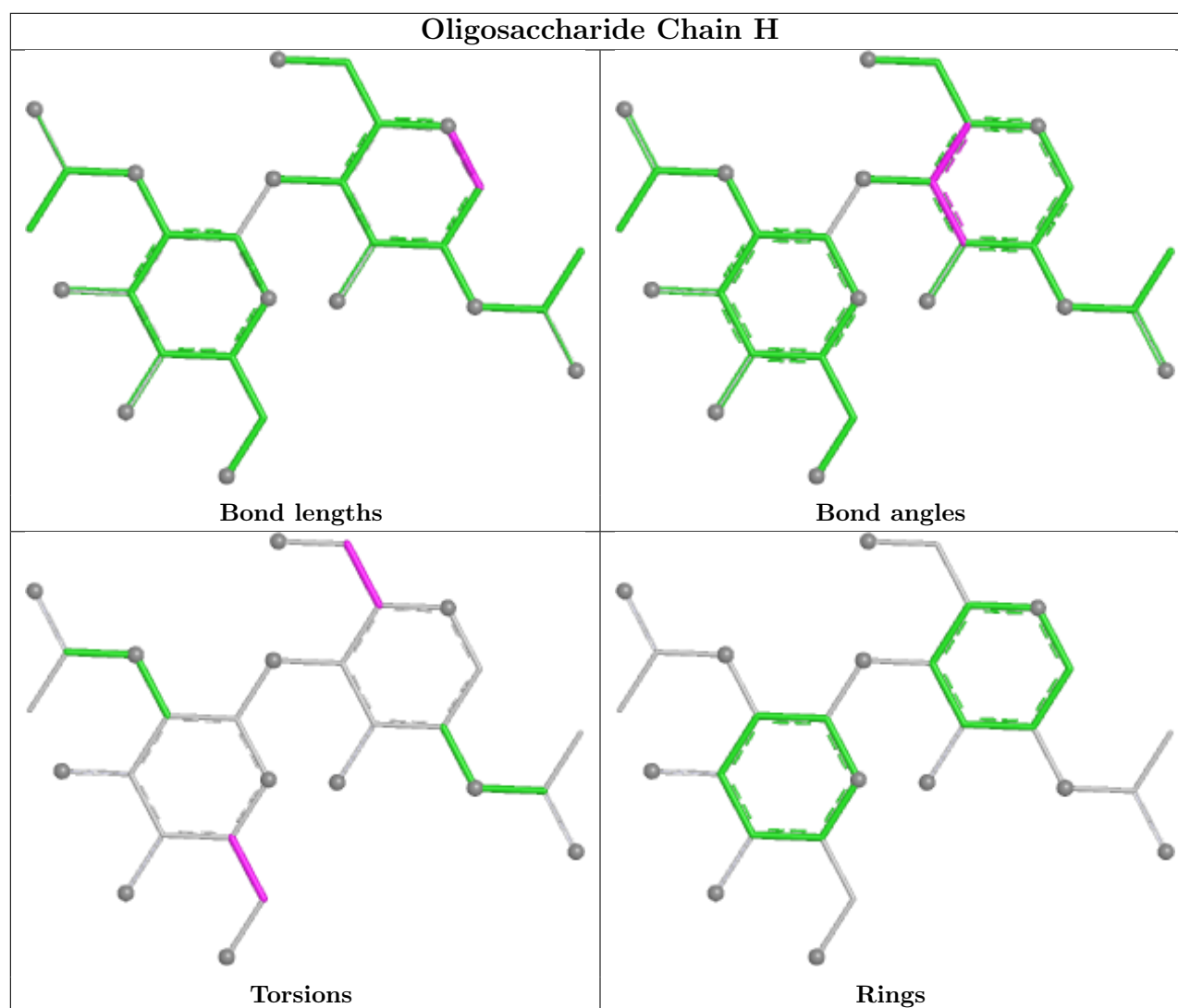












5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1111	1	14,14,15	0.58	0	17,19,21	0.69	1 (5%)
5	NAG	B	1110	1	14,14,15	0.73	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	B	1111	1	14,14,15	0.58	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1110	1	14,14,15	0.73	1 (7%)	17,19,21	1.02	1 (5%)

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	1111	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1110	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1111	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1110	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1110	NAG	O5-C1	2.58	1.48	1.43
5	B	1110	NAG	O5-C1	2.58	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1110	NAG	C1-O5-C5	3.54	116.93	112.19
5	B	1110	NAG	C1-O5-C5	3.54	116.93	112.19
5	A	1111	NAG	C1-O5-C5	2.42	115.43	112.19
5	B	1111	NAG	C1-O5-C5	2.42	115.43	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1110	NAG	O5-C5-C6-O6
5	B	1110	NAG	O5-C5-C6-O6
5	A	1110	NAG	C4-C5-C6-O6
5	B	1110	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1111	NAG	2	0
5	B	1111	NAG	2	0

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.

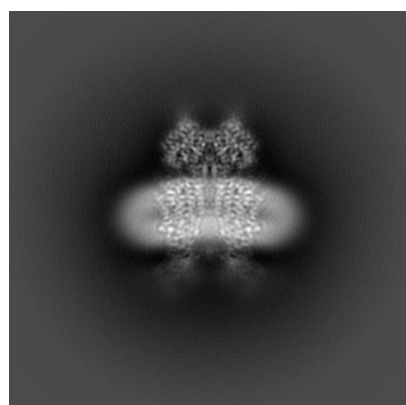
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30049. These allow visual inspection of the internal detail of the map and identification of artifacts.

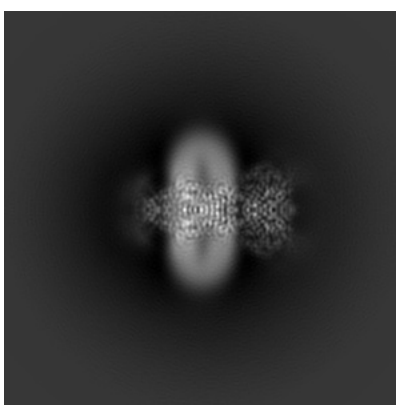
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

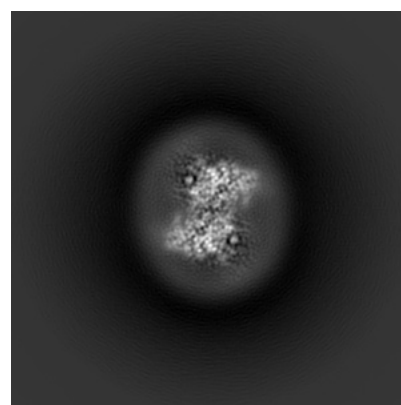
6.1.1 Primary map



X



Y

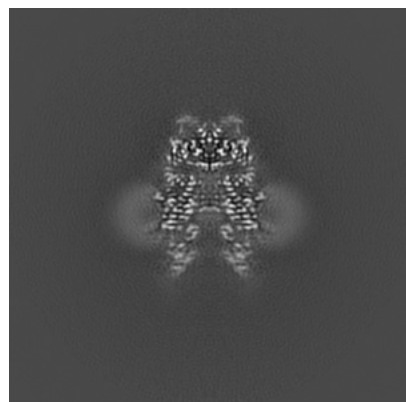


Z

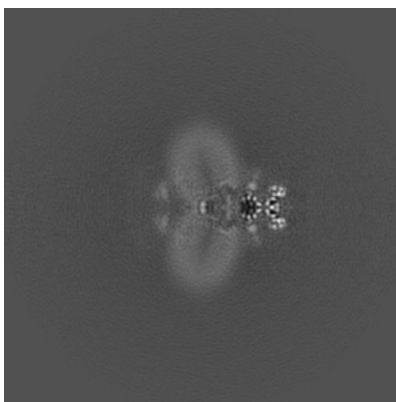
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

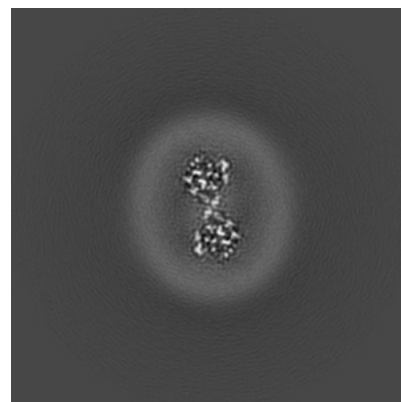
6.2.1 Primary map



X Index: 160



Y Index: 160

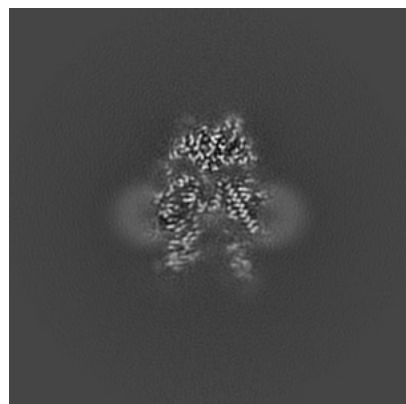


Z Index: 160

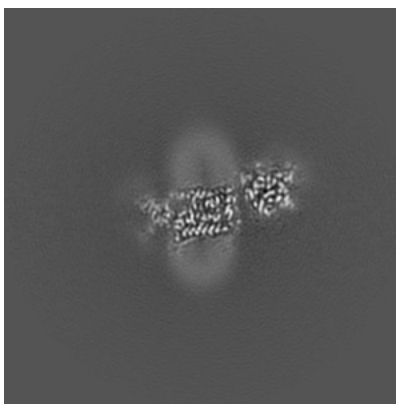
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

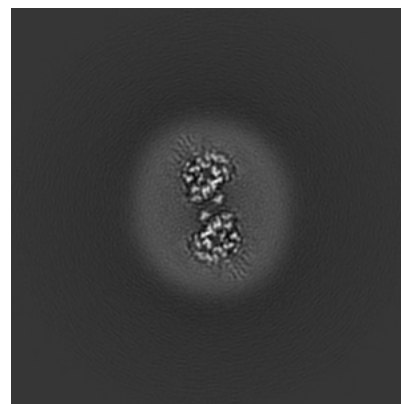
6.3.1 Primary map



X Index: 163



Y Index: 182

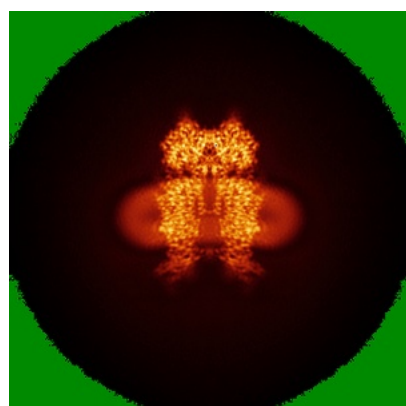


Z Index: 170

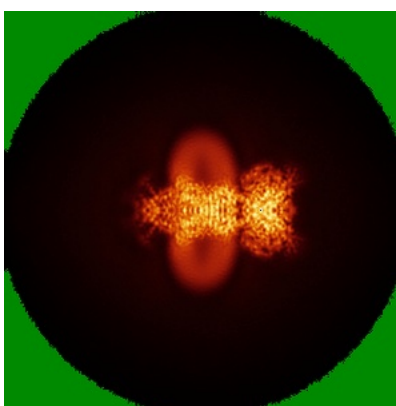
The images above show the largest variance slices of the map in three orthogonal directions.

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

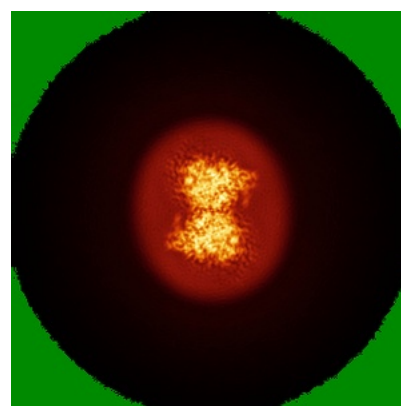
6.4.1 Primary map



X



Y

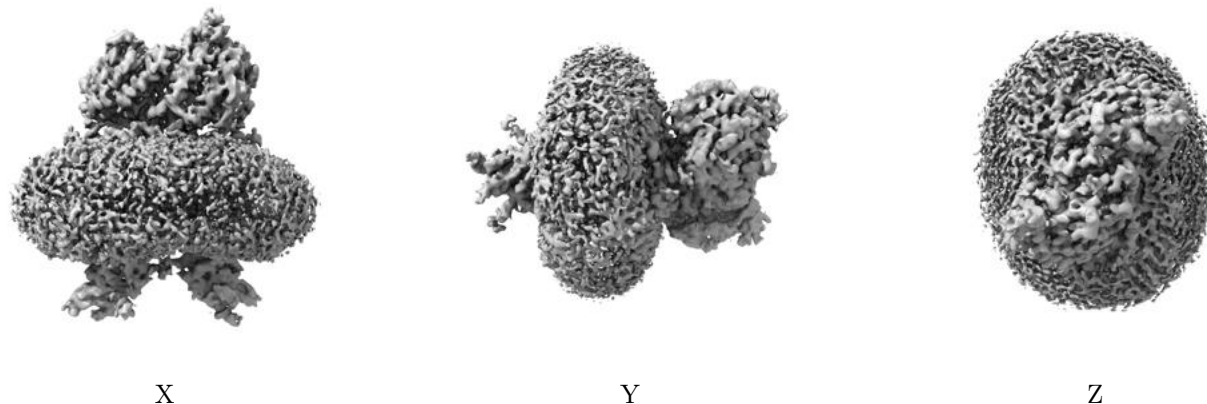


Z

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

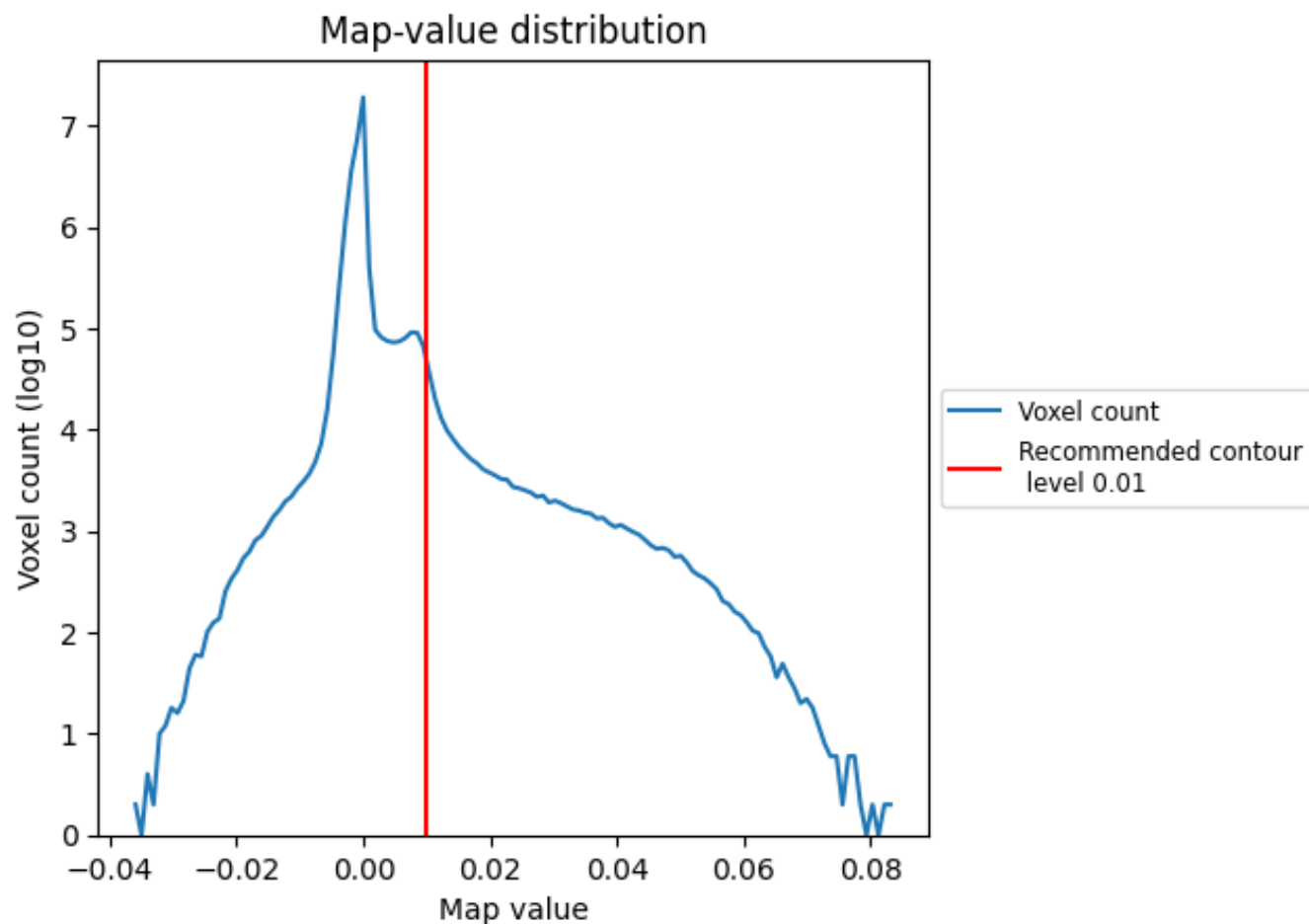
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

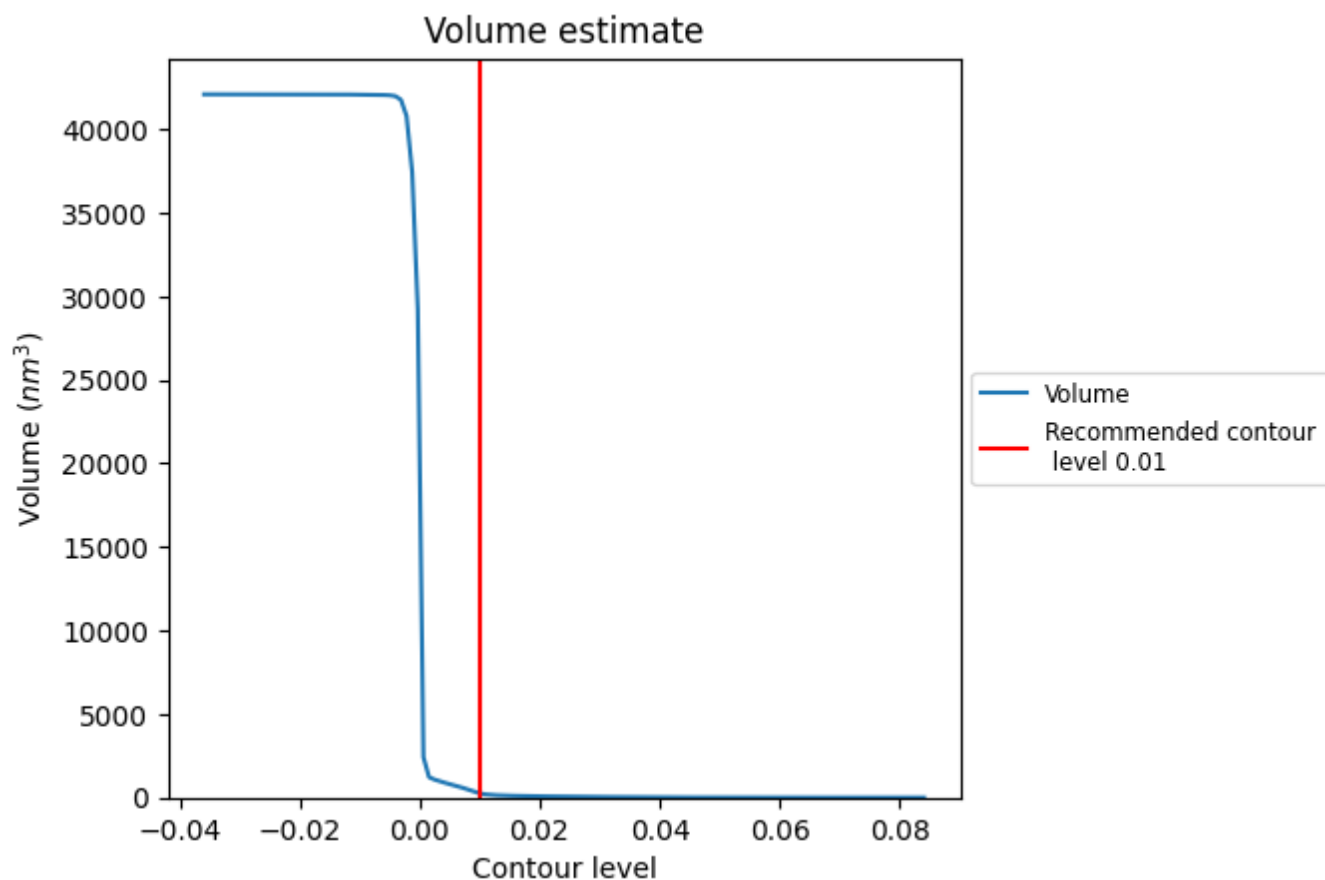
This section contains the results of statistical analysis of the map.

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.

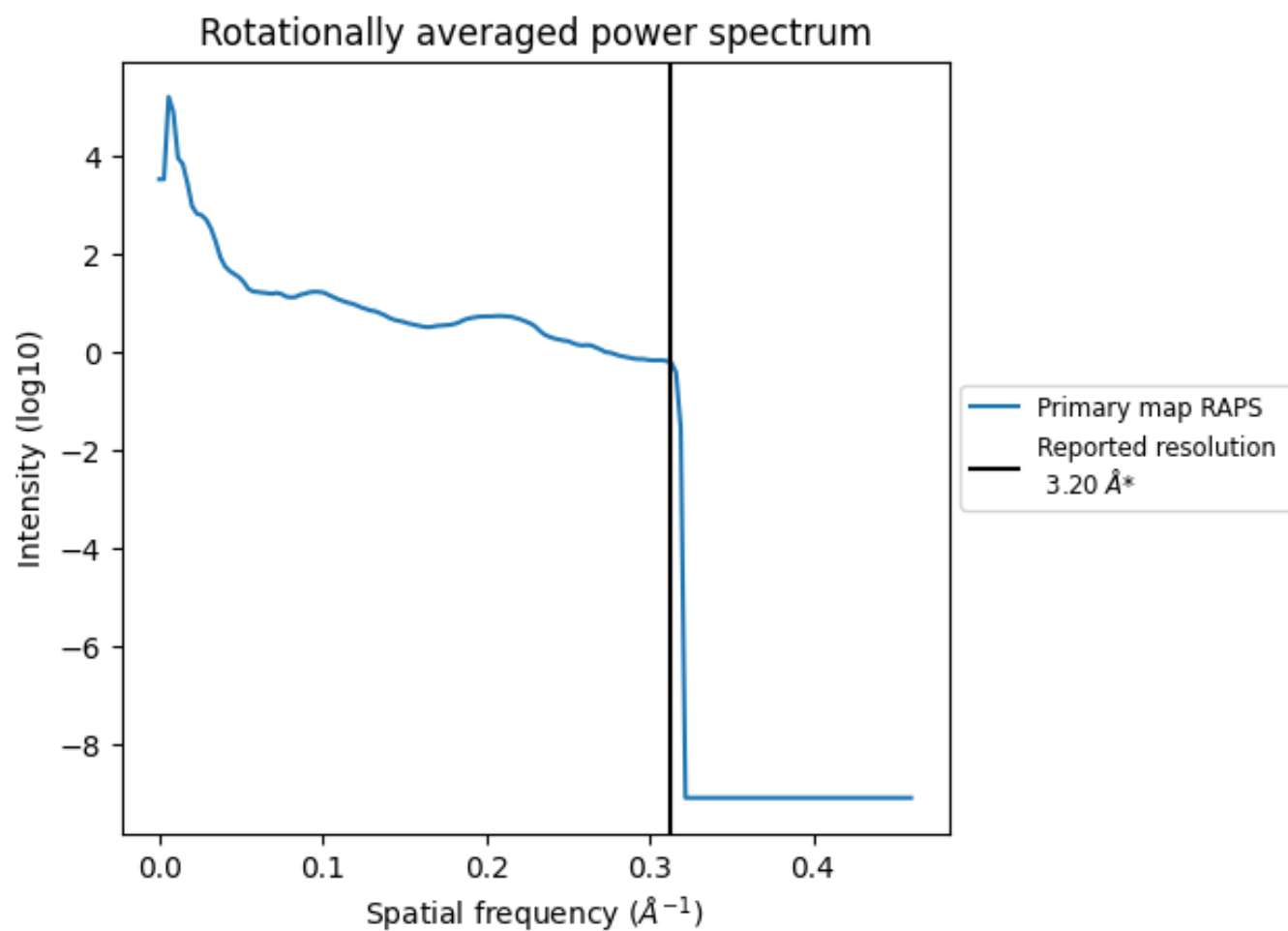
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 228 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 0.312 Å⁻¹

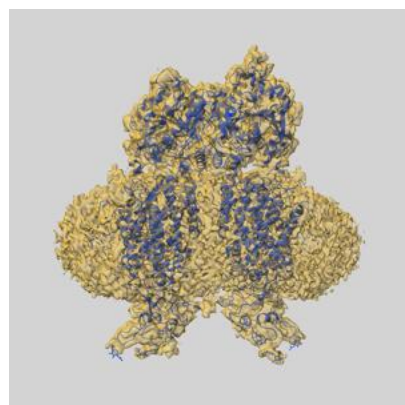
8 Fourier-Shell correlation

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

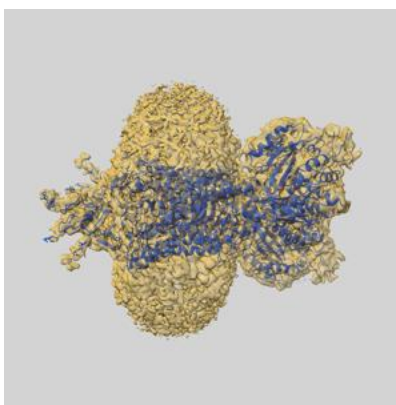
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30049 and PDB model 6M1Y. Per-residue inclusion information can be found in section 3 on page 7.

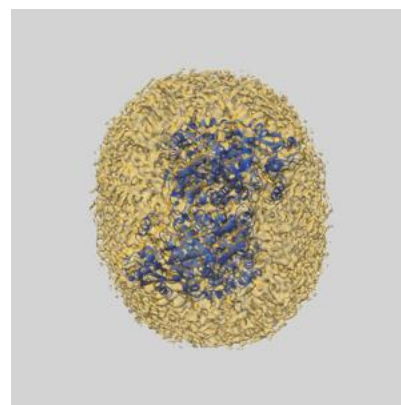
9.1 Map-model overlay [i](#)



X



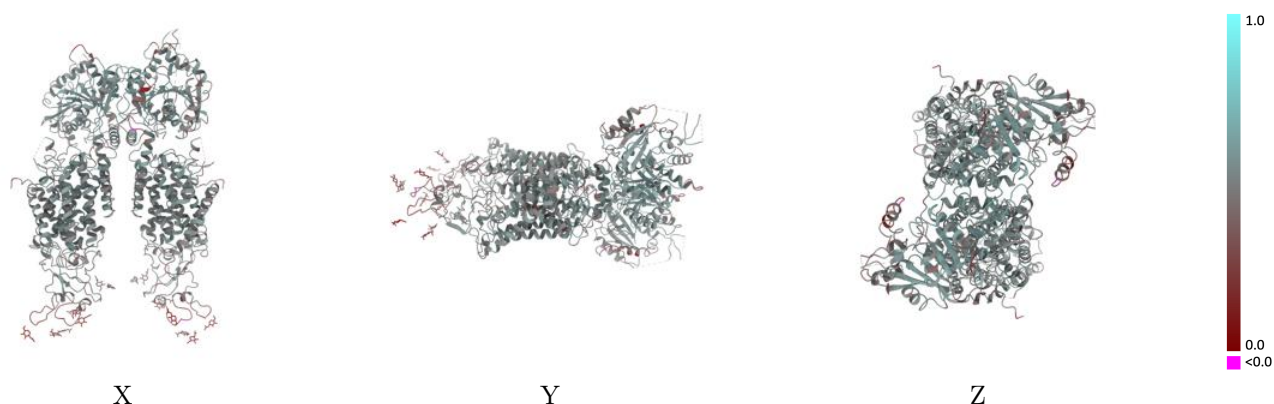
Y



Z

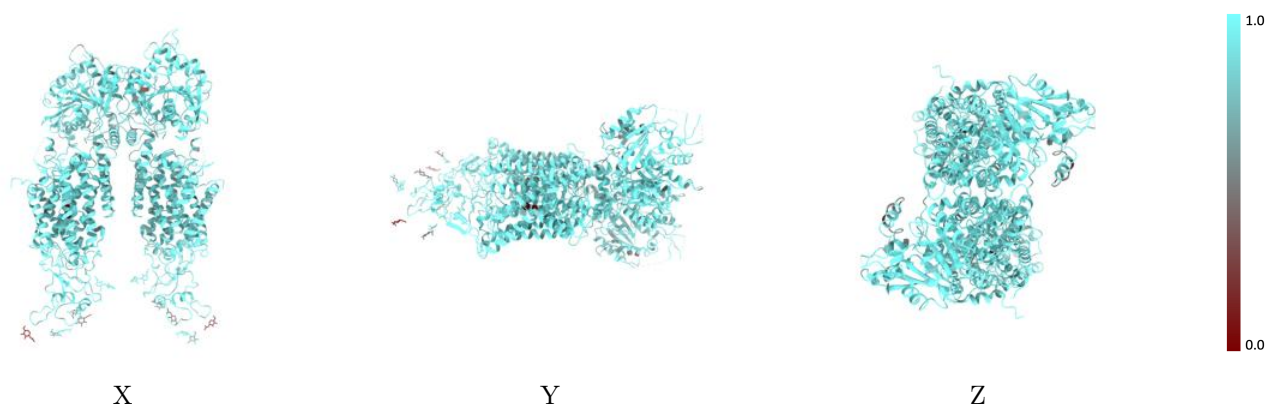
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



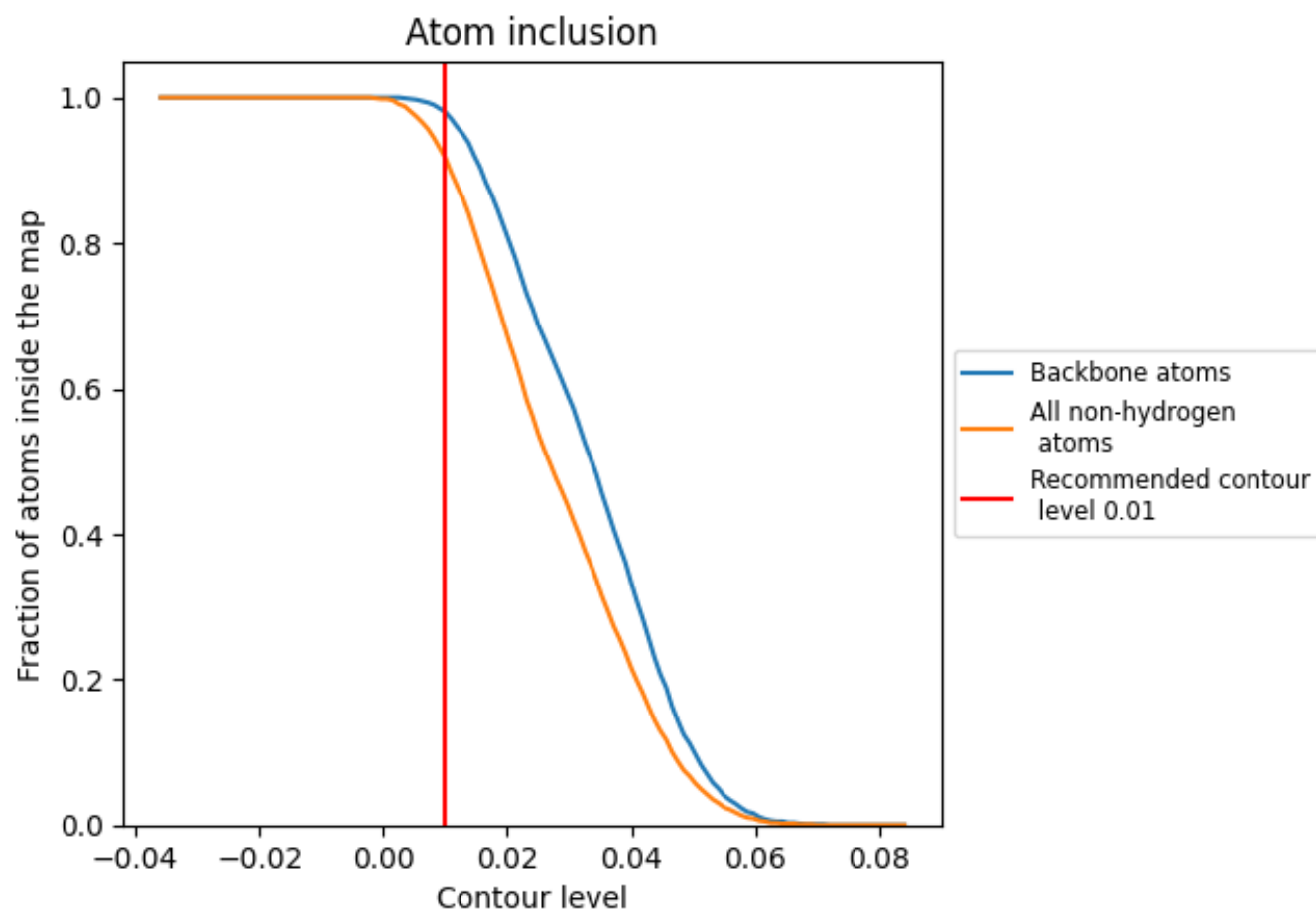
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9170	0.4940
A	0.9210	0.4960
B	0.9210	0.4960
C	0.9290	0.3950
D	0.7860	0.2680
E	0.6070	0.2800
F	0.9290	0.3990
G	0.7860	0.2720
H	0.6070	0.2670

1.0

0.0

<0.0