



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 06:50 PM JST

PDB ID : 7WBH
EMDB ID : EMD-32398
Title : overall structure of hu33 and spike
Authors : Pulan, L.
Deposited on : 2021-12-16
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

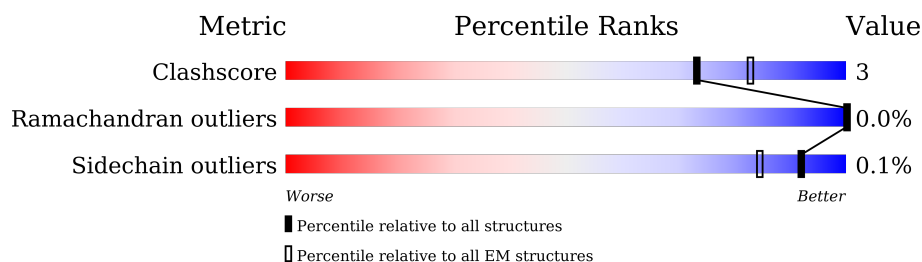
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1120	
2	B	1120	
2	C	1120	
3	O	118	
3	P	118	
3	U	118	
4	Q	107	
4	S	107	

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Mol	Chain	Length	Quality of chain
4	V	107	
5	D	3	
5	E	3	
5	F	3	
6	G	2	
6	H	2	
6	I	2	
6	J	2	
6	K	2	
6	L	2	
6	M	2	
6	N	2	
6	R	2	
6	T	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 29187 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	1006	Total	C	N	O	S	0	0
			7761	4956	1292	1478	35		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	HIS	GLY	conflict	UNP P0DTC2
A	155	GLY	SER	conflict	UNP P0DTC2
A	215	GLY	ASP	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	701	VAL	ALA	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1000	Total	C	N	O	S	0	0
			7732	4938	1283	1476	35		
2	C	1000	Total	C	N	O	S	0	0
			7677	4903	1270	1469	35		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	ALA	ASP	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	215	GLY	ASP	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	701	VAL	ALA	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	80	ALA	ASP	conflict	UNP P0DTC2
C	215	GLY	ASP	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	701	VAL	ALA	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 3 is a protein called heavy chain of hu33.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	118	Total	C	N	O	S	0	0
			928	594	151	178	5		
3	O	118	Total	C	N	O	S	0	0
			928	594	151	178	5		
3	P	118	Total	C	N	O	S	0	0
			928	594	151	178	5		

- Molecule 4 is a protein called light chain of hu33.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	107	Total	C	N	O	S	0	0
			824	520	137	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	107	Total	C	N	O	S	0	0
			824	520	137	164	3		
4	S	107	Total	C	N	O	S	0	0
			824	520	137	164	3		

- Molecule 5 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
5	D	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

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



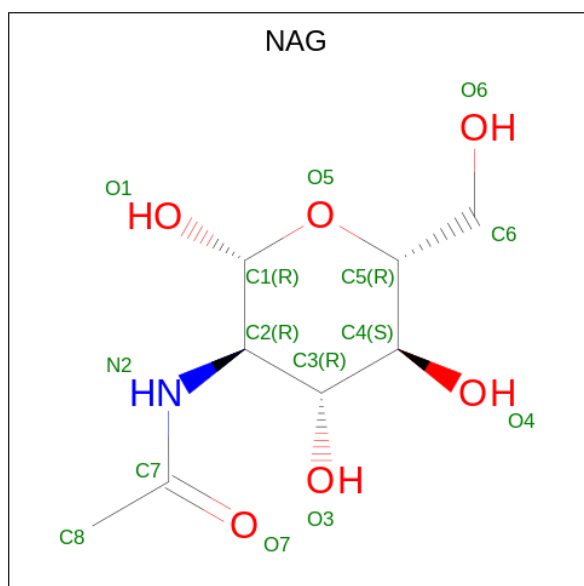
Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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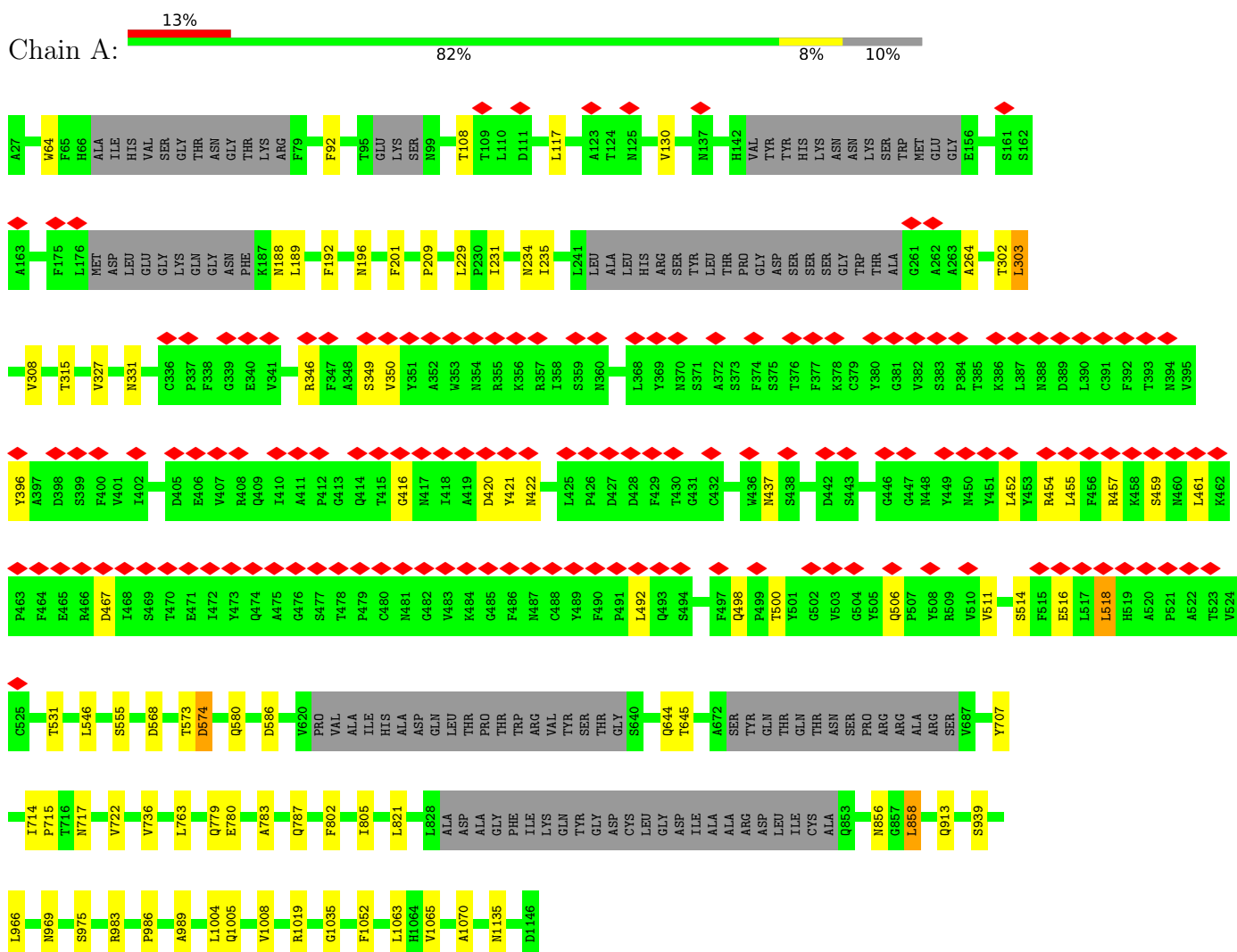
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Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	

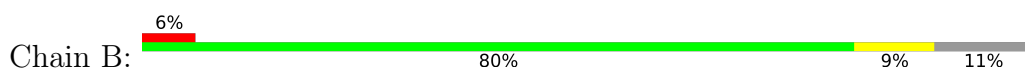
3 Residue-property plots

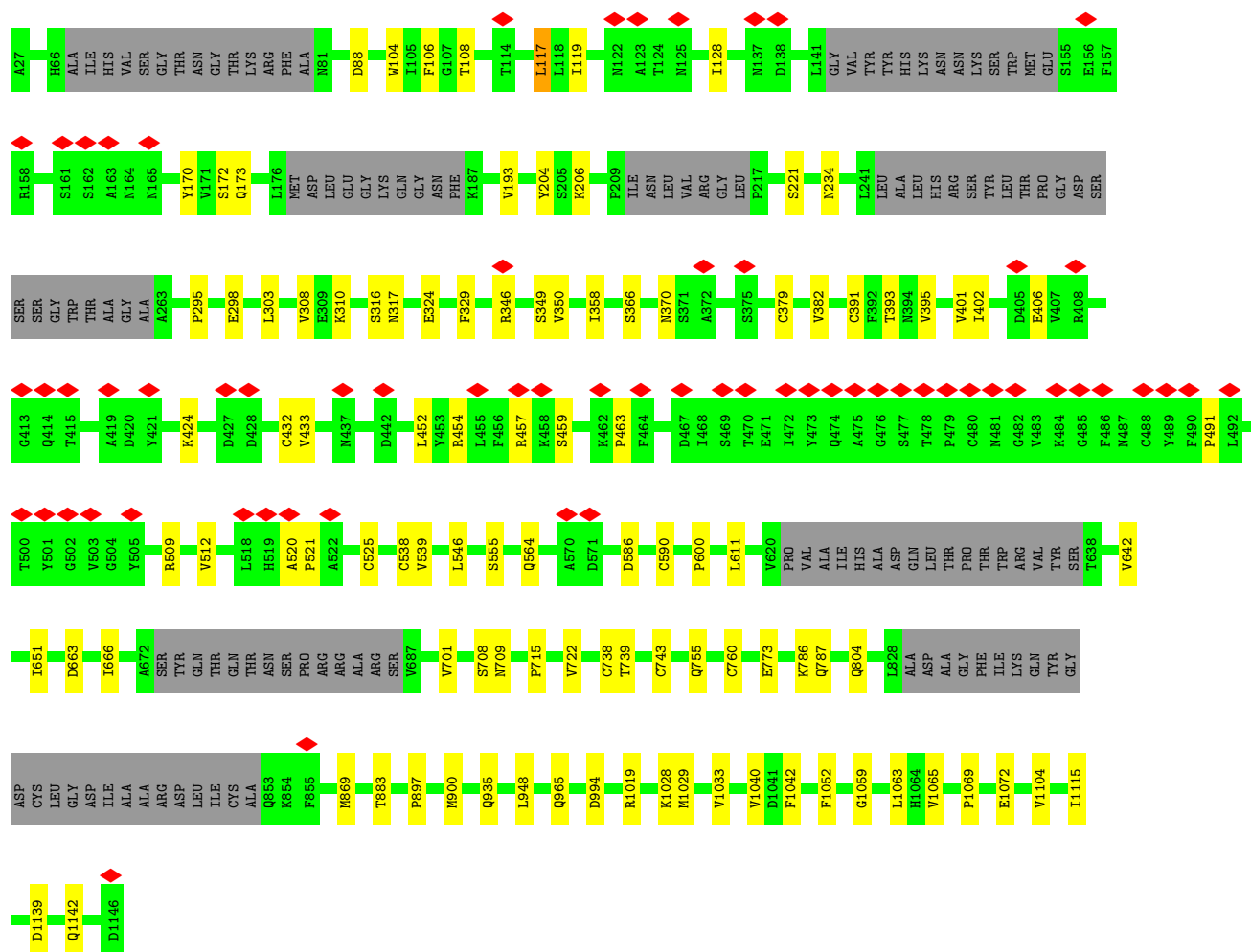
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

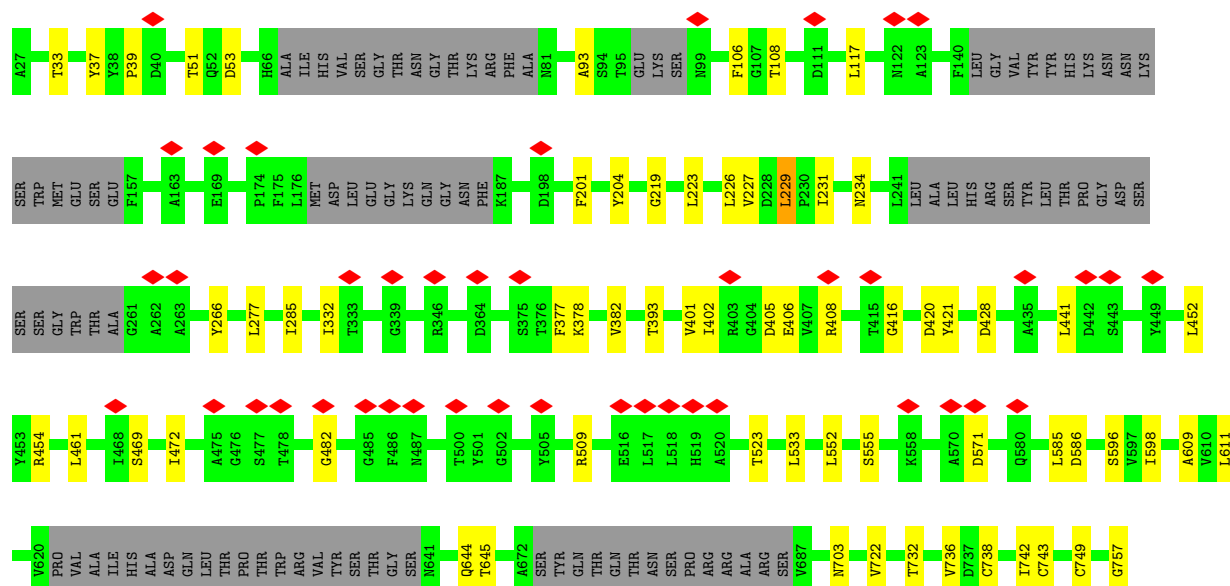
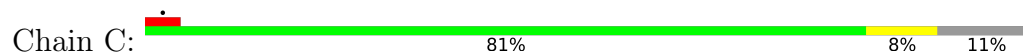


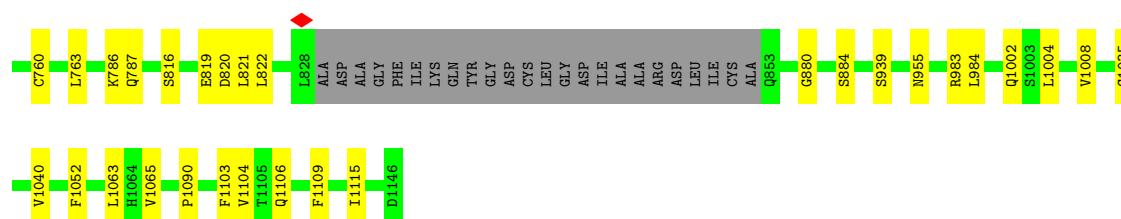
• Molecule 2: Spike glycoprotein



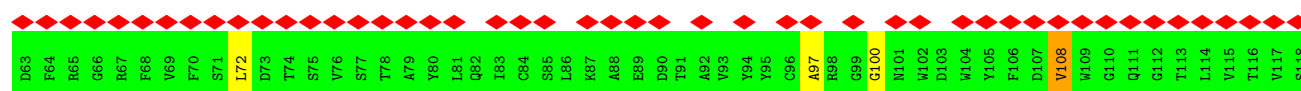
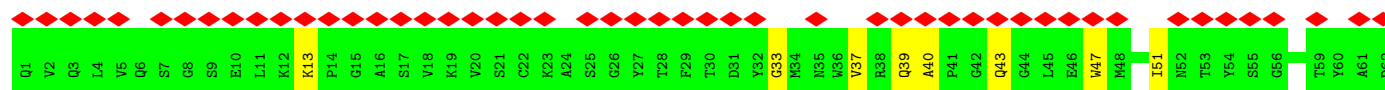
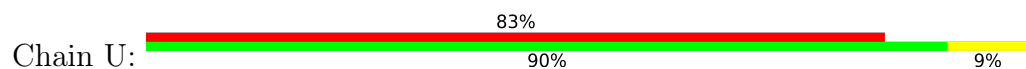


• Molecule 2: Spike glycoprotein

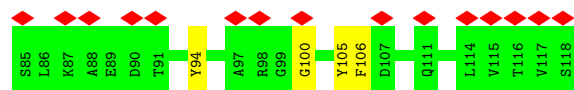
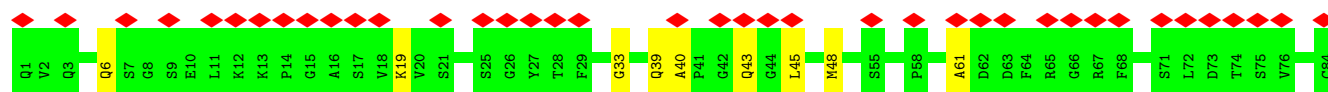
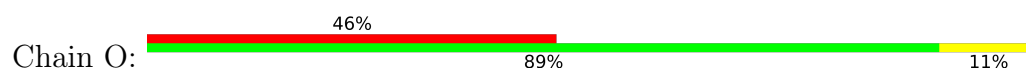




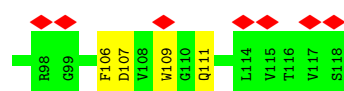
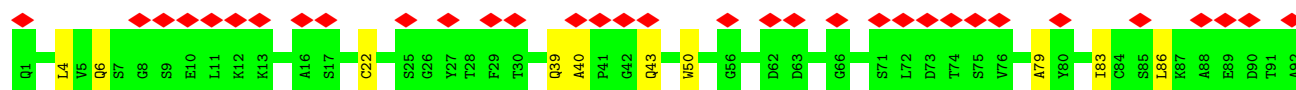
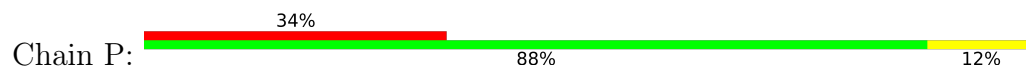
• Molecule 3: heavy chain of hu33



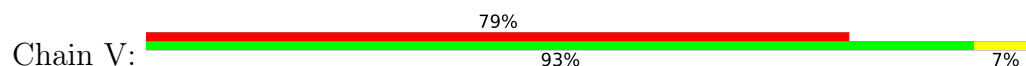
• Molecule 3: heavy chain of hu33

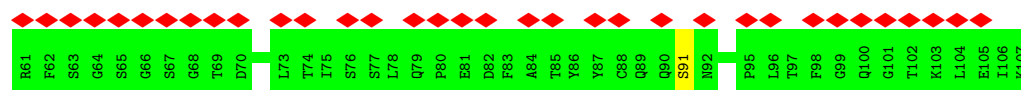


• Molecule 3: heavy chain of hu33

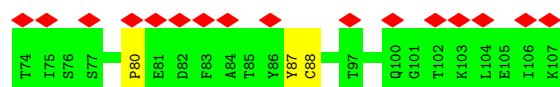
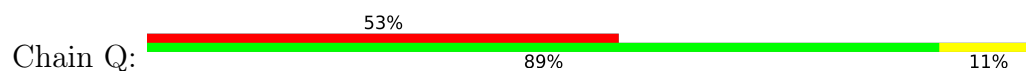


• Molecule 4: light chain of hu33

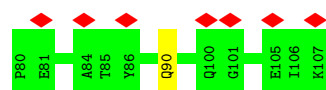
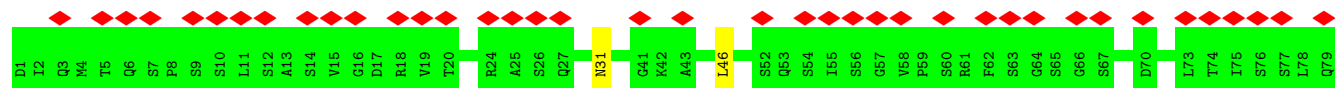
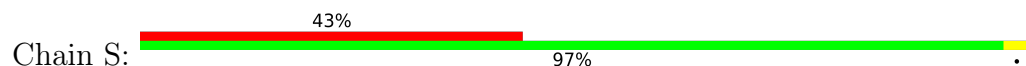




- Molecule 4: light chain of hu33



- Molecule 4: light chain of hu33



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



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



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  100%



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

Chain J:  50% 100%



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

Chain K:  50% 100%



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

Chain L:  100%



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	222776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.657	Depositor
Minimum map value	-0.780	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.177	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/7936	0.64	7/10811 (0.1%)
2	B	0.32	0/7907	0.63	5/10768 (0.0%)
2	C	0.33	0/7851	0.64	5/10703 (0.0%)
3	O	0.33	0/955	0.72	0/1300
3	P	0.36	0/955	0.73	1/1300 (0.1%)
3	U	0.30	0/955	0.64	1/1300 (0.1%)
4	Q	0.31	0/844	0.69	0/1146
4	S	0.32	0/844	0.70	1/1146 (0.1%)
4	V	0.30	0/844	0.70	1/1146 (0.1%)
All	All	0.32	0/29091	0.65	21/39620 (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
2	C	0	2
3	O	0	1
3	P	0	1
4	Q	0	1
All	All	0	5

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	LEU	CA-CB-CG	8.76	135.44	115.30
3	P	107	ASP	CB-CG-OD1	7.73	125.25	118.30
2	B	663	ASP	CB-CG-OD1	6.58	124.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	378	LYS	CA-CB-CG	6.40	127.48	113.40
4	V	23	CYS	CA-CB-SG	6.21	125.18	114.00
2	B	546	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	511	VAL	CG1-CB-CG2	-5.76	101.68	110.90
2	B	117	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	869	MET	CA-CB-CG	5.54	122.71	113.30
2	C	452	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	303	LEU	CA-CB-CG	5.47	127.88	115.30
2	B	994	ASP	CB-CG-OD1	5.34	123.11	118.30
2	C	749	CYS	CA-CB-SG	5.27	123.49	114.00
1	A	189	LEU	CA-CB-CG	5.26	127.40	115.30
3	U	108	VAL	CG1-CB-CG2	-5.14	102.67	110.90
2	C	743	CYS	CA-CB-SG	5.14	123.25	114.00
1	A	117	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	858	LEU	CA-CB-CG	5.04	126.90	115.30
4	S	46	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	574	ASP	CB-CG-OD1	5.03	122.83	118.30
2	C	229	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	377	PHE	Peptide
2	C	742	ILE	Peptide
3	O	106	PHE	Peptide
3	P	106	PHE	Peptide
4	Q	29	VAL	Peptide

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	7761	0	7509	49	0
2	B	7732	0	7493	56	0
2	C	7677	0	7381	53	0
3	O	928	0	869	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	928	0	869	7	0
3	U	928	0	869	7	0
4	Q	824	0	801	7	0
4	S	824	0	801	0	0
4	V	824	0	801	5	0
5	D	39	0	34	1	0
5	E	39	0	34	1	0
5	F	39	0	34	1	0
6	G	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	R	28	0	25	0	0
6	T	28	0	25	0	0
7	A	84	0	78	0	0
7	B	154	0	143	0	0
7	C	112	0	104	1	0
7	S	14	0	13	0	0
All	All	29187	0	28083	177	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 (177) 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:B:739:THR:O	2:B:743:CYS:HB3	1.84	0.77
1:A:568:ASP:HB2	1:A:574:ASP:HB2	1.80	0.64
3:O:33:GLY:H	3:O:100:GLY:HA2	1.62	0.64
2:B:555:SER:HB3	2:B:586:ASP:HB2	1.81	0.62
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.81	0.61
2:C:106:PHE:HB2	2:C:117:LEU:HB2	1.83	0.60
3:U:40:ALA:HB3	3:U:43:GLN:HB2	1.85	0.58
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.86	0.57
4:V:32:PHE:HB3	4:V:91:SER:HB3	1.86	0.57
3:O:40:ALA:HB3	3:O:43:GLN:HB2	1.87	0.56
3:U:33:GLY:H	3:U:100:GLY:HA2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLU:HG2	1:A:518:LEU:H	1.71	0.56
3:O:6:GLN:NE2	3:O:94:TYR:O	2.38	0.56
2:B:106:PHE:HB2	2:B:117:LEU:HB3	1.87	0.56
2:C:763:LEU:HB3	2:C:1008:VAL:HG21	1.88	0.55
4:V:37:GLN:HB2	4:V:47:LEU:HD11	1.89	0.55
2:B:433:VAL:HA	2:B:512:VAL:HG12	1.89	0.55
2:B:642:VAL:HG22	2:B:651:ILE:HG12	1.88	0.55
4:Q:33:LEU:HD11	4:Q:88:CYS:HB2	1.89	0.55
1:A:983:ARG:HD2	2:C:382:VAL:HG22	1.89	0.54
2:C:201:PHE:HB3	2:C:229:LEU:HB2	1.90	0.54
4:Q:6:GLN:NE2	4:Q:88:CYS:SG	2.81	0.54
3:P:40:ALA:HB3	3:P:43:GLN:HB2	1.89	0.54
2:C:454:ARG:NH2	2:C:469:SER:O	2.41	0.53
2:C:226:LEU:HD23	2:C:227:VAL:HG23	1.91	0.53
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.91	0.53
2:C:416:GLY:O	2:C:420:ASP:HB2	2.08	0.53
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.90	0.53
4:Q:36:TYR:HB2	4:Q:87:TYR:HB2	1.90	0.53
2:B:382:VAL:HG22	2:C:983:ARG:HD2	1.91	0.52
3:P:6:GLN:H	3:P:111:GLN:HE22	1.57	0.52
2:B:172:SER:OG	2:B:173:GLN:N	2.42	0.52
2:B:206:LYS:HD3	2:B:221:SER:HB2	1.90	0.52
1:A:707:TYR:HB2	2:B:883:THR:HG23	1.92	0.52
2:B:804:GLN:NE2	2:B:935:GLN:OE1	2.43	0.52
2:B:382:VAL:HG13	2:C:983:ARG:HB2	1.92	0.51
2:B:128:ILE:HB	2:B:170:TYR:HB3	1.92	0.51
1:A:346:ARG:NH2	4:V:50:TYR:OH	2.43	0.51
1:A:349:SER:OG	1:A:350:VAL:N	2.43	0.51
1:A:1035:GLY:HA3	2:C:1040:VAL:HG21	1.92	0.51
2:C:732:THR:OG1	2:C:955:ASN:ND2	2.43	0.51
1:A:130:VAL:HG21	1:A:231:ILE:HG12	1.92	0.51
2:C:598:ILE:HB	2:C:609:ALA:HB3	1.93	0.51
2:C:229:LEU:HB3	2:C:231:ILE:HG12	1.91	0.51
2:B:786:LYS:HG3	2:B:787:GLN:HG3	1.92	0.51
1:A:913:GLN:NE2	2:C:1090:PRO:O	2.44	0.50
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.93	0.50
2:B:1029:MET:O	2:B:1033:VAL:HB	2.12	0.50
2:C:204:TYR:HB3	2:C:223:LEU:HB3	1.93	0.50
1:A:736:VAL:HG21	1:A:1004:LEU:HD11	1.93	0.50
2:B:391:CYS:HA	2:B:525:CYS:HB3	1.94	0.50
2:B:193:VAL:HB	2:B:204:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:THR:HB	2:B:520:ALA:HB3	1.93	0.50
1:A:1005:GLN:OE1	2:C:1002:GLN:NE2	2.45	0.49
1:A:856:ASN:HD22	1:A:966:LEU:HD11	1.76	0.49
2:B:358:ILE:HB	2:B:395:VAL:HB	1.93	0.49
2:B:346:ARG:NH2	4:Q:50:TYR:OH	2.46	0.48
2:B:329:PHE:HE1	2:B:391:CYS:HB2	1.77	0.48
1:A:717:ASN:HB3	1:A:1070:ALA:HB3	1.95	0.48
2:C:1104:VAL:HG23	2:C:1115:ILE:HG12	1.94	0.48
2:B:715:PRO:HG3	2:B:1069:PRO:HB3	1.94	0.48
2:B:1028:LYS:NZ	2:B:1042:PHE:O	2.43	0.48
1:A:331:ASN:HB2	1:A:580:GLN:HG2	1.96	0.48
1:A:452:LEU:HD11	1:A:492:LEU:HB3	1.96	0.48
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	1.96	0.48
2:C:533:LEU:HD11	2:C:585:LEU:HD11	1.96	0.48
2:C:786:LYS:HG3	2:C:787:GLN:HG3	1.96	0.48
3:U:37:VAL:HG12	3:U:47:TRP:HA	1.96	0.47
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.79	0.47
2:B:738:CYS:HB3	2:B:760:CYS:HB3	1.73	0.47
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.79	0.47
2:B:897:PRO:HB2	2:B:900:MET:HG3	1.97	0.47
2:B:310:LYS:HG3	2:B:600:PRO:HA	1.96	0.47
2:C:555:SER:HB3	2:C:586:ASP:HB2	1.97	0.47
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.97	0.47
2:B:1139:ASP:HB3	2:B:1142:GLN:HG2	1.97	0.47
2:B:104:TRP:H	2:B:119:ILE:HB	1.80	0.47
3:P:83:ILE:HD12	3:P:86:LEU:HD13	1.95	0.47
1:A:302:THR:HG21	1:A:315:THR:HA	1.98	0.46
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.43	0.46
2:C:33:THR:OG1	2:C:219:GLY:O	2.33	0.46
2:B:349:SER:OG	2:B:350:VAL:N	2.47	0.46
2:B:1052:PHE:HB2	2:B:1063:LEU:HB2	1.97	0.46
2:C:472:ILE:HD11	2:C:482:GLY:H	1.80	0.46
1:A:188:ASN:HA	1:A:209:PRO:HA	1.97	0.46
2:C:821:LEU:HD11	2:C:939:SER:HB2	1.98	0.46
1:A:969:ASN:HB2	2:B:755:GLN:HB2	1.96	0.46
2:B:349:SER:OG	2:B:452:LEU:O	2.33	0.46
5:D:1:NAG:H4	5:D:2:NAG:H2	1.73	0.46
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.98	0.46
1:A:821:LEU:HD11	1:A:939:SER:HB2	1.98	0.46
2:B:457:ARG:HG3	2:B:459:SER:H	1.81	0.46
2:C:405:ASP:O	2:C:408:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:880:GLY:O	2:C:884:SER:OG	2.31	0.45
2:B:708:SER:OG	2:B:709:ASN:N	2.48	0.45
2:C:1052:PHE:HB2	2:C:1063:LEU:HB2	1.98	0.45
2:C:816:SER:O	2:C:820:ASP:HB2	2.16	0.45
3:U:51:ILE:HD12	3:U:72:LEU:HD12	1.98	0.45
5:E:1:NAG:H4	5:E:2:NAG:H2	1.68	0.45
2:C:39:PRO:HG3	2:C:51:THR:HG21	1.99	0.45
2:B:379:CYS:HA	2:B:432:CYS:HA	1.98	0.45
2:B:965:GLN:HE22	2:C:757:GLY:HA3	1.82	0.45
2:B:303:LEU:HD22	2:B:308:VAL:HG12	1.99	0.45
2:C:644:GLN:NE2	2:C:645:THR:O	2.41	0.44
2:C:738:CYS:HB2	2:C:760:CYS:HB2	1.77	0.44
2:B:424:LYS:HG3	2:B:463:PRO:HG3	1.98	0.44
2:B:948:LEU:HD21	2:B:1059:GLY:HA3	2.00	0.44
2:C:421:TYR:HA	2:C:461:LEU:HD13	2.00	0.44
1:A:108:THR:OG1	1:A:234:ASN:O	2.33	0.44
2:B:108:THR:OG1	2:B:234:ASN:O	2.36	0.44
2:C:1106:GLN:HE21	2:C:1109:PHE:HB3	1.82	0.44
1:A:644:GLN:NE2	1:A:645:THR:O	2.44	0.44
1:A:763:LEU:HB3	1:A:1008:VAL:HG21	2.00	0.44
2:B:1040:VAL:HG21	2:C:1035:GLY:HA3	2.01	0.43
2:C:736:VAL:HG11	2:C:1004:LEU:HD11	1.99	0.43
2:B:295:PRO:HA	2:B:298:GLU:HB2	2.00	0.43
2:C:819:GLU:HA	2:C:822:LEU:HD12	2.00	0.43
3:P:22:CYS:HB3	3:P:79:ALA:HB3	2.00	0.43
2:B:701:VAL:HG23	2:C:787:GLN:HG2	2.00	0.43
3:O:39:GLN:HE22	3:O:45:LEU:HD23	1.84	0.43
1:A:546:LEU:HD21	1:A:573:THR:HG21	2.01	0.43
2:B:715:PRO:HA	2:B:1072:GLU:HA	2.00	0.43
2:C:401:VAL:HG22	2:C:509:ARG:HG2	1.99	0.43
1:A:92:PHE:HB3	1:A:192:PHE:HB2	2.00	0.43
2:B:1104:VAL:HG23	2:B:1115:ILE:HG12	2.01	0.43
2:C:428:ASP:OD1	2:C:428:ASP:N	2.51	0.43
2:C:983:ARG:HG3	2:C:984:LEU:HD12	2.01	0.43
2:B:454:ARG:HG3	2:B:491:PRO:HB2	2.01	0.42
2:C:402:ILE:HD12	2:C:406:GLU:HB2	2.01	0.42
2:B:521:PRO:HA	2:B:564:GLN:HE22	1.83	0.42
1:A:780:GLU:OE1	1:A:1019:ARG:NH2	2.52	0.42
2:B:773:GLU:OE1	2:B:1019:ARG:NH1	2.52	0.42
3:O:48:MET:O	3:O:61:ALA:N	2.52	0.42
2:C:596:SER:HB3	2:C:611:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:PHE:HZ	7:C:1307:NAG:H62	1.84	0.42
1:A:498:GLN:HG3	1:A:500:THR:H	1.84	0.42
2:C:108:THR:OG1	2:C:234:ASN:O	2.38	0.42
3:P:4:LEU:H	3:P:109:TRP:HD1	1.67	0.42
1:A:779:GLN:O	1:A:783:ALA:HB3	2.20	0.42
2:B:316:SER:OG	2:B:317:ASN:N	2.52	0.42
2:B:402:ILE:HD12	2:B:406:GLU:HB2	2.01	0.42
2:C:277:LEU:HD23	2:C:285:ILE:HD13	2.01	0.42
3:U:39:GLN:NE2	3:U:40:ALA:O	2.53	0.42
3:P:39:GLN:NE2	3:P:40:ALA:O	2.52	0.42
1:A:303:LEU:HD13	1:A:308:VAL:HG12	2.01	0.42
2:B:88:ASP:OD2	2:B:88:ASP:N	2.53	0.42
2:C:93:ALA:HB3	2:C:266:TYR:HB2	2.01	0.41
2:C:552:LEU:HD13	2:C:585:LEU:HD13	2.02	0.41
1:A:457:ARG:HG3	1:A:459:SER:H	1.84	0.41
2:B:366:SER:O	2:B:370:ASN:HB2	2.20	0.41
1:A:327:VAL:H	1:A:531:THR:HB	1.85	0.41
1:A:736:VAL:HA	1:A:858:LEU:HA	2.03	0.41
2:C:441:LEU:HD23	3:P:50:TRP:HZ2	1.85	0.41
4:V:46:LEU:HD11	4:V:49:TYR:HB3	2.02	0.41
3:O:19:LYS:HB2	3:O:19:LYS:HE2	1.92	0.41
3:O:105:TYR:HB2	4:Q:46:LEU:HD11	2.03	0.41
2:C:393:THR:O	2:C:523:THR:OG1	2.37	0.41
1:A:416:GLY:O	1:A:420:ASP:HB2	2.20	0.41
1:A:421:TYR:HA	1:A:461:LEU:HD23	2.01	0.41
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.95	0.41
1:A:714:ILE:HA	1:A:715:PRO:HD3	1.95	0.41
2:C:37:TYR:OH	2:C:53:ASP:OD2	2.39	0.41
5:F:1:NAG:H4	5:F:2:NAG:H2	1.84	0.41
1:A:350:VAL:HG11	1:A:422:ASN:HD21	1.85	0.41
2:B:324:GLU:HB3	2:B:539:VAL:HG12	2.03	0.41
3:U:97:ALA:HB2	3:U:108:VAL:HG12	2.02	0.41
1:A:986:PRO:HA	1:A:989:ALA:HB3	2.02	0.40
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.85	0.40
3:U:13:LYS:HA	3:U:13:LYS:HD3	1.89	0.40
4:Q:15:VAL:HG22	4:Q:80:PRO:HG3	2.03	0.40
4:Q:39:LYS:HE2	4:Q:42:LYS:HD3	2.02	0.40
1:A:454:ARG:NH2	1:A:467:ASP:OD1	2.55	0.40
1:A:787:GLN:OE1	2:C:703:ASN:ND2	2.46	0.40
1:A:975:SER:OG	2:C:571:ASP:OD2	2.39	0.40
2:B:538:CYS:HB2	2:B:590:CYS:HB3	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:LEU:HD22	2:B:666:ILE:HG23	2.03	0.40
4:V:46:LEU:HD21	4:V:49:TYR:HB3	2.02	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	988/1120 (88%)	938 (95%)	50 (5%)	0	100	100
2	B	982/1120 (88%)	938 (96%)	44 (4%)	0	100	100
2	C	982/1120 (88%)	938 (96%)	43 (4%)	1 (0%)	48	78
3	O	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
3	P	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	U	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
4	Q	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
4	S	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
4	V	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
All	All	3615/4035 (90%)	3421 (95%)	193 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	332	ILE

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	857/973 (88%)	856 (100%)	1 (0%)	92	96
2	B	858/972 (88%)	858 (100%)	0	100	100
2	C	844/972 (87%)	844 (100%)	0	100	100
3	O	97/97 (100%)	97 (100%)	0	100	100
3	P	97/97 (100%)	97 (100%)	0	100	100
3	U	97/97 (100%)	97 (100%)	0	100	100
4	Q	94/94 (100%)	94 (100%)	0	100	100
4	S	94/94 (100%)	92 (98%)	2 (2%)	48	67
4	V	94/94 (100%)	94 (100%)	0	100	100
All	All	3132/3490 (90%)	3129 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1135	ASN
4	S	31	ASN
4	S	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	804	GLN
2	C	955	ASN
2	C	1011	GLN
4	S	90	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 ⓘ

29 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	D	1	1,5	14,14,15	0.62	0	17,19,21	1.37	2 (11%)
5	NAG	D	2	5	14,14,15	0.89	1 (7%)	17,19,21	0.75	1 (5%)
5	BMA	D	3	5	11,11,12	1.08	1 (9%)	15,15,17	1.02	1 (6%)
5	NAG	E	1	5,2	14,14,15	0.75	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	E	2	5	14,14,15	0.90	1 (7%)	17,19,21	0.76	1 (5%)
5	BMA	E	3	5	11,11,12	1.07	1 (9%)	15,15,17	1.08	1 (6%)
5	NAG	F	1	5,2	14,14,15	0.69	1 (7%)	17,19,21	1.34	1 (5%)
5	NAG	F	2	5	14,14,15	0.92	1 (7%)	17,19,21	0.78	1 (5%)
5	BMA	F	3	5	11,11,12	1.04	0	15,15,17	1.03	1 (6%)
6	NAG	G	1	6	14,14,15	0.54	0	17,19,21	0.69	1 (5%)
6	NAG	G	2	6	14,14,15	1.21	1 (7%)	17,19,21	2.62	4 (23%)
6	NAG	H	1	6,1	14,14,15	0.48	0	17,19,21	0.65	1 (5%)
6	NAG	H	2	6	14,14,15	0.61	0	17,19,21	0.60	1 (5%)
6	NAG	I	1	6,1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
6	NAG	I	2	6	14,14,15	0.64	0	17,19,21	0.65	1 (5%)
6	NAG	J	1	6,1	14,14,15	0.76	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	J	2	6	14,14,15	0.68	1 (7%)	17,19,21	0.59	1 (5%)
6	NAG	K	1	6	14,14,15	0.96	1 (7%)	17,19,21	2.61	4 (23%)
6	NAG	K	2	6	14,14,15	1.10	1 (7%)	17,19,21	2.59	4 (23%)
6	NAG	L	1	6,2	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
6	NAG	L	2	6	14,14,15	0.63	0	17,19,21	0.64	1 (5%)
6	NAG	M	1	6,2	14,14,15	0.37	0	17,19,21	0.86	1 (5%)
6	NAG	M	2	6	14,14,15	0.58	0	17,19,21	0.70	1 (5%)
6	NAG	N	1	6,2	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
6	NAG	N	2	6	14,14,15	0.61	0	17,19,21	0.58	1 (5%)
6	NAG	R	1	6,2	14,14,15	0.33	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	R	2	6	14,14,15	0.63	0	17,19,21	0.56	0
6	NAG	T	1	6,2	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
6	NAG	T	2	6	14,14,15	0.60	0	17,19,21	0.66	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	D	2	5	-	4/6/23/26	0/1/1/1
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
6	NAG	G	1	6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	NAG	K	1	6	-	3/6/23/26	0/1/1/1
6	NAG	K	2	6	-	5/6/23/26	0/1/1/1
6	NAG	L	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	NAG	M	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	2	NAG	C1-C2	3.57	1.57	1.52
6	K	2	NAG	C1-C2	3.00	1.56	1.52
5	F	2	NAG	C1-C2	2.78	1.56	1.52
5	E	2	NAG	C1-C2	2.76	1.56	1.52
6	K	1	NAG	C1-C2	2.63	1.56	1.52
5	D	2	NAG	C1-C2	2.53	1.56	1.52
6	J	1	NAG	O5-C1	2.21	1.47	1.43
5	F	1	NAG	C1-C2	2.14	1.55	1.52
5	E	1	NAG	C1-C2	2.13	1.55	1.52
6	J	2	NAG	O5-C1	2.12	1.47	1.43
5	E	3	BMA	C1-C2	2.10	1.57	1.52
5	D	3	BMA	C2-C3	2.03	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C2-N2-C7	9.05	135.79	122.90
6	K	2	NAG	C2-N2-C7	8.99	135.70	122.90
6	G	2	NAG	C2-N2-C7	8.98	135.69	122.90
6	K	2	NAG	C1-C2-N2	4.34	117.90	110.49
6	K	1	NAG	C1-C2-N2	4.32	117.86	110.49
6	G	2	NAG	C1-C2-N2	4.29	117.81	110.49
5	D	1	NAG	C2-N2-C7	3.99	128.58	122.90
5	E	1	NAG	C2-N2-C7	3.94	128.52	122.90
5	F	1	NAG	C2-N2-C7	3.84	128.37	122.90
5	E	3	BMA	C1-O5-C5	3.11	116.41	112.19
6	I	1	NAG	C1-O5-C5	3.08	116.36	112.19
6	J	1	NAG	C1-O5-C5	3.00	116.26	112.19
5	F	3	BMA	C1-O5-C5	2.93	116.16	112.19
5	D	1	NAG	C1-O5-C5	2.75	115.92	112.19
6	G	2	NAG	C1-O5-C5	2.73	115.90	112.19
6	M	1	NAG	C1-O5-C5	2.67	115.81	112.19
5	D	3	BMA	C1-O5-C5	2.63	115.76	112.19
6	L	1	NAG	C1-O5-C5	2.61	115.73	112.19
6	R	1	NAG	C1-O5-C5	2.60	115.72	112.19
6	M	2	NAG	C1-O5-C5	2.52	115.60	112.19
6	T	1	NAG	C1-O5-C5	2.51	115.60	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	2	NAG	C8-C7-N2	2.50	120.34	116.10
6	N	1	NAG	C1-O5-C5	2.47	115.54	112.19
6	K	1	NAG	C8-C7-N2	2.47	120.27	116.10
6	K	2	NAG	C8-C7-N2	2.45	120.25	116.10
6	T	2	NAG	C1-O5-C5	2.44	115.49	112.19
5	F	2	NAG	C2-N2-C7	2.39	126.30	122.90
6	I	2	NAG	C1-O5-C5	2.37	115.41	112.19
6	L	2	NAG	C1-O5-C5	2.35	115.38	112.19
6	H	1	NAG	C1-O5-C5	2.28	115.28	112.19
5	D	2	NAG	C2-N2-C7	2.23	126.08	122.90
6	H	2	NAG	C1-O5-C5	2.17	115.13	112.19
5	E	2	NAG	C2-N2-C7	2.16	125.98	122.90
6	K	1	NAG	C1-O5-C5	2.14	115.09	112.19
6	J	2	NAG	C1-O5-C5	2.11	115.05	112.19
6	N	2	NAG	C1-O5-C5	2.06	114.99	112.19
6	K	2	NAG	C1-O5-C5	2.06	114.98	112.19
6	G	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C8-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2

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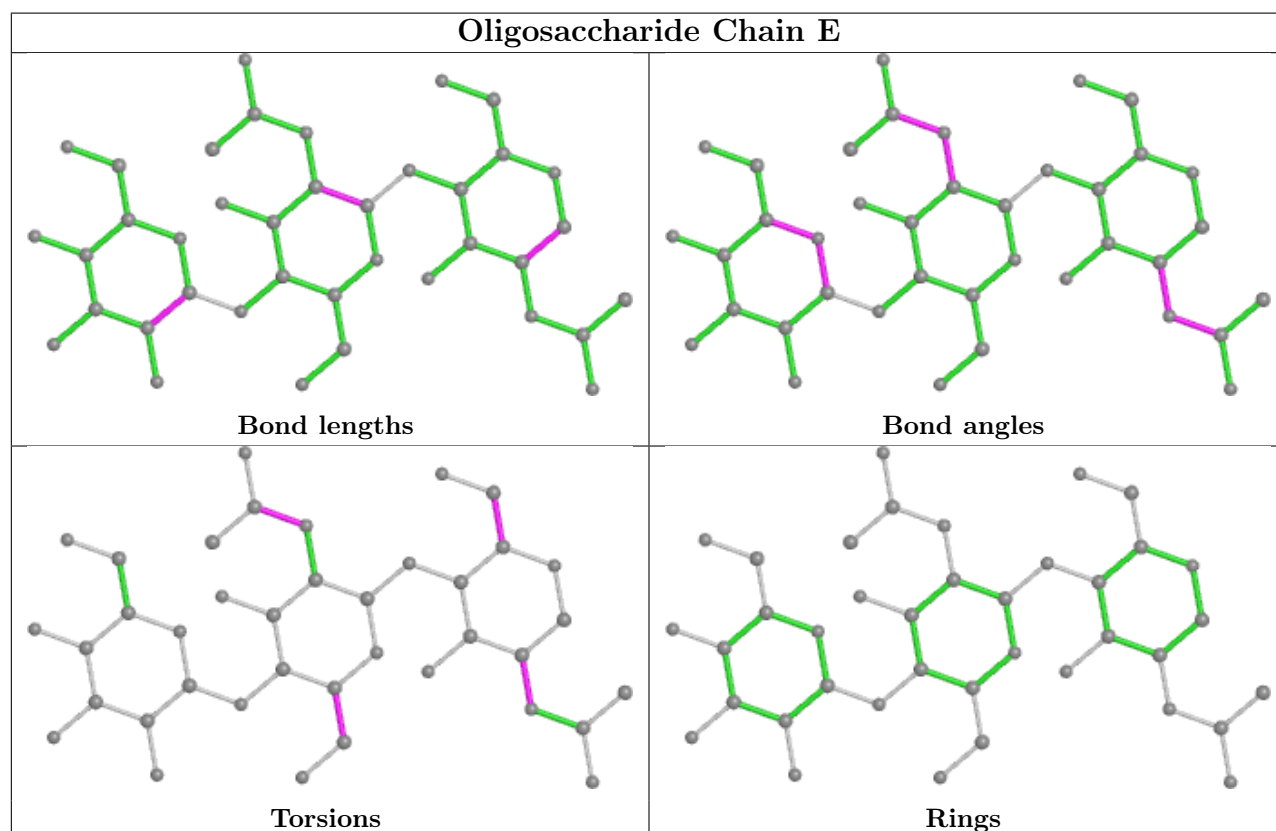
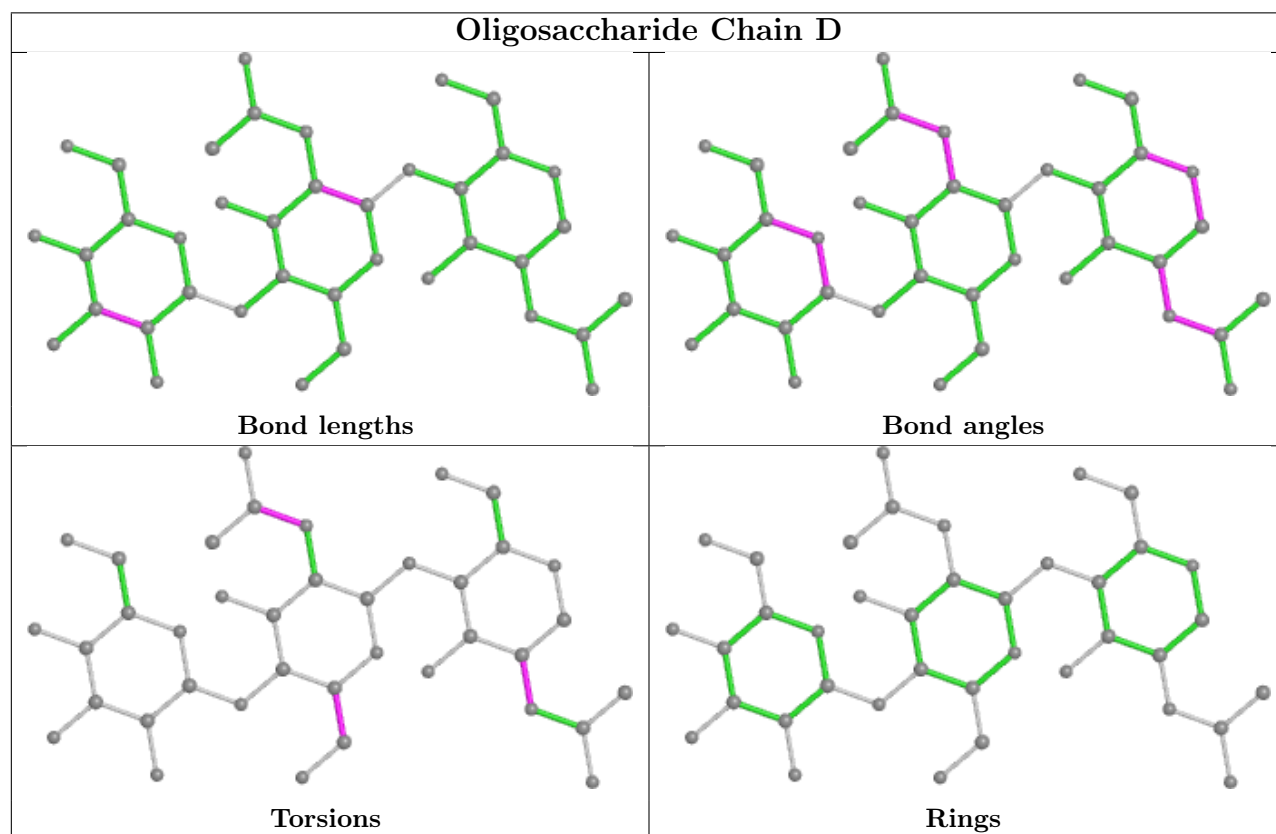
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O7-C7-N2-C2
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
5	D	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C3-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7
6	G	2	NAG	C3-C2-N2-C7
6	K	1	NAG	C3-C2-N2-C7
6	K	2	NAG	C3-C2-N2-C7
6	R	1	NAG	C4-C5-C6-O6

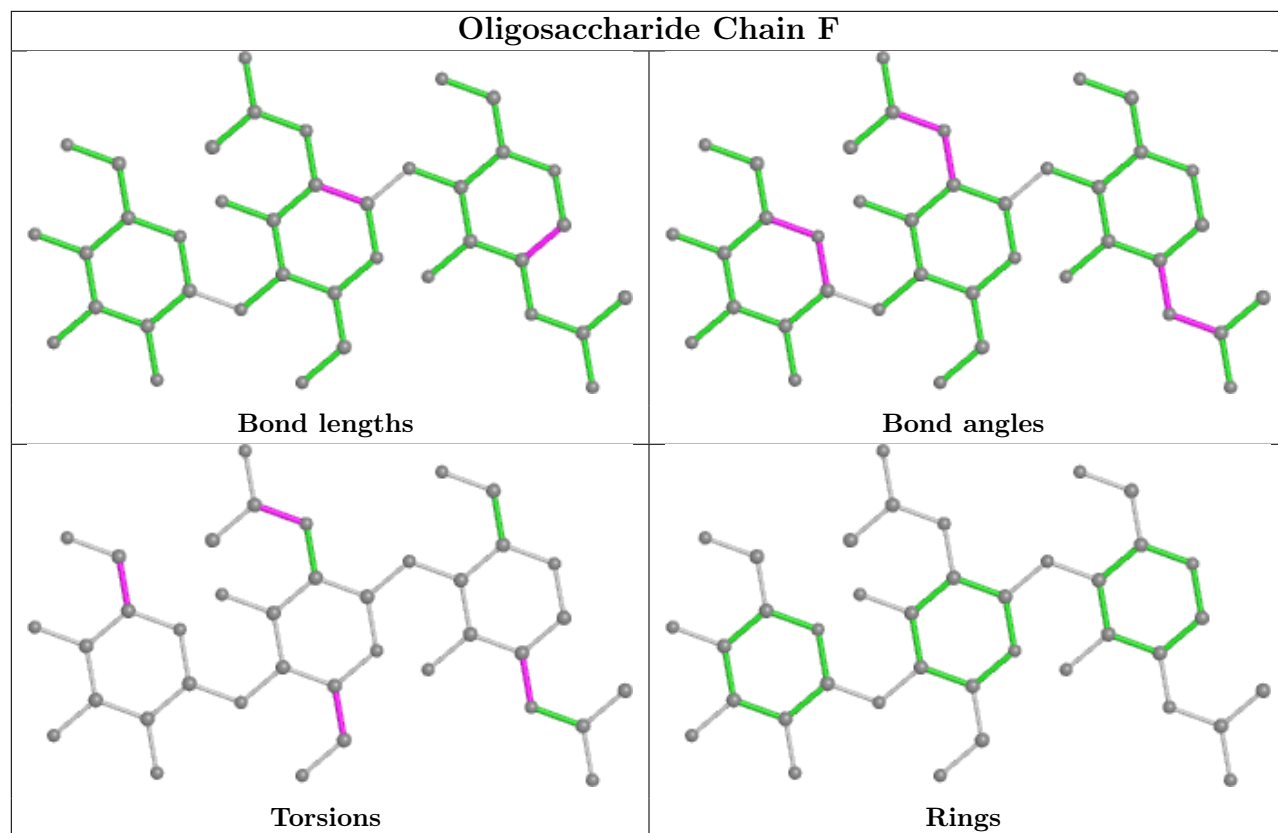
There are no ring outliers.

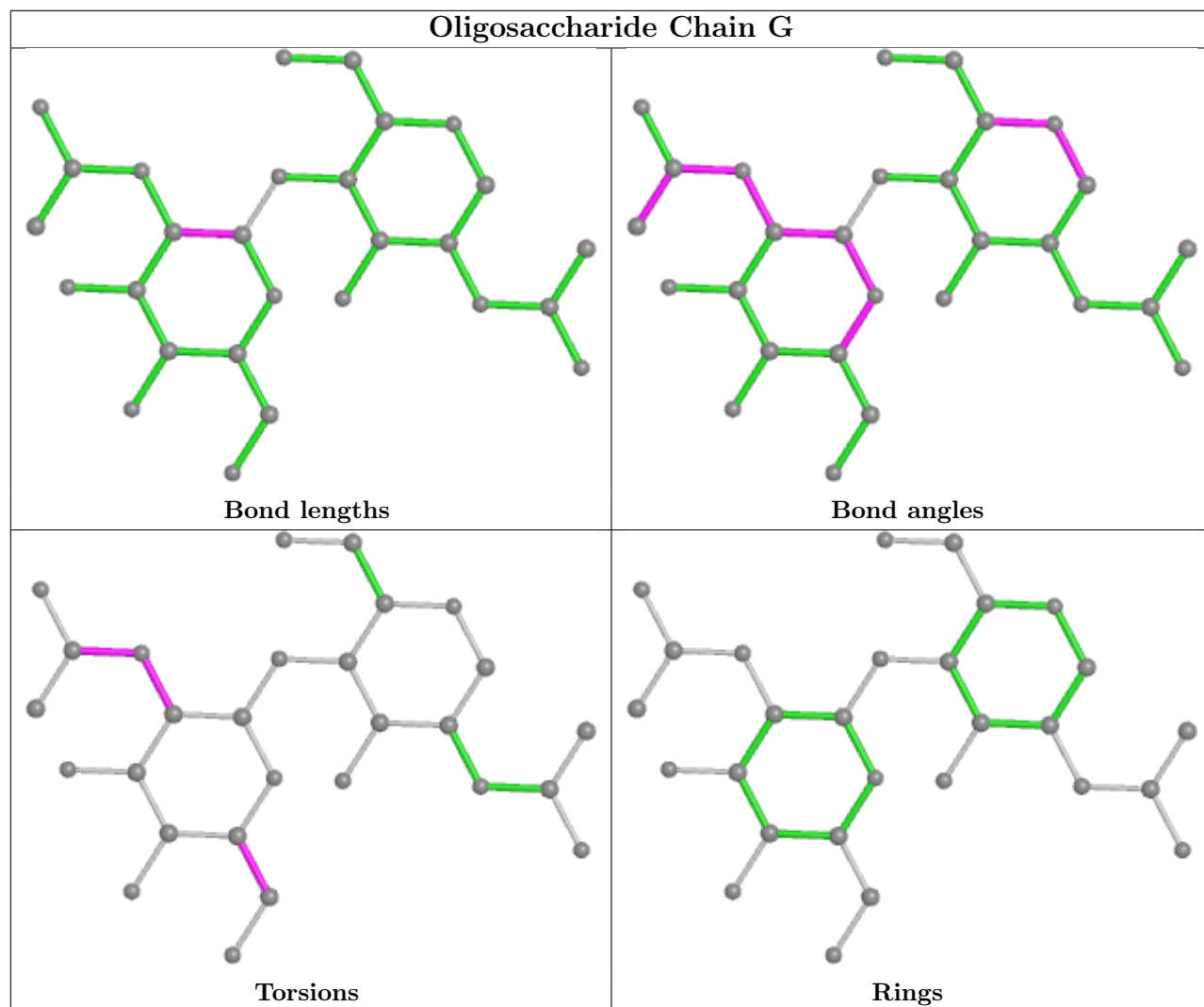
6 monomers are involved in 3 short contacts:

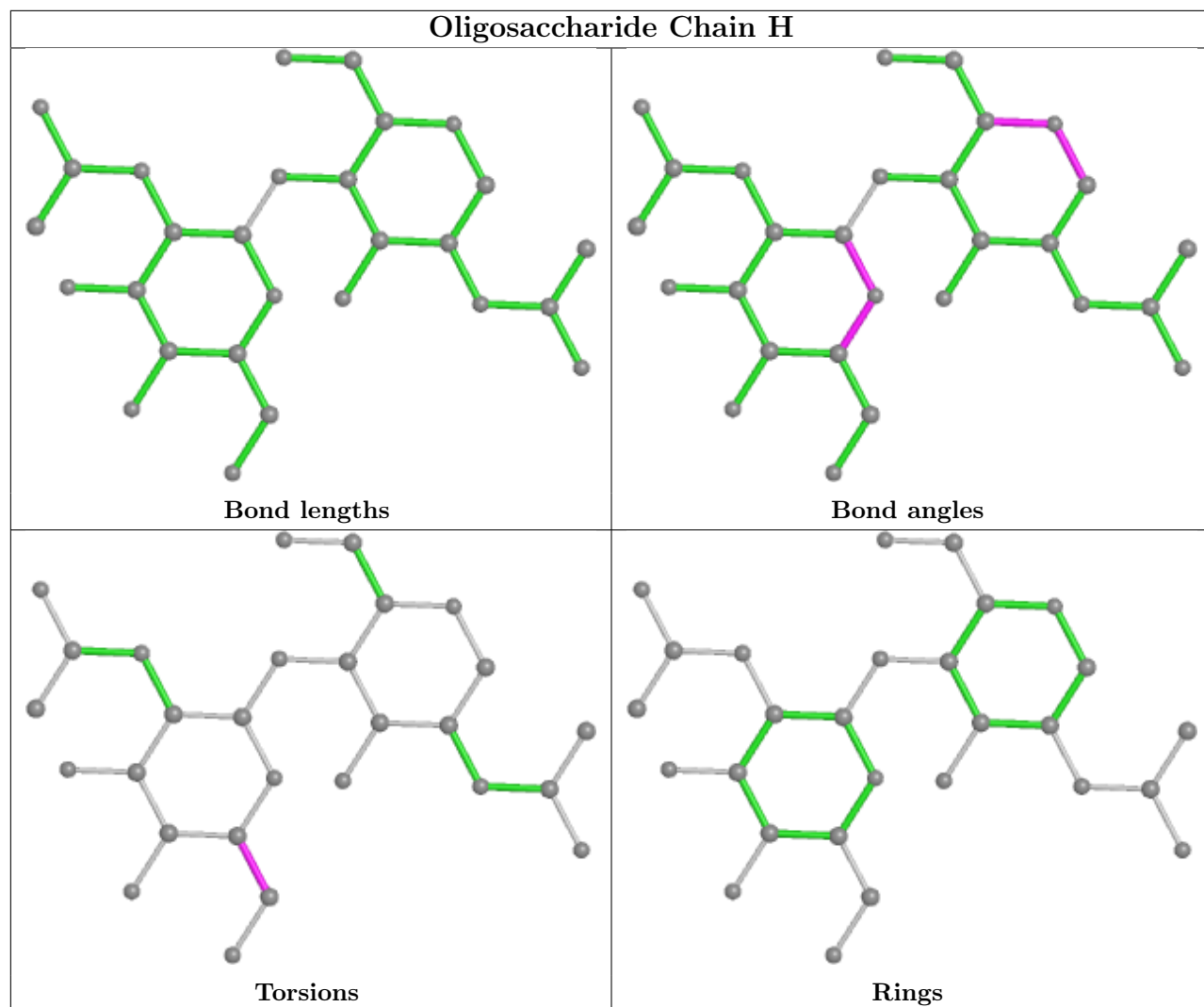
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2	NAG	1	0
5	E	1	NAG	1	0
5	F	1	NAG	1	0
5	E	2	NAG	1	0
5	D	1	NAG	1	0
5	F	2	NAG	1	0

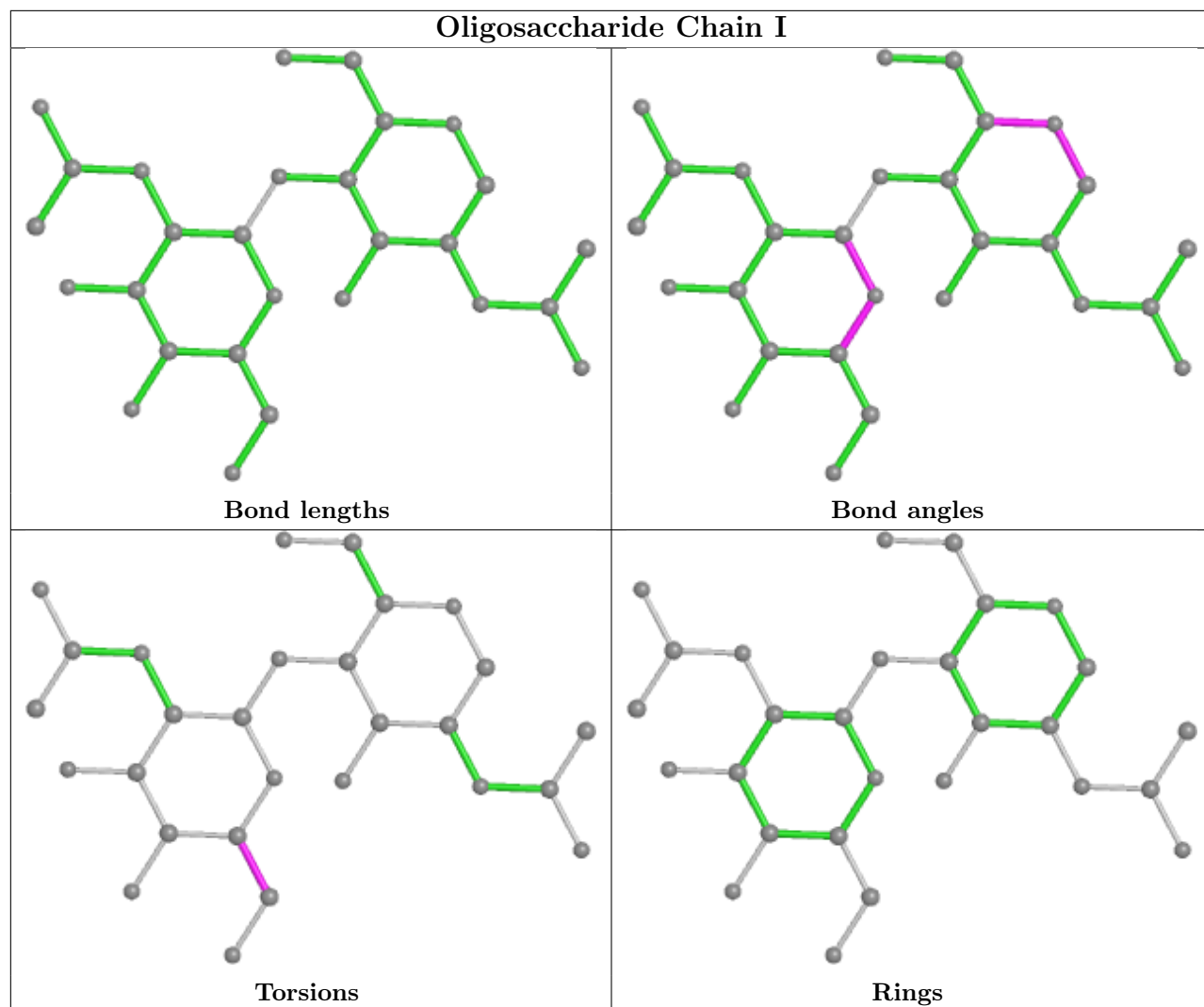
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

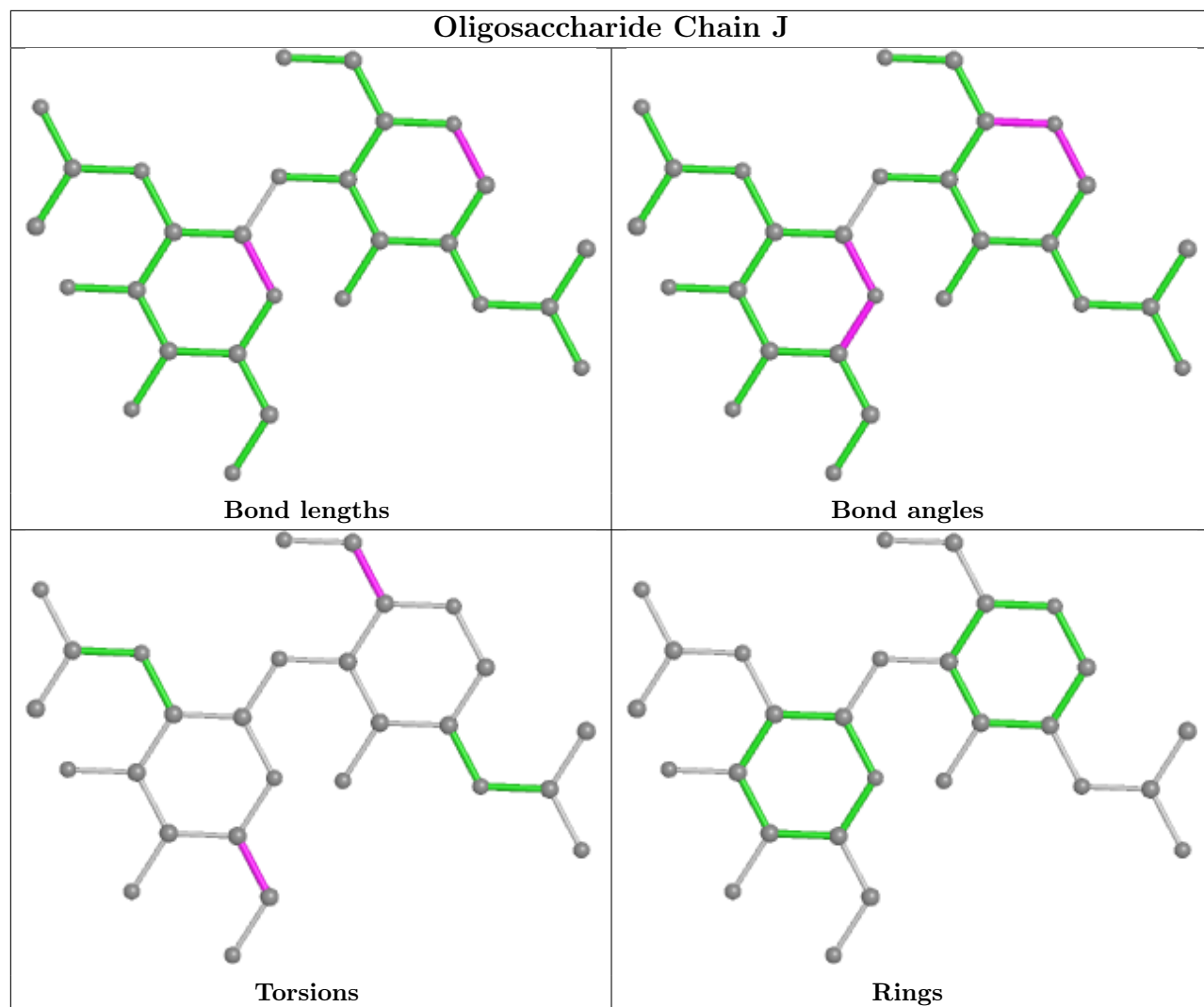


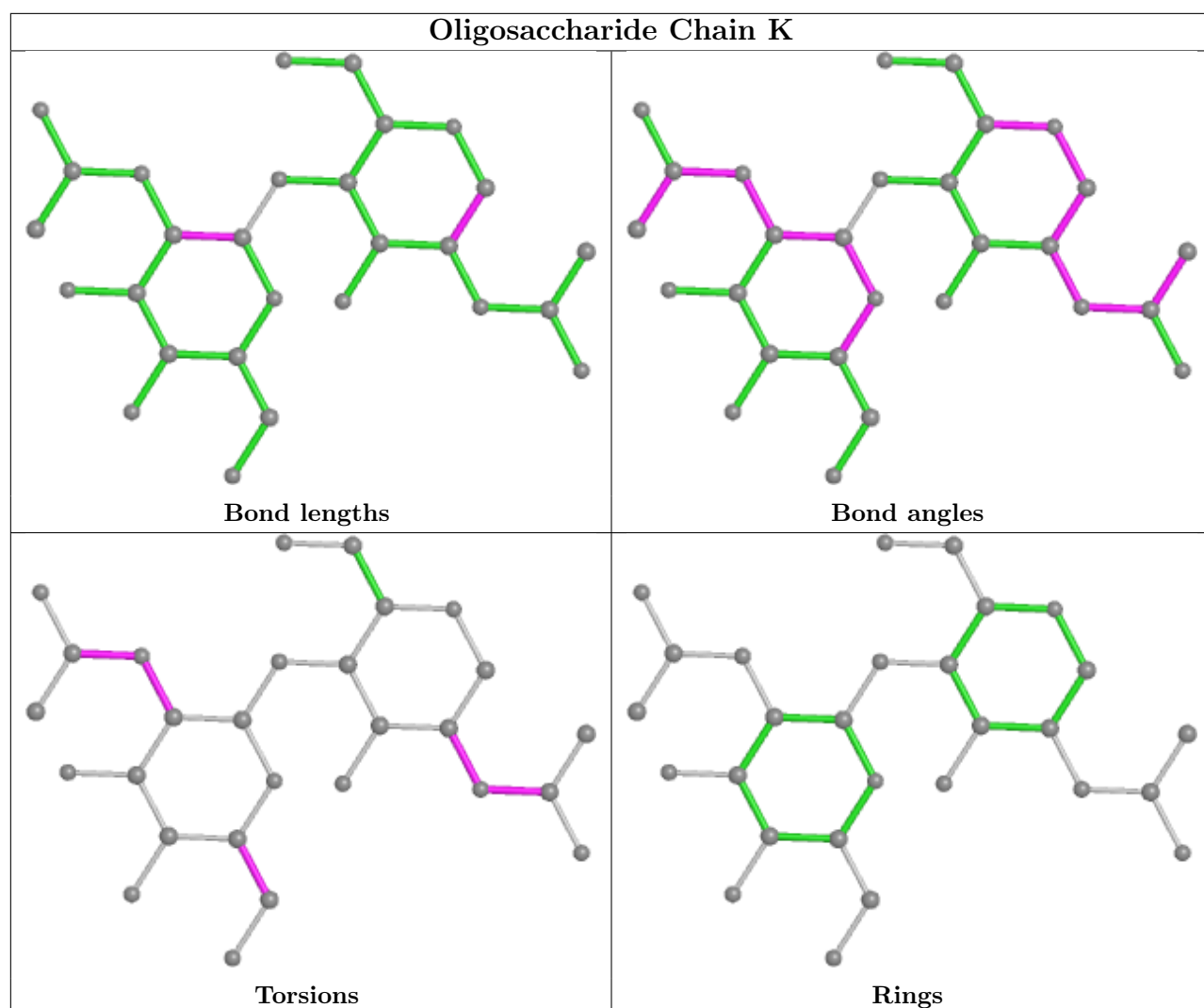


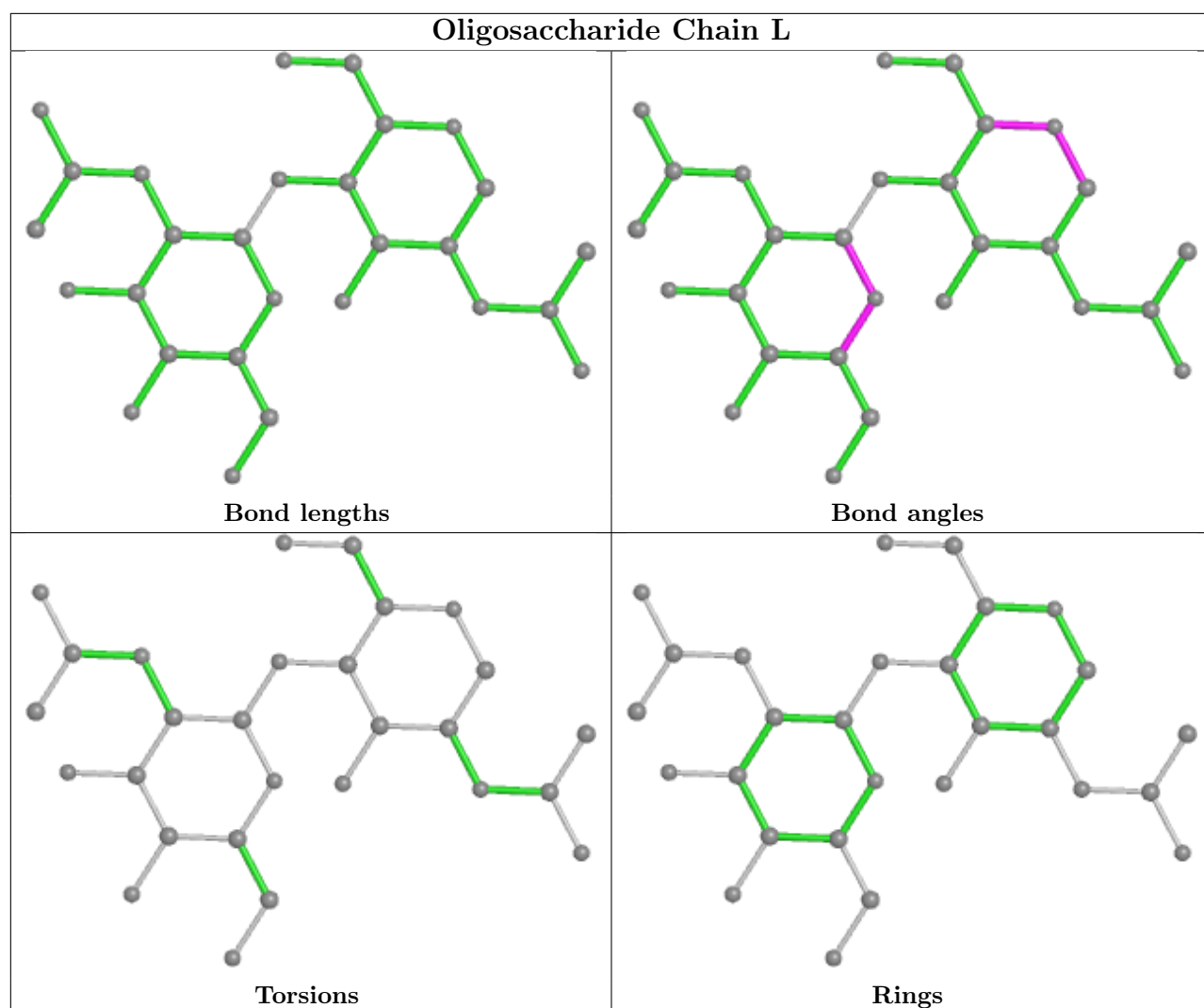


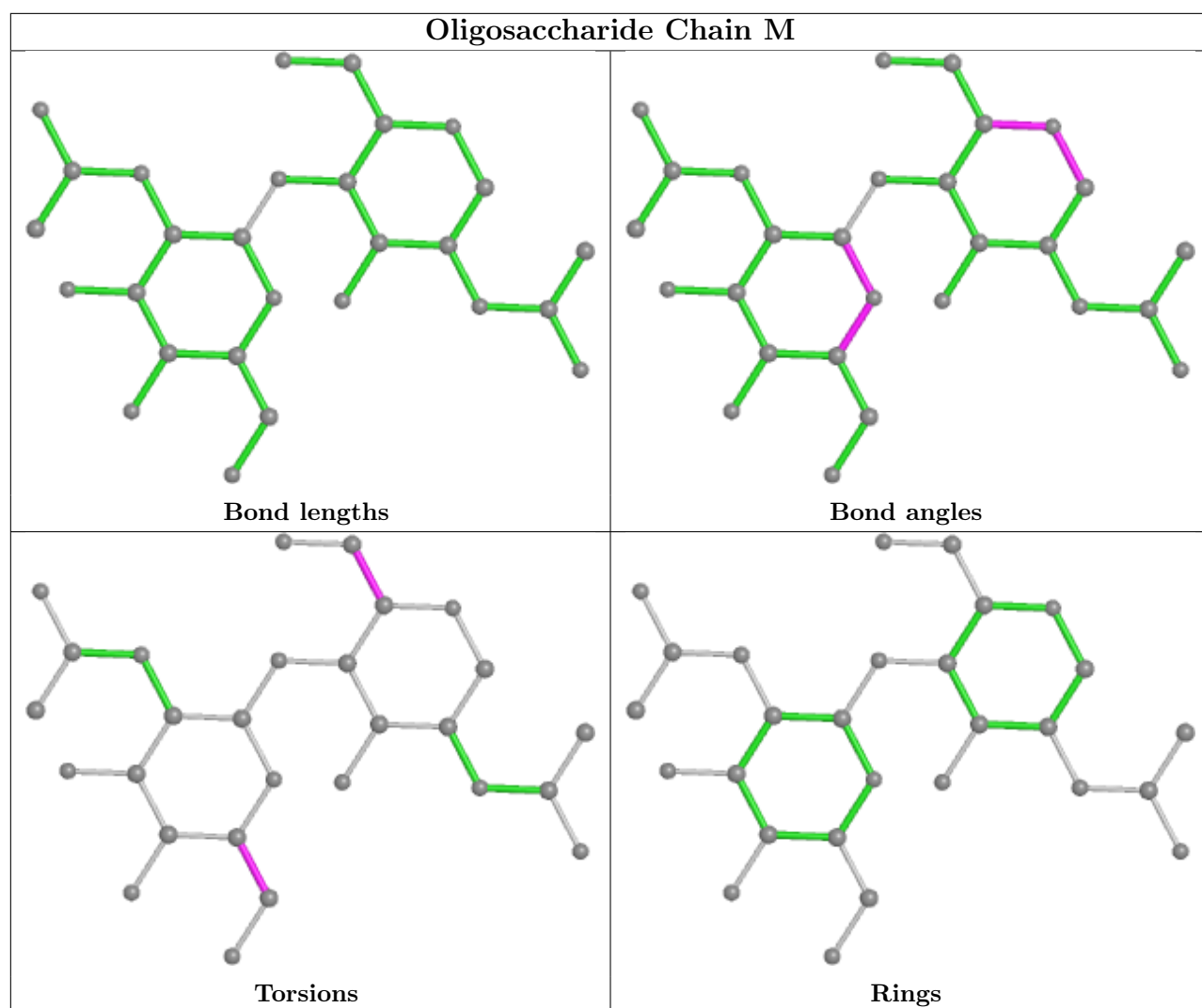


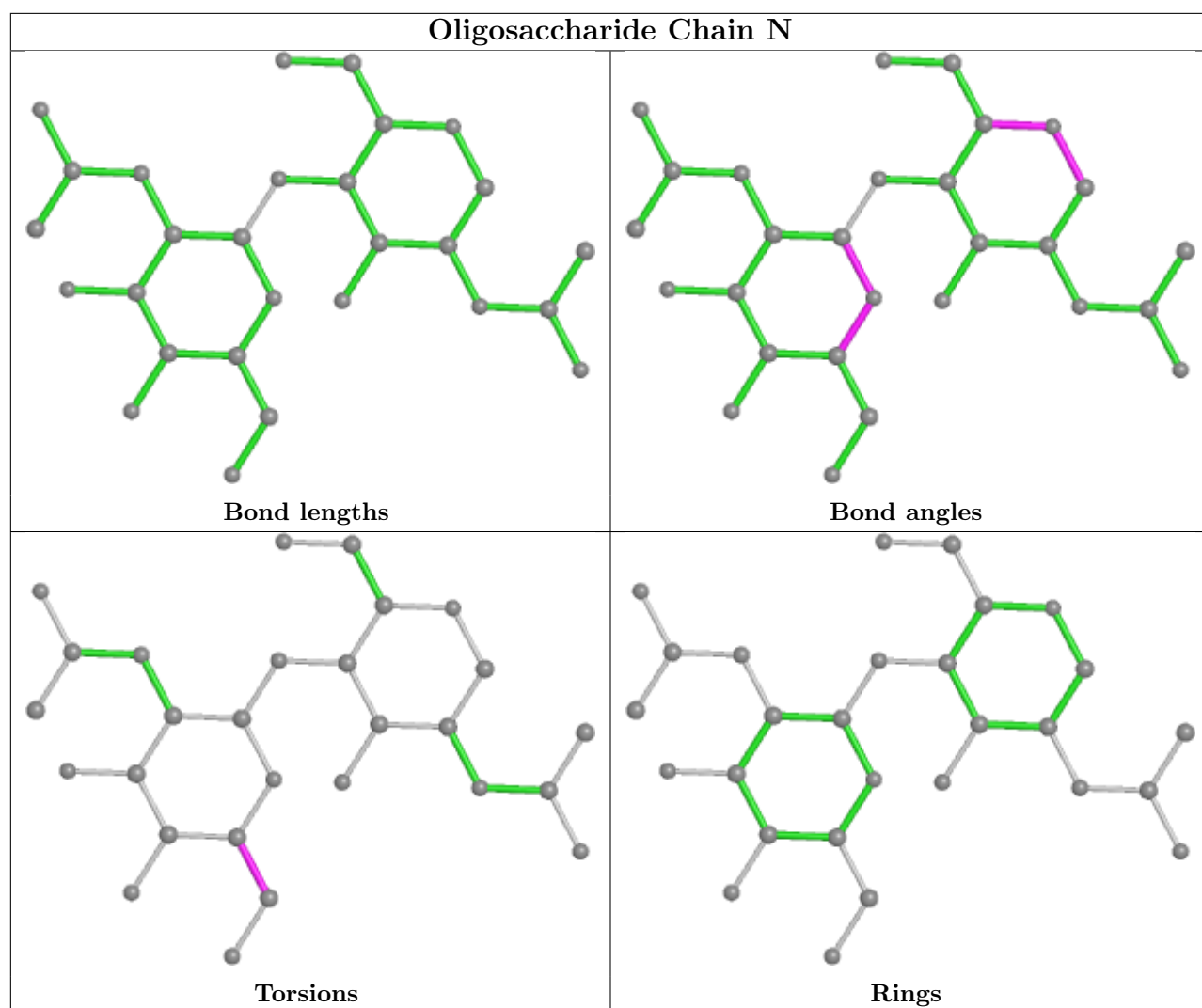


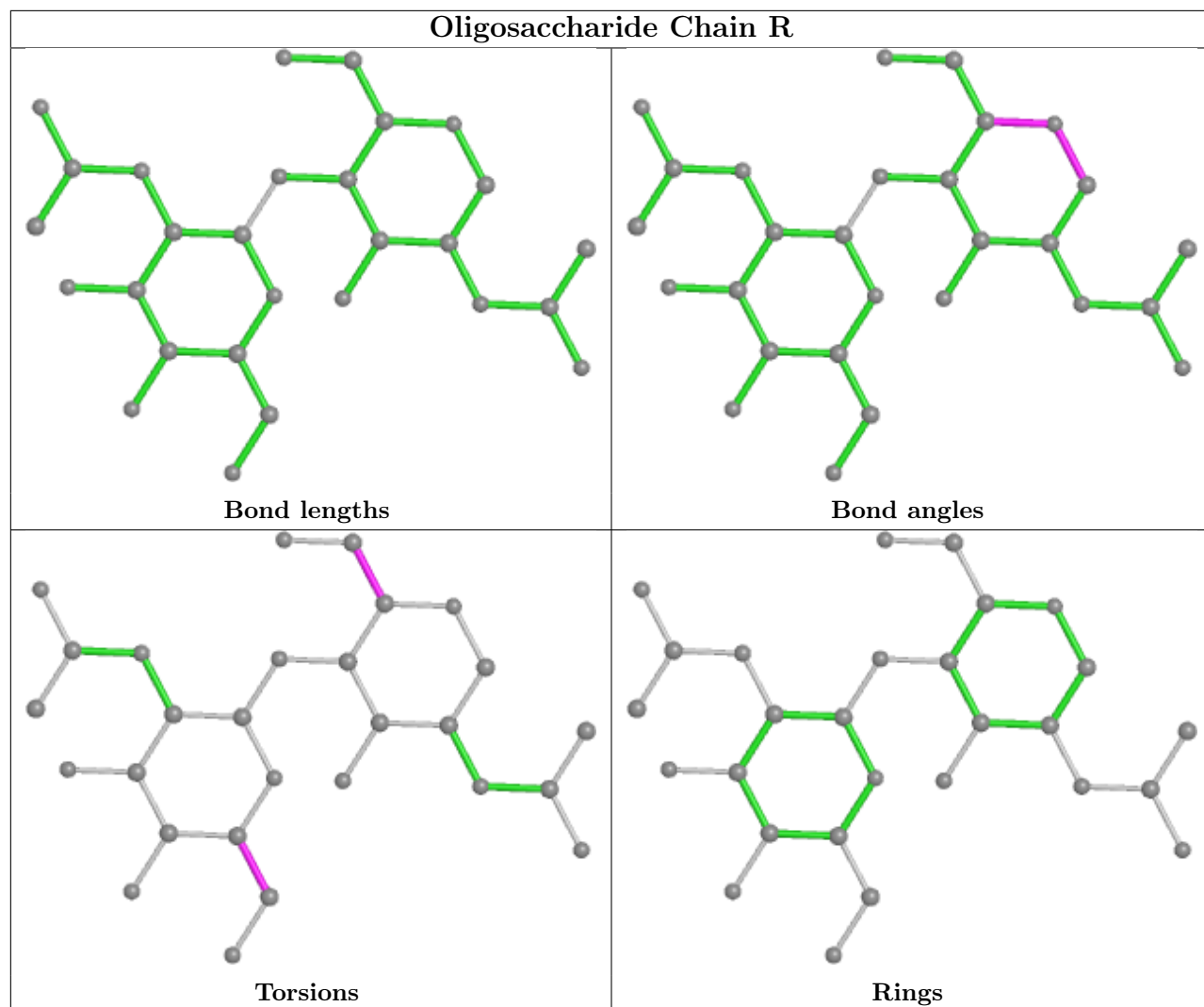


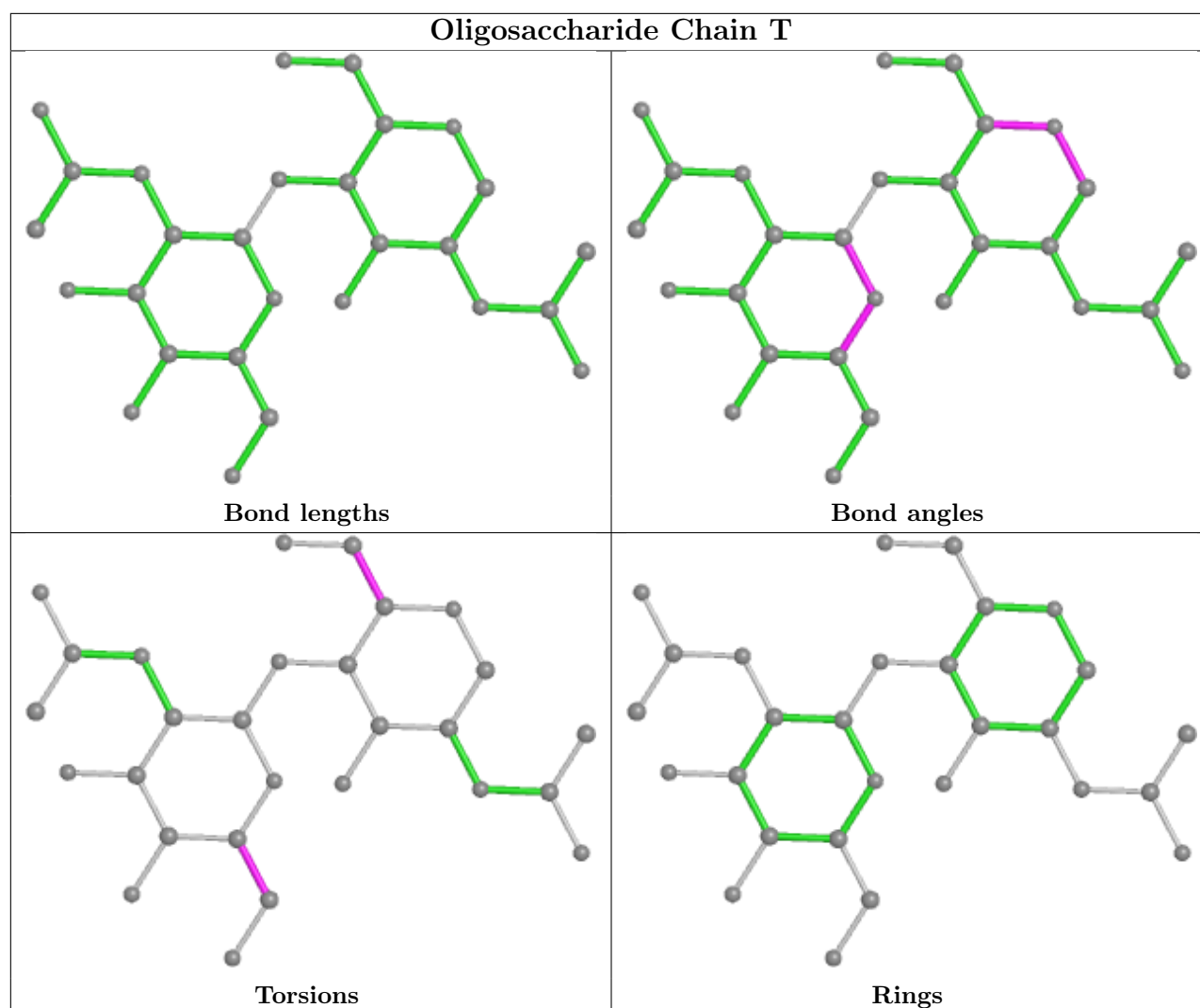












5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
7	NAG	A	1206	-	14,14,15	0.59	0	17,19,21	0.61	1 (5%)
7	NAG	C	1305	2	14,14,15	0.70	1 (7%)	17,19,21	0.66	1 (5%)
7	NAG	B	1302	-	14,14,15	0.75	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1301	-	14,14,15	0.61	0	17,19,21	0.79	1 (5%)
7	NAG	C	1306	2	14,14,15	0.64	0	17,19,21	0.56	0
7	NAG	A	1203	-	14,14,15	0.62	0	17,19,21	0.79	1 (5%)
7	NAG	A	1202	1	14,14,15	0.68	0	17,19,21	0.83	2 (11%)
7	NAG	B	1310	-	14,14,15	0.59	0	17,19,21	0.62	1 (5%)
7	NAG	B	1303	2	14,14,15	0.65	0	17,19,21	0.79	1 (5%)
7	NAG	B	1304	-	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
7	NAG	C	1301	2	14,14,15	0.74	0	17,19,21	0.40	0
7	NAG	C	1308	2	14,14,15	0.66	1 (7%)	17,19,21	0.71	1 (5%)
7	NAG	C	1304	2	14,14,15	0.73	1 (7%)	17,19,21	0.66	1 (5%)
7	NAG	B	1307	-	14,14,15	0.61	0	17,19,21	0.63	1 (5%)
7	NAG	C	1302	2	14,14,15	0.87	2 (14%)	17,19,21	0.91	1 (5%)
7	NAG	S	1301	-	14,14,15	0.58	0	17,19,21	0.66	1 (5%)
7	NAG	B	1311	-	14,14,15	0.59	0	17,19,21	0.63	1 (5%)
7	NAG	B	1309	2	14,14,15	0.60	0	17,19,21	0.66	1 (5%)
7	NAG	B	1305	-	14,14,15	0.74	0	17,19,21	1.27	3 (17%)
7	NAG	B	1308	2	14,14,15	0.68	0	17,19,21	0.48	0
7	NAG	C	1307	2	14,14,15	0.69	1 (7%)	17,19,21	0.58	1 (5%)
7	NAG	A	1201	1	14,14,15	1.15	2 (14%)	17,19,21	1.33	3 (17%)
7	NAG	A	1204	1	14,14,15	0.67	1 (7%)	17,19,21	0.71	1 (5%)
7	NAG	A	1205	1	14,14,15	1.27	1 (7%)	17,19,21	2.61	4 (23%)
7	NAG	C	1303	2	14,14,15	0.67	0	17,19,21	0.65	1 (5%)
7	NAG	B	1306	2	14,14,15	0.65	0	17,19,21	0.59	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
7	NAG	A	1206	-	-	1/6/23/26	0/1/1/1
7	NAG	C	1305	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	-	-	4/6/23/26	0/1/1/1
7	NAG	C	1306	2	-	2/6/23/26	0/1/1/1
7	NAG	A	1203	-	-	4/6/23/26	0/1/1/1
7	NAG	A	1202	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1310	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	2	-	4/6/23/26	0/1/1/1
7	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	2	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	2	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1307	-	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	2	-	3/6/23/26	0/1/1/1
7	NAG	S	1301	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1311	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1309	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	-	-	3/6/23/26	0/1/1/1
7	NAG	B	1308	2	-	0/6/23/26	0/1/1/1
7	NAG	C	1307	2	-	0/6/23/26	0/1/1/1
7	NAG	A	1201	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1205	1	-	5/6/23/26	0/1/1/1
7	NAG	C	1303	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1306	2	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1205	NAG	C1-C2	3.64	1.57	1.52
7	A	1201	NAG	C1-C2	2.99	1.56	1.52
7	A	1201	NAG	O5-C1	2.74	1.48	1.43
7	C	1302	NAG	O5-C1	2.40	1.47	1.43
7	C	1305	NAG	O5-C1	2.21	1.47	1.43
7	C	1304	NAG	O5-C1	2.17	1.47	1.43
7	C	1307	NAG	O5-C1	2.10	1.47	1.43
7	A	1204	NAG	O5-C1	2.05	1.47	1.43
7	C	1308	NAG	O5-C1	2.03	1.47	1.43
7	C	1302	NAG	C1-C2	2.00	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1205	NAG	C2-N2-C7	9.03	135.76	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1205	NAG	C1-C2-N2	4.22	117.69	110.49
7	B	1305	NAG	C2-N2-C7	3.99	128.59	122.90
7	B	1302	NAG	C2-N2-C7	3.92	128.48	122.90
7	A	1201	NAG	C2-N2-C7	3.50	127.88	122.90
7	C	1302	NAG	C1-O5-C5	2.82	116.01	112.19
7	A	1201	NAG	C1-O5-C5	2.71	115.87	112.19
7	C	1308	NAG	C1-O5-C5	2.64	115.77	112.19
7	A	1204	NAG	C1-O5-C5	2.62	115.75	112.19
7	A	1205	NAG	C8-C7-N2	2.50	120.34	116.10
7	C	1305	NAG	C1-O5-C5	2.45	115.51	112.19
7	B	1309	NAG	C1-O5-C5	2.44	115.50	112.19
7	C	1304	NAG	C1-O5-C5	2.41	115.46	112.19
7	S	1301	NAG	C1-O5-C5	2.40	115.44	112.19
7	C	1303	NAG	C1-O5-C5	2.37	115.40	112.19
7	A	1202	NAG	C1-O5-C5	2.32	115.33	112.19
7	A	1205	NAG	C1-O5-C5	2.32	115.33	112.19
7	B	1307	NAG	C1-O5-C5	2.29	115.30	112.19
7	B	1303	NAG	C1-O5-C5	2.27	115.26	112.19
7	B	1311	NAG	C1-O5-C5	2.27	115.26	112.19
7	B	1304	NAG	C1-O5-C5	2.25	115.24	112.19
7	B	1301	NAG	C1-O5-C5	2.25	115.23	112.19
7	A	1203	NAG	C1-O5-C5	2.23	115.22	112.19
7	B	1310	NAG	C1-O5-C5	2.22	115.19	112.19
7	B	1305	NAG	C1-O5-C5	2.21	115.19	112.19
7	A	1206	NAG	C1-O5-C5	2.20	115.17	112.19
7	B	1302	NAG	C1-O5-C5	2.19	115.15	112.19
7	A	1201	NAG	C1-C2-N2	2.18	114.21	110.49
7	B	1306	NAG	C1-O5-C5	2.07	115.00	112.19
7	C	1307	NAG	C1-O5-C5	2.05	114.97	112.19
7	A	1202	NAG	C2-N2-C7	2.05	125.82	122.90
7	B	1305	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1205	NAG	O5-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	A	1201	NAG	C4-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	A	1203	NAG	O5-C5-C6-O6
7	A	1204	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	C	1303	NAG	O5-C5-C6-O6
7	C	1305	NAG	C4-C5-C6-O6
7	B	1301	NAG	O5-C5-C6-O6
7	C	1306	NAG	O5-C5-C6-O6
7	B	1306	NAG	C4-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	B	1305	NAG	C4-C5-C6-O6
7	A	1205	NAG	C4-C5-C6-O6
7	B	1309	NAG	O5-C5-C6-O6
7	B	1311	NAG	O5-C5-C6-O6
7	A	1203	NAG	C4-C5-C6-O6
7	B	1311	NAG	C4-C5-C6-O6
7	C	1306	NAG	C4-C5-C6-O6
7	B	1309	NAG	C4-C5-C6-O6
7	C	1303	NAG	C4-C5-C6-O6
7	A	1202	NAG	C8-C7-N2-C2
7	A	1202	NAG	O7-C7-N2-C2
7	A	1203	NAG	C8-C7-N2-C2
7	A	1203	NAG	O7-C7-N2-C2
7	A	1205	NAG	C8-C7-N2-C2
7	A	1205	NAG	O7-C7-N2-C2
7	B	1301	NAG	C8-C7-N2-C2
7	B	1301	NAG	O7-C7-N2-C2
7	B	1303	NAG	C8-C7-N2-C2
7	B	1303	NAG	O7-C7-N2-C2
7	C	1302	NAG	C8-C7-N2-C2
7	C	1302	NAG	O7-C7-N2-C2
7	A	1204	NAG	C4-C5-C6-O6
7	A	1202	NAG	O5-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	A	1201	NAG	O5-C5-C6-O6
7	C	1308	NAG	O5-C5-C6-O6
7	B	1301	NAG	C4-C5-C6-O6
7	C	1301	NAG	C4-C5-C6-O6
7	C	1308	NAG	C4-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	C	1305	NAG	O5-C5-C6-O6
7	B	1306	NAG	O5-C5-C6-O6
7	B	1303	NAG	C4-C5-C6-O6
7	B	1310	NAG	O5-C5-C6-O6
7	A	1202	NAG	C4-C5-C6-O6
7	S	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	1206	NAG	O5-C5-C6-O6
7	C	1302	NAG	O5-C5-C6-O6
7	S	1301	NAG	O5-C5-C6-O6
7	B	1302	NAG	C4-C5-C6-O6
7	A	1201	NAG	C3-C2-N2-C7
7	B	1304	NAG	C4-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	A	1205	NAG	C3-C2-N2-C7
7	B	1302	NAG	C3-C2-N2-C7
7	B	1305	NAG	C3-C2-N2-C7
7	B	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1307	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.

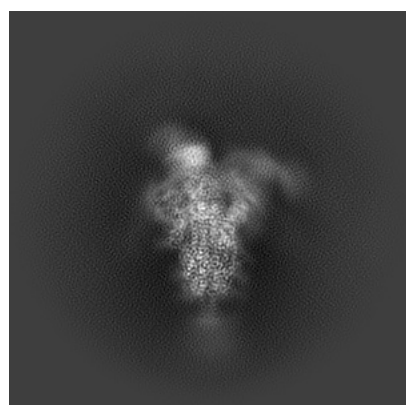
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32398. These allow visual inspection of the internal detail of the map and identification of artifacts.

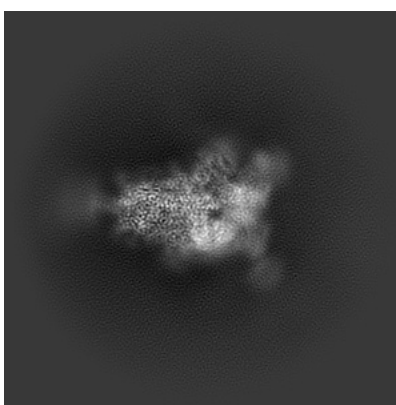
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

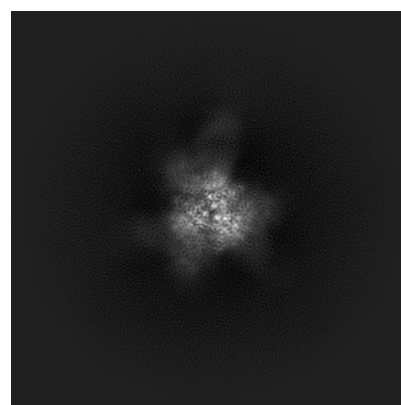
6.1.1 Primary map



X



Y

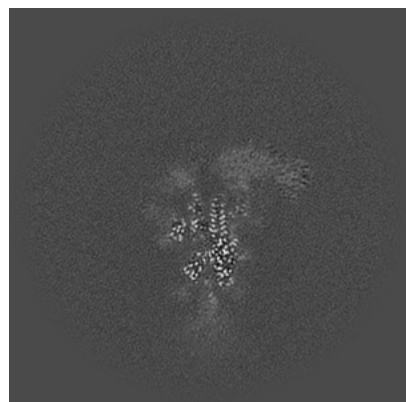


Z

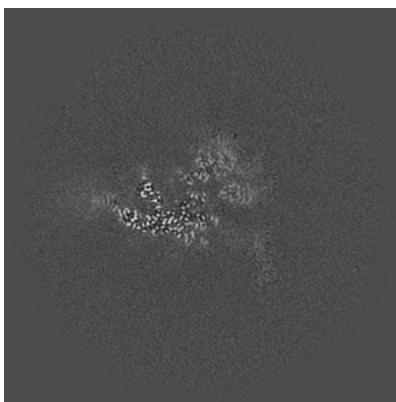
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

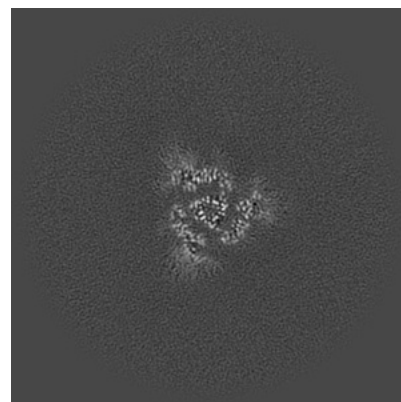
6.2.1 Primary map



X Index: 200



Y Index: 200

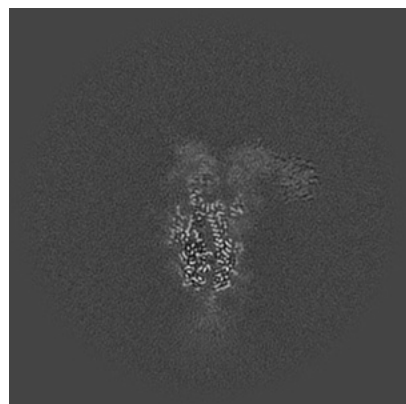


Z Index: 200

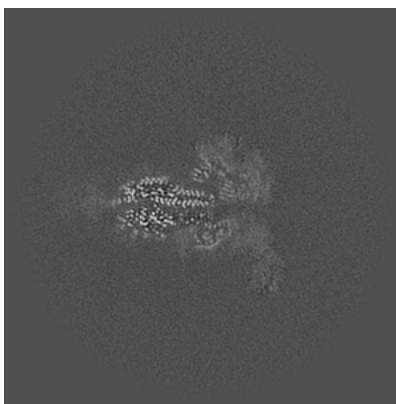
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

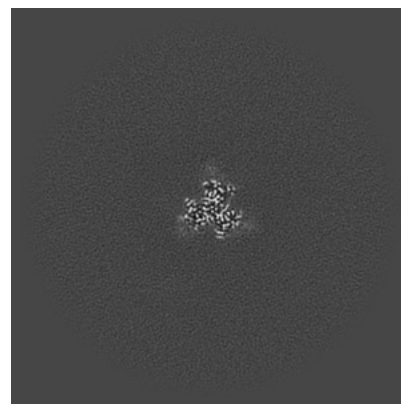
6.3.1 Primary map



X Index: 211



Y Index: 192

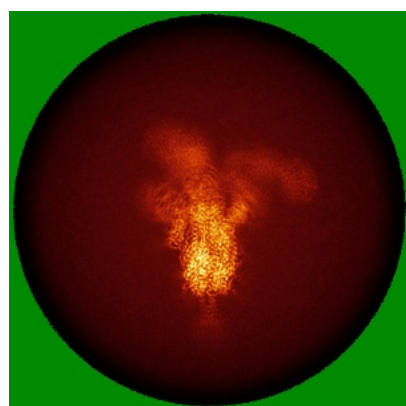


Z Index: 153

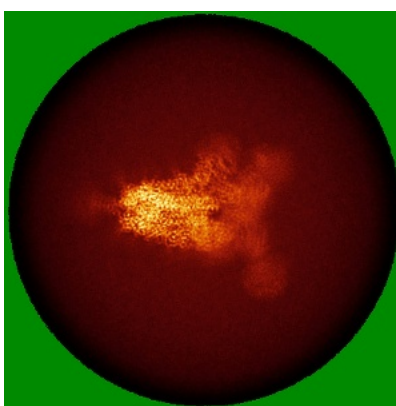
The images above show the largest variance slices of the map in three orthogonal directions.

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

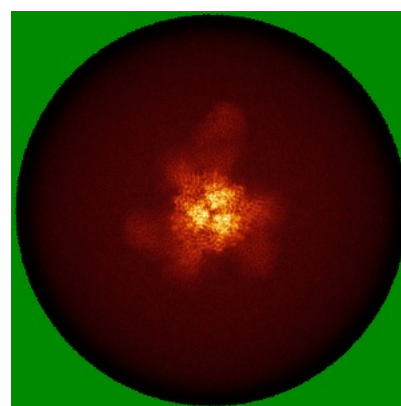
6.4.1 Primary map



X



Y

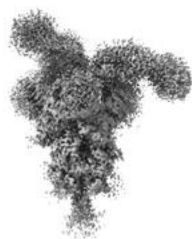


Z

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](#)

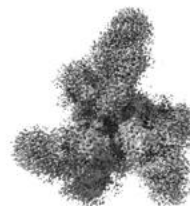
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.177. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

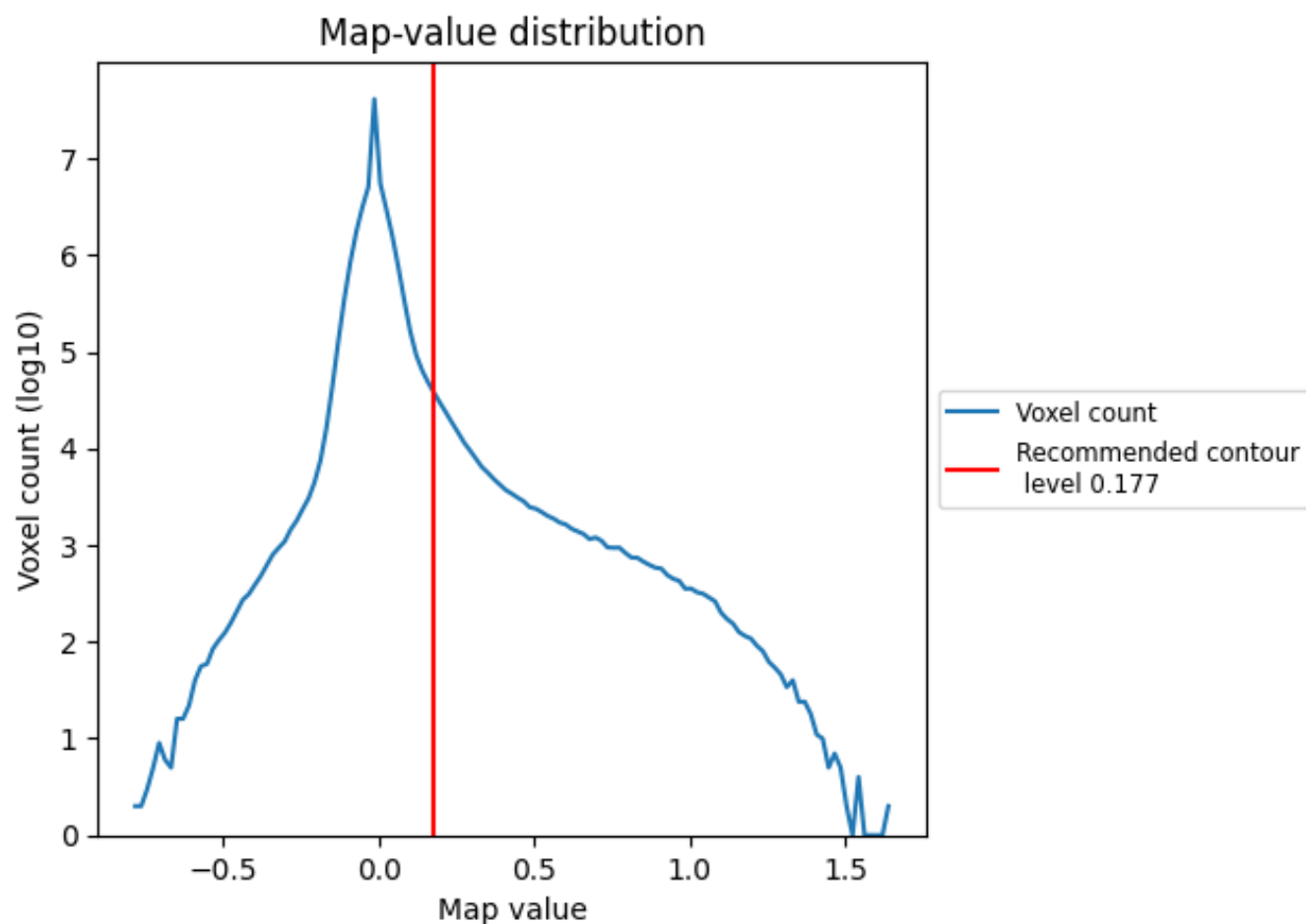
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

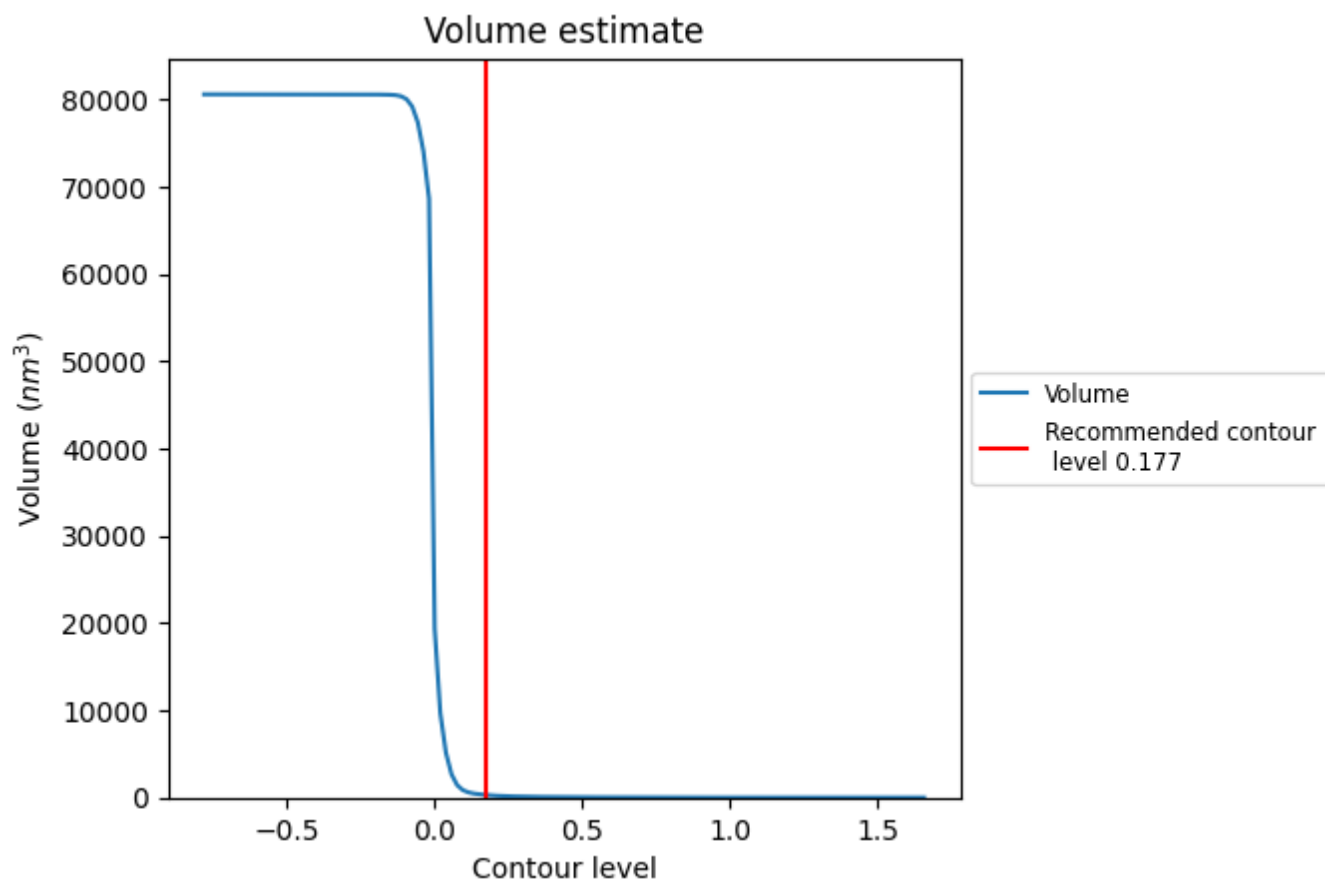
This section contains the results of statistical analysis of the map.

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.

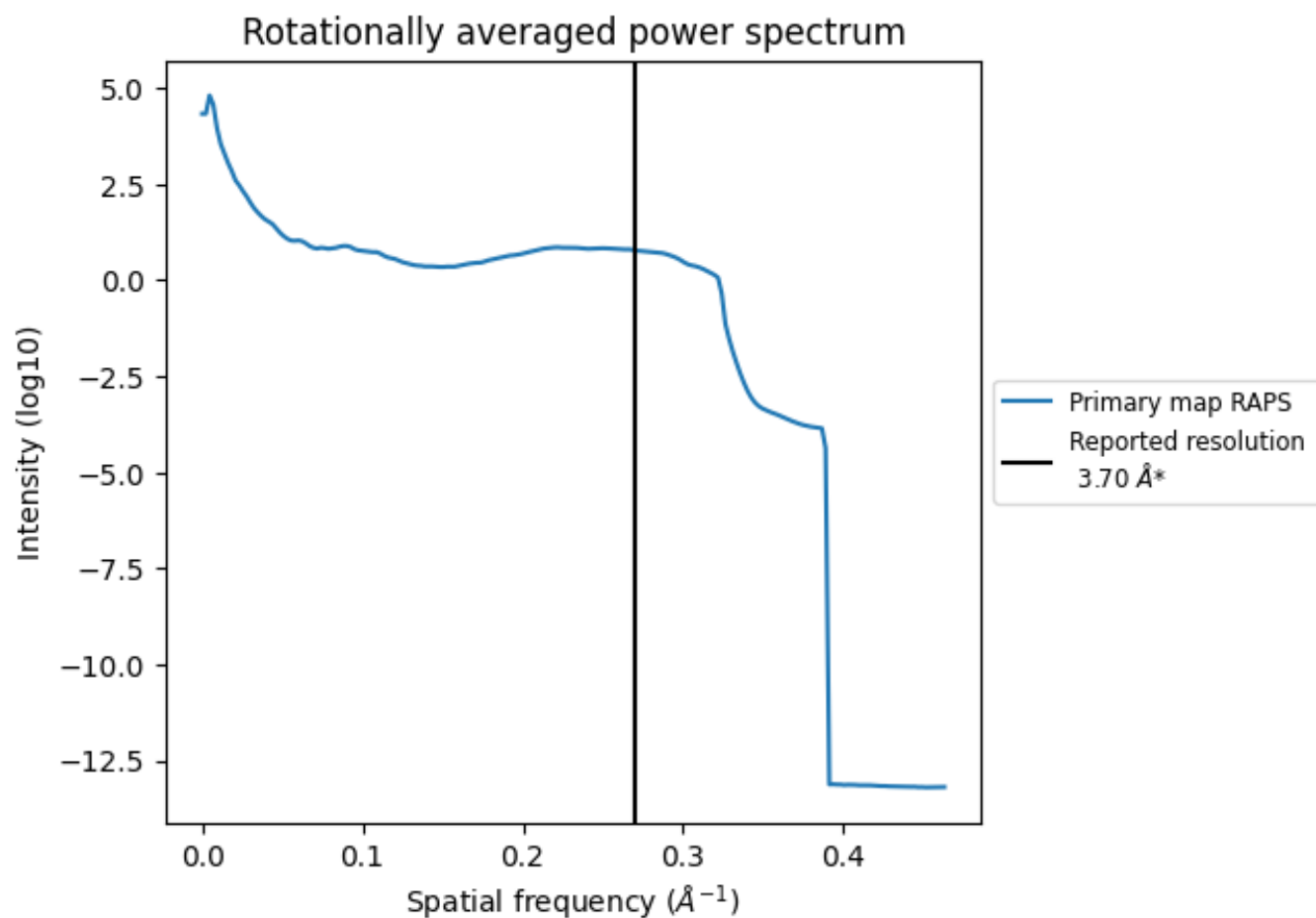
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm³; this corresponds to an approximate mass of 257 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 0.270 Å⁻¹

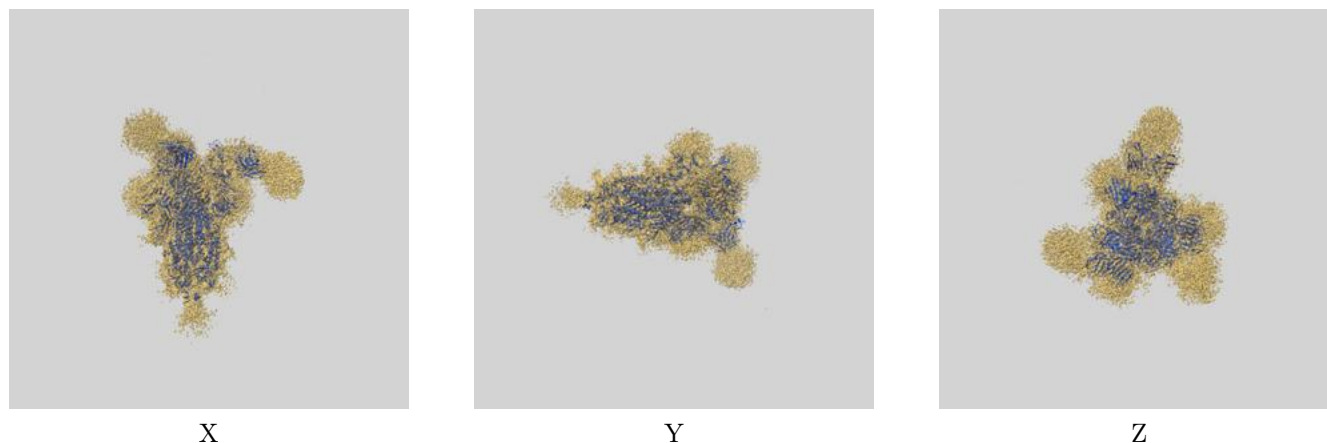
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

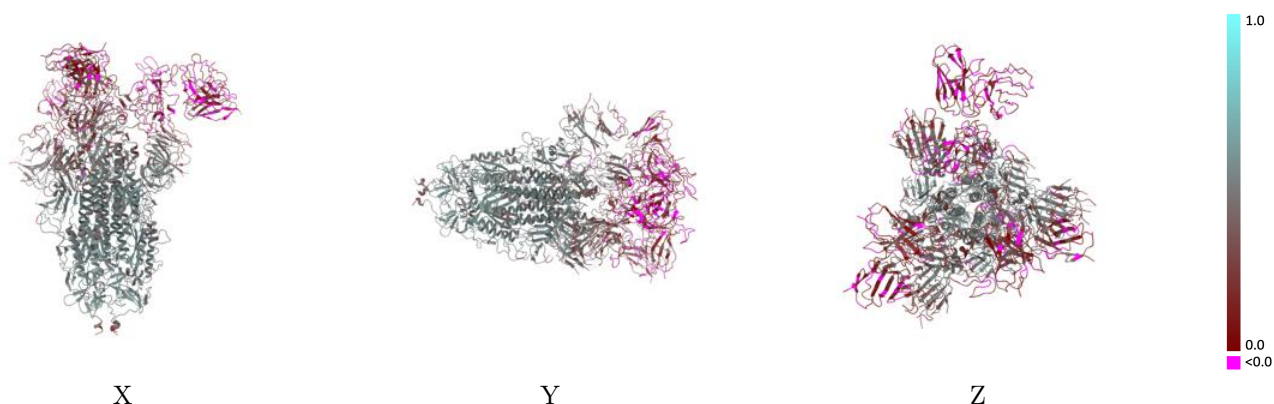
This section contains information regarding the fit between EMDB map EMD-32398 and PDB model 7WBH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



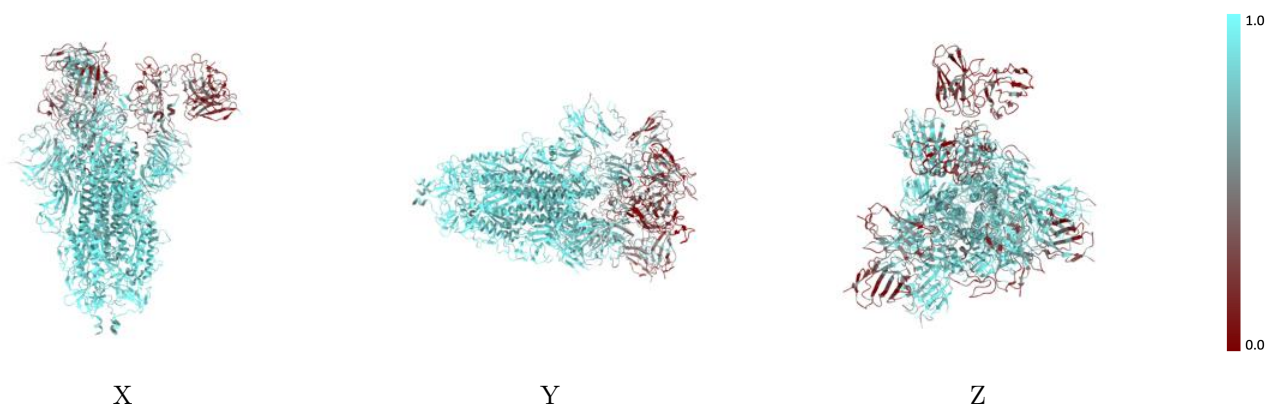
The images above show the 3D surface view of the map at the recommended contour level 0.177 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



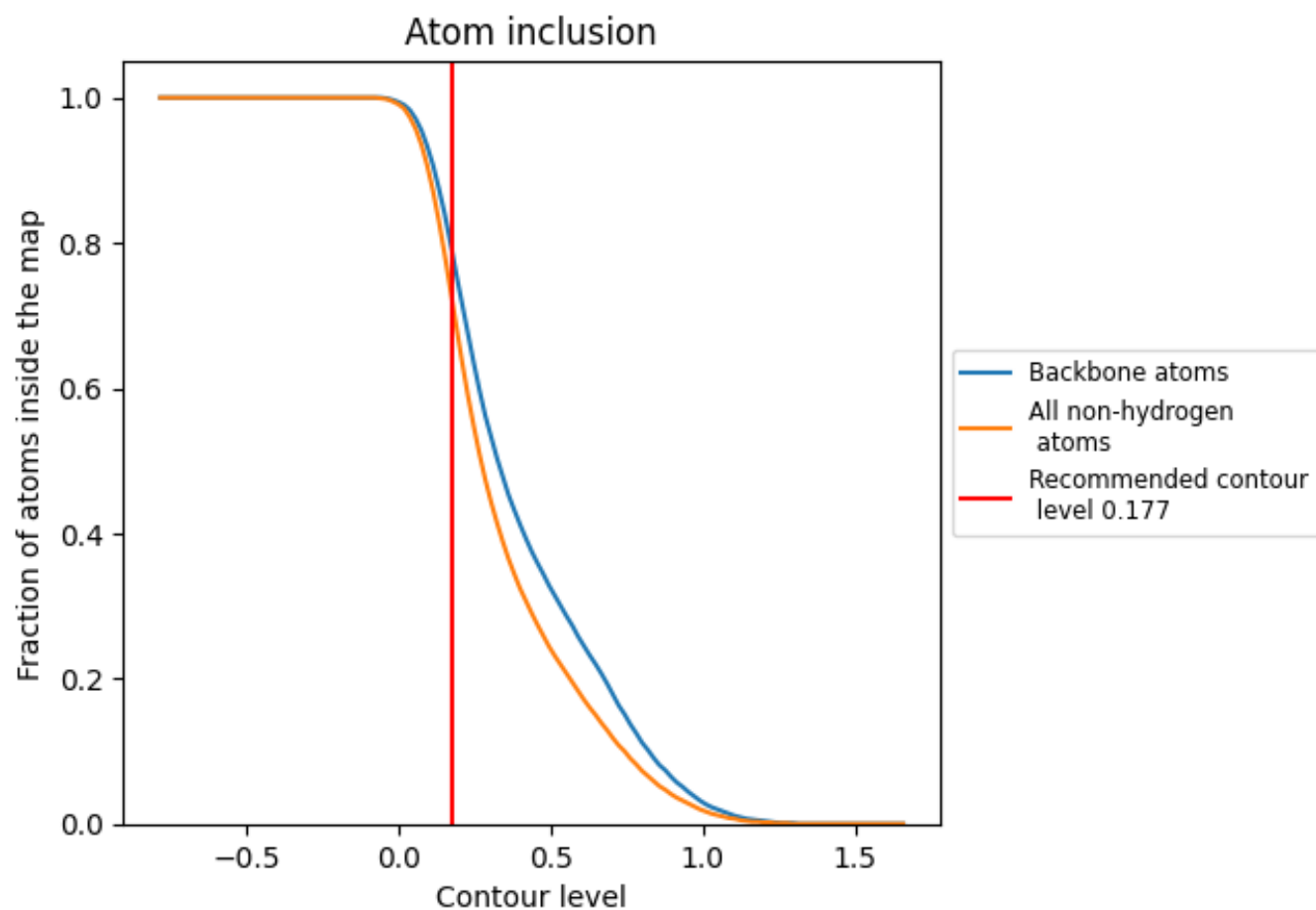
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.177).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 72% 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 (0.177) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.3660
A	 0.7600	 0.4040
B	 0.8080	 0.4230
C	 0.8220	 0.4260
D	 0.4100	 0.1070
E	 0.5640	 0.2080
F	 0.4870	 0.1060
G	 0.5000	 0.0740
H	 0.7500	 0.4510
I	 0.6430	 0.3540
J	 0.3930	 0.2230
K	 0.5710	 0.2100
L	 0.7140	 0.4130
M	 0.4640	 0.2470
N	 0.8210	 0.4830
O	 0.4400	 0.1660
P	 0.5510	 0.1540
Q	 0.4010	 0.1580
R	 0.6790	 0.3520
S	 0.5040	 0.2220
T	 0.3930	 0.3740
U	 0.2320	 0.0760
V	 0.2400	 0.1050

