



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:10 AM UTC

PDB ID : 6M22 / pdb_00006m22
EMDB ID : EMD-30058
Title : KCC3 bound with DIOA
Authors : Chi, X.M.; Li, X.R.; Chen, Y.; Zhang, Y.Y.; Su, Q.; Zhou, Q.
Deposited on : 2020-02-26
Resolution : 2.70 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:

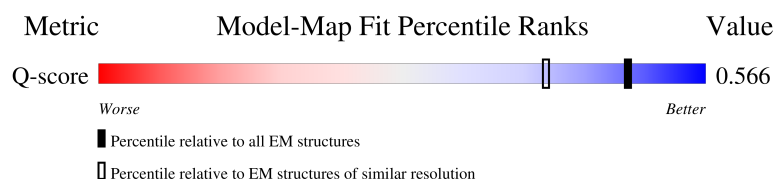
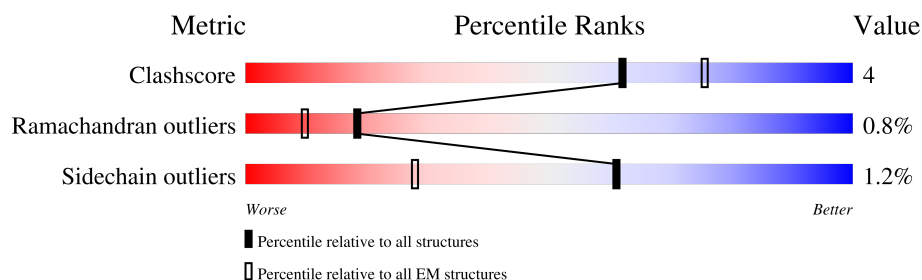
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	 73% 6% • 20%
1	B	1112	 72% 6% • 20%
2	C	2	 50% 50%
2	D	2	 50% 50%

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14028 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	885	Total	C	N	O	S	0	0
			6853	4461	1137	1207	48		
1	B	885	Total	C	N	O	S	0	0
			6853	4461	1137	1207	48		

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).

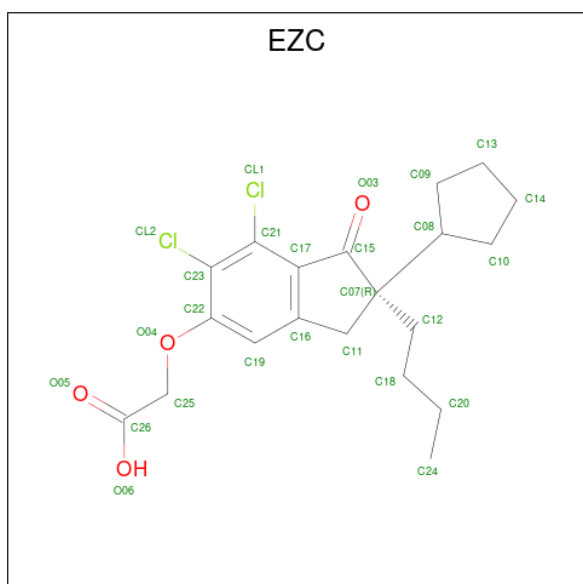
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Cl	0
			2	2	
4	B	2	Total	Cl	0
			2	2	

- 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 2-[[[(2 {R})-2-butyl-6,7-bis(chloranyl)-2-cyclopentyl-1-oxidanylidene-3 {H}-ind en-5-yl]oxy]ethanoic acid (CCD ID: EZC) (formula: C₂₀H₂₄Cl₂O₄).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 26	C 20	Cl 2	O 4	0
6	B	1	Total 26	C 20	Cl 2	O 4	0

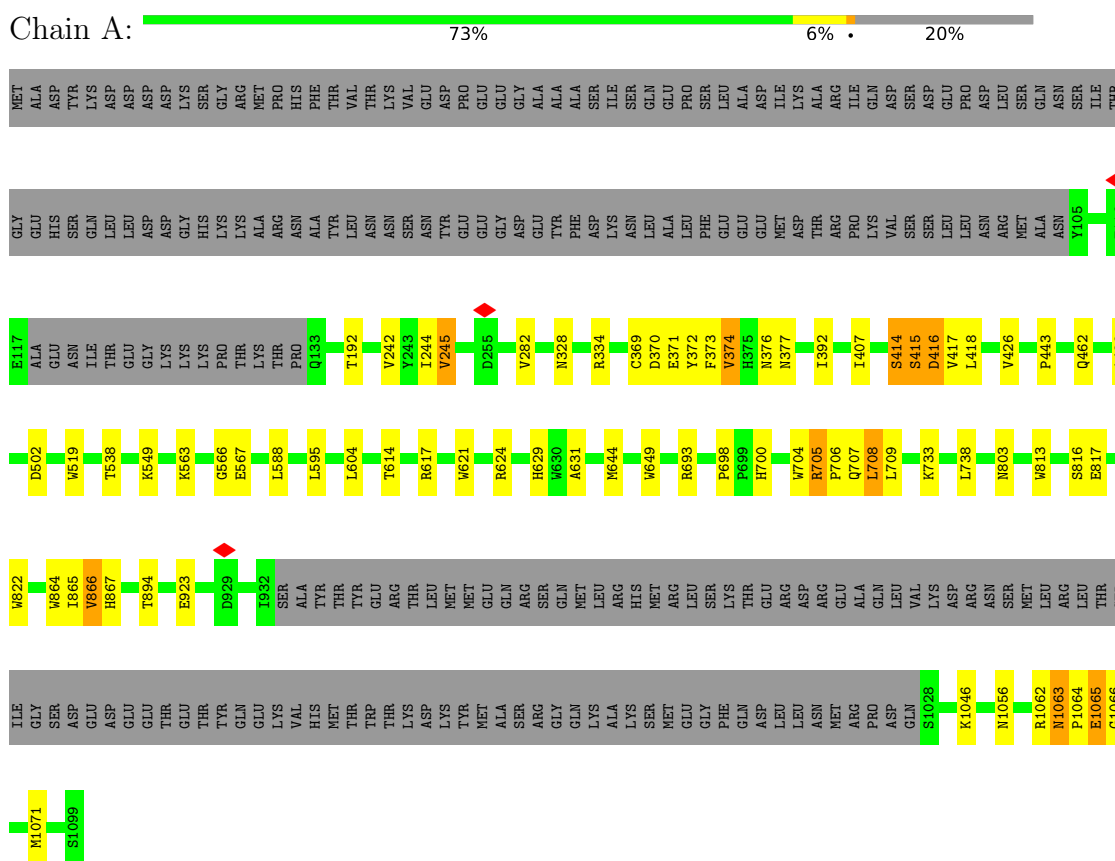
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	20	Total 20	O 20	0
7	B	20	Total 20	O 20	0

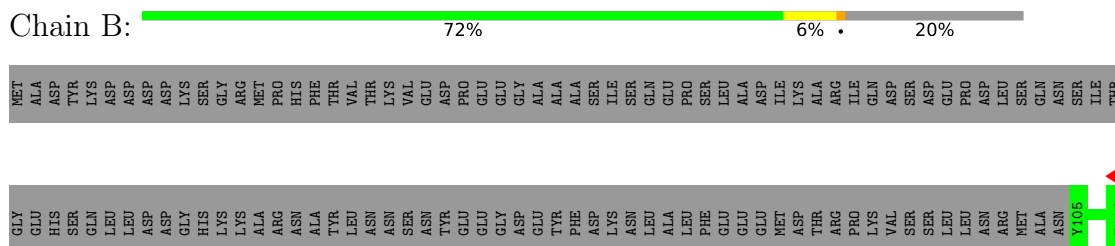
3 Residue-property plots

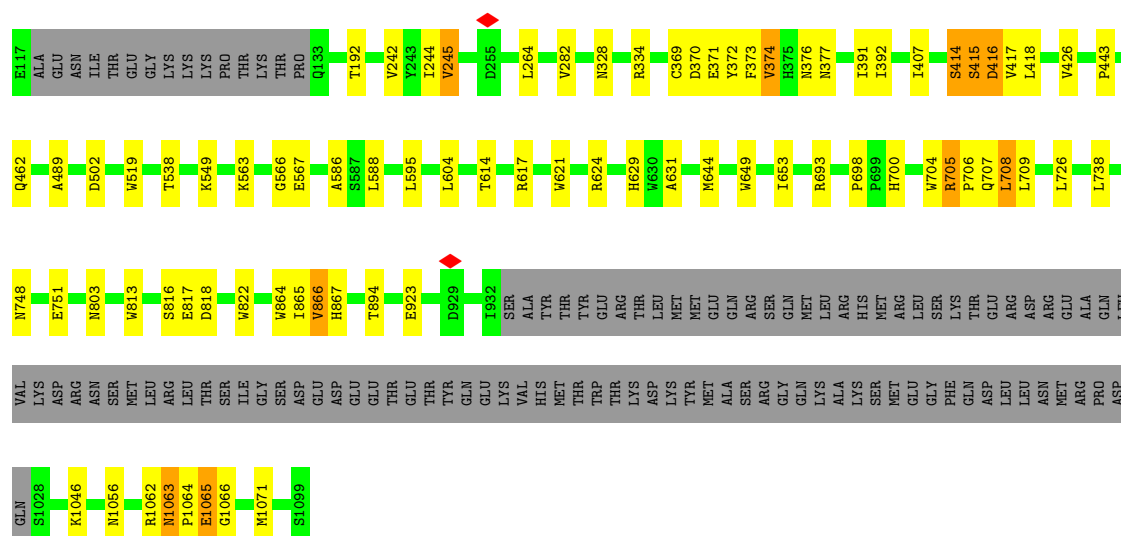
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Solute carrier family 12 member 6



- Molecule 1: Solute carrier family 12 member 6





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

Chain C:  50%

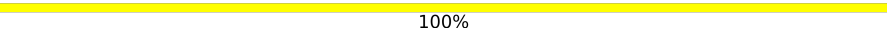


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50%



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

Chain E:  100%



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

Chain F:  50%

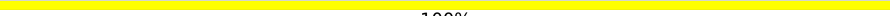


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364959	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	0.161	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	1/7011 (0.0%)	0.61	5/9518 (0.1%)
1	B	0.28	1/7011 (0.0%)	0.61	5/9518 (0.1%)
All	All	0.28	2/14022 (0.0%)	0.61	10/19036 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	ARG	C-N	6.18	1.39	1.33
1	B	705	ARG	C-N	6.18	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	LEU	N-CA-C	8.92	123.69	110.48
1	B	708	LEU	N-CA-C	8.92	123.69	110.48
1	A	374	VAL	N-CA-C	-5.39	105.12	110.62
1	B	374	VAL	N-CA-C	-5.39	105.12	110.62
1	A	709	LEU	N-CA-C	-5.13	98.89	108.02
1	B	709	LEU	N-CA-C	-5.13	98.89	108.02
1	A	549	LYS	CA-C-N	5.04	131.16	121.54
1	A	549	LYS	C-N-CA	5.04	131.16	121.54
1	B	549	LYS	CA-C-N	5.04	131.16	121.54
1	B	549	LYS	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	6853	0	6980	58	0
1	B	6853	0	6980	62	0
2	C	28	0	25	4	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	4	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	0	0
4	B	2	0	0	0	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
6	A	26	0	0	2	0
6	B	26	0	0	1	0
7	A	20	0	0	0	0
7	B	20	0	0	0	0
All	All	14028	0	14162	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (121) 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:328:ASN:ND2	2:F:1:NAG:C1	1.74	1.51
1:A:328:ASN:ND2	2:C:1:NAG:C1	1.74	1.44
1:A:328:ASN:HD22	2:C:1:NAG:C1	1.38	1.24
1:B:328:ASN:HD22	2:F:1:NAG:C1	1.38	1.22
1:B:328:ASN:HD21	2:F:1:NAG:C1	1.65	0.99
1:A:1065:GLU:OE2	1:A:1066:GLY:N	1.96	0.98
1:B:1065:GLU:OE2	1:B:1066:GLY:N	1.96	0.98
1:A:328:ASN:HD21	2:C:1:NAG:C1	1.65	0.93
1:A:417:VAL:HG22	1:A:418:LEU:H	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:VAL:HG22	1:B:418:LEU:H	1.34	0.92
1:A:415:SER:O	1:A:416:ASP:HB2	1.91	0.70
1:B:415:SER:O	1:B:416:ASP:HB2	1.91	0.69
1:A:417:VAL:HG22	1:A:418:LEU:N	2.09	0.67
1:B:417:VAL:HG22	1:B:418:LEU:N	2.09	0.66
1:B:372:TYR:HA	1:B:417:VAL:HG11	1.79	0.64
1:A:372:TYR:HA	1:A:417:VAL:HG11	1.79	0.64
1:A:1063:ASN:OD1	1:A:1063:ASN:N	2.30	0.64
1:B:371:GLU:C	1:B:373:PHE:H	2.07	0.63
1:A:371:GLU:C	1:A:373:PHE:H	2.07	0.63
1:B:1063:ASN:OD1	1:B:1063:ASN:N	2.30	0.63
1:B:328:ASN:HB2	1:B:414:SER:HB2	1.81	0.62
1:A:865:ILE:H	1:A:1056:ASN:HD21	1.47	0.62
1:A:328:ASN:HB2	1:A:414:SER:HB2	1.81	0.62
1:A:813:TRP:HB2	1:A:822:TRP:HB3	1.82	0.61
1:B:1063:ASN:O	1:B:1065:GLU:N	2.33	0.61
1:A:1063:ASN:O	1:A:1065:GLU:N	2.33	0.61
1:B:1063:ASN:C	1:B:1065:GLU:H	2.09	0.61
1:B:865:ILE:H	1:B:1056:ASN:HD21	1.47	0.60
1:B:813:TRP:HB2	1:B:822:TRP:HB3	1.82	0.60
1:B:1063:ASN:HB2	1:B:1065:GLU:HG3	1.85	0.59
1:A:1063:ASN:C	1:A:1065:GLU:H	2.09	0.59
1:A:604:LEU:HD22	1:A:644:MET:HE1	1.84	0.59
1:A:1063:ASN:HB2	1:A:1065:GLU:HG3	1.85	0.59
1:B:604:LEU:HD22	1:B:644:MET:HE1	1.84	0.57
1:B:629:HIS:HD2	1:B:631:ALA:H	1.55	0.55
1:A:629:HIS:HD2	1:A:631:ALA:H	1.55	0.55
6:A:1112:EZC:C15	6:A:1112:EZC:C20	2.85	0.54
1:B:923:GLU:OE1	1:B:1046:LYS:NZ	2.41	0.54
1:A:369:CYS:SG	1:A:373:PHE:HD1	2.31	0.54
1:A:864:TRP:HE3	1:A:894:THR:HG22	1.73	0.53
1:B:369:CYS:SG	1:B:373:PHE:HD1	2.31	0.53
1:B:864:TRP:HE3	1:B:894:THR:HG22	1.73	0.53
1:A:923:GLU:OE1	1:A:1046:LYS:NZ	2.41	0.53
1:B:707:GLN:NE2	1:B:738:LEU:H	2.07	0.53
1:A:462:GLN:HG3	1:A:624:ARG:HH21	1.73	0.53
1:A:707:GLN:NE2	1:A:738:LEU:H	2.07	0.53
1:B:328:ASN:HD21	2:F:1:NAG:C2	2.21	0.53
1:A:392:ILE:HD12	1:A:489:ALA:HB2	1.91	0.52
1:B:462:GLN:HG3	1:B:624:ARG:HH21	1.73	0.52
1:B:614:THR:HB	1:B:621:TRP:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:HD21	2:C:1:NAG:C2	2.21	0.52
1:A:417:VAL:CG2	1:A:418:LEU:H	2.16	0.52
1:B:392:ILE:HD12	1:B:489:ALA:HB2	1.91	0.51
1:A:617:ARG:NH1	6:A:1112:EZC:O05	2.43	0.50
1:A:614:THR:HB	1:A:621:TRP:HE1	1.75	0.50
1:B:617:ARG:NH1	6:B:1112:EZC:O05	2.45	0.50
1:B:372:TYR:HA	1:B:417:VAL:CG1	2.42	0.49
1:A:244:ILE:HG22	1:A:245:VAL:HG22	1.94	0.49
1:B:244:ILE:HD13	1:B:519:TRP:HZ3	1.78	0.48
1:B:369:CYS:SG	1:B:370:ASP:N	2.86	0.48
1:B:244:ILE:HG22	1:B:245:VAL:HG22	1.94	0.48
1:A:372:TYR:HA	1:A:417:VAL:CG1	2.42	0.48
1:A:244:ILE:HD13	1:A:519:TRP:HZ3	1.78	0.48
1:A:369:CYS:SG	1:A:373:PHE:CD1	3.07	0.48
1:A:369:CYS:SG	1:A:370:ASP:N	2.86	0.47
1:A:705:ARG:HD3	1:A:705:ARG:HA	1.61	0.47
1:B:369:CYS:SG	1:B:373:PHE:CD1	3.07	0.47
1:A:1063:ASN:C	1:A:1065:GLU:N	2.73	0.47
1:B:192:THR:HG22	1:B:462:GLN:HG2	1.97	0.47
1:A:371:GLU:C	1:A:373:PHE:N	2.73	0.46
1:B:563:LYS:HB2	1:B:567:GLU:HB2	1.98	0.46
1:A:563:LYS:HB2	1:A:567:GLU:HB2	1.98	0.46
1:A:617:ARG:NH2	1:A:693:ARG:O	2.49	0.45
1:B:1063:ASN:C	1:B:1065:GLU:N	2.73	0.45
1:A:192:THR:HG22	1:A:462:GLN:HG2	1.97	0.45
1:B:817:GLU:HB3	1:B:818:ASP:H	1.60	0.45
1:A:704:TRP:CH2	1:A:706:PRO:HB3	2.52	0.45
1:B:617:ARG:NH2	1:B:693:ARG:O	2.49	0.45
1:B:866:VAL:O	1:B:867:HIS:CD2	2.70	0.45
1:B:704:TRP:CH2	1:B:706:PRO:HB3	2.52	0.45
1:B:748:ASN:ND2	1:B:751:GLU:OE1	2.48	0.44
1:A:866:VAL:O	1:A:867:HIS:CD2	2.70	0.44
1:B:334:ARG:NH1	1:B:502:ASP:OD1	2.51	0.44
1:B:707:GLN:H	1:B:803:ASN:HB2	1.83	0.43
1:A:334:ARG:NH1	1:A:502:ASP:OD1	2.51	0.43
1:B:629:HIS:CD2	1:B:631:ALA:H	2.36	0.43
1:A:700:HIS:O	1:A:700:HIS:ND1	2.51	0.43
1:A:707:GLN:H	1:A:803:ASN:HB2	1.83	0.43
1:B:417:VAL:CG2	1:B:418:LEU:H	2.16	0.43
1:B:443:PRO:HB3	1:B:595:LEU:HD11	2.00	0.43
1:A:443:PRO:HB3	1:A:595:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:VAL:O	1:A:867:HIS:CG	2.72	0.43
1:B:700:HIS:O	1:B:700:HIS:ND1	2.51	0.43
1:B:372:TYR:CA	1:B:417:VAL:HG11	2.46	0.42
1:B:816:SER:OG	1:B:817:GLU:N	2.52	0.42
1:B:866:VAL:O	1:B:867:HIS:CG	2.72	0.42
1:A:1065:GLU:CD	1:A:1066:GLY:N	2.73	0.42
1:A:282:VAL:HG13	1:A:538:THR:HG22	2.01	0.42
1:A:563:LYS:N	1:A:566:GLY:O	2.53	0.42
1:B:563:LYS:N	1:B:566:GLY:O	2.53	0.42
1:A:704:TRP:O	1:A:705:ARG:NH2	2.53	0.42
1:A:816:SER:OG	1:A:817:GLU:N	2.52	0.42
1:A:629:HIS:CD2	1:A:631:ALA:H	2.36	0.42
1:B:282:VAL:HG13	1:B:538:THR:HG22	2.01	0.42
1:B:407:ILE:HD12	1:B:426:VAL:HG12	2.02	0.41
1:B:1065:GLU:CD	1:B:1066:GLY:N	2.73	0.41
1:B:822:TRP:HB2	1:B:1071:MET:HE2	2.02	0.41
1:B:704:TRP:O	1:B:705:ARG:NH2	2.53	0.41
1:A:865:ILE:H	1:A:1056:ASN:ND2	2.17	0.41
1:A:407:ILE:HD12	1:A:426:VAL:HG12	2.02	0.41
1:A:733:LYS:HA	1:A:733:LYS:HD2	1.88	0.41
1:B:370:ASP:O	1:B:374:VAL:HG13	2.21	0.41
1:A:822:TRP:HB2	1:A:1071:MET:HE2	2.02	0.41
1:B:705:ARG:HA	1:B:705:ARG:HD3	1.61	0.41
1:A:370:ASP:O	1:A:374:VAL:HG13	2.21	0.40
1:A:372:TYR:CA	1:A:417:VAL:HG11	2.46	0.40
1:B:865:ILE:H	1:B:1056:ASN:ND2	2.17	0.40
1:B:264:LEU:HD22	1:B:586:ALA:HB3	2.03	0.40
1:B:391:ILE:HD12	1:B:391:ILE:HA	1.98	0.40
1:B:653:ILE:HD13	1:B:653:ILE:HA	1.99	0.40
1:B:726:LEU:HD23	1:B:726: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	879/1112 (79%)	806 (92%)	66 (8%)	7 (1%)	16	37
1	B	879/1112 (79%)	806 (92%)	66 (8%)	7 (1%)	16	37
All	All	1758/2224 (79%)	1612 (92%)	132 (8%)	14 (1%)	18	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	SER
1	A	416	ASP
1	B	415	SER
1	B	416	ASP
1	A	376	ASN
1	A	588	LEU
1	B	376	ASN
1	B	588	LEU
1	A	1064	PRO
1	B	1064	PRO
1	A	866	VAL
1	B	866	VAL
1	A	698	PRO
1	B	698	PRO

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	739/942 (78%)	730 (99%)	9 (1%)	63	84
1	B	739/942 (78%)	730 (99%)	9 (1%)	63	84
All	All	1478/1884 (78%)	1460 (99%)	18 (1%)	61	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	A	245	VAL
1	A	377	ASN
1	A	414	SER
1	A	649	TRP
1	A	708	LEU
1	A	1062	ARG
1	A	1063	ASN
1	A	1065	GLU
1	B	242	VAL
1	B	245	VAL
1	B	377	ASN
1	B	414	SER
1	B	649	TRP
1	B	708	LEU
1	B	1062	ARG
1	B	1063	ASN
1	B	1065	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	320	HIS
1	A	328	ASN
1	A	375	HIS
1	A	607	ASN
1	A	629	HIS
1	A	707	GLN
1	A	761	GLN
1	A	777	GLN
1	A	867	HIS
1	A	1040	ASN
1	A	1056	ASN
1	B	110	GLN
1	B	320	HIS
1	B	328	ASN
1	B	375	HIS
1	B	607	ASN
1	B	629	HIS
1	B	707	GLN
1	B	722	HIS
1	B	752	ASN

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Mol	Chain	Res	Type
1	B	761	GLN
1	B	777	GLN
1	B	793	GLN
1	B	867	HIS
1	B	1040	ASN
1	B	1056	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 ⓘ

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	2	14,14,15	0.48	0	17,19,21	0.61	0
2	NAG	C	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	D	1	2,1	14,14,15	0.66	0	17,19,21	0.76	1 (5%)
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	0.49	0
2	NAG	E	1	2,1	14,14,15	0.73	1 (7%)	17,19,21	0.91	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	NAG	F	1	2	14,14,15	0.48	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	G	1	2,1	14,14,15	0.66	0	17,19,21	0.76	1 (5%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	0.49	0
2	NAG	H	1	2,1	14,14,15	0.73	1 (7%)	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.68	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
2	NAG	C	1	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	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	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	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	-2.49	1.39	1.43
2	H	1	NAG	O5-C1	-2.49	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	G	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	E	2	NAG	C1-O5-C5	2.11	115.01	112.19
2	H	2	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

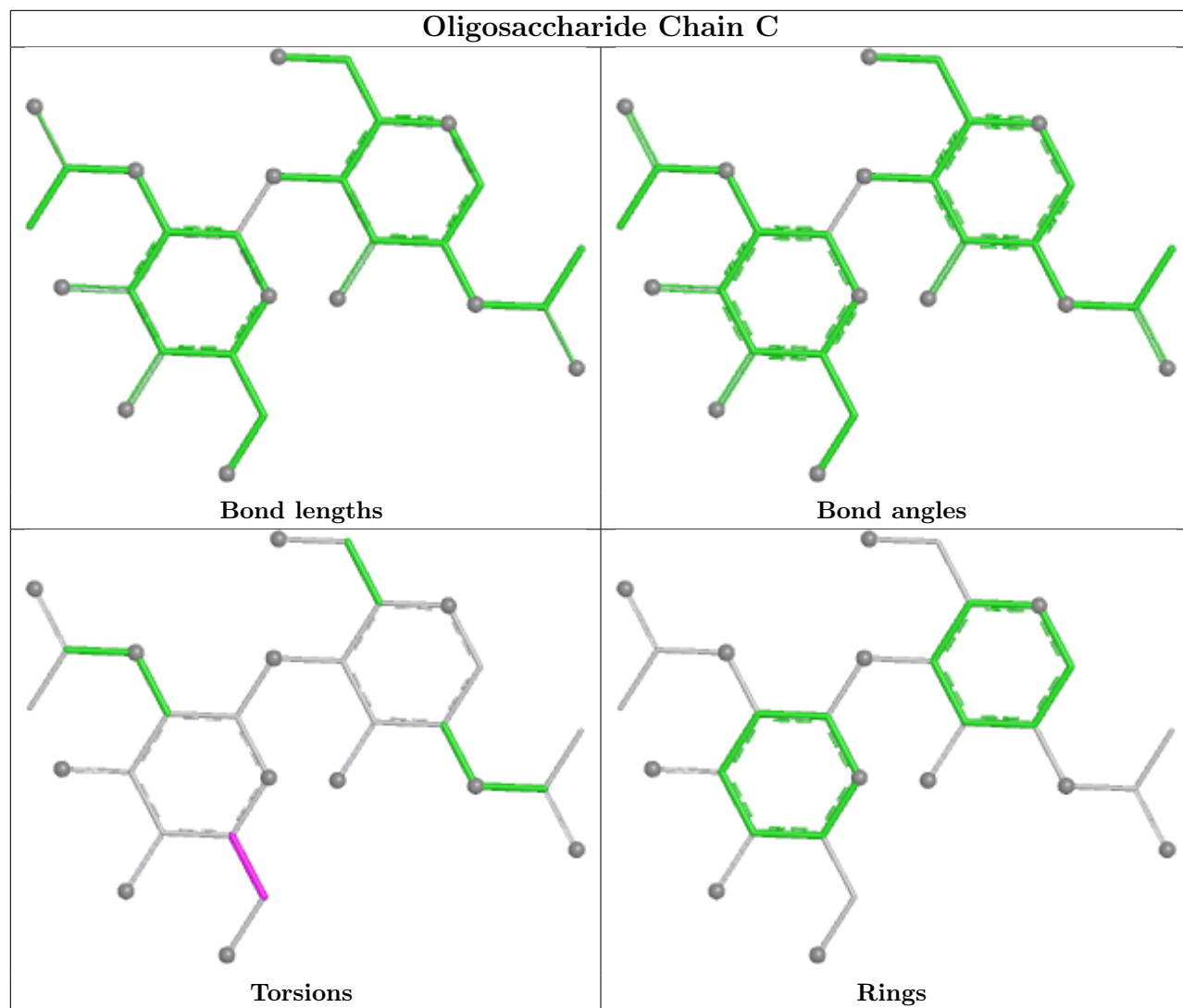
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6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

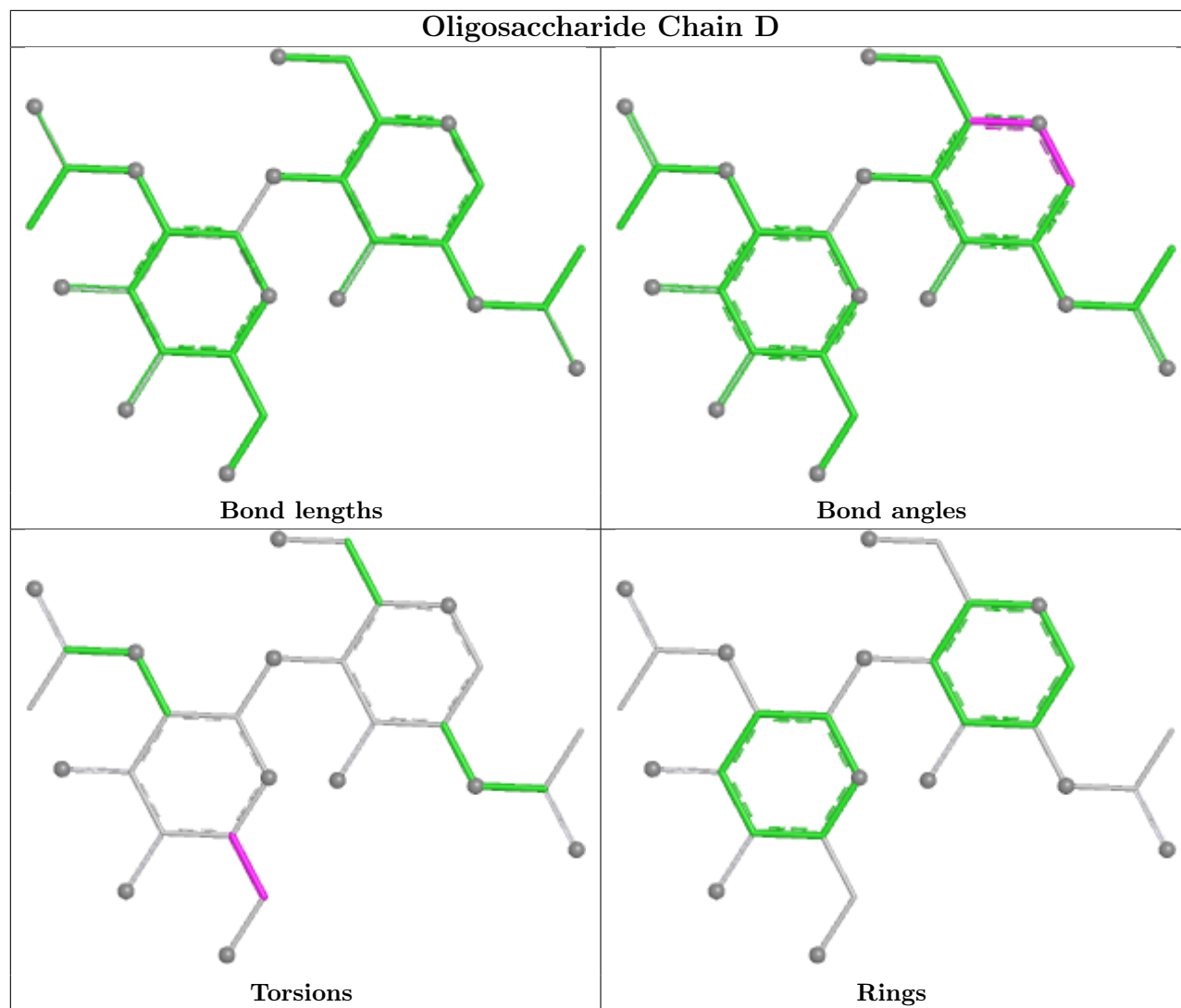
There are no ring outliers.

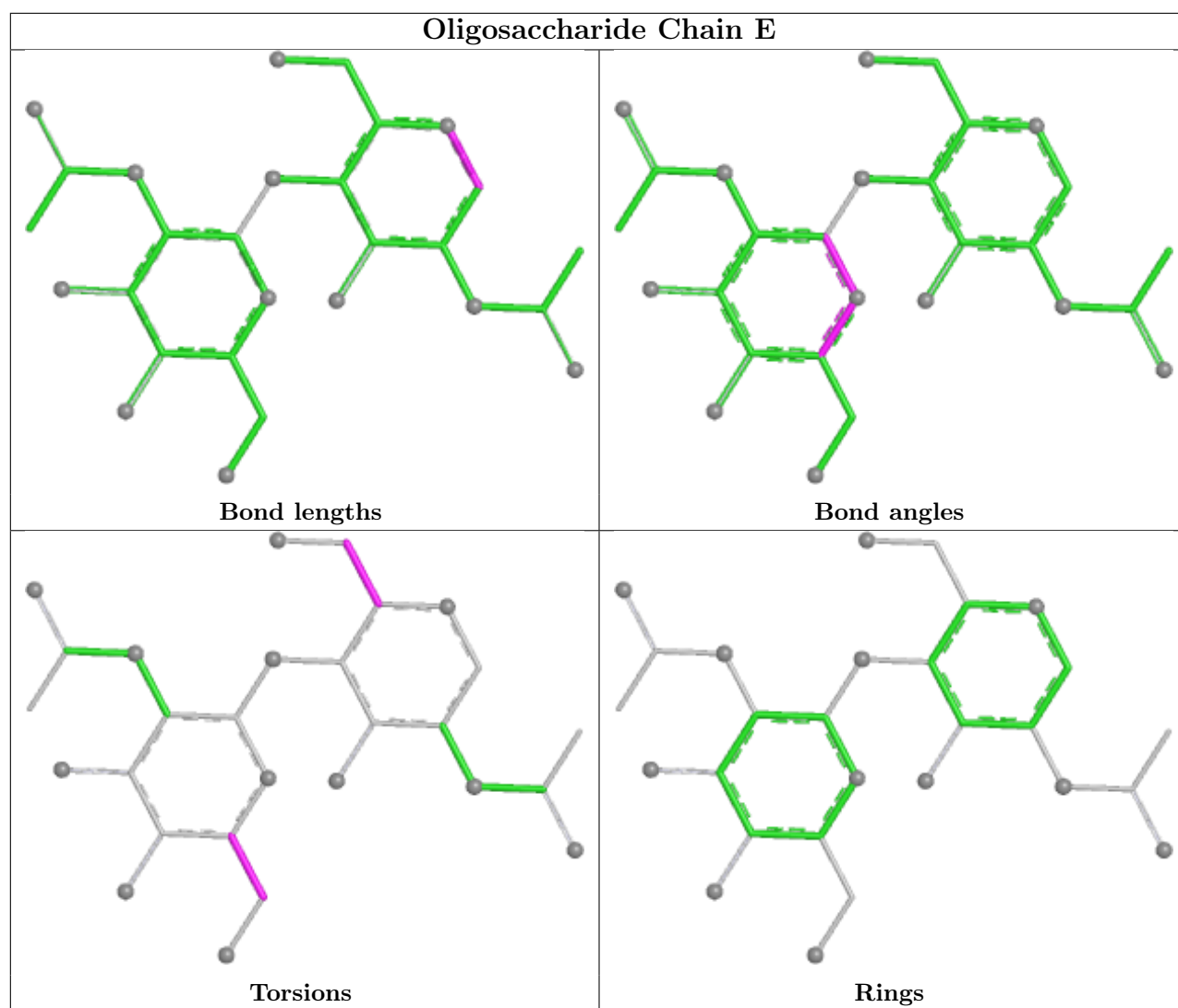
2 monomers are involved in 8 short contacts:

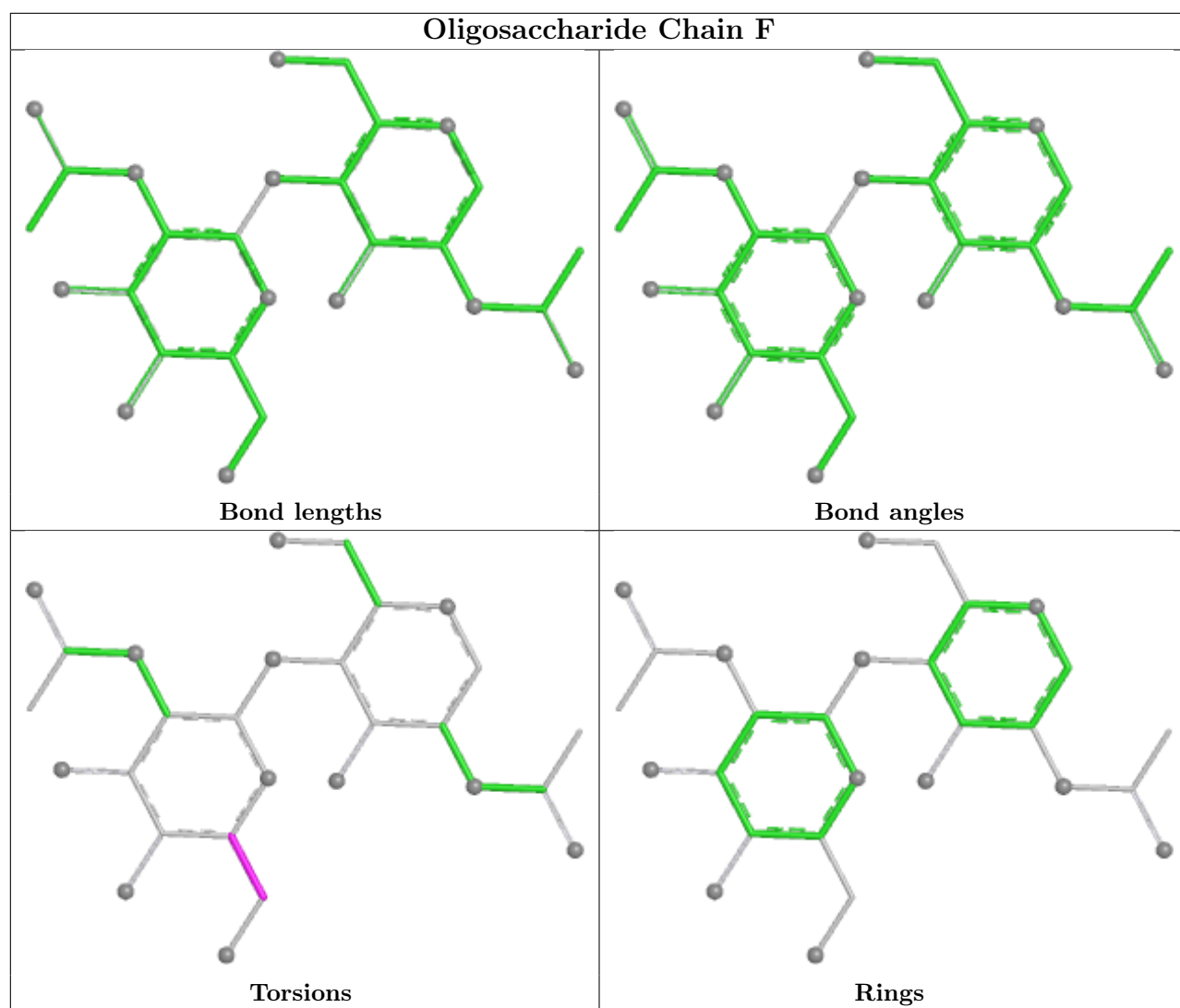
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	4	0
2	F	1	NAG	4	0

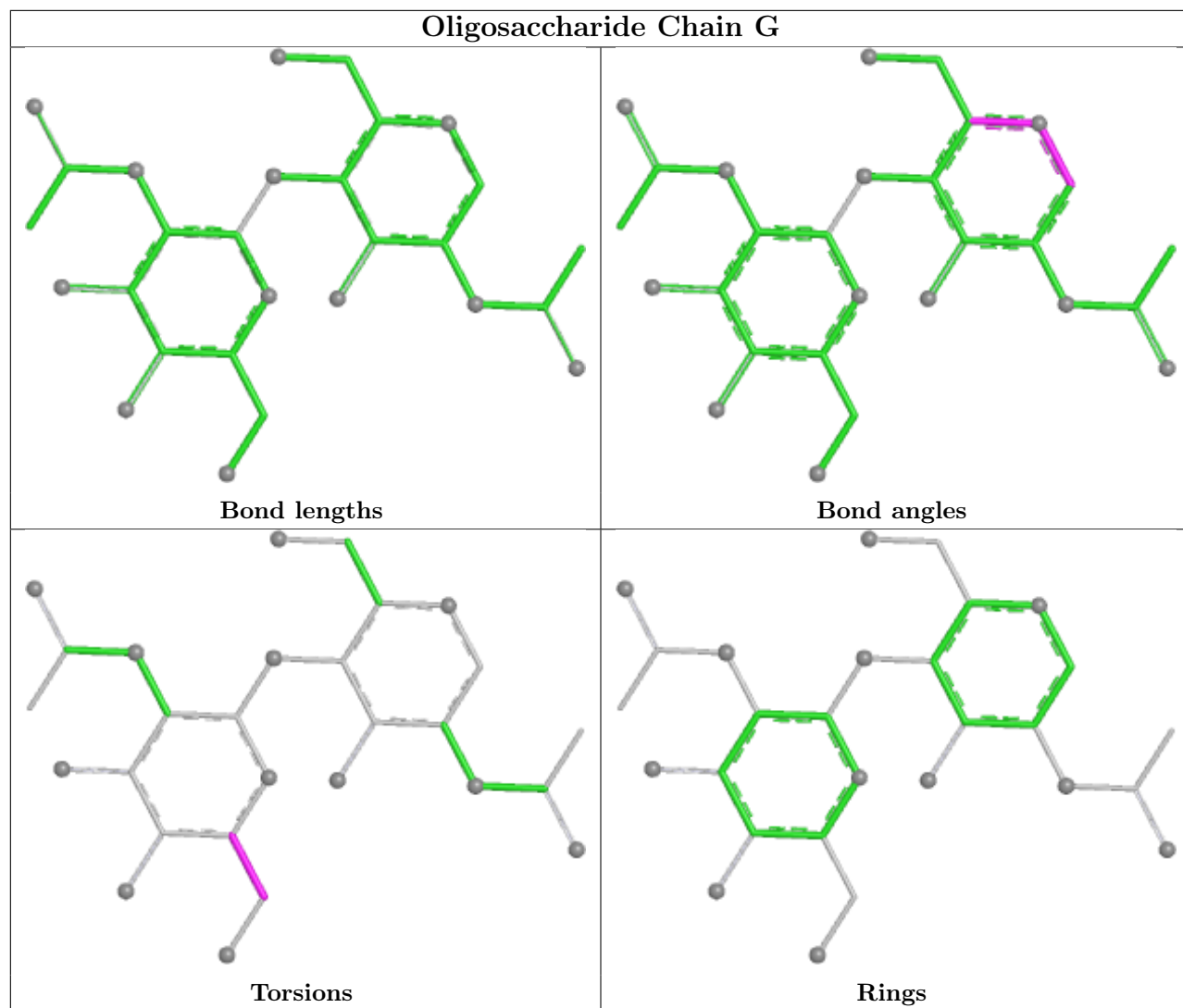
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

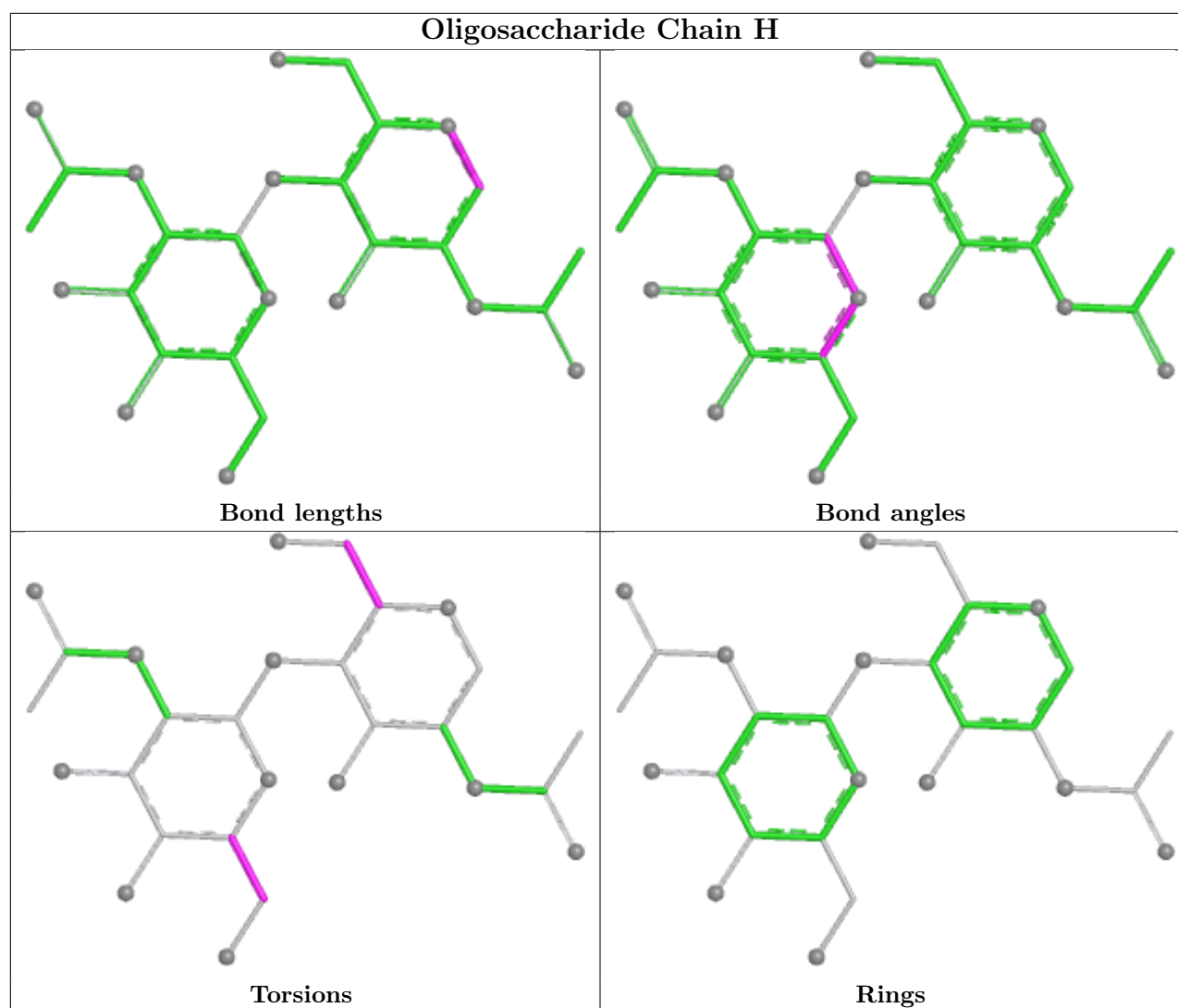












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	0.46	0	17,19,21	0.48	0
5	NAG	A	1110	1	14,14,15	1.32	1 (7%)	17,19,21	1.47	1 (5%)
6	EZC	A	1112	-	26,28,28	5.97	15 (57%)	31,41,41	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EZC	B	1112	-	26,28,28	5.92	15 (57%)	31,41,41	1.29	5 (16%)
5	NAG	B	1111	1	14,14,15	0.46	0	17,19,21	0.48	0
5	NAG	B	1110	1	14,14,15	1.32	1 (7%)	17,19,21	1.47	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	-	1/6/23/26	0/1/1/1
5	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
6	EZC	A	1112	-	-	5/16/38/38	0/3/3/3
6	EZC	B	1112	-	-	3/16/38/38	0/3/3/3
5	NAG	B	1111	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1110	1	-	0/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1112	EZC	C11-C07	-19.41	1.33	1.55
6	B	1112	EZC	C11-C07	-19.39	1.33	1.55
6	A	1112	EZC	C11-C16	10.33	1.63	1.50
6	A	1112	EZC	C19-C16	10.19	1.55	1.39
6	B	1112	EZC	C11-C16	9.96	1.63	1.50
6	B	1112	EZC	C19-C16	9.85	1.55	1.39
6	A	1112	EZC	C19-C22	8.79	1.53	1.38
6	B	1112	EZC	C19-C22	8.70	1.53	1.38
6	B	1112	EZC	C17-C21	7.21	1.56	1.39
6	A	1112	EZC	C17-C21	7.18	1.56	1.39
6	B	1112	EZC	C22-C23	7.10	1.50	1.40
6	A	1112	EZC	C22-C23	7.08	1.50	1.40
6	A	1112	EZC	C10-C08	-6.82	1.35	1.53
6	B	1112	EZC	C10-C08	-6.69	1.35	1.53
6	B	1112	EZC	C23-C21	5.64	1.52	1.39
6	A	1112	EZC	C23-C21	5.55	1.52	1.39
5	A	1110	NAG	O5-C1	4.59	1.51	1.43
5	B	1110	NAG	O5-C1	4.59	1.51	1.43
6	B	1112	EZC	C14-C10	3.96	1.67	1.51
6	A	1112	EZC	C14-C10	3.87	1.67	1.51
6	B	1112	EZC	C23-CL2	3.54	1.80	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1112	EZC	C23-CL2	3.46	1.80	1.72
6	B	1112	EZC	O04-C22	3.18	1.43	1.37
6	A	1112	EZC	O04-C22	3.13	1.43	1.37
6	A	1112	EZC	C09-C08	2.76	1.61	1.53
6	B	1112	EZC	C09-C08	2.73	1.61	1.53
6	A	1112	EZC	C17-C16	2.64	1.44	1.39
6	A	1112	EZC	O03-C15	-2.58	1.18	1.21
6	B	1112	EZC	C17-C16	2.51	1.44	1.39
6	B	1112	EZC	O03-C15	-2.42	1.18	1.21
6	B	1112	EZC	C21-CL1	2.35	1.77	1.72
6	A	1112	EZC	C21-CL1	2.24	1.77	1.72

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1110	NAG	C1-O5-C5	5.82	119.98	112.19
5	B	1110	NAG	C1-O5-C5	5.82	119.98	112.19
6	B	1112	EZC	O04-C22-C23	2.99	120.58	115.77
6	B	1112	EZC	C11-C07-C15	2.97	106.33	103.66
6	A	1112	EZC	O04-C22-C23	2.75	120.20	115.77
6	B	1112	EZC	O03-C15-C17	-2.42	125.55	130.69
6	B	1112	EZC	C13-C09-C08	-2.19	101.67	105.03
6	B	1112	EZC	C25-O04-C22	-2.16	113.09	117.60
6	A	1112	EZC	C25-O04-C22	-2.06	113.30	117.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

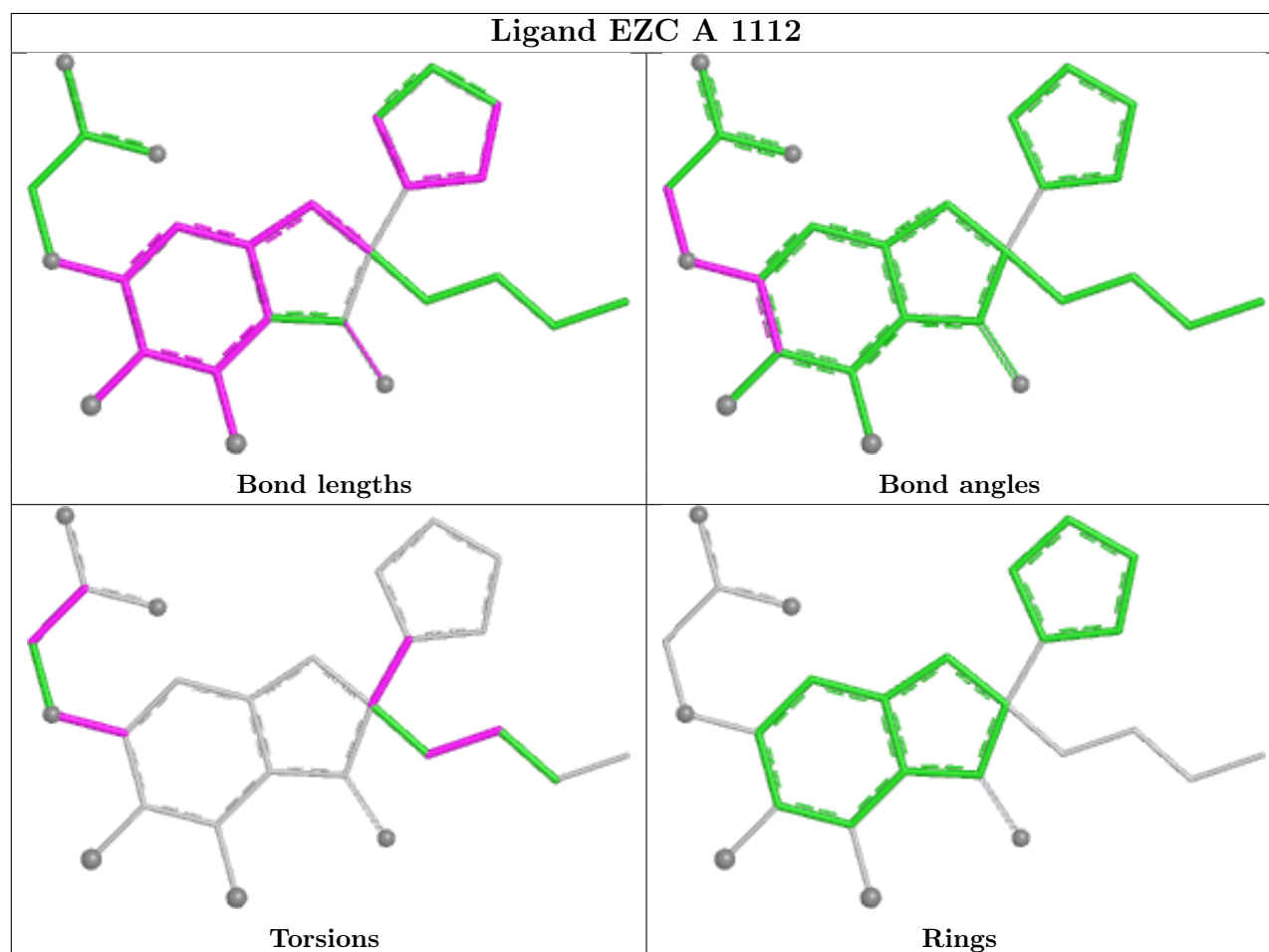
Mol	Chain	Res	Type	Atoms
6	A	1112	EZC	O04-C25-C26-O05
5	A	1111	NAG	O5-C5-C6-O6
5	B	1111	NAG	O5-C5-C6-O6
6	A	1112	EZC	C07-C12-C18-C20
6	A	1112	EZC	O04-C25-C26-O06
6	A	1112	EZC	C12-C07-C08-C09
6	B	1112	EZC	C08-C07-C12-C18
6	A	1112	EZC	C23-C22-O04-C25
6	B	1112	EZC	O04-C25-C26-O05
6	B	1112	EZC	O04-C25-C26-O06

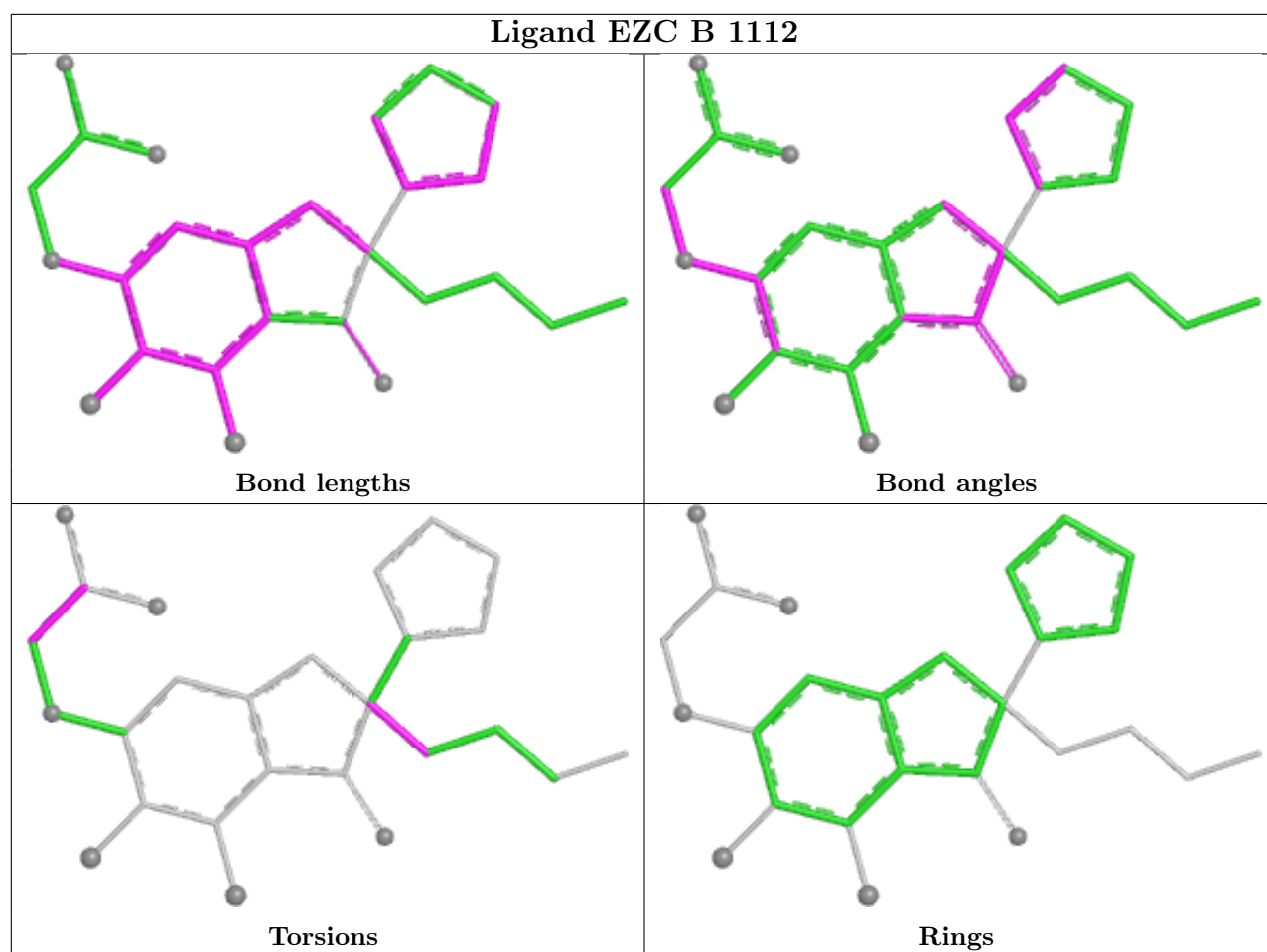
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1112	EZC	2	0
6	B	1112	EZC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

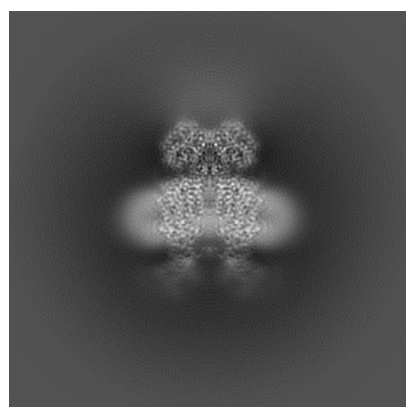
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30058. These allow visual inspection of the internal detail of the map and identification of artifacts.

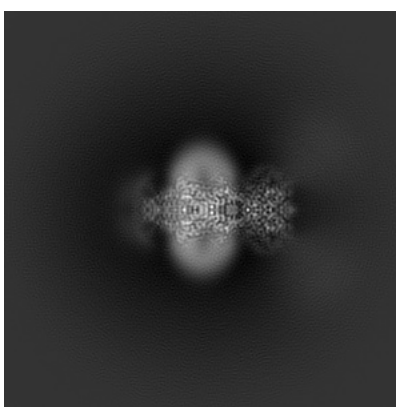
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

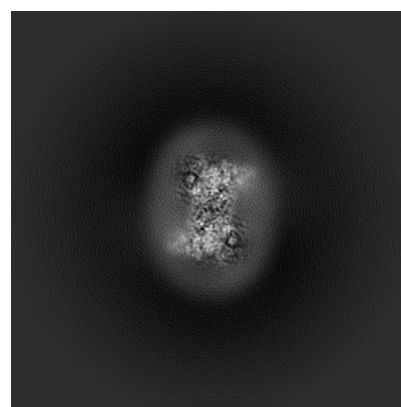
6.1.1 Primary map



X



Y

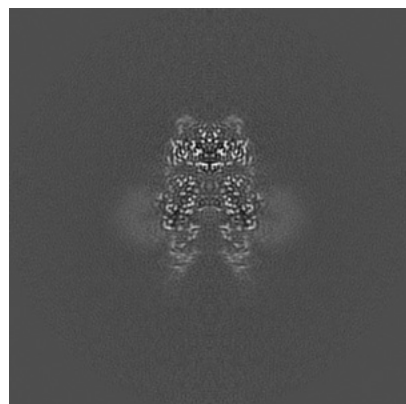


Z

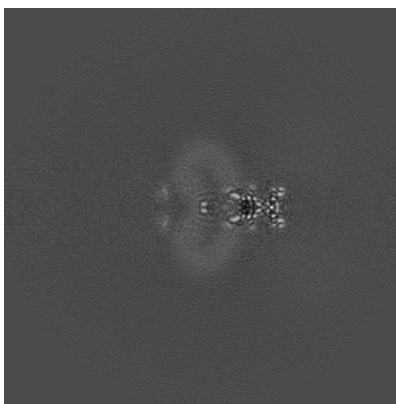
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

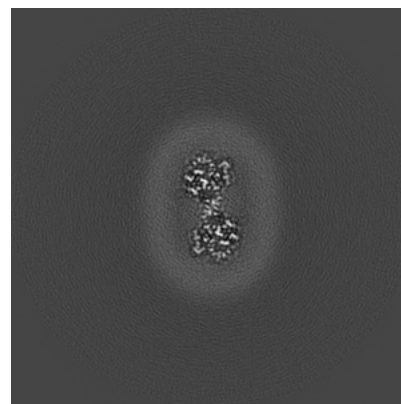
6.2.1 Primary map



X Index: 160



Y Index: 160

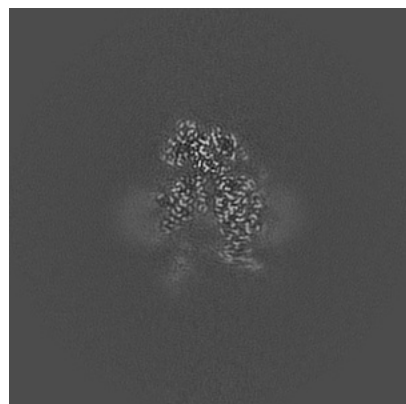


Z Index: 160

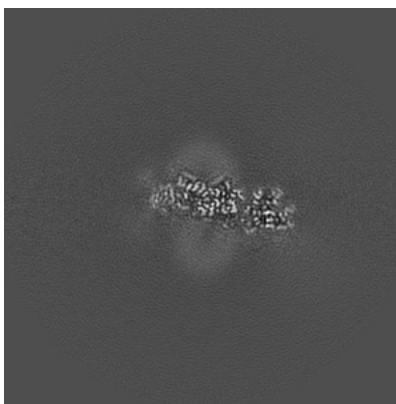
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

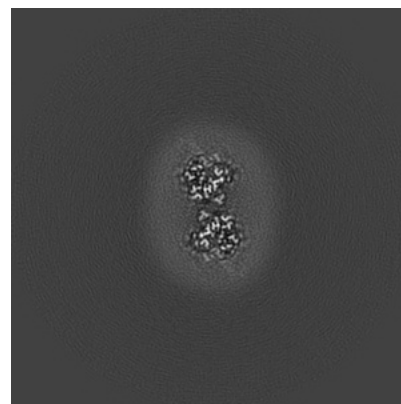
6.3.1 Primary map



X Index: 154



Y Index: 145

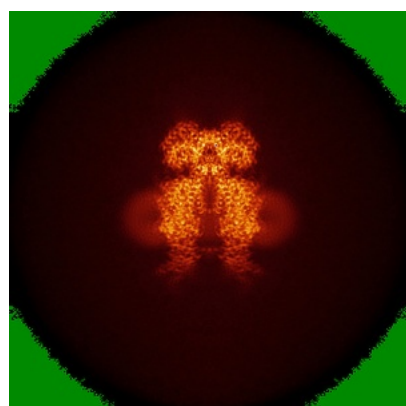


Z Index: 170

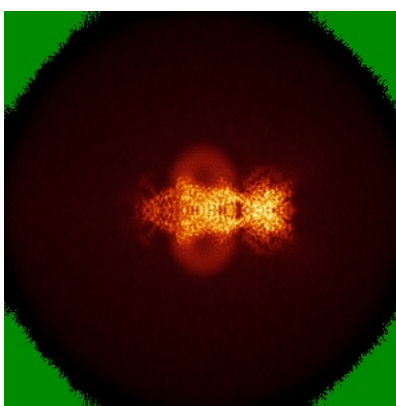
The images above show the largest variance slices of the map in three orthogonal directions.

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

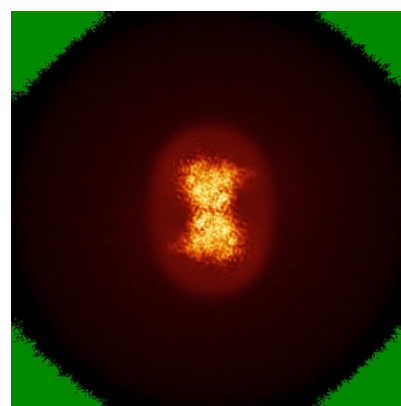
6.4.1 Primary map



X



Y

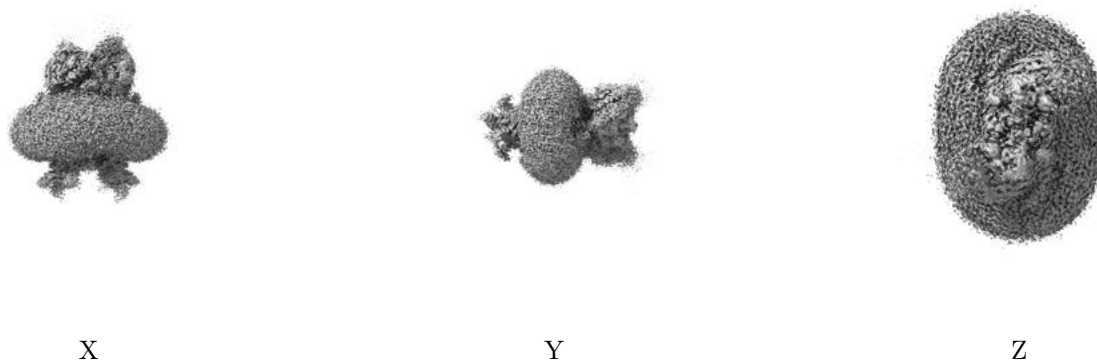


Z

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.

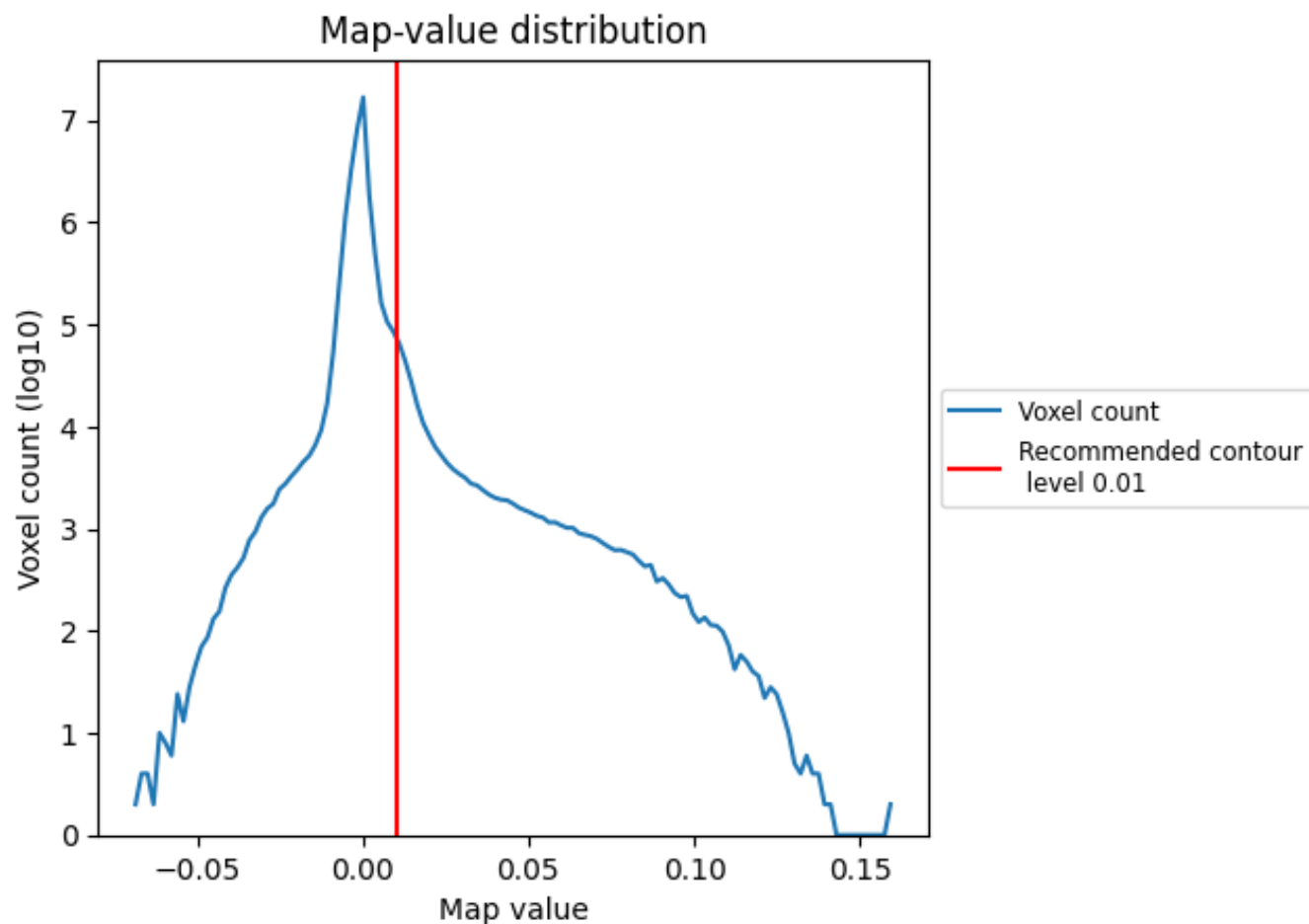
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

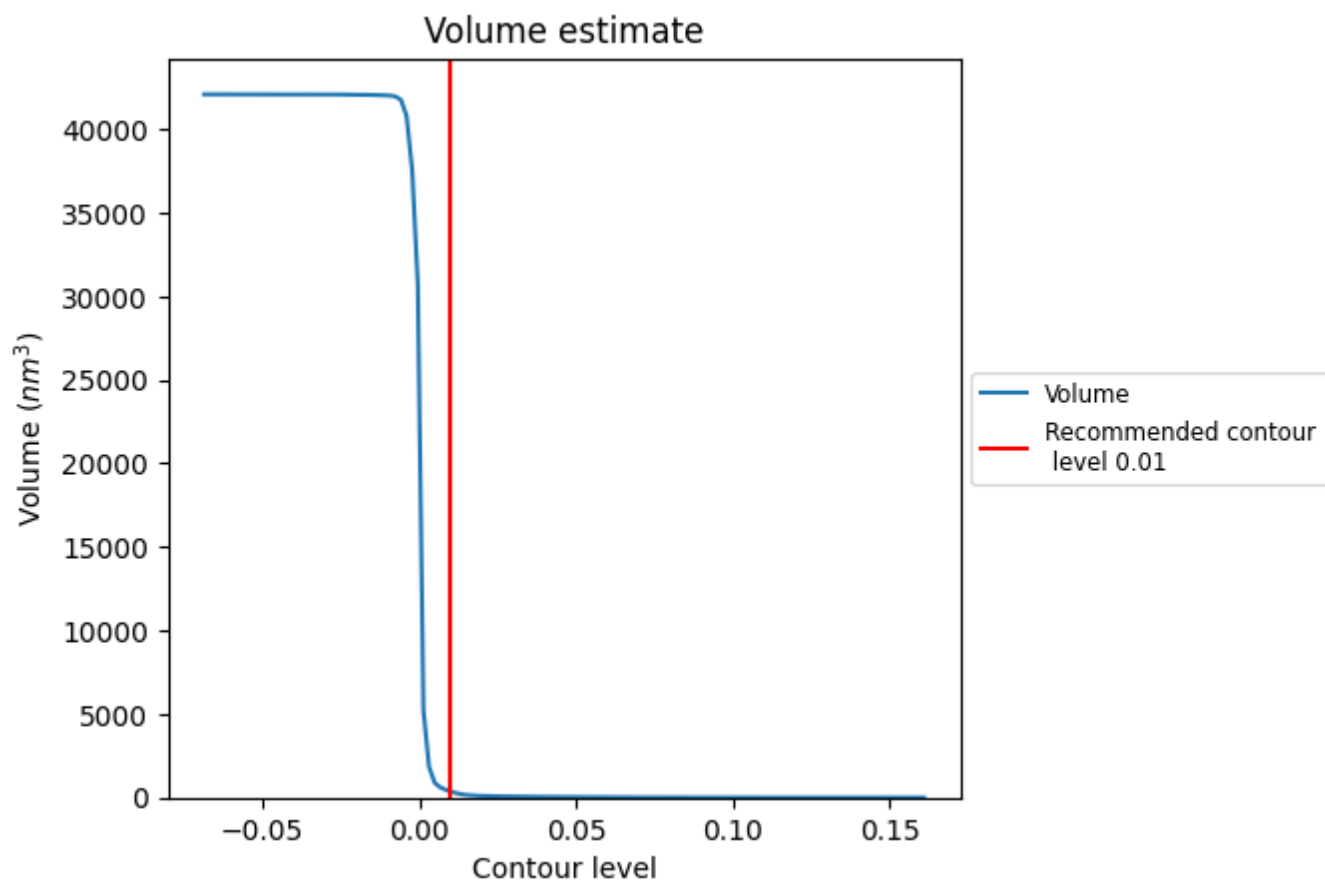
This section contains the results of statistical analysis of the map.

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.

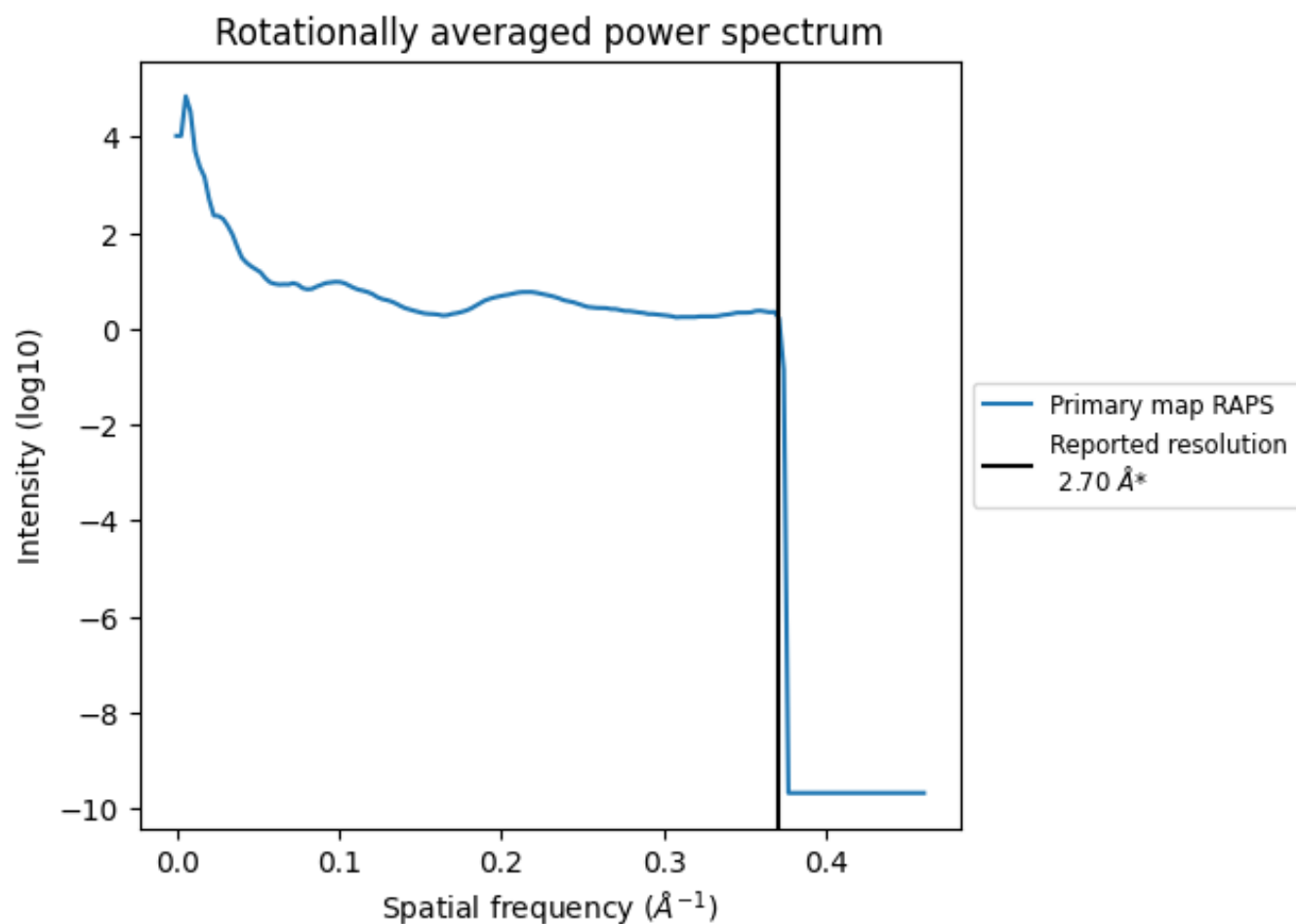
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm^3 ; this corresponds to an approximate mass of 330 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

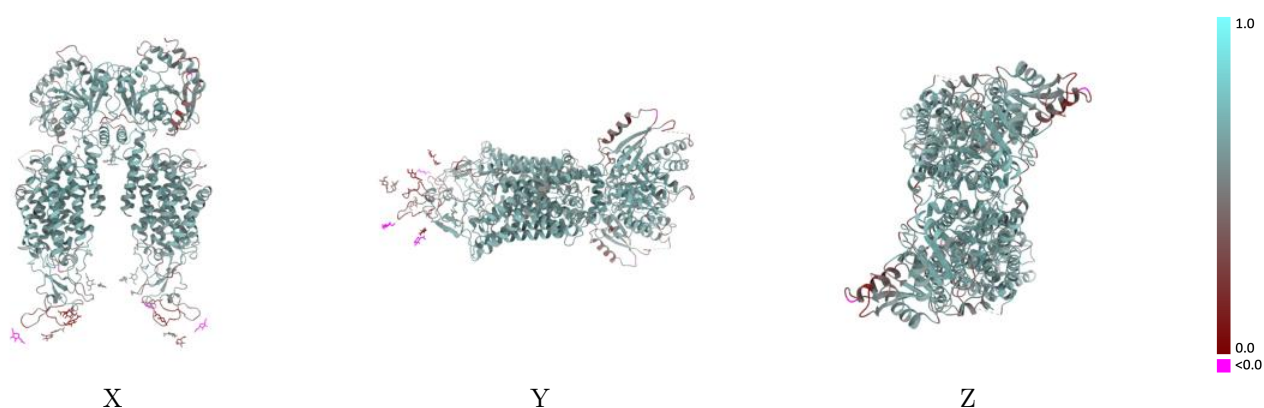
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30058 and PDB model 6M22. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

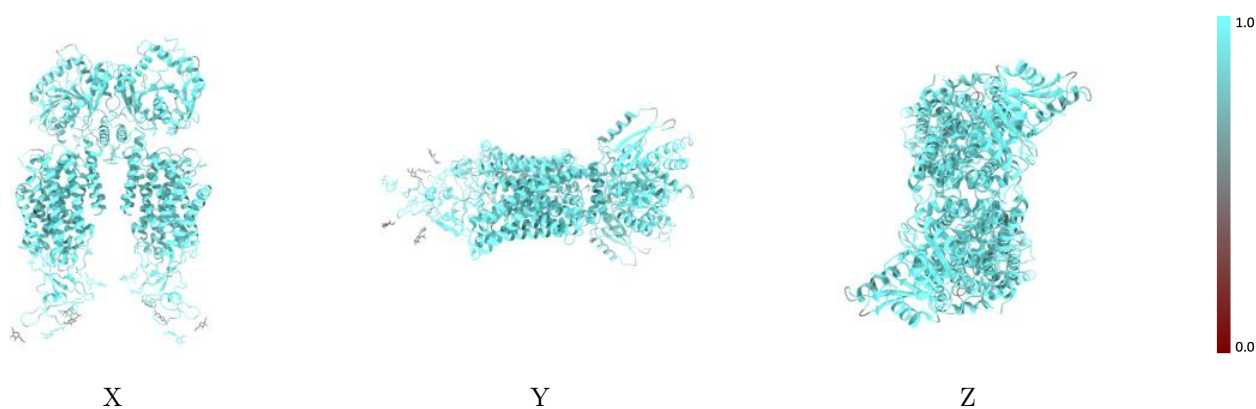
This section was not generated.

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



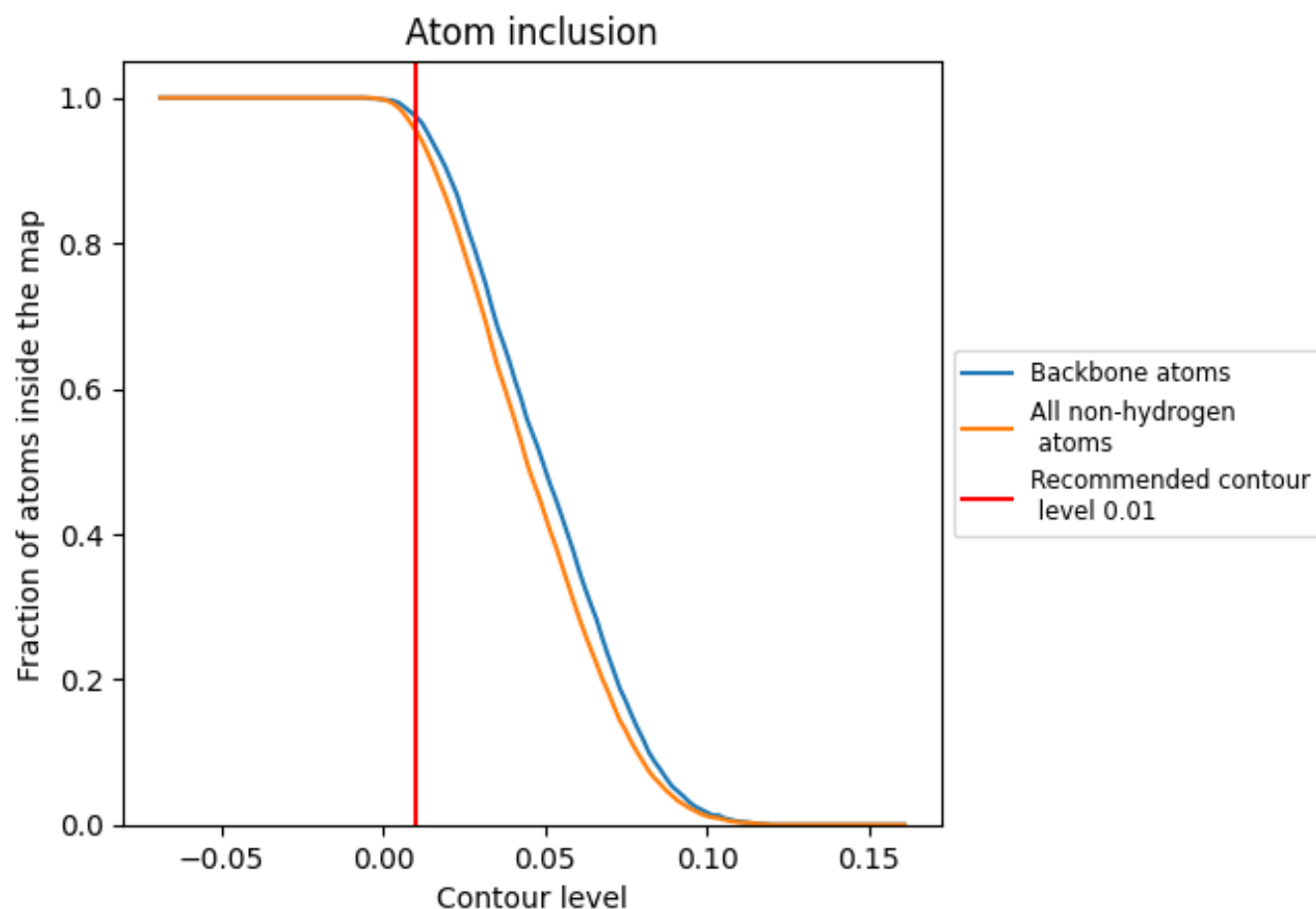
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.9560	0.5660
A	0.9590	0.5690
B	0.9590	0.5700
C	1.0000	0.4990
D	0.8930	0.3340
E	0.5360	0.0510
F	1.0000	0.4970
G	0.8930	0.3250
H	0.5360	0.0620

1.0

0.0

<0.0