



Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 10:20 PM EDT

PDB ID : 6UM6
EMDB ID : EMD-20818
Title : Cryo-EM structure of HIV-1 neutralizing antibody DH270.6 in complex with CH848 10.17DT Env
Authors : Acharya, P.; Henderson, R.C.; Saunderson, K.O.; Haynes, B.F.
Deposited on : 2019-10-09
Resolution : 4.30 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

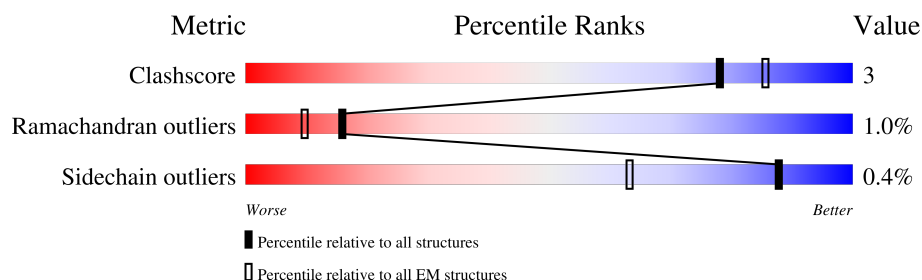
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	463	<div> <div>18%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	E	463	<div> <div>18%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>
1	I	463	<div> <div>18%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
2	B	161	<div> <div>14%</div> <div>75%</div> <div>7%</div> <div>•</div> <div>18%</div> </div>
2	F	161	<div> <div>14%</div> <div>73%</div> <div>8%</div> <div>•</div> <div>18%</div> </div>
2	J	161	<div> <div>15%</div> <div>74%</div> <div>8%</div> <div>•</div> <div>18%</div> </div>
3	C	238	<div> <div>8%</div> <div>50%</div> <div>•</div> <div>47%</div> </div>
3	G	238	<div> <div>7%</div> <div>50%</div> <div>•</div> <div>47%</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	238	
4	D	216	
4	H	216	
4	L	216	
5	M	4	
5	R	4	
5	W	4	
6	N	2	
6	S	2	
6	X	2	
7	O	3	
7	T	3	
7	Y	3	
8	P	2	
8	U	2	
8	Z	2	
9	Q	4	
9	V	4	
9	a	4	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20133 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 CH848 10.17DT gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3612	2261	624	698	29		
1	E	462	Total	C	N	O	S	0	0
			3612	2261	624	698	29		
1	I	462	Total	C	N	O	S	0	0
			3612	2261	624	698	29		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP A0A1W6IPB2
A	32	GLU	-	expression tag	UNP A0A1W6IPB2
A	33	ASN	-	expression tag	UNP A0A1W6IPB2
A	133	ASP	ASN	conflict	UNP A0A1W6IPB2
A	138	THR	ASN	conflict	UNP A0A1W6IPB2
A	201	CYS	VAL	conflict	UNP A0A1W6IPB2
A	433	CYS	ALA	conflict	UNP A0A1W6IPB2
A	490	LYS	GLU	conflict	UNP A0A1W6IPB2
A	492	GLU	GLN	conflict	UNP A0A1W6IPB2
A	496	VAL	ILE	conflict	UNP A0A1W6IPB2
A	500	ARG	GLY	conflict	UNP A0A1W6IPB2
A	501	CYS	ALA	conflict	UNP A0A1W6IPB2
E	31	ALA	-	expression tag	UNP A0A1W6IPB2
E	32	GLU	-	expression tag	UNP A0A1W6IPB2
E	33	ASN	-	expression tag	UNP A0A1W6IPB2
E	133	ASP	ASN	conflict	UNP A0A1W6IPB2
E	138	THR	ASN	conflict	UNP A0A1W6IPB2
E	201	CYS	VAL	conflict	UNP A0A1W6IPB2
E	433	CYS	ALA	conflict	UNP A0A1W6IPB2
E	490	LYS	GLU	conflict	UNP A0A1W6IPB2
E	492	GLU	GLN	conflict	UNP A0A1W6IPB2
E	496	VAL	ILE	conflict	UNP A0A1W6IPB2
E	500	ARG	GLY	conflict	UNP A0A1W6IPB2
E	501	CYS	ALA	conflict	UNP A0A1W6IPB2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	31	ALA	-	expression tag	UNP A0A1W6IPB2
I	32	GLU	-	expression tag	UNP A0A1W6IPB2
I	33	ASN	-	expression tag	UNP A0A1W6IPB2
I	133	ASP	ASN	conflict	UNP A0A1W6IPB2
I	138	THR	ASN	conflict	UNP A0A1W6IPB2
I	201	CYS	VAL	conflict	UNP A0A1W6IPB2
I	433	CYS	ALA	conflict	UNP A0A1W6IPB2
I	490	LYS	GLU	conflict	UNP A0A1W6IPB2
I	492	GLU	GLN	conflict	UNP A0A1W6IPB2
I	496	VAL	ILE	conflict	UNP A0A1W6IPB2
I	500	ARG	GLY	conflict	UNP A0A1W6IPB2
I	501	CYS	ALA	conflict	UNP A0A1W6IPB2

- Molecule 2 is a protein called CH848 10.17DT gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
2	F	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
2	J	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	504	VAL	-	expression tag	UNP Q2N0S7
B	505	GLY	-	expression tag	UNP Q2N0S7
B	506	ARG	-	expression tag	UNP Q2N0S7
B	507	ARG	-	expression tag	UNP Q2N0S7
B	508	ARG	-	expression tag	UNP Q2N0S7
B	509	ARG	-	expression tag	UNP Q2N0S7
B	510	ARG	-	expression tag	UNP Q2N0S7
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
F	504	VAL	-	expression tag	UNP Q2N0S7
F	505	GLY	-	expression tag	UNP Q2N0S7
F	506	ARG	-	expression tag	UNP Q2N0S7
F	507	ARG	-	expression tag	UNP Q2N0S7
F	508	ARG	-	expression tag	UNP Q2N0S7
F	509	ARG	-	expression tag	UNP Q2N0S7
F	510	ARG	-	expression tag	UNP Q2N0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	559	PRO	ILE	conflict	UNP Q2N0S7
F	605	CYS	THR	conflict	UNP Q2N0S7
J	504	VAL	-	expression tag	UNP Q2N0S7
J	505	GLY	-	expression tag	UNP Q2N0S7
J	506	ARG	-	expression tag	UNP Q2N0S7
J	507	ARG	-	expression tag	UNP Q2N0S7
J	508	ARG	-	expression tag	UNP Q2N0S7
J	509	ARG	-	expression tag	UNP Q2N0S7
J	510	ARG	-	expression tag	UNP Q2N0S7
J	559	PRO	ILE	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called DH270.6 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			996	629	170	190	7		
3	G	126	Total	C	N	O	S	0	0
			996	629	170	190	7		
3	K	126	Total	C	N	O	S	0	0
			996	629	170	190	7		

- Molecule 4 is a protein called DH270.6 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	108	Total	C	N	O	S	0	0
			790	491	133	161	5		
4	H	108	Total	C	N	O	S	0	0
			790	491	133	161	5		
4	L	108	Total	C	N	O	S	0	0
			790	491	133	161	5		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



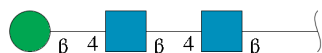
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	4	Total	C	N	O	0	0
			50	28	2	20		
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	W	4	Total	C	N	O	0	0
			50	28	2	20		

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



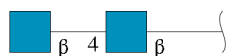
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total	C	N	O	0	0
			39	22	2	15		
7	T	3	Total	C	N	O	0	0
			39	22	2	15		
7	Y	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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
8	P	2	Total	C	N	O	0	0
			28	16	2	10		
8	U	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	4	Total	C	N	O	0	0
			50	28	2	20		
9	V	4	Total	C	N	O	0	0
			50	28	2	20		
9	a	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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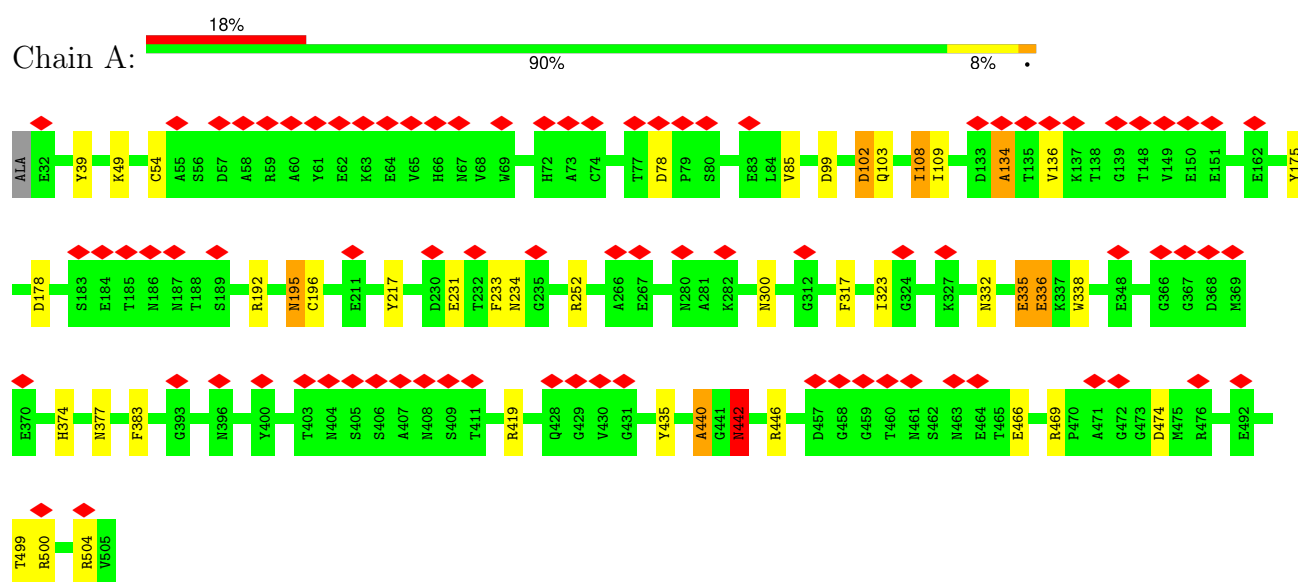
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Mol	Chain	Residues	Atoms				AltConf
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	

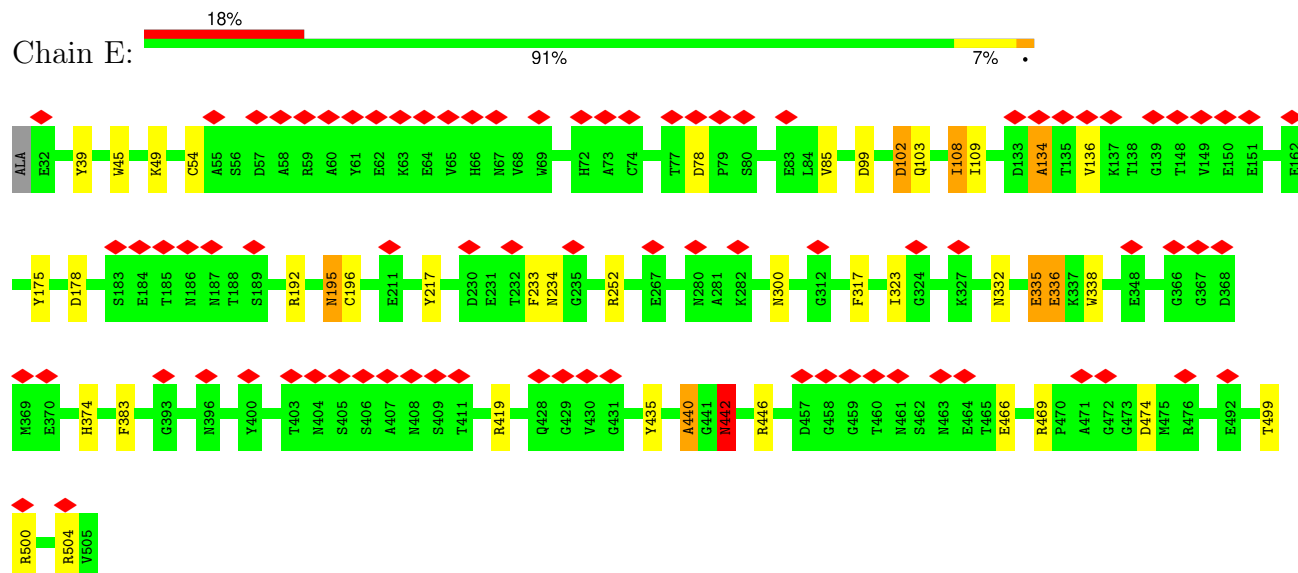
3 Residue-property plots

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.

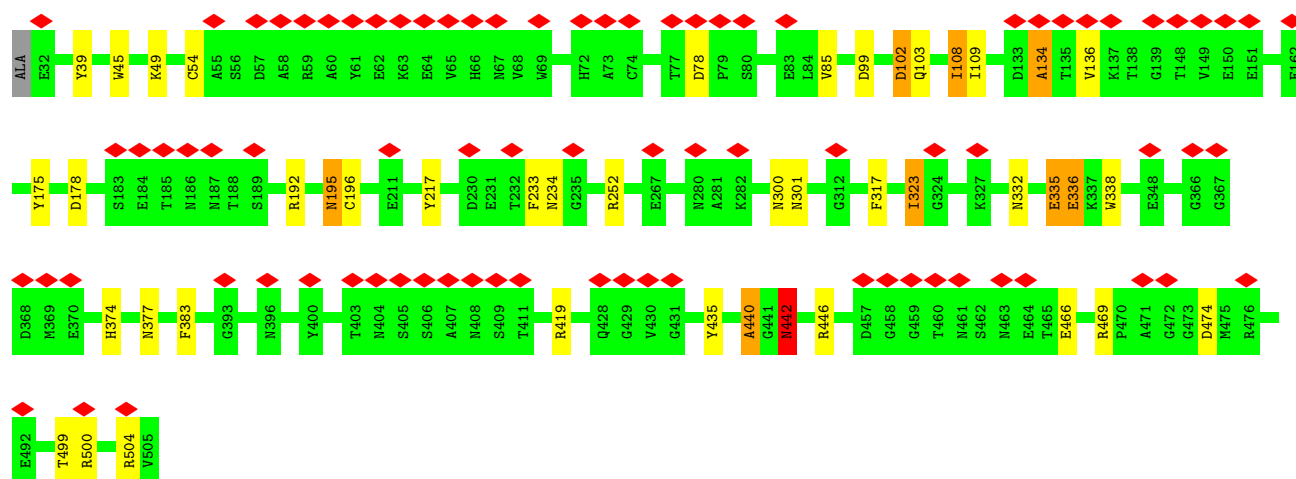
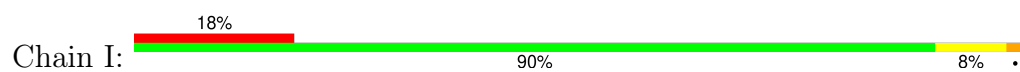
• Molecule 1: CH848 10.17DT gp120



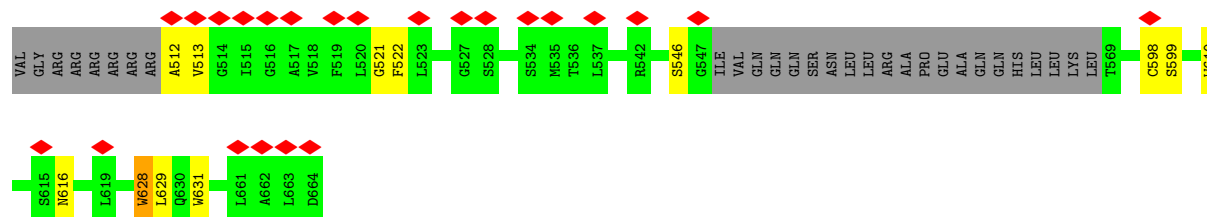
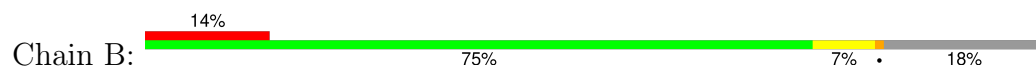
• Molecule 1: CH848 10.17DT gp120



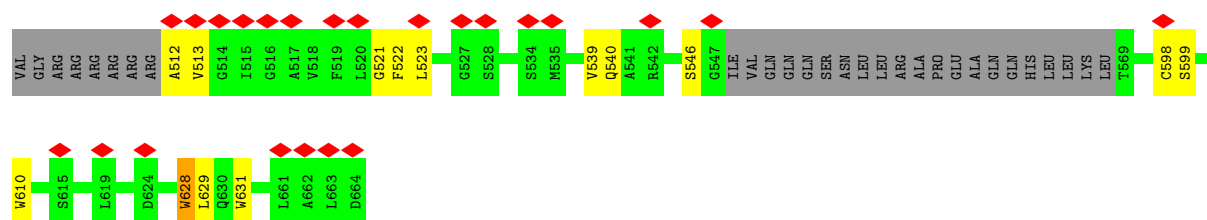
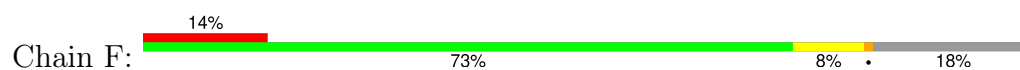
• Molecule 1: CH848 10.17DT gp120



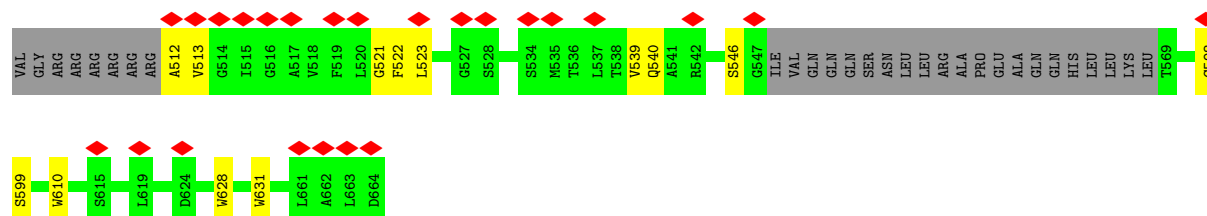
• Molecule 2: CH848 10.17DT gp41



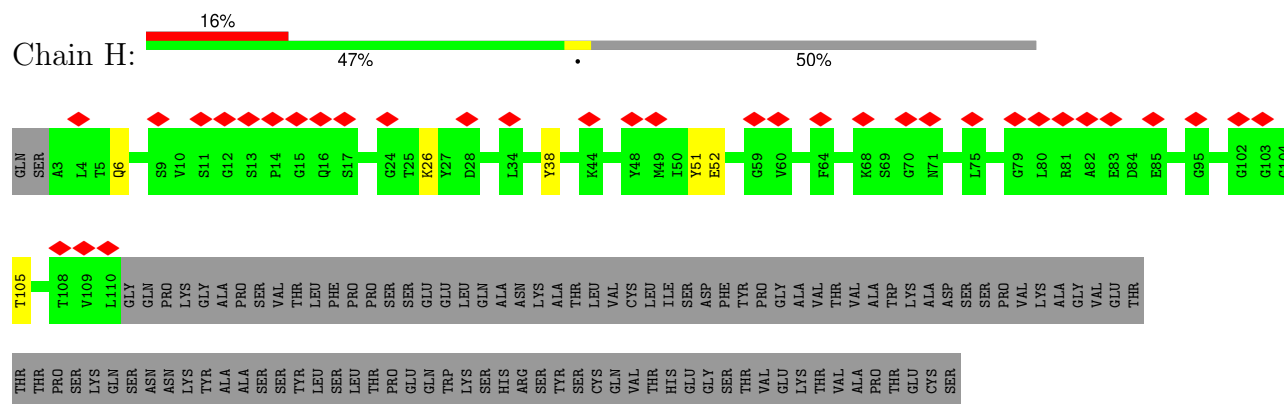
• Molecule 2: CH848 10.17DT gp41



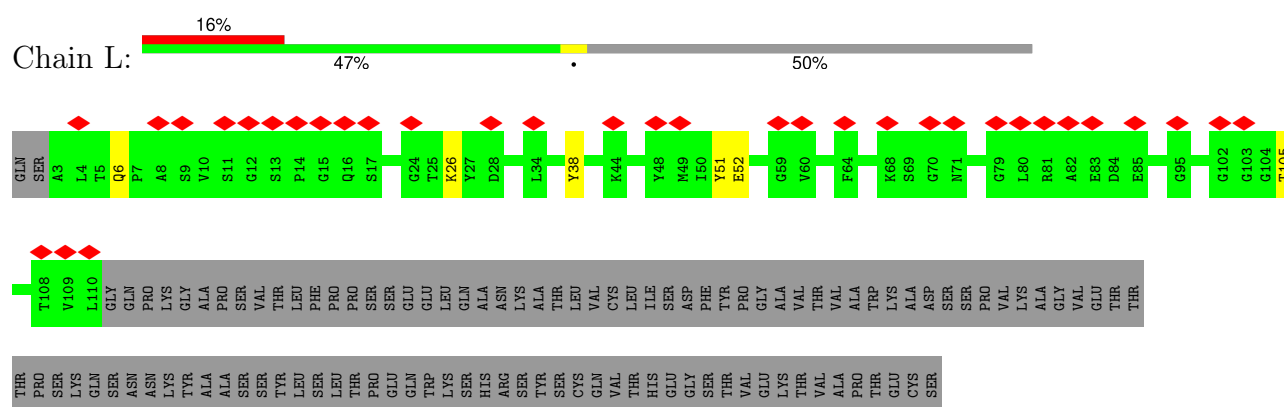
• Molecule 2: CH848 10.17DT gp41



- Molecule 4: DH270.6 Light chain



- Molecule 4: DH270.6 Light chain



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



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



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




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

Chain N: 


NAG1
NAG2

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

Chain S: 

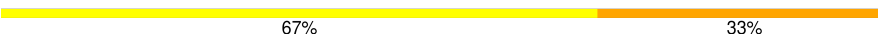

NAG1
NAG2

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

Chain X: 

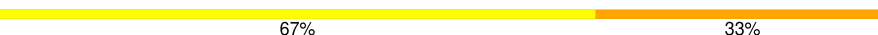

NAG1
NAG2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 

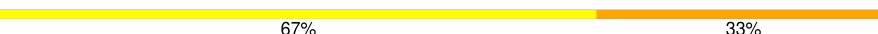

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 


NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 


NAG1
NAG2
BMA3

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	107646	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.058	Depositor
Minimum map value	-1.092	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	12/3689 (0.3%)	1.10	15/5019 (0.3%)
1	E	1.09	10/3689 (0.3%)	1.10	15/5019 (0.3%)
1	I	1.09	11/3689 (0.3%)	1.10	15/5019 (0.3%)
2	B	1.05	3/1052 (0.3%)	1.06	3/1427 (0.2%)
2	F	1.05	3/1052 (0.3%)	1.06	3/1427 (0.2%)
2	J	1.05	3/1052 (0.3%)	1.06	3/1427 (0.2%)
3	C	0.57	0/1025	0.62	0/1397
3	G	0.57	0/1025	0.63	0/1397
3	K	0.57	0/1025	0.62	0/1397
4	D	0.53	0/806	0.67	0/1093
4	H	0.53	0/806	0.67	0/1093
4	L	0.53	0/806	0.67	0/1093
All	All	0.96	42/19716 (0.2%)	0.99	54/26808 (0.2%)

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	7
1	E	0	7
1	I	0	7
2	B	0	2
2	F	0	2
2	J	0	2
All	All	0	27

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	ARG	C-N	9.69	1.52	1.34
1	E	469	ARG	C-N	9.67	1.52	1.34
1	I	469	ARG	C-N	9.66	1.52	1.34
1	I	217	TYR	CB-CG	-6.85	1.41	1.51
1	A	217	TYR	CB-CG	-6.85	1.41	1.51
1	E	217	TYR	CB-CG	-6.85	1.41	1.51
1	A	39	TYR	CB-CG	-6.78	1.41	1.51
1	I	39	TYR	CB-CG	-6.78	1.41	1.51
1	E	39	TYR	CB-CG	-6.77	1.41	1.51
1	I	175	TYR	CB-CG	-6.47	1.42	1.51
1	E	175	TYR	CB-CG	-6.46	1.42	1.51
1	A	175	TYR	CB-CG	-6.46	1.42	1.51
1	I	317	PHE	CB-CG	-6.32	1.40	1.51
1	A	317	PHE	CB-CG	-6.26	1.40	1.51
1	E	317	PHE	CB-CG	-6.24	1.40	1.51
1	I	374	HIS	CB-CG	-6.20	1.38	1.50
1	A	374	HIS	CB-CG	-6.17	1.39	1.50
1	E	374	HIS	CB-CG	-6.15	1.39	1.50
1	I	435	TYR	CE2-CZ	-5.70	1.31	1.38
1	E	435	TYR	CE2-CZ	-5.67	1.31	1.38
1	A	435	TYR	CE2-CZ	-5.67	1.31	1.38
2	F	610	TRP	CD2-CE2	-5.35	1.34	1.41
2	B	610	TRP	CD2-CE2	-5.33	1.34	1.41
2	J	610	TRP	CD2-CE2	-5.29	1.34	1.41
1	E	192	ARG	CG-CD	-5.28	1.38	1.51
1	A	192	ARG	CG-CD	-5.26	1.38	1.51
1	I	192	ARG	CG-CD	-5.26	1.38	1.51
2	J	610	TRP	CB-CG	-5.17	1.41	1.50
1	I	383	PHE	CB-CG	-5.16	1.42	1.51
2	F	610	TRP	CB-CG	-5.15	1.41	1.50
1	A	383	PHE	CB-CG	-5.14	1.42	1.51
2	B	610	TRP	CB-CG	-5.14	1.41	1.50
1	I	466	GLU	CD-OE1	-5.13	1.20	1.25
1	E	383	PHE	CB-CG	-5.12	1.42	1.51
2	J	631	TRP	CB-CG	-5.07	1.41	1.50
2	F	631	TRP	CB-CG	-5.07	1.41	1.50
1	A	466	GLU	CD-OE1	-5.06	1.20	1.25
2	B	631	TRP	CB-CG	-5.06	1.41	1.50
1	E	466	GLU	CD-OE1	-5.05	1.20	1.25
1	A	231	GLU	CD-OE2	-5.04	1.20	1.25
1	I	178	ASP	CB-CG	5.01	1.62	1.51
1	A	178	ASP	CB-CG	5.01	1.62	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	546	SER	C-N-CA	15.55	154.95	122.30
2	J	546	SER	C-N-CA	15.54	154.94	122.30
2	F	546	SER	C-N-CA	15.53	154.91	122.30
1	A	440	ALA	O-C-N	-12.29	102.31	123.20
1	E	440	ALA	O-C-N	-12.29	102.31	123.20
1	I	440	ALA	O-C-N	-12.29	102.31	123.20
1	A	134	ALA	C-N-CA	11.72	151.01	121.70
1	I	134	ALA	C-N-CA	11.72	150.99	121.70
1	E	134	ALA	C-N-CA	11.71	150.96	121.70
1	E	234	ASN	CB-CA-C	-10.53	89.34	110.40
1	I	234	ASN	CB-CA-C	-10.53	89.34	110.40
1	A	234	ASN	CB-CA-C	-10.52	89.35	110.40
1	A	442	ASN	CB-CA-C	10.13	130.66	110.40
1	E	442	ASN	CB-CA-C	10.13	130.65	110.40
1	I	442	ASN	CB-CA-C	10.12	130.64	110.40
1	E	332	ASN	CB-CA-C	-7.20	96.00	110.40
1	A	332	ASN	CB-CA-C	-7.20	96.00	110.40
1	I	332	ASN	CB-CA-C	-7.20	96.01	110.40
1	E	504	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	504	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	I	504	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	I	252	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	252	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	E	252	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	J	512	ALA	C-N-CA	6.57	138.13	121.70
2	B	512	ALA	C-N-CA	6.57	138.12	121.70
2	F	512	ALA	C-N-CA	6.56	138.10	121.70
1	E	442	ASN	N-CA-C	-6.42	93.68	111.00
1	A	442	ASN	N-CA-C	-6.41	93.69	111.00
1	I	442	ASN	N-CA-C	-6.41	93.70	111.00
1	E	196	CYS	CA-CB-SG	-6.08	103.06	114.00
1	I	196	CYS	CA-CB-SG	-6.07	103.07	114.00
1	A	196	CYS	CA-CB-SG	-6.07	103.08	114.00
1	E	178	ASP	N-CA-C	-6.07	94.62	111.00
1	I	178	ASP	N-CA-C	-6.06	94.64	111.00
1	A	178	ASP	N-CA-C	-6.06	94.64	111.00
1	I	435	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	435	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	E	435	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	E	54	CYS	C-N-CA	5.54	135.56	121.70
1	I	54	CYS	C-N-CA	5.54	135.55	121.70
1	A	54	CYS	C-N-CA	5.54	135.54	121.70
1	I	195	ASN	O-C-N	-5.54	113.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASN	O-C-N	-5.53	113.86	122.70
1	E	195	ASN	O-C-N	-5.53	113.86	122.70
1	I	217	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	E	217	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	A	217	TYR	CB-CG-CD2	-5.41	117.76	121.00
2	B	521	GLY	N-CA-C	-5.19	100.12	113.10
2	F	521	GLY	N-CA-C	-5.19	100.11	113.10
2	J	521	GLY	N-CA-C	-5.19	100.12	113.10
1	A	419	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	419	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	I	419	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ASP	Mainchain
1	A	108	ILE	Mainchain
1	A	195	ASN	Mainchain
1	A	335	GLU	Mainchain
1	A	336	GLU	Mainchain
1	A	440	ALA	Mainchain
1	A	446	ARG	Mainchain
2	B	522	PHE	Mainchain
2	B	628	TRP	Mainchain
1	E	102	ASP	Mainchain
1	E	108	ILE	Mainchain
1	E	195	ASN	Mainchain
1	E	335	GLU	Mainchain
1	E	336	GLU	Mainchain
1	E	440	ALA	Mainchain
1	E	446	ARG	Mainchain
2	F	522	PHE	Mainchain
2	F	628	TRP	Mainchain
1	I	102	ASP	Mainchain
1	I	108	ILE	Mainchain
1	I	195	ASN	Mainchain
1	I	335	GLU	Mainchain
1	I	336	GLU	Mainchain
1	I	440	ALA	Mainchain
1	I	446	ARG	Mainchain
2	J	522	PHE	Mainchain

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Mol	Chain	Res	Type	Group
2	J	628	TRP	Mainchain

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	3612	0	3523	14	0
1	E	3612	0	3523	14	0
1	I	3612	0	3523	16	0
2	B	1034	0	1014	3	0
2	F	1034	0	1014	4	0
2	J	1034	0	1014	3	0
3	C	996	0	935	4	0
3	G	996	0	935	5	0
3	K	996	0	935	6	0
4	D	790	0	762	2	0
4	H	790	0	762	2	0
4	L	790	0	762	2	0
5	M	50	0	43	3	0
5	R	50	0	43	3	0
5	W	50	0	43	3	0
6	N	28	0	25	1	0
6	S	28	0	25	1	0
6	X	28	0	25	1	0
7	O	39	0	34	1	0
7	T	39	0	34	2	0
7	Y	39	0	34	2	0
8	P	28	0	25	2	0
8	U	28	0	25	2	0
8	Z	28	0	25	2	0
9	Q	50	0	43	3	0
9	V	50	0	43	4	0
9	a	50	0	43	0	0
10	A	84	0	78	3	0
10	E	84	0	78	4	0
10	I	84	0	78	2	0
All	All	20133	0	19446	106	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 3.

All (106) 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)
9:V:2:NAG:O7	9:V:2:NAG:O3	1.99	0.81
9:Q:2:NAG:O7	9:Q:2:NAG:O3	1.99	0.81
10:E:610:NAG:O6	10:E:610:NAG:O4	2.03	0.75
10:I:610:NAG:O6	10:I:610:NAG:O4	2.03	0.75
10:A:614:NAG:O6	10:A:614:NAG:O4	2.07	0.70
10:A:610:NAG:O6	10:A:610:NAG:O4	2.03	0.68
1:I:499:THR:O	1:I:500:ARG:CB	2.43	0.67
1:E:499:THR:O	1:E:500:ARG:CB	2.43	0.67
10:E:614:NAG:O6	10:E:614:NAG:O4	2.07	0.66
1:A:499:THR:O	1:A:500:ARG:CB	2.43	0.64
10:I:614:NAG:O6	10:I:614:NAG:O4	2.07	0.62
9:V:2:NAG:O7	9:V:2:NAG:C3	2.47	0.62
9:Q:2:NAG:O7	9:Q:2:NAG:C3	2.47	0.62
3:G:112:PRO:O	4:H:38:TYR:OH	2.19	0.60
8:Z:1:NAG:O7	8:Z:1:NAG:C3	2.51	0.58
3:C:112:PRO:O	4:D:38:TYR:OH	2.19	0.58
3:K:112:PRO:O	4:L:38:TYR:OH	2.19	0.58
7:O:1:NAG:O7	7:O:1:NAG:H3	2.03	0.58
8:U:1:NAG:O7	8:U:1:NAG:C3	2.51	0.57
7:T:1:NAG:O7	7:T:1:NAG:H3	2.03	0.57
7:Y:1:NAG:O7	7:Y:1:NAG:H3	2.03	0.57
4:H:6:GLN:NE2	4:H:105:THR:OG1	2.38	0.57
4:L:6:GLN:NE2	4:L:105:THR:OG1	2.38	0.56
8:P:1:NAG:O7	8:P:1:NAG:C3	2.51	0.56
4:D:6:GLN:NE2	4:D:105:THR:OG1	2.38	0.56
1:A:442:ASN:O	1:A:442:ASN:ND2	2.39	0.55
1:E:442:ASN:O	1:E:442:ASN:ND2	2.39	0.55
1:I:442:ASN:O	1:I:442:ASN:ND2	2.39	0.55
1:I:49:LYS:NZ	1:I:99:ASP:OD2	2.39	0.55
1:A:49:LYS:NZ	1:A:99:ASP:OD2	2.39	0.55
1:E:49:LYS:NZ	1:E:99:ASP:OD2	2.39	0.55
10:A:620:NAG:O6	10:A:620:NAG:O4	2.16	0.54
1:E:78:ASP:OD1	1:E:78:ASP:N	2.41	0.53
8:P:1:NAG:O7	8:P:1:NAG:H3	2.08	0.52
8:Z:1:NAG:O7	8:Z:1:NAG:H3	2.08	0.52
1:I:335:GLU:O	1:I:338:TRP:N	2.43	0.52
1:I:78:ASP:OD1	1:I:78:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:1:NAG:O7	8:U:1:NAG:H3	2.09	0.51
10:E:620:NAG:O6	10:E:620:NAG:O4	2.16	0.51
3:K:50:TRP:O	3:K:58:THR:OG1	2.22	0.50
1:I:108:ILE:O	1:I:109:ILE:C	2.48	0.50
1:E:442:ASN:CG	6:S:1:NAG:C7	2.80	0.50
1:I:442:ASN:CG	6:X:1:NAG:C7	2.80	0.49
1:E:335:GLU:O	1:E:338:TRP:N	2.43	0.49
1:A:335:GLU:O	1:A:338:TRP:N	2.43	0.49
1:A:442:ASN:CG	6:N:1:NAG:C7	2.80	0.49
1:E:108:ILE:O	1:E:109:ILE:C	2.48	0.49
3:G:31:ASP:OD1	3:G:101:TRP:NE1	2.45	0.49
1:A:108:ILE:O	1:A:109:ILE:C	2.48	0.49
5:R:1:NAG:O7	5:R:1:NAG:H3	2.14	0.48
10:E:610:NAG:HO4	10:E:610:NAG:HO6	1.52	0.48
5:W:1:NAG:O7	5:W:1:NAG:H3	2.14	0.48
5:M:4:MAN:O6	5:M:4:MAN:O4	2.32	0.48
1:I:442:ASN:HD22	1:I:442:ASN:C	2.18	0.47
1:A:377:ASN:OD1	1:A:377:ASN:N	2.45	0.47
3:C:31:ASP:OD1	3:C:101:TRP:NE1	2.45	0.47
1:E:499:THR:O	1:E:500:ARG:HB2	2.15	0.47
3:G:30:THR:HG22	3:G:30:THR:O	2.15	0.47
1:A:442:ASN:HD22	1:A:442:ASN:C	2.18	0.47
5:M:1:NAG:O7	5:M:1:NAG:H3	2.14	0.46
3:G:50:TRP:O	3:G:58:THR:OG1	2.22	0.46
3:C:30:THR:HG22	3:C:30:THR:O	2.15	0.46
3:K:31:ASP:OD1	3:K:101:TRP:NE1	2.45	0.46
1:E:442:ASN:HD22	1:E:442:ASN:C	2.18	0.46
1:A:102:ASP:O	1:A:103:GLN:C	2.54	0.46
3:G:47:TRP:CZ2	3:G:49:GLY:HA2	2.51	0.46
3:K:30:THR:HG22	3:K:30:THR:O	2.15	0.46
2:B:616:ASN:N	2:B:616:ASN:OD1	2.46	0.45
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.51	0.45
1:A:78:ASP:OD1	1:A:78:ASP:N	2.41	0.45
1:I:499:THR:O	1:I:500:ARG:HB2	2.15	0.45
1:A:499:THR:O	1:A:500:ARG:HB2	2.15	0.45
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.51	0.44
5:R:4:MAN:O6	5:R:4:MAN:O4	2.32	0.44
1:I:377:ASN:OD1	1:I:377:ASN:N	2.45	0.44
1:I:102:ASP:O	1:I:103:GLN:C	2.54	0.43
1:A:499:THR:O	1:A:500:ARG:HB3	2.17	0.43
9:V:2:NAG:O4	9:V:2:NAG:O6	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ASP:O	1:E:103:GLN:C	2.54	0.43
5:W:4:MAN:O6	5:W:4:MAN:O4	2.32	0.42
1:A:335:GLU:O	1:A:336:GLU:C	2.58	0.42
1:E:499:THR:O	1:E:500:ARG:HB3	2.17	0.42
1:E:335:GLU:O	1:E:336:GLU:C	2.58	0.42
5:W:2:NAG:H83	5:W:2:NAG:H2	1.62	0.42
1:I:335:GLU:O	1:I:336:GLU:C	2.58	0.42
7:T:1:NAG:O7	7:T:1:NAG:C1	2.65	0.42
7:Y:1:NAG:O7	7:Y:1:NAG:C1	2.65	0.42
1:I:474:ASP:C	1:I:474:ASP:OD1	2.59	0.41
5:M:2:NAG:H83	5:M:2:NAG:H2	1.62	0.41
2:F:539:VAL:O	2:F:540:GLN:C	2.58	0.41
2:F:628:TRP:O	2:F:629:LEU:C	2.59	0.41
9:V:1:NAG:O7	9:V:1:NAG:H3	2.21	0.41
9:Q:1:NAG:O7	9:Q:1:NAG:H3	2.21	0.41
1:A:474:ASP:OD1	1:A:474:ASP:C	2.59	0.41
5:R:2:NAG:H83	5:R:2:NAG:H2	1.62	0.41
2:J:539:VAL:O	2:J:540:GLN:C	2.58	0.41
2:B:598:CYS:N	2:B:599:SER:HA	2.36	0.41
2:F:598:CYS:N	2:F:599:SER:HA	2.36	0.41
1:I:301:ASN:HD22	1:I:323:ILE:CD1	2.35	0.40
3:K:19:LYS:HA	3:K:81:MET:O	2.22	0.40
1:I:499:THR:O	1:I:500:ARG:HB3	2.17	0.40
1:E:45:TRP:CE3	2:F:523:LEU:HD13	2.56	0.40
1:I:45:TRP:CE3	2:J:523:LEU:HD13	2.56	0.40
2:J:598:CYS:N	2:J:599:SER:HA	2.36	0.40
2:B:628:TRP:O	2:B:629:LEU:C	2.59	0.40
1:E:474:ASP:C	1:E:474:ASP:OD1	2.59	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	460/463 (99%)	424 (92%)	31 (7%)	5 (1%)	12	46
1	E	460/463 (99%)	424 (92%)	31 (7%)	5 (1%)	12	46
1	I	460/463 (99%)	424 (92%)	31 (7%)	5 (1%)	12	46
2	B	128/161 (80%)	121 (94%)	6 (5%)	1 (1%)	16	53
2	F	128/161 (80%)	121 (94%)	6 (5%)	1 (1%)	16	53
2	J	128/161 (80%)	121 (94%)	6 (5%)	1 (1%)	16	53
3	C	124/238 (52%)	120 (97%)	4 (3%)	0	100	100
3	G	124/238 (52%)	120 (97%)	4 (3%)	0	100	100
3	K	124/238 (52%)	120 (97%)	4 (3%)	0	100	100
4	D	106/216 (49%)	96 (91%)	8 (8%)	2 (2%)	6	33
4	H	106/216 (49%)	96 (91%)	8 (8%)	2 (2%)	6	33
4	L	106/216 (49%)	96 (91%)	8 (8%)	2 (2%)	6	33
All	All	2454/3234 (76%)	2283 (93%)	147 (6%)	24 (1%)	16	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ILE
1	E	323	ILE
1	I	323	ILE
1	A	136	VAL
2	B	513	VAL
4	D	52	GLU
1	E	136	VAL
2	F	513	VAL
4	H	52	GLU
1	I	136	VAL
2	J	513	VAL
4	L	52	GLU
1	A	233	PHE
4	D	51	TYR
1	E	233	PHE
4	H	51	TYR
1	I	233	PHE
4	L	51	TYR
1	A	134	ALA
1	E	134	ALA
1	I	134	ALA
1	A	85	VAL

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Mol	Chain	Res	Type
1	E	85	VAL
1	I	85	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	410/411 (100%)	408 (100%)	2 (0%)	86	90
1	E	410/411 (100%)	408 (100%)	2 (0%)	86	90
1	I	410/411 (100%)	408 (100%)	2 (0%)	86	90
2	B	110/136 (81%)	110 (100%)	0	100	100
2	F	110/136 (81%)	110 (100%)	0	100	100
2	J	110/136 (81%)	110 (100%)	0	100	100
3	C	106/203 (52%)	106 (100%)	0	100	100
3	G	106/203 (52%)	106 (100%)	0	100	100
3	K	106/203 (52%)	106 (100%)	0	100	100
4	D	88/181 (49%)	87 (99%)	1 (1%)	70	80
4	H	88/181 (49%)	87 (99%)	1 (1%)	70	80
4	L	88/181 (49%)	87 (99%)	1 (1%)	70	80
All	All	2142/2793 (77%)	2133 (100%)	9 (0%)	88	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	442	ASN
4	D	26	LYS
1	E	300	ASN
1	E	442	ASN
4	H	26	LYS
1	I	300	ASN
1	I	442	ASN

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Mol	Chain	Res	Type
4	L	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	6	GLN
4	D	16	GLN
4	D	39	GLN
2	F	540	GLN
4	H	6	GLN
4	H	16	GLN
2	J	540	GLN
4	L	6	GLN
4	L	16	GLN

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 ⓘ

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	M	1	1,5	14,14,15	2.88	7 (50%)	17,19,21	2.38	8 (47%)
5	NAG	M	2	5	14,14,15	2.42	5 (35%)	17,19,21	3.27	7 (41%)
5	BMA	M	3	5	11,11,12	1.74	4 (36%)	15,15,17	2.64	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	M	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.79	3 (20%)
6	NAG	N	1	6	14,14,15	2.11	5 (35%)	17,19,21	2.29	5 (29%)
6	NAG	N	2	6	14,14,15	1.13	2 (14%)	17,19,21	2.23	7 (41%)
7	NAG	O	1	7	14,14,15	2.11	6 (42%)	17,19,21	2.48	6 (35%)
7	NAG	O	2	7	14,14,15	1.35	3 (21%)	17,19,21	1.91	3 (17%)
7	BMA	O	3	7	11,11,12	0.69	0	15,15,17	1.55	3 (20%)
8	NAG	P	1	8	14,14,15	1.04	0	17,19,21	1.55	2 (11%)
8	NAG	P	2	8	14,14,15	0.92	0	17,19,21	2.15	4 (23%)
9	NAG	Q	1	9	14,14,15	2.63	10 (71%)	17,19,21	2.68	7 (41%)
9	NAG	Q	2	9	14,14,15	1.83	7 (50%)	17,19,21	3.56	9 (52%)
9	BMA	Q	3	9	11,11,12	1.03	1 (9%)	15,15,17	1.65	3 (20%)
9	MAN	Q	4	9	11,11,12	1.21	1 (9%)	15,15,17	2.30	6 (40%)
5	NAG	R	1	1,5	14,14,15	2.87	7 (50%)	17,19,21	2.38	8 (47%)
5	NAG	R	2	5	14,14,15	2.42	5 (35%)	17,19,21	3.27	7 (41%)
5	BMA	R	3	5	11,11,12	1.74	4 (36%)	15,15,17	2.64	5 (33%)
5	MAN	R	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.79	3 (20%)
6	NAG	S	1	6	14,14,15	2.11	5 (35%)	17,19,21	2.30	5 (29%)
6	NAG	S	2	6	14,14,15	1.13	2 (14%)	17,19,21	2.22	7 (41%)
7	NAG	T	1	7	14,14,15	2.12	6 (42%)	17,19,21	2.48	6 (35%)
7	NAG	T	2	7	14,14,15	1.35	3 (21%)	17,19,21	1.91	3 (17%)
7	BMA	T	3	7	11,11,12	0.69	0	15,15,17	1.55	3 (20%)
8	NAG	U	1	8	14,14,15	1.04	0	17,19,21	1.55	2 (11%)
8	NAG	U	2	8	14,14,15	0.91	0	17,19,21	2.15	4 (23%)
9	NAG	V	1	9	14,14,15	2.63	10 (71%)	17,19,21	2.68	7 (41%)
9	NAG	V	2	9	14,14,15	1.83	6 (42%)	17,19,21	3.56	9 (52%)
9	BMA	V	3	9	11,11,12	1.04	1 (9%)	15,15,17	1.65	3 (20%)
9	MAN	V	4	9	11,11,12	1.22	1 (9%)	15,15,17	2.30	6 (40%)
5	NAG	W	1	1,5	14,14,15	2.88	7 (50%)	17,19,21	2.38	8 (47%)
5	NAG	W	2	5	14,14,15	2.42	5 (35%)	17,19,21	3.27	7 (41%)
5	BMA	W	3	5	11,11,12	1.74	4 (36%)	15,15,17	2.64	5 (33%)
5	MAN	W	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.79	3 (20%)
6	NAG	X	1	6	14,14,15	2.11	5 (35%)	17,19,21	2.30	5 (29%)
6	NAG	X	2	6	14,14,15	1.12	2 (14%)	17,19,21	2.23	7 (41%)
7	NAG	Y	1	7	14,14,15	2.11	6 (42%)	17,19,21	2.48	6 (35%)
7	NAG	Y	2	7	14,14,15	1.34	3 (21%)	17,19,21	1.91	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	Y	3	7	11,11,12	0.69	0	15,15,17	1.55	3 (20%)
8	NAG	Z	1	8	14,14,15	1.04	0	17,19,21	1.54	2 (11%)
8	NAG	Z	2	8	14,14,15	0.92	1 (7%)	17,19,21	2.15	4 (23%)
9	NAG	a	1	9	14,14,15	2.63	10 (71%)	17,19,21	2.68	7 (41%)
9	NAG	a	2	9	14,14,15	1.84	7 (50%)	17,19,21	3.56	9 (52%)
9	BMA	a	3	9	11,11,12	1.04	1 (9%)	15,15,17	1.65	3 (20%)
9	MAN	a	4	9	11,11,12	1.21	1 (9%)	15,15,17	2.30	6 (40%)

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	M	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
5	MAN	M	4	5	-	1/2/19/22	0/1/1/1
6	NAG	N	1	6	-	5/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
7	NAG	O	1	7	-	3/6/23/26	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
8	NAG	P	1	8	-	3/6/23/26	0/1/1/1
8	NAG	P	2	8	-	4/6/23/26	0/1/1/1
9	NAG	Q	1	9	-	5/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	4/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Q	4	9	-	0/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	1/2/19/22	0/1/1/1
6	NAG	S	1	6	-	5/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
7	NAG	T	1	7	-	3/6/23/26	0/1/1/1
7	NAG	T	2	7	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
8	NAG	U	1	8	-	3/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
9	NAG	V	1	9	-	5/6/23/26	0/1/1/1
9	NAG	V	2	9	-	4/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	-	1/2/19/22	0/1/1/1
6	NAG	X	1	6	-	5/6/23/26	0/1/1/1
6	NAG	X	2	6	-	4/6/23/26	0/1/1/1
7	NAG	Y	1	7	-	3/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	3/6/23/26	0/1/1/1
7	BMA	Y	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	8	-	3/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	4/6/23/26	0/1/1/1
9	NAG	a	1	9	-	5/6/23/26	0/1/1/1
9	NAG	a	2	9	-	4/6/23/26	0/1/1/1
9	BMA	a	3	9	-	2/2/19/22	0/1/1/1
9	MAN	a	4	9	-	0/2/19/22	0/1/1/1

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	1	NAG	C1-C2	-5.97	1.44	1.52
5	M	1	NAG	C1-C2	-5.93	1.44	1.52
5	R	1	NAG	C1-C2	-5.91	1.44	1.52
5	M	1	NAG	O5-C1	-5.08	1.35	1.43
5	R	1	NAG	O5-C1	-5.06	1.35	1.43
5	W	1	NAG	O5-C1	-5.06	1.35	1.43
5	R	2	NAG	C1-C2	-4.80	1.45	1.52
5	W	2	NAG	C1-C2	-4.78	1.45	1.52
5	M	2	NAG	C1-C2	-4.78	1.45	1.52
6	X	1	NAG	C1-C2	-4.67	1.46	1.52
6	S	1	NAG	C1-C2	-4.66	1.46	1.52
6	N	1	NAG	C1-C2	-4.66	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	2	NAG	O5-C1	-4.21	1.36	1.43
5	R	2	NAG	O5-C1	-4.19	1.36	1.43
5	W	2	NAG	O5-C1	-4.17	1.36	1.43
9	a	1	NAG	C2-N2	-4.14	1.39	1.46
9	Q	1	NAG	C2-N2	-4.14	1.39	1.46
9	V	1	NAG	C2-N2	-4.11	1.39	1.46
5	W	2	NAG	C2-N2	-4.04	1.39	1.46
5	M	2	NAG	C2-N2	-4.01	1.39	1.46
5	R	2	NAG	C2-N2	-4.00	1.39	1.46
9	Q	1	NAG	C3-C2	-3.68	1.44	1.52
9	a	1	NAG	C3-C2	-3.67	1.44	1.52
9	V	1	NAG	C3-C2	-3.67	1.44	1.52
5	W	1	NAG	O5-C5	-3.41	1.36	1.43
5	M	1	NAG	O5-C5	-3.41	1.36	1.43
5	R	1	NAG	O5-C5	-3.41	1.36	1.43
9	a	1	NAG	O5-C1	-3.38	1.38	1.43
9	Q	1	NAG	O5-C1	-3.35	1.38	1.43
9	V	1	NAG	O5-C1	-3.34	1.38	1.43
7	Y	1	NAG	C2-N2	-3.33	1.40	1.46
7	O	1	NAG	C2-N2	-3.30	1.40	1.46
7	T	1	NAG	O5-C1	-3.30	1.38	1.43
7	T	1	NAG	C2-N2	-3.29	1.40	1.46
7	O	1	NAG	O5-C1	-3.25	1.38	1.43
6	X	1	NAG	O5-C5	-3.23	1.37	1.43
7	Y	1	NAG	O5-C1	-3.22	1.38	1.43
6	N	1	NAG	O5-C5	-3.22	1.37	1.43
6	S	1	NAG	O5-C5	-3.19	1.37	1.43
9	a	1	NAG	C1-C2	-3.10	1.48	1.52
9	Q	1	NAG	C1-C2	-3.08	1.48	1.52
9	V	1	NAG	C1-C2	-3.07	1.48	1.52
9	V	1	NAG	O5-C5	-3.03	1.37	1.43
9	Q	1	NAG	O5-C5	-3.01	1.37	1.43
9	a	1	NAG	O5-C5	-3.00	1.37	1.43
5	W	1	NAG	C4-C5	-2.92	1.46	1.53
5	R	1	NAG	C4-C5	-2.92	1.46	1.53
5	M	1	NAG	C4-C5	-2.91	1.46	1.53
5	R	3	BMA	C4-C5	-2.90	1.46	1.53
5	M	3	BMA	C4-C5	-2.89	1.46	1.53
5	W	3	BMA	C4-C5	-2.89	1.46	1.53
9	a	2	NAG	O5-C1	-2.89	1.38	1.43
9	Q	2	NAG	O5-C1	-2.86	1.38	1.43
9	V	2	NAG	C1-C2	-2.85	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	2	NAG	C1-C2	-2.85	1.48	1.52
9	V	2	NAG	O5-C1	-2.83	1.38	1.43
9	a	2	NAG	C1-C2	-2.83	1.48	1.52
5	M	1	NAG	C3-C2	-2.82	1.46	1.52
5	W	1	NAG	C3-C2	-2.82	1.46	1.52
5	R	1	NAG	C3-C2	-2.81	1.46	1.52
5	M	3	BMA	O5-C5	-2.80	1.38	1.43
5	R	3	BMA	O5-C5	-2.79	1.38	1.43
7	T	2	NAG	C2-N2	-2.79	1.41	1.46
5	W	3	BMA	O5-C5	-2.78	1.38	1.43
7	T	1	NAG	C3-C2	-2.78	1.46	1.52
5	W	2	NAG	C3-C2	-2.77	1.46	1.52
7	O	1	NAG	C3-C2	-2.77	1.46	1.52
5	M	2	NAG	C3-C2	-2.77	1.46	1.52
5	R	2	NAG	C3-C2	-2.77	1.46	1.52
7	Y	2	NAG	C2-N2	-2.76	1.41	1.46
7	O	2	NAG	C2-N2	-2.76	1.41	1.46
7	Y	1	NAG	C3-C2	-2.73	1.46	1.52
5	W	3	BMA	O5-C1	-2.71	1.39	1.43
5	R	3	BMA	O5-C1	-2.70	1.39	1.43
7	O	1	NAG	C4-C3	-2.69	1.45	1.52
7	Y	1	NAG	C4-C3	-2.68	1.45	1.52
5	M	3	BMA	O5-C1	-2.68	1.39	1.43
7	T	1	NAG	C4-C3	-2.66	1.45	1.52
6	X	1	NAG	C3-C2	-2.66	1.46	1.52
6	N	1	NAG	C3-C2	-2.66	1.46	1.52
6	S	1	NAG	C3-C2	-2.63	1.47	1.52
9	V	4	MAN	O5-C1	-2.62	1.39	1.43
9	V	1	NAG	C4-C5	-2.62	1.47	1.53
9	a	1	NAG	C4-C5	-2.62	1.47	1.53
9	Q	1	NAG	C4-C5	-2.62	1.47	1.53
9	V	1	NAG	C4-C3	-2.60	1.45	1.52
5	R	2	NAG	O5-C5	-2.59	1.38	1.43
9	Q	4	MAN	O5-C1	-2.59	1.39	1.43
9	a	1	NAG	C4-C3	-2.58	1.45	1.52
9	Q	1	NAG	C4-C3	-2.58	1.45	1.52
5	W	2	NAG	O5-C5	-2.57	1.38	1.43
9	a	4	MAN	O5-C1	-2.57	1.39	1.43
5	M	2	NAG	O5-C5	-2.55	1.38	1.43
6	X	2	NAG	O5-C5	-2.54	1.38	1.43
6	N	2	NAG	O5-C5	-2.53	1.38	1.43
5	W	1	NAG	C2-N2	-2.53	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	2	NAG	O5-C5	-2.53	1.38	1.43
5	M	1	NAG	C2-N2	-2.52	1.42	1.46
5	R	1	NAG	C2-N2	-2.52	1.42	1.46
9	Q	2	NAG	O5-C5	-2.47	1.38	1.43
9	V	2	NAG	O5-C5	-2.47	1.38	1.43
9	a	2	NAG	O5-C5	-2.46	1.38	1.43
9	V	1	NAG	C7-N2	-2.45	1.26	1.34
6	N	1	NAG	C2-N2	-2.45	1.42	1.46
9	a	1	NAG	C7-N2	-2.44	1.26	1.34
6	S	1	NAG	C2-N2	-2.44	1.42	1.46
9	Q	1	NAG	C7-N2	-2.44	1.26	1.34
6	S	1	NAG	O5-C1	-2.44	1.39	1.43
6	X	1	NAG	C2-N2	-2.43	1.42	1.46
9	Q	1	NAG	O4-C4	-2.41	1.37	1.43
9	a	1	NAG	O4-C4	-2.41	1.37	1.43
6	N	1	NAG	O5-C1	-2.41	1.39	1.43
9	V	1	NAG	O4-C4	-2.40	1.37	1.43
7	Y	1	NAG	C1-C2	-2.40	1.49	1.52
6	S	2	NAG	C4-C5	-2.39	1.47	1.53
9	a	2	NAG	C4-C5	-2.38	1.48	1.53
7	T	1	NAG	C1-C2	-2.38	1.49	1.52
6	N	2	NAG	C4-C5	-2.38	1.48	1.53
7	O	1	NAG	C1-C2	-2.37	1.49	1.52
9	Q	2	NAG	C4-C5	-2.37	1.48	1.53
6	X	1	NAG	O5-C1	-2.37	1.39	1.43
9	V	2	NAG	C4-C5	-2.37	1.48	1.53
6	X	2	NAG	C4-C5	-2.35	1.48	1.53
7	Y	1	NAG	O3-C3	-2.31	1.37	1.43
7	O	1	NAG	O3-C3	-2.28	1.37	1.43
7	T	1	NAG	O3-C3	-2.28	1.37	1.43
5	M	1	NAG	C4-C3	-2.22	1.46	1.52
5	R	1	NAG	C4-C3	-2.20	1.46	1.52
5	W	1	NAG	C4-C3	-2.19	1.46	1.52
5	M	4	MAN	C4-C5	-2.16	1.48	1.53
5	R	4	MAN	C4-C5	-2.15	1.48	1.53
9	Q	1	NAG	C8-C7	-2.15	1.46	1.50
9	V	1	NAG	C8-C7	-2.15	1.46	1.50
5	W	4	MAN	C4-C5	-2.13	1.48	1.53
9	a	1	NAG	C8-C7	-2.12	1.46	1.50
7	T	2	NAG	C1-C2	-2.11	1.49	1.52
7	O	2	NAG	C1-C2	-2.10	1.49	1.52
5	W	3	BMA	C4-C3	-2.10	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	2	NAG	O5-C1	-2.10	1.40	1.43
7	O	2	NAG	O5-C1	-2.10	1.40	1.43
7	Y	2	NAG	O5-C1	-2.08	1.40	1.43
9	V	2	NAG	C2-N2	-2.08	1.42	1.46
5	M	3	BMA	C4-C3	-2.08	1.46	1.52
5	R	3	BMA	C4-C3	-2.08	1.47	1.52
7	Y	2	NAG	C1-C2	-2.06	1.49	1.52
9	Q	3	BMA	C2-C3	-2.06	1.49	1.52
9	Q	2	NAG	C2-N2	-2.05	1.42	1.46
9	V	3	BMA	C2-C3	-2.05	1.49	1.52
9	Q	2	NAG	O4-C4	-2.04	1.37	1.43
9	a	3	BMA	C2-C3	-2.04	1.49	1.52
9	a	2	NAG	C2-N2	-2.04	1.42	1.46
8	Z	2	NAG	C2-N2	-2.04	1.42	1.46
9	a	2	NAG	C4-C3	-2.03	1.47	1.52
9	V	2	NAG	O4-C4	-2.03	1.37	1.43
9	a	2	NAG	O4-C4	-2.02	1.37	1.43
9	Q	2	NAG	C4-C3	-2.02	1.47	1.52

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2	NAG	C2-N2-C7	-8.48	111.53	122.90
5	W	2	NAG	C2-N2-C7	-8.48	111.53	122.90
5	M	2	NAG	C2-N2-C7	-8.47	111.54	122.90
9	a	2	NAG	C3-C4-C5	-8.14	95.47	110.23
9	Q	2	NAG	C3-C4-C5	-8.14	95.48	110.23
9	V	2	NAG	C3-C4-C5	-8.12	95.51	110.23
5	R	3	BMA	O3-C3-C2	6.55	123.43	110.05
5	M	3	BMA	O3-C3-C2	6.55	123.42	110.05
5	W	3	BMA	O3-C3-C2	6.53	123.38	110.05
9	Q	1	NAG	O5-C1-C2	-6.45	101.31	111.29
9	V	1	NAG	O5-C1-C2	-6.44	101.32	111.29
9	a	1	NAG	O5-C1-C2	-6.44	101.33	111.29
8	U	2	NAG	C2-N2-C7	-6.30	114.46	122.90
8	P	2	NAG	C2-N2-C7	-6.29	114.47	122.90
8	Z	2	NAG	C2-N2-C7	-6.28	114.48	122.90
5	R	2	NAG	C4-C3-C2	-6.27	101.82	111.02
5	M	2	NAG	C4-C3-C2	-6.25	101.86	111.02
9	V	2	NAG	O5-C5-C6	6.25	119.82	107.66
9	a	2	NAG	O5-C5-C6	6.24	119.82	107.66
9	Q	2	NAG	O5-C5-C6	6.24	119.80	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	2	NAG	C4-C3-C2	-6.24	101.88	111.02
9	V	2	NAG	O6-C6-C5	-5.60	92.26	111.33
7	Y	1	NAG	C2-N2-C7	-5.59	115.40	122.90
9	Q	2	NAG	O6-C6-C5	-5.59	92.28	111.33
7	T	1	NAG	C2-N2-C7	-5.59	115.41	122.90
9	a	2	NAG	O6-C6-C5	-5.58	92.32	111.33
7	O	1	NAG	C2-N2-C7	-5.58	115.42	122.90
5	M	1	NAG	C3-C4-C5	-4.79	101.55	110.23
5	W	1	NAG	C3-C4-C5	-4.79	101.55	110.23
5	R	1	NAG	C3-C4-C5	-4.79	101.56	110.23
7	Y	2	NAG	O5-C1-C2	-4.76	103.93	111.29
7	O	2	NAG	O5-C1-C2	-4.76	103.93	111.29
5	R	2	NAG	O5-C1-C2	-4.75	103.94	111.29
7	T	2	NAG	O5-C1-C2	-4.75	103.94	111.29
5	M	2	NAG	O5-C1-C2	-4.74	103.95	111.29
6	X	1	NAG	C4-C3-C2	-4.73	104.08	111.02
5	W	2	NAG	O5-C1-C2	-4.73	103.97	111.29
6	S	1	NAG	C4-C3-C2	-4.73	104.09	111.02
6	N	1	NAG	C4-C3-C2	-4.73	104.09	111.02
5	R	1	NAG	C2-N2-C7	-4.63	116.70	122.90
5	W	1	NAG	C2-N2-C7	-4.62	116.71	122.90
5	M	1	NAG	C2-N2-C7	-4.62	116.71	122.90
9	Q	4	MAN	O5-C5-C6	-4.55	98.82	107.66
9	a	4	MAN	O5-C5-C6	-4.54	98.82	107.66
9	V	4	MAN	O5-C5-C6	-4.54	98.83	107.66
9	V	4	MAN	C6-C5-C4	-4.53	101.89	113.02
9	a	4	MAN	C6-C5-C4	-4.53	101.90	113.02
9	Q	4	MAN	C6-C5-C4	-4.53	101.90	113.02
5	M	3	BMA	C6-C5-C4	-4.40	102.22	113.02
5	R	3	BMA	C6-C5-C4	-4.39	102.23	113.02
5	W	3	BMA	C6-C5-C4	-4.39	102.23	113.02
9	V	2	NAG	C1-C2-N2	-4.38	103.54	110.43
9	Q	2	NAG	C1-C2-N2	-4.36	103.56	110.43
9	a	2	NAG	C1-C2-N2	-4.36	103.57	110.43
7	O	1	NAG	O5-C1-C2	-4.35	104.56	111.29
7	T	1	NAG	O5-C1-C2	-4.34	104.57	111.29
7	Y	1	NAG	O5-C1-C2	-4.33	104.58	111.29
6	X	1	NAG	O5-C1-C2	-4.13	104.90	111.29
6	X	2	NAG	C1-C2-N2	4.13	116.94	110.43
6	N	2	NAG	C1-C2-N2	4.12	116.93	110.43
6	N	1	NAG	O5-C1-C2	-4.12	104.92	111.29
6	S	1	NAG	O5-C1-C2	-4.12	104.92	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	2	NAG	C1-C2-N2	4.12	116.92	110.43
6	N	2	NAG	C8-C7-N2	4.08	122.89	116.12
8	Z	2	NAG	C1-C2-N2	4.08	116.86	110.43
6	X	2	NAG	C8-C7-N2	4.07	122.87	116.12
8	P	2	NAG	C1-C2-N2	4.07	116.85	110.43
8	U	2	NAG	C1-C2-N2	4.07	116.84	110.43
8	U	1	NAG	C1-C2-N2	-4.05	104.05	110.43
6	S	2	NAG	C8-C7-N2	4.05	122.84	116.12
8	P	1	NAG	C1-C2-N2	-4.04	104.07	110.43
6	S	1	NAG	O6-C6-C5	-4.04	97.58	111.33
8	Z	1	NAG	C1-C2-N2	-4.03	104.08	110.43
6	N	1	NAG	O6-C6-C5	-4.03	97.62	111.33
6	X	1	NAG	O6-C6-C5	-4.03	97.62	111.33
9	Q	2	NAG	C1-O5-C5	-3.99	106.84	112.19
9	a	2	NAG	C1-O5-C5	-3.99	106.84	112.19
9	V	2	NAG	C1-O5-C5	-3.99	106.84	112.19
7	T	1	NAG	O3-C3-C4	-3.98	100.99	110.38
7	O	1	NAG	O3-C3-C4	-3.97	101.01	110.38
7	Y	1	NAG	O3-C3-C4	-3.97	101.02	110.38
9	V	1	NAG	C6-C5-C4	-3.83	103.62	113.02
9	Q	1	NAG	C6-C5-C4	-3.83	103.62	113.02
9	a	1	NAG	C6-C5-C4	-3.82	103.63	113.02
9	V	2	NAG	O4-C4-C3	-3.77	101.48	110.38
9	Q	2	NAG	O4-C4-C3	-3.76	101.51	110.38
9	a	2	NAG	O4-C4-C3	-3.76	101.51	110.38
9	a	1	NAG	C2-N2-C7	-3.72	117.91	122.90
9	Q	1	NAG	C3-C4-C5	-3.69	103.54	110.23
9	Q	1	NAG	C2-N2-C7	-3.69	117.95	122.90
5	M	2	NAG	O4-C4-C5	-3.69	100.23	109.32
9	V	1	NAG	C3-C4-C5	-3.69	103.54	110.23
5	R	2	NAG	O4-C4-C5	-3.68	100.25	109.32
9	V	1	NAG	C2-N2-C7	-3.68	117.96	122.90
5	R	4	MAN	O5-C5-C6	3.68	114.83	107.66
9	a	1	NAG	C3-C4-C5	-3.68	103.56	110.23
5	W	2	NAG	O4-C4-C5	-3.68	100.26	109.32
5	W	4	MAN	O5-C5-C6	3.68	114.82	107.66
5	M	4	MAN	O5-C5-C6	3.66	114.79	107.66
5	W	2	NAG	C6-C5-C4	-3.64	104.08	113.02
9	V	1	NAG	C4-C3-C2	-3.64	105.69	111.02
5	R	2	NAG	C6-C5-C4	-3.64	104.09	113.02
9	Q	1	NAG	C4-C3-C2	-3.63	105.69	111.02
5	M	2	NAG	C6-C5-C4	-3.63	104.10	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	1	NAG	C4-C3-C2	-3.62	105.71	111.02
9	a	4	MAN	O3-C3-C2	3.59	117.38	110.05
9	V	4	MAN	O3-C3-C2	3.58	117.36	110.05
9	Q	4	MAN	O3-C3-C2	3.58	117.35	110.05
7	T	2	NAG	C3-C4-C5	-3.47	103.93	110.23
7	Y	2	NAG	C3-C4-C5	-3.46	103.95	110.23
7	O	2	NAG	C3-C4-C5	-3.46	103.95	110.23
5	W	4	MAN	O4-C4-C5	-3.44	100.86	109.32
5	M	4	MAN	O4-C4-C5	-3.44	100.86	109.32
5	R	4	MAN	O4-C4-C5	-3.43	100.88	109.32
5	W	3	BMA	C3-C4-C5	-3.34	104.17	110.23
9	a	3	BMA	O2-C2-C3	-3.34	103.24	110.15
5	M	3	BMA	C3-C4-C5	-3.33	104.19	110.23
9	V	3	BMA	O2-C2-C3	-3.33	103.25	110.15
9	Q	3	BMA	O2-C2-C3	-3.33	103.26	110.15
5	R	3	BMA	C3-C4-C5	-3.32	104.21	110.23
7	Y	3	BMA	O4-C4-C3	-3.29	102.63	110.38
7	O	3	BMA	O4-C4-C3	-3.28	102.65	110.38
7	T	3	BMA	O4-C4-C3	-3.27	102.66	110.38
5	W	3	BMA	O4-C4-C5	-3.27	101.28	109.32
5	M	3	BMA	O4-C4-C5	-3.26	101.30	109.32
5	R	3	BMA	O4-C4-C5	-3.26	101.31	109.32
6	S	1	NAG	O5-C5-C6	-3.22	101.40	107.66
6	N	1	NAG	O5-C5-C6	-3.21	101.41	107.66
9	a	2	NAG	O5-C1-C2	-3.21	106.32	111.29
6	X	1	NAG	O5-C5-C6	-3.21	101.42	107.66
9	Q	2	NAG	O5-C1-C2	-3.20	106.33	111.29
9	V	2	NAG	O5-C1-C2	-3.20	106.34	111.29
6	X	2	NAG	C1-O5-C5	3.03	116.24	112.19
6	N	2	NAG	C1-O5-C5	3.02	116.24	112.19
6	S	2	NAG	C1-O5-C5	3.01	116.22	112.19
9	V	4	MAN	O4-C4-C3	-2.97	103.36	110.38
9	Q	4	MAN	O4-C4-C3	-2.97	103.37	110.38
5	W	1	NAG	C4-C3-C2	-2.97	106.67	111.02
9	a	4	MAN	O4-C4-C3	-2.96	103.39	110.38
5	R	1	NAG	C4-C3-C2	-2.96	106.68	111.02
5	M	1	NAG	C4-C3-C2	-2.95	106.70	111.02
5	R	1	NAG	C1-O5-C5	-2.95	108.24	112.19
7	Y	1	NAG	O5-C5-C6	-2.93	101.95	107.66
7	O	1	NAG	O5-C5-C6	-2.93	101.96	107.66
5	M	1	NAG	C1-O5-C5	-2.92	108.27	112.19
7	T	1	NAG	O5-C5-C6	-2.92	101.98	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	1	NAG	C1-O5-C5	-2.92	108.28	112.19
9	V	3	BMA	C2-C3-C4	-2.89	105.78	110.86
9	Q	3	BMA	C2-C3-C4	-2.88	105.79	110.86
9	a	3	BMA	C2-C3-C4	-2.88	105.80	110.86
5	W	1	NAG	O5-C1-C2	-2.86	106.87	111.29
5	R	1	NAG	O5-C1-C2	-2.85	106.88	111.29
5	M	1	NAG	O5-C1-C2	-2.85	106.88	111.29
8	P	2	NAG	C6-C5-C4	-2.83	106.07	113.02
9	Q	2	NAG	O5-C5-C4	2.83	117.70	110.83
8	U	2	NAG	C6-C5-C4	-2.82	106.08	113.02
8	Z	2	NAG	C6-C5-C4	-2.82	106.09	113.02
9	a	2	NAG	O5-C5-C4	2.82	117.69	110.83
9	V	2	NAG	O5-C5-C4	2.82	117.68	110.83
9	Q	4	MAN	O2-C2-C1	-2.79	102.83	109.22
9	V	4	MAN	O2-C2-C1	-2.78	102.86	109.22
9	a	4	MAN	O2-C2-C1	-2.78	102.87	109.22
7	Y	1	NAG	O3-C3-C2	-2.77	103.65	109.40
7	O	1	NAG	O3-C3-C2	-2.77	103.65	109.40
7	T	1	NAG	O3-C3-C2	-2.76	103.66	109.40
9	a	1	NAG	C8-C7-N2	-2.75	111.56	116.12
7	Y	3	BMA	C2-C3-C4	-2.74	106.03	110.86
9	Q	1	NAG	C8-C7-N2	-2.74	111.58	116.12
7	O	3	BMA	C2-C3-C4	-2.74	106.05	110.86
7	T	3	BMA	C2-C3-C4	-2.73	106.06	110.86
9	V	1	NAG	C8-C7-N2	-2.72	111.60	116.12
7	T	2	NAG	C6-C5-C4	-2.67	106.47	113.02
7	O	2	NAG	C6-C5-C4	-2.65	106.50	113.02
7	Y	2	NAG	C6-C5-C4	-2.65	106.50	113.02
9	a	4	MAN	C2-C3-C4	-2.61	106.26	110.86
5	W	3	BMA	C1-C2-C3	-2.61	105.84	109.64
9	V	4	MAN	C2-C3-C4	-2.61	106.26	110.86
5	R	3	BMA	C1-C2-C3	-2.61	105.84	109.64
9	Q	4	MAN	C2-C3-C4	-2.61	106.27	110.86
5	M	3	BMA	C1-C2-C3	-2.60	105.85	109.64
8	U	2	NAG	C4-C3-C2	-2.58	107.23	111.02
8	P	2	NAG	C4-C3-C2	-2.57	107.25	111.02
8	Z	2	NAG	C4-C3-C2	-2.57	107.25	111.02
6	X	2	NAG	C6-C5-C4	-2.57	106.72	113.02
6	S	1	NAG	O3-C3-C2	-2.56	104.08	109.40
6	S	2	NAG	C6-C5-C4	-2.56	106.72	113.02
6	N	2	NAG	C6-C5-C4	-2.56	106.73	113.02
6	N	1	NAG	O3-C3-C2	-2.56	104.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	1	NAG	O3-C3-C2	-2.56	104.08	109.40
7	T	1	NAG	C3-C4-C5	-2.54	105.63	110.23
7	O	1	NAG	C3-C4-C5	-2.52	105.66	110.23
7	Y	1	NAG	C3-C4-C5	-2.52	105.66	110.23
6	S	2	NAG	O5-C1-C2	-2.50	107.42	111.29
6	N	2	NAG	O5-C1-C2	-2.50	107.42	111.29
5	M	1	NAG	O3-C3-C2	-2.49	104.23	109.40
5	W	1	NAG	O3-C3-C2	-2.49	104.23	109.40
6	X	2	NAG	O5-C1-C2	-2.48	107.45	111.29
5	R	1	NAG	O3-C3-C2	-2.48	104.26	109.40
5	W	1	NAG	C1-C2-N2	-2.47	106.53	110.43
5	M	1	NAG	C1-C2-N2	-2.47	106.54	110.43
5	W	2	NAG	C8-C7-N2	2.47	120.21	116.12
5	R	2	NAG	C8-C7-N2	2.46	120.20	116.12
5	R	1	NAG	C1-C2-N2	-2.46	106.56	110.43
6	X	2	NAG	O3-C3-C4	-2.45	104.59	110.38
5	M	2	NAG	C8-C7-N2	2.45	120.19	116.12
8	Z	1	NAG	C4-C3-C2	-2.45	107.43	111.02
6	N	2	NAG	O3-C3-C4	-2.45	104.61	110.38
8	P	1	NAG	C4-C3-C2	-2.45	107.43	111.02
8	U	1	NAG	C4-C3-C2	-2.45	107.43	111.02
6	S	2	NAG	O3-C3-C4	-2.44	104.61	110.38
7	T	3	BMA	O2-C2-C3	-2.43	105.12	110.15
7	O	3	BMA	O2-C2-C3	-2.43	105.12	110.15
7	Y	3	BMA	O2-C2-C3	-2.42	105.15	110.15
9	a	2	NAG	O4-C4-C5	-2.32	103.61	109.32
9	V	2	NAG	O4-C4-C5	-2.31	103.62	109.32
9	Q	2	NAG	O4-C4-C5	-2.31	103.63	109.32
5	M	4	MAN	C1-C2-C3	-2.30	106.29	109.64
5	R	4	MAN	C1-C2-C3	-2.30	106.29	109.64
5	W	4	MAN	C1-C2-C3	-2.29	106.31	109.64
9	Q	3	BMA	O5-C1-C2	-2.20	105.55	110.79
9	a	3	BMA	O5-C1-C2	-2.19	105.55	110.79
9	V	3	BMA	O5-C1-C2	-2.19	105.57	110.79
5	W	2	NAG	O5-C5-C6	-2.18	103.41	107.66
5	M	2	NAG	O5-C5-C6	-2.17	103.44	107.66
5	R	1	NAG	O4-C4-C3	2.17	115.49	110.38
5	M	1	NAG	O4-C4-C3	2.16	115.48	110.38
5	R	2	NAG	O5-C5-C6	-2.15	103.48	107.66
5	W	1	NAG	O4-C4-C3	2.15	115.44	110.38
9	V	1	NAG	O6-C6-C5	-2.09	104.22	111.33
9	Q	1	NAG	O6-C6-C5	-2.09	104.23	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	1	NAG	O6-C6-C5	-2.09	104.23	111.33
6	X	2	NAG	O7-C7-C8	-2.05	118.41	122.05
6	N	2	NAG	O7-C7-C8	-2.04	118.43	122.05
6	S	2	NAG	O7-C7-C8	-2.01	118.47	122.05
7	Y	2	NAG	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C3-C2-N2-C7
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C3-C2-N2-C7
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C3-C2-N2-C7
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C1-C2-N2-C7
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	S	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	X	1	NAG	C1-C2-N2-C7
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
7	O	1	NAG	C1-C2-N2-C7
7	O	2	NAG	C1-C2-N2-C7
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	T	1	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C8-C7-N2-C2
7	T	2	NAG	O7-C7-N2-C2
7	Y	1	NAG	C1-C2-N2-C7
7	Y	2	NAG	C1-C2-N2-C7
7	Y	2	NAG	C8-C7-N2-C2
7	Y	2	NAG	O7-C7-N2-C2
8	P	1	NAG	C3-C2-N2-C7
8	U	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	Z	1	NAG	C3-C2-N2-C7
9	Q	1	NAG	C3-C2-N2-C7
9	Q	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C3-C2-N2-C7
9	V	2	NAG	C3-C2-N2-C7
9	a	1	NAG	C3-C2-N2-C7
9	a	2	NAG	C3-C2-N2-C7
7	O	1	NAG	C8-C7-N2-C2
7	T	1	NAG	C8-C7-N2-C2
7	Y	1	NAG	C8-C7-N2-C2
9	Q	2	NAG	C8-C7-N2-C2
9	V	2	NAG	C8-C7-N2-C2
9	a	2	NAG	C8-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
9	Q	2	NAG	O7-C7-N2-C2
9	V	2	NAG	O7-C7-N2-C2
9	a	2	NAG	O7-C7-N2-C2
6	N	2	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O7-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
8	P	1	NAG	C8-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2
8	U	1	NAG	C8-C7-N2-C2
8	U	1	NAG	O7-C7-N2-C2
8	Z	1	NAG	C8-C7-N2-C2
8	Z	1	NAG	O7-C7-N2-C2
5	M	3	BMA	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	a	2	NAG	O5-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	W	3	BMA	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
9	Q	3	BMA	C4-C5-C6-O6
9	V	3	BMA	C4-C5-C6-O6
9	a	3	BMA	C4-C5-C6-O6
6	N	2	NAG	C8-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	X	2	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
7	Y	1	NAG	O7-C7-N2-C2
9	Q	1	NAG	O5-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
9	a	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O7-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
9	V	1	NAG	C4-C5-C6-O6
9	a	1	NAG	C4-C5-C6-O6
9	Q	1	NAG	C8-C7-N2-C2
9	Q	1	NAG	O7-C7-N2-C2
9	V	1	NAG	C8-C7-N2-C2
9	V	1	NAG	O7-C7-N2-C2
9	a	1	NAG	C8-C7-N2-C2
9	a	1	NAG	O7-C7-N2-C2
9	a	3	BMA	O5-C5-C6-O6
9	Q	3	BMA	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
8	P	2	NAG	C8-C7-N2-C2
8	U	2	NAG	C8-C7-N2-C2

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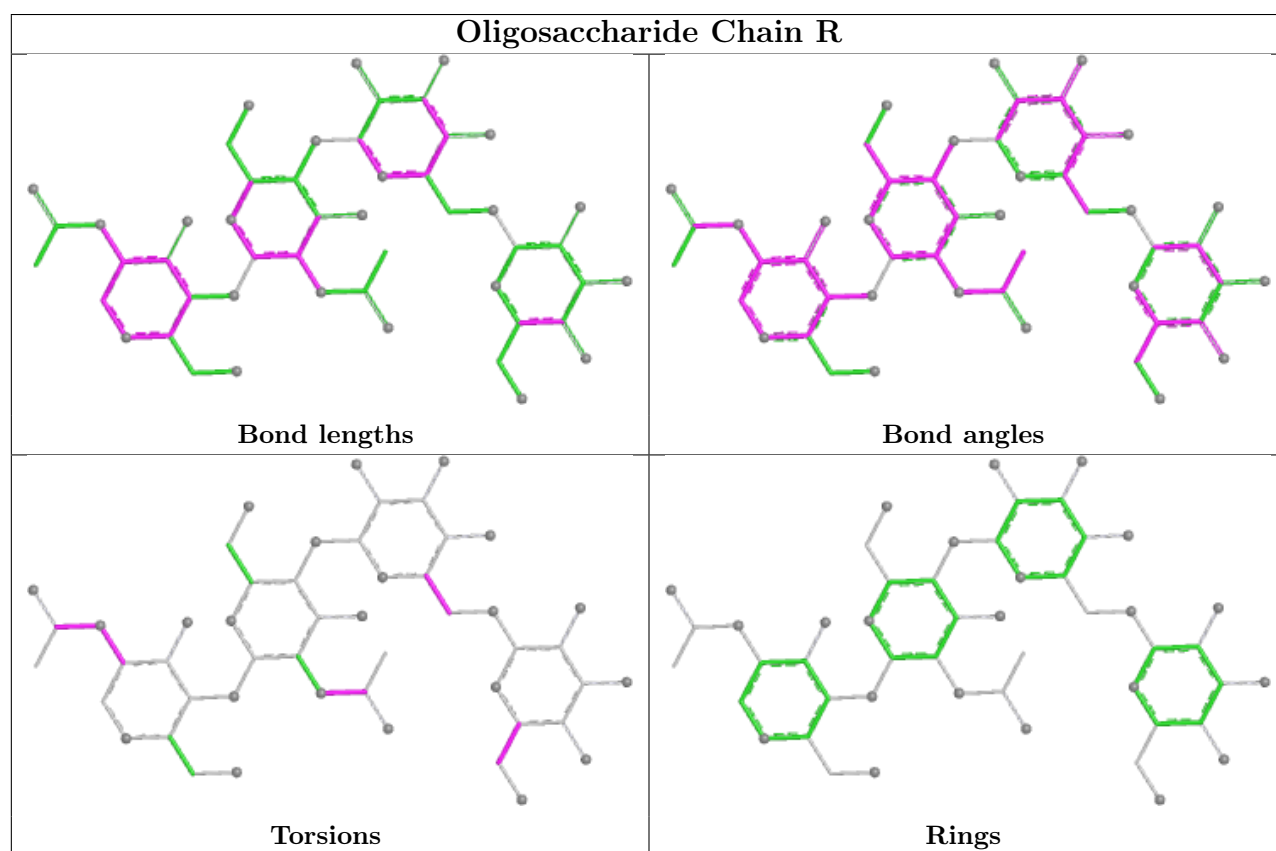
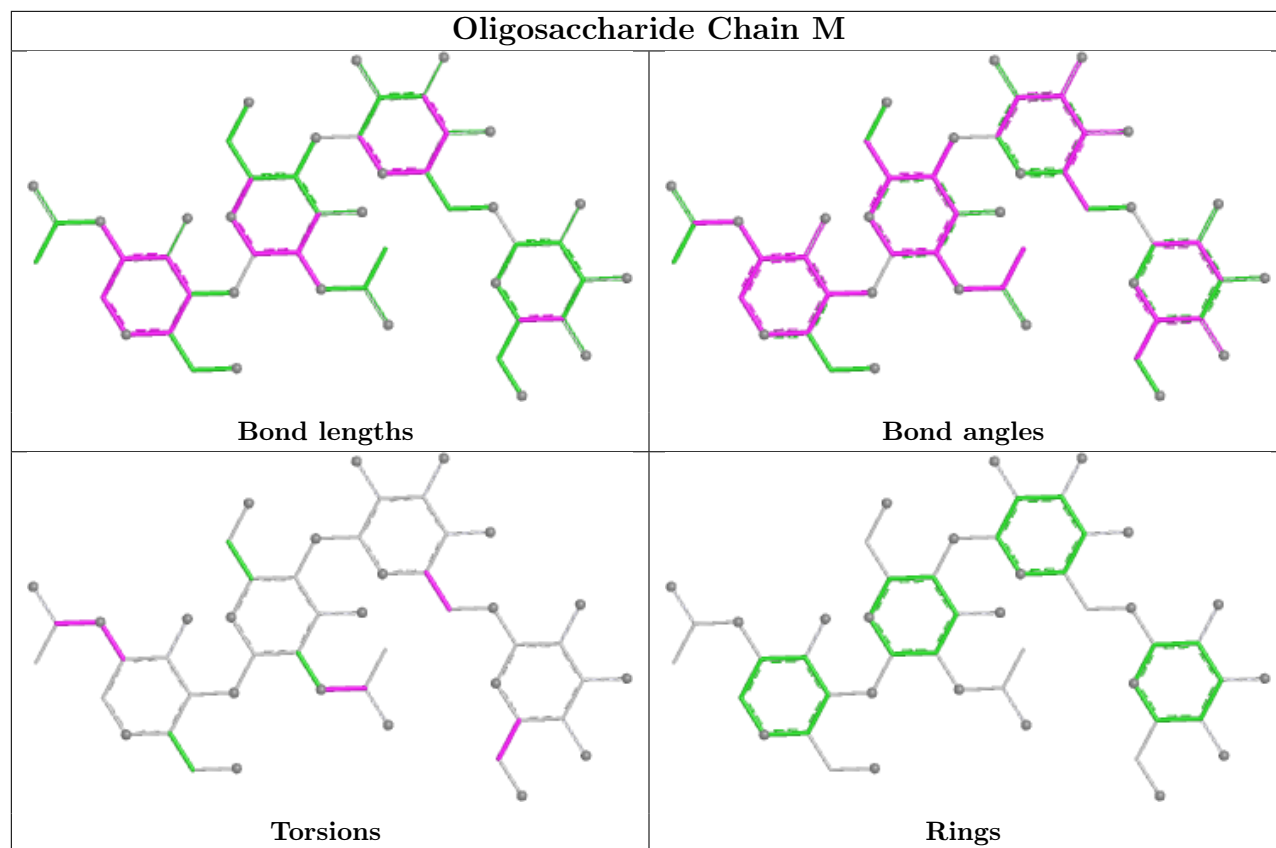
Mol	Chain	Res	Type	Atoms
8	Z	2	NAG	C8-C7-N2-C2
8	U	2	NAG	C4-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6
8	P	2	NAG	C4-C5-C6-O6
8	P	2	NAG	O7-C7-N2-C2
8	U	2	NAG	O7-C7-N2-C2
8	Z	2	NAG	O7-C7-N2-C2

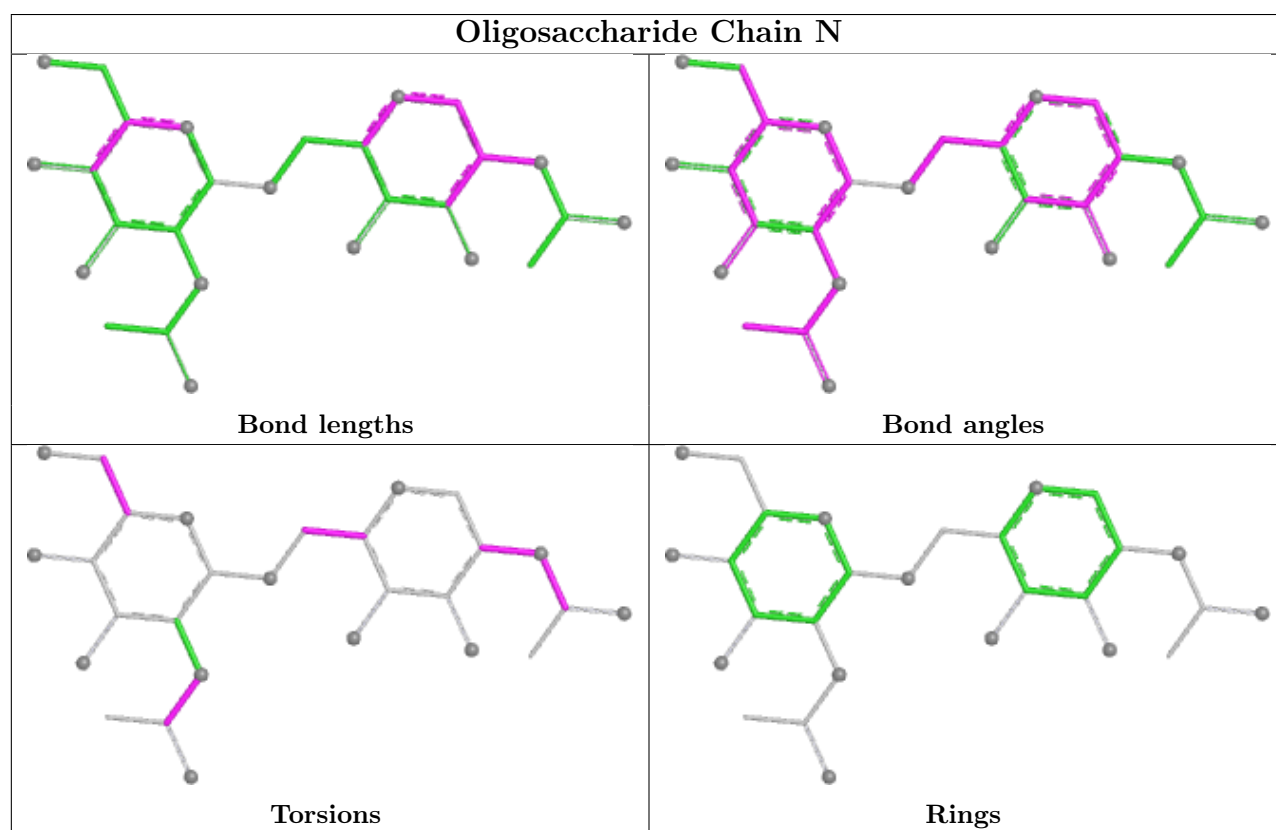
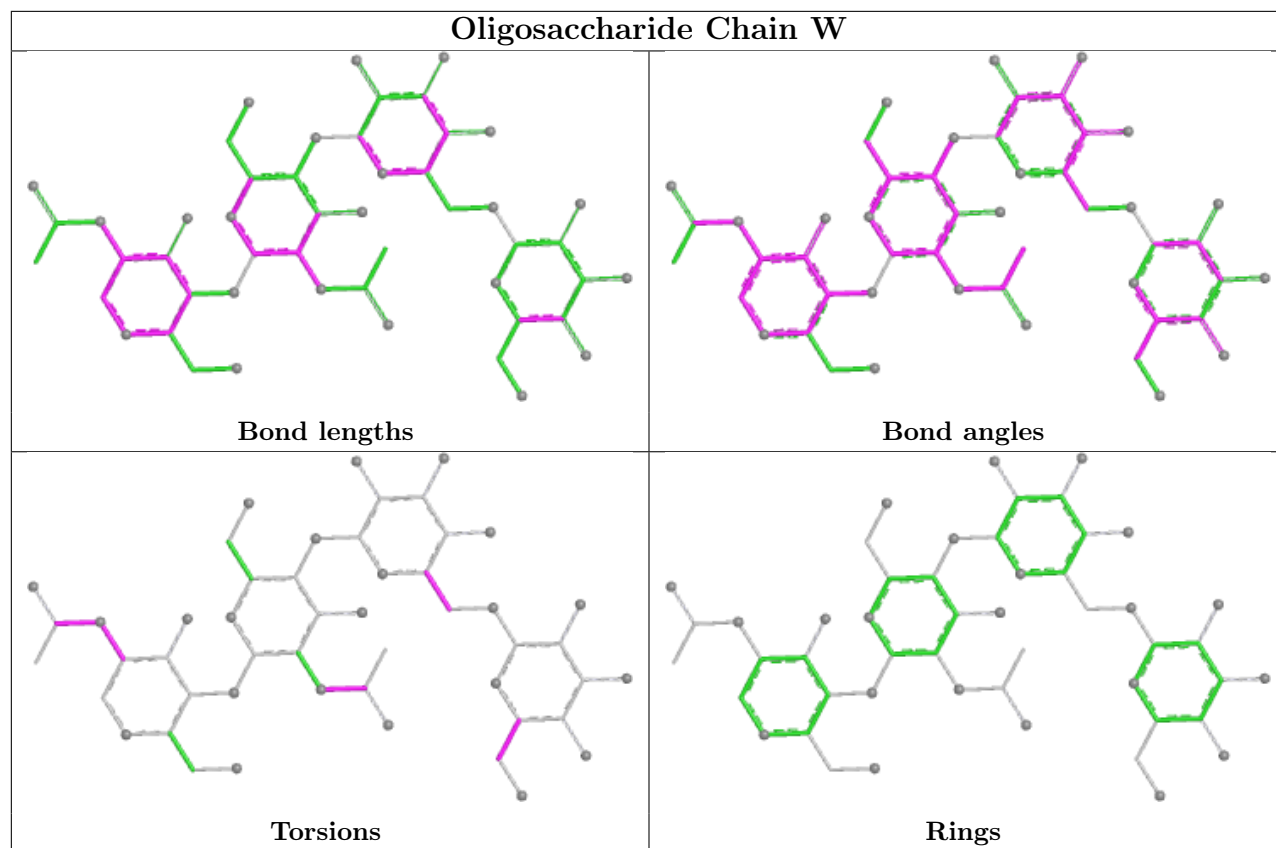
There are no ring outliers.

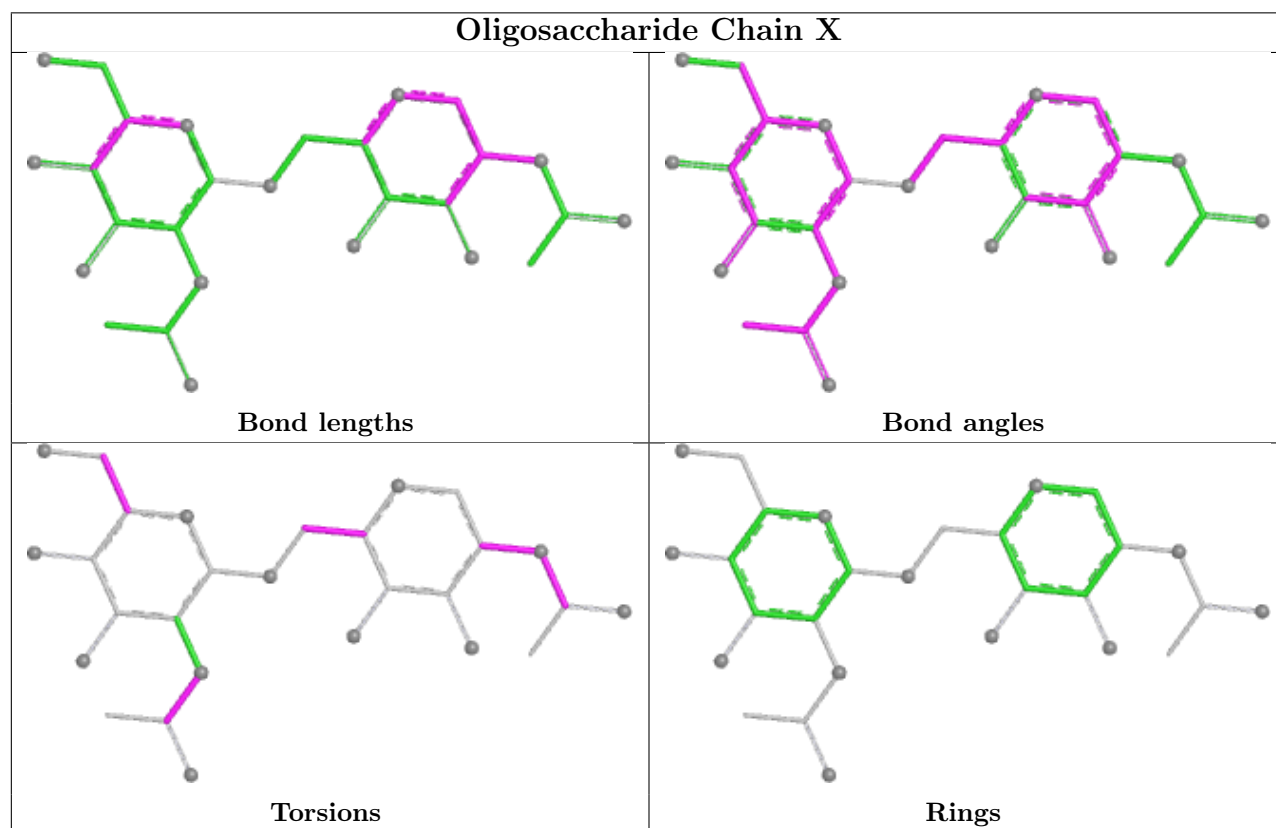
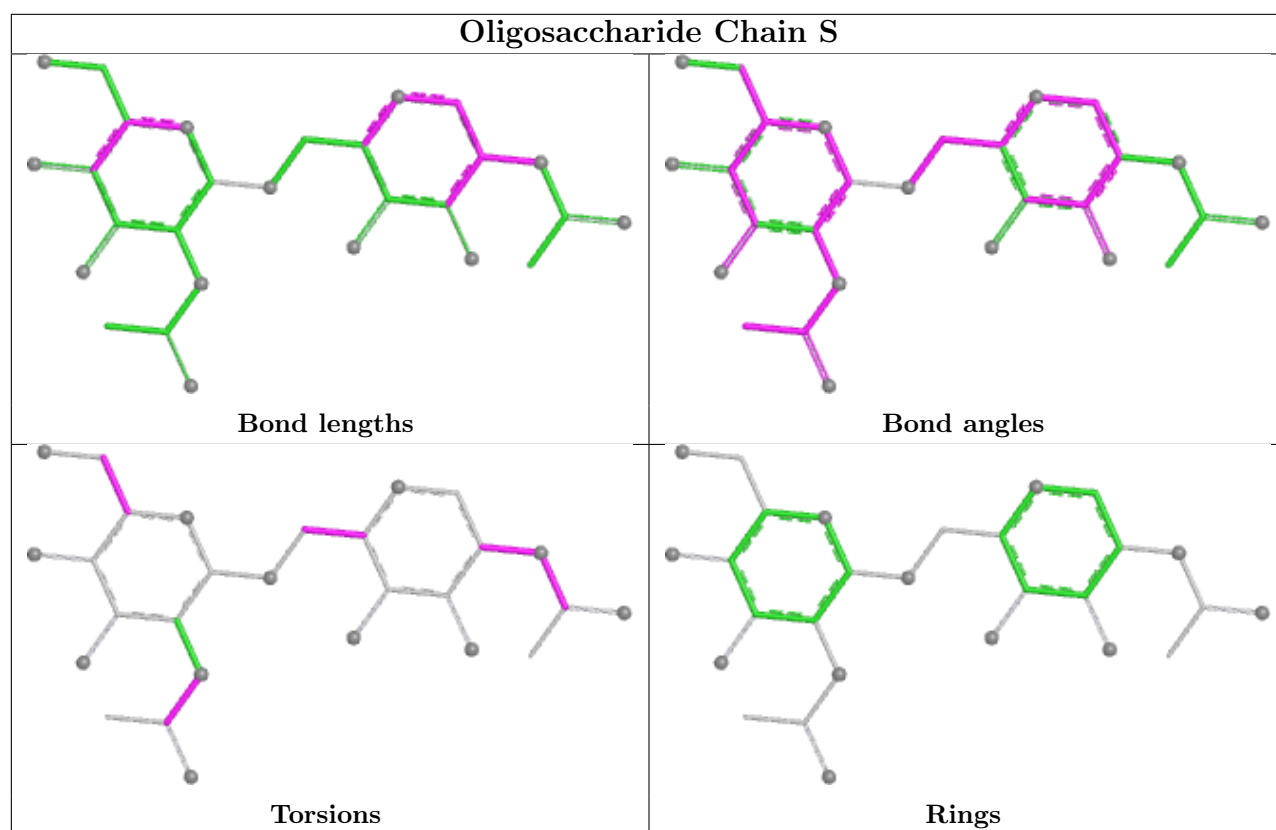
22 monomers are involved in 30 short contacts:

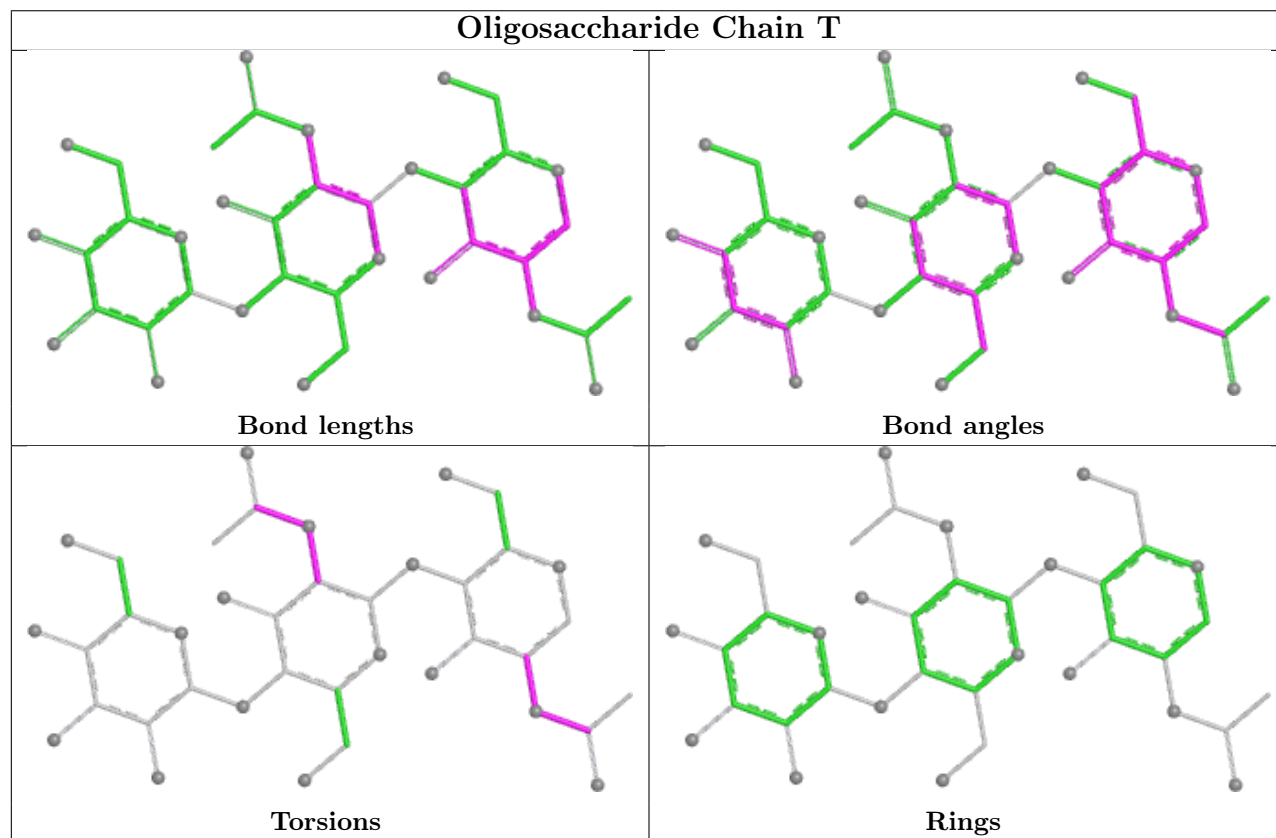
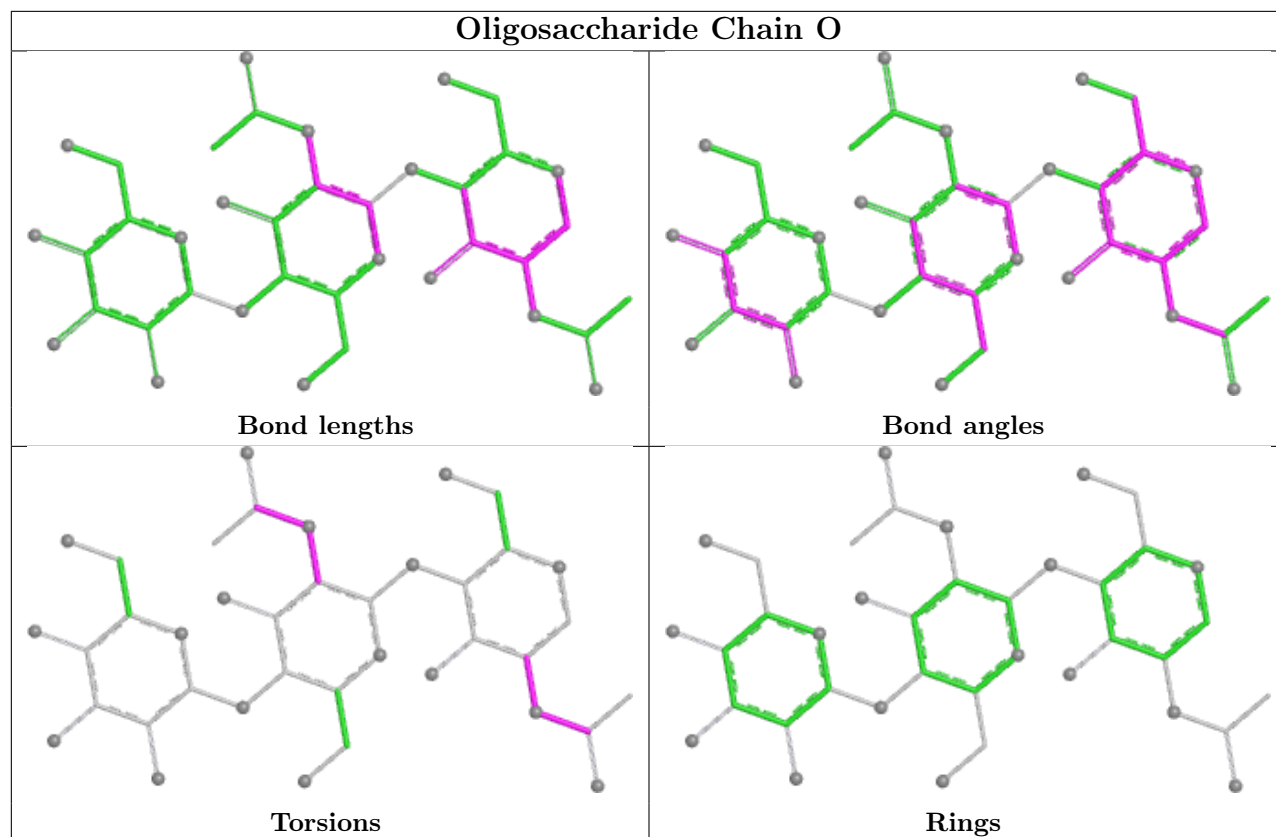
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	2	NAG	1	0
8	Z	1	NAG	2	0
9	V	2	NAG	3	0
6	S	1	NAG	1	0
5	R	1	NAG	1	0
6	X	1	NAG	1	0
7	O	1	NAG	1	0
5	M	1	NAG	1	0
5	W	4	MAN	1	0
8	U	1	NAG	2	0
5	R	4	MAN	1	0
7	Y	1	NAG	2	0
9	Q	2	NAG	2	0
5	W	1	NAG	1	0
5	R	2	NAG	1	0
8	P	1	NAG	2	0
6	N	1	NAG	1	0
9	V	1	NAG	1	0
5	W	2	NAG	1	0
9	Q	1	NAG	1	0
7	T	1	NAG	2	0
5	M	4	MAN	1	0

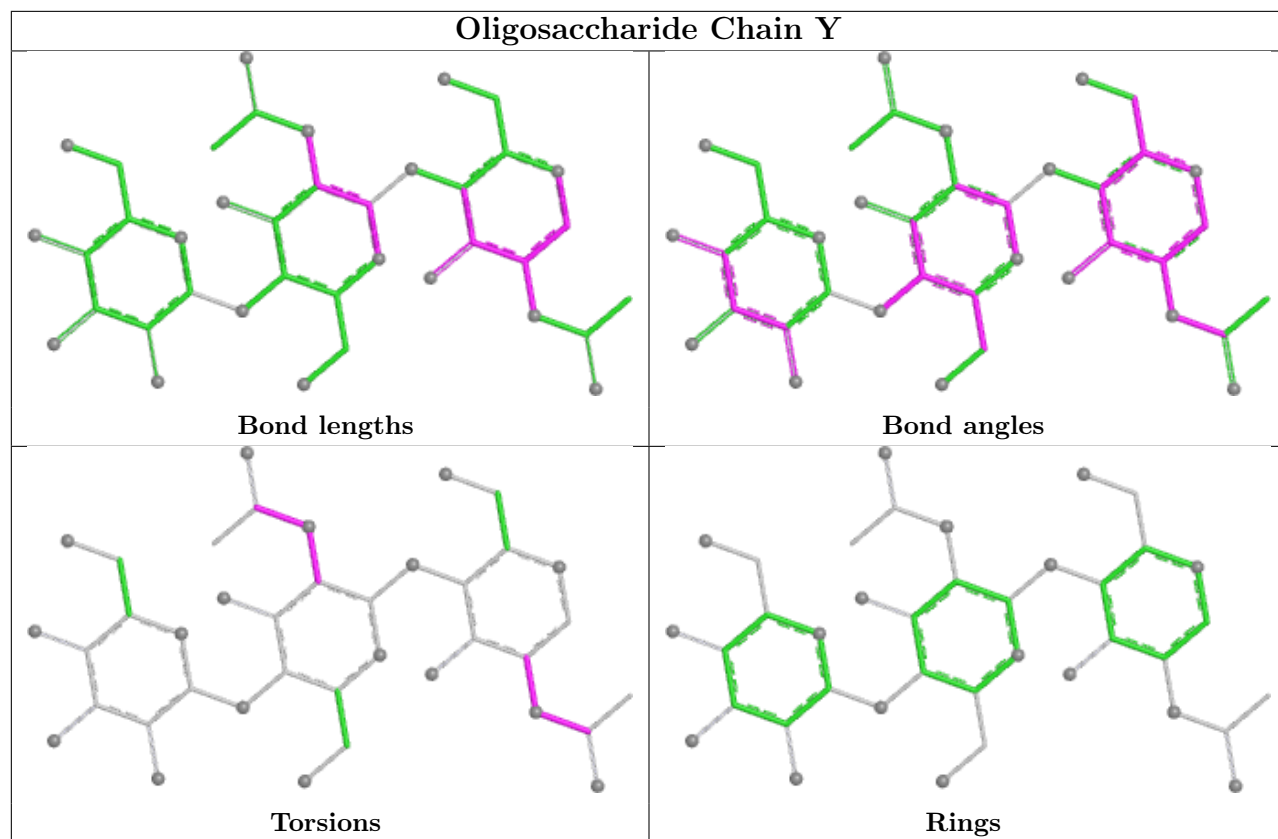
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

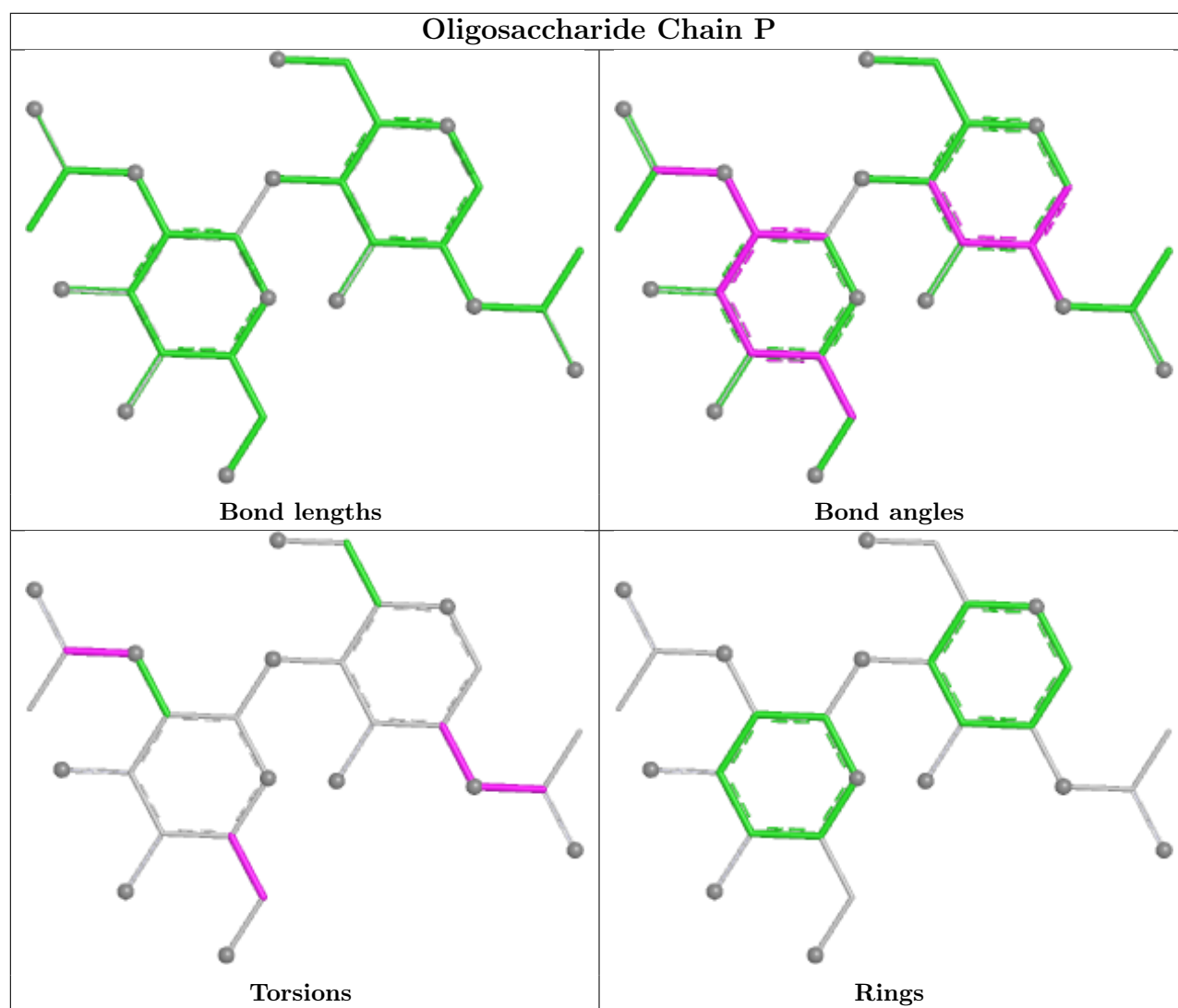


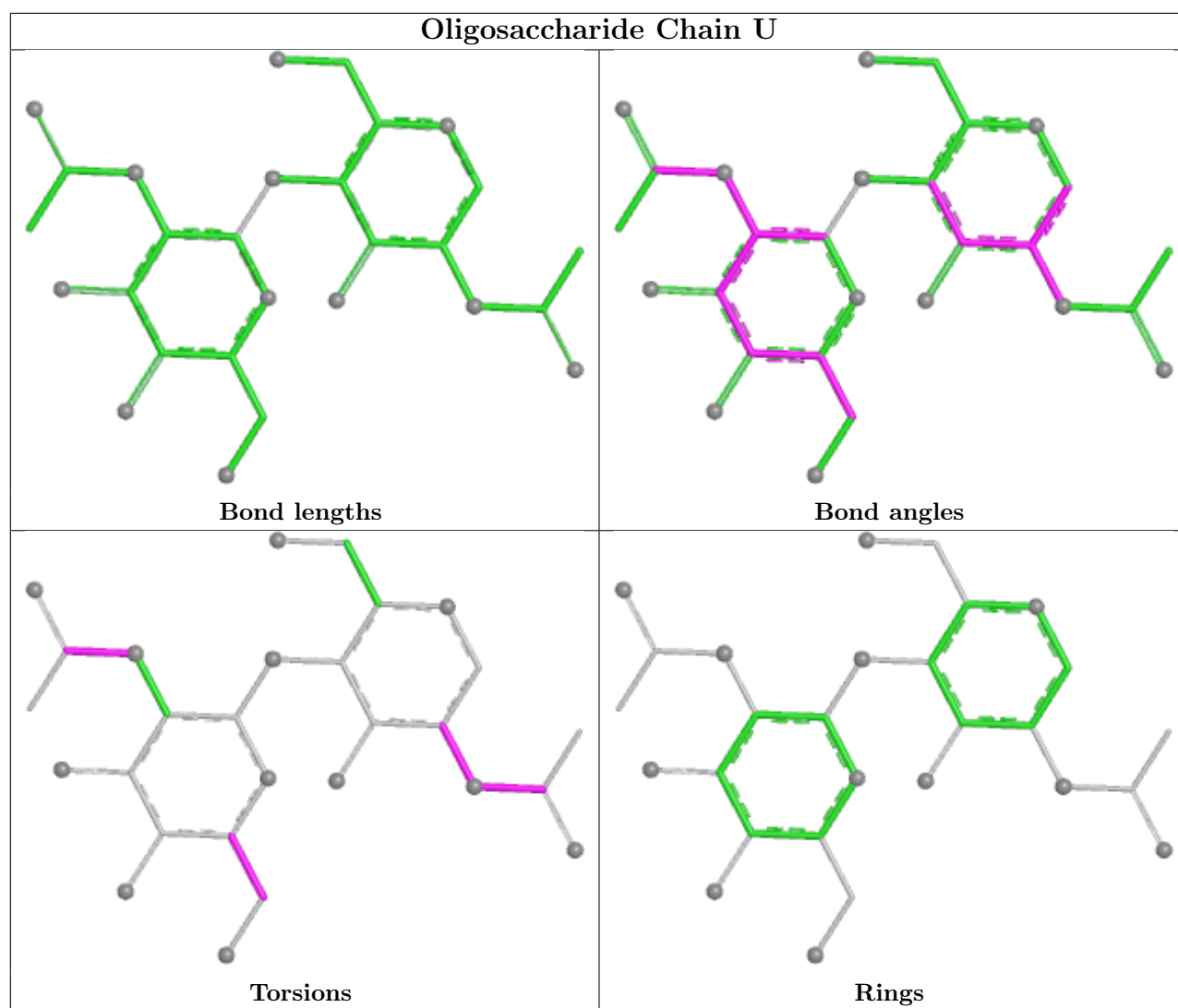


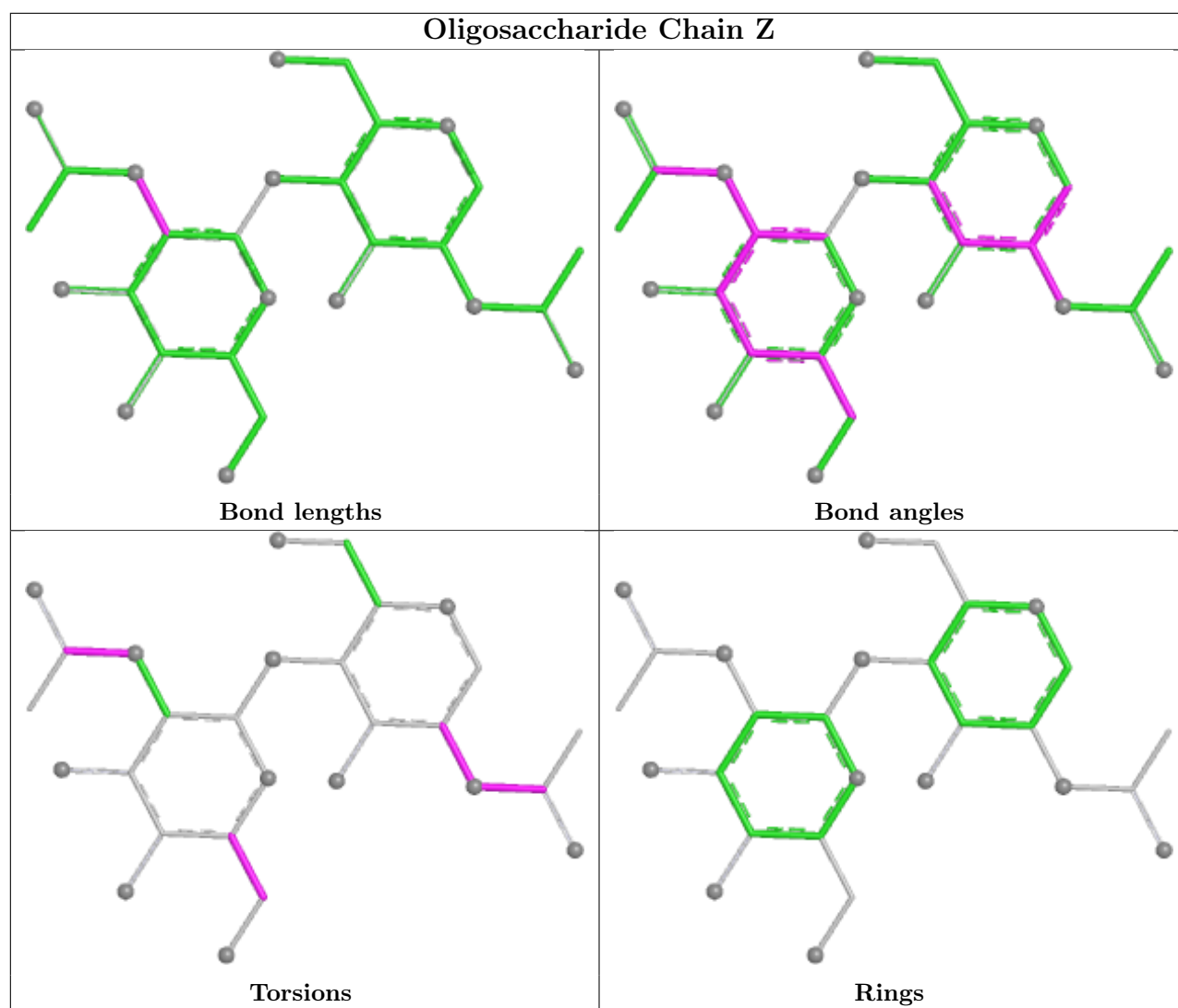


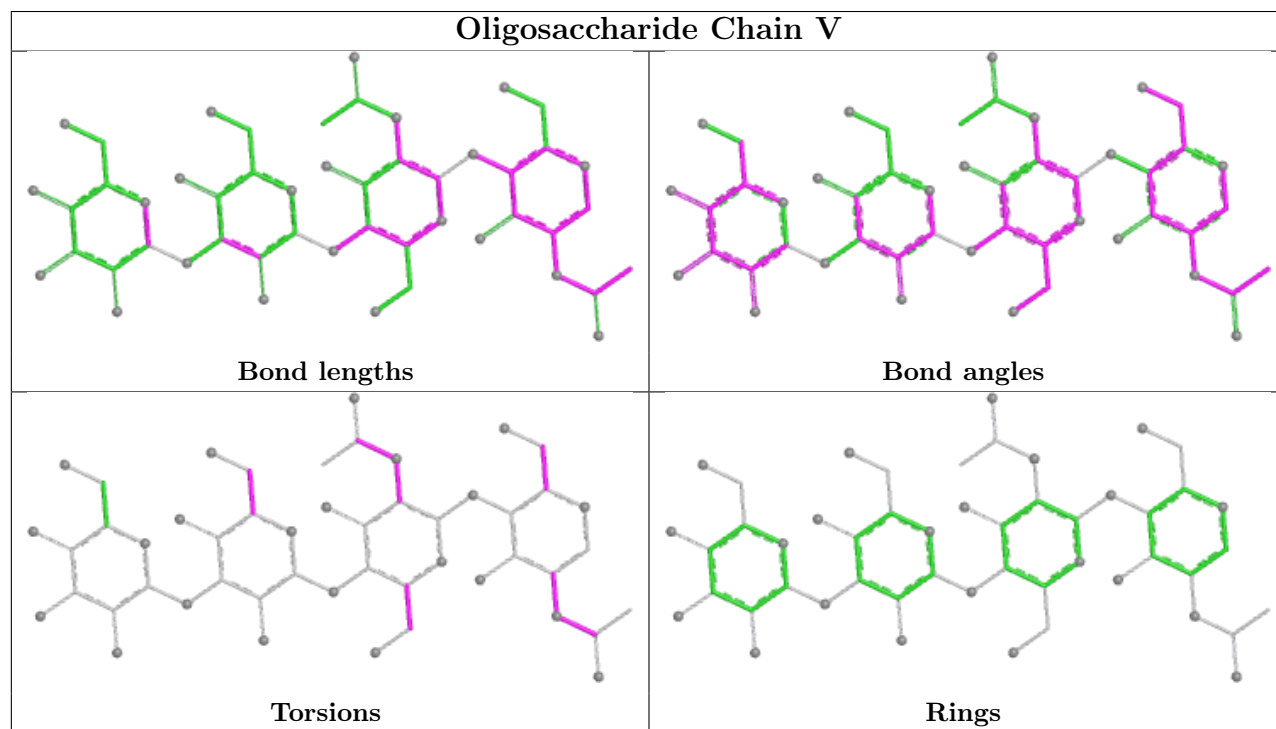
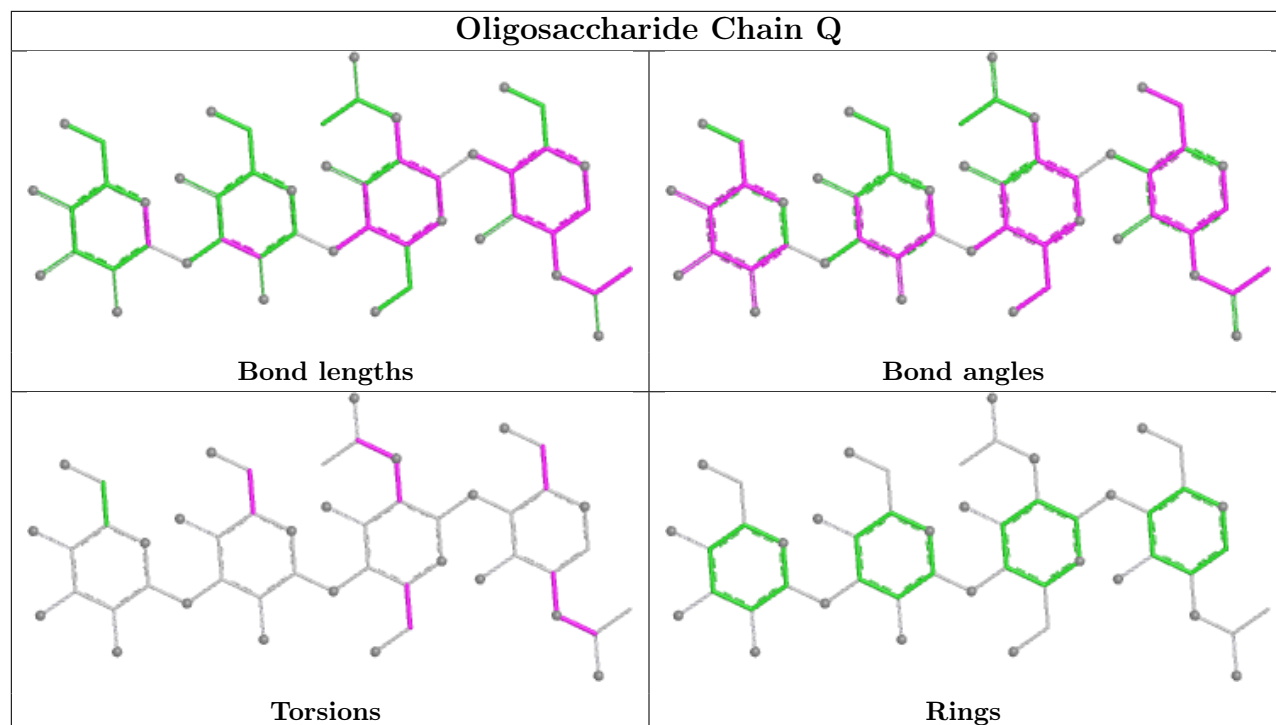


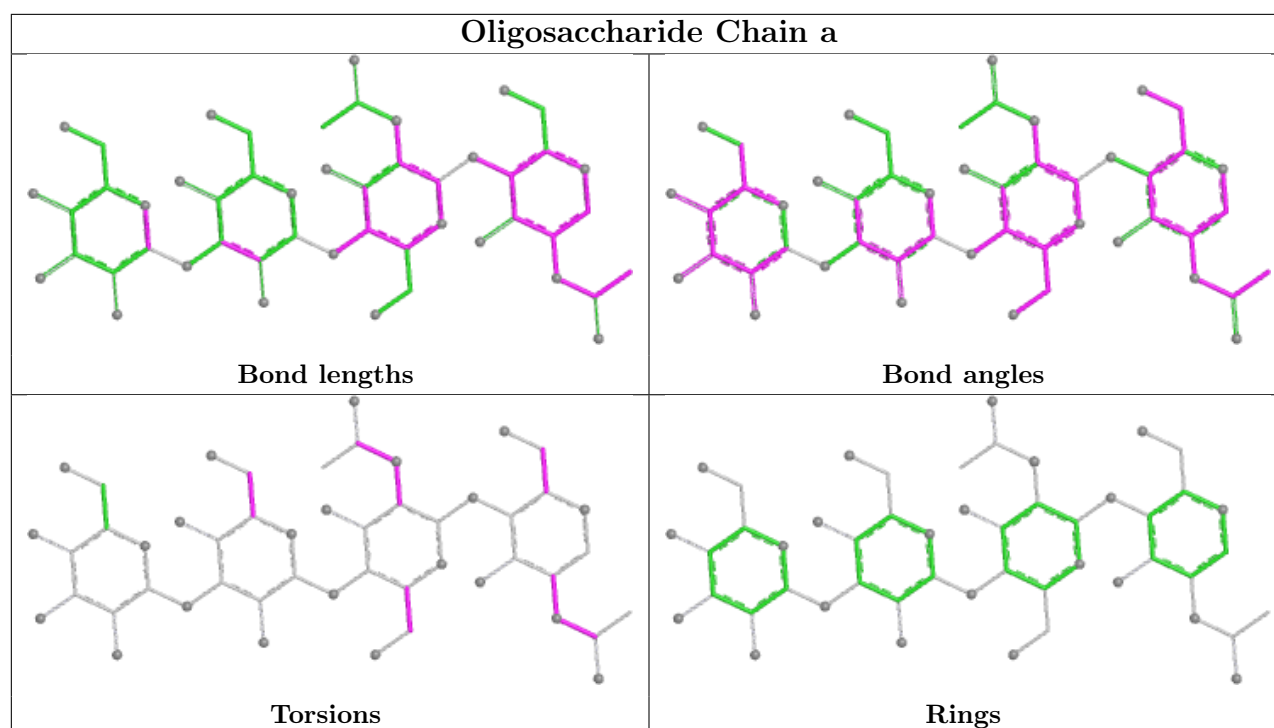












5.6 Ligand geometry [i](#)

18 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
10	NAG	E	620	-	14,14,15	0.93	0	17,19,21	2.41	6 (35%)
10	NAG	A	613	-	14,14,15	1.61	3 (21%)	17,19,21	3.05	7 (41%)
10	NAG	A	620	-	14,14,15	0.93	0	17,19,21	2.41	6 (35%)
10	NAG	A	614	-	14,14,15	1.55	3 (21%)	17,19,21	3.28	10 (58%)
10	NAG	E	614	-	14,14,15	1.55	3 (21%)	17,19,21	3.28	10 (58%)
10	NAG	E	610	1	14,14,15	1.63	3 (21%)	17,19,21	3.08	8 (47%)
10	NAG	E	615	-	14,14,15	0.47	0	17,19,21	1.12	0
10	NAG	E	621	-	14,14,15	1.12	1 (7%)	17,19,21	2.51	7 (41%)
10	NAG	I	620	-	14,14,15	0.92	0	17,19,21	2.41	6 (35%)
10	NAG	I	621	-	14,14,15	1.12	1 (7%)	17,19,21	2.51	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	E	613	-	14,14,15	1.61	3 (21%)	17,19,21	3.05	7 (41%)
10	NAG	I	614	-	14,14,15	1.55	3 (21%)	17,19,21	3.29	10 (58%)
10	NAG	I	610	1	14,14,15	1.65	3 (21%)	17,19,21	3.07	8 (47%)
10	NAG	I	613	-	14,14,15	1.60	3 (21%)	17,19,21	3.05	7 (41%)
10	NAG	A	615	-	14,14,15	0.47	0	17,19,21	1.13	0
10	NAG	A	610	1	14,14,15	1.64	3 (21%)	17,19,21	3.08	8 (47%)
10	NAG	A	621	-	14,14,15	1.12	1 (7%)	17,19,21	2.51	6 (35%)
10	NAG	I	615	-	14,14,15	0.47	0	17,19,21	1.13	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
10	NAG	E	620	-	-	1/6/23/26	0/1/1/1
10	NAG	A	613	-	-	2/6/23/26	0/1/1/1
10	NAG	A	620	-	-	1/6/23/26	0/1/1/1
10	NAG	A	614	-	-	1/6/23/26	0/1/1/1
10	NAG	E	614	-	-	1/6/23/26	0/1/1/1
10	NAG	E	610	1	-	3/6/23/26	0/1/1/1
10	NAG	E	615	-	-	4/6/23/26	0/1/1/1
10	NAG	E	621	-	-	4/6/23/26	0/1/1/1
10	NAG	I	620	-	-	1/6/23/26	0/1/1/1
10	NAG	I	621	-	-	4/6/23/26	0/1/1/1
10	NAG	E	613	-	-	2/6/23/26	0/1/1/1
10	NAG	I	614	-	-	1/6/23/26	0/1/1/1
10	NAG	I	610	1	-	3/6/23/26	0/1/1/1
10	NAG	I	613	-	-	2/6/23/26	0/1/1/1
10	NAG	A	615	-	-	4/6/23/26	0/1/1/1
10	NAG	A	610	1	-	3/6/23/26	0/1/1/1
10	NAG	A	621	-	-	4/6/23/26	0/1/1/1
10	NAG	I	615	-	-	4/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	610	NAG	C1-C2	-3.43	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	610	NAG	C1-C2	-3.40	1.47	1.52
10	E	610	NAG	C1-C2	-3.36	1.47	1.52
10	E	613	NAG	C2-N2	-3.17	1.41	1.46
10	I	613	NAG	C2-N2	-3.16	1.41	1.46
10	A	613	NAG	C2-N2	-3.16	1.41	1.46
10	E	614	NAG	C1-C2	-2.88	1.48	1.52
10	I	614	NAG	C2-N2	-2.86	1.41	1.46
10	A	614	NAG	C2-N2	-2.86	1.41	1.46
10	E	614	NAG	C2-N2	-2.85	1.41	1.46
10	I	614	NAG	C1-C2	-2.85	1.48	1.52
10	A	614	NAG	C1-C2	-2.83	1.48	1.52
10	I	610	NAG	C2-N2	-2.56	1.42	1.46
10	A	610	NAG	C2-N2	-2.56	1.42	1.46
10	E	610	NAG	C2-N2	-2.55	1.42	1.46
10	E	614	NAG	C3-C2	-2.50	1.47	1.52
10	A	614	NAG	C3-C2	-2.48	1.47	1.52
10	I	614	NAG	C3-C2	-2.47	1.47	1.52
10	A	613	NAG	C1-C2	-2.39	1.49	1.52
10	I	613	NAG	C1-C2	-2.38	1.49	1.52
10	A	613	NAG	C3-C2	-2.38	1.47	1.52
10	E	613	NAG	C1-C2	-2.38	1.49	1.52
10	E	613	NAG	C3-C2	-2.37	1.47	1.52
10	I	613	NAG	C3-C2	-2.37	1.47	1.52
10	I	610	NAG	C3-C2	-2.24	1.47	1.52
10	E	610	NAG	C3-C2	-2.24	1.47	1.52
10	A	610	NAG	C3-C2	-2.23	1.47	1.52
10	I	621	NAG	C3-C2	-2.19	1.47	1.52
10	A	621	NAG	C3-C2	-2.18	1.48	1.52
10	E	621	NAG	C3-C2	-2.17	1.48	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	613	NAG	C2-N2-C7	-8.51	111.50	122.90
10	A	613	NAG	C2-N2-C7	-8.50	111.52	122.90
10	E	613	NAG	C2-N2-C7	-8.49	111.52	122.90
10	A	610	NAG	C2-N2-C7	-7.61	112.71	122.90
10	I	610	NAG	C2-N2-C7	-7.60	112.71	122.90
10	E	610	NAG	C2-N2-C7	-7.60	112.71	122.90
10	E	621	NAG	C2-N2-C7	-7.56	112.77	122.90
10	A	621	NAG	C2-N2-C7	-7.53	112.81	122.90
10	I	621	NAG	C2-N2-C7	-7.53	112.81	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	614	NAG	C1-C2-N2	-7.44	98.70	110.43
10	A	614	NAG	C1-C2-N2	-7.44	98.71	110.43
10	I	614	NAG	C1-C2-N2	-7.44	98.71	110.43
10	I	614	NAG	O5-C5-C6	6.19	119.71	107.66
10	E	610	NAG	O5-C5-C6	6.19	119.70	107.66
10	A	614	NAG	O5-C5-C6	6.18	119.70	107.66
10	E	614	NAG	O5-C5-C6	6.18	119.70	107.66
10	A	610	NAG	O5-C5-C6	6.15	119.64	107.66
10	I	610	NAG	O5-C5-C6	6.15	119.64	107.66
10	I	620	NAG	O5-C1-C2	-5.37	102.99	111.29
10	A	620	NAG	O5-C1-C2	-5.36	103.00	111.29
10	E	620	NAG	O5-C1-C2	-5.35	103.01	111.29
10	E	620	NAG	C2-N2-C7	-5.08	116.09	122.90
10	A	620	NAG	C2-N2-C7	-5.07	116.11	122.90
10	I	620	NAG	C2-N2-C7	-5.06	116.11	122.90
10	A	614	NAG	O5-C1-C2	-4.80	103.87	111.29
10	E	614	NAG	O5-C1-C2	-4.79	103.88	111.29
10	I	614	NAG	O5-C1-C2	-4.79	103.88	111.29
10	E	613	NAG	O5-C1-C2	-4.77	103.92	111.29
10	A	613	NAG	O5-C1-C2	-4.76	103.92	111.29
10	I	613	NAG	O5-C1-C2	-4.76	103.93	111.29
10	E	610	NAG	O5-C1-C2	-4.51	104.31	111.29
10	A	610	NAG	O5-C1-C2	-4.50	104.33	111.29
10	I	610	NAG	O5-C1-C2	-4.49	104.34	111.29
10	A	621	NAG	O3-C3-C2	-4.27	100.53	109.40
10	E	621	NAG	O3-C3-C2	-4.27	100.53	109.40
10	I	621	NAG	O3-C3-C2	-4.27	100.54	109.40
10	I	614	NAG	O3-C3-C2	-4.20	100.68	109.40
10	A	614	NAG	O3-C3-C2	-4.18	100.71	109.40
10	E	614	NAG	O3-C3-C2	-4.17	100.75	109.40
10	E	613	NAG	O3-C3-C2	-3.97	101.16	109.40
10	I	613	NAG	O3-C3-C2	-3.96	101.17	109.40
10	A	613	NAG	O3-C3-C2	-3.96	101.18	109.40
10	I	620	NAG	C4-C3-C2	-3.67	105.64	111.02
10	A	620	NAG	C4-C3-C2	-3.66	105.66	111.02
10	E	620	NAG	C4-C3-C2	-3.65	105.66	111.02
10	A	610	NAG	O3-C3-C4	-3.20	102.84	110.38
10	E	610	NAG	O3-C3-C4	-3.20	102.84	110.38
10	I	610	NAG	O3-C3-C4	-3.19	102.86	110.38
10	A	610	NAG	O3-C3-C2	-3.16	102.85	109.40
10	E	610	NAG	O3-C3-C2	-3.15	102.85	109.40
10	I	610	NAG	O3-C3-C2	-3.14	102.89	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	614	NAG	C6-C5-C4	-3.06	105.51	113.02
10	A	614	NAG	C6-C5-C4	-3.05	105.53	113.02
10	E	614	NAG	C6-C5-C4	-3.04	105.55	113.02
10	E	613	NAG	C6-C5-C4	-3.02	105.61	113.02
10	A	613	NAG	C6-C5-C4	-3.02	105.61	113.02
10	I	613	NAG	C6-C5-C4	-3.02	105.61	113.02
10	I	613	NAG	C4-C3-C2	-3.02	106.60	111.02
10	E	613	NAG	C1-O5-C5	3.02	116.23	112.19
10	A	613	NAG	C4-C3-C2	-3.01	106.60	111.02
10	E	613	NAG	C4-C3-C2	-3.00	106.61	111.02
10	I	613	NAG	C1-O5-C5	3.00	116.21	112.19
10	A	613	NAG	C1-O5-C5	2.98	116.18	112.19
10	E	620	NAG	C6-C5-C4	-2.84	106.04	113.02
10	A	620	NAG	C6-C5-C4	-2.84	106.04	113.02
10	I	620	NAG	C6-C5-C4	-2.83	106.06	113.02
10	I	614	NAG	C3-C4-C5	-2.81	105.13	110.23
10	A	614	NAG	C3-C4-C5	-2.81	105.14	110.23
10	E	614	NAG	C3-C4-C5	-2.81	105.14	110.23
10	E	610	NAG	C3-C4-C5	-2.77	105.22	110.23
10	A	610	NAG	C3-C4-C5	-2.76	105.23	110.23
10	I	610	NAG	C3-C4-C5	-2.75	105.25	110.23
10	A	613	NAG	O3-C3-C4	-2.70	104.01	110.38
10	E	613	NAG	O3-C3-C4	-2.70	104.01	110.38
10	I	613	NAG	O3-C3-C4	-2.70	104.02	110.38
10	E	614	NAG	O3-C3-C4	-2.65	104.12	110.38
10	A	614	NAG	O3-C3-C4	-2.65	104.14	110.38
10	I	614	NAG	O3-C3-C4	-2.65	104.14	110.38
10	I	614	NAG	C2-N2-C7	-2.56	119.46	122.90
10	E	614	NAG	C2-N2-C7	-2.56	119.47	122.90
10	A	614	NAG	C2-N2-C7	-2.56	119.47	122.90
10	A	621	NAG	C4-C3-C2	-2.47	107.39	111.02
10	E	621	NAG	C4-C3-C2	-2.47	107.39	111.02
10	I	621	NAG	C4-C3-C2	-2.46	107.42	111.02
10	E	610	NAG	C6-C5-C4	-2.36	107.22	113.02
10	I	610	NAG	C6-C5-C4	-2.34	107.27	113.02
10	A	610	NAG	C6-C5-C4	-2.34	107.27	113.02
10	A	614	NAG	C8-C7-N2	-2.33	112.25	116.12
10	E	614	NAG	C8-C7-N2	-2.33	112.25	116.12
10	I	614	NAG	C8-C7-N2	-2.33	112.26	116.12
10	I	614	NAG	O7-C7-C8	2.32	126.19	122.05
10	A	614	NAG	O7-C7-C8	2.32	126.18	122.05
10	I	620	NAG	C1-O5-C5	2.32	115.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	620	NAG	C1-O5-C5	2.31	115.28	112.19
10	E	614	NAG	O7-C7-C8	2.31	126.16	122.05
10	E	620	NAG	C1-O5-C5	2.30	115.27	112.19
10	E	621	NAG	O3-C3-C4	-2.22	105.15	110.38
10	I	621	NAG	O3-C3-C4	-2.22	105.15	110.38
10	A	621	NAG	O3-C3-C4	-2.21	105.16	110.38
10	I	621	NAG	O7-C7-C8	2.19	125.95	122.05
10	A	621	NAG	O7-C7-C8	2.16	125.90	122.05
10	E	621	NAG	O7-C7-C8	2.16	125.90	122.05
10	A	620	NAG	O5-C5-C6	2.14	111.83	107.66
10	I	620	NAG	O5-C5-C6	2.13	111.81	107.66
10	E	620	NAG	O5-C5-C6	2.13	111.81	107.66
10	A	621	NAG	O5-C1-C2	-2.13	108.00	111.29
10	I	621	NAG	O5-C1-C2	-2.13	108.00	111.29
10	E	621	NAG	O5-C1-C2	-2.12	108.02	111.29
10	E	610	NAG	O4-C4-C3	2.09	115.31	110.38
10	A	610	NAG	O4-C4-C3	2.09	115.31	110.38
10	I	610	NAG	O4-C4-C3	2.09	115.29	110.38
10	E	621	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	615	NAG	C4-C5-C6-O6
10	E	615	NAG	C4-C5-C6-O6
10	I	615	NAG	C4-C5-C6-O6
10	A	621	NAG	C4-C5-C6-O6
10	E	621	NAG	C4-C5-C6-O6
10	I	621	NAG	C4-C5-C6-O6
10	A	615	NAG	C8-C7-N2-C2
10	E	615	NAG	C8-C7-N2-C2
10	I	615	NAG	C8-C7-N2-C2
10	A	613	NAG	C8-C7-N2-C2
10	A	615	NAG	O7-C7-N2-C2
10	A	621	NAG	C8-C7-N2-C2
10	E	613	NAG	C8-C7-N2-C2
10	E	615	NAG	O7-C7-N2-C2
10	E	621	NAG	C8-C7-N2-C2
10	I	613	NAG	C8-C7-N2-C2
10	I	615	NAG	O7-C7-N2-C2
10	I	621	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
10	A	615	NAG	O5-C5-C6-O6
10	A	620	NAG	O5-C5-C6-O6
10	E	615	NAG	O5-C5-C6-O6
10	E	620	NAG	O5-C5-C6-O6
10	I	615	NAG	O5-C5-C6-O6
10	I	620	NAG	O5-C5-C6-O6
10	I	621	NAG	O5-C5-C6-O6
10	A	621	NAG	O5-C5-C6-O6
10	E	621	NAG	O5-C5-C6-O6
10	A	613	NAG	O7-C7-N2-C2
10	E	613	NAG	O7-C7-N2-C2
10	I	613	NAG	O7-C7-N2-C2
10	A	610	NAG	O5-C5-C6-O6
10	E	610	NAG	O5-C5-C6-O6
10	I	610	NAG	O5-C5-C6-O6
10	A	614	NAG	O5-C5-C6-O6
10	I	614	NAG	O5-C5-C6-O6
10	E	614	NAG	O5-C5-C6-O6
10	A	621	NAG	O7-C7-N2-C2
10	E	621	NAG	O7-C7-N2-C2
10	I	621	NAG	O7-C7-N2-C2
10	A	610	NAG	C8-C7-N2-C2
10	E	610	NAG	C8-C7-N2-C2
10	I	610	NAG	C8-C7-N2-C2
10	E	610	NAG	O7-C7-N2-C2
10	A	610	NAG	O7-C7-N2-C2
10	I	610	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	620	NAG	1	0
10	A	620	NAG	1	0
10	A	614	NAG	1	0
10	E	614	NAG	1	0
10	E	610	NAG	2	0
10	I	614	NAG	1	0
10	I	610	NAG	1	0
10	A	610	NAG	1	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.

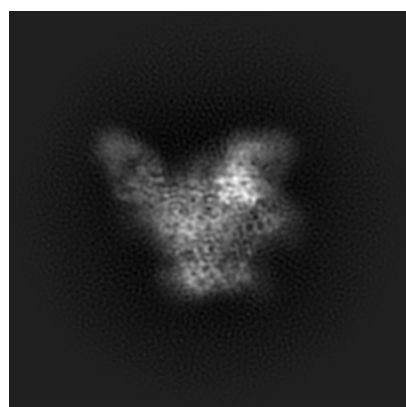
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20818. These allow visual inspection of the internal detail of the map and identification of artifacts.

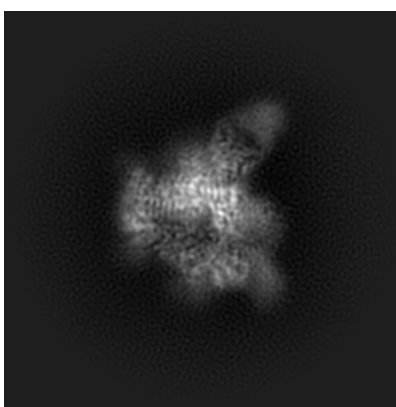
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

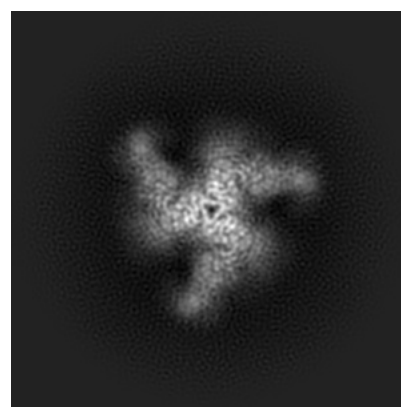
6.1.1 Primary map



X



Y

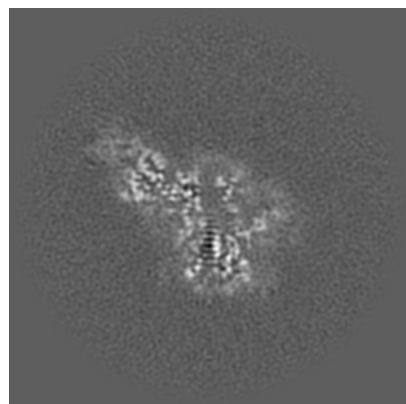


Z

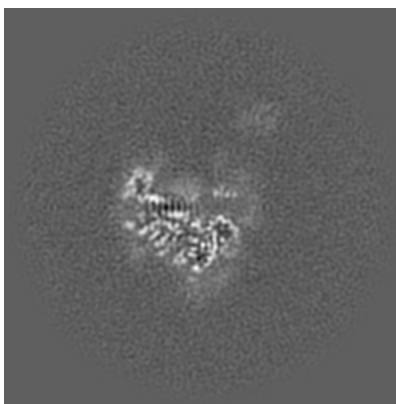
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

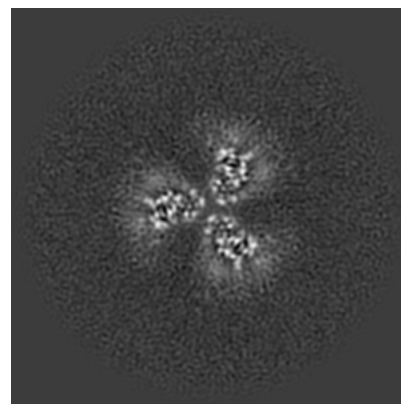
6.2.1 Primary map



X Index: 160



Y Index: 160

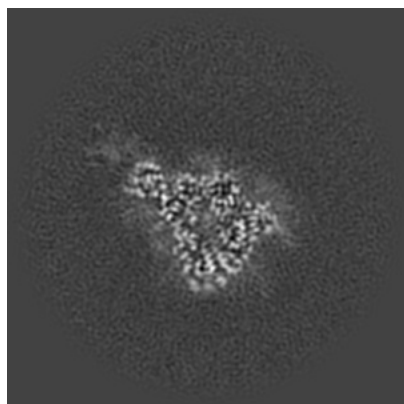


Z Index: 160

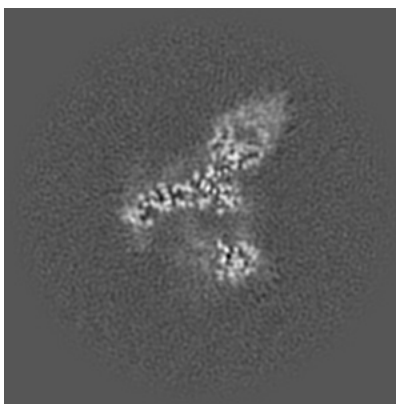
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

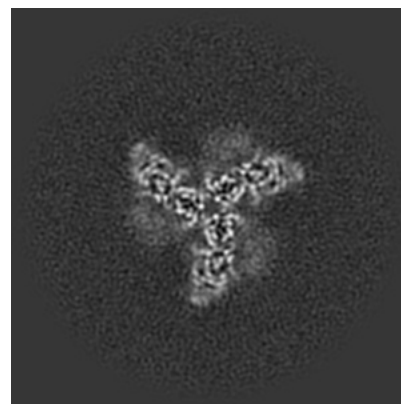
6.3.1 Primary map



X Index: 169



Y Index: 181

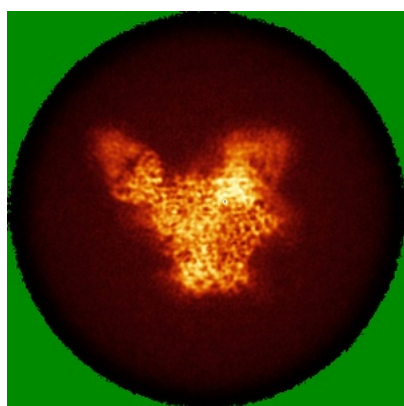


Z Index: 173

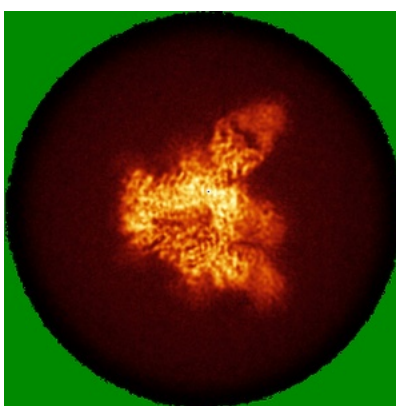
The images above show the largest variance slices of the map in three orthogonal directions.

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

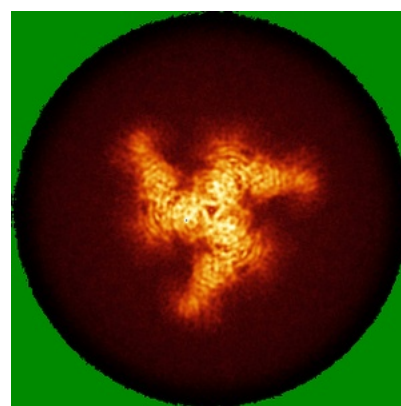
6.4.1 Primary map



X



Y

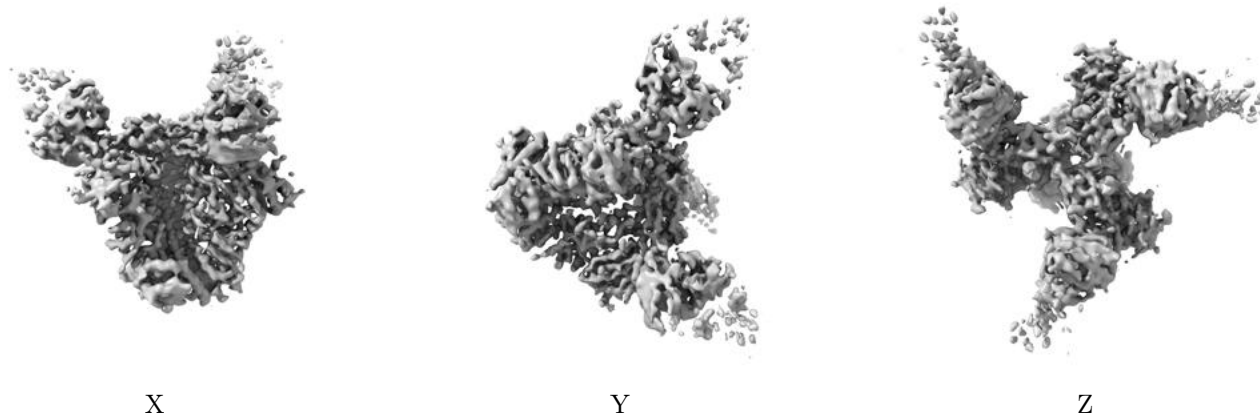


Z

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

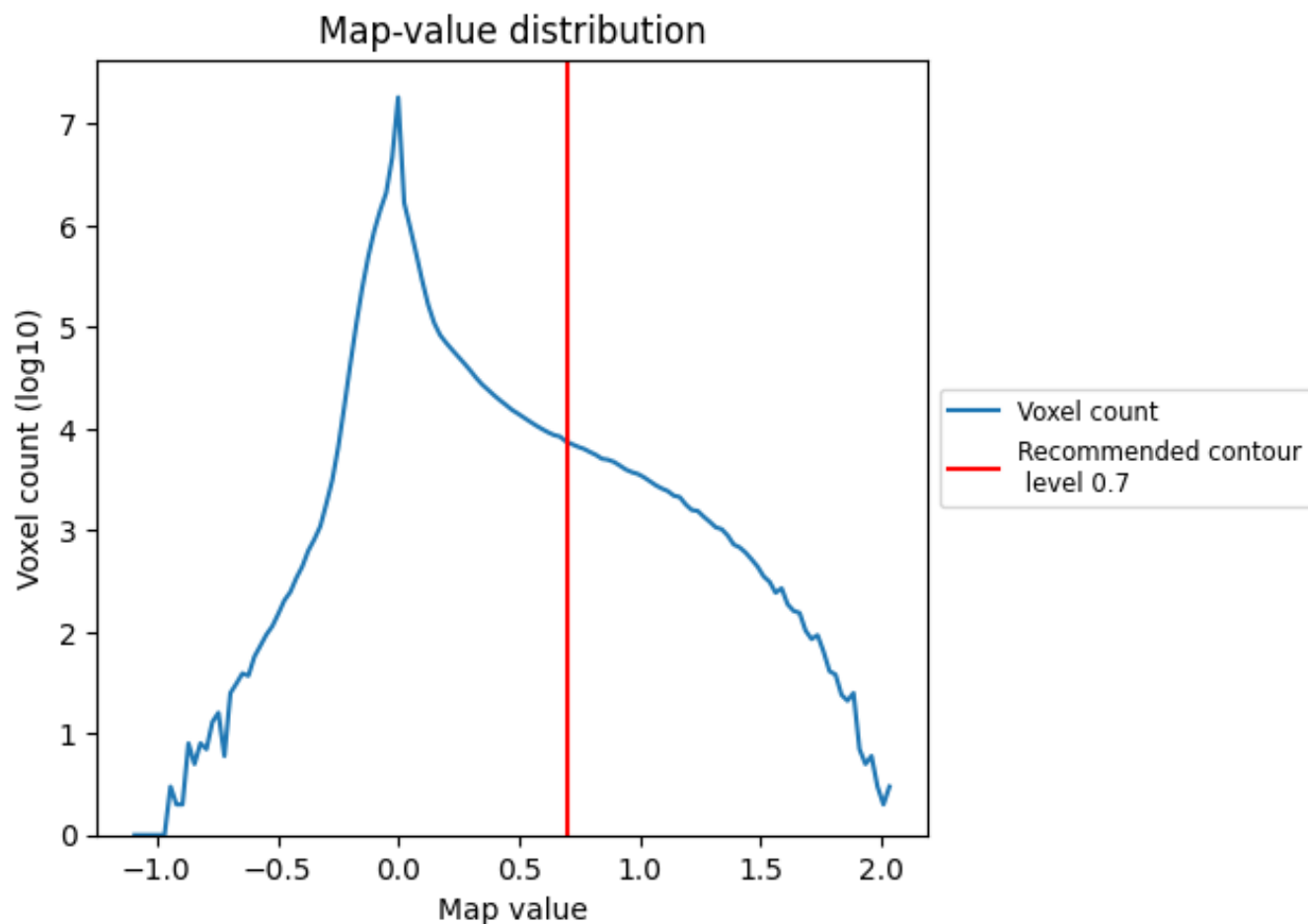
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

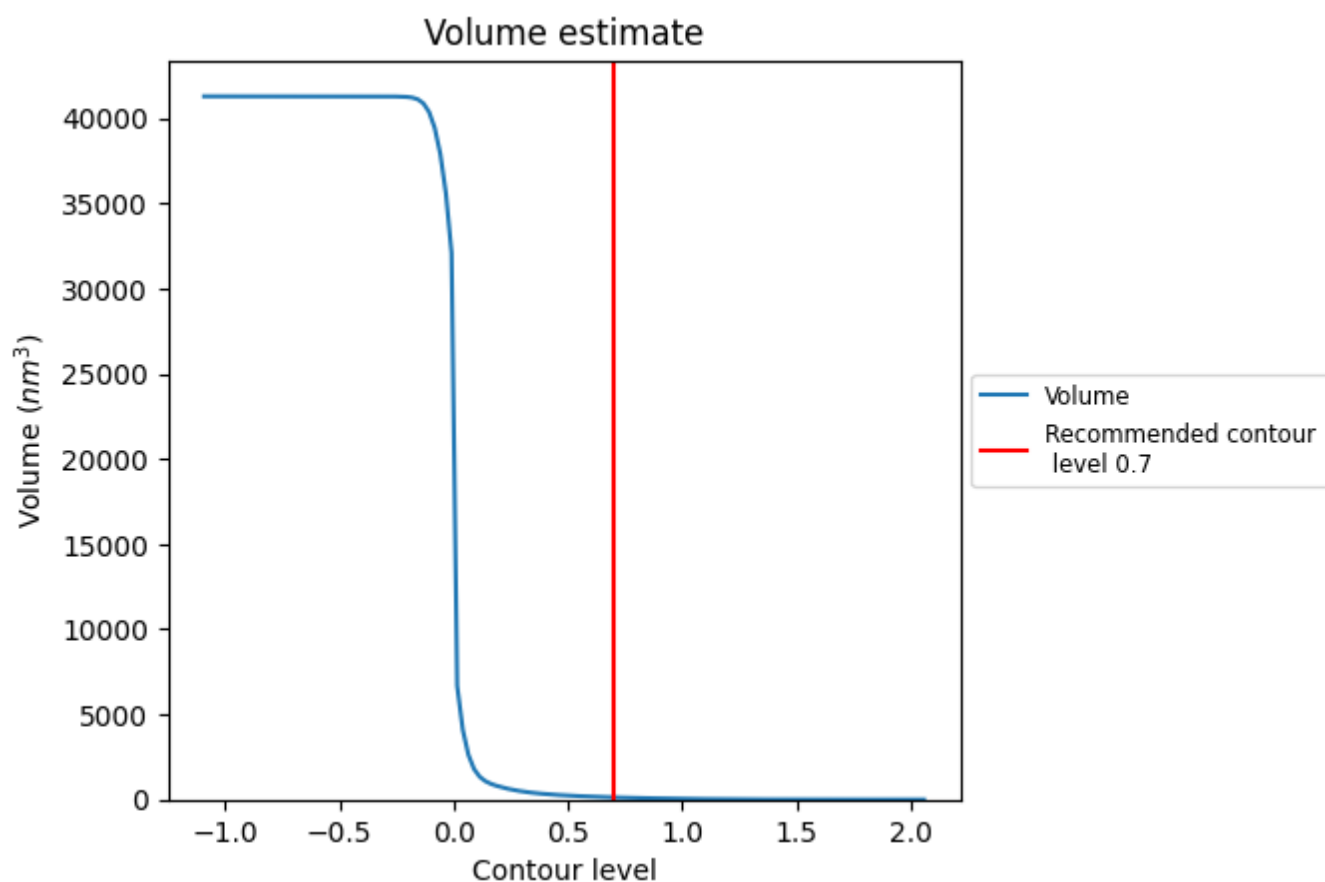
This section contains the results of statistical analysis of the map.

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.

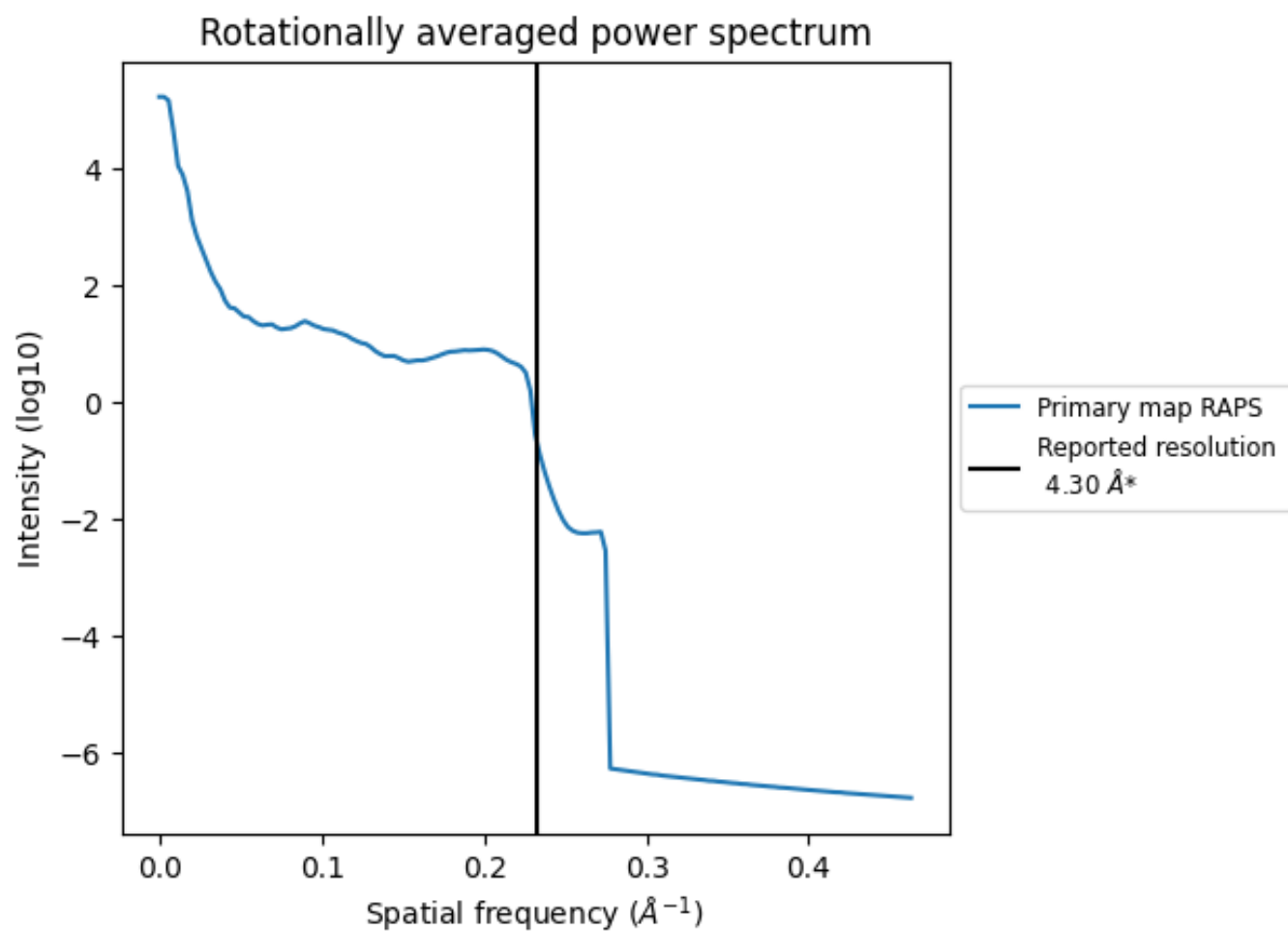
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 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 0.233 Å⁻¹

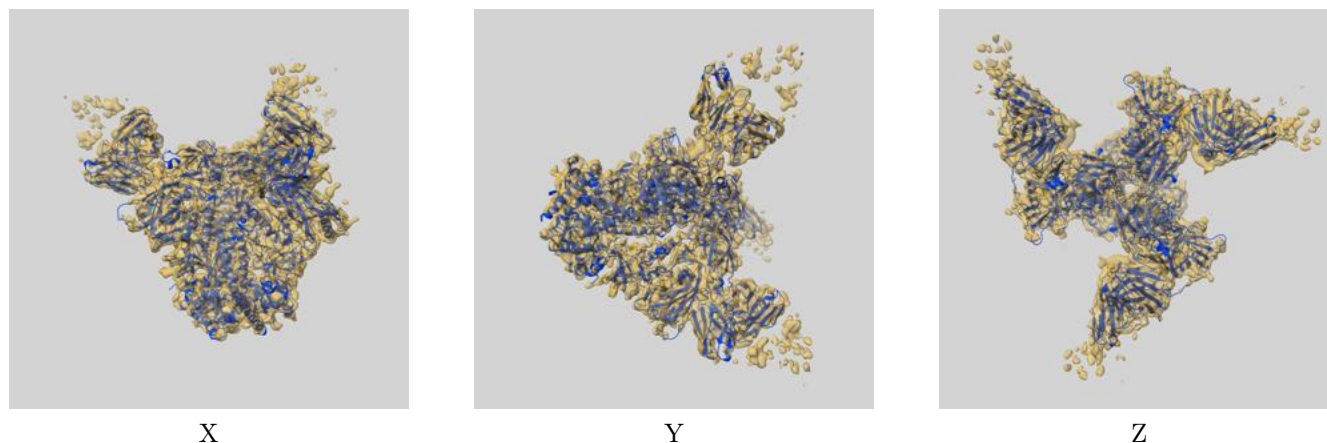
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

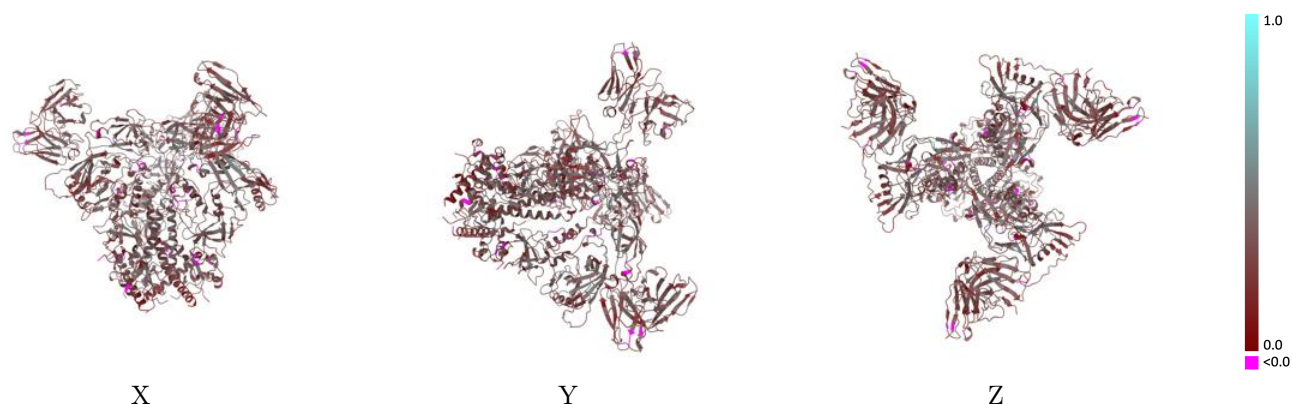
This section contains information regarding the fit between EMDB map EMD-20818 and PDB model 6UM6. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



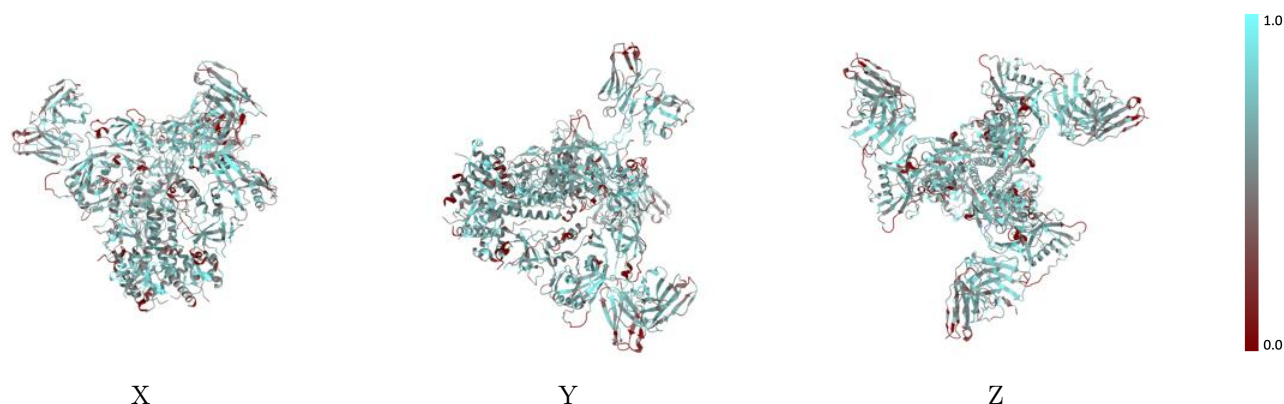
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



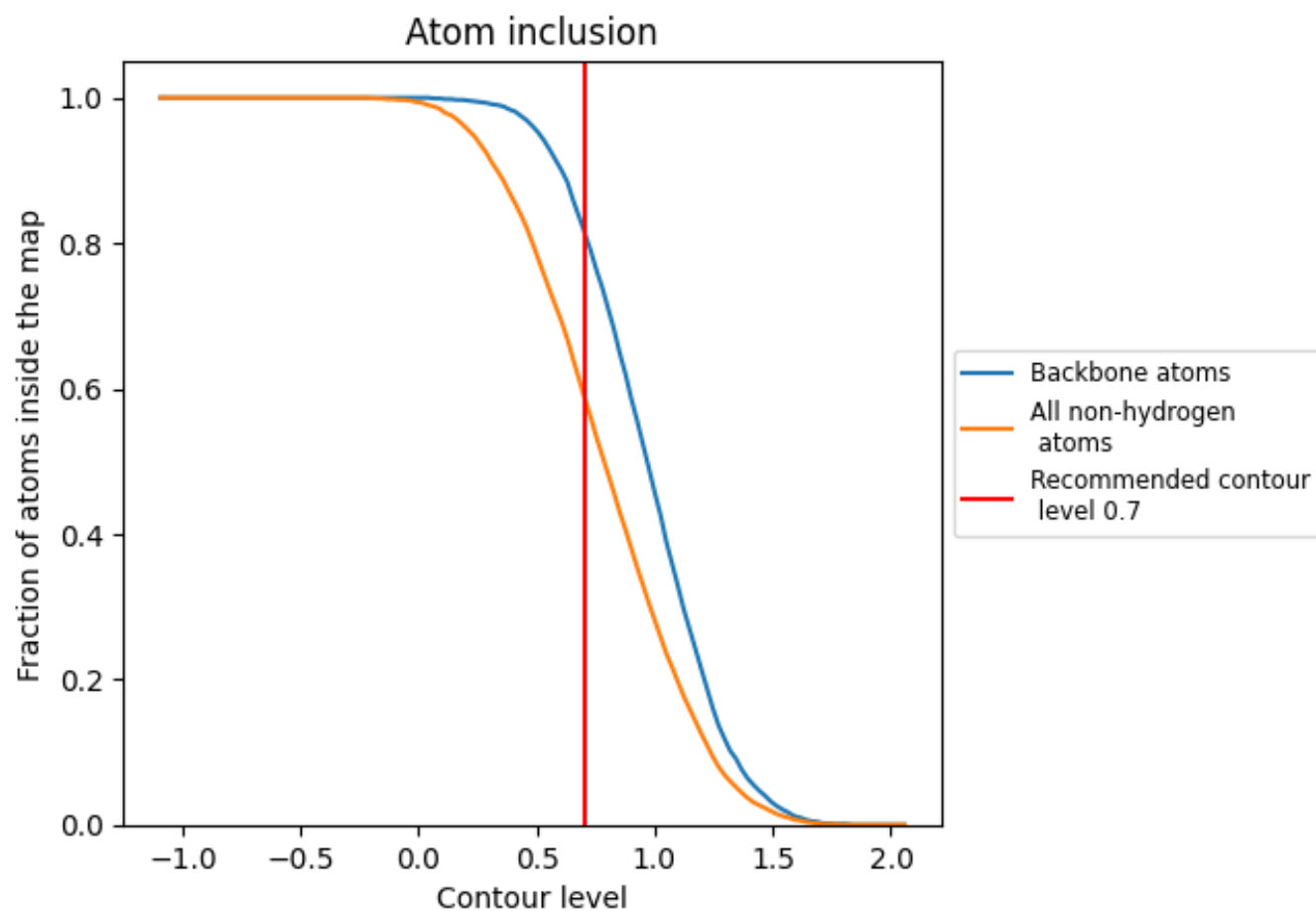
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 59% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5910	 0.3180
A	 0.5900	 0.3290
B	 0.5910	 0.2770
C	 0.6270	 0.3290
D	 0.5270	 0.2680
E	 0.5910	 0.3290
F	 0.5940	 0.2800
G	 0.6360	 0.3300
H	 0.5270	 0.2700
I	 0.5900	 0.3290
J	 0.5890	 0.2790
K	 0.6360	 0.3320
L	 0.5230	 0.2700
M	 0.8800	 0.4930
N	 0.5360	 0.4030
O	 0.6670	 0.3950
P	 0.3210	 0.4130
Q	 0.6800	 0.4760
R	 0.8800	 0.4940
S	 0.5360	 0.4020
T	 0.6670	 0.4020
U	 0.3210	 0.4240
V	 0.6600	 0.4770
W	 0.8800	 0.4930
X	 0.5000	 0.4000
Y	 0.6670	 0.4010
Z	 0.3210	 0.4250
a	 0.6600	 0.4810

