



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:54 AM UTC

PDB ID : 7LD1 / pdb_00007ld1
EMDB ID : EMD-23279
Title : Structure of SARS-CoV-2 S protein in complex with Receptor Binding Domain antibody DH1047
Authors : Manne, K.; Acharya, P.
Deposited on : 2021-01-12
Resolution : 3.40 Å(reported)
Based on initial model : 6VXX

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

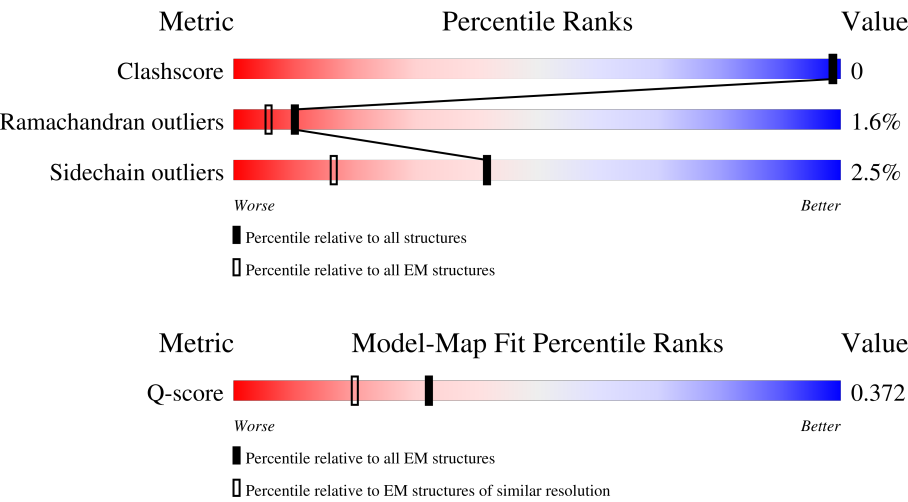
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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 <=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	1121	5% 83% 13%
1	B	1121	83% 13%
1	C	1121	82% 15%
2	H	232	47% 97%

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Mol	Chain	Length	Quality of chain
2	M	232	
2	P	232	
3	L	220	
3	N	220	
3	O	220	
4	D	3	
4	F	3	
4	G	3	
4	I	3	
4	J	3	
4	K	3	
4	R	3	
4	S	3	
4	T	3	
4	U	3	
4	V	3	
4	W	3	
4	X	3	
5	E	2	
5	Q	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29444 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	973	Total	C	N	O	S	0	0
			7046	4478	1189	1345	34		
1	B	973	Total	C	N	O	S	0	0
			7046	4478	1189	1345	34		
1	C	949	Total	C	N	O	S	0	0
			7026	4477	1186	1331	32		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	GLU	THR	conflict	UNP P0DTC2
A	471	ALA	GLU	conflict	UNP P0DTC2
A	486	TYR	PHE	conflict	UNP P0DTC2
A	607	GLU	GLN	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	470	GLU	THR	conflict	UNP P0DTC2
B	471	ALA	GLU	conflict	UNP P0DTC2
B	486	TYR	PHE	conflict	UNP P0DTC2
B	607	GLU	GLN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	470	GLU	THR	conflict	UNP P0DTC2
C	471	ALA	GLU	conflict	UNP P0DTC2
C	486	TYR	PHE	conflict	UNP P0DTC2
C	607	GLU	GLN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

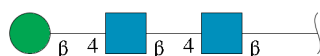
- Molecule 2 is a protein called DH1047 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	232	Total	C	N	O	S	0	0
			1248	761	236	249	2		
2	P	232	Total	C	N	O	S	0	0
			1235	755	236	242	2		
2	H	232	Total	C	N	O	S	0	0
			1235	755	236	242	2		

- Molecule 3 is a protein called DH1047 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	219	Total	C	N	O	S	0	0
			1245	761	233	248	3		
3	O	220	Total	C	N	O	S	0	0
			1235	753	230	249	3		
3	L	219	Total	C	N	O	S	0	0
			1229	750	229	247	3		

- Molecule 4 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
4	D	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		

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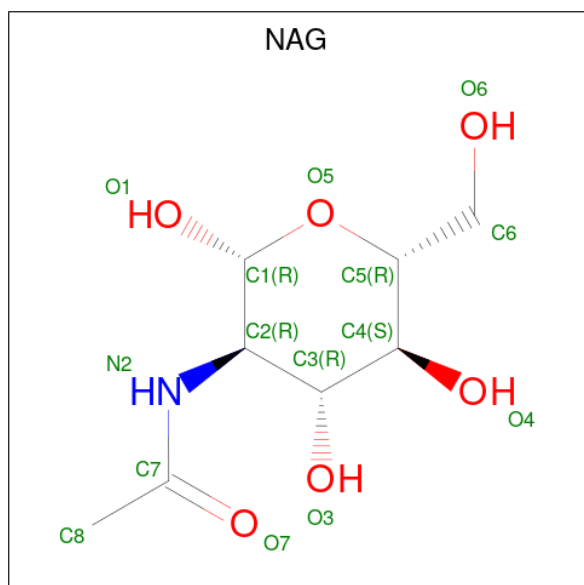
Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	3	Total	C	N	O	0	0
			39	22	2	15		
4	W	3	Total	C	N	O	0	0
			39	22	2	15		
4	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 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
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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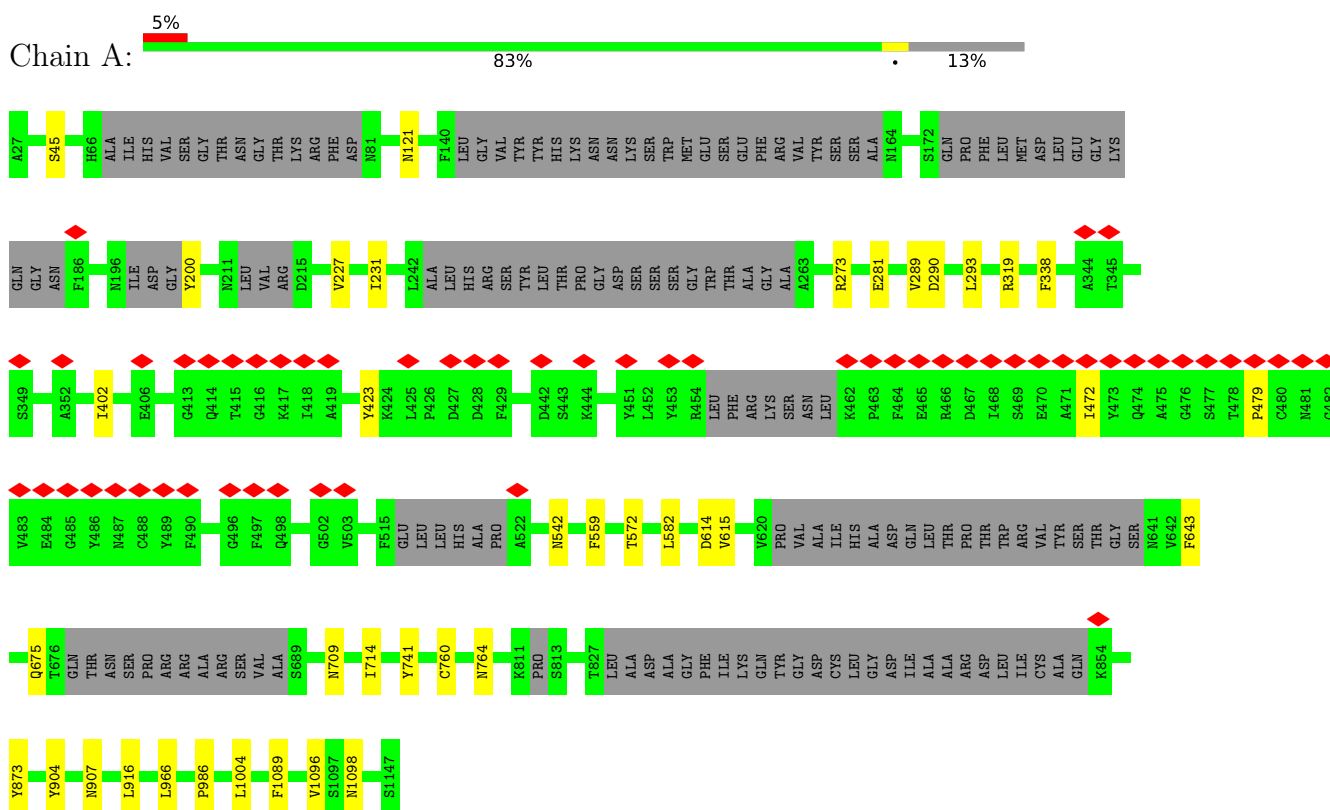
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

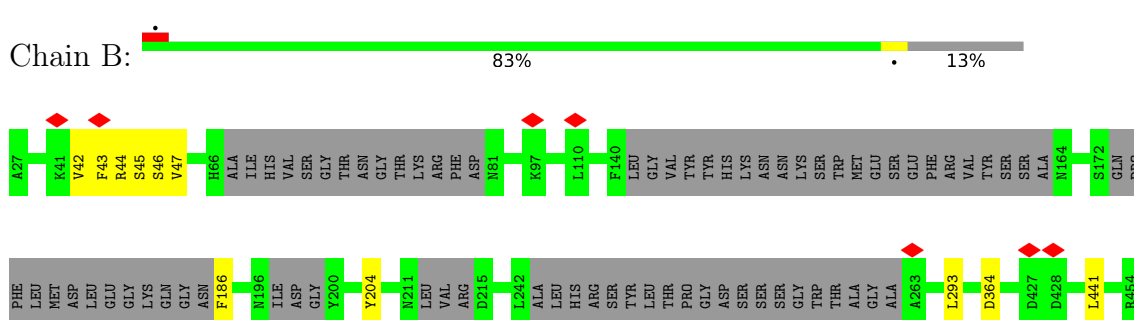
3 Residue-property plots

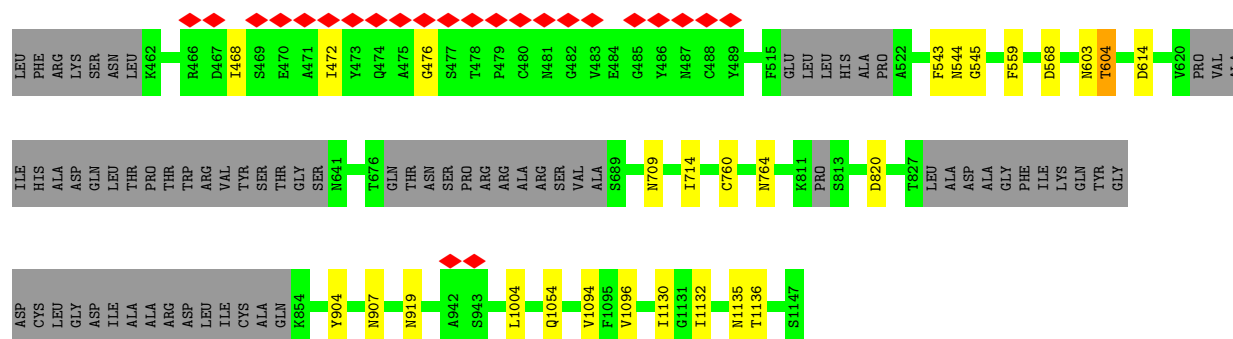
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



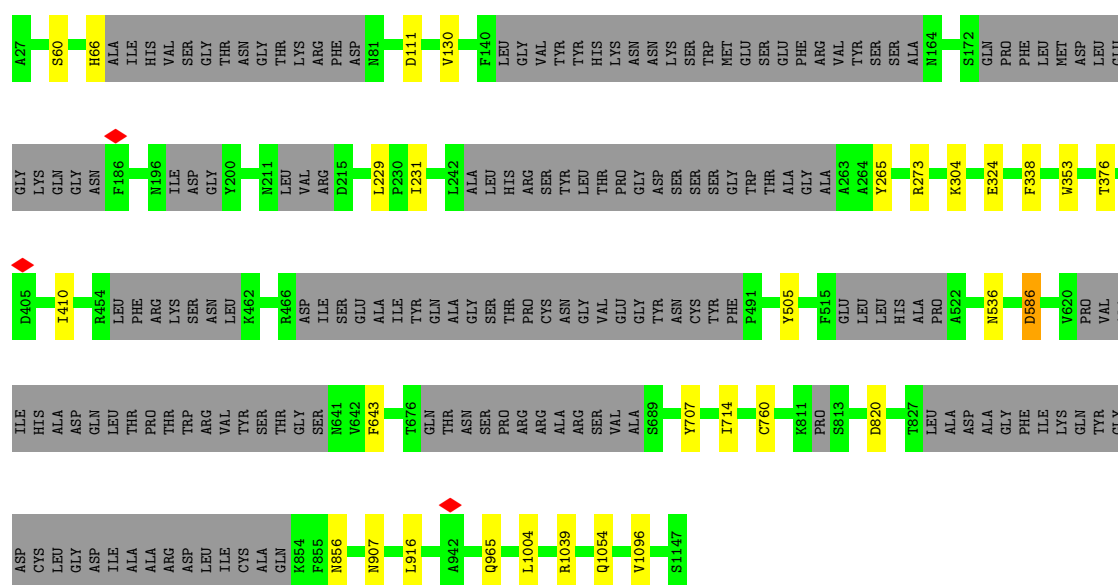
• Molecule 1: Spike glycoprotein





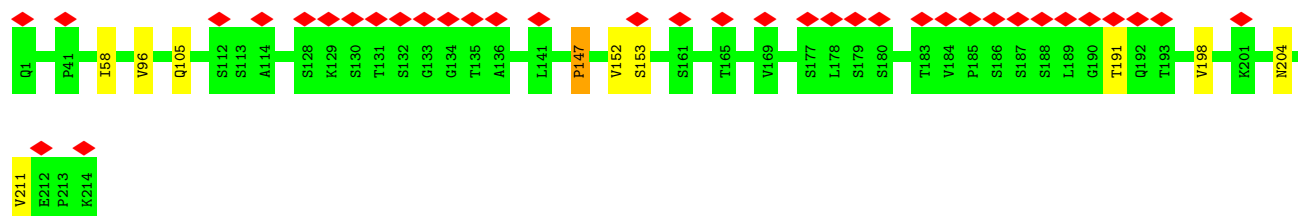
• Molecule 1: Spike glycoprotein

Chain C: 82% 15%



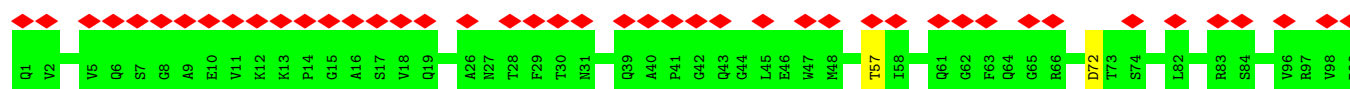
• Molecule 2: DH1047 heavy chain

Chain M: 16% 96%



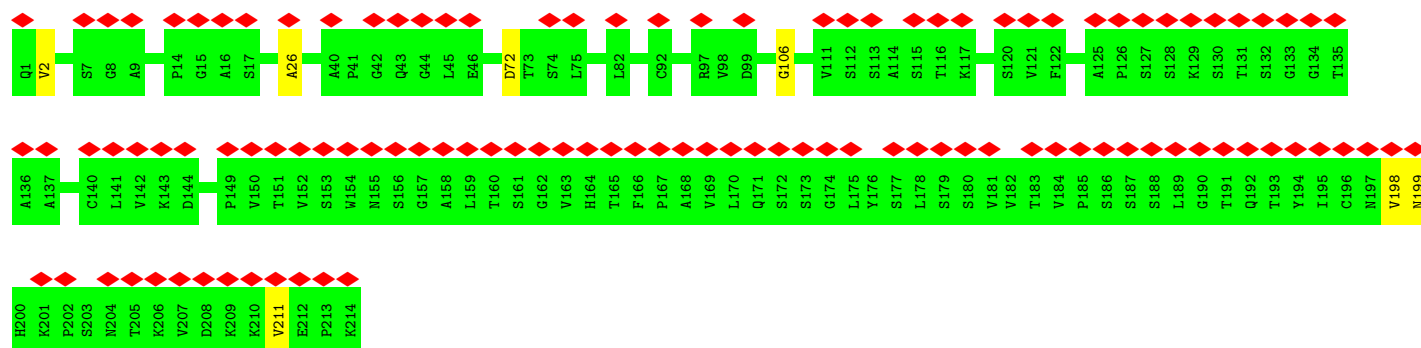
• Molecule 2: DH1047 heavy chain

Chain P: 66% 98%

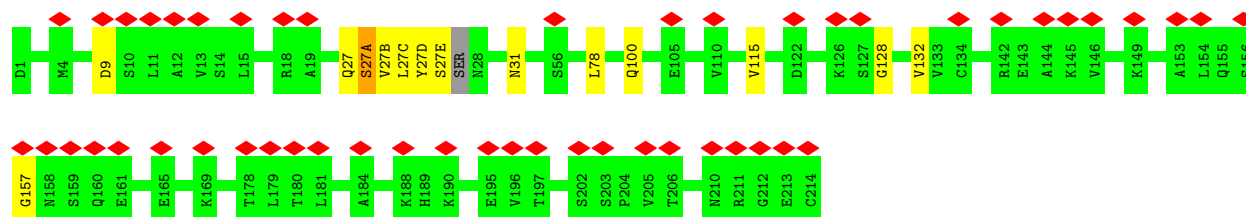
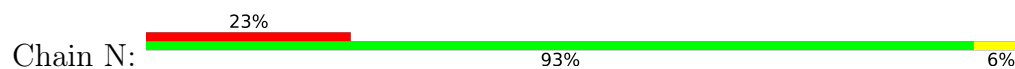




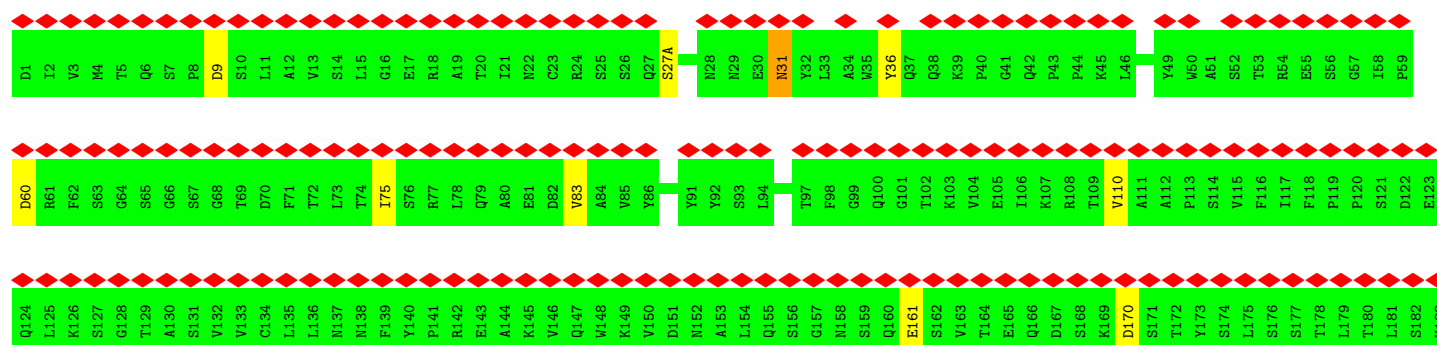
• Molecule 2: DH1047 heavy chain

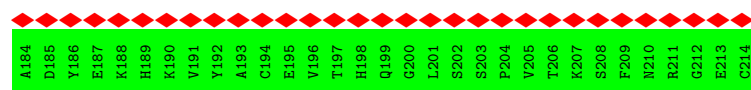


• Molecule 3: DH1047 light chain



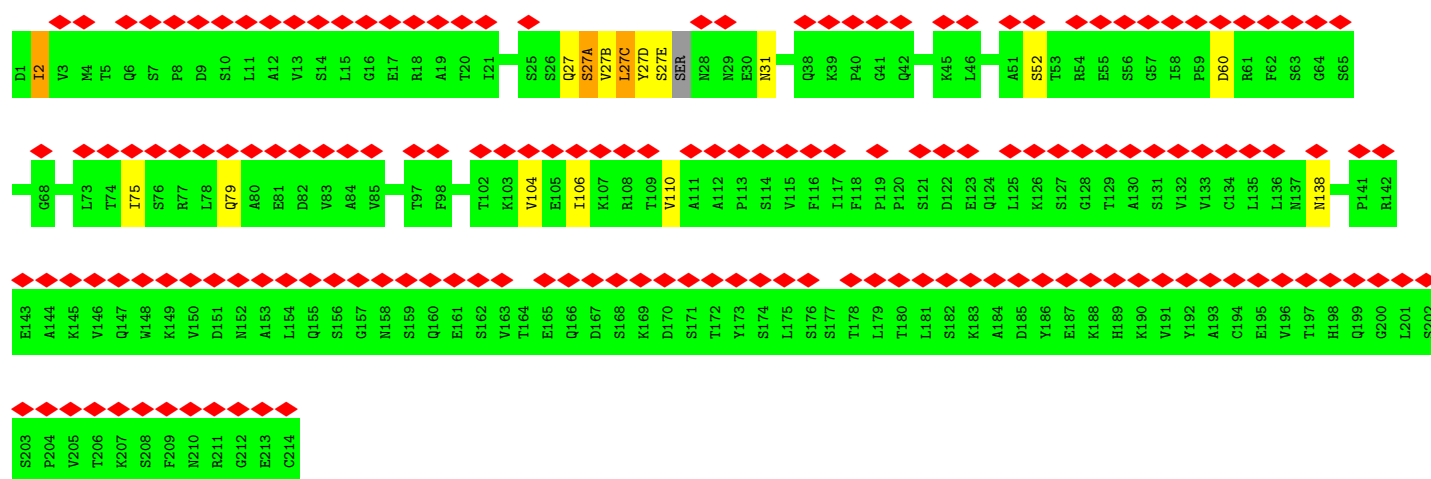
• Molecule 3: DH1047 light chain





- Molecule 3: DH1047 light chain

Chain L: 74% 92% 6%



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

Chain D: 33% 100%



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

Chain F: 33% 100%



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

Chain G: 67% 100%



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



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



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



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



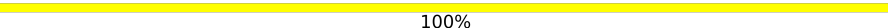
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

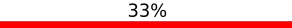


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

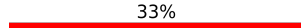
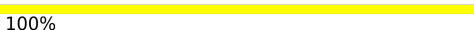
NAG1
NAG2
BMA3

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

Chain V:  33%  100%

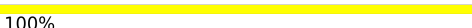
NAG1
NAG2
BMA3

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

Chain W:  33%  100%

NAG1
NAG2
BMA3

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

Chain X:  33%  100%

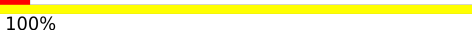
NAG1
NAG2
BMA3

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

Chain E:  50%  100%

NAG1
NAG2

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

Chain Q:  50%  100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127401	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 ($e^-/\text{\AA}^2$)	66.77	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.267	Depositor
Minimum map value	-0.507	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.243	Depositor
Map size ($\text{\AA}$)	338.56, 338.56, 338.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	0/7185	1.29	11/9811 (0.1%)
1	B	0.73	0/7185	1.29	10/9811 (0.1%)
1	C	0.72	0/7169	1.27	5/9777 (0.1%)
2	H	0.76	0/1252	1.49	0/1742
2	M	0.76	0/1265	1.51	3/1759 (0.2%)
2	P	0.78	0/1252	1.48	0/1742
3	L	0.80	0/1244	1.51	0/1729
3	N	0.74	0/1260	1.42	1/1749 (0.1%)
3	O	0.83	0/1251	1.55	3/1740 (0.2%)
All	All	0.74	0/29063	1.34	33/39860 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	5
All	All	0	11

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	289	VAL	N-CA-C	6.71	117.33	111.90
1	B	45	SER	CA-C-N	6.39	129.91	120.90
1	B	45	SER	C-N-CA	6.39	129.91	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	PHE	CA-CB-CG	6.37	120.17	113.80
1	B	46	SER	N-CA-C	6.02	118.73	110.24
1	C	586	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	186	PHE	CA-CB-CG	5.86	119.66	113.80
1	C	643	PHE	CA-CB-CG	5.86	119.66	113.80
3	N	27(A)	SER	N-CA-C	5.81	119.95	112.86
1	A	764	ASN	CA-CB-CG	-5.78	106.82	112.60
1	A	200	TYR	CA-C-N	5.73	129.40	120.75
1	A	200	TYR	C-N-CA	5.73	129.40	120.75
1	C	1054	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	559	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	338	PHE	CA-CB-CG	5.52	119.32	113.80
2	M	153	SER	N-CA-C	5.52	119.31	112.47
1	B	568	ASP	CA-CB-CG	5.30	117.90	112.60
3	O	161	GLU	N-CA-C	5.28	117.09	109.07
1	A	986	PRO	N-CA-C	5.25	117.10	110.70
1	B	1054	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	231	ILE	N-CA-C	5.23	117.59	111.05
1	C	965	GLN	OE1-CD-NE2	-5.21	117.39	122.60
3	O	27(A)	SER	N-CA-C	5.20	121.88	110.80
1	C	66	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	B	919	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	46	SER	CA-C-N	5.18	131.30	121.97
1	B	46	SER	C-N-CA	5.18	131.30	121.97
3	O	31	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	1089	PHE	CA-CB-CG	5.10	118.90	113.80
2	M	147	PRO	CA-C-N	5.06	126.41	120.09
2	M	147	PRO	C-N-CA	5.06	126.41	120.09
1	A	1098	ASN	CB-CA-C	5.03	118.97	111.88

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain
1	A	873	TYR	Sidechain
1	A	904	TYR	Sidechain
1	B	204	TYR	Sidechain
1	B	43	PHE	Sidechain
1	B	904	TYR	Sidechain
1	C	1039	ARG	Sidechain
1	C	265	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	273	ARG	Sidechain
1	C	505	TYR	Sidechain
1	C	707	TYR	Sidechain

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	7046	0	6450	2	0
1	B	7046	0	6450	2	0
1	C	7026	0	6571	1	0
2	H	1235	0	715	0	0
2	M	1248	0	733	0	0
2	P	1235	0	715	2	0
3	L	1229	0	771	0	0
3	N	1245	0	806	0	0
3	O	1235	0	777	0	0
4	D	39	0	34	0	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
4	J	39	0	34	0	0
4	K	39	0	34	0	0
4	R	39	0	34	0	0
4	S	39	0	34	0	0
4	T	39	0	34	0	0
4	U	39	0	34	0	0
4	V	39	0	34	0	0
4	W	39	0	34	0	0
4	X	39	0	34	0	0
5	E	28	0	25	0	0
5	Q	28	0	25	0	0
6	A	112	0	104	0	0
6	B	126	0	117	0	0
6	C	98	0	91	0	0
All	All	29444	0	24792	7	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 0.

All (7) 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)
2:P:118:GLY:H	2:P:119:PRO:CD	2.27	0.47
2:P:118:GLY:H	2:P:119:PRO:HD3	1.79	0.47
1:B:543:PHE:CG	1:B:544:ASN:N	2.85	0.45
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	2.00	0.44
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	2.00	0.42
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.55	0.41
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	2.03	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	947/1121 (84%)	873 (92%)	66 (7%)	8 (1%)	16	44
1	B	947/1121 (84%)	879 (93%)	58 (6%)	10 (1%)	11	38
1	C	921/1121 (82%)	850 (92%)	66 (7%)	5 (0%)	24	54
2	H	230/232 (99%)	187 (81%)	36 (16%)	7 (3%)	3	18
2	M	230/232 (99%)	186 (81%)	36 (16%)	8 (4%)	3	16
2	P	230/232 (99%)	195 (85%)	32 (14%)	3 (1%)	9	33
3	L	215/220 (98%)	176 (82%)	27 (13%)	12 (6%)	1	9
3	N	215/220 (98%)	181 (84%)	26 (12%)	8 (4%)	2	16
3	O	218/220 (99%)	176 (81%)	36 (16%)	6 (3%)	4	19
All	All	4153/4719 (88%)	3703 (89%)	383 (9%)	67 (2%)	10	29

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	ASN
1	B	709	ASN
1	B	47	VAL
1	C	410	ILE
2	M	152	VAL
2	M	198	VAL
2	M	211	VAL
2	H	2	VAL
2	H	106	GLY
3	L	106	ILE
1	B	604	THR
1	C	338	PHE
2	M	105	GLN
3	N	9	ASP
3	N	78	LEU
3	N	100	GLN
3	O	9	ASP
3	O	60	ASP
3	O	75	ILE
2	H	26	ALA
2	H	199	ASN
3	L	27(C)	LEU
3	L	60	ASP
3	L	79	GLN
1	A	290	ASP
1	A	402	ILE
1	A	423	TYR
1	B	42	VAL
1	B	476	GLY
1	C	536	ASN
2	M	96	VAL
2	M	191	THR
2	M	204	ASN
3	N	31	ASN
3	N	157	GLY
2	P	72	ASP
2	H	72	ASP
2	H	198	VAL
3	L	75	ILE
3	L	104	VAL
3	L	110	VAL
1	A	45	SER
1	A	582	LEU

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Mol	Chain	Res	Type
1	A	614	ASP
1	B	364	ASP
1	B	614	ASP
1	C	111	ASP
1	C	304	LYS
3	N	115	VAL
3	N	132	VAL
2	P	118	GLY
3	O	170	ASP
3	L	27(A)	SER
3	L	52	SER
1	A	479	PRO
1	B	441	LEU
3	L	31	ASN
3	L	138	ASN
1	B	468	ILE
1	B	545	GLY
2	M	147	PRO
2	P	181	VAL
3	O	110	VAL
3	L	2	ILE
3	O	83	VAL
2	H	211	VAL
3	N	128	GLY

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	701/971 (72%)	687 (98%)	14 (2%)	48	65
1	B	701/971 (72%)	686 (98%)	15 (2%)	47	64
1	C	725/971 (75%)	711 (98%)	14 (2%)	50	66
2	H	31/196 (16%)	31 (100%)	0	100	100
2	M	36/196 (18%)	35 (97%)	1 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	31/196 (16%)	30 (97%)	1 (3%)	34 58
3	L	51/195 (26%)	44 (86%)	7 (14%)	3 14
3	N	55/195 (28%)	49 (89%)	6 (11%)	6 22
3	O	52/195 (27%)	50 (96%)	2 (4%)	29 54
All	All	2383/4086 (58%)	2323 (98%)	60 (2%)	42 62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	227	VAL
1	A	273	ARG
1	A	281	GLU
1	A	293	LEU
1	A	472	ILE
1	A	542	ASN
1	A	572	THR
1	A	615	VAL
1	A	675	GLN
1	A	760	CYS
1	A	907	ASN
1	A	916	LEU
1	A	1004	LEU
1	B	44	ARG
1	B	293	LEU
1	B	472	ILE
1	B	603	ASN
1	B	604	THR
1	B	760	CYS
1	B	764	ASN
1	B	820	ASP
1	B	907	ASN
1	B	1004	LEU
1	B	1094	VAL
1	B	1130	ILE
1	B	1132	ILE
1	B	1135	ASN
1	B	1136	THR
1	C	60	SER
1	C	130	VAL
1	C	229	LEU

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Mol	Chain	Res	Type
1	C	231	ILE
1	C	324	GLU
1	C	353	TRP
1	C	376	THR
1	C	586	ASP
1	C	760	CYS
1	C	820	ASP
1	C	856	ASN
1	C	907	ASN
1	C	916	LEU
1	C	1004	LEU
2	M	58	ILE
3	N	27	GLN
3	N	27(A)	SER
3	N	27(B)	VAL
3	N	27(C)	LEU
3	N	27(D)	TYR
3	N	27(E)	SER
2	P	57	THR
3	O	31	ASN
3	O	36	TYR
3	L	2	ILE
3	L	27	GLN
3	L	27(A)	SER
3	L	27(B)	VAL
3	L	27(C)	LEU
3	L	27(D)	TYR
3	L	27(E)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	ASN
1	A	658	ASN
1	A	690	GLN
1	A	762	GLN
1	A	1002	GLN
1	A	1005	GLN
1	A	1058	HIS
1	A	1135	ASN
1	B	188	ASN
1	B	536	ASN

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Mol	Chain	Res	Type
1	B	542	ASN
1	B	564	GLN
1	B	690	GLN
1	B	914	ASN
1	B	919	ASN
1	B	935	GLN
1	C	49	HIS
1	C	196	ASN
1	C	314	GLN
1	C	317	ASN
1	C	540	ASN
1	C	675	GLN
1	C	690	GLN
1	C	764	ASN
1	C	856	ASN
1	C	872	GLN
1	C	907	ASN
1	C	913	GLN
1	C	919	ASN
1	C	969	ASN
1	C	1002	GLN
1	C	1010	GLN
1	C	1134	ASN
2	M	61	GLN
2	M	64	GLN
2	H	64	GLN
3	L	31	ASN
3	L	37	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 ⓘ

43 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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.98	0	17,19,21	0.92	1 (5%)
4	NAG	D	2	4	14,14,15	1.29	2 (14%)	17,19,21	0.95	1 (5%)
4	BMA	D	3	4	11,11,12	1.21	1 (9%)	15,15,17	1.08	1 (6%)
5	NAG	E	1	5,1	14,14,15	1.34	2 (14%)	17,19,21	1.53	2 (11%)
5	NAG	E	2	5	14,14,15	1.15	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	F	1	4,1	14,14,15	1.15	2 (14%)	17,19,21	0.82	1 (5%)
4	NAG	F	2	4	14,14,15	1.34	2 (14%)	17,19,21	1.02	1 (5%)
4	BMA	F	3	4	11,11,12	1.44	2 (18%)	15,15,17	0.85	1 (6%)
4	NAG	G	1	4,1	14,14,15	1.30	2 (14%)	17,19,21	1.32	2 (11%)
4	NAG	G	2	4	14,14,15	1.31	3 (21%)	17,19,21	1.03	1 (5%)
4	BMA	G	3	4	11,11,12	1.46	2 (18%)	15,15,17	0.95	1 (6%)
4	NAG	I	1	4,1	14,14,15	1.06	2 (14%)	17,19,21	0.92	1 (5%)
4	NAG	I	2	4	14,14,15	1.31	2 (14%)	17,19,21	0.99	2 (11%)
4	BMA	I	3	4	11,11,12	1.45	2 (18%)	15,15,17	0.65	0
4	NAG	J	1	4,1	14,14,15	1.17	2 (14%)	17,19,21	1.05	1 (5%)
4	NAG	J	2	4	14,14,15	1.23	2 (14%)	17,19,21	0.79	1 (5%)
4	BMA	J	3	4	11,11,12	1.25	1 (9%)	15,15,17	0.73	1 (6%)
4	NAG	K	1	4,1	14,14,15	1.26	3 (21%)	17,19,21	0.95	1 (5%)
4	NAG	K	2	4	14,14,15	1.31	2 (14%)	17,19,21	0.83	1 (5%)
4	BMA	K	3	4	11,11,12	1.33	2 (18%)	15,15,17	0.76	0
5	NAG	Q	1	5,1	14,14,15	1.18	2 (14%)	17,19,21	0.77	0
5	NAG	Q	2	5	14,14,15	1.25	2 (14%)	17,19,21	0.75	0
4	NAG	R	1	4,1	14,14,15	1.24	2 (14%)	17,19,21	1.85	3 (17%)
4	NAG	R	2	4	14,14,15	1.41	3 (21%)	17,19,21	1.49	3 (17%)
4	BMA	R	3	4	11,11,12	1.30	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	S	1	4,1	14,14,15	1.31	2 (14%)	17,19,21	1.05	0
4	NAG	S	2	4	14,14,15	1.38	3 (21%)	17,19,21	1.14	1 (5%)
4	BMA	S	3	4	11,11,12	1.28	1 (9%)	15,15,17	0.93	1 (6%)
4	NAG	T	1	4,1	14,14,15	1.09	2 (14%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	T	2	4	14,14,15	1.40	3 (21%)	17,19,21	0.75	0
4	BMA	T	3	4	11,11,12	1.46	1 (9%)	15,15,17	1.68	3 (20%)
4	NAG	U	1	4,1	14,14,15	1.18	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	U	2	4	14,14,15	1.19	1 (7%)	17,19,21	0.87	1 (5%)
4	BMA	U	3	4	11,11,12	1.25	2 (18%)	15,15,17	0.88	1 (6%)
4	NAG	V	1	4	14,14,15	1.10	2 (14%)	17,19,21	0.96	2 (11%)
4	NAG	V	2	4	14,14,15	1.28	2 (14%)	17,19,21	1.10	1 (5%)
4	BMA	V	3	4	11,11,12	1.27	2 (18%)	15,15,17	1.25	1 (6%)
4	NAG	W	1	4,1	14,14,15	1.18	2 (14%)	17,19,21	0.88	1 (5%)
4	NAG	W	2	4	14,14,15	1.47	3 (21%)	17,19,21	1.15	1 (5%)
4	BMA	W	3	4	11,11,12	1.32	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	X	1	4,1	14,14,15	1.08	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	X	2	4	14,14,15	1.30	2 (14%)	17,19,21	1.06	1 (5%)
4	BMA	X	3	4	11,11,12	1.26	2 (18%)	15,15,17	0.82	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
4	NAG	D	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	2/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	BMA	S	3	4	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	BMA	U	3	4	-	1/2/19/22	0/1/1/1
4	NAG	V	1	4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	1/6/23/26	0/1/1/1
4	BMA	V	3	4	-	1/2/19/22	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	1/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	BMA	O5-C5	3.09	1.49	1.43
4	F	3	BMA	O5-C5	3.04	1.49	1.43
4	T	2	NAG	O4-C4	3.03	1.50	1.43
4	G	3	BMA	O5-C5	2.98	1.49	1.43
5	E	1	NAG	O5-C5	2.90	1.49	1.43
4	S	3	BMA	O5-C5	2.89	1.49	1.43
4	W	2	NAG	O5-C5	2.81	1.48	1.43
4	I	2	NAG	O5-C5	2.81	1.48	1.43
4	K	3	BMA	O5-C5	2.81	1.48	1.43
4	R	2	NAG	O4-C4	2.77	1.49	1.43
4	S	2	NAG	O5-C5	2.76	1.48	1.43
4	S	1	NAG	O5-C5	2.68	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	O5-C5	2.66	1.48	1.43
4	K	2	NAG	O4-C4	2.66	1.49	1.43
4	W	3	BMA	O5-C5	2.66	1.48	1.43
4	D	2	NAG	O4-C4	2.65	1.49	1.43
4	I	3	BMA	O5-C1	2.63	1.48	1.43
5	Q	2	NAG	O5-C5	2.62	1.48	1.43
4	V	3	BMA	O5-C5	2.60	1.48	1.43
4	T	3	BMA	O5-C5	2.60	1.48	1.43
4	R	3	BMA	O5-C5	2.57	1.48	1.43
4	F	3	BMA	O5-C1	2.56	1.48	1.43
4	R	2	NAG	C1-C2	2.54	1.55	1.52
4	W	2	NAG	O4-C4	2.53	1.49	1.43
4	X	2	NAG	O5-C5	2.53	1.48	1.43
4	D	3	BMA	O5-C5	2.52	1.48	1.43
4	X	3	BMA	O5-C5	2.50	1.48	1.43
4	W	2	NAG	O5-C1	2.50	1.47	1.43
4	U	3	BMA	O5-C5	2.49	1.48	1.43
4	R	1	NAG	C1-C2	2.48	1.55	1.52
4	S	2	NAG	O4-C4	2.48	1.49	1.43
4	X	2	NAG	O4-C4	2.45	1.49	1.43
5	E	2	NAG	O5-C5	2.45	1.48	1.43
4	G	3	BMA	O5-C1	2.45	1.47	1.43
4	G	2	NAG	O5-C5	2.44	1.48	1.43
4	T	2	NAG	O5-C5	2.43	1.48	1.43
4	G	1	NAG	O5-C5	2.42	1.48	1.43
4	F	1	NAG	O5-C5	2.42	1.48	1.43
4	U	2	NAG	O5-C5	2.42	1.48	1.43
4	K	1	NAG	O5-C1	2.41	1.47	1.43
4	U	1	NAG	O5-C5	2.41	1.48	1.43
4	R	1	NAG	O4-C4	2.39	1.48	1.43
4	F	2	NAG	O5-C5	2.39	1.48	1.43
4	W	1	NAG	O5-C5	2.39	1.48	1.43
4	V	2	NAG	O5-C5	2.37	1.48	1.43
4	T	1	NAG	O5-C5	2.35	1.48	1.43
4	J	2	NAG	O5-C5	2.32	1.48	1.43
4	I	2	NAG	O4-C4	2.32	1.48	1.43
5	E	1	NAG	O4-C4	2.32	1.48	1.43
4	J	3	BMA	O5-C5	2.30	1.47	1.43
4	I	1	NAG	O5-C5	2.28	1.47	1.43
5	Q	1	NAG	O4-C4	2.27	1.48	1.43
4	D	2	NAG	O5-C5	2.26	1.47	1.43
4	K	2	NAG	O5-C5	2.25	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	1	NAG	O5-C5	2.24	1.47	1.43
4	S	1	NAG	C1-C2	2.19	1.55	1.52
4	T	1	NAG	O4-C4	2.19	1.48	1.43
4	W	3	BMA	O5-C1	2.18	1.47	1.43
4	K	1	NAG	O4-C4	2.18	1.48	1.43
4	F	2	NAG	C1-C2	2.16	1.55	1.52
4	G	2	NAG	C1-C2	2.16	1.55	1.52
4	V	2	NAG	O4-C4	2.16	1.48	1.43
4	X	3	BMA	O5-C1	2.16	1.47	1.43
4	J	2	NAG	O4-C4	2.15	1.48	1.43
4	G	1	NAG	O4-C4	2.14	1.48	1.43
4	X	1	NAG	O5-C5	2.14	1.47	1.43
4	R	2	NAG	O5-C5	2.14	1.47	1.43
5	E	2	NAG	C1-C2	2.12	1.55	1.52
4	K	3	BMA	O5-C1	2.12	1.47	1.43
5	Q	2	NAG	O5-C1	2.11	1.47	1.43
4	F	1	NAG	O4-C4	2.11	1.48	1.43
4	V	1	NAG	O5-C1	2.09	1.47	1.43
4	V	3	BMA	O5-C1	2.09	1.47	1.43
4	T	2	NAG	C1-C2	2.09	1.55	1.52
4	J	1	NAG	C1-C2	2.07	1.55	1.52
4	W	1	NAG	O4-C4	2.07	1.48	1.43
4	I	1	NAG	O4-C4	2.07	1.48	1.43
4	V	1	NAG	O5-C5	2.06	1.47	1.43
4	U	3	BMA	O5-C1	2.06	1.47	1.43
4	R	3	BMA	O5-C1	2.05	1.47	1.43
4	G	2	NAG	O4-C4	2.03	1.48	1.43
4	S	2	NAG	C1-C2	2.03	1.55	1.52
4	J	1	NAG	O5-C5	2.01	1.47	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	1	NAG	O5-C1-C2	6.09	120.71	111.29
5	E	1	NAG	C1-O5-C5	5.07	118.98	112.19
4	R	2	NAG	C1-O5-C5	4.34	118.00	112.19
4	V	3	BMA	C1-O5-C5	4.29	117.93	112.19
4	S	2	NAG	C1-O5-C5	3.90	117.41	112.19
4	T	3	BMA	O2-C2-C1	3.79	117.89	109.22
4	T	3	BMA	O5-C1-C2	3.51	119.17	110.79
4	W	2	NAG	C1-O5-C5	3.38	116.71	112.19
4	G	1	NAG	O4-C4-C3	-3.21	102.81	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	3.01	116.22	112.19
5	E	2	NAG	C1-O5-C5	2.90	116.08	112.19
4	F	2	NAG	C2-N2-C7	2.87	126.74	122.90
4	X	2	NAG	O5-C1-C2	-2.83	106.91	111.29
4	D	3	BMA	C1-O5-C5	2.83	115.97	112.19
4	W	3	BMA	C1-O5-C5	2.82	115.97	112.19
4	T	3	BMA	C1-C2-C3	-2.80	105.56	109.64
4	R	3	BMA	C1-O5-C5	2.73	115.84	112.19
4	D	1	NAG	O4-C4-C5	-2.72	102.64	109.32
4	G	2	NAG	O5-C1-C2	-2.68	107.14	111.29
4	T	1	NAG	O4-C4-C3	-2.67	104.09	110.38
4	U	3	BMA	C1-O5-C5	2.64	115.73	112.19
4	V	2	NAG	O5-C1-C2	-2.59	107.28	111.29
4	K	2	NAG	C1-O5-C5	2.58	115.65	112.19
4	G	3	BMA	C1-O5-C5	2.55	115.61	112.19
4	K	1	NAG	C4-C3-C2	2.54	114.74	111.02
4	J	2	NAG	C1-O5-C5	2.54	115.59	112.19
5	E	1	NAG	O4-C4-C3	-2.52	104.44	110.38
4	F	1	NAG	C1-O5-C5	2.51	115.55	112.19
4	V	1	NAG	O4-C4-C5	-2.50	103.18	109.32
4	I	1	NAG	O4-C4-C5	-2.49	103.20	109.32
4	G	1	NAG	C4-C3-C2	2.47	114.64	111.02
4	X	1	NAG	C1-O5-C5	2.43	115.44	112.19
4	R	1	NAG	C2-N2-C7	2.43	126.15	122.90
4	S	3	BMA	C1-O5-C5	2.42	115.44	112.19
4	F	3	BMA	C1-O5-C5	2.37	115.36	112.19
4	R	1	NAG	C4-C3-C2	2.26	114.32	111.02
4	R	2	NAG	C3-C4-C5	2.24	114.29	110.23
4	W	1	NAG	O5-C1-C2	-2.24	107.83	111.29
4	V	1	NAG	O5-C1-C2	-2.23	107.84	111.29
4	U	1	NAG	O4-C4-C3	-2.21	105.16	110.38
4	U	2	NAG	O5-C1-C2	-2.16	107.94	111.29
4	R	2	NAG	C1-C2-N2	2.11	113.76	110.43
4	I	2	NAG	C4-C3-C2	-2.09	107.96	111.02
4	I	2	NAG	O4-C4-C3	2.04	115.18	110.38
4	J	1	NAG	C3-C4-C5	2.03	113.91	110.23
4	J	3	BMA	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

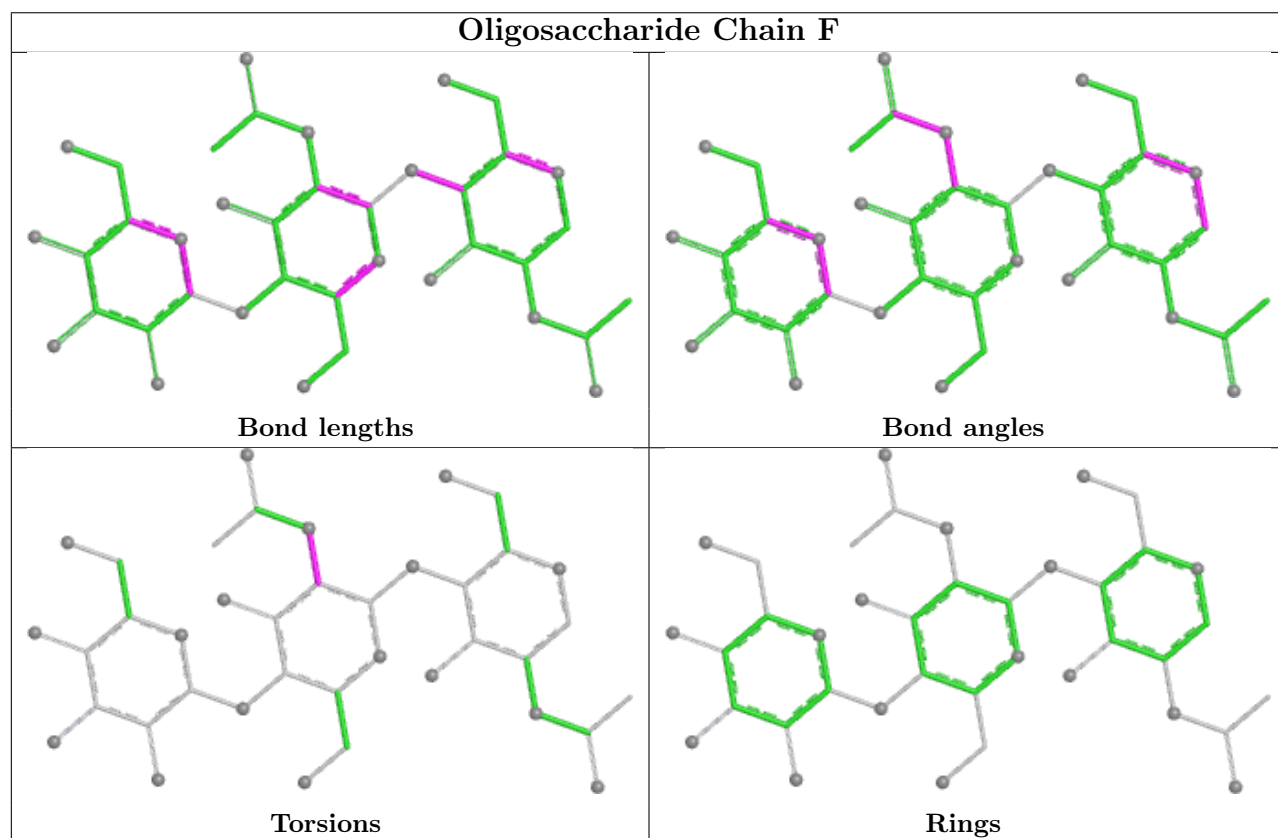
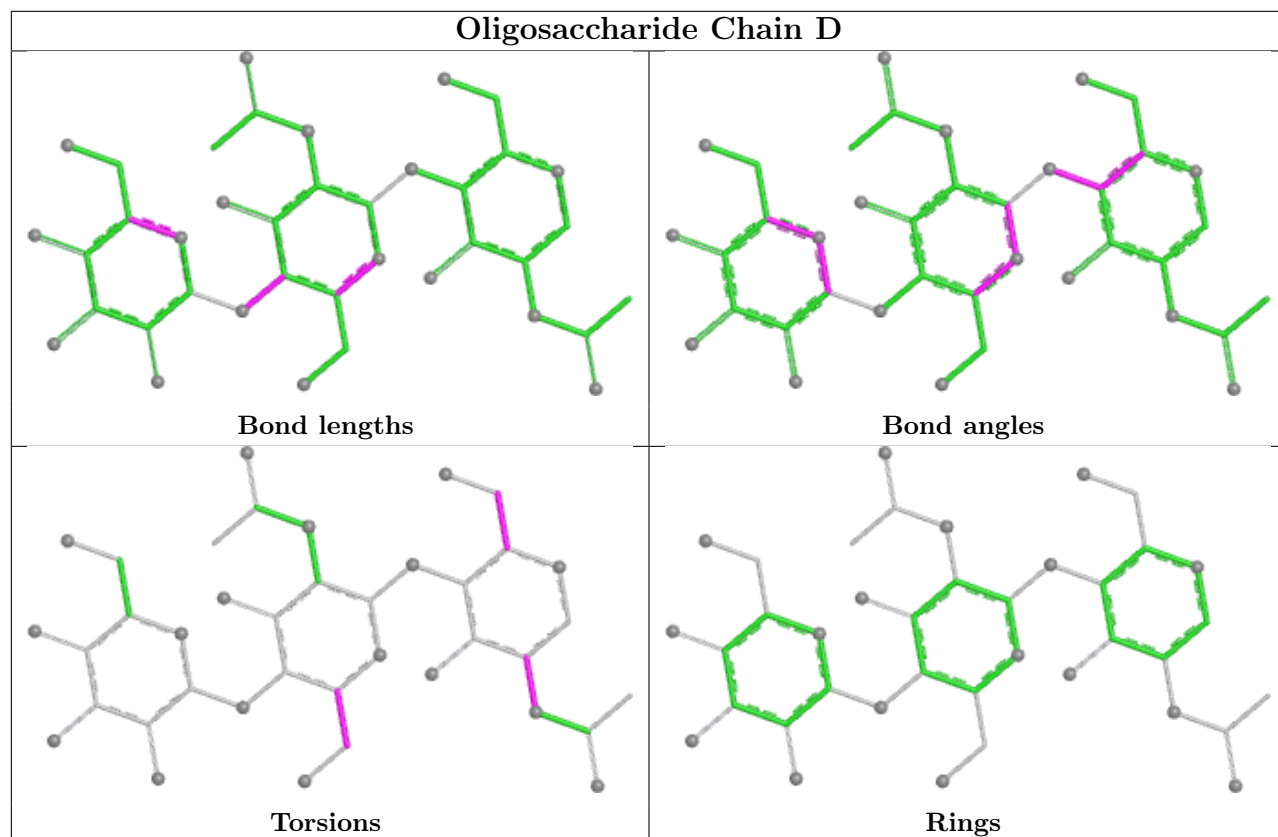
All (28) torsion outliers are listed below:

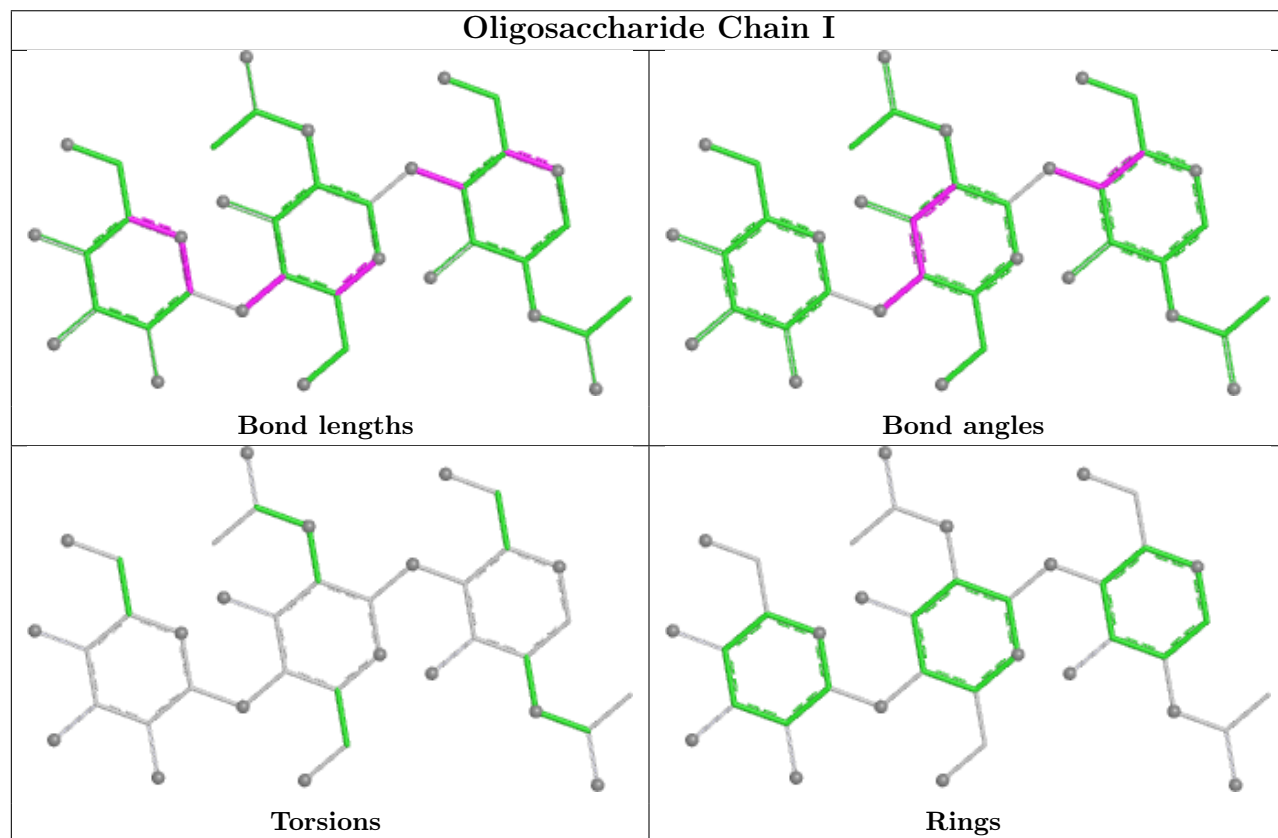
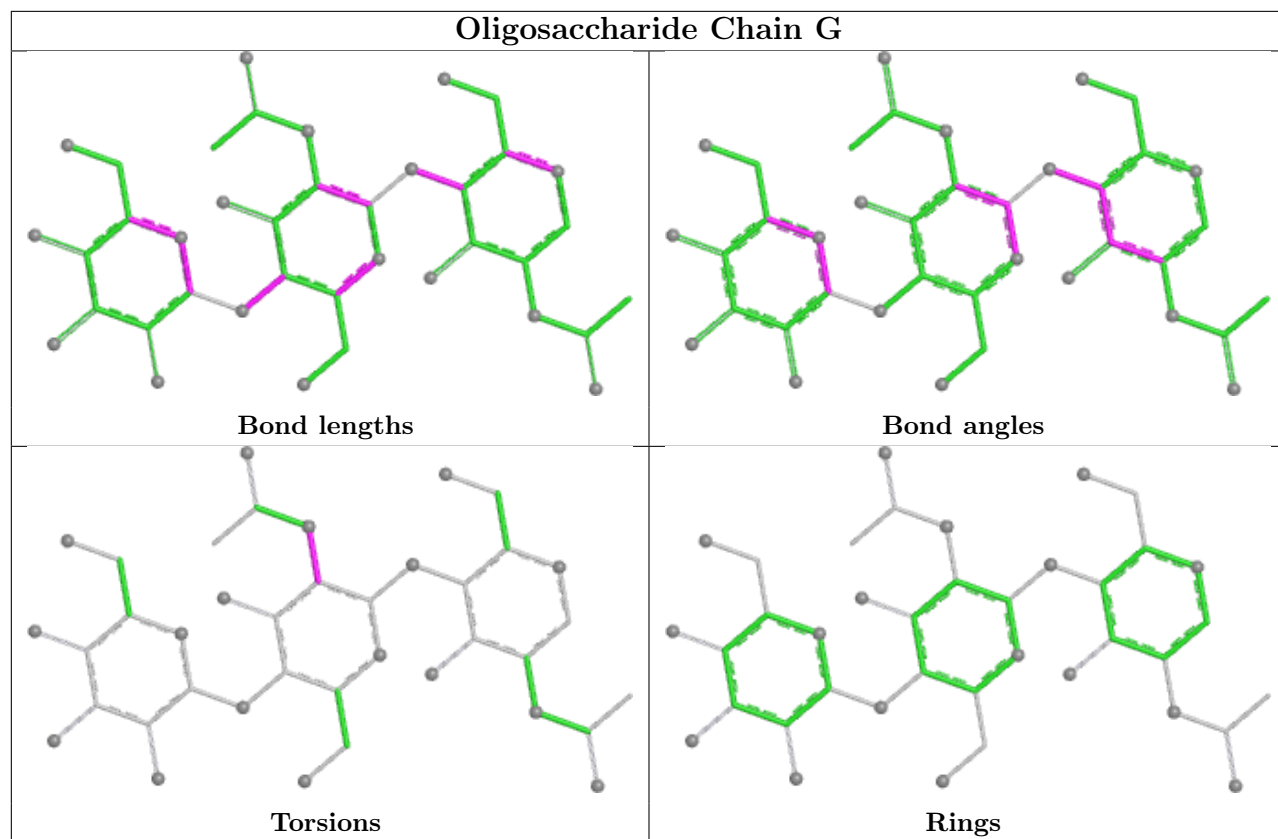
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	F	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	V	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	R	3	BMA	O5-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	R	2	NAG	C1-C2-N2-C7
4	W	2	NAG	C1-C2-N2-C7
4	S	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
4	X	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
4	S	1	NAG	C1-C2-N2-C7
4	W	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	W	2	NAG	C3-C2-N2-C7
4	D	2	NAG	O5-C5-C6-O6
4	R	3	BMA	C4-C5-C6-O6

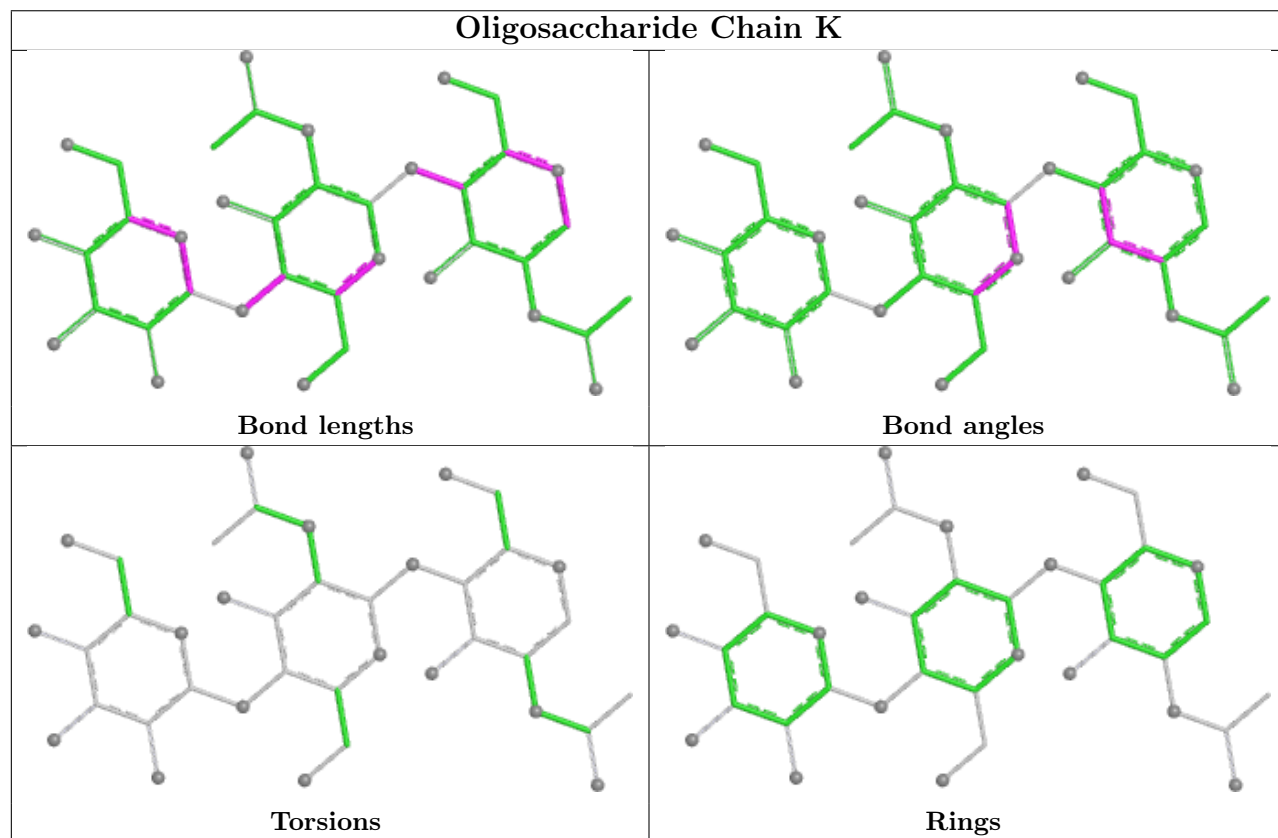
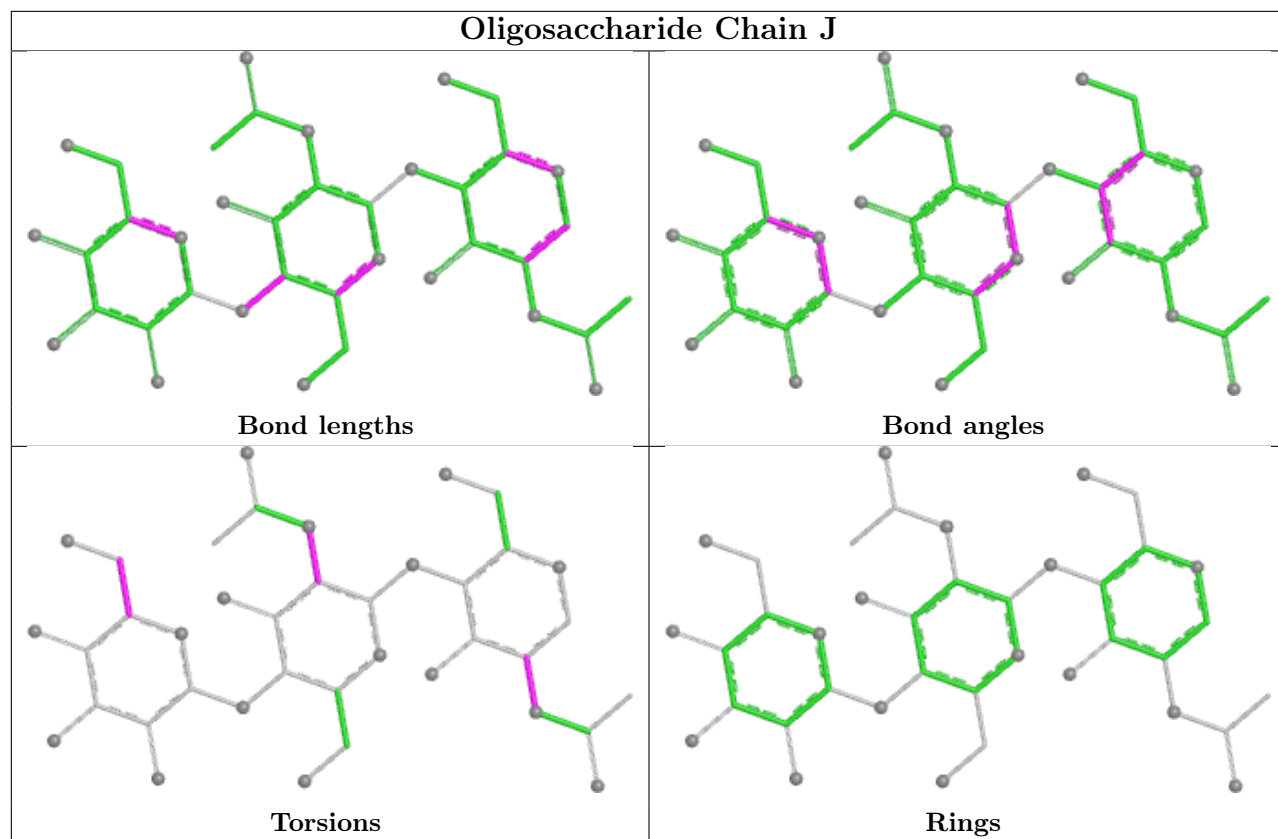
There are no ring outliers.

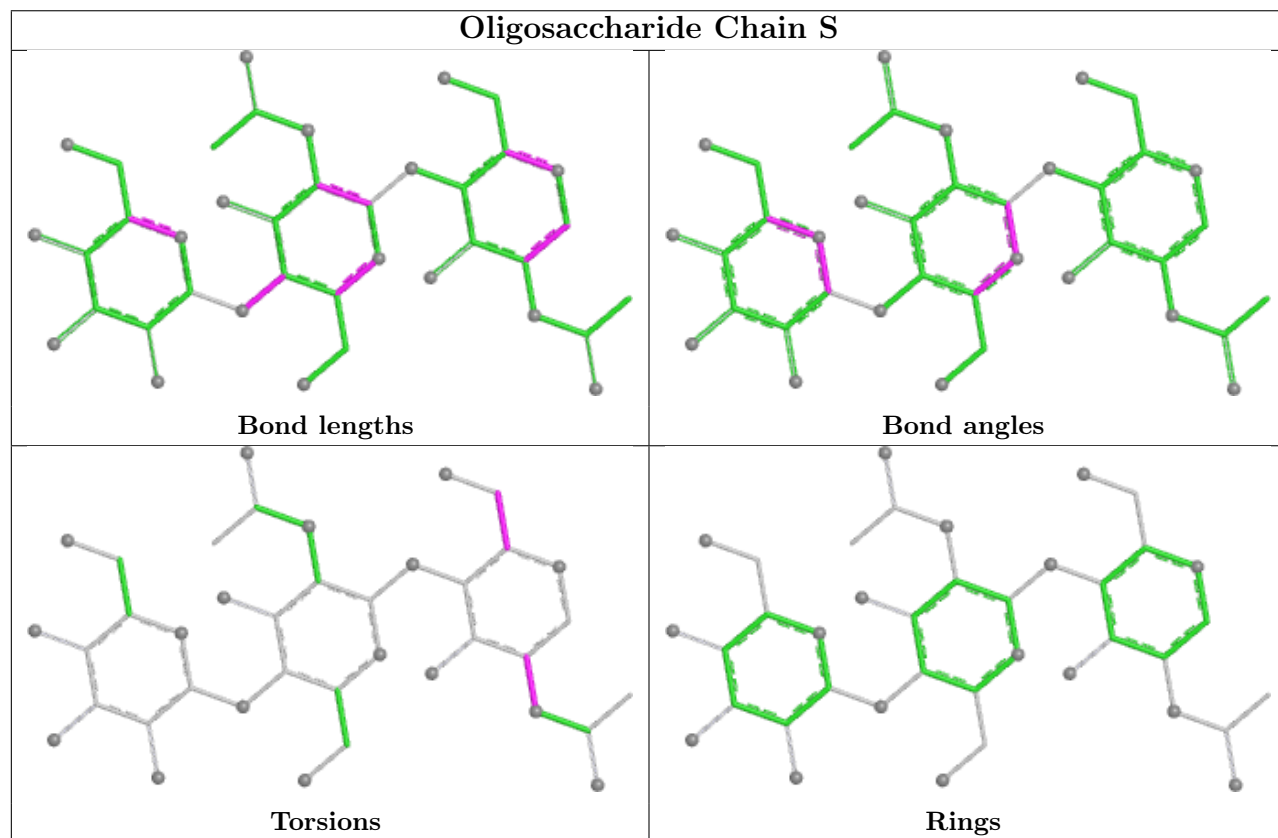
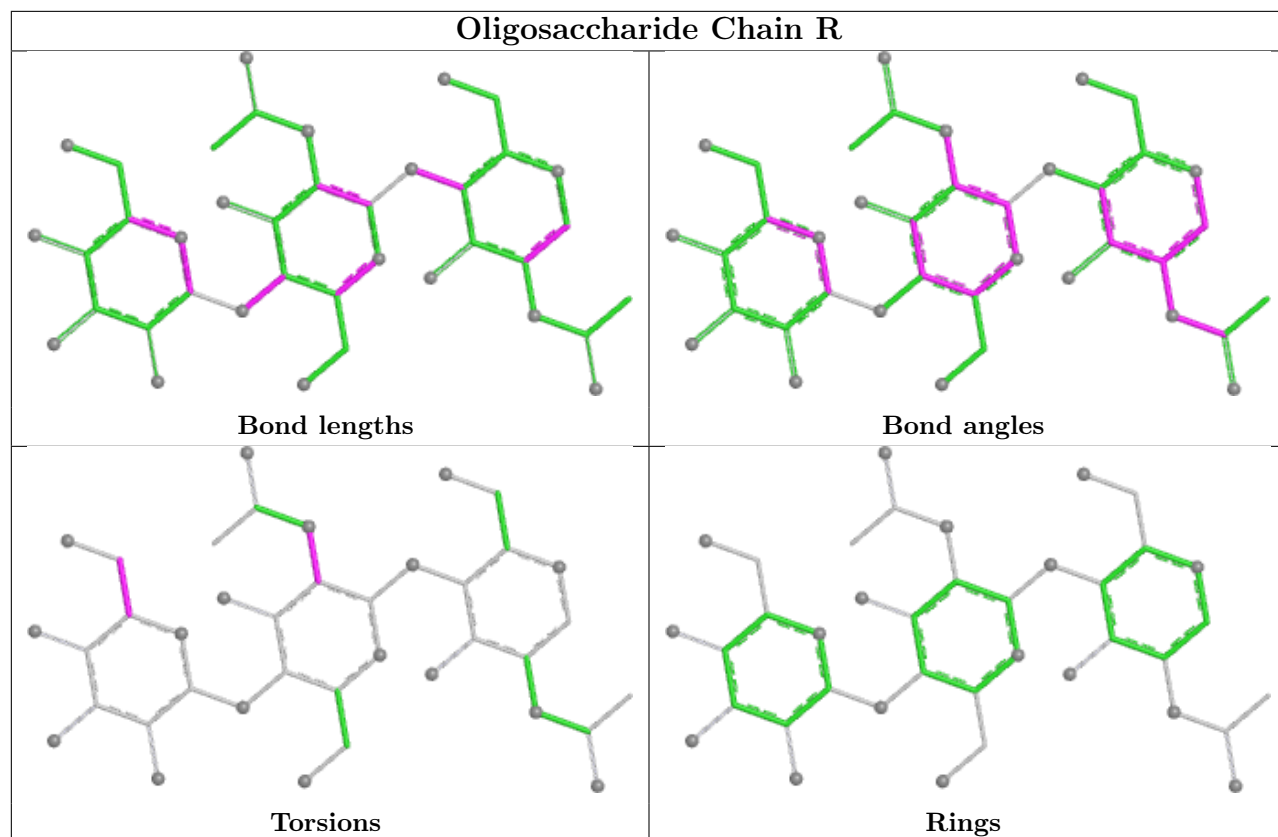
No monomer is involved in short contacts.

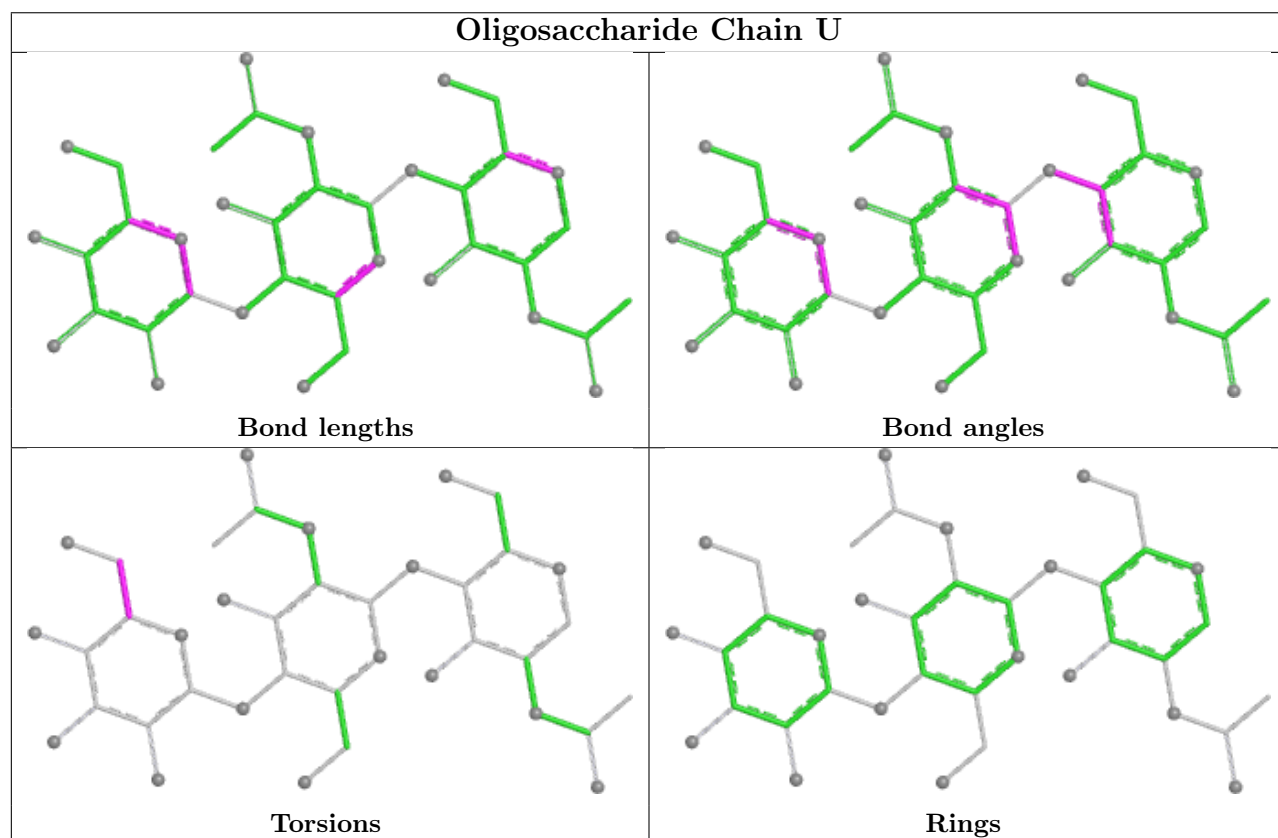
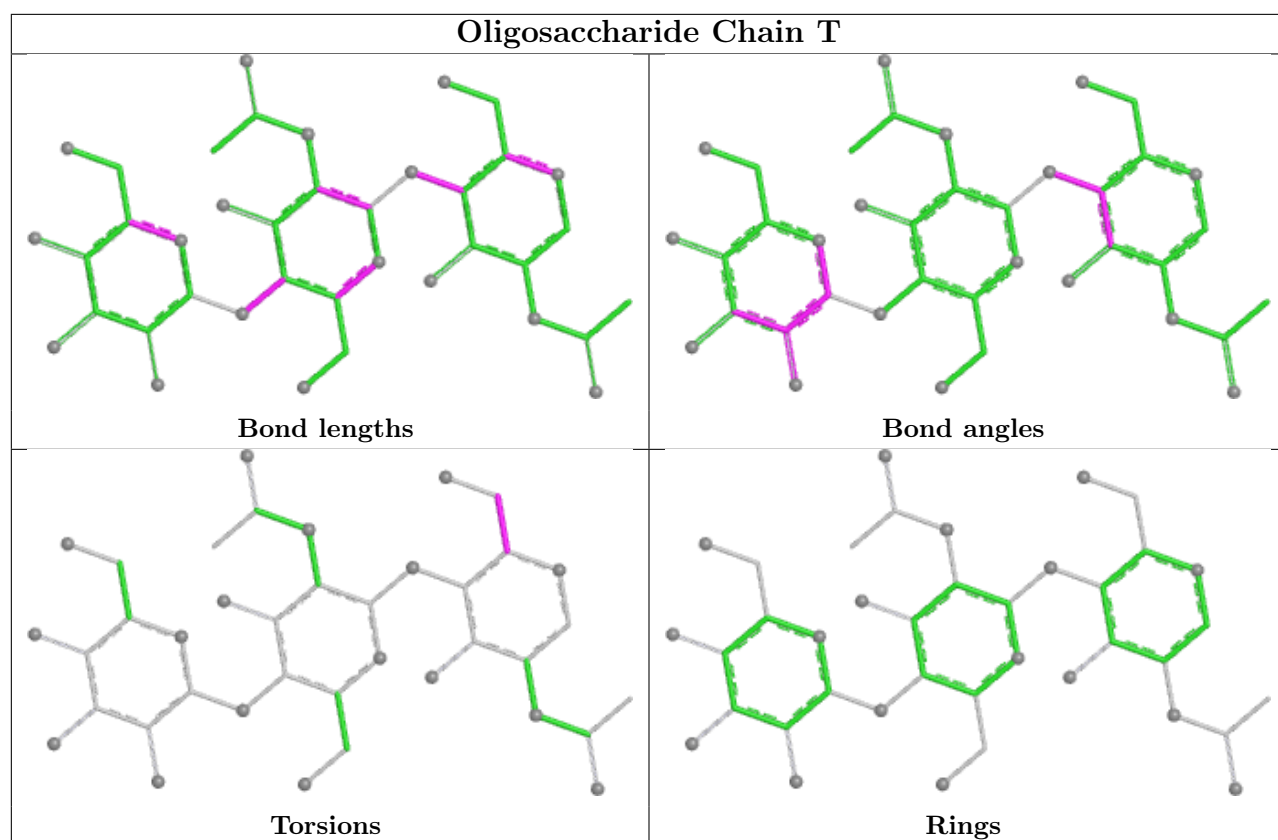
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

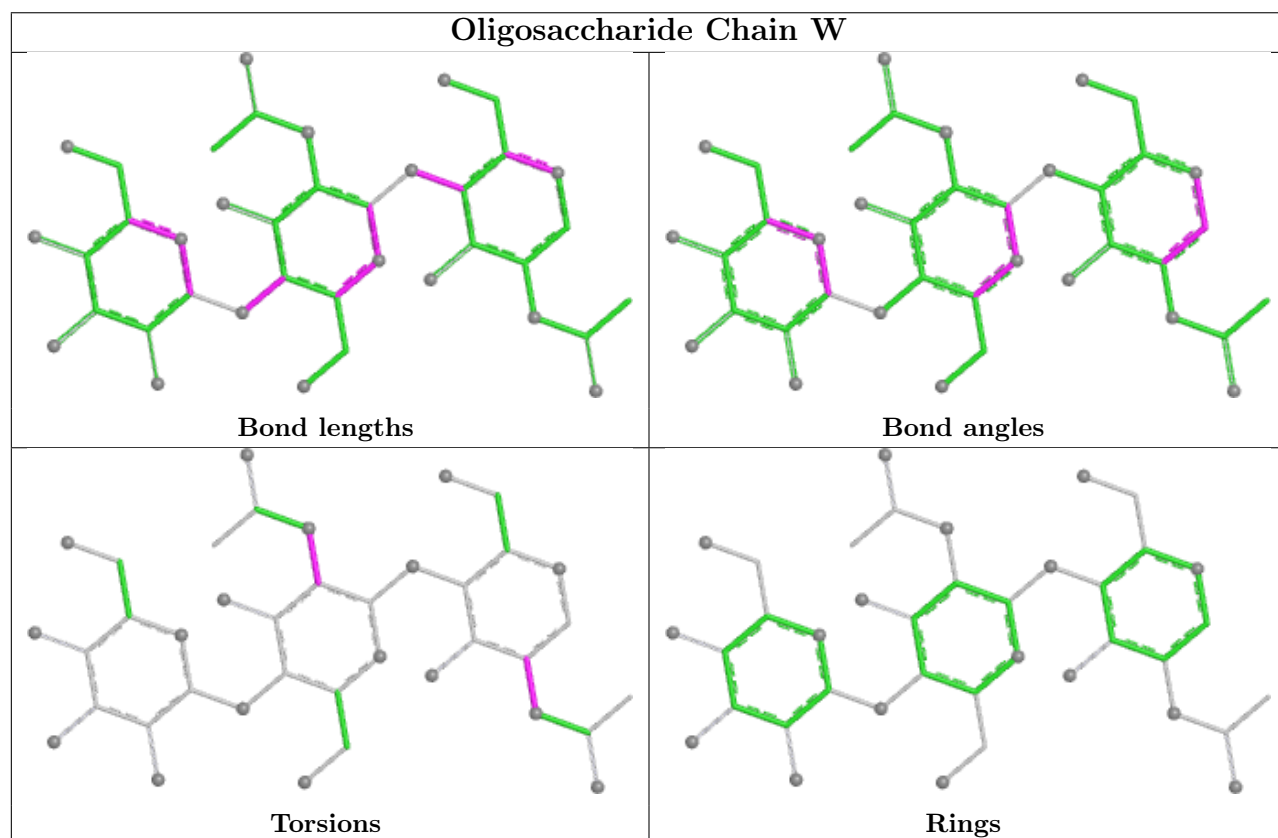
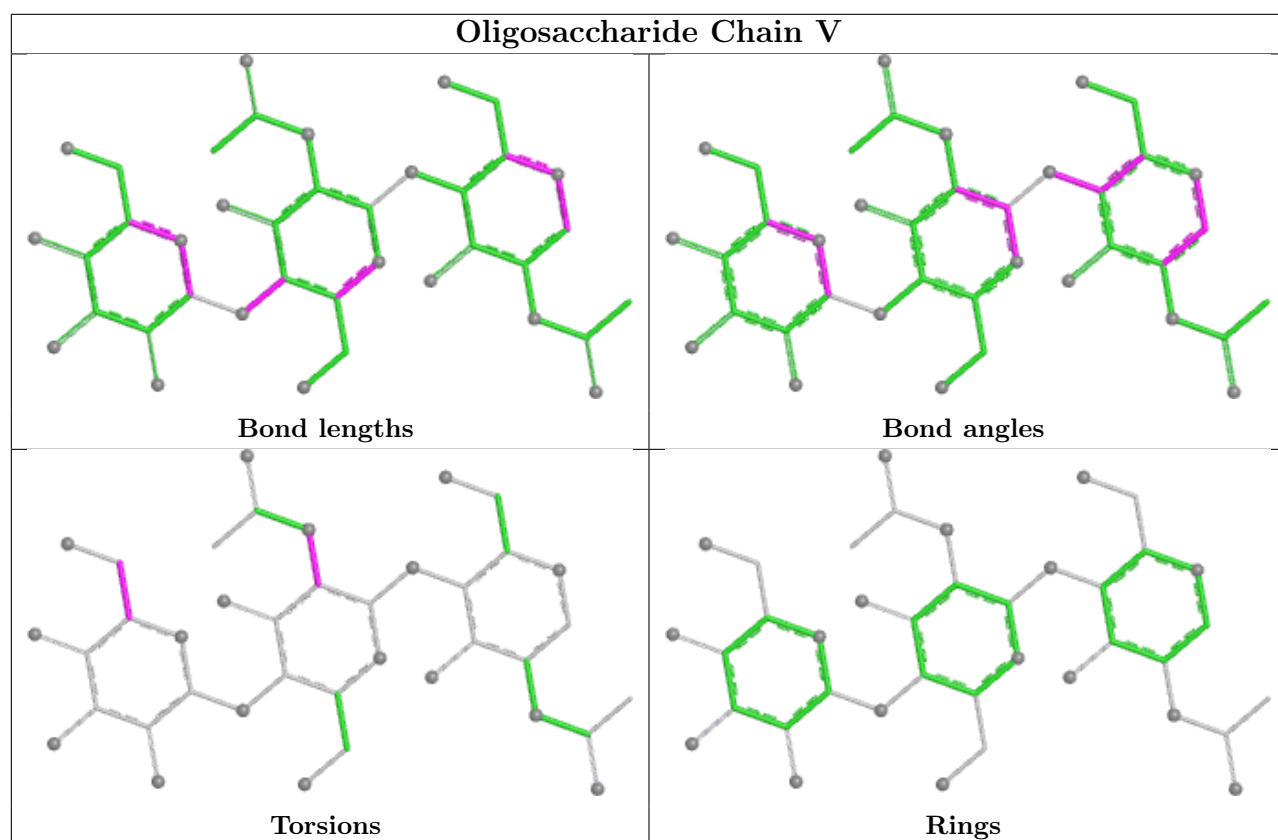


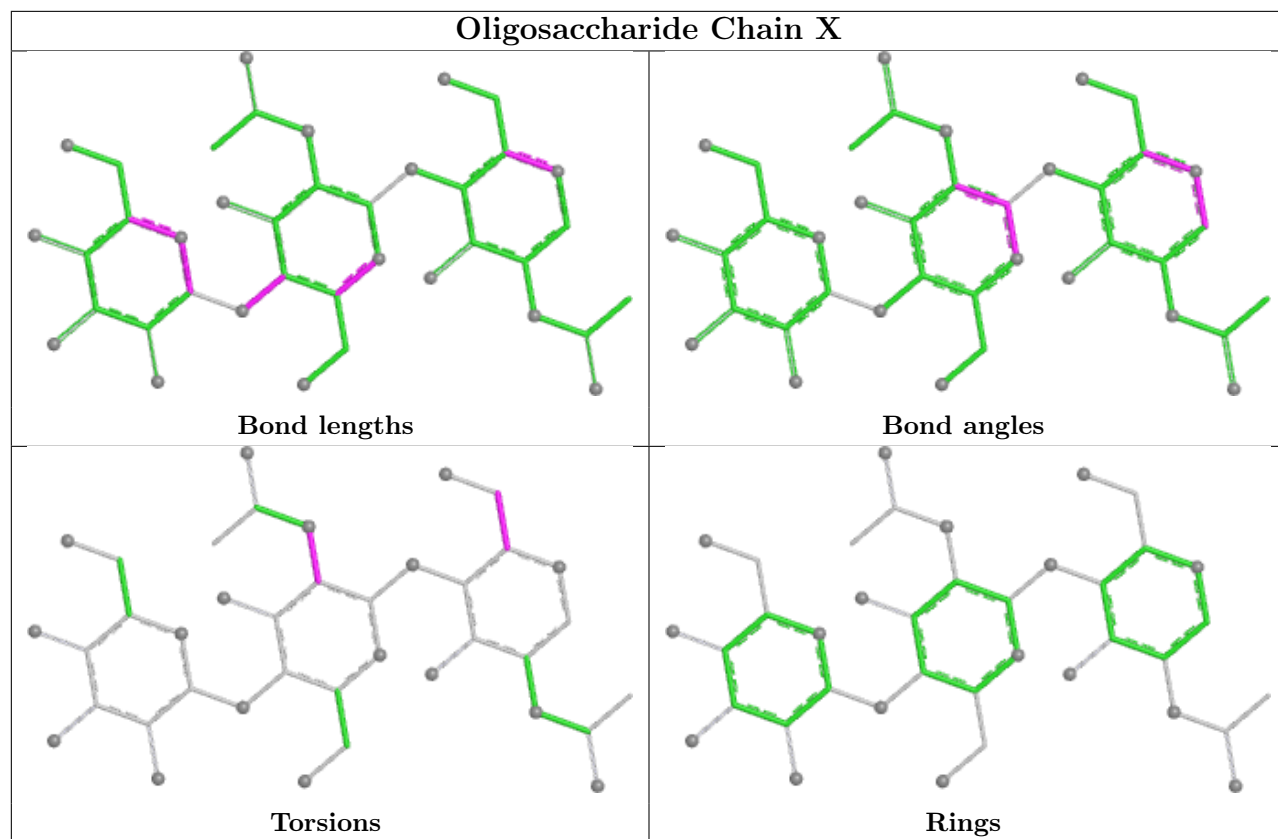


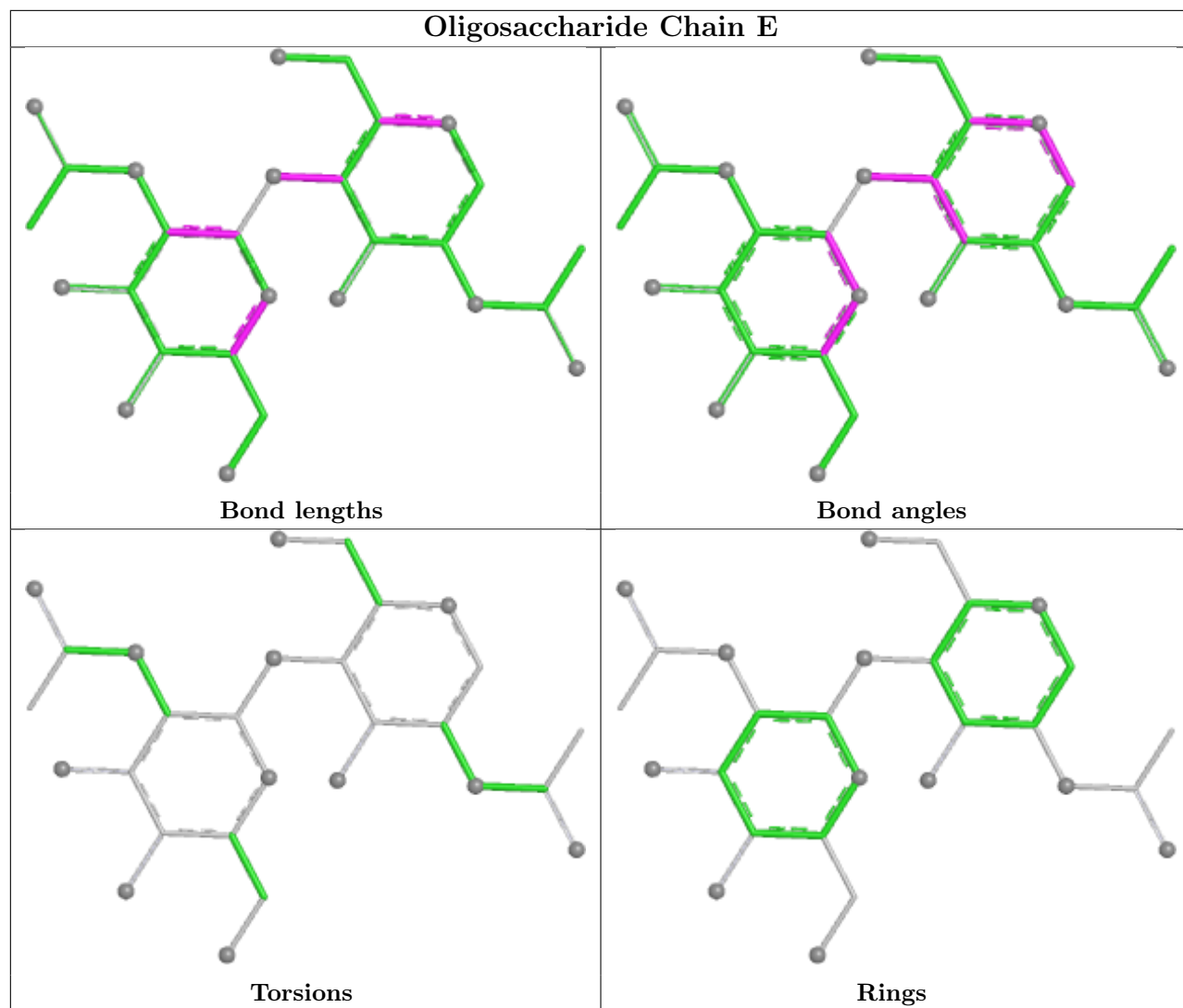


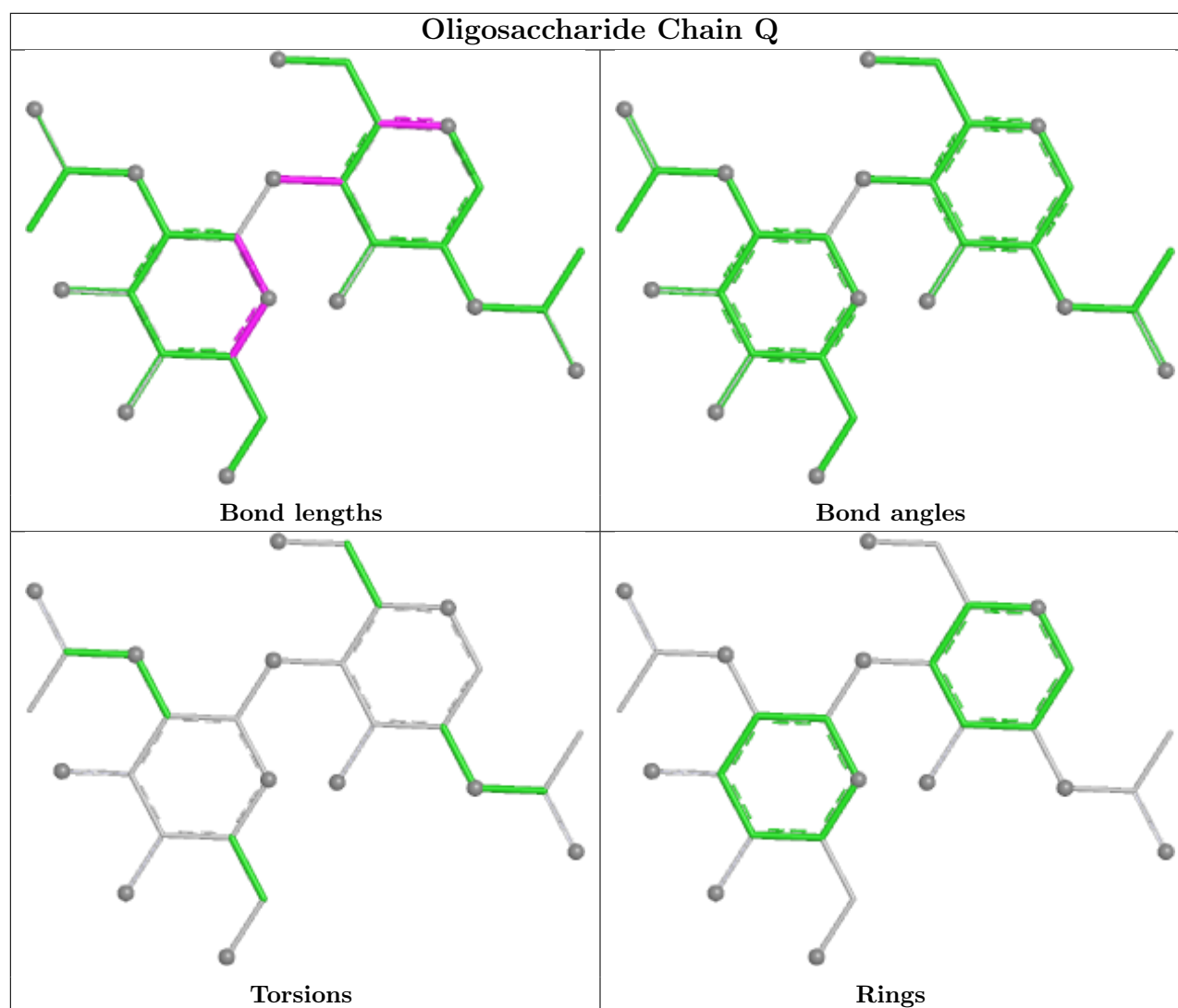












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
6	NAG	A	1204	1	14,14,15	1.29	2 (14%)	17,19,21	0.68	0
6	NAG	C	1201	-	14,14,15	1.19	2 (14%)	17,19,21	0.92	1 (5%)
6	NAG	B	1201	1	14,14,15	1.27	2 (14%)	17,19,21	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1205	1	14,14,15	1.38	3 (21%)	17,19,21	1.12	2 (11%)
6	NAG	A	1203	1	14,14,15	1.24	2 (14%)	17,19,21	0.95	1 (5%)
6	NAG	B	1205	1	14,14,15	1.18	2 (14%)	17,19,21	0.87	0
6	NAG	C	1207	1	14,14,15	1.31	2 (14%)	17,19,21	0.95	1 (5%)
6	NAG	B	1203	1	14,14,15	1.22	2 (14%)	17,19,21	1.34	1 (5%)
6	NAG	C	1205	1	14,14,15	1.16	2 (14%)	17,19,21	0.71	0
6	NAG	C	1202	1	14,14,15	1.29	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	C	1206	1	14,14,15	1.10	1 (7%)	17,19,21	0.58	0
6	NAG	A	1206	1	14,14,15	1.26	2 (14%)	17,19,21	1.16	1 (5%)
6	NAG	A	1201	1	14,14,15	1.28	1 (7%)	17,19,21	1.57	1 (5%)
6	NAG	C	1204	1	14,14,15	1.04	1 (7%)	17,19,21	0.71	0
6	NAG	B	1204	1	14,14,15	1.24	1 (7%)	17,19,21	0.91	1 (5%)
6	NAG	A	1207	1	14,14,15	1.21	2 (14%)	17,19,21	0.66	0
6	NAG	B	1207	1	14,14,15	1.26	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	A	1202	1	14,14,15	1.14	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	B	1202	1	14,14,15	1.20	2 (14%)	17,19,21	1.57	1 (5%)
6	NAG	B	1208	1	14,14,15	1.22	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	B	1206	1	14,14,15	1.29	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	A	1208	1	14,14,15	1.23	2 (14%)	17,19,21	1.00	1 (5%)
6	NAG	B	1209	1	14,14,15	1.45	3 (21%)	17,19,21	0.85	0
6	NAG	C	1203	1	14,14,15	1.26	2 (14%)	17,19,21	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1201	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1201	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1205	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1205	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1206	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1207	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1208	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1209	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	1/6/23/26	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1207	NAG	O5-C5	3.26	1.49	1.43
6	A	1201	NAG	C1-C2	3.14	1.56	1.52
6	A	1205	NAG	C1-C2	3.04	1.56	1.52
6	C	1203	NAG	O5-C5	2.98	1.49	1.43
6	B	1201	NAG	O5-C5	2.94	1.49	1.43
6	B	1209	NAG	O5-C5	2.88	1.49	1.43
6	A	1203	NAG	O5-C5	2.87	1.49	1.43
6	A	1204	NAG	O5-C5	2.80	1.48	1.43
6	B	1209	NAG	C1-C2	2.79	1.56	1.52
6	B	1207	NAG	O5-C5	2.76	1.48	1.43
6	C	1201	NAG	O5-C1	2.75	1.48	1.43
6	B	1206	NAG	O5-C5	2.74	1.48	1.43
6	B	1208	NAG	O5-C5	2.73	1.48	1.43
6	B	1204	NAG	O5-C5	2.70	1.48	1.43
6	A	1205	NAG	O5-C5	2.69	1.48	1.43
6	A	1208	NAG	C1-C2	2.67	1.56	1.52
6	C	1202	NAG	O5-C5	2.59	1.48	1.43
6	B	1202	NAG	C1-C2	2.58	1.55	1.52
6	B	1205	NAG	O5-C5	2.55	1.48	1.43
6	B	1206	NAG	C1-C2	2.52	1.55	1.52
6	A	1206	NAG	O5-C5	2.51	1.48	1.43
6	B	1203	NAG	C1-C2	2.50	1.55	1.52
6	A	1207	NAG	O5-C5	2.50	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1204	NAG	O5-C5	2.47	1.48	1.43
6	C	1201	NAG	O5-C5	2.44	1.48	1.43
6	A	1202	NAG	O5-C5	2.42	1.48	1.43
6	C	1206	NAG	O5-C5	2.39	1.48	1.43
6	A	1203	NAG	C1-C2	2.38	1.55	1.52
6	B	1202	NAG	O5-C5	2.37	1.48	1.43
6	A	1207	NAG	C1-C2	2.37	1.55	1.52
6	A	1206	NAG	C1-C2	2.29	1.55	1.52
6	B	1208	NAG	C1-C2	2.28	1.55	1.52
6	C	1203	NAG	C1-C2	2.22	1.55	1.52
6	A	1204	NAG	C1-C2	2.22	1.55	1.52
6	B	1209	NAG	O5-C1	2.21	1.47	1.43
6	C	1205	NAG	O5-C5	2.19	1.47	1.43
6	C	1207	NAG	O5-C1	2.17	1.47	1.43
6	B	1203	NAG	O5-C5	2.17	1.47	1.43
6	C	1205	NAG	C1-C2	2.17	1.55	1.52
6	C	1202	NAG	C1-C2	2.13	1.55	1.52
6	B	1201	NAG	C1-C2	2.11	1.55	1.52
6	A	1208	NAG	O5-C5	2.10	1.47	1.43
6	B	1205	NAG	C1-C2	2.04	1.55	1.52
6	A	1205	NAG	O5-C1	2.00	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1202	NAG	O5-C1-C2	5.56	119.89	111.29
6	A	1201	NAG	O5-C1-C2	5.33	119.54	111.29
6	B	1203	NAG	C1-O5-C5	4.84	118.67	112.19
6	A	1205	NAG	C1-O5-C5	3.36	116.69	112.19
6	A	1208	NAG	C1-O5-C5	3.28	116.58	112.19
6	A	1206	NAG	C1-O5-C5	3.25	116.55	112.19
6	C	1203	NAG	C1-O5-C5	3.16	116.42	112.19
6	A	1202	NAG	C1-O5-C5	3.04	116.25	112.19
6	B	1204	NAG	C1-O5-C5	2.85	116.01	112.19
6	C	1207	NAG	C1-O5-C5	2.70	115.80	112.19
6	C	1201	NAG	C1-O5-C5	2.63	115.71	112.19
6	C	1202	NAG	C1-O5-C5	2.56	115.61	112.19
6	A	1203	NAG	C1-O5-C5	2.53	115.57	112.19
6	B	1206	NAG	C1-O5-C5	2.47	115.50	112.19
6	B	1207	NAG	C1-O5-C5	2.29	115.26	112.19
6	B	1208	NAG	C1-O5-C5	2.22	115.16	112.19
6	A	1205	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1206	NAG	O5-C5-C6-O6
6	C	1205	NAG	O5-C5-C6-O6
6	A	1202	NAG	O5-C5-C6-O6
6	C	1201	NAG	O5-C5-C6-O6
6	A	1208	NAG	O5-C5-C6-O6
6	B	1203	NAG	O5-C5-C6-O6
6	B	1202	NAG	O5-C5-C6-O6
6	B	1201	NAG	O5-C5-C6-O6
6	C	1206	NAG	C4-C5-C6-O6
6	A	1205	NAG	C1-C2-N2-C7
6	B	1201	NAG	C1-C2-N2-C7
6	A	1203	NAG	C4-C5-C6-O6
6	B	1208	NAG	C4-C5-C6-O6
6	A	1203	NAG	O5-C5-C6-O6
6	A	1206	NAG	C4-C5-C6-O6
6	B	1208	NAG	O5-C5-C6-O6
6	B	1201	NAG	C3-C2-N2-C7
6	A	1206	NAG	O5-C5-C6-O6
6	A	1206	NAG	C1-C2-N2-C7
6	A	1207	NAG	C1-C2-N2-C7
6	C	1202	NAG	C1-C2-N2-C7
6	A	1205	NAG	C3-C2-N2-C7
6	A	1206	NAG	C3-C2-N2-C7
6	B	1209	NAG	C4-C5-C6-O6
6	C	1203	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

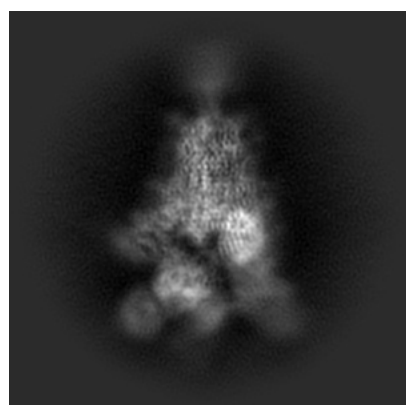
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23279. These allow visual inspection of the internal detail of the map and identification of artifacts.

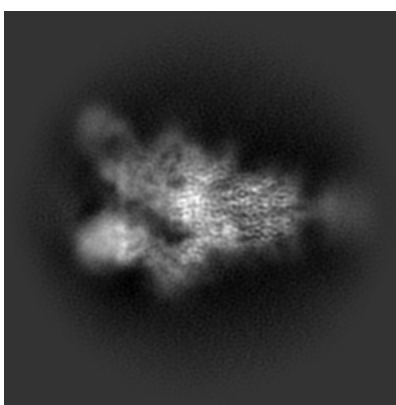
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

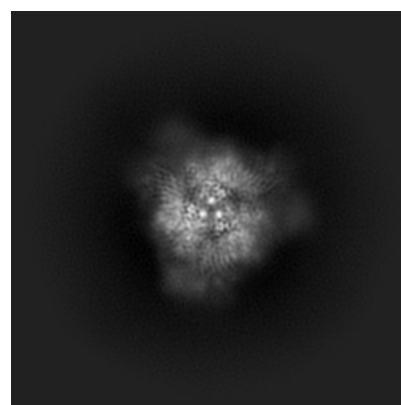
6.1.1 Primary map



X



Y

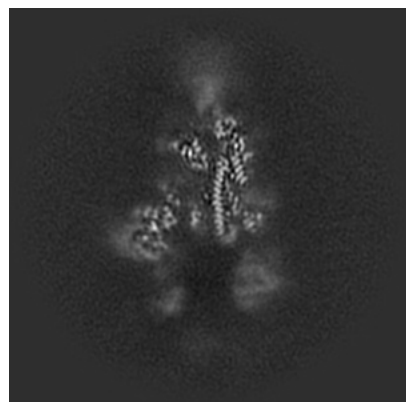


Z

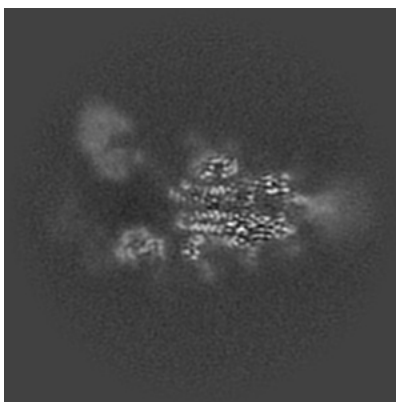
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

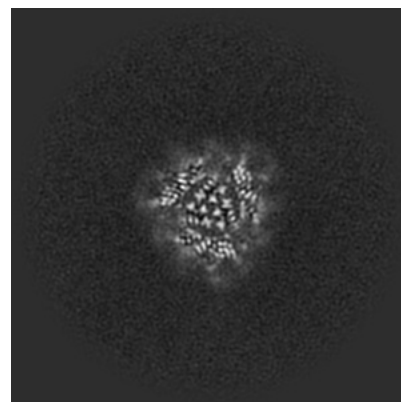
6.2.1 Primary map



X Index: 160



Y Index: 160

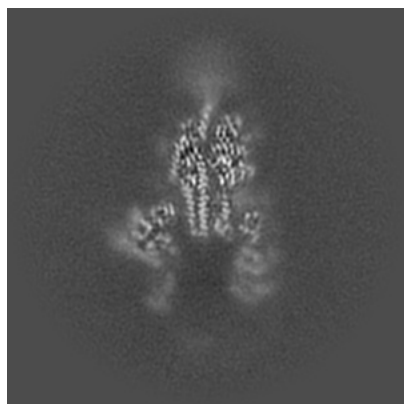


Z Index: 160

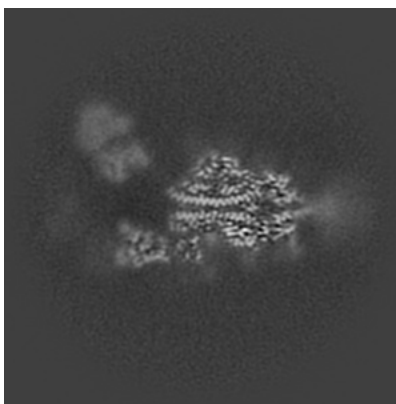
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

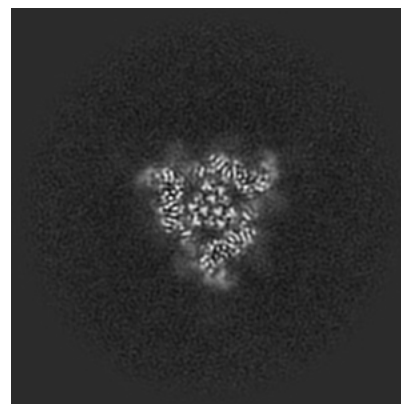
6.3.1 Primary map



X Index: 166



Y Index: 156

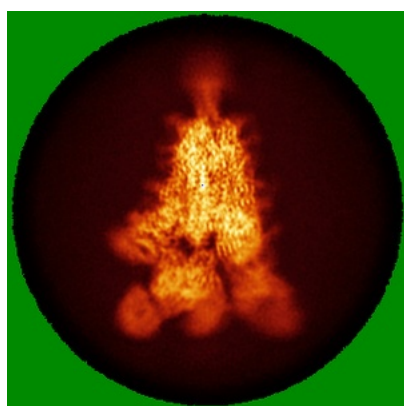


Z Index: 154

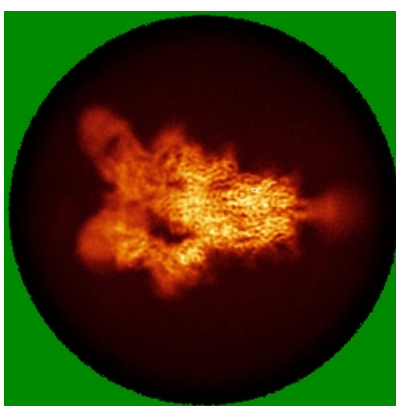
The images above show the largest variance slices of the map in three orthogonal directions.

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

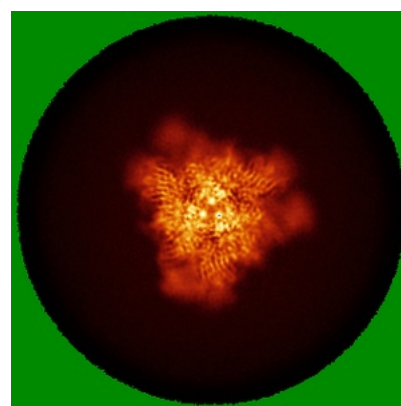
6.4.1 Primary map



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

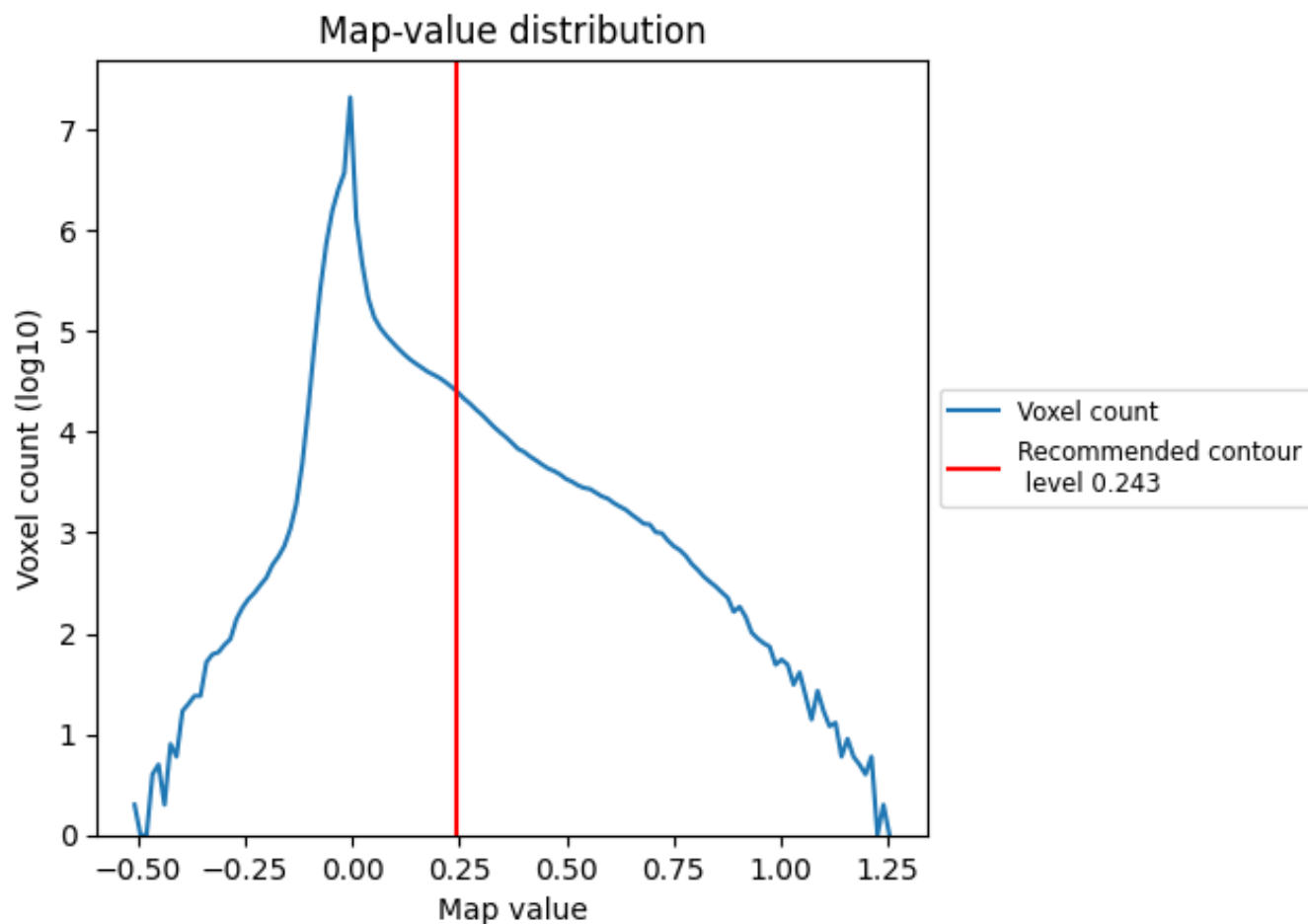
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

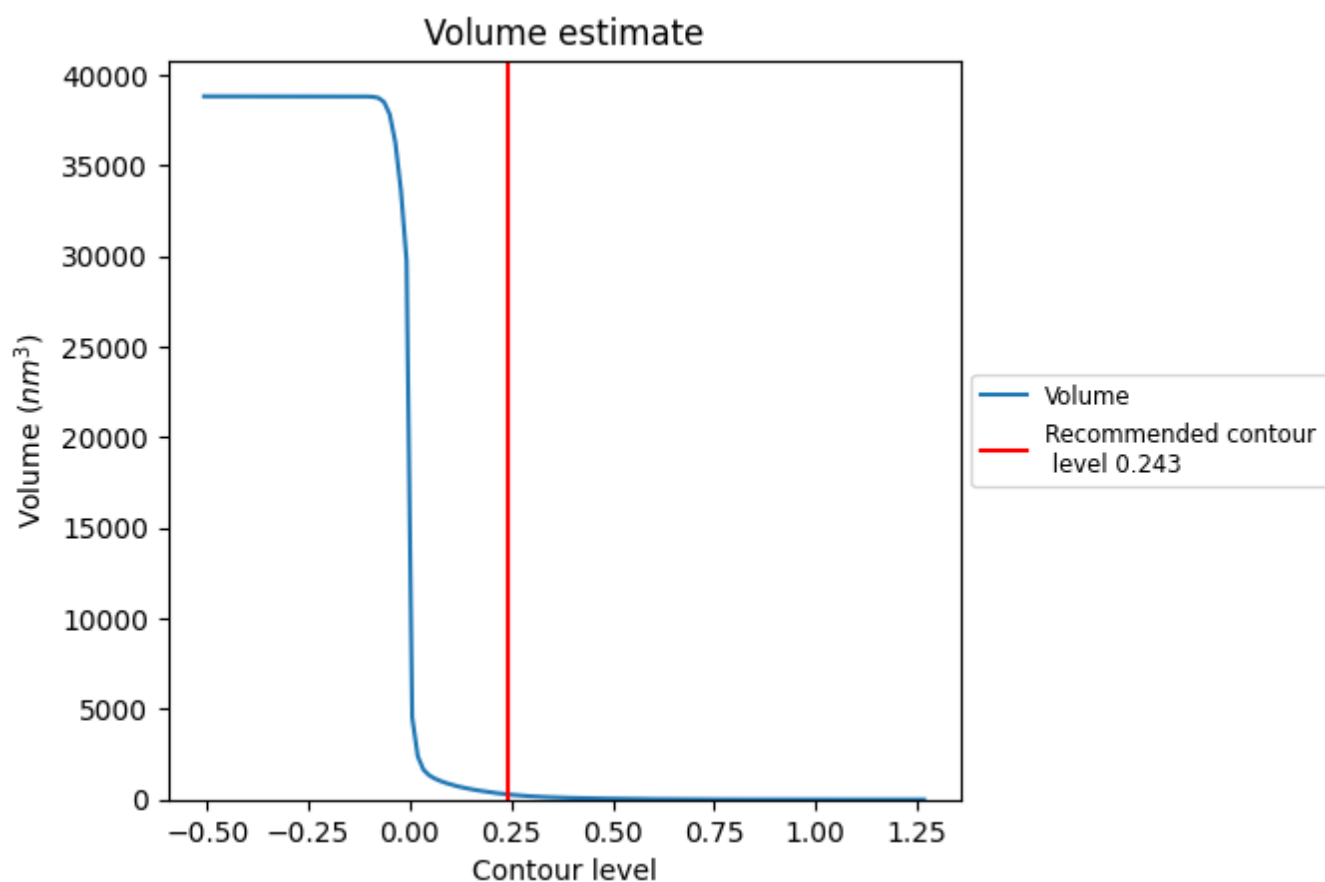
This section contains the results of statistical analysis of the map.

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.

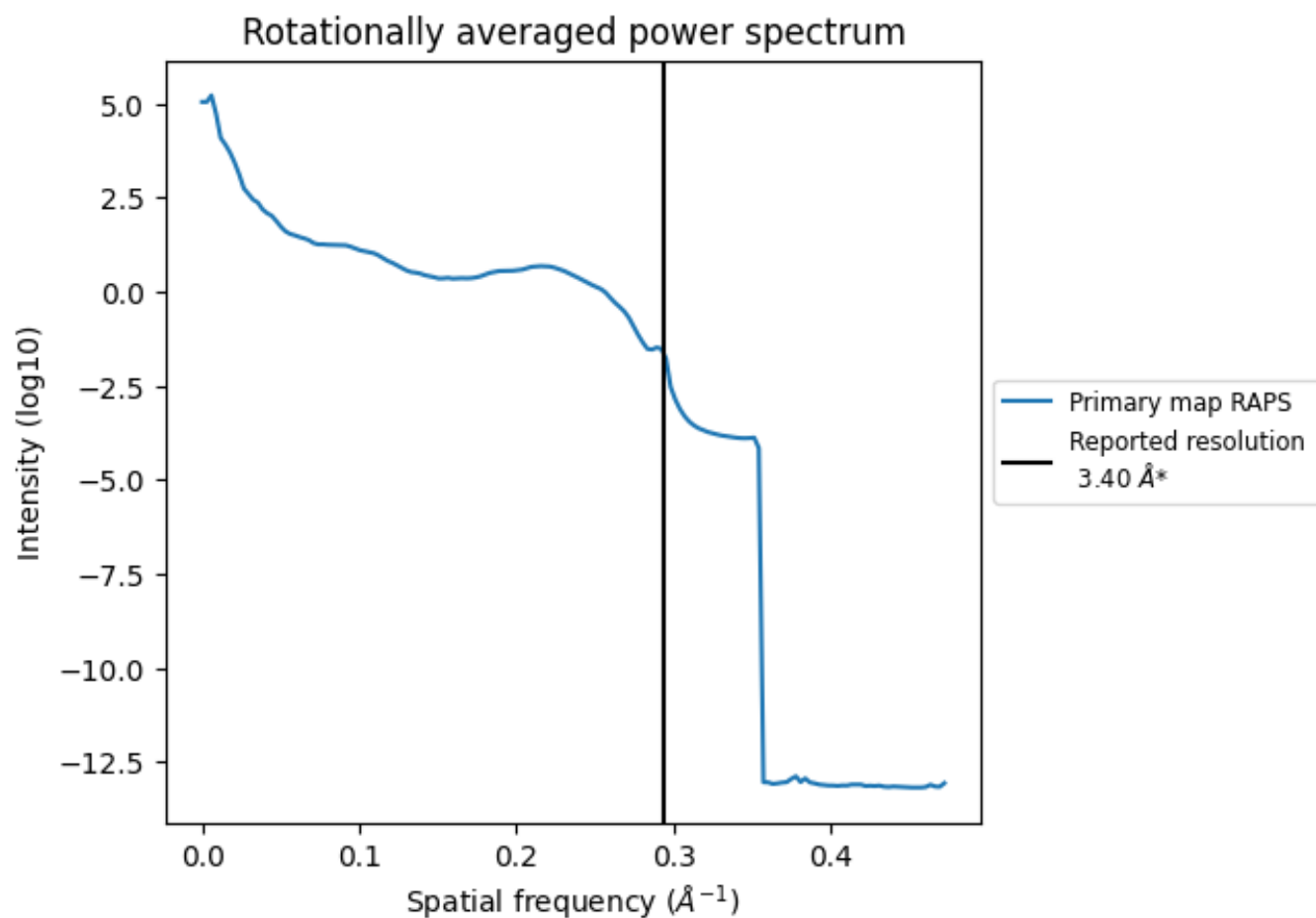
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 253 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 0.294 Å⁻¹

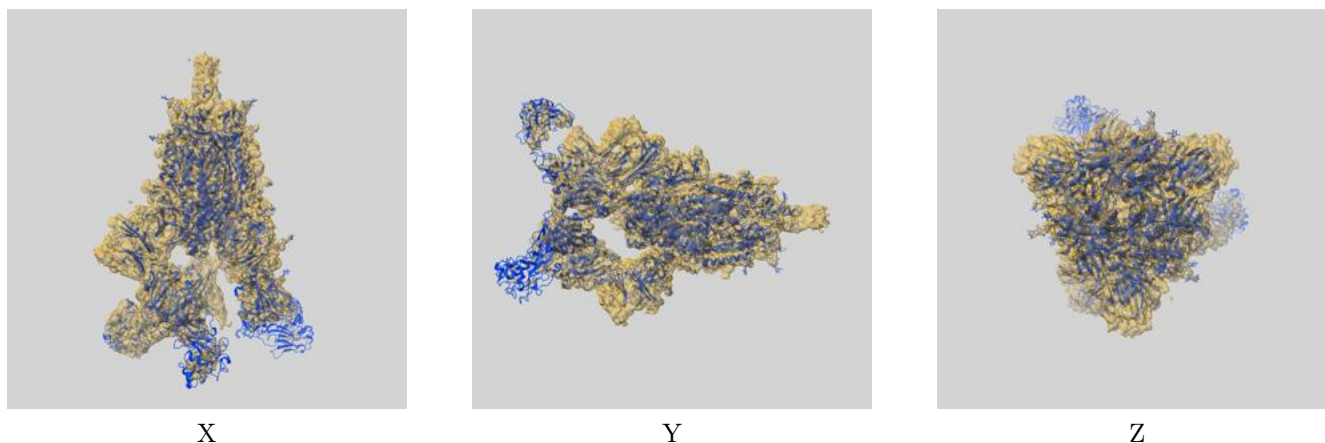
8 Fourier-Shell correlation ⓘ

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-23279 and PDB model 7LD1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



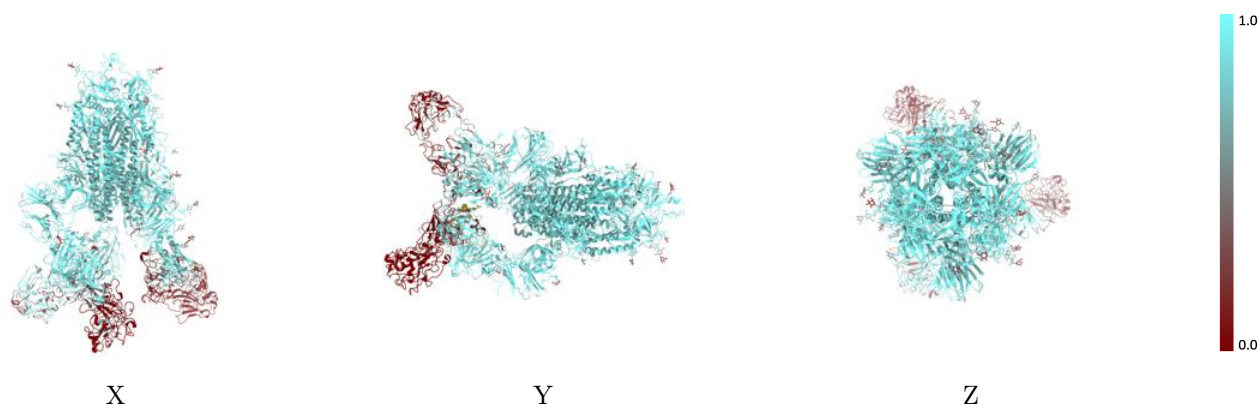
The images above show the 3D surface view of the map at the recommended contour level 0.243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



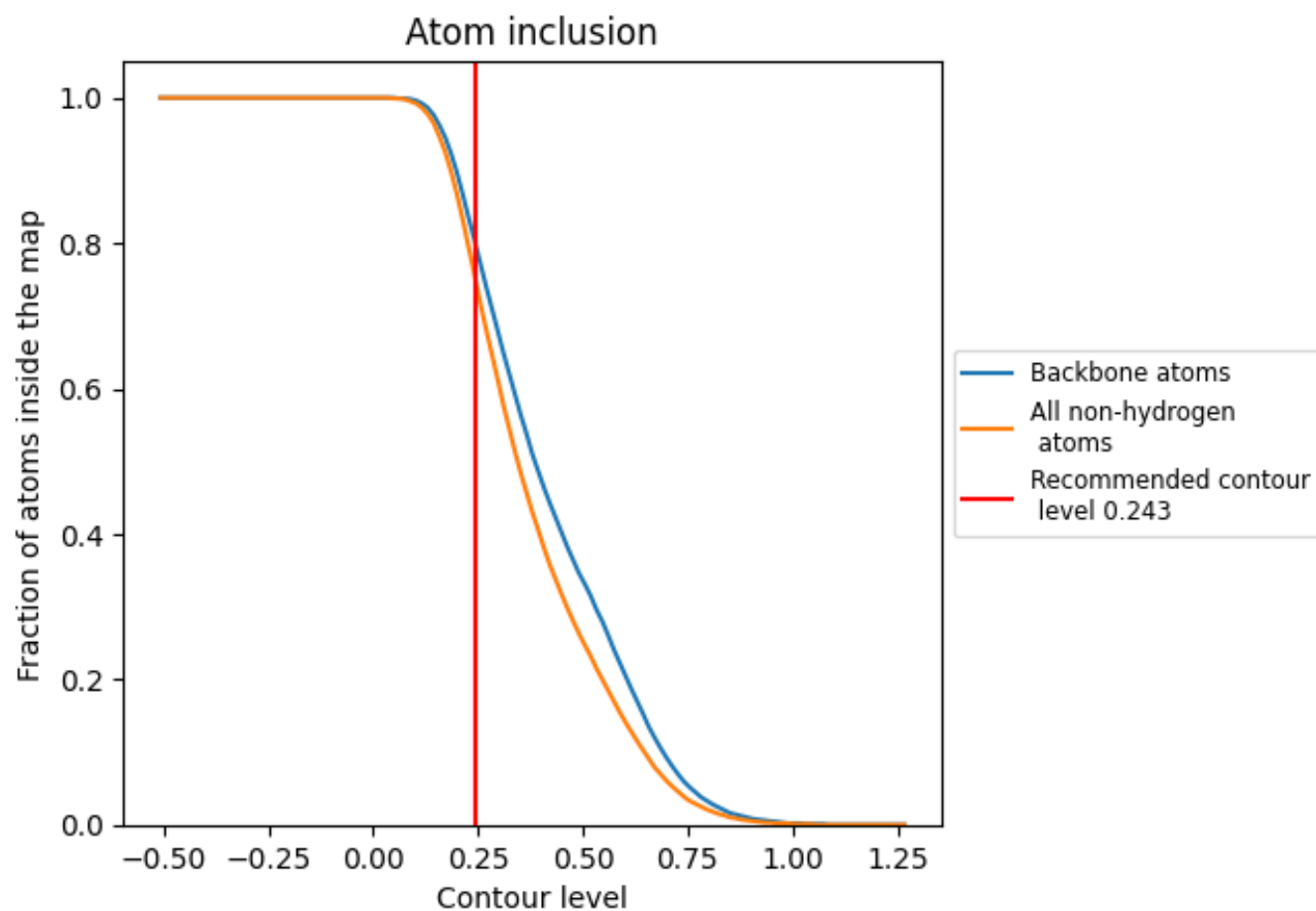
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.243).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.3720
A	 0.8480	 0.4190
B	 0.8650	 0.4170
C	 0.8900	 0.4340
D	 0.6920	 0.4100
E	 0.5360	 0.2830
F	 0.6410	 0.4130
G	 0.2310	 0.3150
H	 0.4750	 0.2370
I	 0.6150	 0.4130
J	 0.5640	 0.3900
K	 0.5900	 0.4080
L	 0.2870	 0.1930
M	 0.7780	 0.3190
N	 0.7010	 0.2640
O	 0.0930	 0.1450
P	 0.2880	 0.1740
Q	 0.2860	 0.2390
R	 0.5130	 0.3540
S	 0.3850	 0.3680
T	 0.5900	 0.3920
U	 0.7440	 0.4820
V	 0.4870	 0.3930
W	 0.5130	 0.3740
X	 0.6150	 0.4380

